



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:18 AM GMT

PDB ID : 3A5C
Title : Inter-subunit interaction and quaternary rearrangement defined by the central stalk of prokaryotic V1-ATPase
Authors : Numoto, N.; Hasegawa, Y.; Takeda, K.; Miki, K.
Deposited on : 2009-08-06
Resolution : 4.51 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

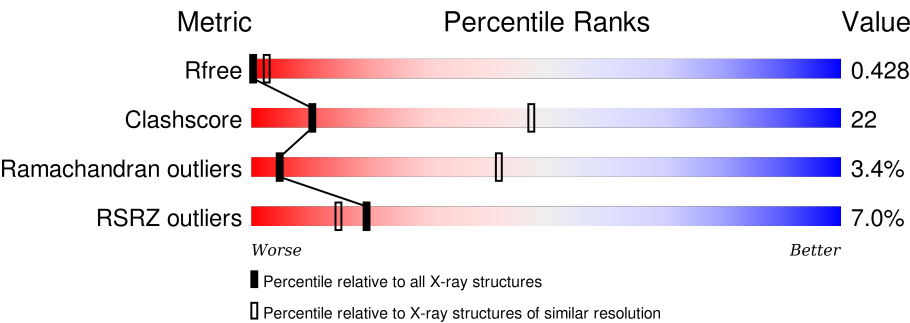
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.51 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1071 (5.40-3.60)
Clashscore	102246	1004 (5.40-3.62)
Ramachandran outliers	100387	1117 (5.40-3.60)
RSRZ outliers	91569	1075 (5.40-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	578	
1	B	578	
1	C	578	
1	I	578	
1	J	578	
1	K	578	
2	D	478	

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Mol	Chain	Length	Quality of chain
2	E	478	
2	F	478	
2	L	478	
2	M	478	
2	N	478	
3	G	223	
3	O	223	
4	H	104	
4	P	104	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ADP	K	600	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32188 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called V-type ATP synthase alpha chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	B	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	C	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	I	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	J	561	Total	C	N	O	0	0	0
			2752	1630	561	561			
1	K	561	Total	C	N	O	0	0	0
			2752	1630	561	561			

- Molecule 2 is a protein called V-type ATP synthase beta chain.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	E	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	F	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	L	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	M	450	Total	C	N	O	0	0	0
			2212	1312	450	450			
2	N	450	Total	C	N	O	0	0	0
			2212	1312	450	450			

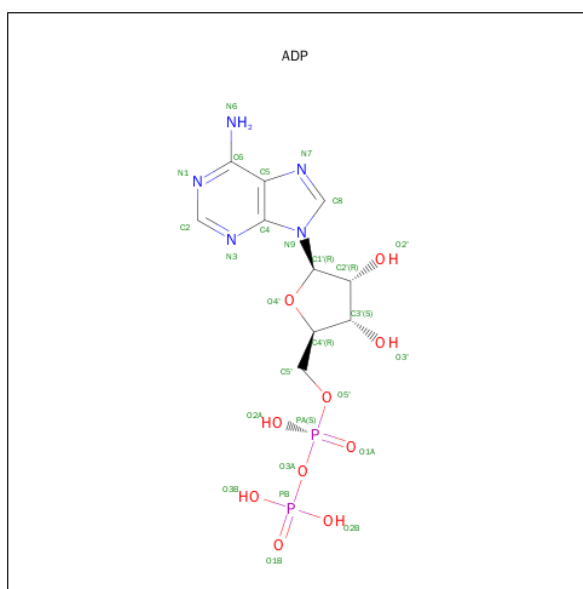
- Molecule 3 is a protein called V-type ATP synthase subunit D.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	129	Total	C	N	O	0	0	0
			639	381	129	129			
3	O	129	Total	C	N	O	0	0	0
			639	381	129	129			

- Molecule 4 is a protein called V-type ATP synthase subunit F.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	104	Total	C	N	O	0	0	0
			509	301	104	104			
4	P	104	Total	C	N	O	0	0	0
			509	301	104	104			

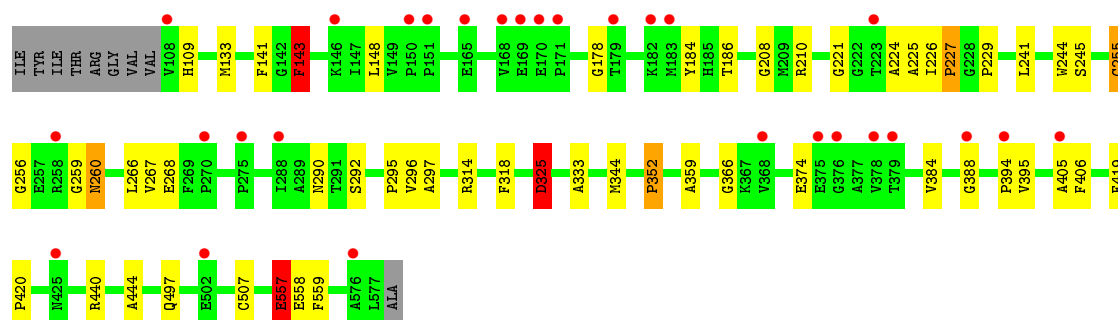
- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



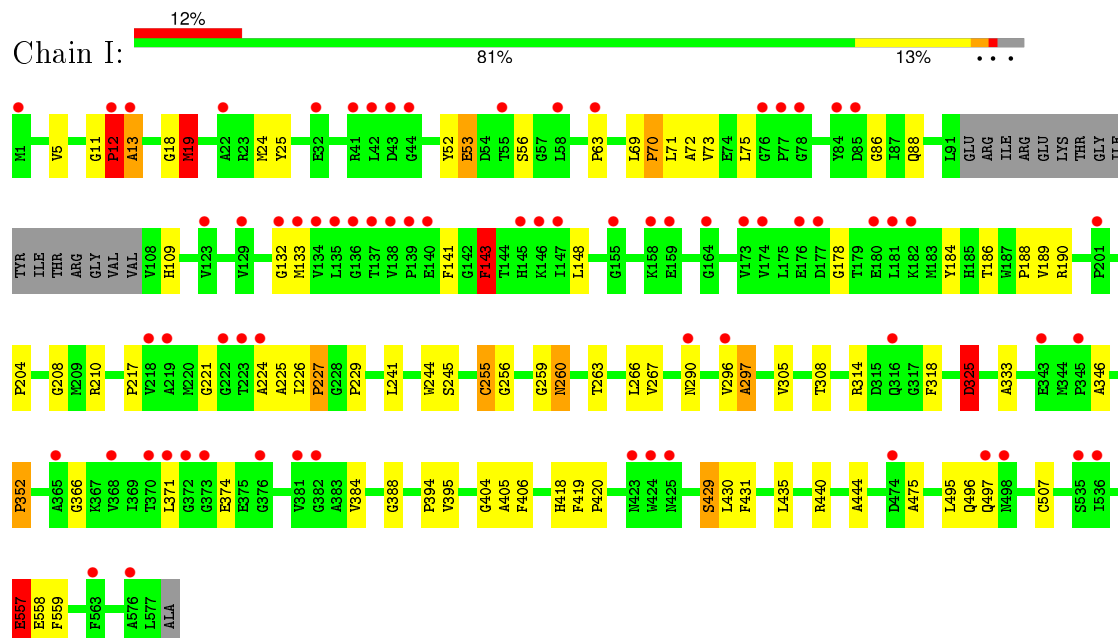
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
5	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 1: V-type ATP synthase alpha chain

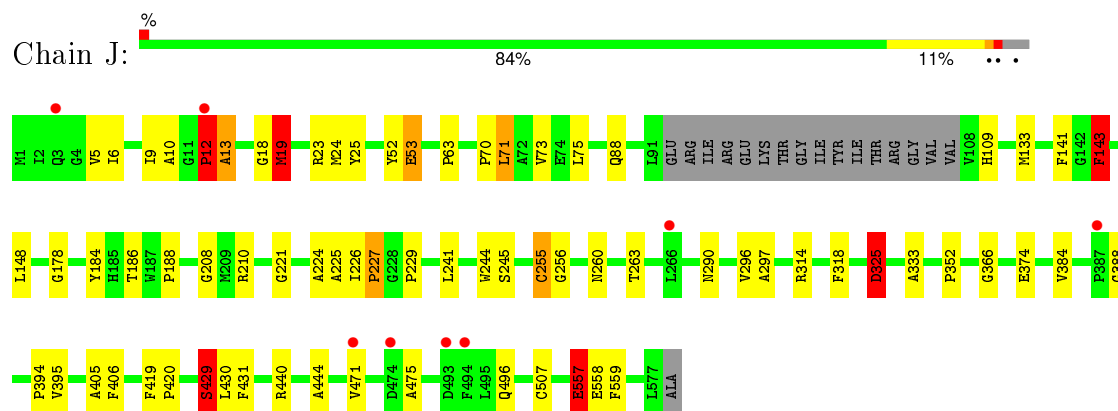




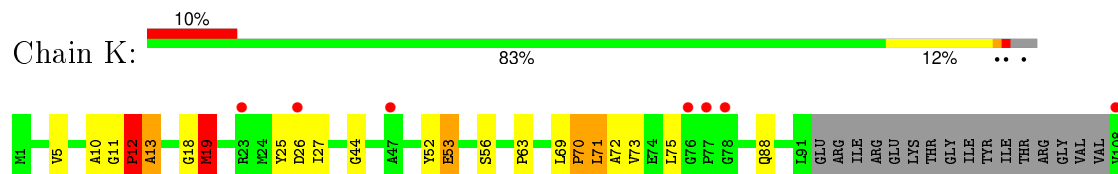
• Molecule 1: V-type ATP synthase alpha chain

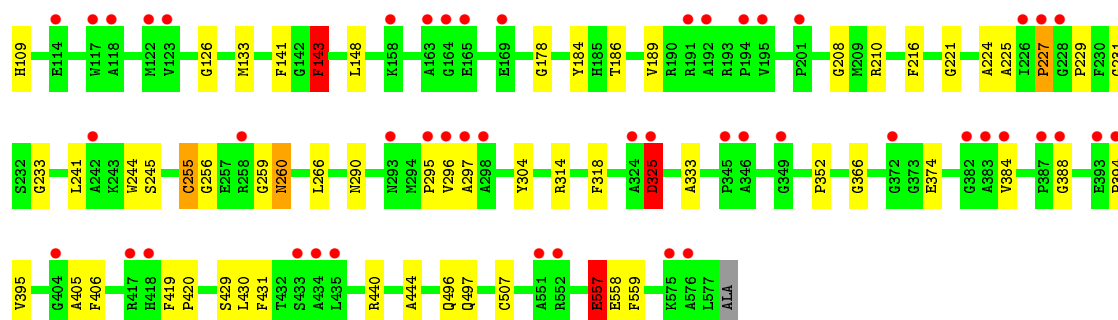


• Molecule 1: V-type ATP synthase alpha chain

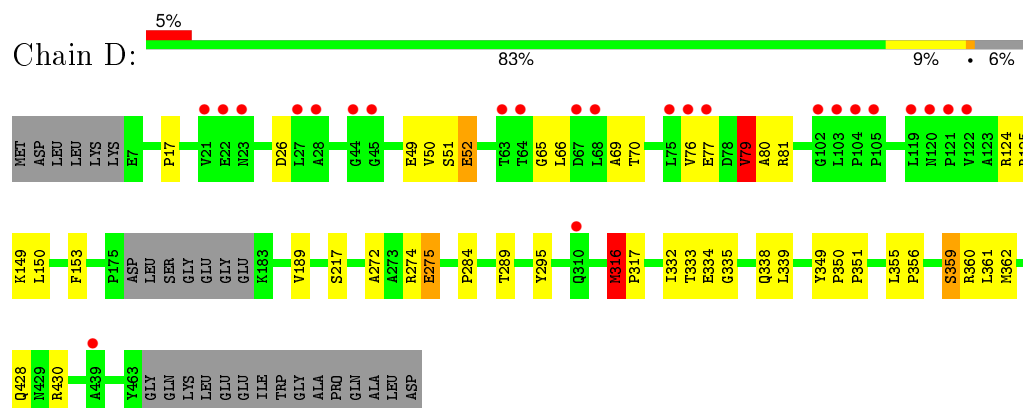


• Molecule 1: V-type ATP synthase alpha chain

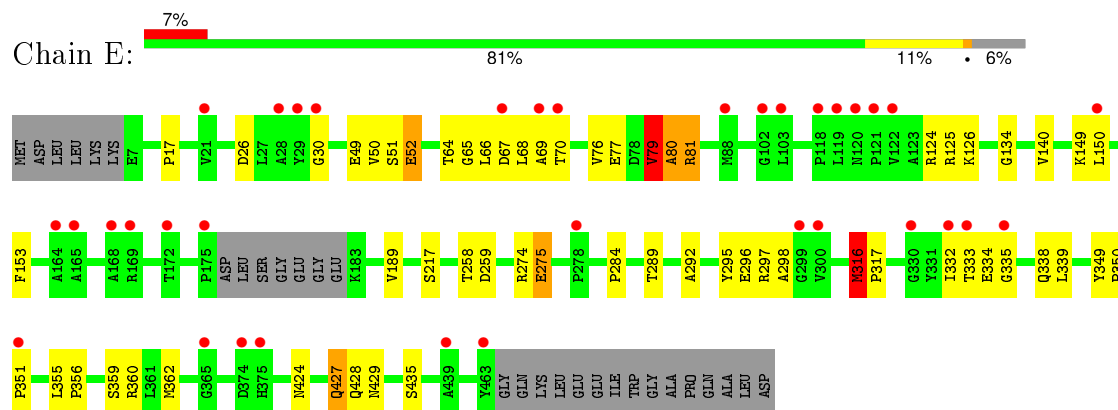




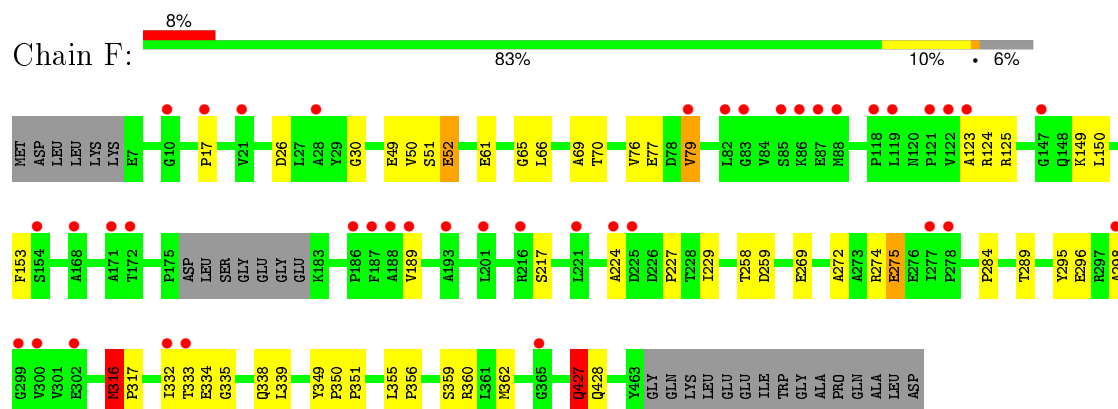
• Molecule 2: V-type ATP synthase beta chain



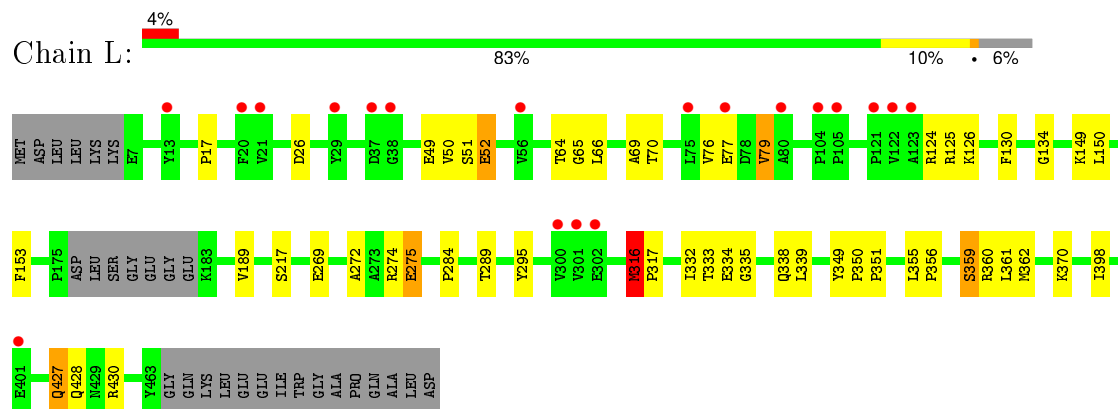
• Molecule 2: V-type ATP synthase beta chain



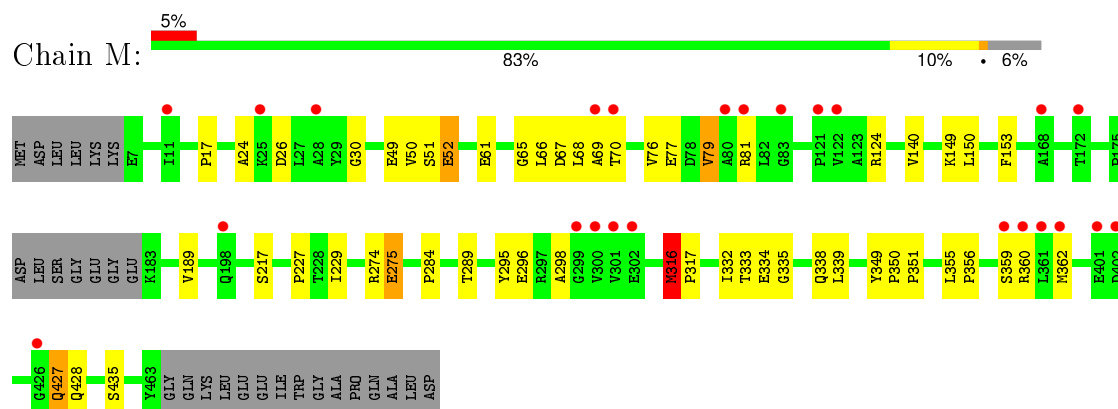
• Molecule 2: V-type ATP synthase beta chain



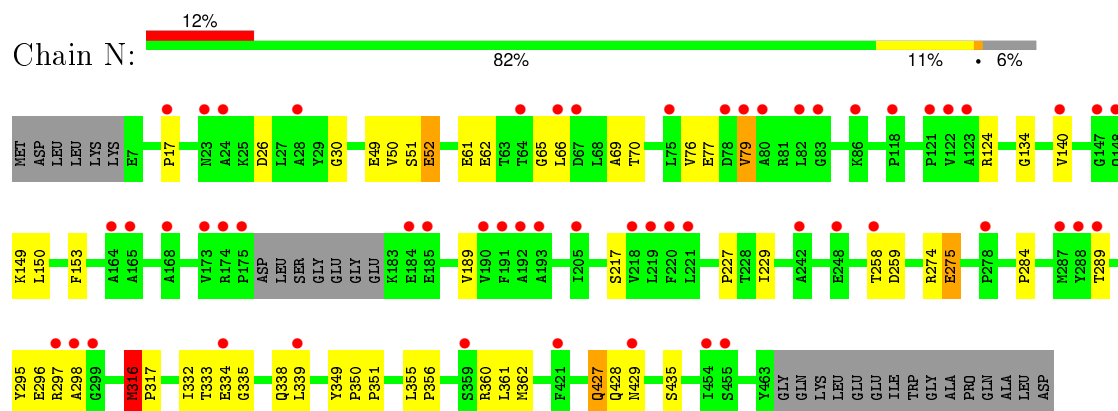
- Molecule 2: V-type ATP synthase beta chain



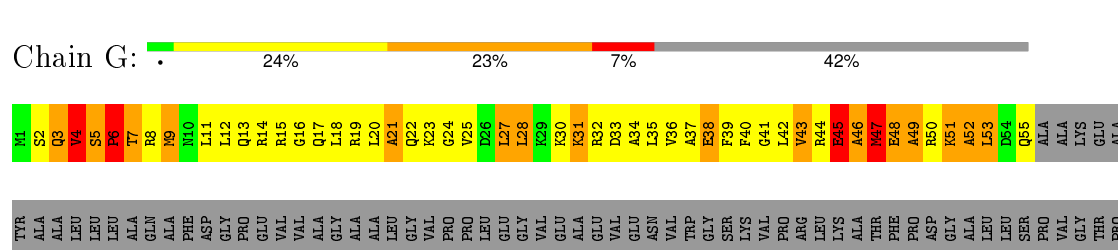
- Molecule 2: V-type ATP synthase beta chain



- Molecule 2: V-type ATP synthase beta chain



- Molecule 3: V-type ATP synthase subunit D



ALA TYR THR LEU GLU ALA SER ARG ALA ARG
 Q181 V182 L183 E184 Q185 R186 E187 R188 E189 D190 T191 F192 Y193 R193 A194 E195 A196 I197 L197 K198 I198 R199 R200 V140 A141 I201 E202 N142 T143 E204 R204 E205 R146 L147 K148 K149 I150 G151 E152 E153 I154 PRO K155 K156 T157 T158 T159 R160 V161 N162 N163 A163 L164 E165 Q166 V167 V168 I169 P170 G171 G172 R173 A174 Q175 I176 R177 F178 I179 Q180

Q181 V182 L183 E184 Q185 R186 E187 R188 E189 D190 T191 F192 Y193 R193 A194 E195 A196 I197 L197 K198 I198 R199 R200 V140 A141 I201 E202 N142 T143 E204 R204 E205 R146 L147 K148 K149 I150 G151 E152 E153 I154 PRO K155 K156 T157 T158 T159 R160 V161 N162 N163 A163 L164 E165 Q166 V167 V168 I169 P170 G171 G172 R173 A174 Q175 I176 R177 F178 I179 Q180

• Molecule 3: V-type ATP synthase subunit D

Chain O: 23% 24% 8% 42%

R1 S2 Q3 V4 S5 P6 T7 R8 M9 N10 L11 F192 Y193 R193 A194 E195 A196 I197 L197 K198 I198 R199 R200 V140 A141 I201 E202 N142 T143 E204 R204 E205 R146 L147 K148 K149 I150 G151 E152 E153 I154 PRO K155 K156 T157 T158 T159 R160 V161 N162 N163 A163 L164 E165 Q166 V167 V168 I169 P170 G171 G172 R173 A174 Q175 I176 R177 F178 I179 Q180

TYR ALA ALA LEU LEU LEU ALA ALA GLN ALA PHE ASP ARG R132 Y193 R193 A194 E195 A196 I197 L197 K198 I198 R199 R200 V140 A141 I201 E202 N142 T143 E204 R204 E205 R146 L147 K148 K149 I150 G151 E152 E153 I154 PRO K155 K156 T157 T158 T159 R160 V161 N162 N163 A163 L164 E165 Q166 V167 V168 I169 P170 G171 G172 R173 A174 Q175 I176 R177 F178 I179 Q180

ALA TYR THR LEU GLU ALA SER ARG ALA ARG
 Q181 V182 L183 E184 Q185 R186 E187 R188 E189 D190 T191 F192 Y193 R193 A194 E195 A196 I197 L197 K198 I198 R199 R200 V140 A141 I201 E202 N142 T143 E204 R204 E205 R146 L147 K148 K149 I150 G151 E152 E153 I154 PRO K155 K156 T157 T158 T159 R160 V161 N162 N163 A163 L164 E165 Q166 V167 V168 I169 P170 G171 G172 R173 A174 Q175 I176 R177 F178 I179 Q180

Q181 V182 L183 E184 Q185 R186 E187 R188 E189 D190 T191 F192 Y193 R193 A194 E195 A196 I197 L197 K198 I198 R199 R200 V140 A141 I201 E202 N142 T143 E204 R204 E205 R146 L147 K148 K149 I150 G151 E152 E153 I154 PRO K155 K156 T157 T158 T159 R160 V161 N162 N163 A163 L164 E165 Q166 V167 V168 I169 P170 G171 G172 R173 A174 Q175 I176 R177 F178 I179 Q180

• Molecule 4: V-type ATP synthase subunit F

Chain H: 6% 79% 18%

V1 A16 S25 A29 E34 T35 R39 G40 M63 R64 G65 R66 I74 A75 G76 L77 K78 Q82 G83 D84 V86 I98 G99 F100 L104

• Molecule 4: V-type ATP synthase subunit F

Chain P: 7% 77% 16% 7%

V1 A16 S25 A29 E34 T35 R39 G40 M63 R64 G65 R66 I74 A75 G76 L77 K78 Q82 G83 D84 V86 I98 G99 F100 L104

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	381.58Å 381.58Å 147.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.92 – 4.51 49.81 – 4.51	Depositor EDS
% Data completeness (in resolution range)	96.7 (29.92-4.51) 96.8 (49.81-4.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 4.45Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.429 , 0.437 0.421 , 0.428	Depositor DCC
R_{free} test set	3582 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	145.8	Xtriage
Anisotropy	0.008	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.01 , -10.0	EDS
Estimated twinning fraction	0.217 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.28$, $\langle L^2 \rangle = 0.13$	Xtriage
Outliers	1 of 70593 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.69	EDS
Total number of atoms	32188	wwPDB-VP
Average B, all atoms (Å ²)	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.61% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.59	3/2750 (0.1%)	1.20	9/3815 (0.2%)
1	B	0.59	3/2750 (0.1%)	1.21	12/3815 (0.3%)
1	C	0.59	3/2750 (0.1%)	1.20	10/3815 (0.3%)
1	I	0.59	3/2750 (0.1%)	1.38	13/3815 (0.3%)
1	J	0.59	3/2750 (0.1%)	1.21	11/3815 (0.3%)
1	K	0.60	3/2750 (0.1%)	1.34	13/3815 (0.3%)
2	D	0.80	7/2210 (0.3%)	1.03	13/3068 (0.4%)
2	E	0.85	7/2210 (0.3%)	1.04	10/3068 (0.3%)
2	F	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
2	L	0.74	3/2210 (0.1%)	1.01	9/3068 (0.3%)
2	M	0.75	3/2210 (0.1%)	1.00	8/3068 (0.3%)
2	N	0.73	3/2210 (0.1%)	0.99	7/3068 (0.2%)
3	G	4.09	122/637 (19.2%)	2.62	48/885 (5.4%)
3	O	4.09	126/637 (19.8%)	2.63	50/885 (5.6%)
4	H	1.48	6/508 (1.2%)	1.43	9/703 (1.3%)
4	P	1.78	10/508 (2.0%)	2.16	15/703 (2.1%)
All	All	1.08	308/32050 (1.0%)	1.27	244/44474 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	B	0	5
1	C	0	5
1	I	0	6
1	J	0	6
1	K	0	6
2	D	0	4

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	4
2	F	0	3
2	L	0	4
2	M	0	3
2	N	0	3
4	H	0	3
4	P	0	2
All	All	0	60

All (308) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	47	MET	CA-CB	-25.00	0.98	1.53
3	G	47	MET	CA-CB	-24.93	0.99	1.53
3	O	27	LEU	CA-CB	14.81	1.87	1.53
3	G	27	LEU	CA-CB	14.78	1.87	1.53
4	P	75	ALA	N-CA	13.48	1.73	1.46
3	O	7	THR	CA-CB	12.79	1.86	1.53
3	G	7	THR	CA-CB	12.64	1.86	1.53
3	O	31	LYS	N-CA	12.38	1.71	1.46
3	G	31	LYS	N-CA	12.15	1.70	1.46
3	G	196	ARG	CA-C	12.11	1.84	1.52
3	G	138	ILE	CA-CB	-12.09	1.27	1.54
3	O	138	ILE	CA-CB	-12.06	1.27	1.54
3	O	196	ARG	CA-C	12.06	1.84	1.52
4	P	76	GLY	CA-C	11.97	1.71	1.51
3	O	205	GLU	CA-CB	11.22	1.78	1.53
3	O	52	ALA	CA-CB	11.20	1.75	1.52
3	G	52	ALA	CA-CB	11.16	1.75	1.52
3	G	168	VAL	CA-CB	-11.09	1.31	1.54
3	G	16	GLY	CA-C	11.05	1.69	1.51
3	O	16	GLY	CA-C	11.05	1.69	1.51
4	P	75	ALA	CA-C	11.02	1.81	1.52
3	O	168	VAL	CA-CB	-11.01	1.31	1.54
3	G	205	GLU	CA-CB	10.98	1.78	1.53
3	G	167	VAL	CA-C	10.92	1.81	1.52
3	O	167	VAL	CA-C	10.87	1.81	1.52
2	E	81	ARG	N-CA	10.68	1.67	1.46
4	H	34	GLU	C-O	10.58	1.43	1.23
3	O	171	GLY	CA-C	10.58	1.68	1.51
4	P	34	GLU	C-O	10.56	1.43	1.23
3	G	171	GLY	CA-C	10.52	1.68	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	16	GLY	C-O	10.30	1.40	1.23
3	G	189	GLU	CA-CB	10.27	1.76	1.53
3	O	189	GLU	CA-CB	10.16	1.76	1.53
3	G	16	GLY	C-O	9.98	1.39	1.23
2	E	80	ALA	CA-C	9.83	1.78	1.52
3	O	4	VAL	CA-C	9.79	1.78	1.52
4	P	76	GLY	N-CA	9.77	1.60	1.46
3	G	4	VAL	CA-C	9.76	1.78	1.52
2	E	80	ALA	N-CA	9.63	1.65	1.46
2	E	81	ARG	CA-C	9.58	1.77	1.52
3	O	19	ARG	N-CA	9.50	1.65	1.46
3	G	19	ARG	N-CA	9.48	1.65	1.46
3	O	50	ARG	C-O	9.25	1.41	1.23
3	G	32	ARG	C-O	9.14	1.40	1.23
3	O	32	ARG	C-O	9.14	1.40	1.23
3	G	164	LEU	C-O	9.13	1.40	1.23
3	O	164	LEU	C-O	9.08	1.40	1.23
3	G	50	ARG	C-O	9.07	1.40	1.23
3	G	184	GLU	CA-CB	9.05	1.73	1.53
3	O	184	GLU	CA-CB	9.05	1.73	1.53
3	O	163	ALA	C-O	8.95	1.40	1.23
3	G	184	GLU	N-CA	8.95	1.64	1.46
3	G	6	PRO	C-O	8.93	1.41	1.23
3	O	184	GLU	N-CA	8.92	1.64	1.46
3	G	163	ALA	C-O	8.87	1.40	1.23
3	O	169	ILE	C-O	8.76	1.40	1.23
3	G	169	ILE	C-O	8.71	1.40	1.23
3	O	6	PRO	C-O	8.69	1.40	1.23
3	O	142	ASN	CA-CB	8.65	1.75	1.53
3	G	142	ASN	CA-CB	8.62	1.75	1.53
3	G	183	LEU	C-O	8.62	1.39	1.23
3	G	194	LEU	CA-C	8.56	1.75	1.52
3	O	183	LEU	C-O	8.54	1.39	1.23
3	O	194	LEU	CA-C	8.47	1.75	1.52
3	G	163	ALA	CA-C	8.46	1.75	1.52
3	O	38	GLU	N-CA	8.39	1.63	1.46
3	O	163	ALA	CA-C	8.36	1.74	1.52
3	G	38	GLU	N-CA	8.33	1.63	1.46
3	G	182	VAL	N-CA	8.28	1.62	1.46
3	O	182	VAL	N-CA	8.26	1.62	1.46
2	D	81	ARG	N-CA	8.25	1.62	1.46
4	P	40	GLY	C-O	8.24	1.36	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	40	GLY	C-O	8.09	1.36	1.23
3	O	155	LYS	N-CA	8.04	1.62	1.46
3	O	34	ALA	CA-CB	-8.03	1.35	1.52
3	G	34	ALA	CA-CB	-8.01	1.35	1.52
3	G	155	LYS	N-CA	8.00	1.62	1.46
3	G	195	LYS	N-CA	7.95	1.62	1.46
3	O	185	GLN	C-O	7.89	1.38	1.23
3	O	205	GLU	CA-C	7.89	1.73	1.52
3	O	195	LYS	N-CA	7.88	1.62	1.46
3	O	170	PRO	CA-C	7.88	1.68	1.52
3	G	185	GLN	C-O	7.83	1.38	1.23
3	G	205	GLU	CA-C	7.82	1.73	1.52
3	G	24	GLY	CA-C	7.72	1.64	1.51
3	G	170	PRO	CA-C	7.71	1.68	1.52
3	O	198	LYS	C-O	7.70	1.38	1.23
3	G	198	LYS	C-O	7.67	1.38	1.23
3	G	46	ALA	C-O	7.62	1.37	1.23
3	G	192	PHE	C-O	7.60	1.37	1.23
3	O	24	GLY	CA-C	7.57	1.64	1.51
2	D	80	ALA	CA-C	7.57	1.72	1.52
3	O	192	PHE	C-O	7.56	1.37	1.23
3	O	46	ALA	C-O	7.54	1.37	1.23
3	O	51	LYS	C-O	7.48	1.37	1.23
3	G	134	ALA	CA-CB	7.44	1.68	1.52
3	O	4	VAL	CA-CB	7.43	1.70	1.54
3	G	4	VAL	CA-CB	7.41	1.70	1.54
3	G	33	ASP	N-CA	7.39	1.61	1.46
3	O	33	ASP	N-CA	7.39	1.61	1.46
3	O	134	ALA	N-CA	7.37	1.61	1.46
3	O	134	ALA	CA-CB	7.36	1.67	1.52
3	G	51	LYS	C-O	7.33	1.37	1.23
3	G	134	ALA	N-CA	7.31	1.60	1.46
3	O	146	ARG	CA-CB	7.30	1.70	1.53
3	G	6	PRO	CA-CB	7.28	1.68	1.53
3	G	167	VAL	CA-CB	7.28	1.70	1.54
3	G	22	GLN	C-O	7.27	1.37	1.23
3	G	146	ARG	CA-CB	7.26	1.70	1.53
3	O	53	LEU	N-CA	7.24	1.60	1.46
3	O	22	GLN	C-O	7.22	1.37	1.23
3	O	20	LEU	CA-C	7.20	1.71	1.52
3	G	20	LEU	CA-C	7.20	1.71	1.52
3	O	167	VAL	CA-CB	7.14	1.69	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	6	PRO	CA-CB	7.14	1.67	1.53
3	O	172	ILE	N-CA	7.14	1.60	1.46
3	G	193	ARG	N-CA	7.13	1.60	1.46
3	O	193	ARG	N-CA	7.11	1.60	1.46
3	G	172	ILE	N-CA	7.09	1.60	1.46
3	G	53	LEU	N-CA	7.08	1.60	1.46
3	O	27	LEU	N-CA	7.08	1.60	1.46
3	G	188	ARG	N-CA	7.06	1.60	1.46
3	G	154	ILE	C-O	7.04	1.36	1.23
2	D	81	ARG	CA-C	7.03	1.71	1.52
3	G	27	LEU	N-CA	7.02	1.60	1.46
3	O	52	ALA	N-CA	7.02	1.60	1.46
3	O	188	ARG	N-CA	7.01	1.60	1.46
3	G	199	GLY	N-CA	6.96	1.56	1.46
3	G	179	ILE	C-O	6.95	1.36	1.23
3	G	4	VAL	C-O	6.95	1.36	1.23
3	O	11	LEU	CA-CB	6.94	1.69	1.53
3	G	52	ALA	N-CA	6.93	1.60	1.46
3	G	156	LYS	CA-C	6.92	1.71	1.52
3	G	32	ARG	CA-C	6.91	1.71	1.52
3	G	11	LEU	CA-CB	6.91	1.69	1.53
3	O	179	ILE	C-O	6.88	1.36	1.23
3	O	156	LYS	CA-C	6.88	1.70	1.52
3	O	32	ARG	CA-C	6.87	1.70	1.52
3	O	4	VAL	C-O	6.84	1.36	1.23
3	O	154	ILE	C-O	6.80	1.36	1.23
3	O	199	GLY	N-CA	6.71	1.56	1.46
4	P	75	ALA	C-N	6.69	1.45	1.33
3	O	169	ILE	N-CA	6.62	1.59	1.46
2	D	80	ALA	N-CA	6.61	1.59	1.46
3	G	204	ARG	N-CA	6.60	1.59	1.46
3	O	175	GLN	CA-CB	-6.60	1.39	1.53
3	G	5	SER	CA-CB	6.58	1.62	1.52
3	G	17	GLN	CA-CB	-6.57	1.39	1.53
3	O	204	ARG	N-CA	6.56	1.59	1.46
3	G	169	ILE	N-CA	6.54	1.59	1.46
3	O	32	ARG	C-N	6.53	1.49	1.34
3	G	189	GLU	CA-C	6.49	1.69	1.52
3	G	32	ARG	C-N	6.48	1.49	1.34
3	G	175	GLN	CA-CB	-6.47	1.39	1.53
3	O	17	GLN	CA-CB	-6.47	1.39	1.53
3	G	148	LYS	CA-CB	6.46	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	O	148	LYS	CA-CB	6.43	1.68	1.53
3	G	14	ARG	N-CA	6.42	1.59	1.46
3	O	189	GLU	CA-C	6.41	1.69	1.52
3	O	9	MET	CA-C	-6.39	1.36	1.52
3	O	5	SER	CA-CB	6.38	1.62	1.52
3	O	31	LYS	C-O	6.35	1.35	1.23
3	O	196	ARG	CA-CB	6.34	1.68	1.53
3	G	28	LEU	CA-C	6.33	1.69	1.52
3	G	14	ARG	C-O	6.32	1.35	1.23
3	G	196	ARG	CA-CB	6.31	1.67	1.53
3	O	14	ARG	C-O	6.29	1.35	1.23
3	G	9	MET	CA-C	-6.28	1.36	1.52
4	H	40	GLY	C-N	6.22	1.44	1.33
3	O	14	ARG	N-CA	6.20	1.58	1.46
3	O	28	LEU	CA-C	6.19	1.69	1.52
3	O	192	PHE	CA-C	6.19	1.69	1.52
3	G	31	LYS	C-O	6.18	1.35	1.23
3	O	24	GLY	C-O	6.17	1.33	1.23
3	G	192	PHE	CA-C	6.16	1.69	1.52
4	P	40	GLY	C-N	6.14	1.44	1.33
3	O	45	GLU	C-O	6.11	1.34	1.23
1	J	13	ALA	CA-CB	-6.09	1.39	1.52
1	B	13	ALA	CA-CB	-6.08	1.39	1.52
3	G	164	LEU	N-CA	6.08	1.58	1.46
1	K	13	ALA	CA-CB	-6.07	1.39	1.52
1	C	13	ALA	CA-CB	-6.05	1.39	1.52
3	O	164	LEU	N-CA	6.03	1.58	1.46
3	O	201	ILE	CA-CB	-6.03	1.41	1.54
1	A	13	ALA	CA-CB	-6.02	1.39	1.52
3	O	203	ALA	N-CA	-6.01	1.34	1.46
3	G	205	GLU	C-O	6.01	1.34	1.23
3	G	201	ILE	CA-CB	-6.00	1.41	1.54
1	I	13	ALA	CA-CB	-6.00	1.39	1.52
3	G	45	GLU	C-O	6.00	1.34	1.23
3	O	194	LEU	C-O	6.00	1.34	1.23
3	G	194	LEU	C-O	5.98	1.34	1.23
3	O	205	GLU	C-O	5.98	1.34	1.23
3	G	7	THR	CA-C	5.96	1.68	1.52
3	G	166	GLN	CA-CB	-5.95	1.40	1.53
3	O	7	THR	CA-C	5.95	1.68	1.52
3	O	166	GLN	CA-CB	-5.91	1.41	1.53
3	G	24	GLY	C-O	5.86	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	203	ALA	N-CA	-5.80	1.34	1.46
3	G	21	ALA	C-O	5.80	1.34	1.23
3	O	14	ARG	CA-CB	5.79	1.66	1.53
3	G	37	ALA	CA-CB	-5.79	1.40	1.52
3	O	141	ALA	CA-CB	5.75	1.64	1.52
3	G	23	LYS	N-CA	5.72	1.57	1.46
3	O	23	LYS	N-CA	5.72	1.57	1.46
3	G	52	ALA	C-O	5.70	1.34	1.23
3	G	170	PRO	N-CA	5.70	1.56	1.47
3	O	21	ALA	C-O	5.69	1.34	1.23
3	O	52	ALA	C-O	5.69	1.34	1.23
3	G	49	ALA	N-CA	5.66	1.57	1.46
2	L	275	GLU	CA-CB	-5.65	1.41	1.53
3	O	37	ALA	CA-CB	-5.64	1.40	1.52
2	N	275	GLU	CA-CB	-5.64	1.41	1.53
4	H	25	SER	CA-CB	5.62	1.61	1.52
3	G	49	ALA	CA-CB	-5.62	1.40	1.52
3	O	170	PRO	N-CA	5.61	1.56	1.47
3	G	141	ALA	CA-CB	5.60	1.64	1.52
3	O	47	MET	C-O	5.59	1.33	1.23
3	G	47	MET	C-O	5.59	1.33	1.23
2	M	275	GLU	CA-CB	-5.59	1.41	1.53
3	G	14	ARG	CA-CB	5.58	1.66	1.53
3	G	158	THR	CA-CB	-5.58	1.38	1.53
2	F	275	GLU	CA-CB	-5.57	1.41	1.53
2	E	275	GLU	CA-CB	-5.56	1.41	1.53
3	G	15	ARG	CA-CB	5.56	1.66	1.53
3	G	25	VAL	N-CA	5.55	1.57	1.46
3	O	25	VAL	N-CA	5.54	1.57	1.46
3	O	158	THR	CA-CB	-5.54	1.39	1.53
3	O	171	GLY	C-O	5.53	1.32	1.23
3	G	148	LYS	N-CA	5.52	1.57	1.46
3	O	49	ALA	N-CA	5.52	1.57	1.46
3	O	148	LYS	N-CA	5.51	1.57	1.46
3	O	15	ARG	CA-CB	5.51	1.66	1.53
2	L	289	THR	C-N	5.51	1.46	1.34
4	P	25	SER	CA-CB	5.48	1.61	1.52
3	G	171	GLY	C-O	5.48	1.32	1.23
2	D	275	GLU	CA-CB	-5.47	1.42	1.53
3	O	187	GLU	CA-C	5.47	1.67	1.52
3	G	36	VAL	CA-C	5.46	1.67	1.52
3	O	49	ALA	CA-CB	-5.46	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7	THR	C-O	5.44	1.33	1.23
3	G	187	GLU	CA-C	5.43	1.67	1.52
3	G	163	ALA	C-N	5.43	1.46	1.34
3	O	163	ALA	C-N	5.43	1.46	1.34
2	L	316	MET	C-N	-5.42	1.24	1.34
2	E	316	MET	C-N	-5.42	1.24	1.34
3	O	7	THR	C-O	5.42	1.33	1.23
3	O	36	VAL	CA-C	5.39	1.67	1.52
1	J	19	MET	CA-CB	-5.38	1.42	1.53
2	N	316	MET	C-N	-5.38	1.24	1.34
1	K	19	MET	CA-CB	-5.36	1.42	1.53
2	M	289	THR	C-N	5.36	1.46	1.34
1	I	19	MET	CA-CB	-5.35	1.42	1.53
3	O	28	LEU	C-O	5.35	1.33	1.23
1	C	19	MET	CA-CB	-5.34	1.42	1.53
1	I	352	PRO	CA-CB	-5.33	1.42	1.53
2	M	316	MET	C-N	-5.33	1.24	1.34
1	J	352	PRO	CA-CB	-5.32	1.43	1.53
2	N	289	THR	C-N	5.32	1.46	1.34
2	E	289	THR	C-N	5.31	1.46	1.34
2	F	289	THR	C-N	5.31	1.46	1.34
1	A	19	MET	CA-CB	-5.30	1.42	1.53
1	B	19	MET	CA-CB	-5.30	1.42	1.53
2	D	289	THR	C-N	5.30	1.46	1.34
3	G	15	ARG	C-O	5.29	1.33	1.23
4	H	75	ALA	N-CA	5.29	1.56	1.46
2	F	316	MET	C-N	-5.26	1.24	1.34
3	O	7	THR	N-CA	5.26	1.56	1.46
1	B	352	PRO	CA-CB	-5.25	1.43	1.53
3	G	28	LEU	C-O	5.25	1.33	1.23
1	K	352	PRO	CA-CB	-5.25	1.43	1.53
4	P	29	ALA	CA-CB	-5.24	1.41	1.52
1	A	352	PRO	CA-CB	-5.23	1.43	1.53
3	G	7	THR	N-CA	5.22	1.56	1.46
3	O	196	ARG	C-O	5.21	1.33	1.23
3	G	153	GLU	N-CA	5.21	1.56	1.46
3	O	138	ILE	CA-C	-5.20	1.39	1.52
3	O	49	ALA	CA-C	-5.19	1.39	1.52
3	G	162	ASN	C-O	5.19	1.33	1.23
4	H	29	ALA	CA-CB	-5.19	1.41	1.52
3	G	200	LYS	CA-C	5.17	1.66	1.52
3	O	153	GLU	N-CA	5.17	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	143	THR	N-CA	5.17	1.56	1.46
3	G	201	ILE	C-O	5.17	1.33	1.23
3	G	49	ALA	CA-C	-5.16	1.39	1.52
3	G	196	ARG	C-O	5.16	1.33	1.23
3	G	36	VAL	C-O	5.15	1.33	1.23
3	G	37	ALA	C-O	5.15	1.33	1.23
3	O	201	ILE	C-O	5.13	1.33	1.23
3	O	15	ARG	C-O	5.13	1.33	1.23
2	D	316	MET	C-N	-5.13	1.24	1.34
3	O	143	THR	N-CA	5.12	1.56	1.46
3	G	165	GLU	C-O	5.12	1.33	1.23
3	G	139	ARG	CA-CB	5.12	1.65	1.53
3	O	36	VAL	CA-CB	5.12	1.65	1.54
3	O	162	ASN	C-O	5.12	1.33	1.23
3	G	22	GLN	C-N	5.11	1.45	1.34
3	O	165	GLU	C-O	5.10	1.33	1.23
3	O	200	LYS	CA-C	5.08	1.66	1.52
3	O	165	GLU	N-CA	5.08	1.56	1.46
3	G	138	ILE	CA-C	-5.06	1.39	1.52
1	C	352	PRO	CA-CB	-5.05	1.43	1.53
3	O	160	ARG	C-O	5.04	1.32	1.23
3	O	22	GLN	C-N	5.04	1.45	1.34
3	O	132	ARG	C-O	5.04	1.32	1.23
3	O	37	ALA	C-O	5.03	1.32	1.23
3	O	36	VAL	C-O	5.03	1.32	1.23
3	O	41	GLY	C-O	5.00	1.31	1.23

All (244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	325	ASP	O-C-N	-39.90	58.86	122.70
1	J	325	ASP	O-C-N	-39.89	58.87	122.70
1	C	325	ASP	O-C-N	-39.89	58.87	122.70
1	A	325	ASP	O-C-N	-39.88	58.89	122.70
1	K	325	ASP	O-C-N	-39.85	58.94	122.70
1	B	325	ASP	O-C-N	-39.85	58.95	122.70
1	K	70	PRO	C-N-CA	-27.45	53.06	121.70
4	P	76	GLY	N-CA-C	26.75	179.98	113.10
1	I	429	SER	O-C-N	25.71	163.84	122.70
1	I	429	SER	CA-C-N	-25.54	61.02	117.20
1	I	429	SER	C-N-CA	-21.28	68.49	121.70
1	K	70	PRO	CA-C-N	-19.68	73.90	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	P	74	ILE	O-C-N	-18.90	92.46	122.70
1	C	325	ASP	C-N-CA	-18.30	75.94	121.70
1	A	325	ASP	C-N-CA	-18.27	76.03	121.70
1	K	325	ASP	C-N-CA	-18.24	76.09	121.70
1	B	325	ASP	C-N-CA	-18.22	76.15	121.70
1	J	325	ASP	C-N-CA	-18.21	76.16	121.70
1	I	325	ASP	C-N-CA	-18.17	76.27	121.70
2	D	316	MET	O-C-N	-15.68	91.31	121.10
2	L	316	MET	O-C-N	-15.62	91.42	121.10
2	E	316	MET	O-C-N	-15.62	91.42	121.10
2	F	316	MET	O-C-N	-15.60	91.47	121.10
2	N	316	MET	O-C-N	-15.55	91.55	121.10
2	M	316	MET	O-C-N	-15.55	91.56	121.10
1	I	325	ASP	CA-C-N	15.11	150.44	117.20
1	B	325	ASP	CA-C-N	15.10	150.42	117.20
1	J	325	ASP	CA-C-N	15.07	150.36	117.20
1	A	325	ASP	CA-C-N	15.01	150.22	117.20
1	K	325	ASP	CA-C-N	15.00	150.20	117.20
1	C	325	ASP	CA-C-N	14.99	150.17	117.20
4	P	76	GLY	CA-C-N	14.65	149.44	117.20
1	K	70	PRO	O-C-N	13.39	144.13	122.70
4	H	77	LEU	C-N-CA	-13.22	88.66	121.70
4	P	74	ILE	CA-C-N	12.92	145.62	117.20
4	P	75	ALA	N-CA-C	12.21	143.98	111.00
4	P	77	LEU	C-N-CA	-11.86	92.06	121.70
4	P	76	GLY	CA-C-O	-11.47	99.96	120.60
3	O	47	MET	N-CA-C	10.66	139.78	111.00
3	G	47	MET	N-CA-C	10.63	139.70	111.00
3	O	139	ARG	N-CA-C	-10.47	82.73	111.00
3	G	139	ARG	N-CA-C	-10.45	82.78	111.00
4	P	76	GLY	C-N-CA	10.11	146.97	121.70
3	O	6	PRO	C-N-CA	-9.82	97.15	121.70
3	G	6	PRO	C-N-CA	-9.73	97.38	121.70
3	G	6	PRO	N-CA-CB	9.70	114.94	103.30
2	D	316	MET	CA-C-N	9.48	143.66	117.10
2	F	316	MET	CA-C-N	9.45	143.57	117.10
2	L	316	MET	CA-C-N	9.45	143.57	117.10
2	N	316	MET	CA-C-N	9.46	143.57	117.10
2	M	316	MET	CA-C-N	9.45	143.55	117.10
3	O	6	PRO	N-CA-CB	9.45	114.64	103.30
2	E	79	VAL	O-C-N	-9.44	107.59	122.70
2	E	316	MET	CA-C-N	9.44	143.53	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	9	MET	C-N-CA	-9.37	98.27	121.70
3	G	9	MET	C-N-CA	-9.36	98.31	121.70
1	J	429	SER	O-C-N	-9.29	107.84	122.70
3	O	49	ALA	C-N-CA	-9.14	98.84	121.70
4	P	75	ALA	C-N-CA	9.12	141.44	122.30
3	G	49	ALA	C-N-CA	-9.11	98.92	121.70
4	P	77	LEU	CA-C-N	8.73	136.40	117.20
1	I	63	PRO	N-CA-CB	8.72	113.76	103.30
1	C	63	PRO	N-CA-CB	8.68	113.71	103.30
1	K	63	PRO	N-CA-CB	8.64	113.67	103.30
1	B	63	PRO	N-CA-CB	8.60	113.62	103.30
3	G	47	MET	C-N-CA	-8.57	100.27	121.70
3	O	47	MET	C-N-CA	-8.57	100.28	121.70
1	A	63	PRO	N-CA-CB	8.55	113.56	103.30
1	J	63	PRO	N-CA-CB	8.55	113.56	103.30
3	G	187	GLU	N-CA-C	8.43	133.77	111.00
3	O	187	GLU	N-CA-C	8.36	133.58	111.00
3	G	31	LYS	CA-C-N	-8.29	98.97	117.20
3	O	31	LYS	CA-C-N	-8.27	99.00	117.20
1	B	429	SER	O-C-N	8.27	135.93	122.70
4	H	74	ILE	O-C-N	-8.23	109.53	122.70
2	E	81	ARG	N-CA-C	8.18	133.09	111.00
4	P	76	GLY	O-C-N	-8.06	109.81	122.70
4	H	76	GLY	C-N-CA	8.02	141.74	121.70
3	O	186	ARG	C-N-CA	-7.85	102.08	121.70
3	O	203	ALA	N-CA-C	-7.81	89.91	111.00
3	G	203	ALA	N-CA-C	-7.79	89.96	111.00
4	H	75	ALA	N-CA-C	7.75	131.93	111.00
3	G	186	ARG	C-N-CA	-7.65	102.56	121.70
3	G	167	VAL	O-C-N	-7.49	110.72	122.70
3	O	167	VAL	O-C-N	-7.47	110.74	122.70
4	H	77	LEU	CA-C-N	7.45	133.59	117.20
4	P	63	MET	N-CA-C	7.37	130.90	111.00
3	G	31	LYS	O-C-N	7.32	134.40	122.70
3	O	31	LYS	O-C-N	7.30	134.37	122.70
3	G	167	VAL	C-N-CA	-7.27	103.53	121.70
3	O	167	VAL	C-N-CA	-7.27	103.53	121.70
2	L	289	THR	O-C-N	-7.24	111.11	122.70
3	G	7	THR	C-N-CA	-7.20	103.71	121.70
2	D	289	THR	O-C-N	-7.18	111.21	122.70
2	E	289	THR	O-C-N	-7.18	111.22	122.70
2	M	289	THR	O-C-N	-7.15	111.27	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	289	THR	O-C-N	-7.14	111.27	122.70
3	O	7	THR	C-N-CA	-7.14	103.85	121.70
2	E	80	ALA	N-CA-C	7.10	130.17	111.00
3	O	170	PRO	N-CA-CB	7.10	111.82	103.30
3	O	30	LYS	C-N-CA	7.09	139.44	121.70
2	F	289	THR	O-C-N	-7.09	111.35	122.70
3	O	133	TYR	N-CA-C	-7.09	91.85	111.00
3	G	153	GLU	N-CA-C	7.09	130.14	111.00
3	G	30	LYS	C-N-CA	7.09	139.41	121.70
3	G	133	TYR	N-CA-C	-7.06	91.95	111.00
3	O	157	THR	N-CA-C	-7.01	92.07	111.00
3	O	153	GLU	N-CA-C	7.01	129.91	111.00
3	G	157	THR	N-CA-C	-6.99	92.12	111.00
3	G	170	PRO	N-CA-CB	6.99	111.69	103.30
3	G	202	GLU	CA-C-N	-6.97	101.87	117.20
3	O	182	VAL	O-C-N	6.97	133.85	122.70
4	P	77	LEU	O-C-N	-6.93	111.61	122.70
3	O	156	LYS	N-CA-C	6.90	129.63	111.00
3	O	202	GLU	CA-C-N	-6.90	102.03	117.20
3	G	151	GLY	N-CA-C	-6.89	95.88	113.10
3	G	156	LYS	N-CA-C	6.88	129.58	111.00
3	O	151	GLY	N-CA-C	-6.83	96.02	113.10
3	G	182	VAL	O-C-N	6.79	133.56	122.70
1	C	12	PRO	N-CA-CB	6.75	111.39	103.30
3	G	167	VAL	CA-C-N	6.73	132.01	117.20
3	G	12	LEU	N-CA-C	-6.70	92.92	111.00
3	O	167	VAL	CA-C-N	6.69	131.91	117.20
1	K	12	PRO	N-CA-CB	6.67	111.30	103.30
3	O	12	LEU	N-CA-C	-6.66	93.02	111.00
1	A	12	PRO	N-CA-CB	6.60	111.22	103.30
1	J	12	PRO	N-CA-CB	6.59	111.21	103.30
1	B	12	PRO	N-CA-CB	6.59	111.21	103.30
1	I	12	PRO	N-CA-CB	6.55	111.16	103.30
3	G	49	ALA	CA-C-N	-6.51	102.87	117.20
3	O	49	ALA	CA-C-N	-6.51	102.88	117.20
4	H	76	GLY	CA-C-N	6.50	131.49	117.20
3	G	154	ILE	N-CA-C	-6.47	93.52	111.00
2	D	289	THR	CA-C-N	6.47	131.44	117.20
2	E	289	THR	CA-C-N	6.47	131.43	117.20
3	G	156	LYS	C-N-CA	-6.46	105.54	121.70
3	O	156	LYS	C-N-CA	-6.45	105.58	121.70
3	O	154	ILE	N-CA-C	-6.44	93.61	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	143	PHE	N-CA-C	6.44	128.38	111.00
3	G	196	ARG	CB-CA-C	6.43	123.27	110.40
2	L	289	THR	CA-C-N	6.42	131.33	117.20
2	N	289	THR	CA-C-N	6.42	131.32	117.20
3	O	196	ARG	N-CA-CB	-6.40	99.08	110.60
1	C	143	PHE	N-CA-C	6.39	128.25	111.00
3	G	196	ARG	N-CA-CB	-6.39	99.10	110.60
1	J	143	PHE	N-CA-C	6.38	128.24	111.00
1	C	229	PRO	N-CA-CB	6.38	110.96	103.30
3	O	196	ARG	CB-CA-C	6.38	123.17	110.40
1	K	143	PHE	N-CA-C	6.38	128.21	111.00
1	B	143	PHE	N-CA-C	6.37	128.20	111.00
2	M	289	THR	CA-C-N	6.37	131.21	117.20
2	D	81	ARG	N-CA-C	6.35	128.15	111.00
2	F	289	THR	CA-C-N	6.34	131.14	117.20
1	B	429	SER	CA-C-N	-6.32	103.31	117.20
1	I	229	PRO	N-CA-CB	6.31	110.87	103.30
1	A	143	PHE	N-CA-C	6.29	127.97	111.00
1	B	229	PRO	N-CA-CB	6.28	110.84	103.30
3	G	199	GLY	N-CA-C	-6.27	97.42	113.10
1	J	229	PRO	N-CA-CB	6.26	110.82	103.30
3	O	199	GLY	N-CA-C	-6.25	97.47	113.10
1	K	229	PRO	N-CA-CB	6.23	110.77	103.30
2	L	360	ARG	N-CA-C	-6.16	94.36	111.00
3	O	21	ALA	O-C-N	6.14	132.53	122.70
1	A	229	PRO	N-CA-CB	6.09	110.61	103.30
3	G	21	ALA	O-C-N	6.06	132.40	122.70
2	D	17	PRO	N-CA-CB	6.00	110.50	103.30
2	F	17	PRO	N-CA-CB	5.99	110.49	103.30
2	E	17	PRO	N-CA-CB	5.99	110.49	103.30
3	G	194	LEU	N-CA-C	5.97	127.12	111.00
3	O	149	LYS	N-CA-C	-5.93	94.98	111.00
3	O	194	LEU	N-CA-C	5.93	127.02	111.00
2	L	284	PRO	N-CA-CB	5.92	110.40	103.30
2	N	351	PRO	N-CA-CB	5.92	110.40	103.30
2	L	17	PRO	N-CA-CB	5.91	110.39	103.30
2	D	284	PRO	N-CA-CB	5.90	110.38	103.30
2	N	284	PRO	N-CA-CB	5.90	110.38	103.30
2	N	17	PRO	N-CA-CB	5.89	110.37	103.30
2	M	351	PRO	N-CA-CB	5.89	110.36	103.30
3	G	149	LYS	N-CA-C	-5.87	95.15	111.00
2	E	284	PRO	N-CA-CB	5.87	110.34	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	M	17	PRO	N-CA-CB	5.86	110.33	103.30
3	G	188	ARG	N-CA-CB	5.85	121.13	110.60
2	D	351	PRO	N-CA-CB	5.84	110.31	103.30
2	D	79	VAL	CA-C-N	-5.83	104.37	117.20
2	M	284	PRO	N-CA-CB	5.82	110.29	103.30
3	O	21	ALA	CB-CA-C	-5.79	101.42	110.10
1	J	557	GLU	O-C-N	-5.78	113.45	122.70
2	F	284	PRO	N-CA-CB	5.77	110.23	103.30
2	L	351	PRO	N-CA-CB	5.77	110.22	103.30
3	O	136	ALA	N-CA-C	-5.76	95.45	111.00
1	C	557	GLU	O-C-N	-5.76	113.49	122.70
3	O	188	ARG	N-CA-CB	5.74	120.93	110.60
2	F	351	PRO	N-CA-CB	5.73	110.18	103.30
1	B	557	GLU	O-C-N	-5.73	113.54	122.70
1	A	557	GLU	O-C-N	-5.72	113.54	122.70
2	E	351	PRO	N-CA-CB	5.72	110.17	103.30
3	G	21	ALA	CB-CA-C	-5.72	101.52	110.10
1	I	557	GLU	O-C-N	-5.71	113.56	122.70
1	C	70	PRO	N-CA-C	-5.71	97.26	112.10
1	K	557	GLU	O-C-N	-5.69	113.60	122.70
3	G	47	MET	N-CA-CB	-5.69	100.36	110.60
3	O	47	MET	N-CA-CB	-5.67	100.40	110.60
3	G	142	ASN	N-CA-C	-5.66	95.71	111.00
3	G	136	ALA	N-CA-C	-5.64	95.77	111.00
1	B	429	SER	C-N-CA	-5.64	107.60	121.70
1	C	244	TRP	N-CA-C	5.63	126.21	111.00
1	K	244	TRP	N-CA-C	5.63	126.19	111.00
1	J	244	TRP	N-CA-C	5.62	126.17	111.00
1	I	244	TRP	N-CA-C	5.61	126.15	111.00
1	A	244	TRP	N-CA-C	5.61	126.13	111.00
1	B	244	TRP	N-CA-C	5.60	126.12	111.00
3	O	142	ASN	N-CA-C	-5.58	95.94	111.00
2	D	79	VAL	O-C-N	-5.57	113.79	122.70
3	G	47	MET	CA-C-O	5.45	131.55	120.10
1	J	429	SER	CA-C-N	5.44	129.17	117.20
4	H	76	GLY	CA-C-O	-5.43	110.83	120.60
3	G	174	ALA	C-N-CA	-5.42	108.14	121.70
2	L	359	SER	N-CA-C	-5.41	96.40	111.00
4	P	35	THR	CB-CA-C	-5.40	97.01	111.60
4	H	74	ILE	CA-C-N	5.40	129.08	117.20
4	H	35	THR	CB-CA-C	-5.40	97.03	111.60
2	D	360	ARG	N-CA-C	-5.38	96.47	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	155	LYS	C-N-CA	-5.37	108.27	121.70
3	O	174	ALA	C-N-CA	-5.37	108.27	121.70
3	O	140	VAL	N-CA-C	5.37	125.49	111.00
3	O	47	MET	CA-C-O	5.36	131.36	120.10
3	G	155	LYS	C-N-CA	-5.34	108.36	121.70
3	G	140	VAL	N-CA-C	5.33	125.38	111.00
1	I	70	PRO	N-CA-C	-5.28	98.37	112.10
3	O	171	GLY	N-CA-C	-5.22	100.04	113.10
3	G	31	LYS	CB-CA-C	-5.20	100.00	110.40
1	K	430	LEU	N-CA-C	-5.19	97.00	111.00
3	O	31	LYS	CB-CA-C	-5.18	100.03	110.40
2	D	80	ALA	N-CA-C	5.16	124.92	111.00
3	G	171	GLY	N-CA-C	-5.14	100.25	113.10
3	O	137	LEU	O-C-N	-5.13	114.48	122.70
3	O	156	LYS	CA-C-N	5.09	128.40	117.20
3	G	156	LYS	CA-C-N	5.09	128.39	117.20
2	M	81	ARG	N-CA-C	5.07	124.69	111.00
3	O	21	ALA	CA-C-N	-5.06	106.06	117.20
2	D	359	SER	N-CA-C	-5.05	97.35	111.00
3	G	21	ALA	CA-C-N	-5.04	106.11	117.20
3	O	47	MET	CB-CA-C	-5.03	100.35	110.40
4	P	62	LEU	C-N-CA	-5.02	109.16	121.70

There are no chirality outliers.

All (60) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	178	GLY	Peptide
1	A	210	ARG	Mainchain
1	A	297	ALA	Mainchain
1	A	325	ASP	Mainchain
1	A	557	GLU	Mainchain
1	A	69	LEU	Peptide
1	B	178	GLY	Peptide
1	B	210	ARG	Mainchain
1	B	297	ALA	Mainchain
1	B	325	ASP	Mainchain
1	B	557	GLU	Mainchain
1	C	178	GLY	Peptide
1	C	210	ARG	Mainchain
1	C	297	ALA	Mainchain
1	C	325	ASP	Mainchain

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Mol	Chain	Res	Type	Group
1	C	557	GLU	Mainchain
2	D	316	MET	Mainchain
2	D	427	GLN	Peptide
2	D	79	VAL	Mainchain,Peptide
2	E	316	MET	Mainchain
2	E	427	GLN	Peptide
2	E	79	VAL	Mainchain,Peptide
2	F	316	MET	Mainchain
2	F	427	GLN	Peptide
2	F	79	VAL	Mainchain
4	H	39	ARG	Peptide
4	H	76	GLY	Peptide
4	H	82	GLN	Peptide
1	I	178	GLY	Peptide
1	I	210	ARG	Mainchain
1	I	297	ALA	Mainchain
1	I	325	ASP	Mainchain
1	I	557	GLU	Mainchain
1	I	69	LEU	Peptide
1	J	178	GLY	Peptide
1	J	210	ARG	Mainchain
1	J	297	ALA	Mainchain
1	J	325	ASP	Mainchain
1	J	429	SER	Mainchain
1	J	557	GLU	Mainchain
1	K	178	GLY	Peptide
1	K	210	ARG	Mainchain
1	K	297	ALA	Mainchain
1	K	325	ASP	Mainchain
1	K	557	GLU	Mainchain
1	K	70	PRO	Mainchain
2	L	316	MET	Mainchain
2	L	427	GLN	Peptide
2	L	79	VAL	Mainchain,Peptide
2	M	316	MET	Mainchain
2	M	427	GLN	Peptide
2	M	79	VAL	Mainchain
2	N	316	MET	Mainchain
2	N	427	GLN	Peptide
2	N	79	VAL	Mainchain
4	P	39	ARG	Peptide
4	P	82	GLN	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	1302	92	0
1	B	2752	0	1303	65	0
1	C	2752	0	1303	100	0
1	I	2752	0	1300	122	0
1	J	2752	0	1303	61	2
1	K	2752	0	1302	94	0
2	D	2212	0	1009	66	0
2	E	2212	0	1008	80	0
2	F	2212	0	1009	94	0
2	L	2212	0	1009	80	0
2	M	2212	0	1009	59	2
2	N	2212	0	1009	76	0
3	G	639	0	299	131	0
3	O	639	0	299	136	0
4	H	509	0	255	12	0
4	P	509	0	255	23	0
5	A	27	0	12	2	0
5	C	27	0	12	1	0
5	I	27	0	12	0	0
5	K	27	0	12	5	0
All	All	32188	0	15022	1021	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (1021) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:142:ASN:CB	3:O:142:ASN:CA	1.75	1.65
3:O:189:GLU:CA	3:O:189:GLU:CB	1.76	1.64
3:G:205:GLU:CA	3:G:205:GLU:CB	1.78	1.62
3:O:52:ALA:CB	3:O:52:ALA:CA	1.76	1.59
3:G:189:GLU:CB	3:G:189:GLU:CA	1.76	1.58
1:C:352:PRO:CB	2:F:269:GLU:CA	1.80	1.58
3:O:205:GLU:CB	3:O:205:GLU:CA	1.78	1.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:475:ALA:HB1	4:P:100:PHE:CB	1.33	1.57
3:G:52:ALA:CB	3:G:52:ALA:CA	1.75	1.57
1:I:71:LEU:CB	1:I:188:PRO:HA	1.09	1.56
3:O:163:ALA:C	3:O:163:ALA:CA	1.74	1.55
3:G:163:ALA:CA	3:G:163:ALA:C	1.74	1.55
2:E:81:ARG:CA	2:E:81:ARG:N	1.67	1.54
1:K:52:TYR:HA	1:K:295:PRO:CB	1.08	1.54
3:G:7:THR:CB	3:G:7:THR:CA	1.86	1.54
3:G:142:ASN:CB	3:G:142:ASN:CA	1.75	1.54
3:O:31:LYS:N	3:O:31:LYS:CA	1.71	1.53
2:E:81:ARG:CA	2:E:81:ARG:C	1.77	1.53
1:I:24:MET:HA	2:L:66:LEU:CA	1.38	1.53
3:G:194:LEU:C	3:G:194:LEU:CA	1.75	1.52
1:K:52:TYR:CA	1:K:295:PRO:CB	1.85	1.51
2:N:140:VAL:CB	2:N:435:SER:CB	1.84	1.51
3:O:7:THR:CB	3:O:7:THR:CA	1.86	1.51
3:O:27:LEU:CB	3:O:27:LEU:CA	1.87	1.51
3:O:4:VAL:C	3:O:4:VAL:CA	1.78	1.51
3:O:194:LEU:C	3:O:194:LEU:CA	1.75	1.51
3:G:31:LYS:CA	3:G:31:LYS:N	1.70	1.50
3:G:27:LEU:CA	3:G:27:LEU:CB	1.87	1.50
2:E:80:ALA:C	2:E:80:ALA:CA	1.78	1.50
1:I:267:VAL:N	2:N:124:ARG:CB	1.70	1.49
3:G:4:VAL:C	3:G:4:VAL:CA	1.78	1.49
3:G:167:VAL:C	3:G:167:VAL:CA	1.81	1.49
1:C:344:MET:CB	2:F:272:ALA:HB1	1.42	1.49
4:P:75:ALA:C	4:P:75:ALA:CA	1.81	1.49
3:O:167:VAL:C	3:O:167:VAL:CA	1.81	1.49
4:P:75:ALA:N	4:P:75:ALA:CA	1.73	1.47
1:C:352:PRO:CB	2:F:269:GLU:HA	1.00	1.46
3:O:196:ARG:C	3:O:196:ARG:CA	1.84	1.46
1:C:25:TYR:CB	2:F:65:GLY:HA2	1.42	1.46
1:I:25:TYR:N	2:L:66:LEU:H	0.97	1.44
1:B:471:VAL:CB	4:H:98:ILE:CB	1.95	1.43
3:G:196:ARG:CA	3:G:196:ARG:C	1.84	1.42
1:I:24:MET:CA	2:L:66:LEU:HA	1.48	1.42
1:I:25:TYR:H	2:L:66:LEU:N	1.16	1.40
2:E:359:SER:CB	2:E:362:MET:CB	1.99	1.40
1:J:475:ALA:CB	4:P:100:PHE:CB	1.99	1.38
1:I:11:GLY:CA	2:N:50:VAL:H	1.36	1.36
1:I:266:LEU:C	2:N:124:ARG:CB	1.93	1.36

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:44:ARG:O	3:G:47:MET:CB	1.71	1.36
4:P:75:ALA:HB3	4:P:85:ASP:CB	1.53	1.35
3:O:44:ARG:O	3:O:47:MET:CB	1.72	1.34
1:C:11:GLY:HA3	2:E:50:VAL:N	1.38	1.34
1:J:9:ILE:CB	2:L:50:VAL:O	1.75	1.34
1:I:71:LEU:CB	1:I:188:PRO:CA	2.05	1.33
1:A:266:LEU:CB	2:F:124:ARG:CB	2.08	1.31
1:K:259:GLY:N	2:M:296:GLU:CA	1.83	1.31
1:B:25:TYR:O	2:E:65:GLY:HA2	1.15	1.29
1:K:69:LEU:CB	1:K:72:ALA:HB3	1.61	1.29
1:C:11:GLY:CA	2:E:50:VAL:H	1.45	1.28
1:C:344:MET:CB	2:F:272:ALA:CB	2.11	1.27
1:I:259:GLY:O	2:N:296:GLU:C	1.73	1.27
1:C:25:TYR:N	2:F:66:LEU:H	1.33	1.27
1:K:44:GLY:HA2	2:N:69:ALA:CB	1.64	1.27
1:I:11:GLY:HA3	2:N:50:VAL:CA	1.63	1.26
2:F:427:GLN:CB	1:K:126:GLY:HA3	1.66	1.26
1:I:224:ALA:CB	1:I:405:ALA:HB3	1.65	1.25
1:J:224:ALA:CB	1:J:405:ALA:HB3	1.65	1.25
1:J:419:PHE:O	1:J:496:GLN:HA	1.25	1.25
1:C:224:ALA:CB	1:C:405:ALA:HB3	1.65	1.25
4:H:84:HIS:O	4:H:86:VAL:N	1.67	1.25
1:B:224:ALA:CB	1:B:405:ALA:HB3	1.65	1.24
2:N:360:ARG:O	2:N:362:MET:N	1.70	1.24
1:C:25:TYR:H	2:F:66:LEU:N	1.30	1.24
1:I:11:GLY:HA3	2:N:50:VAL:C	1.58	1.24
1:A:224:ALA:CB	1:A:405:ALA:HB3	1.65	1.24
1:K:224:ALA:CB	1:K:405:ALA:HB3	1.66	1.23
1:B:25:TYR:O	2:E:65:GLY:CA	1.87	1.22
1:I:11:GLY:CA	2:N:50:VAL:N	2.00	1.22
1:B:419:PHE:O	1:B:496:GLN:HA	1.37	1.22
4:P:74:ILE:O	4:P:75:ALA:HA	1.35	1.21
1:C:44:GLY:HA2	2:F:69:ALA:CB	1.69	1.21
4:P:75:ALA:CB	4:P:85:ASP:CB	2.18	1.20
1:A:11:GLY:CA	2:F:50:VAL:H	1.56	1.19
2:N:61:GLU:O	2:N:227:PRO:CB	1.90	1.18
1:A:11:GLY:HA3	2:F:50:VAL:O	1.42	1.17
1:I:11:GLY:HA3	2:N:50:VAL:N	1.60	1.16
1:I:11:GLY:HA3	2:N:50:VAL:O	1.47	1.15
1:K:44:GLY:HA2	2:N:69:ALA:HB3	1.15	1.15
1:C:208:GLY:HA2	1:C:507:CYS:O	1.46	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:25:TYR:N	2:L:66:LEU:N	1.76	1.13
4:P:84:HIS:O	4:P:86:VAL:N	1.81	1.13
1:J:263:THR:CB	2:L:125:ARG:C	2.15	1.12
1:A:11:GLY:HA2	2:F:50:VAL:H	1.02	1.12
1:K:266:LEU:CB	2:M:124:ARG:CB	2.26	1.12
1:B:10:ALA:H	2:D:50:VAL:CB	1.62	1.11
1:K:69:LEU:CB	1:K:72:ALA:CB	2.27	1.11
1:A:11:GLY:HA3	2:F:50:VAL:C	1.72	1.11
1:I:24:MET:C	2:L:66:LEU:H	1.53	1.10
1:I:259:GLY:C	2:N:296:GLU:C	2.05	1.10
1:J:419:PHE:O	1:J:496:GLN:CA	1.99	1.09
1:I:266:LEU:CB	2:N:124:ARG:CB	2.30	1.09
1:J:24:MET:HA	2:M:67:ASP:O	1.52	1.09
2:L:334:GLU:O	2:L:361:LEU:N	1.86	1.08
2:D:149:LYS:O	2:D:334:GLU:N	1.87	1.07
1:A:259:GLY:N	2:F:296:GLU:HA	1.59	1.07
1:C:24:MET:HA	2:F:66:LEU:HA	1.32	1.07
1:K:10:ALA:O	2:M:50:VAL:CB	2.03	1.07
3:O:176:ILE:O	3:O:179:ILE:CB	2.03	1.06
2:F:149:LYS:O	2:F:334:GLU:N	1.87	1.06
2:L:149:LYS:O	2:L:334:GLU:N	1.87	1.06
2:N:149:LYS:O	2:N:334:GLU:N	1.87	1.06
3:G:176:ILE:O	3:G:179:ILE:CB	2.03	1.06
1:I:24:MET:CA	2:L:66:LEU:CA	2.18	1.06
1:C:344:MET:CB	2:F:272:ALA:CA	2.32	1.06
2:E:149:LYS:O	2:E:334:GLU:N	1.87	1.06
1:K:52:TYR:CB	1:K:295:PRO:CB	2.34	1.06
1:B:10:ALA:O	2:D:50:VAL:N	1.89	1.06
1:B:9:ILE:CB	2:D:50:VAL:O	2.04	1.05
2:M:149:LYS:O	2:M:334:GLU:N	1.87	1.05
1:C:208:GLY:O	1:C:507:CYS:CB	2.04	1.04
1:K:259:GLY:O	2:M:296:GLU:C	1.96	1.03
2:F:61:GLU:O	2:F:227:PRO:CB	2.06	1.03
1:K:259:GLY:O	2:M:296:GLU:O	1.74	1.03
1:A:259:GLY:N	2:F:296:GLU:CA	2.17	1.03
1:I:11:GLY:HA2	2:N:50:VAL:N	1.67	1.03
1:C:12:PRO:N	2:E:49:GLU:CB	2.22	1.02
1:C:224:ALA:HB1	1:C:405:ALA:HB3	1.41	1.02
1:I:224:ALA:HB1	1:I:405:ALA:HB3	1.41	1.01
1:A:224:ALA:HB1	1:A:405:ALA:HB3	1.41	1.01
1:C:52:TYR:CB	1:C:295:PRO:CB	2.38	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:TYR:CB	2:F:65:GLY:CA	2.38	1.01
1:A:11:GLY:CA	2:F:50:VAL:N	2.22	1.01
1:K:44:GLY:CA	2:N:69:ALA:CB	2.38	1.01
1:A:352:PRO:CB	2:D:272:ALA:HB3	1.90	1.01
1:I:11:GLY:CA	2:N:50:VAL:O	2.07	1.01
1:A:11:GLY:HA3	2:F:50:VAL:CA	1.89	1.01
1:K:224:ALA:HB1	1:K:405:ALA:HB3	1.42	1.00
1:K:208:GLY:O	1:K:507:CYS:O	1.79	1.00
3:O:7:THR:O	3:O:8:ARG:C	1.98	0.99
1:C:352:PRO:CB	2:F:269:GLU:CB	2.39	0.99
1:K:259:GLY:N	2:M:296:GLU:HA	1.36	0.99
1:J:224:ALA:HB1	1:J:405:ALA:HB3	1.41	0.99
1:B:224:ALA:HB2	1:B:405:ALA:HB3	1.45	0.99
1:I:24:MET:CA	2:L:66:LEU:N	2.25	0.98
1:A:11:GLY:HA3	2:F:50:VAL:N	1.78	0.98
1:B:11:GLY:HA3	2:D:49:GLU:HA	1.45	0.98
1:I:267:VAL:N	2:N:124:ARG:CA	2.22	0.98
1:I:25:TYR:O	2:L:65:GLY:HA2	1.62	0.98
1:C:292:SER:CB	2:E:292:ALA:HB3	1.93	0.98
2:N:360:ARG:C	2:N:362:MET:H	1.67	0.98
1:A:259:GLY:H	2:F:296:GLU:CA	1.75	0.97
1:B:224:ALA:HB1	1:B:405:ALA:HB3	1.42	0.97
2:D:134:GLY:HA2	2:D:430:ARG:O	1.61	0.97
3:G:199:GLY:O	3:G:203:ALA:HB2	1.63	0.97
3:G:7:THR:O	3:G:8:ARG:C	1.98	0.97
1:C:224:ALA:HB2	1:C:405:ALA:HB3	1.45	0.97
1:K:25:TYR:CB	2:N:65:GLY:HA2	1.94	0.97
1:I:224:ALA:HB2	1:I:405:ALA:HB3	1.45	0.96
2:L:334:GLU:CB	2:L:361:LEU:CB	2.44	0.96
3:G:199:GLY:C	3:G:203:ALA:HB2	1.86	0.96
2:F:149:LYS:O	2:F:333:THR:HA	1.66	0.96
1:I:259:GLY:O	2:N:296:GLU:O	1.82	0.96
2:F:427:GLN:CB	1:K:126:GLY:CA	2.43	0.96
1:J:224:ALA:HB2	1:J:405:ALA:HB3	1.45	0.96
1:A:224:ALA:HB2	1:A:405:ALA:HB3	1.46	0.96
3:O:199:GLY:O	3:O:203:ALA:HB2	1.63	0.96
2:L:150:LEU:HA	2:L:335:GLY:O	1.66	0.96
1:I:11:GLY:HA2	2:N:50:VAL:H	0.81	0.96
1:A:11:GLY:CA	2:F:50:VAL:O	2.13	0.95
1:C:259:GLY:H	2:E:296:GLU:N	1.64	0.95
1:B:11:GLY:HA3	2:D:49:GLU:CB	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:224:ALA:HB2	1:K:405:ALA:HB3	1.46	0.95
2:F:150:LEU:HA	2:F:335:GLY:O	1.66	0.95
3:G:148:LYS:O	3:G:152:GLU:CB	2.15	0.95
2:D:150:LEU:HA	2:D:335:GLY:O	1.67	0.95
2:N:150:LEU:HA	2:N:335:GLY:O	1.67	0.94
2:N:149:LYS:O	2:N:333:THR:HA	1.66	0.94
1:C:259:GLY:N	2:E:296:GLU:N	1.86	0.94
3:O:47:MET:O	3:O:49:ALA:N	2.00	0.94
2:M:150:LEU:HA	2:M:335:GLY:O	1.67	0.94
3:O:199:GLY:C	3:O:203:ALA:HB2	1.86	0.94
1:K:259:GLY:H	2:M:296:GLU:CA	1.51	0.94
2:L:149:LYS:O	2:L:333:THR:HA	1.66	0.94
1:K:11:GLY:HA3	2:M:50:VAL:H	1.31	0.94
2:E:150:LEU:HA	2:E:335:GLY:O	1.66	0.94
2:D:149:LYS:O	2:D:333:THR:HA	1.66	0.94
1:C:266:LEU:CB	2:E:124:ARG:HA	1.97	0.93
3:O:148:LYS:O	3:O:152:GLU:CB	2.15	0.93
3:O:135:GLU:C	3:O:137:LEU:N	2.17	0.93
3:G:47:MET:O	3:G:49:ALA:N	2.00	0.93
2:N:149:LYS:O	2:N:333:THR:CA	2.16	0.93
1:I:70:PRO:CB	1:I:190:ARG:CB	2.46	0.93
2:E:149:LYS:O	2:E:333:THR:HA	1.66	0.93
2:L:149:LYS:O	2:L:333:THR:CA	2.17	0.93
1:I:11:GLY:CA	2:N:50:VAL:CA	2.45	0.93
1:C:44:GLY:HA2	2:F:69:ALA:HB1	1.50	0.93
2:D:149:LYS:O	2:D:333:THR:CA	2.16	0.93
2:F:149:LYS:O	2:F:333:THR:CA	2.16	0.93
2:M:149:LYS:O	2:M:333:THR:HA	1.66	0.93
1:I:25:TYR:O	2:L:65:GLY:CA	2.17	0.93
2:E:149:LYS:O	2:E:333:THR:CA	2.17	0.92
1:B:11:GLY:HA3	2:D:49:GLU:CA	1.98	0.92
3:O:48:GLU:O	3:O:51:LYS:CB	2.18	0.92
3:G:48:GLU:O	3:G:51:LYS:CB	2.18	0.92
1:I:267:VAL:H	2:N:124:ARG:CA	1.83	0.92
2:M:149:LYS:O	2:M:333:THR:CA	2.17	0.92
1:I:260:ASN:CB	2:N:298:ALA:O	2.19	0.91
1:C:208:GLY:CA	1:C:507:CYS:O	2.19	0.91
1:B:263:THR:CB	2:D:124:ARG:C	2.39	0.90
3:G:49:ALA:O	3:G:52:ALA:HB3	1.72	0.90
1:I:25:TYR:CA	2:L:65:GLY:HA2	2.02	0.90
3:O:141:ALA:O	3:O:145:THR:CB	2.20	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:419:PHE:CB	1:I:497:GLN:O	2.20	0.89
1:J:263:THR:CB	2:L:125:ARG:CA	2.51	0.89
3:O:49:ALA:O	3:O:52:ALA:HB3	1.72	0.88
5:C:600:ADP:O3'	2:E:360:ARG:HA	1.73	0.88
1:I:25:TYR:CB	2:L:64:THR:O	2.21	0.88
3:G:141:ALA:O	3:G:145:THR:CB	2.21	0.88
3:O:51:LYS:CB	3:O:136:ALA:HB1	2.04	0.88
1:J:24:MET:CB	2:M:66:LEU:HA	2.03	0.88
2:F:295:TYR:CB	2:F:332:ILE:CB	2.52	0.87
1:K:259:GLY:C	2:M:296:GLU:C	2.33	0.87
1:C:11:GLY:HA3	2:E:50:VAL:H	0.86	0.87
2:N:295:TYR:CB	2:N:332:ILE:CB	2.53	0.87
2:M:295:TYR:CB	2:M:332:ILE:CB	2.52	0.87
1:I:419:PHE:N	1:I:496:GLN:HA	1.89	0.87
3:G:135:GLU:C	3:G:137:LEU:N	2.17	0.87
2:D:295:TYR:CB	2:D:332:ILE:CB	2.53	0.86
2:L:295:TYR:CB	2:L:332:ILE:CB	2.53	0.86
2:L:153:PHE:O	2:L:339:LEU:N	2.08	0.86
4:P:74:ILE:O	4:P:75:ALA:CA	2.19	0.86
2:L:150:LEU:CA	2:L:335:GLY:O	2.24	0.86
3:G:47:MET:O	3:G:48:GLU:C	2.09	0.86
1:I:217:PRO:O	1:I:431:PHE:CB	2.24	0.86
2:F:153:PHE:O	2:F:339:LEU:N	2.09	0.86
1:A:11:GLY:HA2	2:F:50:VAL:N	1.87	0.86
2:M:153:PHE:O	2:M:339:LEU:N	2.09	0.86
1:J:263:THR:CB	2:L:125:ARG:N	2.40	0.85
3:G:174:ALA:O	3:G:175:GLN:C	2.09	0.85
1:I:12:PRO:N	2:N:49:GLU:CB	2.38	0.85
2:E:295:TYR:CB	2:E:332:ILE:CB	2.53	0.85
2:M:150:LEU:CA	2:M:335:GLY:O	2.24	0.85
2:F:150:LEU:CA	2:F:335:GLY:O	2.24	0.85
2:N:153:PHE:O	2:N:339:LEU:N	2.09	0.85
3:O:174:ALA:O	3:O:175:GLN:C	2.09	0.85
3:O:47:MET:O	3:O:48:GLU:C	2.09	0.85
2:E:150:LEU:CA	2:E:335:GLY:O	2.24	0.85
2:D:150:LEU:CA	2:D:335:GLY:O	2.24	0.85
1:I:267:VAL:CA	2:N:124:ARG:CB	2.50	0.84
1:B:25:TYR:C	2:E:65:GLY:HA2	1.97	0.84
3:O:199:GLY:O	3:O:203:ALA:CB	2.25	0.84
2:D:153:PHE:O	2:D:339:LEU:N	2.09	0.84
2:N:150:LEU:CA	2:N:335:GLY:O	2.24	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:352:PRO:CB	2:L:269:GLU:O	2.26	0.84
1:B:419:PHE:O	1:B:496:GLN:CA	2.23	0.84
2:M:140:VAL:CB	2:M:435:SER:CB	2.56	0.83
1:I:25:TYR:CB	2:L:65:GLY:HA2	2.08	0.83
2:D:134:GLY:O	2:D:430:ARG:N	2.11	0.83
2:E:153:PHE:O	2:E:339:LEU:N	2.09	0.83
3:O:158:THR:O	3:O:161:VAL:CB	2.27	0.83
1:J:475:ALA:HB3	4:P:100:PHE:CB	2.05	0.83
1:B:263:THR:CB	2:D:125:ARG:N	2.42	0.83
1:C:344:MET:CB	2:F:272:ALA:HA	2.09	0.82
3:G:158:THR:O	3:G:161:VAL:CB	2.27	0.82
1:B:10:ALA:N	2:D:50:VAL:CB	2.41	0.82
1:C:18:GLY:O	1:C:19:MET:CB	2.28	0.82
3:G:199:GLY:O	3:G:203:ALA:CB	2.26	0.82
1:I:266:LEU:CA	2:N:124:ARG:CB	2.57	0.82
1:I:25:TYR:C	2:L:65:GLY:HA2	1.98	0.82
4:P:75:ALA:HA	4:P:75:ALA:C	1.95	0.82
1:A:189:VAL:HA	1:A:308:THR:CB	2.10	0.82
1:I:18:GLY:O	1:I:19:MET:CB	2.27	0.81
1:K:231:GLY:HA2	5:K:600:ADP:H5'1	1.61	0.81
2:E:81:ARG:HA	2:E:81:ARG:N	1.94	0.81
3:G:167:VAL:O	3:G:168:VAL:C	2.19	0.80
1:C:292:SER:CB	2:E:292:ALA:CB	2.59	0.80
1:K:18:GLY:O	1:K:19:MET:CB	2.27	0.80
3:O:167:VAL:O	3:O:169:ILE:N	2.14	0.80
1:A:259:GLY:O	2:F:296:GLU:O	1.99	0.80
2:L:134:GLY:HA2	2:L:430:ARG:O	1.81	0.80
1:J:18:GLY:O	1:J:19:MET:CB	2.28	0.80
1:K:44:GLY:HA2	2:N:69:ALA:HB2	1.62	0.80
1:K:44:GLY:CA	2:N:69:ALA:HB2	2.12	0.80
1:J:224:ALA:HB1	1:J:405:ALA:CB	2.12	0.80
3:G:167:VAL:O	3:G:169:ILE:N	2.14	0.79
1:B:18:GLY:O	1:B:19:MET:CB	2.28	0.79
2:N:134:GLY:O	2:N:429:ASN:HA	1.82	0.79
1:A:224:ALA:HB1	1:A:405:ALA:CB	2.12	0.79
1:C:224:ALA:HB1	1:C:405:ALA:CB	2.12	0.79
1:B:224:ALA:HB1	1:B:405:ALA:CB	2.12	0.79
3:G:132:ARG:N	3:G:134:ALA:HB3	1.98	0.79
1:I:267:VAL:H	2:N:124:ARG:CB	1.90	0.79
1:K:259:GLY:C	2:M:296:GLU:HA	1.81	0.79
1:I:71:LEU:CB	1:I:72:ALA:HA	2.12	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:224:ALA:HB1	1:I:405:ALA:CB	2.12	0.79
1:K:224:ALA:HB1	1:K:405:ALA:CB	2.13	0.79
1:C:52:TYR:HA	1:C:295:PRO:CB	2.13	0.78
1:C:352:PRO:CB	2:F:269:GLU:C	2.51	0.78
3:O:167:VAL:O	3:O:168:VAL:C	2.19	0.78
3:O:132:ARG:N	3:O:134:ALA:HB3	1.98	0.78
1:A:259:GLY:O	2:F:296:GLU:C	2.21	0.78
1:A:44:GLY:HA2	2:D:69:ALA:CB	2.13	0.78
1:A:18:GLY:O	1:A:19:MET:CB	2.28	0.78
3:G:28:LEU:O	3:G:31:LYS:CB	2.32	0.77
1:A:12:PRO:N	2:F:49:GLU:CB	2.47	0.77
1:A:81:ASN:HA	1:A:282:MET:O	1.84	0.77
3:O:28:LEU:O	3:O:31:LYS:CB	2.32	0.77
2:F:51:SER:O	2:F:52:GLU:CB	2.33	0.77
1:C:224:ALA:CB	1:C:405:ALA:CB	2.58	0.76
2:M:51:SER:O	2:M:52:GLU:CB	2.33	0.76
2:L:51:SER:O	2:L:52:GLU:CB	2.33	0.76
2:D:51:SER:O	2:D:52:GLU:CB	2.33	0.76
1:A:43:ASP:C	2:D:69:ALA:CB	2.54	0.76
1:K:11:GLY:HA3	2:M:50:VAL:N	2.00	0.76
1:K:259:GLY:C	2:M:296:GLU:CA	2.38	0.75
3:G:39:PHE:O	3:G:42:LEU:CB	2.34	0.75
2:N:51:SER:O	2:N:52:GLU:CB	2.33	0.75
3:O:39:PHE:O	3:O:42:LEU:CB	2.34	0.75
3:O:194:LEU:HA	3:O:194:LEU:C	2.03	0.75
1:C:52:TYR:CA	1:C:295:PRO:CB	2.65	0.75
1:I:259:GLY:O	2:N:297:ARG:N	2.18	0.75
1:I:224:ALA:CB	1:I:405:ALA:CB	2.58	0.75
1:I:24:MET:CB	2:L:66:LEU:N	2.49	0.75
2:E:149:LYS:CB	2:E:332:ILE:O	2.35	0.75
4:P:65:GLY:CA	4:P:66:ARG:CB	2.65	0.75
2:L:149:LYS:CB	2:L:332:ILE:O	2.35	0.75
2:F:149:LYS:CB	2:F:332:ILE:O	2.35	0.75
2:E:51:SER:O	2:E:52:GLU:CB	2.33	0.75
1:B:224:ALA:CB	1:B:405:ALA:CB	2.58	0.74
1:C:56:SER:CB	2:E:30:GLY:O	2.35	0.74
3:O:140:VAL:O	3:O:144:GLU:CB	2.35	0.74
1:K:52:TYR:C	1:K:295:PRO:CB	2.56	0.74
3:G:132:ARG:C	3:G:134:ALA:N	2.37	0.74
1:J:419:PHE:O	1:J:496:GLN:CB	2.35	0.74
1:J:263:THR:CB	2:L:125:ARG:O	2.35	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:24:MET:CB	2:L:66:LEU:CA	2.65	0.74
3:G:199:GLY:C	3:G:203:ALA:CB	2.56	0.74
3:O:199:GLY:C	3:O:203:ALA:CB	2.56	0.74
2:M:149:LYS:CB	2:M:332:ILE:O	2.35	0.74
3:G:140:VAL:O	3:G:144:GLU:CB	2.35	0.74
3:O:132:ARG:C	3:O:134:ALA:N	2.37	0.73
1:K:69:LEU:CB	1:K:72:ALA:HB2	2.19	0.73
2:N:69:ALA:O	2:N:70:THR:CB	2.36	0.73
3:O:142:ASN:O	3:O:146:ARG:CB	2.36	0.73
3:G:142:ASN:O	3:G:146:ARG:CB	2.36	0.73
1:B:25:TYR:N	2:E:66:LEU:H	1.86	0.73
3:G:196:ARG:HA	3:G:196:ARG:C	2.05	0.73
1:C:11:GLY:HA2	2:E:49:GLU:HA	1.70	0.73
2:N:149:LYS:CB	2:N:332:ILE:O	2.35	0.73
1:I:52:TYR:CB	1:I:297:ALA:HB3	2.19	0.73
4:P:75:ALA:HB2	4:P:85:ASP:CB	2.19	0.73
3:G:45:GLU:O	3:G:46:ALA:C	2.27	0.73
2:D:149:LYS:CB	2:D:332:ILE:O	2.35	0.73
1:I:56:SER:CB	2:N:30:GLY:N	2.52	0.73
3:O:45:GLU:O	3:O:46:ALA:C	2.27	0.73
2:F:69:ALA:O	2:F:70:THR:CB	2.37	0.73
2:L:69:ALA:O	2:L:70:THR:CB	2.36	0.73
1:C:44:GLY:CA	2:F:69:ALA:CB	2.61	0.73
1:C:11:GLY:CA	2:E:50:VAL:N	2.21	0.72
1:A:224:ALA:CB	1:A:405:ALA:CB	2.58	0.72
2:E:69:ALA:O	2:E:70:THR:CB	2.37	0.72
3:O:150:ILE:O	3:O:151:GLY:O	2.07	0.72
3:G:163:ALA:HA	3:G:163:ALA:C	2.04	0.72
3:G:150:ILE:O	3:G:151:GLY:O	2.08	0.72
1:I:11:GLY:CA	2:N:50:VAL:CB	2.65	0.72
1:C:344:MET:CA	2:F:272:ALA:HB1	2.18	0.72
1:B:86:GLY:HA2	1:B:302:SER:CB	2.19	0.72
2:F:359:SER:CB	2:F:362:MET:CB	2.67	0.72
1:C:267:VAL:O	2:E:125:ARG:HA	1.84	0.72
2:D:69:ALA:O	2:D:70:THR:CB	2.36	0.72
2:M:69:ALA:O	2:M:70:THR:CB	2.37	0.72
3:O:135:GLU:O	3:O:136:ALA:C	2.28	0.71
2:N:65:GLY:O	2:N:66:LEU:CB	2.38	0.71
3:G:4:VAL:C	3:G:4:VAL:HA	2.07	0.71
3:O:196:ARG:C	3:O:196:ARG:HA	2.05	0.71
1:K:259:GLY:H	2:M:296:GLU:CB	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:HA	2:D:50:VAL:CB	2.21	0.71
3:G:135:GLU:O	3:G:136:ALA:C	2.28	0.71
1:C:260:ASN:CB	2:E:298:ALA:HB3	2.21	0.71
4:H:77:LEU:H	4:H:80:ALA:HB3	1.55	0.71
1:B:10:ALA:C	2:D:50:VAL:H	1.94	0.71
2:L:359:SER:C	2:L:361:LEU:N	2.39	0.71
1:I:204:PRO:CB	1:I:435:LEU:CB	2.68	0.71
2:F:65:GLY:O	2:F:66:LEU:CB	2.39	0.70
2:E:65:GLY:O	2:E:66:LEU:CB	2.38	0.70
1:B:11:GLY:CA	2:D:49:GLU:HA	2.20	0.70
1:I:225:ALA:N	1:I:405:ALA:O	2.25	0.70
2:E:81:ARG:HA	2:E:81:ARG:C	2.05	0.70
1:K:44:GLY:CA	2:N:69:ALA:HB3	2.07	0.70
2:M:65:GLY:O	2:M:66:LEU:CB	2.38	0.70
1:I:56:SER:CB	2:N:30:GLY:O	2.40	0.70
2:L:274:ARG:O	2:L:275:GLU:CB	2.37	0.70
1:A:225:ALA:N	1:A:405:ALA:O	2.25	0.70
2:N:61:GLU:HA	2:N:229:ILE:CB	2.22	0.70
2:F:274:ARG:O	2:F:275:GLU:CB	2.37	0.70
1:A:71:LEU:CB	1:A:188:PRO:HA	2.22	0.70
1:K:225:ALA:N	1:K:405:ALA:O	2.25	0.69
1:A:44:GLY:N	2:D:69:ALA:CB	2.54	0.69
2:N:274:ARG:O	2:N:275:GLU:CB	2.37	0.69
2:D:65:GLY:O	2:D:66:LEU:CB	2.38	0.69
4:P:75:ALA:C	4:P:75:ALA:CB	2.60	0.69
1:J:225:ALA:N	1:J:405:ALA:O	2.25	0.69
1:A:44:GLY:HA2	2:D:69:ALA:HB1	1.74	0.69
1:C:225:ALA:N	1:C:405:ALA:O	2.25	0.69
1:I:11:GLY:HA3	2:N:50:VAL:CB	2.23	0.69
2:F:427:GLN:O	1:K:126:GLY:N	2.25	0.69
1:B:225:ALA:N	1:B:405:ALA:O	2.25	0.69
1:J:24:MET:CB	2:M:66:LEU:CA	2.69	0.69
3:O:48:GLU:C	3:O:51:LYS:H	1.97	0.69
2:E:140:VAL:CB	2:E:435:SER:CB	2.71	0.69
1:I:25:TYR:O	2:L:65:GLY:HA3	1.93	0.69
2:L:65:GLY:O	2:L:66:LEU:CB	2.39	0.69
2:M:274:ARG:O	2:M:275:GLU:CB	2.38	0.69
3:O:31:LYS:N	3:O:31:LYS:HA	2.02	0.68
3:O:197:ILE:O	3:O:200:LYS:CB	2.41	0.68
1:A:71:LEU:HA	1:A:188:PRO:HA	1.75	0.68
1:J:224:ALA:CB	1:J:405:ALA:CB	2.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:197:ILE:O	3:G:200:LYS:CB	2.40	0.68
1:A:5:VAL:CB	1:A:18:GLY:O	2.42	0.68
3:O:4:VAL:HA	3:O:4:VAL:C	2.07	0.68
1:A:352:PRO:CB	2:D:272:ALA:CB	2.70	0.68
1:J:419:PHE:C	1:J:496:GLN:HA	2.13	0.68
1:J:5:VAL:CB	1:J:18:GLY:O	2.42	0.68
1:I:5:VAL:CB	1:I:18:GLY:O	2.42	0.68
1:K:5:VAL:CB	1:K:18:GLY:O	2.42	0.68
1:J:10:ALA:O	2:L:49:GLU:HA	1.93	0.68
1:C:259:GLY:O	2:E:296:GLU:C	2.32	0.68
1:K:224:ALA:CB	1:K:405:ALA:CB	2.58	0.68
1:C:44:GLY:HA2	2:F:69:ALA:HB3	1.70	0.68
1:K:189:VAL:O	1:K:304:TYR:CB	2.42	0.67
1:A:11:GLY:CA	2:F:50:VAL:CA	2.68	0.67
3:G:48:GLU:C	3:G:51:LYS:H	1.97	0.67
2:E:274:ARG:O	2:E:275:GLU:CB	2.37	0.67
1:C:5:VAL:CB	1:C:18:GLY:O	2.42	0.67
1:B:5:VAL:CB	1:B:18:GLY:O	2.42	0.67
1:I:419:PHE:H	1:I:496:GLN:HA	1.59	0.67
1:A:196:GLN:N	1:A:369:ILE:O	2.28	0.67
1:B:24:MET:C	2:E:66:LEU:H	1.96	0.67
3:G:151:GLY:HA2	3:G:155:LYS:CB	2.25	0.67
3:G:31:LYS:N	3:G:31:LYS:HA	2.02	0.67
1:C:24:MET:CA	2:F:66:LEU:HA	2.18	0.67
3:G:194:LEU:HA	3:G:194:LEU:C	2.04	0.66
1:C:44:GLY:HA2	2:F:69:ALA:HB2	1.74	0.66
3:O:151:GLY:HA2	3:O:155:LYS:CB	2.26	0.66
3:G:3:GLN:O	3:G:5:SER:N	2.29	0.66
4:P:74:ILE:C	4:P:75:ALA:CA	2.62	0.66
2:D:274:ARG:O	2:D:275:GLU:CB	2.38	0.66
3:O:141:ALA:HA	3:O:144:GLU:CB	2.26	0.66
1:A:44:GLY:CA	2:D:69:ALA:HB1	2.25	0.66
1:K:27:ILE:HA	1:K:71:LEU:H	1.61	0.66
3:O:3:GLN:O	3:O:5:SER:N	2.29	0.66
1:C:419:PHE:C	1:C:497:GLN:H	1.97	0.66
2:M:61:GLU:O	2:M:227:PRO:CB	2.44	0.66
1:A:44:GLY:CA	2:D:69:ALA:CB	2.74	0.66
3:G:141:ALA:HA	3:G:144:GLU:CB	2.26	0.65
2:E:80:ALA:HA	2:E:80:ALA:C	2.06	0.65
1:C:266:LEU:C	2:E:124:ARG:CB	2.64	0.65
4:H:65:GLY:HA2	4:H:66:ARG:CB	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:GLY:HA2	2:D:69:ALA:HB3	1.78	0.65
2:L:334:GLU:O	2:L:361:LEU:CB	2.45	0.65
2:M:149:LYS:O	2:M:333:THR:C	2.35	0.65
1:K:56:SER:CB	2:M:30:GLY:O	2.44	0.65
2:L:334:GLU:CA	2:L:361:LEU:CB	2.75	0.65
1:I:260:ASN:N	2:N:296:GLU:HA	1.99	0.65
2:N:149:LYS:O	2:N:333:THR:C	2.35	0.65
2:F:149:LYS:O	2:F:333:THR:C	2.35	0.65
2:E:149:LYS:O	2:E:333:THR:C	2.35	0.65
4:P:65:GLY:HA2	4:P:66:ARG:CB	2.27	0.65
1:J:24:MET:CA	2:M:67:ASP:O	2.38	0.64
3:O:172:ILE:O	3:O:176:ILE:CB	2.45	0.64
1:C:11:GLY:HA3	2:E:49:GLU:C	2.15	0.64
2:L:149:LYS:O	2:L:333:THR:C	2.35	0.64
1:A:43:ASP:C	2:D:69:ALA:HB2	2.18	0.64
3:O:163:ALA:C	3:O:163:ALA:HA	2.04	0.64
3:G:141:ALA:HA	3:G:145:THR:H	1.62	0.64
3:O:156:LYS:C	3:O:158:THR:N	2.44	0.64
1:A:260:ASN:CB	2:F:298:ALA:O	2.45	0.64
3:O:156:LYS:O	3:O:157:THR:C	2.33	0.64
2:E:81:ARG:CB	2:E:81:ARG:N	2.60	0.64
2:D:149:LYS:O	2:D:333:THR:C	2.35	0.64
3:G:156:LYS:C	3:G:158:THR:N	2.44	0.64
3:G:172:ILE:O	3:G:176:ILE:CB	2.45	0.64
3:O:141:ALA:HA	3:O:145:THR:H	1.62	0.63
4:H:84:HIS:O	4:H:85:ASP:C	2.34	0.63
1:K:11:GLY:CA	2:M:49:GLU:HA	2.28	0.63
3:G:151:GLY:O	3:G:152:GLU:C	2.36	0.63
3:O:151:GLY:O	3:O:152:GLU:C	2.36	0.63
1:C:11:GLY:CA	2:E:49:GLU:CA	2.77	0.63
1:A:259:GLY:C	2:F:296:GLU:HA	2.10	0.63
1:K:259:GLY:C	2:M:296:GLU:O	2.35	0.63
1:A:81:ASN:CA	1:A:282:MET:O	2.47	0.63
3:G:18:LEU:O	3:G:21:ALA:HB3	1.99	0.63
2:N:76:VAL:O	2:N:77:GLU:CB	2.47	0.63
3:O:156:LYS:HA	3:O:159:ARG:H	1.64	0.63
3:O:148:LYS:O	3:O:149:LYS:O	2.17	0.62
1:C:25:TYR:CA	2:F:65:GLY:HA2	2.27	0.62
2:E:76:VAL:O	2:E:77:GLU:CB	2.47	0.62
2:L:76:VAL:O	2:L:77:GLU:CB	2.47	0.62
2:F:76:VAL:O	2:F:77:GLU:CB	2.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:25:TYR:CB	2:N:65:GLY:CA	2.75	0.62
3:G:156:LYS:HA	3:G:159:ARG:H	1.64	0.62
3:G:156:LYS:O	3:G:157:THR:C	2.33	0.62
3:O:18:LEU:O	3:O:21:ALA:HB3	1.99	0.62
2:D:334:GLU:O	2:D:361:LEU:N	2.31	0.62
1:I:208:GLY:O	1:I:507:CYS:O	2.18	0.62
1:I:259:GLY:C	2:N:296:GLU:O	2.31	0.62
2:D:134:GLY:CA	2:D:430:ARG:O	2.42	0.62
3:O:135:GLU:C	3:O:137:LEU:H	2.03	0.62
3:O:41:GLY:O	3:O:42:LEU:C	2.38	0.62
3:G:41:GLY:O	3:G:42:LEU:C	2.38	0.61
1:K:429:SER:C	1:K:431:PHE:H	2.03	0.61
3:G:148:LYS:O	3:G:149:LYS:O	2.17	0.61
2:D:76:VAL:O	2:D:77:GLU:CB	2.47	0.61
4:P:75:ALA:N	4:P:75:ALA:CB	2.56	0.61
1:I:25:TYR:H	2:L:65:GLY:C	1.96	0.61
1:A:266:LEU:CB	2:F:124:ARG:CA	2.78	0.61
1:B:25:TYR:N	2:E:66:LEU:N	2.48	0.61
2:M:76:VAL:O	2:M:77:GLU:CB	2.47	0.61
3:O:170:PRO:O	3:O:174:ALA:HB2	2.00	0.61
2:L:134:GLY:O	2:L:430:ARG:N	2.34	0.61
2:F:61:GLU:HA	2:F:229:ILE:CB	2.31	0.61
3:G:170:PRO:O	3:G:174:ALA:HB2	2.00	0.60
2:E:349:TYR:O	2:E:424:ASN:HA	2.01	0.60
1:C:359:ALA:HB3	2:F:224:ALA:HB1	1.83	0.60
3:G:135:GLU:O	3:G:137:LEU:N	2.33	0.60
3:O:158:THR:C	3:O:161:VAL:CB	2.70	0.60
1:I:12:PRO:O	1:I:13:ALA:HB3	2.01	0.60
1:C:12:PRO:O	1:C:13:ALA:HB3	2.02	0.60
3:G:158:THR:C	3:G:161:VAL:CB	2.70	0.60
1:C:259:GLY:O	2:E:297:ARG:N	2.35	0.60
1:A:12:PRO:O	1:A:13:ALA:HB3	2.02	0.60
3:G:160:ARG:O	3:G:164:LEU:CB	2.50	0.60
1:J:12:PRO:O	1:J:13:ALA:HB3	2.02	0.60
1:K:12:PRO:O	1:K:13:ALA:HB3	2.02	0.59
3:G:135:GLU:HA	3:G:138:ILE:N	2.16	0.59
3:O:150:ILE:C	3:O:151:GLY:O	2.39	0.59
1:J:9:ILE:CA	2:L:50:VAL:O	2.48	0.59
1:C:266:LEU:CB	2:E:124:ARG:CA	2.78	0.59
3:O:135:GLU:HA	3:O:138:ILE:N	2.17	0.59
1:B:12:PRO:O	1:B:13:ALA:HB3	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:ILE:CB	2:D:50:VAL:C	2.70	0.59
4:H:77:LEU:N	4:H:80:ALA:HB3	2.18	0.59
3:O:160:ARG:O	3:O:164:LEU:CB	2.50	0.59
1:A:419:PHE:C	1:A:497:GLN:O	2.41	0.59
2:F:427:GLN:O	1:K:126:GLY:CA	2.50	0.59
1:I:429:SER:CB	1:I:431:PHE:H	2.16	0.59
4:P:62:LEU:O	4:P:63:MET:CB	2.46	0.59
3:O:135:GLU:O	3:O:137:LEU:N	2.33	0.59
1:I:25:TYR:N	2:L:65:GLY:HA2	2.18	0.58
2:D:359:SER:C	2:D:361:LEU:N	2.49	0.58
3:G:150:ILE:C	3:G:151:GLY:O	2.39	0.58
1:A:43:ASP:O	2:D:69:ALA:HB3	2.04	0.58
1:I:189:VAL:HA	1:I:308:THR:CB	2.34	0.58
2:L:134:GLY:CA	2:L:430:ARG:O	2.51	0.58
1:A:56:SER:CB	2:F:30:GLY:N	2.67	0.58
2:E:80:ALA:CB	2:E:80:ALA:C	2.70	0.57
1:C:11:GLY:CA	2:E:49:GLU:HA	2.34	0.57
3:G:47:MET:C	3:G:49:ALA:N	2.57	0.57
1:A:259:GLY:C	2:F:296:GLU:C	2.63	0.57
3:O:186:ARG:O	3:O:190:ASP:CB	2.53	0.57
1:K:241:LEU:O	1:K:245:SER:N	2.31	0.57
3:G:47:MET:C	3:G:49:ALA:H	2.08	0.57
1:K:260:ASN:CB	2:M:298:ALA:O	2.52	0.57
2:E:134:GLY:O	2:E:429:ASN:HA	2.04	0.57
1:A:81:ASN:N	1:A:282:MET:O	2.36	0.57
1:C:266:LEU:C	2:E:124:ARG:CA	2.68	0.57
3:G:135:GLU:C	3:G:137:LEU:H	2.03	0.57
3:O:132:ARG:O	3:O:133:TYR:C	2.38	0.56
3:O:48:GLU:O	3:O:51:LYS:N	2.38	0.56
1:K:11:GLY:HA3	2:M:49:GLU:CA	2.35	0.56
3:G:186:ARG:O	3:G:190:ASP:CB	2.53	0.56
1:J:23:ARG:O	2:M:68:LEU:HA	2.05	0.56
3:O:47:MET:C	3:O:49:ALA:H	2.09	0.56
3:G:189:GLU:CB	3:G:189:GLU:HA	2.18	0.56
1:I:419:PHE:HA	1:I:420:PRO:C	2.25	0.56
1:A:241:LEU:O	1:A:245:SER:N	2.31	0.56
1:C:241:LEU:O	1:C:245:SER:N	2.31	0.56
3:O:47:MET:C	3:O:49:ALA:N	2.57	0.56
1:C:419:PHE:HA	1:C:420:PRO:C	2.25	0.56
1:C:344:MET:CB	2:F:272:ALA:C	2.73	0.56
1:K:419:PHE:CB	1:K:497:GLN:O	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:137:LEU:O	3:G:140:VAL:CB	2.54	0.56
1:I:24:MET:CB	2:L:66:LEU:HA	2.29	0.56
1:B:419:PHE:HA	1:B:420:PRO:C	2.25	0.56
1:K:419:PHE:HA	1:K:420:PRO:C	2.25	0.56
3:G:132:ARG:N	3:G:134:ALA:CB	2.68	0.56
1:A:419:PHE:HA	1:A:420:PRO:C	2.25	0.56
1:J:241:LEU:O	1:J:245:SER:N	2.32	0.56
3:O:45:GLU:C	3:O:47:MET:N	2.58	0.56
1:C:352:PRO:CB	2:F:269:GLU:O	2.54	0.56
1:I:241:LEU:O	1:I:245:SER:N	2.31	0.56
2:E:81:ARG:CB	2:E:81:ARG:C	2.67	0.55
3:O:158:THR:HA	3:O:161:VAL:CB	2.37	0.55
3:O:137:LEU:O	3:O:140:VAL:CB	2.54	0.55
3:O:142:ASN:HA	3:O:142:ASN:CB	2.16	0.55
3:G:44:ARG:C	3:G:47:MET:CB	2.72	0.55
1:A:199:LEU:O	1:A:200:ASP:C	2.45	0.55
1:J:419:PHE:HA	1:J:420:PRO:C	2.25	0.55
2:D:334:GLU:CB	2:D:361:LEU:CB	2.84	0.55
3:G:48:GLU:O	3:G:51:LYS:N	2.39	0.55
3:O:55:GLN:CB	3:O:133:TYR:CB	2.85	0.55
3:G:142:ASN:CB	3:G:142:ASN:HA	2.17	0.55
1:A:199:LEU:O	1:A:200:ASP:O	2.24	0.55
1:I:71:LEU:HA	1:I:189:VAL:H	1.72	0.55
3:G:132:ARG:O	3:G:133:TYR:C	2.37	0.55
3:O:136:ALA:O	3:O:140:VAL:CB	2.55	0.55
1:I:71:LEU:CB	1:I:72:ALA:CA	2.83	0.54
2:L:334:GLU:O	2:L:361:LEU:CA	2.54	0.54
3:O:137:LEU:O	3:O:140:VAL:N	2.40	0.54
1:C:260:ASN:N	2:E:296:GLU:HA	2.22	0.54
3:G:158:THR:HA	3:G:161:VAL:CB	2.37	0.54
1:B:241:LEU:O	1:B:245:SER:N	2.31	0.54
1:A:11:GLY:CA	2:F:50:VAL:CB	2.85	0.54
3:G:137:LEU:O	3:G:140:VAL:N	2.40	0.54
2:E:334:GLU:O	2:E:360:ARG:N	2.39	0.54
1:A:259:GLY:C	2:F:296:GLU:CA	2.69	0.54
3:G:136:ALA:O	3:G:140:VAL:CB	2.55	0.54
1:I:225:ALA:O	1:I:406:PHE:HA	2.07	0.54
4:H:84:HIS:C	4:H:86:VAL:N	2.53	0.54
1:K:225:ALA:O	1:K:406:PHE:HA	2.07	0.54
1:C:259:GLY:H	2:E:296:GLU:H	1.51	0.54
1:I:404:GLY:O	1:I:430:LEU:CB	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:132:ARG:N	3:O:134:ALA:CB	2.68	0.54
3:O:7:THR:O	3:O:9:MET:N	2.41	0.54
3:G:167:VAL:C	3:G:169:ILE:N	2.61	0.53
1:A:225:ALA:O	1:A:406:PHE:HA	2.08	0.53
2:E:153:PHE:CB	2:E:338:GLN:HA	2.38	0.53
1:J:296:VAL:HA	1:J:333:ALA:HB1	1.90	0.53
1:C:225:ALA:O	1:C:406:PHE:HA	2.08	0.53
1:B:225:ALA:O	1:B:406:PHE:HA	2.07	0.53
1:B:224:ALA:CA	1:B:405:ALA:HB3	2.37	0.53
1:K:224:ALA:CA	1:K:405:ALA:HB3	2.37	0.53
2:L:359:SER:C	2:L:361:LEU:H	2.07	0.53
1:K:11:GLY:CA	2:M:50:VAL:H	2.14	0.53
3:O:44:ARG:C	3:O:47:MET:CB	2.72	0.53
3:G:138:ILE:O	3:G:139:ARG:O	2.27	0.53
1:K:11:GLY:HA2	2:M:49:GLU:HA	1.89	0.53
1:K:429:SER:C	1:K:431:PHE:N	2.60	0.53
1:A:296:VAL:HA	1:A:333:ALA:HB1	1.90	0.53
1:J:227:PRO:HA	1:J:384:VAL:CB	2.39	0.53
3:O:145:THR:O	3:O:149:LYS:CB	2.57	0.53
2:L:153:PHE:CB	2:L:338:GLN:HA	2.39	0.53
1:B:296:VAL:HA	1:B:333:ALA:HB1	1.90	0.53
1:A:233:GLY:HA2	5:A:600:ADP:O1A	2.09	0.53
1:C:25:TYR:N	2:F:66:LEU:N	2.14	0.53
2:M:153:PHE:CB	2:M:338:GLN:HA	2.39	0.53
1:A:227:PRO:HA	1:A:384:VAL:CB	2.39	0.53
3:O:42:LEU:O	3:O:45:GLU:CB	2.57	0.53
1:I:352:PRO:CB	2:L:272:ALA:HB3	2.39	0.53
3:G:166:GLN:O	3:G:169:ILE:CB	2.57	0.53
2:D:153:PHE:CB	2:D:338:GLN:HA	2.39	0.53
1:B:86:GLY:O	1:B:302:SER:HA	2.09	0.53
3:O:138:ILE:O	3:O:139:ARG:O	2.27	0.53
2:N:153:PHE:CB	2:N:338:GLN:HA	2.39	0.53
1:I:227:PRO:HA	1:I:384:VAL:CB	2.39	0.53
1:C:296:VAL:HA	1:C:333:ALA:HB1	1.90	0.53
2:F:153:PHE:CB	2:F:338:GLN:HA	2.39	0.53
3:G:145:THR:O	3:G:149:LYS:CB	2.57	0.52
1:C:419:PHE:C	1:C:497:GLN:N	2.58	0.52
1:B:227:PRO:HA	1:B:384:VAL:CB	2.39	0.52
1:A:224:ALA:CA	1:A:405:ALA:HB3	2.37	0.52
4:H:77:LEU:O	4:H:78:LYS:C	2.35	0.52
1:C:227:PRO:HA	1:C:384:VAL:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:296:VAL:HA	1:I:333:ALA:HB1	1.91	0.52
1:C:11:GLY:C	2:E:49:GLU:CB	2.75	0.52
2:L:359:SER:CA	2:L:362:MET:H	2.22	0.52
1:K:69:LEU:CA	1:K:72:ALA:HB2	2.40	0.52
1:J:225:ALA:O	1:J:406:PHE:HA	2.08	0.52
1:A:71:LEU:CA	1:A:188:PRO:HA	2.39	0.52
1:C:420:PRO:N	1:C:497:GLN:H	2.07	0.52
3:G:138:ILE:C	3:G:139:ARG:O	2.45	0.52
3:G:165:GLU:O	3:G:166:GLN:C	2.47	0.52
3:O:166:GLN:O	3:O:169:ILE:CB	2.57	0.52
3:O:173:ARG:O	3:O:177:ARG:CB	2.58	0.52
3:G:45:GLU:C	3:G:47:MET:N	2.58	0.52
4:P:74:ILE:C	4:P:75:ALA:HA	2.16	0.52
1:K:227:PRO:HA	1:K:384:VAL:CB	2.40	0.52
3:G:42:LEU:O	3:G:45:GLU:CB	2.57	0.52
3:O:167:VAL:C	3:O:169:ILE:N	2.61	0.52
1:I:259:GLY:O	2:N:298:ALA:N	2.42	0.52
1:A:44:GLY:N	2:D:69:ALA:HB1	2.22	0.52
1:A:233:GLY:HA2	5:A:600:ADP:PA	2.49	0.52
2:N:62:GLU:HA	2:N:227:PRO:CB	2.39	0.52
2:D:359:SER:C	2:D:362:MET:H	2.13	0.52
1:A:52:TYR:O	1:A:53:GLU:CB	2.58	0.52
1:C:52:TYR:O	1:C:53:GLU:CB	2.58	0.52
1:J:263:THR:CB	2:L:124:ARG:C	2.78	0.52
1:I:52:TYR:O	1:I:53:GLU:CB	2.58	0.52
1:K:52:TYR:O	1:K:53:GLU:CB	2.58	0.51
1:I:25:TYR:CB	2:L:65:GLY:CA	2.84	0.51
1:A:419:PHE:O	1:A:497:GLN:O	2.27	0.51
1:B:71:LEU:O	1:B:188:PRO:HA	2.10	0.51
3:O:141:ALA:CA	3:O:145:THR:H	2.22	0.51
1:I:263:THR:O	2:N:124:ARG:HA	2.10	0.51
1:I:224:ALA:CA	1:I:405:ALA:HB3	2.37	0.51
1:I:132:GLY:HA3	1:I:371:LEU:C	2.30	0.51
1:K:296:VAL:HA	1:K:333:ALA:HB1	1.90	0.51
3:O:165:GLU:O	3:O:166:GLN:C	2.47	0.51
1:C:11:GLY:CA	2:E:49:GLU:CB	2.88	0.51
3:O:171:GLY:O	3:O:174:ALA:HB3	2.11	0.51
1:B:52:TYR:O	1:B:53:GLU:CB	2.59	0.51
3:O:205:GLU:CB	3:O:205:GLU:N	2.67	0.51
3:G:7:THR:O	3:G:9:MET:N	2.42	0.51
3:G:141:ALA:CA	3:G:145:THR:H	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ALA:HB2	1:B:405:ALA:CB	2.31	0.51
3:G:173:ARG:O	3:G:177:ARG:CB	2.58	0.51
2:M:359:SER:CB	2:M:362:MET:CB	2.88	0.51
1:B:9:ILE:CA	2:D:50:VAL:CB	2.87	0.51
3:G:171:GLY:O	3:G:174:ALA:HB3	2.11	0.51
3:G:52:ALA:CB	3:G:52:ALA:C	2.74	0.51
3:O:138:ILE:C	3:O:139:ARG:O	2.45	0.51
1:I:346:ALA:HB2	2:L:272:ALA:CB	2.40	0.51
3:O:52:ALA:CB	3:O:52:ALA:C	2.74	0.51
3:O:183:LEU:O	3:O:186:ARG:CB	2.59	0.50
3:G:183:LEU:O	3:G:186:ARG:CB	2.59	0.50
1:A:132:GLY:HA3	1:A:371:LEU:O	2.11	0.50
3:G:194:LEU:CB	3:G:194:LEU:C	2.73	0.50
4:P:77:LEU:O	4:P:78:LYS:C	2.37	0.50
1:C:73:VAL:O	1:C:186:THR:HA	2.12	0.50
2:L:130:PHE:CB	2:L:370:LYS:O	2.60	0.50
3:O:148:LYS:O	3:O:152:GLU:CA	2.59	0.50
1:I:418:HIS:HA	1:I:496:GLN:CB	2.42	0.50
1:J:52:TYR:O	1:J:53:GLU:CB	2.58	0.50
3:O:132:ARG:C	3:O:134:ALA:H	2.13	0.50
1:J:224:ALA:CA	1:J:405:ALA:HB3	2.37	0.50
1:A:73:VAL:O	1:A:186:THR:HA	2.12	0.50
3:G:205:GLU:N	3:G:205:GLU:CB	2.66	0.50
3:G:146:ARG:O	3:G:147:LEU:C	2.50	0.50
1:J:224:ALA:HB2	1:J:405:ALA:CB	2.31	0.50
3:G:132:ARG:C	3:G:134:ALA:H	2.13	0.49
2:N:149:LYS:O	2:N:333:THR:CB	2.59	0.49
2:L:150:LEU:CB	2:L:335:GLY:O	2.60	0.49
1:K:231:GLY:CA	5:K:600:ADP:H5'1	2.37	0.49
1:K:73:VAL:O	1:K:186:THR:HA	2.12	0.49
1:J:73:VAL:O	1:J:186:THR:HA	2.11	0.49
1:B:73:VAL:O	1:B:186:THR:HA	2.12	0.49
1:J:9:ILE:HA	2:L:50:VAL:CB	2.42	0.49
3:O:43:VAL:O	3:O:44:ARG:C	2.51	0.49
3:G:146:ARG:O	3:G:149:LYS:N	2.45	0.49
2:F:149:LYS:O	2:F:333:THR:CB	2.59	0.49
3:G:148:LYS:O	3:G:152:GLU:CA	2.59	0.49
1:C:11:GLY:HA3	2:E:49:GLU:CA	2.42	0.49
2:E:149:LYS:O	2:E:333:THR:CB	2.59	0.49
3:O:146:ARG:O	3:O:149:LYS:N	2.45	0.49
3:O:49:ALA:O	3:O:52:ALA:CB	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:7:THR:O	3:O:8:ARG:O	2.30	0.49
2:D:149:LYS:O	2:D:333:THR:CB	2.59	0.49
2:E:150:LEU:CB	2:E:335:GLY:O	2.61	0.49
1:K:557:GLU:C	1:K:559:PHE:N	2.66	0.49
3:O:142:ASN:CB	3:O:142:ASN:N	2.67	0.49
2:N:150:LEU:CB	2:N:335:GLY:O	2.61	0.49
1:A:557:GLU:C	1:A:559:PHE:N	2.66	0.49
1:J:557:GLU:C	1:J:559:PHE:N	2.66	0.49
2:D:150:LEU:CB	2:D:335:GLY:O	2.60	0.49
2:M:150:LEU:CB	2:M:335:GLY:O	2.61	0.49
1:K:216:PHE:HA	1:K:429:SER:CB	2.43	0.49
1:I:475:ALA:HB1	2:L:398:ILE:O	2.13	0.49
3:O:146:ARG:O	3:O:147:LEU:C	2.50	0.49
3:G:43:VAL:O	3:G:44:ARG:C	2.51	0.49
3:O:198:LYS:O	3:O:199:GLY:O	2.31	0.49
1:B:21:GLY:O	2:E:68:LEU:CB	2.61	0.49
3:O:134:ALA:O	4:P:16:ALA:HB2	2.13	0.49
1:I:71:LEU:CB	1:I:188:PRO:CB	2.87	0.49
2:D:134:GLY:HA2	2:D:430:ARG:C	2.30	0.49
1:J:429:SER:C	1:J:431:PHE:H	2.17	0.49
3:O:134:ALA:O	3:O:137:LEU:CB	2.61	0.49
1:I:24:MET:HA	2:L:66:LEU:HA	0.57	0.49
2:L:149:LYS:O	2:L:333:THR:CB	2.59	0.49
2:M:149:LYS:O	2:M:333:THR:CB	2.60	0.48
1:A:81:ASN:HA	1:A:282:MET:C	2.33	0.48
3:G:198:LYS:O	3:G:199:GLY:O	2.31	0.48
4:H:65:GLY:CA	4:H:66:ARG:CB	2.91	0.48
1:B:557:GLU:C	1:B:559:PHE:N	2.66	0.48
1:I:73:VAL:O	1:I:186:THR:HA	2.12	0.48
1:C:224:ALA:CA	1:C:405:ALA:HB3	2.37	0.48
1:C:208:GLY:O	1:C:507:CYS:CA	2.61	0.48
3:O:198:LYS:O	3:O:199:GLY:C	2.52	0.48
1:I:557:GLU:C	1:I:559:PHE:N	2.66	0.48
3:O:3:GLN:O	3:O:6:PRO:N	2.46	0.48
3:O:200:LYS:HA	3:O:203:ALA:HB3	1.96	0.48
1:I:440:ARG:HA	1:I:444:ALA:O	2.14	0.48
1:J:440:ARG:HA	1:J:444:ALA:O	2.14	0.48
1:J:471:VAL:CB	4:P:98:ILE:O	2.61	0.48
3:O:138:ILE:O	3:O:142:ASN:CB	2.62	0.48
1:C:352:PRO:C	2:F:269:GLU:CB	2.81	0.48
3:G:134:ALA:O	3:G:137:LEU:CB	2.62	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:259:GLY:N	2:M:296:GLU:CB	2.68	0.48
1:C:266:LEU:O	2:E:124:ARG:CB	2.62	0.48
3:O:48:GLU:CB	3:O:51:LYS:CB	2.92	0.48
1:I:24:MET:CB	2:L:66:LEU:CB	2.92	0.48
3:G:3:GLN:O	3:G:6:PRO:N	2.47	0.48
2:F:150:LEU:CB	2:F:335:GLY:O	2.61	0.48
1:C:557:GLU:C	1:C:559:PHE:N	2.66	0.48
3:G:135:GLU:HA	3:G:138:ILE:H	1.79	0.48
3:G:198:LYS:O	3:G:199:GLY:C	2.52	0.48
1:I:404:GLY:O	1:I:430:LEU:N	2.47	0.48
1:A:43:ASP:C	2:D:69:ALA:HB3	2.34	0.48
2:M:61:GLU:HA	2:M:229:ILE:CB	2.44	0.47
3:O:153:GLU:O	3:O:154:ILE:O	2.32	0.47
3:G:153:GLU:O	3:G:154:ILE:O	2.32	0.47
3:G:4:VAL:CA	3:G:5:SER:N	2.68	0.47
1:I:25:TYR:N	2:L:65:GLY:C	2.60	0.47
3:G:167:VAL:C	3:G:169:ILE:H	2.18	0.47
3:O:167:VAL:C	3:O:169:ILE:H	2.17	0.47
1:K:233:GLY:CA	5:K:600:ADP:C8	2.97	0.47
1:A:440:ARG:HA	1:A:444:ALA:O	2.14	0.47
3:G:48:GLU:CB	3:G:51:LYS:CB	2.92	0.47
3:G:138:ILE:O	3:G:142:ASN:CB	2.62	0.47
2:E:150:LEU:C	2:E:335:GLY:O	2.53	0.47
1:K:440:ARG:HA	1:K:444:ALA:O	2.14	0.47
1:B:25:TYR:CB	2:E:64:THR:O	2.63	0.47
2:F:150:LEU:C	2:F:335:GLY:O	2.53	0.47
2:M:150:LEU:C	2:M:335:GLY:O	2.53	0.47
3:O:135:GLU:HA	3:O:138:ILE:H	1.80	0.47
1:I:25:TYR:N	2:L:65:GLY:CA	2.77	0.47
1:B:429:SER:C	1:B:431:PHE:H	2.19	0.47
1:C:440:ARG:HA	1:C:444:ALA:O	2.14	0.47
1:C:352:PRO:O	2:F:269:GLU:CB	2.63	0.47
3:G:200:LYS:HA	3:G:203:ALA:HB3	1.96	0.47
2:D:150:LEU:C	2:D:335:GLY:O	2.53	0.47
1:C:266:LEU:CB	2:E:124:ARG:CB	2.93	0.47
1:B:440:ARG:HA	1:B:444:ALA:O	2.14	0.47
2:D:359:SER:CA	2:D:362:MET:H	2.27	0.46
2:L:150:LEU:C	2:L:335:GLY:O	2.52	0.46
1:I:346:ALA:HB2	2:L:272:ALA:HB2	1.97	0.46
3:O:200:LYS:CA	3:O:203:ALA:HB3	2.45	0.46
3:G:49:ALA:O	3:G:52:ALA:CB	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:132:GLY:HA3	1:I:371:LEU:O	2.16	0.46
2:L:134:GLY:C	2:L:430:ARG:O	2.54	0.46
1:J:24:MET:CB	2:M:66:LEU:C	2.83	0.46
1:A:43:ASP:O	2:D:69:ALA:CB	2.63	0.46
1:B:23:ARG:O	2:E:67:ASP:O	2.34	0.46
2:F:427:GLN:O	1:K:126:GLY:HA2	2.15	0.46
1:B:10:ALA:O	2:D:49:GLU:HA	2.16	0.46
2:N:150:LEU:C	2:N:335:GLY:O	2.53	0.46
1:I:419:PHE:O	1:I:495:LEU:O	2.34	0.46
1:A:198:LYS:HA	1:A:368:VAL:HA	1.98	0.46
3:G:7:THR:O	3:G:8:ARG:O	2.30	0.46
4:H:84:HIS:C	4:H:86:VAL:H	2.10	0.46
3:G:200:LYS:CA	3:G:203:ALA:HB3	2.45	0.46
1:A:56:SER:CB	2:F:30:GLY:H	2.28	0.46
1:A:224:ALA:HB2	1:A:405:ALA:CB	2.31	0.46
1:C:359:ALA:CB	2:F:224:ALA:HB1	2.46	0.46
1:K:419:PHE:N	1:K:496:GLN:HA	2.31	0.46
1:I:217:PRO:C	1:I:431:PHE:CB	2.84	0.46
1:C:268:GLU:CB	2:E:126:LYS:CB	2.94	0.46
3:O:52:ALA:O	3:O:55:GLN:O	2.34	0.45
1:I:419:PHE:H	1:I:496:GLN:CA	2.27	0.45
3:O:194:LEU:C	3:O:194:LEU:CB	2.73	0.45
1:I:11:GLY:N	2:N:50:VAL:O	2.47	0.45
1:A:197:ARG:O	1:A:369:ILE:N	2.38	0.45
3:G:35:LEU:O	3:G:38:GLU:CB	2.65	0.45
3:O:35:LEU:O	3:O:38:GLU:CB	2.65	0.45
3:G:52:ALA:O	3:G:55:GLN:O	2.34	0.45
1:J:71:LEU:O	1:J:188:PRO:HA	2.15	0.45
3:G:142:ASN:CB	3:G:142:ASN:N	2.67	0.45
1:K:44:GLY:N	2:N:69:ALA:HB2	2.32	0.45
1:K:296:VAL:CA	1:K:333:ALA:HB1	2.47	0.45
3:G:151:GLY:O	3:G:152:GLU:O	2.35	0.45
1:A:11:GLY:HA3	2:F:50:VAL:CB	2.42	0.45
1:J:208:GLY:O	1:J:507:CYS:CB	2.65	0.45
1:I:24:MET:CA	2:L:66:LEU:H	1.93	0.45
1:I:11:GLY:C	2:N:50:VAL:O	2.54	0.45
3:O:179:ILE:O	3:O:180:GLN:C	2.55	0.45
3:G:179:ILE:O	3:G:180:GLN:C	2.56	0.45
1:J:70:PRO:O	1:J:71:LEU:C	2.55	0.45
1:A:44:GLY:CA	2:D:69:ALA:HB3	2.44	0.45
1:I:56:SER:CB	2:N:30:GLY:CA	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:296:VAL:CA	1:C:333:ALA:HB1	2.47	0.45
3:G:141:ALA:HB1	3:G:145:THR:CB	2.47	0.44
3:O:4:VAL:CA	3:O:5:SER:N	2.68	0.44
1:K:26:ASP:O	1:K:71:LEU:N	2.50	0.44
1:J:296:VAL:CA	1:J:333:ALA:HB1	2.47	0.44
3:O:141:ALA:HB1	3:O:145:THR:CB	2.47	0.44
2:D:153:PHE:O	2:D:338:GLN:HA	2.17	0.44
1:A:263:THR:CB	2:F:123:ALA:O	2.66	0.44
1:B:296:VAL:CA	1:B:333:ALA:HB1	2.47	0.44
1:C:314:ARG:HA	1:C:318:PHE:O	2.18	0.44
3:G:45:GLU:O	3:G:47:MET:N	2.50	0.44
1:K:11:GLY:HA3	2:M:49:GLU:HA	1.94	0.44
3:G:189:GLU:CB	3:G:189:GLU:N	2.69	0.44
1:K:259:GLY:CA	2:M:296:GLU:C	2.60	0.44
3:G:175:GLN:O	3:G:177:ARG:N	2.51	0.44
1:J:314:ARG:HA	1:J:318:PHE:O	2.18	0.44
3:O:151:GLY:O	3:O:152:GLU:O	2.35	0.44
1:J:10:ALA:O	2:L:49:GLU:CA	2.65	0.44
1:J:25:TYR:O	2:M:65:GLY:HA2	2.17	0.44
3:O:175:GLN:O	3:O:177:ARG:N	2.51	0.44
1:A:314:ARG:HA	1:A:318:PHE:O	2.18	0.44
1:K:233:GLY:HA2	5:K:600:ADP:C8	2.52	0.44
1:A:296:VAL:CA	1:A:333:ALA:HB1	2.47	0.44
1:I:296:VAL:CA	1:I:333:ALA:HB1	2.47	0.44
1:B:314:ARG:HA	1:B:318:PHE:O	2.18	0.44
1:I:86:GLY:O	1:I:305:VAL:CB	2.66	0.44
1:K:314:ARG:HA	1:K:318:PHE:O	2.18	0.44
3:O:45:GLU:O	3:O:47:MET:N	2.50	0.44
2:L:153:PHE:O	2:L:338:GLN:HA	2.18	0.44
2:E:153:PHE:O	2:E:338:GLN:HA	2.18	0.44
1:K:224:ALA:HB2	1:K:405:ALA:CB	2.32	0.43
2:N:153:PHE:O	2:N:338:GLN:HA	2.18	0.43
2:N:349:TYR:HA	2:N:350:PRO:C	2.38	0.43
2:D:349:TYR:HA	2:D:350:PRO:C	2.38	0.43
3:O:167:VAL:C	3:O:167:VAL:HA	2.16	0.43
2:M:153:PHE:O	2:M:338:GLN:HA	2.18	0.43
1:I:314:ARG:HA	1:I:318:PHE:O	2.18	0.43
3:O:189:GLU:N	3:O:189:GLU:CB	2.69	0.43
2:M:349:TYR:HA	2:M:350:PRO:C	2.39	0.43
1:J:75:LEU:O	1:J:184:TYR:HA	2.19	0.43
1:I:255:CYS:HA	1:I:290:ASN:CB	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:258:THR:HA	2:F:259:ASP:HA	1.85	0.43
1:B:241:LEU:O	1:B:245:SER:CB	2.67	0.43
2:D:334:GLU:CA	2:D:361:LEU:CB	2.97	0.43
3:O:135:GLU:O	3:O:139:ARG:CB	2.67	0.43
1:C:292:SER:CB	2:E:292:ALA:HB1	2.45	0.43
3:G:175:GLN:O	3:G:178:PHE:N	2.51	0.43
1:I:56:SER:CB	2:N:30:GLY:H	2.29	0.43
1:J:241:LEU:O	1:J:245:SER:CB	2.67	0.43
1:K:75:LEU:O	1:K:184:TYR:HA	2.19	0.43
1:A:255:CYS:HA	1:A:290:ASN:CB	2.49	0.43
2:F:349:TYR:HA	2:F:350:PRO:C	2.38	0.43
3:O:140:VAL:O	3:O:144:GLU:N	2.47	0.43
3:G:135:GLU:O	3:G:139:ARG:CB	2.67	0.43
1:K:189:VAL:CB	1:K:304:TYR:CB	2.97	0.43
2:E:258:THR:HA	2:E:259:ASP:HA	1.85	0.43
3:O:189:GLU:HA	3:O:189:GLU:CB	2.18	0.42
2:F:427:GLN:C	1:K:126:GLY:HA2	2.40	0.42
1:B:9:ILE:CB	2:D:52:GLU:N	2.82	0.42
1:A:241:LEU:O	1:A:245:SER:CB	2.67	0.42
1:K:255:CYS:HA	1:K:290:ASN:CB	2.49	0.42
1:B:255:CYS:HA	1:B:290:ASN:CB	2.49	0.42
2:F:427:GLN:CB	1:K:126:GLY:HA2	2.43	0.42
2:M:334:GLU:O	2:M:360:ARG:N	2.49	0.42
2:F:153:PHE:O	2:F:338:GLN:HA	2.18	0.42
3:O:174:ALA:O	3:O:175:GLN:O	2.37	0.42
1:K:241:LEU:O	1:K:245:SER:CB	2.67	0.42
1:C:241:LEU:O	1:C:245:SER:CB	2.67	0.42
1:I:241:LEU:O	1:I:245:SER:CB	2.67	0.42
1:B:75:LEU:O	1:B:184:TYR:HA	2.19	0.42
2:L:349:TYR:HA	2:L:350:PRO:C	2.38	0.42
1:J:255:CYS:HA	1:J:290:ASN:CB	2.49	0.42
4:H:77:LEU:H	4:H:80:ALA:CB	2.28	0.42
2:E:189:VAL:O	2:E:217:SER:HA	2.20	0.42
2:L:189:VAL:O	2:L:217:SER:HA	2.20	0.42
2:D:189:VAL:O	2:D:217:SER:HA	2.20	0.42
1:K:12:PRO:N	2:M:49:GLU:CB	2.83	0.42
2:N:360:ARG:C	2:N:362:MET:N	2.38	0.42
1:A:11:GLY:N	2:F:50:VAL:O	2.53	0.42
2:E:349:TYR:HA	2:E:350:PRO:C	2.39	0.42
1:C:75:LEU:O	1:C:184:TYR:HA	2.19	0.42
3:G:4:VAL:C	3:G:6:PRO:N	2.71	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:189:VAL:O	2:F:217:SER:HA	2.20	0.42
1:A:267:VAL:CB	2:F:125:ARG:HA	2.50	0.42
1:A:266:LEU:CB	2:F:124:ARG:HA	2.49	0.42
1:B:25:TYR:O	2:E:65:GLY:HA3	2.02	0.42
1:K:11:GLY:CA	2:M:49:GLU:CA	2.95	0.42
1:A:133:MET:O	1:A:148:LEU:HA	2.20	0.42
1:I:75:LEU:O	1:I:184:TYR:HA	2.19	0.42
3:O:175:GLN:O	3:O:178:PHE:N	2.51	0.41
1:B:227:PRO:CB	1:B:384:VAL:CB	2.98	0.41
1:J:133:MET:O	1:J:148:LEU:HA	2.20	0.41
1:A:221:GLY:O	1:A:366:GLY:HA2	2.20	0.41
1:A:75:LEU:O	1:A:184:TYR:HA	2.19	0.41
3:O:48:GLU:O	3:O:51:LYS:CA	2.67	0.41
2:F:334:GLU:O	2:F:360:ARG:N	2.53	0.41
1:B:22:ALA:HA	2:E:68:LEU:CB	2.50	0.41
2:M:189:VAL:O	2:M:217:SER:HA	2.20	0.41
1:C:133:MET:O	1:C:148:LEU:HA	2.20	0.41
1:J:10:ALA:O	2:L:50:VAL:N	2.47	0.41
1:K:227:PRO:CB	1:K:384:VAL:CB	2.99	0.41
1:C:255:CYS:HA	1:C:290:ASN:CB	2.49	0.41
3:G:43:VAL:O	3:G:45:GLU:N	2.54	0.41
2:N:189:VAL:O	2:N:217:SER:HA	2.20	0.41
1:K:133:MET:O	1:K:148:LEU:HA	2.21	0.41
2:L:334:GLU:C	2:L:361:LEU:CB	2.88	0.41
2:D:149:LYS:CB	2:D:333:THR:HA	2.51	0.41
1:I:133:MET:O	1:I:148:LEU:HA	2.21	0.41
1:B:221:GLY:O	1:B:366:GLY:HA2	2.21	0.41
1:B:133:MET:O	1:B:148:LEU:HA	2.20	0.41
3:O:148:LYS:C	3:O:149:LYS:O	2.59	0.41
2:F:149:LYS:CB	2:F:333:THR:HA	2.51	0.41
1:B:263:THR:CB	2:D:124:ARG:CA	2.97	0.41
1:B:141:PHE:O	1:B:143:PHE:O	2.39	0.41
1:K:221:GLY:O	1:K:366:GLY:HA2	2.21	0.41
1:I:227:PRO:CB	1:I:384:VAL:CB	2.99	0.41
1:J:221:GLY:O	1:J:366:GLY:HA2	2.20	0.41
1:C:221:GLY:O	1:C:366:GLY:HA2	2.21	0.41
3:O:40:PHE:O	3:O:43:VAL:CB	2.69	0.41
3:O:43:VAL:O	3:O:45:GLU:N	2.54	0.41
2:F:427:GLN:C	1:K:126:GLY:CA	2.89	0.41
2:N:149:LYS:CB	2:N:333:THR:HA	2.51	0.41
1:I:346:ALA:HB2	2:L:272:ALA:HB1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:141:PHE:O	1:K:143:PHE:O	2.39	0.41
1:C:141:PHE:O	1:C:143:PHE:O	2.39	0.41
2:D:130:PHE:CB	2:D:370:LYS:O	2.68	0.41
3:G:146:ARG:O	3:G:149:LYS:CB	2.69	0.41
1:A:227:PRO:CB	1:A:384:VAL:CB	2.99	0.41
3:G:48:GLU:O	3:G:51:LYS:CA	2.68	0.40
1:C:44:GLY:CA	2:F:69:ALA:HB2	2.42	0.40
3:G:174:ALA:O	3:G:175:GLN:O	2.36	0.40
1:C:227:PRO:CB	1:C:384:VAL:CB	2.99	0.40
2:N:258:THR:HA	2:N:259:ASP:HA	1.85	0.40
1:I:221:GLY:O	1:I:366:GLY:HA2	2.21	0.40
3:O:146:ARG:O	3:O:149:LYS:CB	2.69	0.40
2:M:149:LYS:CB	2:M:333:THR:HA	2.51	0.40
1:I:226:ILE:O	1:I:384:VAL:N	2.55	0.40
4:H:63:MET:CB	4:H:64:ARG:HA	2.52	0.40
3:G:40:PHE:O	3:G:43:VAL:CB	2.69	0.40
1:J:263:THR:CB	2:L:126:LYS:N	2.77	0.40
1:A:226:ILE:O	1:A:384:VAL:N	2.55	0.40
4:P:94:VAL:O	4:P:95:ARG:C	2.58	0.40
3:G:148:LYS:C	3:G:149:LYS:O	2.60	0.40
3:O:4:VAL:C	3:O:6:PRO:N	2.71	0.40
2:L:149:LYS:CB	2:L:333:THR:HA	2.51	0.40
1:K:233:GLY:HA2	5:K:600:ADP:O1A	2.21	0.40
1:J:227:PRO:CB	1:J:384:VAL:CB	2.99	0.40
1:C:226:ILE:O	1:C:384:VAL:N	2.54	0.40
1:I:141:PHE:O	1:I:143:PHE:O	2.39	0.40
1:C:259:GLY:C	2:E:296:GLU:C	2.80	0.40
1:B:263:THR:CB	2:D:124:ARG:HA	2.51	0.40
1:J:226:ILE:O	1:J:384:VAL:N	2.55	0.40
1:J:141:PHE:O	1:J:143:PHE:O	2.39	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:6:ILE:CB	2:M:24:ALA:O[5_555]	2.04	0.16
1:J:5:VAL:CA	2:M:24:ALA:CB[5_555]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	557/578 (96%)	491 (88%)	48 (9%)	18 (3%)	5	43
1	B	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	5	43
1	C	557/578 (96%)	492 (88%)	48 (9%)	17 (3%)	5	44
1	I	557/578 (96%)	493 (88%)	48 (9%)	16 (3%)	6	45
1	J	557/578 (96%)	492 (88%)	47 (8%)	18 (3%)	5	43
1	K	557/578 (96%)	493 (88%)	47 (8%)	17 (3%)	5	44
2	D	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	9	53
2	E	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	9	53
2	F	446/478 (93%)	421 (94%)	16 (4%)	9 (2%)	9	53
2	L	446/478 (93%)	420 (94%)	17 (4%)	9 (2%)	9	53
2	M	446/478 (93%)	422 (95%)	15 (3%)	9 (2%)	9	53
2	N	446/478 (93%)	420 (94%)	16 (4%)	10 (2%)	8	51
3	G	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
3	O	125/223 (56%)	76 (61%)	20 (16%)	29 (23%)	0	1
4	H	102/104 (98%)	89 (87%)	11 (11%)	2 (2%)	9	53
4	P	102/104 (98%)	90 (88%)	10 (10%)	2 (2%)	9	53
All	All	6472/6990 (93%)	5808 (90%)	443 (7%)	221 (3%)	5	42

All (221) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	12	PRO
1	A	19	MET
1	A	53	GLU
1	A	143	PHE
1	A	227	PRO
1	A	256	GLY

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Mol	Chain	Res	Type
1	A	260	ASN
1	A	325	ASP
1	A	394	PRO
1	A	395	VAL
1	A	558	GLU
1	B	12	PRO
1	B	19	MET
1	B	53	GLU
1	B	143	PHE
1	B	227	PRO
1	B	256	GLY
1	B	260	ASN
1	B	325	ASP
1	B	394	PRO
1	B	395	VAL
1	B	558	GLU
1	C	12	PRO
1	C	19	MET
1	C	53	GLU
1	C	143	PHE
1	C	227	PRO
1	C	256	GLY
1	C	260	ASN
1	C	325	ASP
1	C	394	PRO
1	C	395	VAL
1	C	558	GLU
2	D	52	GLU
2	D	79	VAL
2	D	316	MET
2	D	356	PRO
2	D	427	GLN
2	E	52	GLU
2	E	79	VAL
2	E	316	MET
2	E	356	PRO
2	E	427	GLN
2	F	52	GLU
2	F	316	MET
2	F	356	PRO
2	F	427	GLN
3	G	3	GLN

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Mol	Chain	Res	Type
3	G	4	VAL
3	G	43	VAL
3	G	47	MET
3	G	48	GLU
3	G	140	VAL
3	G	149	LYS
3	G	152	GLU
3	G	161	VAL
3	G	172	ILE
3	G	174	ALA
4	H	85	ASP
4	H	100	PHE
1	I	12	PRO
1	I	19	MET
1	I	53	GLU
1	I	143	PHE
1	I	227	PRO
1	I	256	GLY
1	I	260	ASN
1	I	325	ASP
1	I	394	PRO
1	I	395	VAL
1	I	558	GLU
1	J	12	PRO
1	J	19	MET
1	J	53	GLU
1	J	143	PHE
1	J	227	PRO
1	J	256	GLY
1	J	260	ASN
1	J	325	ASP
1	J	394	PRO
1	J	395	VAL
1	J	558	GLU
1	K	12	PRO
1	K	19	MET
1	K	53	GLU
1	K	71	LEU
1	K	143	PHE
1	K	227	PRO
1	K	256	GLY
1	K	260	ASN

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Mol	Chain	Res	Type
1	K	325	ASP
1	K	394	PRO
1	K	395	VAL
1	K	558	GLU
2	L	52	GLU
2	L	79	VAL
2	L	316	MET
2	L	356	PRO
2	L	427	GLN
2	M	52	GLU
2	M	316	MET
2	M	356	PRO
2	M	427	GLN
2	N	52	GLU
2	N	316	MET
2	N	356	PRO
2	N	361	LEU
2	N	427	GLN
3	O	3	GLN
3	O	4	VAL
3	O	43	VAL
3	O	47	MET
3	O	48	GLU
3	O	140	VAL
3	O	149	LYS
3	O	152	GLU
3	O	161	VAL
3	O	172	ILE
3	O	174	ALA
3	O	200	LYS
4	P	85	ASP
4	P	100	PHE
1	A	88	GLN
1	A	255	CYS
1	A	431	PHE
1	B	71	LEU
1	B	88	GLN
1	B	255	CYS
1	C	88	GLN
1	C	255	CYS
2	D	26	ASP
2	D	428	GLN

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Mol	Chain	Res	Type
2	E	26	ASP
2	E	428	GLN
2	F	26	ASP
2	F	428	GLN
3	G	2	SER
3	G	6	PRO
3	G	150	ILE
3	G	151	GLY
3	G	185	GLN
3	G	200	LYS
1	I	88	GLN
1	I	255	CYS
1	J	71	LEU
1	J	88	GLN
1	J	255	CYS
1	J	430	LEU
1	K	88	GLN
1	K	255	CYS
2	L	26	ASP
2	L	428	GLN
2	M	26	ASP
2	M	79	VAL
2	M	428	GLN
2	N	26	ASP
2	N	428	GLN
3	O	2	SER
3	O	6	PRO
3	O	13	GLN
3	O	150	ILE
3	O	151	GLY
3	O	185	GLN
1	A	109	HIS
1	B	109	HIS
1	C	109	HIS
3	G	13	GLN
3	G	139	ARG
3	G	155	LYS
3	G	162	ASN
3	G	165	GLU
1	I	109	HIS
1	J	109	HIS
1	K	109	HIS

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Mol	Chain	Res	Type
2	N	79	VAL
3	O	139	ARG
3	O	155	LYS
3	O	162	ASN
3	O	165	GLU
1	A	200	ASP
2	F	79	VAL
3	G	45	GLU
3	G	186	ARG
3	O	45	GLU
3	O	137	LEU
3	O	186	ARG
1	A	374	GLU
1	B	70	PRO
1	B	374	GLU
1	C	71	LEU
1	C	374	GLU
2	D	317	PRO
2	E	317	PRO
2	F	317	PRO
3	G	53	LEU
3	G	137	LEU
3	G	197	ILE
1	I	374	GLU
1	J	374	GLU
1	K	374	GLU
2	L	317	PRO
2	M	317	PRO
2	N	317	PRO
3	O	53	LEU
3	O	197	ILE
2	D	355	LEU
2	E	355	LEU
2	F	355	LEU
2	L	355	LEU
2	M	355	LEU
2	N	355	LEU
1	A	388	GLY
1	B	388	GLY
1	C	388	GLY
3	G	179	ILE
1	I	388	GLY

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Mol	Chain	Res	Type
1	J	388	GLY
1	K	388	GLY
3	O	179	ILE
3	G	168	VAL
3	O	168	VAL

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	ADP	A	600	-	22,29,29	1.17	3 (13%)	27,45,45	0.88	1 (3%)
5	ADP	C	600	-	22,29,29	1.04	2 (9%)	27,45,45	1.15	3 (11%)
5	ADP	I	600	-	22,29,29	1.16	3 (13%)	27,45,45	0.88	1 (3%)
5	ADP	K	600	-	22,29,29	1.04	2 (9%)	27,45,45	1.15	3 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	A	600	-	-	0/12/32/32	0/3/3/3
5	ADP	C	600	-	-	0/12/32/32	0/3/3/3
5	ADP	I	600	-	-	0/12/32/32	0/3/3/3
5	ADP	K	600	-	-	0/12/32/32	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	600	ADP	PB-O2B	-2.58	1.45	1.54
5	C	600	ADP	PB-O2B	-2.58	1.45	1.54
5	A	600	ADP	PB-O2B	-2.49	1.45	1.54
5	I	600	ADP	PB-O2B	-2.47	1.45	1.54
5	C	600	ADP	PA-O1A	-2.33	1.42	1.51
5	K	600	ADP	PA-O1A	-2.33	1.42	1.51
5	I	600	ADP	PB-O3B	-2.04	1.47	1.54
5	A	600	ADP	PB-O3B	-2.02	1.47	1.54
5	I	600	ADP	O4'-C1'	2.77	1.44	1.41
5	A	600	ADP	O4'-C1'	2.80	1.44	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	600	ADP	C2'-C1'-N9	-3.03	109.66	114.29
5	K	600	ADP	C2'-C1'-N9	-3.03	109.66	114.29
5	I	600	ADP	C2'-C1'-N9	-2.32	110.75	114.29
5	A	600	ADP	C2'-C1'-N9	-2.29	110.79	114.29
5	K	600	ADP	O4'-C4'-C3'	-2.02	101.08	105.15
5	C	600	ADP	O4'-C4'-C3'	-2.01	101.09	105.15
5	C	600	ADP	O3B-PB-O2B	2.45	116.71	107.38
5	K	600	ADP	O3B-PB-O2B	2.45	116.72	107.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ADP	2	0
5	C	600	ADP	1	0
5	K	600	ADP	5	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	561/578 (97%)	0.24	47 (8%) 14 11	103, 162, 214, 214	0
1	B	561/578 (97%)	-0.14	13 (2%) 64 54	79, 130, 144, 144	0
1	C	561/578 (97%)	0.28	48 (8%) 13 11	137, 189, 210, 210	0
1	I	561/578 (97%)	0.48	72 (12%) 5 6	172, 172, 232, 232	0
1	J	561/578 (97%)	-0.33	8 (1%) 78 69	50, 58, 104, 104	0
1	K	561/578 (97%)	0.39	55 (9%) 10 8	146, 177, 189, 189	0
2	D	450/478 (94%)	0.05	25 (5%) 28 21	118, 118, 188, 188	0
2	E	450/478 (94%)	0.18	35 (7%) 16 12	122, 130, 162, 162	0
2	F	450/478 (94%)	0.28	40 (8%) 12 9	109, 217, 217, 217	0
2	L	450/478 (94%)	0.00	19 (4%) 40 31	98, 98, 158, 158	0
2	M	450/478 (94%)	0.07	24 (5%) 30 23	99, 99, 148, 148	0
2	N	450/478 (94%)	0.54	55 (12%) 5 6	158, 250, 250, 250	0
3	G	129/223 (57%)	-0.68	0 100 100	34, 34, 49, 49	0
3	O	129/223 (57%)	-0.60	1 (0%) 87 82	84, 85, 85, 85	0
4	H	104/104 (100%)	0.14	6 (5%) 26 20	110, 110, 134, 134	0
4	P	104/104 (100%)	0.03	7 (6%) 21 15	94, 94, 141, 141	0
All	All	6532/6990 (93%)	0.13	455 (6%) 19 15	34, 137, 232, 250	0

All (455) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	77	PRO	10.8
2	N	191	PHE	9.9
1	I	372	GLY	9.6
2	N	192	ALA	9.3
1	C	379	THR	8.8

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Mol	Chain	Res	Type	RSRZ
2	D	67	ASP	8.7
2	M	121	PRO	8.5
4	H	24	SER	8.5
4	H	76	GLY	8.3
2	N	122	VAL	8.3
2	L	121	PRO	8.2
1	K	382	GLY	8.0
2	L	122	VAL	7.9
2	E	120	ASN	7.4
1	C	36	VAL	7.2
1	I	77	PRO	7.2
1	C	47	ALA	7.1
1	K	383	ALA	7.1
4	P	104	LEU	6.9
1	K	76	GLY	6.7
2	M	302	GLU	6.7
2	N	190	VAL	6.5
2	M	122	VAL	6.5
1	C	37	GLY	6.5
1	I	78	GLY	6.4
1	C	29	LYS	6.3
1	I	180	GLU	6.2
4	P	85	ASP	6.2
1	A	128	GLU	6.2
1	K	324	ALA	6.2
1	K	195	VAL	6.0
2	E	29	TYR	6.0
1	A	61	GLY	5.9
2	D	28	ALA	5.9
2	E	119	LEU	5.8
1	K	78	GLY	5.8
1	B	109	HIS	5.8
2	N	218	VAL	5.8
2	D	68	LEU	5.7
2	E	118	PRO	5.7
2	F	225	ASP	5.7
2	N	121	PRO	5.6
2	F	122	VAL	5.6
2	D	102	GLY	5.6
1	I	134	VAL	5.5
2	N	67	ASP	5.5
1	A	147	ILE	5.5

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Mol	Chain	Res	Type	RSRZ
1	I	63	PRO	5.4
2	F	86	LYS	5.4
2	N	118	PRO	5.3
1	K	122	MET	5.3
1	I	145	HIS	5.2
2	F	121	PRO	5.2
1	K	117	TRP	5.1
2	L	56	VAL	5.1
2	F	278	PRO	5.0
1	K	394	PRO	5.0
1	A	346	ALA	5.0
2	E	28	ALA	4.9
1	I	181	LEU	4.9
2	E	172	THR	4.9
2	E	70	THR	4.9
1	A	146	LYS	4.8
1	A	77	PRO	4.8
1	I	576	ALA	4.8
1	C	77	PRO	4.7
1	A	162	PRO	4.7
2	F	221	LEU	4.7
1	K	194	PRO	4.7
2	N	242	ALA	4.6
2	E	168	ALA	4.6
1	B	110	ALA	4.6
1	I	177	ASP	4.6
1	I	424	TRP	4.5
2	D	21	VAL	4.5
1	I	373	GLY	4.5
2	D	22	GLU	4.5
4	P	75	ALA	4.5
4	H	75	ALA	4.5
2	F	83	GLY	4.5
1	C	150	PRO	4.5
1	I	146	LYS	4.5
2	M	301	VAL	4.4
1	C	1	MET	4.4
1	I	219	ALA	4.4
2	F	28	ALA	4.3
1	I	135	LEU	4.3
1	A	193	ARG	4.3
2	L	21	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	12	PRO	4.3
2	M	300	VAL	4.3
1	C	376	GLY	4.3
1	I	218	VAL	4.3
1	K	227	PRO	4.3
2	D	310	GLN	4.3
1	I	371	LEU	4.2
1	A	134	VAL	4.2
2	L	20	PHE	4.2
1	A	194	PRO	4.2
2	F	188	ALA	4.2
1	I	12	PRO	4.2
1	K	345	PRO	4.2
2	F	189	VAL	4.2
2	N	148	GLN	4.2
1	K	297	ALA	4.1
2	F	332	ILE	4.1
1	B	108	VAL	4.1
1	I	155	GLY	4.0
1	I	497	GLN	4.0
2	E	69	ALA	4.0
2	N	220	PHE	4.0
1	K	165	GLU	3.9
2	E	299	GLY	3.9
1	K	164	GLY	3.9
2	F	299	GLY	3.9
2	N	164	ALA	3.9
1	A	86	GLY	3.9
1	C	2	ILE	3.8
1	I	42	LEU	3.8
2	N	80	ALA	3.8
2	D	121	PRO	3.8
1	A	201	PRO	3.8
2	D	75	LEU	3.8
2	F	365	GLY	3.8
2	E	351	PRO	3.7
1	K	226	ILE	3.7
2	N	123	ALA	3.7
1	I	563	PHE	3.7
2	N	298	ALA	3.7
1	A	155	GLY	3.7
2	F	187	PHE	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	62	GLU	3.6
1	I	176	GLU	3.6
1	K	118	ALA	3.6
1	K	108	VAL	3.6
2	N	83	GLY	3.6
1	I	138	VAL	3.6
1	K	123	VAL	3.6
1	C	502	GLU	3.5
2	E	333	THR	3.5
2	M	11	ILE	3.5
2	N	28	ALA	3.5
2	E	121	PRO	3.5
1	K	393	GLU	3.5
2	E	463	TYR	3.5
2	M	402	ASP	3.5
2	F	298	ALA	3.5
2	M	168	ALA	3.4
1	C	368	VAL	3.4
2	F	224	ALA	3.4
1	K	417	ARG	3.4
2	D	23	ASN	3.4
1	K	433	SER	3.4
4	H	25	SER	3.4
2	N	184	GLU	3.4
1	I	173	VAL	3.4
1	I	55	THR	3.4
1	I	139	PRO	3.3
2	N	66	LEU	3.3
1	K	325	ASP	3.3
1	C	183	MET	3.3
1	C	165	GLU	3.3
1	I	164	GLY	3.3
1	K	576	ALA	3.3
2	D	64	THR	3.3
2	N	205	ILE	3.3
2	N	173	VAL	3.3
1	K	551	ALA	3.2
2	D	27	LEU	3.2
1	J	494	PHE	3.2
1	A	13	ALA	3.2
2	N	429	ASN	3.2
2	D	45	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	55	THR	3.2
1	A	222	GLY	3.2
1	A	577	LEU	3.2
2	M	360	ARG	3.2
2	F	87	GLU	3.2
1	C	73	VAL	3.2
1	K	169	GLU	3.2
1	K	384	VAL	3.2
1	I	224	ALA	3.2
2	M	359	SER	3.2
1	K	434	ALA	3.1
2	D	44	GLY	3.1
2	F	147	GLY	3.1
1	A	1	MET	3.1
2	N	82	LEU	3.1
2	M	299	GLY	3.1
3	O	143	THR	3.1
1	K	47	ALA	3.1
1	K	295	PRO	3.1
2	E	88	MET	3.1
2	E	335	GLY	3.1
1	A	163	ALA	3.1
1	A	60	VAL	3.1
2	D	120	ASN	3.1
1	B	388	GLY	3.1
1	C	43	ASP	3.1
1	C	151	PRO	3.1
2	N	174	ARG	3.1
2	F	88	MET	3.1
1	J	471	VAL	3.0
2	N	165	ALA	3.0
4	P	98	ILE	3.0
1	K	114	GLU	3.0
2	E	102	GLY	3.0
1	A	218	VAL	3.0
2	E	332	ILE	3.0
2	N	359	SER	3.0
2	M	80	ALA	3.0
1	A	200	ASP	3.0
2	N	339	LEU	3.0
1	C	74	GLU	3.0
1	C	78	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	288	ILE	3.0
1	B	471	VAL	2.9
1	B	267	VAL	2.9
2	F	193	ALA	2.9
1	C	275	PRO	2.9
1	I	140	GLU	2.9
2	E	165	ALA	2.9
1	C	394	PRO	2.9
2	M	401	GLU	2.9
1	A	347	GLU	2.9
2	N	185	GLU	2.9
2	M	83	GLY	2.9
2	L	302	GLU	2.9
1	C	168	VAL	2.9
1	B	345	PRO	2.9
1	C	179	THR	2.9
1	K	346	ALA	2.9
2	M	25	LYS	2.9
1	I	137	THR	2.9
2	M	81	ARG	2.9
1	I	13	ALA	2.8
1	C	58	LEU	2.8
1	I	201	PRO	2.8
1	I	368	VAL	2.8
2	M	362	MET	2.8
2	N	219	LEU	2.8
1	C	258	ARG	2.8
1	C	270	PRO	2.8
2	F	172	THR	2.8
1	J	266	LEU	2.8
2	N	193	ALA	2.8
1	I	296	VAL	2.8
1	I	84	TYR	2.8
1	C	44	GLY	2.8
1	A	78	GLY	2.8
1	I	41	ARG	2.8
2	F	277	ILE	2.8
2	F	21	VAL	2.7
2	M	28	ALA	2.7
1	K	296	VAL	2.7
1	A	181	LEU	2.7
2	M	361	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	K	418	HIS	2.7
2	N	75	LEU	2.7
2	E	300	VAL	2.7
1	I	136	GLY	2.7
1	A	223	THR	2.7
1	C	388	GLY	2.7
1	K	349	GLY	2.7
2	E	375	HIS	2.7
1	K	242	ALA	2.7
2	L	77	GLU	2.7
2	N	168	ALA	2.7
2	F	119	LEU	2.7
2	D	77	GLU	2.7
2	F	201	LEU	2.7
2	L	37	ASP	2.7
1	K	192	ALA	2.6
1	B	387	PRO	2.6
2	D	103	LEU	2.6
1	A	57	GLY	2.6
2	N	421	PHE	2.6
1	C	3	GLN	2.6
1	I	85	ASP	2.6
1	A	63	PRO	2.6
1	K	201	PRO	2.6
2	E	439	ALA	2.6
1	C	375	GLU	2.6
2	N	454	ILE	2.6
1	C	108	VAL	2.6
2	E	150	LEU	2.6
1	J	12	PRO	2.6
2	L	38	GLY	2.6
1	A	349	GLY	2.6
1	I	425	ASN	2.6
4	P	64	ARG	2.6
2	N	86	LYS	2.6
4	P	78	LYS	2.6
2	N	140	VAL	2.6
2	D	104	PRO	2.5
1	I	382	GLY	2.5
2	L	29	TYR	2.5
2	N	78	ASP	2.5
1	I	370	THR	2.5

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Mol	Chain	Res	Type	RSRZ
2	L	13	TYR	2.5
1	I	182	LYS	2.5
1	A	129	VAL	2.5
1	K	404	GLY	2.5
1	C	17	LYS	2.5
1	I	158	LYS	2.5
1	J	493	ASP	2.5
1	I	132	GLY	2.5
1	I	498	ASN	2.5
2	N	297	ARG	2.5
1	A	87	ILE	2.5
1	C	169	GLU	2.5
2	N	64	THR	2.5
1	I	159	GLU	2.5
2	F	118	PRO	2.5
1	I	365	ALA	2.5
1	I	345	PRO	2.4
1	J	474	ASP	2.4
4	P	103	LYS	2.4
1	I	44	GLY	2.4
1	K	552	ARG	2.4
1	A	208	GLY	2.4
1	A	345	PRO	2.4
1	I	381	VAL	2.4
1	I	133	MET	2.4
2	E	278	PRO	2.4
2	F	17	PRO	2.4
2	N	23	ASN	2.4
2	N	287	MET	2.4
2	N	17	PRO	2.4
1	I	376	GLY	2.4
2	F	216	ARG	2.4
2	F	123	ALA	2.4
2	L	75	LEU	2.4
2	F	10	GLY	2.4
2	F	302	GLU	2.4
2	L	301	VAL	2.4
2	M	172	THR	2.4
2	N	24	ALA	2.4
1	I	290	ASN	2.4
2	L	300	VAL	2.4
1	A	76	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	76	VAL	2.4
1	A	210	ARG	2.4
1	C	378	VAL	2.3
1	C	171	PRO	2.3
1	I	22	ALA	2.3
1	I	316	GLN	2.3
1	I	43	ASP	2.3
1	I	147	ILE	2.3
2	F	168	ALA	2.3
2	L	105	PRO	2.3
1	C	59	LYS	2.3
1	C	182	LYS	2.3
1	C	52	TYR	2.3
2	E	374	ASP	2.3
2	D	63	THR	2.3
2	F	186	PRO	2.3
2	E	67	ASP	2.3
2	M	70	THR	2.3
1	A	21	GLY	2.3
1	K	191	ARG	2.3
2	E	122	VAL	2.3
1	C	4	GLY	2.3
1	K	228	GLY	2.3
2	F	85	SER	2.3
2	N	289	THR	2.3
1	I	76	GLY	2.3
2	E	365	GLY	2.3
2	N	455	SER	2.3
1	C	170	GLU	2.3
2	D	365	GLY	2.3
2	E	175	PRO	2.3
1	J	387	PRO	2.3
1	I	423	ASN	2.3
1	K	388	GLY	2.3
1	C	28	CYS	2.2
2	F	82	LEU	2.2
1	C	146	LYS	2.2
2	L	123	ALA	2.2
2	M	426	GLY	2.2
1	A	116	LYS	2.2
1	I	222	GLY	2.2
2	N	248	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	M	198	GLN	2.2
1	A	209	MET	2.2
1	I	32	GLU	2.2
1	I	343	GLU	2.2
2	N	175	PRO	2.2
2	N	278	PRO	2.2
1	C	405	ALA	2.2
1	K	372	GLY	2.2
1	B	58	LEU	2.2
2	D	105	PRO	2.2
1	I	58	LEU	2.2
1	I	129	VAL	2.2
2	M	69	ALA	2.2
1	B	552	ARG	2.2
1	C	16	ALA	2.2
2	E	21	VAL	2.2
1	A	381	VAL	2.2
1	C	425	ASN	2.2
1	B	503	VAL	2.2
2	N	147	GLY	2.2
2	D	439	ALA	2.2
2	L	80	ALA	2.2
1	I	474	ASP	2.2
2	E	30	GLY	2.1
2	F	300	VAL	2.1
1	K	158	LYS	2.1
1	K	387	PRO	2.1
1	I	123	VAL	2.1
1	A	325	ASP	2.1
2	E	330	GLY	2.1
1	K	293	ASN	2.1
1	A	180	GLU	2.1
1	I	536	ILE	2.1
2	F	333	THR	2.1
2	F	171	ALA	2.1
1	A	165	GLU	2.1
2	N	334	GLU	2.1
2	N	288	TYR	2.1
1	I	535	SER	2.1
1	K	23	ARG	2.1
2	N	79	VAL	2.1
1	I	223	THR	2.1

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Mol	Chain	Res	Type	RSRZ
1	K	26	ASP	2.1
2	L	104	PRO	2.1
1	C	223	THR	2.1
1	I	174	VAL	2.1
1	K	575	LYS	2.1
2	F	79	VAL	2.1
1	A	182	LYS	2.1
1	J	3	GLN	2.1
1	B	111	LEU	2.1
1	K	435	LEU	2.1
2	N	221	LEU	2.1
2	D	122	VAL	2.1
1	C	576	ALA	2.1
2	N	258	THR	2.1
4	H	16	ALA	2.1
1	B	12	PRO	2.1
1	A	144	THR	2.1
1	A	177	ASP	2.1
1	K	163	ALA	2.1
2	N	299	GLY	2.0
1	K	298	ALA	2.0
4	H	99	GLY	2.0
2	F	154	SER	2.0
2	L	401	GLU	2.0
2	E	164	ALA	2.0
2	E	169	ARG	2.0
1	K	258	ARG	2.0
2	E	103	LEU	2.0
1	I	1	MET	2.0
2	D	119	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	ADP	K	600	27/27	0.63	0.47	0.17	112,112,112,112	0
5	ADP	C	600	27/27	0.79	0.28	-0.27	116,116,116,116	0
5	ADP	A	600	27/27	0.82	0.26	-0.38	109,109,109,109	0
5	ADP	I	600	27/27	0.80	0.28	-0.96	110,110,110,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.