



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:39 PM GMT

PDB ID : 4M9S
Title : crystal structure of CED-4 bound CED-3 fragment
Authors : Huang, W.J.; Jinag, T.Y.; Choi, W.Y.; Wang, J.W.; Shi, Y.G.
Deposited on : 2013-08-15
Resolution : 3.21 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

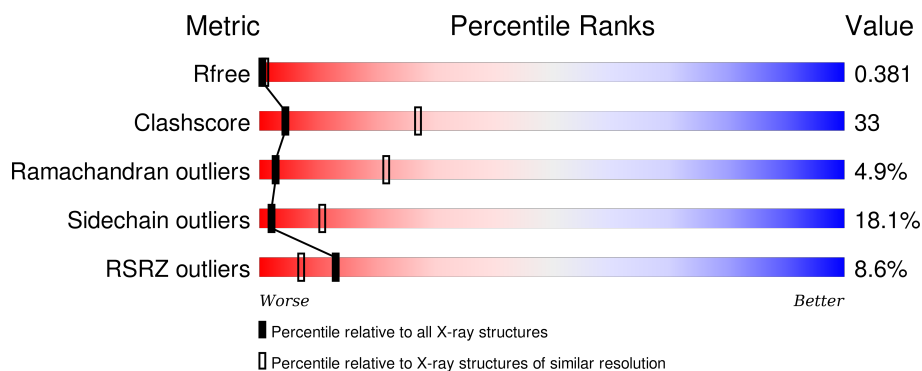
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.21 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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	549	 4% 37% 45% 10% • 7%
1	B	549	 9% 35% 45% 11% • 7%
1	C	549	 7% 35% 45% 12% • 7%
1	D	549	 12% 35% 45% 12% • 7%
2	E	8	 13% 25% 38% 25%

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Mol	Chain	Length	Quality of chain
2	F	8	
2	G	8	
2	H	8	

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
3	MG	A	601	-	-	-	X
3	MG	D	601	-	-	-	X

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 16687 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 Cell death protein 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	510	Total	C	N	O	S	Se	0	0	0
			4088	2606	685	767	13	17			
1	B	511	Total	C	N	O	S	Se	0	0	0
			4094	2607	688	768	14	17			
1	C	510	Total	C	N	O	S	Se	0	0	0
			4088	2606	685	767	13	17			
1	D	511	Total	C	N	O	S	Se	0	0	0
			4094	2607	688	768	14	17			

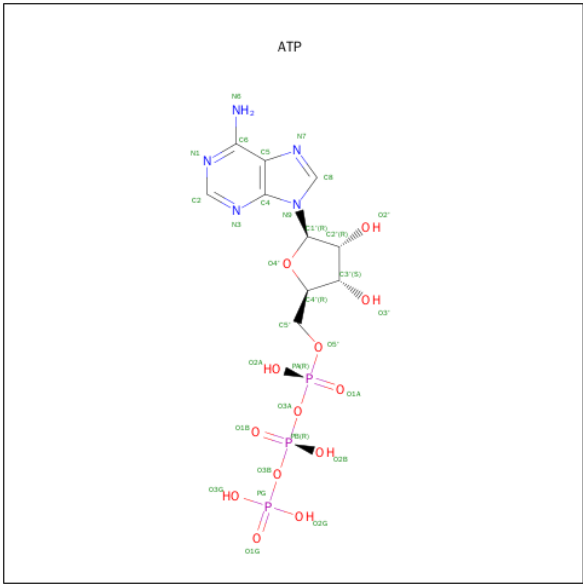
- Molecule 2 is a protein called CED-3 fragment.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	6	Total	C	N	O	Se	0	0	0
			50	34	7	7	2			
2	F	5	Total	C	N	O	Se	0	0	0
			46	32	6	6	2			
2	G	5	Total	C	N	O	Se	0	0	0
			46	32	6	6	2			
2	H	6	Total	C	N	O	Se	0	0	0
			53	37	7	7	2			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

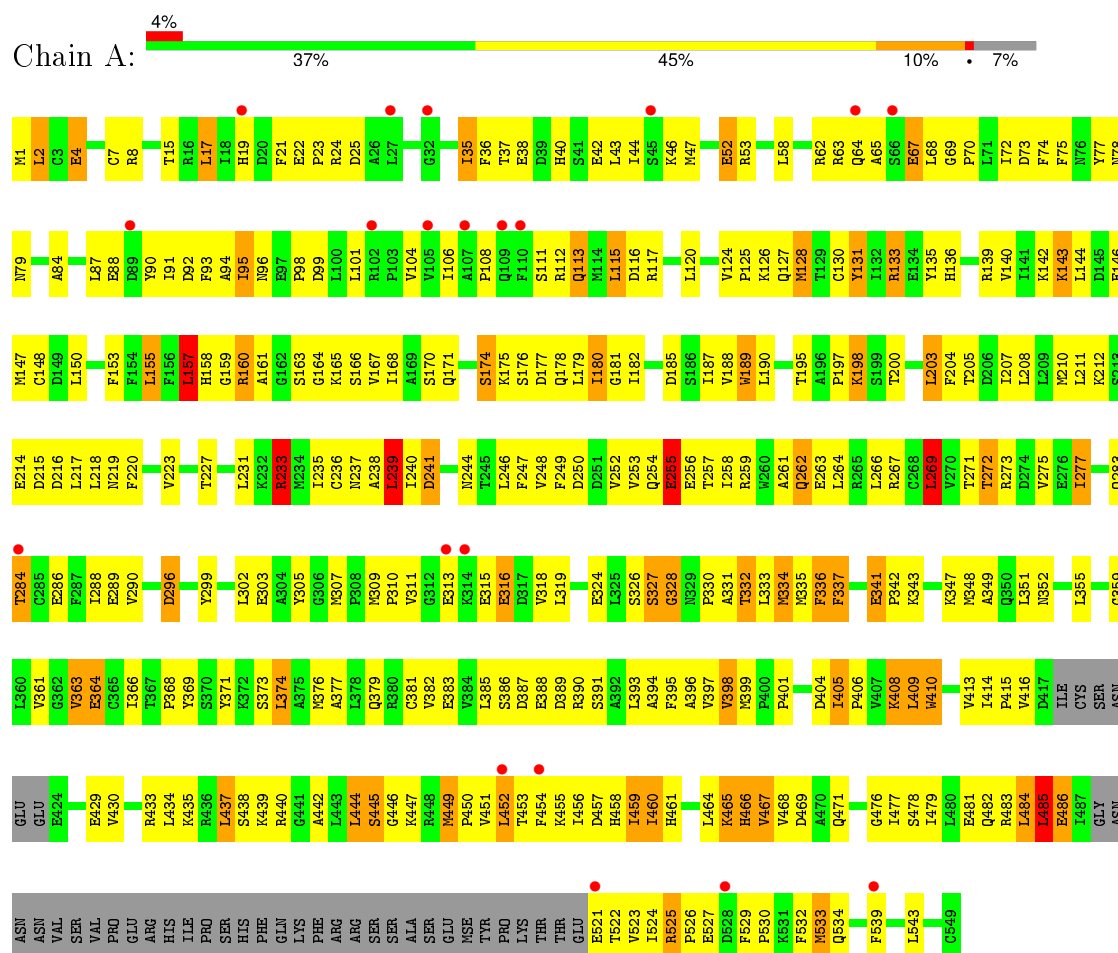


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
4	D	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

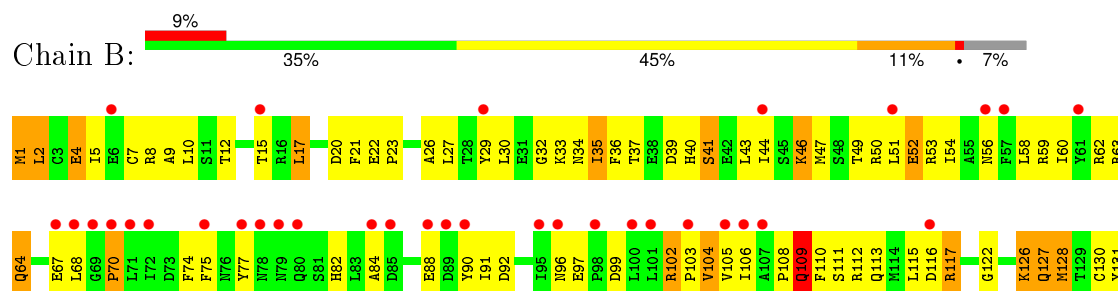
3 Residue-property plots

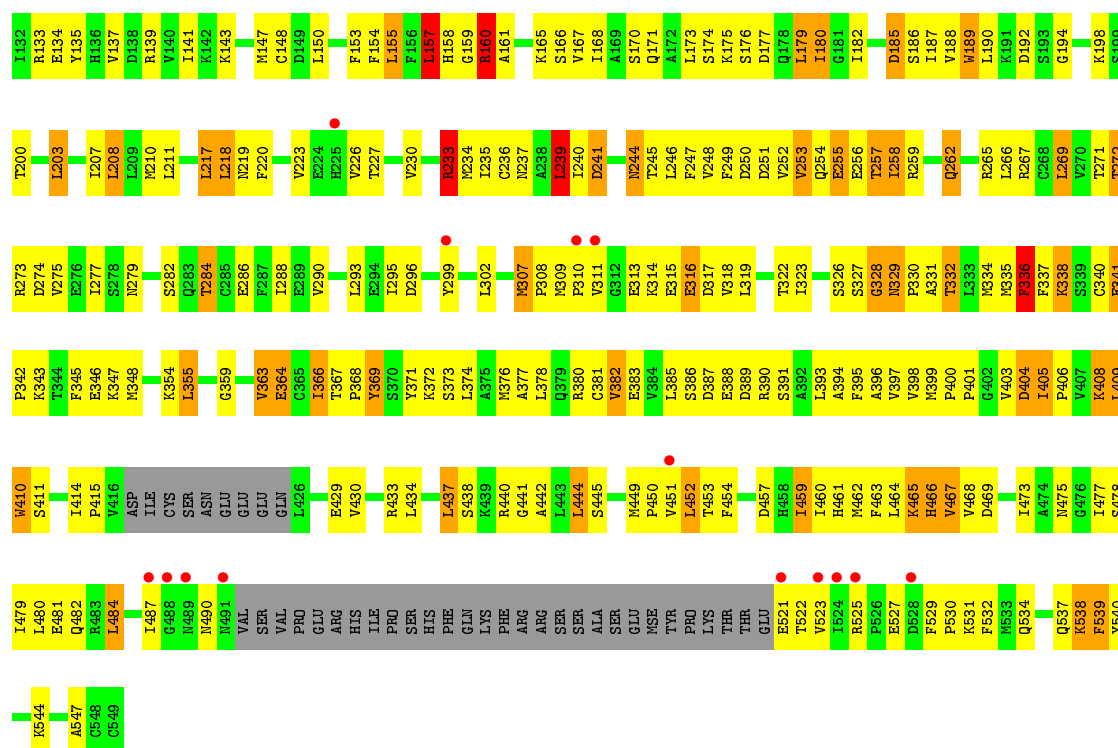
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cell death protein 4

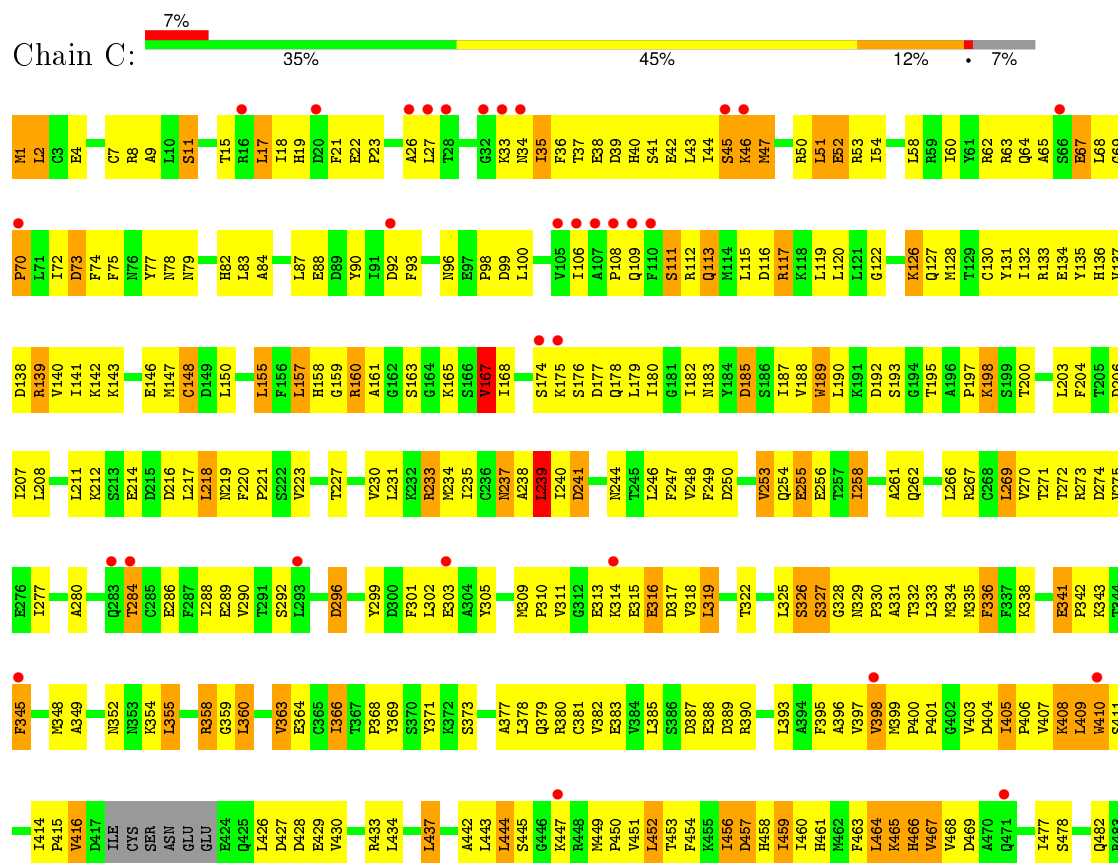


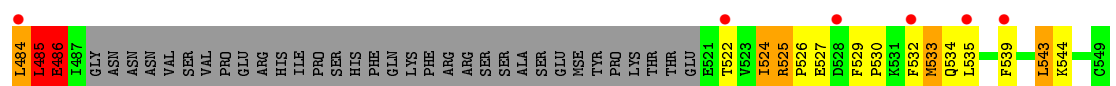
• Molecule 1: Cell death protein 4



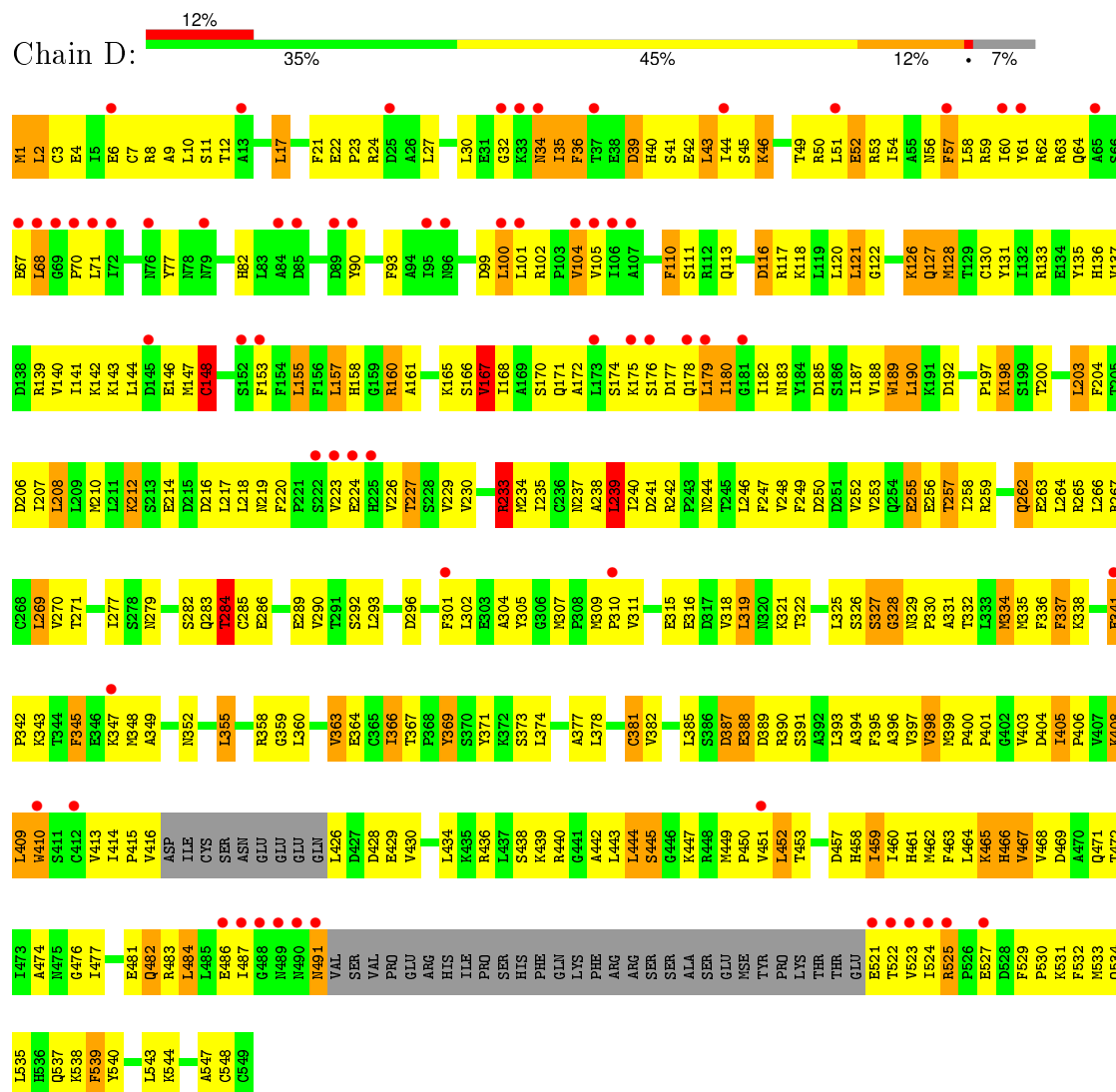


• Molecule 1: Cell death protein 4





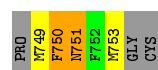
• Molecule 1: Cell death protein 4



• Molecule 2: CED-3 fragment



• Molecule 2: CED-3 fragment



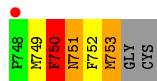
- Molecule 2: CED-3 fragment

Chain G: 



- Molecule 2: CED-3 fragment

Chain H: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	178.81Å 178.81Å 201.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.85 – 3.21 40.85 – 3.21	Depositor EDS
% Data completeness (in resolution range)	55.5 (40.85-3.21) 69.2 (40.85-3.21)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.87 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.283 , 0.334 0.332 , 0.381	Depositor DCC
R_{free} test set	1877 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	73.7	Xtriage
Anisotropy	0.377	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 69.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	2 of 37332 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	16687	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.62 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.6626e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.82	1/4147 (0.0%)	1.12	14/5577 (0.3%)
1	B	0.80	0/4153	1.13	11/5585 (0.2%)
1	C	0.77	1/4147 (0.0%)	1.05	5/5577 (0.1%)
1	D	0.79	2/4153 (0.0%)	1.08	8/5585 (0.1%)
2	E	1.02	0/50	1.00	0/62
2	F	1.00	0/46	1.11	0/57
2	G	0.87	0/46	1.14	0/57
2	H	1.11	0/53	1.15	0/65
All	All	0.80	4/16795 (0.0%)	1.09	38/22565 (0.2%)

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	B	0	1
2	G	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	381	CYS	CB-SG	6.49	1.93	1.82
1	C	167	VAL	CB-CG2	-6.25	1.39	1.52
1	A	236	CYS	CB-SG	5.96	1.92	1.82
1	D	167	VAL	CB-CG2	-5.10	1.42	1.52

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	LEU	CA-CB-CG	7.72	133.06	115.30
1	A	409	LEU	CA-CB-CG	7.60	132.78	115.30
1	D	239	LEU	CA-CB-CG	7.53	132.63	115.30
1	B	239	LEU	CA-CB-CG	6.87	131.10	115.30
1	C	360	LEU	CA-CB-CG	6.84	131.03	115.30
1	A	239	LEU	CA-CB-CG	6.83	131.00	115.30
1	D	484	LEU	CA-CB-CG	6.77	130.88	115.30
1	A	43	LEU	CA-CB-CG	6.58	130.44	115.30
1	A	236	CYS	CA-CB-SG	6.39	125.51	114.00
1	D	121	LEU	CA-CB-CG	-6.27	100.88	115.30
1	A	255	GLU	CA-CB-CG	6.12	126.88	113.40
1	C	258	ILE	CG1-CB-CG2	-6.05	98.08	111.40
1	B	336	PHE	CB-CG-CD2	-5.98	116.62	120.80
1	C	464	LEU	CB-CG-CD2	-5.70	101.31	111.00
1	A	133	ARG	NE-CZ-NH1	-5.63	117.49	120.30
1	B	307	MSE	CB-CG-SE	5.62	129.57	112.70
1	D	190	LEU	CB-CG-CD1	-5.54	101.59	111.00
1	D	233	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	143	LYS	CD-CE-NZ	5.50	124.35	111.70
1	B	538	LYS	CA-CB-CG	-5.49	101.33	113.40
1	B	338	LYS	CB-CG-CD	5.46	125.79	111.60
1	D	535	LEU	CA-CB-CG	5.44	127.81	115.30
1	D	212	LYS	CA-CB-CG	5.42	125.31	113.40
1	B	233	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	C	212	LYS	CA-CB-CG	5.23	124.91	113.40
1	A	269	LEU	N-CA-C	-5.22	96.90	111.00
1	D	148	CYS	CA-CB-SG	5.19	123.34	114.00
1	A	233	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	239	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	440	ARG	CG-CD-NE	5.16	122.63	111.80
1	B	157	LEU	CB-CG-CD1	-5.14	102.26	111.00
1	A	164	GLY	N-CA-C	5.13	125.94	113.10
1	B	258	ILE	CG1-CB-CG2	-5.13	100.11	111.40
1	B	236	CYS	CA-CB-SG	5.12	123.22	114.00
1	A	333	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	A	157	LEU	CA-CB-CG	5.06	126.94	115.30
1	B	251	ASP	CB-CG-OD1	-5.05	113.76	118.30
1	A	333	LEU	CA-CB-CG	-5.05	103.69	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	346	GLU	Sidechain
2	G	752	PHE	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	4088	0	4107	277	0
1	B	4094	0	4115	267	0
1	C	4088	0	4108	287	1
1	D	4094	0	4115	274	1
2	E	50	0	44	6	0
2	F	46	0	41	6	0
2	G	46	0	41	6	0
2	H	53	0	49	7	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	12	4	0
4	B	31	0	12	5	0
4	C	31	0	12	1	0
4	D	31	0	12	1	0
All	All	16687	0	16668	1091	1

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 33.

All (1091) 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)
1:A:63:ARG:HE	1:A:240:ILE:HD11	1.24	1.02
1:D:128:MSE:HG3	1:D:167:VAL:HG22	1.48	0.94
1:D:364:GLU:HB2	1:D:373:SER:HB3	1.54	0.89
1:A:484:LEU:HD11	1:A:533:MSE:HG2	1.52	0.89
1:C:63:ARG:HE	1:C:240:ILE:HD11	1.39	0.88
1:A:334:MSE:HE1	1:A:337:PHE:HD2	1.39	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:366:ILE:HD12	1:D:366:ILE:H	1.42	0.85
1:C:190:LEU:HD12	1:C:207:ILE:HG13	1.59	0.84
1:C:150:LEU:O	1:C:267:ARG:NH1	2.10	0.84
1:B:366:ILE:HD12	1:B:366:ILE:H	1.43	0.84
1:D:160:ARG:HG2	1:D:161:ALA:H	1.44	0.83
1:D:397:VAL:HG21	1:D:468:VAL:HG21	1.60	0.82
1:B:75:PHE:HB2	1:B:84:ALA:HB2	1.62	0.82
1:C:138:ASP:OD1	1:C:175:LYS:NZ	2.12	0.82
1:A:128:MSE:HG3	1:A:167:VAL:HG22	1.60	0.82
1:D:160:ARG:NH1	1:D:442:ALA:O	2.12	0.81
1:B:20:ASP:OD2	1:B:82:HIS:NE2	2.13	0.81
1:B:478:SER:O	1:B:482:GLN:HG2	1.80	0.81
1:A:190:LEU:HD12	1:A:207:ILE:HG13	1.62	0.81
1:D:8:ARG:NH1	1:D:90:TYR:OH	2.14	0.81
1:B:165:LYS:HG2	1:B:290:VAL:HG21	1.61	0.81
1:D:190:LEU:HD11	1:D:207:ILE:HG13	1.63	0.81
1:C:484:LEU:HD11	1:C:533:MSE:HG2	1.62	0.80
1:B:128:MSE:HG3	1:B:167:VAL:HG22	1.62	0.80
1:C:47:MSE:HB2	1:C:53:ARG:HG3	1.63	0.79
1:B:102:ARG:HG3	1:B:103:PRO:HD2	1.64	0.79
1:A:75:PHE:HB2	1:A:84:ALA:HB2	1.64	0.79
1:D:42:GLU:O	1:D:46:LYS:NZ	2.15	0.79
1:D:462:MSE:H	1:D:462:MSE:SE	2.16	0.78
1:C:90:TYR:HE2	1:C:106:ILE:HD11	1.48	0.78
1:C:155:LEU:HB3	1:C:269:LEU:HD23	1.65	0.78
1:B:147:MSE:HE1	1:B:286:GLU:HG2	1.63	0.78
1:C:465:LYS:HD3	1:C:466:HIS:CE1	2.19	0.78
1:C:309:MSE:HG3	1:C:310:PRO:HD2	1.65	0.77
1:C:327:SER:HB2	1:C:459:ILE:HG13	1.66	0.77
1:A:190:LEU:CD1	1:A:207:ILE:HG13	2.16	0.76
1:B:397:VAL:HG21	1:B:468:VAL:HG21	1.66	0.76
1:C:366:ILE:H	1:C:366:ILE:HD12	1.51	0.76
1:C:355:LEU:HD21	1:C:363:VAL:HB	1.69	0.75
1:A:90:TYR:HE2	1:A:106:ILE:HD11	1.48	0.75
1:A:410:TRP:HD1	1:A:414:ILE:HD13	1.52	0.75
1:A:72:ILE:HG21	1:A:88:GLU:HG3	1.67	0.75
1:A:452:LEU:H	1:A:452:LEU:HD23	1.49	0.75
1:D:148:CYS:SG	1:D:183:ASN:ND2	2.58	0.75
1:C:75:PHE:HB2	1:C:84:ALA:HB2	1.68	0.74
2:G:750:PHE:O	2:G:752:PHE:N	2.20	0.74
1:B:92:ASP:OD1	1:B:96:ASN:ND2	2.20	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:449:MSE:HE3	1:B:450:PRO:HA	1.68	0.73
2:F:751:ASN:ND2	2:F:751:ASN:O	2.21	0.73
1:C:41:SER:O	1:C:45:SER:OG	2.07	0.73
1:C:465:LYS:HD3	1:C:466:HIS:HE1	1.54	0.72
1:A:8:ARG:HG2	1:A:8:ARG:HH11	1.55	0.72
1:D:250:ASP:HA	1:D:271:THR:OG1	1.89	0.72
1:A:334:MSE:HA	1:A:334:MSE:HE3	1.71	0.72
1:A:414:ILE:HG21	1:A:430:VAL:HG13	1.72	0.72
1:B:332:THR:O	1:B:336:PHE:HB2	1.90	0.72
1:A:67:GLU:HG2	1:A:69:GLY:H	1.55	0.72
1:B:335:MSE:HE3	1:B:364:GLU:HA	1.71	0.72
1:C:447:LYS:HE2	1:C:450:PRO:HD2	1.71	0.72
1:A:309:MSE:HG3	1:A:310:PRO:HD2	1.71	0.72
1:D:487:ILE:O	1:D:531:LYS:NZ	2.23	0.72
1:C:8:ARG:HG2	1:C:8:ARG:HH11	1.55	0.72
1:D:406:PRO:HA	1:D:453:THR:HG22	1.72	0.72
1:A:128:MSE:HG3	1:A:167:VAL:CG2	2.20	0.71
1:C:128:MSE:HE3	1:D:282:SER:HB2	1.73	0.71
1:C:443:LEU:O	1:C:460:ILE:HG12	1.90	0.71
1:D:40:HIS:HA	1:D:43:LEU:HB2	1.72	0.71
1:A:393:LEU:HB2	1:A:437:LEU:HD11	1.73	0.71
1:A:150:LEU:O	1:A:267:ARG:NH1	2.24	0.71
1:C:397:VAL:HG22	1:C:464:LEU:HB3	1.71	0.71
1:C:532:PHE:HB2	1:C:534:GLN:HG2	1.73	0.71
1:B:190:LEU:HD12	1:B:207:ILE:HG13	1.71	0.71
1:D:190:LEU:CD1	1:D:207:ILE:HG13	2.20	0.71
1:A:532:PHE:HB2	1:A:534:GLN:HG2	1.72	0.71
1:C:128:MSE:HG3	1:C:167:VAL:HG22	1.72	0.71
1:C:58:LEU:O	1:C:62:ARG:HG3	1.90	0.70
2:E:750:PHE:O	2:E:752:PHE:N	2.24	0.70
1:A:187:ILE:HD13	1:A:246:LEU:HB3	1.73	0.70
1:D:230:VAL:HG12	1:D:234:MSE:HE2	1.74	0.70
1:D:292:SER:HB3	1:D:328:GLY:HA3	1.74	0.70
1:B:335:MSE:HE2	1:B:363:VAL:HG13	1.74	0.70
1:B:1:MSE:HA	1:B:62:ARG:O	1.92	0.70
1:A:449:MSE:HE2	1:A:450:PRO:HA	1.74	0.70
1:A:157:LEU:HD11	1:A:168:ILE:HG22	1.74	0.70
1:A:401:PRO:HB2	1:A:458:HIS:ND1	2.07	0.70
1:B:405:ILE:HG12	1:B:410:TRP:CZ3	2.26	0.69
1:A:47:MSE:HB2	1:A:53:ARG:HG3	1.74	0.69
1:B:403:VAL:HG12	1:B:405:ILE:HG22	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:PRO:HA	1:A:453:THR:HG22	1.74	0.69
1:C:211:LEU:HD13	1:C:239:LEU:HD23	1.75	0.69
1:A:72:ILE:HD11	1:A:87:LEU:HB2	1.74	0.69
1:A:447:LYS:HE2	1:A:450:PRO:HD2	1.74	0.69
1:C:247:PHE:CE2	1:C:266:LEU:HD13	2.28	0.68
1:C:96:ASN:O	1:C:98:PRO:HD3	1.93	0.68
1:B:160:ARG:HG2	1:B:161:ALA:H	1.58	0.68
1:B:102:ARG:HG3	1:B:103:PRO:CD	2.24	0.68
1:D:128:MSE:HG3	1:D:167:VAL:CG2	2.22	0.68
1:C:133:ARG:O	1:C:137:VAL:HG23	1.94	0.68
1:A:160:ARG:HG2	1:A:161:ALA:H	1.58	0.68
1:C:35:ILE:HG12	1:C:65:ALA:HA	1.74	0.68
1:A:334:MSE:HE1	1:A:337:PHE:CD2	2.28	0.67
1:A:389:ASP:HB3	1:A:437:LEU:HD21	1.76	0.67
1:A:247:PHE:CE2	1:A:266:LEU:HD13	2.30	0.67
1:D:155:LEU:HB3	1:D:269:LEU:HD23	1.74	0.67
1:D:403:VAL:HG12	1:D:405:ILE:HG22	1.76	0.67
1:A:386:SER:OG	1:A:388:GLU:OE1	2.12	0.67
1:D:214:GLU:N	1:D:214:GLU:OE1	2.26	0.67
1:B:529:PHE:HB3	1:B:532:PHE:CZ	2.30	0.67
1:A:35:ILE:HG12	1:A:65:ALA:HA	1.76	0.67
1:B:438:SER:O	1:B:442:ALA:HA	1.95	0.67
1:B:247:PHE:CE2	1:B:266:LEU:HD13	2.29	0.67
1:B:157:LEU:HD11	1:B:168:ILE:HG21	1.75	0.67
1:B:388:GLU:HB3	1:B:433:ARG:HH21	1.59	0.67
1:A:96:ASN:O	1:A:98:PRO:HD3	1.94	0.67
1:B:4:GLU:O	1:B:8:ARG:HB2	1.95	0.66
1:D:262:GLN:HE21	1:D:283:GLN:HG3	1.60	0.66
1:A:397:VAL:HG22	1:A:464:LEU:HB3	1.77	0.66
1:C:128:MSE:SE	1:C:167:VAL:HG21	2.45	0.66
1:C:247:PHE:CD2	1:C:266:LEU:HD13	2.31	0.65
1:B:302:LEU:HD13	1:B:319:LEU:HD11	1.76	0.65
1:C:90:TYR:CE2	1:C:106:ILE:HD11	2.32	0.65
1:C:249:PHE:HE2	1:C:261:ALA:HB2	1.61	0.65
1:D:452:LEU:HD23	1:D:452:LEU:H	1.61	0.65
1:A:438:SER:O	1:A:442:ALA:HA	1.97	0.65
1:A:366:ILE:HD12	1:A:366:ILE:H	1.62	0.65
1:B:464:LEU:O	1:B:468:VAL:HG22	1.97	0.65
1:D:327:SER:HB2	1:D:459:ILE:HG13	1.77	0.65
1:A:165:LYS:N	4:A:602:ATP:O2B	2.30	0.64
1:C:44:ILE:O	1:C:53:ARG:HG2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LYS:HD3	1:A:466:HIS:CE1	2.32	0.64
1:C:67:GLU:HG2	1:C:69:GLY:H	1.63	0.64
1:B:406:PRO:HA	1:B:453:THR:HG22	1.80	0.64
1:C:326:SER:O	1:C:328:GLY:N	2.30	0.64
1:A:47:MSE:HE2	1:A:52:GLU:HG2	1.80	0.64
1:C:126:LYS:NZ	1:D:283:GLN:HG2	2.13	0.64
1:D:447:LYS:NZ	1:D:449:MSE:O	2.25	0.64
1:D:2:LEU:HD11	1:D:62:ARG:HE	1.63	0.64
1:C:197:PRO:HD2	1:C:198:LYS:HE2	1.80	0.63
1:B:410:TRP:HD1	1:B:414:ILE:HD13	1.64	0.63
1:A:117:ARG:HH21	1:A:120:LEU:HD23	1.62	0.63
1:C:434:LEU:HD22	1:C:444:LEU:CD2	2.29	0.63
1:C:341:GLU:HB2	1:C:342:PRO:HD3	1.80	0.63
1:C:160:ARG:NH1	1:C:442:ALA:O	2.32	0.63
1:C:527:GLU:HA	1:C:530:PRO:HG3	1.80	0.63
1:D:30:LEU:HD21	1:D:70:PRO:HB2	1.81	0.63
1:C:214:GLU:OE1	1:C:214:GLU:N	2.27	0.63
1:C:349:ALA:HA	1:C:352:ASN:HD22	1.63	0.63
1:B:143:LYS:O	1:B:147:MSE:HE3	1.99	0.63
1:B:128:MSE:HG3	1:B:167:VAL:CG2	2.28	0.63
1:A:255:GLU:HA	1:A:277:ILE:HG22	1.80	0.62
1:B:334:MSE:HE2	1:B:338:LYS:CD	2.29	0.62
1:C:132:ILE:HG23	1:C:137:VAL:HG21	1.80	0.62
1:A:335:MSE:HE2	1:A:363:VAL:HG13	1.81	0.62
1:D:341:GLU:HB2	1:D:342:PRO:HD3	1.80	0.62
1:B:135:TYR:O	1:B:139:ARG:HG3	2.00	0.62
1:B:371:TYR:CD2	1:B:377:ALA:HB2	2.34	0.62
1:D:374:LEU:HD13	1:D:374:LEU:O	1.99	0.62
1:D:462:MSE:N	1:D:462:MSE:SE	2.83	0.62
1:D:283:GLN:C	1:D:285:CYS:H	2.03	0.62
1:A:178:GLN:O	1:A:182:ILE:HB	1.98	0.62
1:A:233:ARG:HH11	1:A:233:ARG:HG3	1.65	0.62
1:B:50:ARG:HA	1:B:53:ARG:HE	1.64	0.62
1:A:8:ARG:NH2	1:A:181:GLY:O	2.29	0.62
1:C:434:LEU:HD22	1:C:444:LEU:HD21	1.81	0.62
1:C:469:ASP:HB2	2:G:749:MSE:HA	1.81	0.62
1:A:216:ASP:HA	1:A:219:ASN:HB2	1.81	0.62
1:D:371:TYR:CD2	1:D:377:ALA:HB2	2.34	0.62
1:B:309:MSE:HG3	1:B:310:PRO:HD2	1.81	0.62
1:D:178:GLN:HA	1:D:182:ILE:HB	1.82	0.62
1:D:309:MSE:HG3	1:D:310:PRO:HD2	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:527:GLU:OE1	1:B:527:GLU:N	2.33	0.62
1:C:464:LEU:O	1:C:468:VAL:HG22	2.00	0.61
1:D:342:PRO:O	1:D:343:LYS:HB3	2.00	0.61
1:C:63:ARG:HE	1:C:240:ILE:CD1	2.12	0.61
1:C:147:MSE:O	1:C:150:LEU:HB2	2.00	0.61
1:C:211:LEU:CD1	1:C:239:LEU:HD23	2.31	0.61
1:A:252:VAL:HG21	1:A:257:THR:HG21	1.82	0.61
1:D:24:ARG:HG3	1:D:27:LEU:HD12	1.81	0.61
1:C:143:LYS:O	1:C:147:MSE:HG3	2.00	0.61
1:C:410:TRP:HD1	1:C:414:ILE:HD13	1.64	0.61
1:A:477:ILE:HD11	1:A:543:LEU:HB3	1.83	0.61
1:A:401:PRO:HB2	1:A:458:HIS:CE1	2.36	0.61
1:C:17:LEU:HD23	1:C:21:PHE:CD2	2.35	0.61
1:A:397:VAL:O	1:A:461:HIS:NE2	2.29	0.61
1:A:481:GLU:HA	1:A:484:LEU:HD22	1.82	0.61
1:A:247:PHE:HE2	1:A:266:LEU:HD22	1.65	0.61
1:C:142:LYS:O	1:C:146:GLU:HG3	2.00	0.61
1:A:435:LYS:NZ	1:A:446:GLY:HA3	2.16	0.61
1:A:116:ASP:N	1:A:116:ASP:OD1	2.33	0.60
1:A:430:VAL:O	1:A:434:LEU:HG	2.02	0.60
1:A:364:GLU:HB2	1:A:373:SER:HB3	1.83	0.60
1:C:136:HIS:O	1:C:140:VAL:HG23	2.01	0.60
1:B:23:PRO:HG2	1:B:53:ARG:C	2.21	0.60
1:C:178:GLN:HA	1:C:182:ILE:HB	1.82	0.60
1:B:430:VAL:O	1:B:434:LEU:HG	2.02	0.60
1:C:397:VAL:HG21	1:C:468:VAL:HG21	1.82	0.60
1:D:430:VAL:O	1:D:434:LEU:HG	2.02	0.60
1:B:364:GLU:HB2	1:B:373:SER:HB3	1.84	0.60
1:C:250:ASP:HA	1:C:271:THR:OG1	2.02	0.60
1:A:211:LEU:HD11	1:A:239:LEU:HD23	1.83	0.60
1:D:360:LEU:HD11	1:D:459:ILE:HG22	1.84	0.59
1:C:477:ILE:HG21	1:C:544:LYS:HE3	1.84	0.59
1:B:8:ARG:HG2	1:B:8:ARG:HH11	1.65	0.59
1:B:385:LEU:O	1:B:390:ARG:NH2	2.35	0.59
1:D:464:LEU:O	1:D:468:VAL:HG22	2.03	0.59
1:D:141:ILE:HD12	1:D:175:LYS:HE3	1.85	0.59
1:C:414:ILE:HG21	1:C:430:VAL:HG13	1.83	0.59
1:C:233:ARG:HH11	1:C:233:ARG:HG3	1.67	0.59
1:C:40:HIS:O	1:C:44:ILE:HG13	2.02	0.59
1:B:147:MSE:CE	1:B:286:GLU:HG2	2.33	0.59
1:B:4:GLU:HG3	1:B:5:ILE:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:491:ASN:N	1:D:491:ASN:OD1	2.36	0.59
1:B:165:LYS:N	4:B:602:ATP:O2B	2.36	0.58
1:A:143:LYS:O	1:A:147:MSE:HG3	2.03	0.58
1:D:459:ILE:HD12	1:D:460:ILE:H	1.68	0.58
1:A:36:PHE:CD2	1:A:40:HIS:HB3	2.38	0.58
1:A:385:LEU:HD22	1:A:389:ASP:CB	2.33	0.58
1:A:157:LEU:HD11	1:A:168:ILE:CG2	2.32	0.58
1:A:247:PHE:HB2	1:A:267:ARG:O	2.03	0.58
1:B:190:LEU:CD1	1:B:207:ILE:HG13	2.33	0.58
1:D:189:TRP:CE3	1:D:248:VAL:HG11	2.38	0.58
1:A:341:GLU:HB2	1:A:342:PRO:HD3	1.85	0.58
1:A:305:TYR:OH	4:A:602:ATP:H2	1.87	0.58
1:A:40:HIS:O	1:A:44:ILE:HG13	2.03	0.58
1:D:319:LEU:HD12	1:D:345:PHE:CE1	2.37	0.58
1:A:257:THR:HG22	1:A:258:ILE:HD12	1.85	0.58
1:D:477:ILE:HD13	1:D:544:LYS:HG3	1.85	0.58
1:D:310:PRO:HA	1:D:345:PHE:HE2	1.67	0.58
1:B:374:LEU:HD13	1:B:374:LEU:O	2.04	0.58
1:C:529:PHE:HB3	1:C:532:PHE:CZ	2.39	0.58
1:B:315:GLU:HA	1:B:318:VAL:HG23	1.85	0.58
1:B:47:MSE:HB2	1:B:53:ARG:HG3	1.85	0.58
1:A:262:GLN:HG2	1:A:262:GLN:O	2.02	0.58
1:B:395:PHE:HD2	1:B:415:PRO:HD3	1.69	0.58
1:A:176:SER:OG	1:A:178:GLN:HB2	2.04	0.58
1:A:332:THR:HG23	1:A:374:LEU:HB2	1.85	0.58
1:C:216:ASP:H	1:C:218:LEU:HD23	1.68	0.58
1:A:327:SER:HB2	1:A:459:ILE:HG13	1.85	0.58
1:B:399:MSE:HE1	1:B:409:LEU:O	2.03	0.58
1:A:410:TRP:CD1	1:A:414:ILE:HD13	2.36	0.58
1:A:529:PHE:HB3	1:A:532:PHE:CZ	2.38	0.58
1:B:299:TYR:HA	1:B:302:LEU:HD12	1.86	0.58
1:C:301:PHE:CE1	1:C:305:TYR:HE2	2.21	0.58
1:B:341:GLU:HB2	1:B:342:PRO:HD3	1.86	0.58
1:B:35:ILE:HD12	1:B:70:PRO:HG2	1.86	0.58
1:B:30:LEU:HB3	1:B:36:PHE:CD1	2.39	0.58
1:A:128:MSE:HE3	1:B:282:SER:HB2	1.84	0.57
1:A:385:LEU:HD22	1:A:389:ASP:HB3	1.84	0.57
1:C:126:LYS:HZ3	1:D:283:GLN:HG2	1.68	0.57
1:B:185:ASP:N	1:B:244:ASN:O	2.31	0.57
1:C:139:ARG:NH2	1:C:143:LYS:HE3	2.19	0.57
1:C:395:PHE:CD2	1:C:415:PRO:HD3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:VAL:HG22	1:B:269:LEU:HB3	1.86	0.57
1:C:23:PRO:HG2	1:C:53:ARG:HB3	1.86	0.57
1:A:143:LYS:HB3	1:A:147:MSE:HE2	1.85	0.57
1:A:189:TRP:CD2	1:A:248:VAL:HG11	2.39	0.57
1:C:26:ALA:HA	1:C:74:PHE:CE1	2.39	0.57
1:B:158:HIS:CD2	1:B:275:VAL:HG13	2.38	0.57
1:D:235:ILE:O	1:D:239:LEU:HB2	2.04	0.57
1:B:235:ILE:O	1:B:239:LEU:HB2	2.05	0.57
1:B:111:SER:O	1:B:115:LEU:HB3	2.04	0.57
1:C:93:PHE:CE2	1:C:100:LEU:HD23	2.40	0.57
1:A:67:GLU:HG2	1:A:69:GLY:N	2.18	0.57
1:B:469:ASP:HB2	2:F:749:MSE:HA	1.87	0.57
1:B:157:LEU:HD11	1:B:168:ILE:CG2	2.35	0.57
1:B:314:LYS:HA	1:B:317:ASP:HB2	1.87	0.57
1:A:393:LEU:O	1:A:393:LEU:HD23	2.04	0.56
1:C:160:ARG:HG2	1:C:161:ALA:H	1.68	0.56
1:D:401:PRO:HB2	1:D:458:HIS:CE1	2.41	0.56
1:C:327:SER:HB2	1:C:459:ILE:CG1	2.35	0.56
1:D:374:LEU:HD13	1:D:378:LEU:HG	1.86	0.56
1:B:382:VAL:HA	1:B:385:LEU:HD12	1.86	0.56
1:C:177:ASP:O	1:C:182:ILE:HD13	2.05	0.56
1:D:200:THR:HG21	1:D:256:GLU:HB3	1.87	0.56
1:D:21:PHE:O	1:D:50:ARG:NE	2.38	0.56
1:D:436:ARG:O	1:D:440:ARG:HG3	2.06	0.56
1:B:293:LEU:HG	1:B:330:PRO:HD3	1.87	0.56
1:B:233:ARG:HG3	1:B:233:ARG:HH11	1.71	0.56
1:C:216:ASP:HA	1:C:219:ASN:HB2	1.87	0.56
1:D:334:MSE:CE	1:D:337:PHE:HB3	2.36	0.56
1:A:23:PRO:HG2	1:A:53:ARG:HB3	1.87	0.56
1:D:7:CYS:O	1:D:11:SER:OG	2.11	0.56
1:B:133:ARG:O	1:B:137:VAL:HG23	2.06	0.56
1:D:157:LEU:HD11	1:D:168:ILE:HG22	1.87	0.56
1:C:247:PHE:HB2	1:C:267:ARG:O	2.07	0.55
1:C:37:THR:O	1:C:40:HIS:HB2	2.05	0.55
1:B:257:THR:HG22	1:B:258:ILE:N	2.21	0.55
1:A:158:HIS:CE1	1:A:289:GLU:HB2	2.39	0.55
1:B:473:ILE:HG22	1:B:547:ALA:HB2	1.87	0.55
1:C:274:ASP:O	1:C:277:ILE:HG12	2.06	0.55
1:D:388:GLU:O	1:D:391:SER:OG	2.13	0.55
1:C:200:THR:HG21	1:C:256:GLU:HB3	1.88	0.55
1:A:147:MSE:O	1:A:150:LEU:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:LYS:O	1:C:343:LYS:HG2	2.05	0.55
1:A:58:LEU:O	1:A:62:ARG:HG3	2.05	0.55
1:C:467:VAL:O	2:G:751:ASN:HB2	2.06	0.55
1:D:187:ILE:HD13	1:D:246:LEU:HB3	1.88	0.55
1:A:273:ARG:NH2	1:A:377:ALA:HB1	2.22	0.55
1:C:35:ILE:HD12	1:C:70:PRO:HG2	1.87	0.55
1:B:334:MSE:HE2	1:B:338:LYS:HD3	1.89	0.55
1:D:458:HIS:O	1:D:462:MSE:SE	2.74	0.55
1:D:177:ASP:O	1:D:182:ILE:HD13	2.07	0.55
1:A:214:GLU:HG3	1:B:237:ASN:CG	2.27	0.55
1:A:44:ILE:O	1:A:53:ARG:HG2	2.06	0.55
1:D:160:ARG:HG2	1:D:161:ALA:N	2.18	0.55
1:B:334:MSE:HE2	1:B:338:LYS:HD2	1.89	0.55
1:D:126:LYS:HE2	1:D:126:LYS:O	2.06	0.55
1:B:405:ILE:HG12	1:B:410:TRP:CE3	2.42	0.54
1:C:341:GLU:CB	1:C:342:PRO:HD3	2.37	0.54
1:A:189:TRP:CE3	1:A:248:VAL:HG11	2.42	0.54
1:A:163:SER:C	1:A:330:PRO:HG2	2.28	0.54
1:D:208:LEU:HD23	1:D:235:ILE:HA	1.88	0.54
1:C:21:PHE:CD1	1:C:75:PHE:HE1	2.25	0.54
1:D:529:PHE:HB3	1:D:532:PHE:CZ	2.42	0.54
1:A:259:ARG:O	1:A:263:GLU:HG3	2.07	0.54
1:C:334:MSE:HE2	1:C:338:LYS:CD	2.38	0.54
1:C:159:GLY:N	1:C:165:LYS:HD3	2.22	0.54
1:C:39:ASP:HA	1:C:42:GLU:HB2	1.89	0.54
1:B:463:PHE:O	1:B:467:VAL:HB	2.06	0.54
1:D:190:LEU:HD13	1:D:203:LEU:HD22	1.90	0.54
1:A:395:PHE:O	1:A:397:VAL:N	2.40	0.54
1:D:342:PRO:HD2	1:D:347:LYS:HG3	1.89	0.54
1:A:211:LEU:CD1	1:A:239:LEU:HD23	2.37	0.54
1:A:342:PRO:O	1:A:343:LYS:HB3	2.07	0.54
1:B:166:SER:OG	1:B:250:ASP:OD1	2.26	0.54
1:C:368:PRO:HD3	1:D:279:ASN:O	2.06	0.54
1:D:233:ARG:HG3	1:D:233:ARG:HH11	1.72	0.54
1:B:414:ILE:HG21	1:B:430:VAL:HG13	1.90	0.54
1:C:128:MSE:SE	1:C:167:VAL:CG2	3.06	0.54
1:D:301:PHE:CE1	1:D:305:TYR:HE1	2.26	0.54
1:D:264:LEU:HD12	1:D:266:LEU:HD11	1.90	0.54
1:C:188:VAL:HB	1:C:247:PHE:CE1	2.42	0.54
1:D:189:TRP:CZ3	1:D:248:VAL:HG11	2.43	0.54
1:B:35:ILE:O	1:B:64:GLN:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:ILE:HD11	1:A:249:PHE:CE1	2.42	0.54
1:C:235:ILE:O	1:C:239:LEU:HB2	2.08	0.54
1:B:40:HIS:O	1:B:43:LEU:HB2	2.08	0.54
1:B:255:GLU:O	1:B:259:ARG:HG3	2.07	0.54
1:A:406:PRO:CA	1:A:453:THR:HG22	2.37	0.54
1:B:310:PRO:HA	1:B:345:PHE:HE1	1.72	0.54
1:D:364:GLU:CB	1:D:373:SER:HB3	2.33	0.54
1:A:452:LEU:H	1:A:452:LEU:CD2	2.17	0.54
1:C:139:ARG:HH21	1:C:143:LYS:HE3	1.73	0.53
2:G:752:PHE:O	2:G:753:MSE:HG2	2.08	0.53
1:A:233:ARG:HH11	1:A:233:ARG:CG	2.20	0.53
1:B:10:LEU:HB3	1:B:58:LEU:HD22	1.90	0.53
1:C:395:PHE:HD2	1:C:415:PRO:HD3	1.74	0.53
1:A:382:VAL:O	1:A:385:LEU:HB2	2.08	0.53
1:B:188:VAL:HB	1:B:247:PHE:CD1	2.43	0.53
1:C:253:VAL:HG11	1:C:380:ARG:HD3	1.90	0.53
1:D:395:PHE:O	1:D:397:VAL:N	2.42	0.53
1:A:465:LYS:HD3	1:A:466:HIS:HE1	1.72	0.53
1:B:159:GLY:N	1:B:165:LYS:HD3	2.23	0.53
1:B:128:MSE:HB2	1:B:171:GLN:NE2	2.23	0.53
1:D:447:LYS:HE3	1:D:450:PRO:HD2	1.91	0.53
1:A:90:TYR:CE2	1:A:106:ILE:HD11	2.38	0.53
1:D:477:ILE:HG21	1:D:544:LYS:HG3	1.91	0.53
1:D:188:VAL:HB	1:D:247:PHE:HD1	1.74	0.53
1:C:313:GLU:O	1:C:316:GLU:HG3	2.09	0.53
1:A:331:ALA:HB2	4:A:602:ATP:H5'1	1.88	0.53
1:A:207:ILE:HD11	1:A:249:PHE:HE1	1.73	0.53
1:C:33:LYS:HD3	1:C:70:PRO:HG3	1.89	0.53
1:B:50:ARG:CA	1:B:53:ARG:HH21	2.21	0.53
1:B:155:LEU:HB3	1:B:269:LEU:HD23	1.91	0.53
1:C:452:LEU:H	1:C:452:LEU:HD23	1.72	0.53
1:D:359:GLY:N	1:D:466:HIS:NE2	2.56	0.53
1:C:240:ILE:HG13	1:C:241:ASP:N	2.24	0.53
1:D:206:ASP:O	1:D:210:MSE:HG2	2.09	0.53
1:A:326:SER:O	1:A:328:GLY:N	2.42	0.53
1:C:157:LEU:HD11	1:C:168:ILE:HG22	1.91	0.53
1:D:10:LEU:HB3	1:D:58:LEU:HD22	1.91	0.53
1:B:2:LEU:HB2	1:B:7:CYS:SG	2.49	0.53
1:A:444:LEU:O	1:A:445:SER:HB2	2.09	0.52
1:C:327:SER:O	1:C:459:ILE:HD11	2.08	0.52
1:D:248:VAL:HG22	1:D:269:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:MSE:HE1	1:B:233:ARG:HD3	1.91	0.52
1:A:7:CYS:SG	1:A:62:ARG:HD3	2.48	0.52
1:D:393:LEU:O	1:D:393:LEU:HD23	2.10	0.52
1:A:155:LEU:HB3	1:A:269:LEU:HD23	1.91	0.52
1:C:406:PRO:HA	1:C:453:THR:HG22	1.90	0.52
1:B:388:GLU:O	1:B:391:SER:HB3	2.10	0.52
1:B:108:PRO:O	1:B:109:GLN:HB2	2.08	0.52
1:A:170:SER:O	1:A:174:SER:HB2	2.09	0.52
1:C:230:VAL:O	1:C:234:MSE:HB2	2.09	0.52
1:B:411:SER:HA	1:B:430:VAL:HG21	1.91	0.52
1:B:230:VAL:HG12	1:B:234:MSE:HE2	1.91	0.52
1:A:166:SER:OG	1:A:250:ASP:OD1	2.28	0.52
1:B:383:GLU:HG2	2:F:753:MSE:HG2	1.90	0.52
1:A:527:GLU:OE1	1:A:527:GLU:N	2.41	0.52
1:B:105:VAL:HG22	1:B:110:PHE:CE2	2.44	0.52
1:C:47:MSE:HE2	1:C:52:GLU:HG2	1.91	0.52
1:A:72:ILE:HG23	1:A:84:ALA:HB1	1.90	0.52
1:B:342:PRO:O	1:B:343:LYS:HB3	2.10	0.52
1:A:93:PHE:CE2	1:A:104:VAL:HG11	2.45	0.52
1:A:464:LEU:O	1:A:468:VAL:HG22	2.10	0.52
1:A:359:GLY:N	1:A:466:HIS:NE2	2.58	0.52
1:B:49:THR:HG22	1:B:50:ARG:N	2.24	0.52
1:B:452:LEU:HD23	1:B:452:LEU:H	1.75	0.52
1:B:273:ARG:NE	4:B:602:ATP:O3G	2.41	0.52
1:B:273:ARG:CZ	1:B:380:ARG:HH21	2.22	0.52
1:A:37:THR:H	1:A:40:HIS:HB2	1.74	0.52
1:C:7:CYS:SG	1:C:62:ARG:HD3	2.50	0.52
1:A:187:ILE:HD12	1:A:246:LEU:O	2.10	0.52
1:C:230:VAL:HG12	1:C:234:MSE:HE3	1.91	0.52
1:C:456:ILE:HG13	1:C:460:ILE:CG2	2.40	0.52
1:C:461:HIS:O	1:C:464:LEU:N	2.43	0.52
1:A:195:THR:O	1:A:254:GLN:NE2	2.43	0.52
1:C:23:PRO:O	1:C:27:LEU:HG	2.09	0.51
1:A:188:VAL:HB	1:A:247:PHE:CE1	2.45	0.51
1:C:230:VAL:CG1	1:C:234:MSE:HE3	2.40	0.51
1:D:216:ASP:HA	1:D:219:ASN:HB2	1.92	0.51
1:C:247:PHE:HE2	1:C:266:LEU:HD22	1.75	0.51
1:C:47:MSE:HB2	1:C:53:ARG:CG	2.38	0.51
1:C:529:PHE:N	1:C:530:PRO:HD3	2.26	0.51
1:B:8:ARG:O	1:B:12:THR:OG1	2.12	0.51
1:C:195:THR:O	1:C:254:GLN:NE2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:GLU:HA	1:B:484:LEU:HG	1.92	0.51
1:A:376:MSE:O	1:A:379:GLN:HB3	2.09	0.51
1:A:159:GLY:N	1:A:165:LYS:HD3	2.25	0.51
1:C:401:PRO:HB2	1:C:458:HIS:CE1	2.46	0.51
1:C:443:LEU:O	1:C:460:ILE:HG21	2.10	0.51
1:D:341:GLU:CB	1:D:342:PRO:HD3	2.40	0.51
1:C:148:CYS:SG	1:C:183:ASN:ND2	2.81	0.51
1:C:9:ALA:HB2	1:C:90:TYR:CD1	2.46	0.51
1:B:399:MSE:O	1:B:539:PHE:CZ	2.64	0.51
1:C:122:GLY:HA3	1:C:187:ILE:HG23	1.92	0.51
1:B:395:PHE:CD2	1:B:415:PRO:HD3	2.46	0.51
1:C:314:LYS:HA	1:C:317:ASP:HB2	1.93	0.51
1:B:177:ASP:O	1:B:182:ILE:HD13	2.10	0.51
1:D:413:VAL:HG23	1:D:414:ILE:HD12	1.92	0.51
1:D:43:LEU:HD23	1:D:60:ILE:HD11	1.92	0.51
1:B:343:LYS:O	1:B:343:LYS:HG2	2.09	0.51
1:A:250:ASP:OD1	1:A:271:THR:OG1	2.25	0.51
1:A:272:THR:OG1	1:A:273:ARG:N	2.43	0.51
1:D:326:SER:O	1:D:328:GLY:N	2.44	0.51
1:D:269:LEU:HD22	1:D:270:VAL:H	1.76	0.51
1:C:410:TRP:CZ3	1:C:454:PHE:HB2	2.46	0.51
1:D:390:ARG:HH11	2:H:753:MSE:SE	2.44	0.51
1:C:484:LEU:HD21	1:C:533:MSE:CG	2.41	0.51
1:B:410:TRP:CD1	1:B:414:ILE:HD13	2.45	0.51
1:A:255:GLU:CA	1:A:277:ILE:HG22	2.40	0.51
1:B:334:MSE:HE3	1:B:337:PHE:HB2	1.93	0.51
1:C:72:ILE:HG21	1:C:88:GLU:HG3	1.91	0.51
1:D:142:LYS:O	1:D:146:GLU:HG3	2.10	0.51
1:C:364:GLU:HB3	1:C:373:SER:HB3	1.93	0.51
1:B:391:SER:OG	1:B:415:PRO:HG2	2.11	0.51
1:D:214:GLU:N	1:D:214:GLU:CD	2.64	0.51
1:B:37:THR:OG1	1:B:40:HIS:ND1	2.33	0.51
1:A:248:VAL:HG22	1:A:269:LEU:HB3	1.92	0.51
1:D:59:ARG:NH1	1:D:63:ARG:HH22	2.08	0.51
1:C:292:SER:HB3	1:C:328:GLY:HA3	1.92	0.51
1:B:30:LEU:HD13	1:B:36:PHE:CE1	2.46	0.51
1:D:385:LEU:HD22	1:D:389:ASP:HB3	1.93	0.50
1:A:335:MSE:HE3	1:A:364:GLU:HA	1.93	0.50
1:D:180:ILE:HD12	1:D:187:ILE:HB	1.91	0.50
1:C:117:ARG:HH21	1:C:120:LEU:HD23	1.76	0.50
1:A:4:GLU:OE2	1:A:267:ARG:NH2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PRO:O	1:A:416:VAL:HG23	2.11	0.50
1:D:337:PHE:C	1:D:337:PHE:HD1	2.14	0.50
1:C:36:PHE:HD2	1:C:40:HIS:HB3	1.76	0.50
1:C:269:LEU:HD22	1:C:270:VAL:H	1.76	0.50
1:B:40:HIS:O	1:B:44:ILE:HG13	2.10	0.50
1:D:337:PHE:C	1:D:337:PHE:CD1	2.85	0.50
1:A:264:LEU:HB2	1:A:266:LEU:HG	1.94	0.50
1:B:334:MSE:CE	1:B:337:PHE:HB2	2.41	0.50
1:C:411:SER:OG	1:C:430:VAL:HG21	2.12	0.50
1:B:473:ILE:CG2	1:B:547:ALA:HB2	2.41	0.50
1:C:399:MSE:HE1	1:C:409:LEU:O	2.11	0.50
1:B:43:LEU:O	1:B:47:MSE:SE	2.80	0.50
1:D:400:PRO:HB2	1:D:403:VAL:HB	1.94	0.50
1:C:415:PRO:O	1:C:416:VAL:HG13	2.11	0.50
1:C:165:LYS:HG2	1:C:290:VAL:HG21	1.93	0.50
1:C:23:PRO:HG2	1:C:53:ARG:CB	2.42	0.50
1:D:40:HIS:O	1:D:44:ILE:HG13	2.11	0.50
1:A:177:ASP:O	1:A:182:ILE:HD13	2.12	0.50
1:D:315:GLU:HB3	1:D:345:PHE:CE2	2.46	0.50
1:B:255:GLU:HB3	1:B:277:ILE:HG22	1.93	0.50
1:A:197:PRO:HD2	1:A:198:LYS:HE2	1.92	0.50
1:D:226:VAL:HG11	1:D:234:MSE:HE1	1.94	0.50
1:C:50:ARG:HE	1:C:54:ILE:HD11	1.76	0.50
1:C:233:ARG:HH11	1:C:233:ARG:CG	2.25	0.50
1:A:379:GLN:O	1:A:383:GLU:HG3	2.12	0.49
1:B:88:GLU:O	1:B:91:ILE:HG22	2.11	0.49
1:B:466:HIS:ND1	1:B:466:HIS:N	2.59	0.49
1:A:273:ARG:NE	4:A:602:ATP:O3G	2.39	0.49
1:A:406:PRO:HD3	1:A:524:ILE:HD11	1.93	0.49
1:B:189:TRP:CE3	1:B:248:VAL:HG11	2.47	0.49
1:D:247:PHE:CE2	1:D:266:LEU:HD13	2.48	0.49
1:D:135:TYR:CE1	1:D:139:ARG:HD2	2.47	0.49
1:D:399:MSE:HG3	1:D:410:TRP:CE2	2.47	0.49
1:A:324:GLU:HG3	1:A:458:HIS:CD2	2.47	0.49
1:B:9:ALA:HB2	1:B:90:TYR:CE1	2.47	0.49
1:B:318:VAL:HG12	1:B:348:MSE:HE3	1.95	0.49
1:C:410:TRP:CD1	1:C:414:ILE:HD13	2.46	0.49
1:B:359:GLY:N	1:B:466:HIS:NE2	2.59	0.49
1:D:135:TYR:CZ	1:D:139:ARG:HD2	2.47	0.49
1:C:322:THR:OG1	1:C:348:MSE:SE	2.79	0.49
1:C:157:LEU:HD11	1:C:168:ILE:CG2	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:LYS:HG2	1:A:290:VAL:HG21	1.93	0.49
1:A:150:LEU:HD13	1:A:153:PHE:HB3	1.94	0.49
1:A:529:PHE:HB3	1:A:532:PHE:CE2	2.46	0.49
1:D:342:PRO:CD	1:D:347:LYS:HG3	2.42	0.49
1:B:17:LEU:HD23	1:B:21:PHE:CD2	2.46	0.49
1:C:447:LYS:CE	1:C:450:PRO:HD2	2.40	0.49
1:D:21:PHE:H	1:D:50:ARG:NH2	2.10	0.49
1:A:379:GLN:HE22	2:E:754:GLY:N	2.11	0.49
1:A:171:GLN:O	1:A:175:LYS:N	2.45	0.49
1:C:189:TRP:CE3	1:C:248:VAL:HG21	2.47	0.49
1:B:404:ASP:OD2	1:B:453:THR:OG1	2.27	0.49
1:A:351:LEU:HD13	1:A:363:VAL:HG23	1.94	0.49
1:A:214:GLU:HG3	1:B:237:ASN:ND2	2.27	0.49
1:C:403:VAL:HG12	1:C:405:ILE:HG22	1.93	0.49
1:B:153:PHE:CE2	1:B:267:ARG:HB3	2.47	0.49
1:D:467:VAL:HG13	2:H:750:PHE:HD1	1.78	0.49
1:C:296:ASP:O	1:C:299:TYR:HB2	2.13	0.49
1:C:484:LEU:CD1	1:C:533:MSE:HG2	2.37	0.49
1:B:233:ARG:CG	1:B:233:ARG:HH11	2.25	0.49
1:B:383:GLU:HG2	2:F:753:MSE:HB3	1.93	0.49
1:C:262:GLN:O	1:C:262:GLN:HG2	2.12	0.49
1:D:237:ASN:C	1:D:239:LEU:H	2.16	0.49
1:C:526:PRO:HG2	1:C:529:PHE:CD2	2.48	0.49
1:A:127:GLN:CD	1:A:174:SER:HB3	2.33	0.49
1:C:388:GLU:HG2	1:C:433:ARG:HH21	1.77	0.49
1:C:190:LEU:CD1	1:C:207:ILE:HG13	2.35	0.49
1:C:466:HIS:N	1:C:466:HIS:ND1	2.61	0.49
1:A:8:ARG:NH1	1:A:8:ARG:HG2	2.25	0.49
1:D:465:LYS:HD3	1:D:466:HIS:CE1	2.48	0.49
1:C:303:GLU:HA	1:C:309:MSE:HE1	1.94	0.49
1:A:143:LYS:HB3	1:A:147:MSE:CE	2.42	0.49
1:B:190:LEU:HD13	1:B:203:LEU:HD22	1.95	0.49
1:C:214:GLU:N	1:C:214:GLU:CD	2.66	0.49
1:A:435:LYS:HZ1	1:A:446:GLY:HA3	1.77	0.49
1:A:374:LEU:HD13	1:A:374:LEU:O	2.13	0.49
1:B:326:SER:O	1:B:328:GLY:N	2.46	0.49
1:B:127:GLN:HA	1:B:170:SER:OG	2.13	0.49
1:A:200:THR:HG21	1:A:256:GLU:HB3	1.95	0.49
1:A:205:THR:HA	1:A:231:LEU:HD11	1.94	0.49
1:C:527:GLU:C	1:C:530:PRO:HD3	2.33	0.48
1:B:529:PHE:N	1:B:530:PRO:HD3	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:319:LEU:HA	1:B:348:MSE:HE1	1.95	0.48
1:C:349:ALA:HA	1:C:352:ASN:HB2	1.94	0.48
2:F:749:MSE:O	2:F:750:PHE:HB2	2.13	0.48
1:A:368:PRO:HD3	1:B:279:ASN:O	2.12	0.48
1:B:59:ARG:HH11	1:B:63:ARG:HH22	1.60	0.48
1:A:275:VAL:HG12	1:A:275:VAL:O	2.12	0.48
1:B:141:ILE:HD12	1:B:175:LYS:NZ	2.28	0.48
1:C:128:MSE:HE3	1:D:282:SER:CB	2.43	0.48
1:A:160:ARG:HD3	1:A:460:ILE:HD13	1.95	0.48
1:B:487:ILE:O	1:B:531:LYS:NZ	2.46	0.48
1:B:154:PHE:CE2	1:B:262:GLN:HG3	2.49	0.48
1:B:29:TYR:OH	1:B:33:LYS:HD2	2.13	0.48
1:D:394:ALA:O	1:D:468:VAL:HG11	2.14	0.48
1:B:355:LEU:HD21	1:B:363:VAL:HB	1.95	0.48
1:B:521:GLU:C	1:B:523:VAL:H	2.16	0.48
1:C:188:VAL:HB	1:C:247:PHE:CD1	2.48	0.48
1:D:178:GLN:HB3	1:D:183:ASN:OD1	2.13	0.48
1:B:47:MSE:HB3	1:B:52:GLU:HB3	1.96	0.48
1:A:343:LYS:HG2	1:A:343:LYS:O	2.12	0.48
1:D:233:ARG:CG	1:D:233:ARG:HH11	2.27	0.48
1:B:400:PRO:HA	1:B:401:PRO:HD3	1.73	0.48
1:D:6:GLU:O	1:D:9:ALA:HB3	2.14	0.48
1:D:335:MSE:HE2	1:D:363:VAL:CG1	2.43	0.48
1:A:334:MSE:HA	1:A:334:MSE:CE	2.41	0.48
1:B:335:MSE:HE2	1:B:363:VAL:CG1	2.43	0.48
1:D:30:LEU:C	1:D:36:PHE:HB2	2.34	0.48
1:C:18:ILE:HD11	1:C:51:LEU:HD21	1.95	0.48
1:A:315:GLU:HA	1:A:318:VAL:HG23	1.96	0.48
1:D:405:ILE:HG13	1:D:409:LEU:HB3	1.95	0.48
1:B:165:LYS:HE3	1:B:272:THR:O	2.13	0.48
1:A:72:ILE:CD1	1:A:87:LEU:HB2	2.42	0.48
1:D:532:PHE:C	1:D:534:GLN:H	2.17	0.48
1:C:397:VAL:HG22	1:C:464:LEU:CB	2.40	0.48
1:C:434:LEU:HA	1:C:437:LEU:HB2	1.95	0.48
1:C:406:PRO:CA	1:C:453:THR:HG22	2.44	0.48
1:A:135:TYR:O	1:A:139:ARG:HG3	2.13	0.48
1:B:17:LEU:O	1:B:54:ILE:HD13	2.13	0.48
1:A:529:PHE:N	1:A:530:PRO:HD3	2.29	0.48
1:A:395:PHE:O	1:A:398:VAL:HG22	2.13	0.48
1:A:215:ASP:O	1:A:216:ASP:HB2	2.14	0.48
1:D:23:PRO:HG2	1:D:53:ARG:C	2.33	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LEU:HD21	1:A:180:ILE:HB	1.94	0.48
1:D:415:PRO:O	1:D:416:VAL:HG23	2.13	0.48
1:B:187:ILE:HD13	1:B:246:LEU:HB3	1.95	0.48
1:A:23:PRO:HG2	1:A:53:ARG:CB	2.44	0.48
1:C:189:TRP:CE3	1:C:248:VAL:HG11	2.49	0.48
1:D:466:HIS:ND1	1:D:466:HIS:N	2.62	0.48
1:D:133:ARG:CZ	1:D:293:LEU:HD23	2.43	0.48
1:B:27:LEU:HD22	1:B:41:SER:HB2	1.96	0.48
1:B:157:LEU:HD23	1:B:288:ILE:O	2.14	0.48
1:D:22:GLU:OE1	1:D:53:ARG:NH1	2.47	0.48
1:C:453:THR:HG21	1:C:524:ILE:HD12	1.96	0.48
1:B:165:LYS:HG2	1:B:290:VAL:CG2	2.39	0.47
1:A:72:ILE:C	1:A:74:PHE:H	2.17	0.47
1:B:200:THR:HG21	1:B:256:GLU:HB3	1.95	0.47
1:D:410:TRP:HD1	1:D:414:ILE:HD13	1.79	0.47
1:C:36:PHE:CD2	1:C:40:HIS:HB3	2.48	0.47
1:C:7:CYS:O	1:C:11:SER:HB2	2.14	0.47
1:C:315:GLU:HA	1:C:318:VAL:HG23	1.96	0.47
1:B:341:GLU:CB	1:B:342:PRO:HD3	2.44	0.47
1:C:400:PRO:HB2	1:C:403:VAL:HB	1.95	0.47
1:D:367:THR:HG23	1:D:369:TYR:HB3	1.94	0.47
1:C:543:LEU:HA	1:C:543:LEU:HD23	1.69	0.47
1:A:37:THR:O	1:A:40:HIS:HB2	2.14	0.47
1:D:302:LEU:CD1	1:D:319:LEU:HD21	2.45	0.47
1:D:398:VAL:HG11	1:D:477:ILE:N	2.29	0.47
1:D:158:HIS:NE2	1:D:289:GLU:HB2	2.29	0.47
1:B:460:ILE:HD12	1:B:460:ILE:HA	1.76	0.47
1:D:21:PHE:CE2	1:D:23:PRO:HG3	2.50	0.47
1:C:165:LYS:HG2	1:C:290:VAL:CG2	2.43	0.47
1:C:189:TRP:CD2	1:C:248:VAL:HG11	2.50	0.47
1:B:399:MSE:CE	1:B:410:TRP:HA	2.44	0.47
1:A:410:TRP:CZ3	1:A:454:PHE:HB2	2.49	0.47
1:A:361:VAL:HG13	1:A:364:GLU:OE1	2.14	0.47
1:A:178:GLN:HA	1:A:182:ILE:HD13	1.97	0.47
1:A:444:LEU:HD12	1:A:444:LEU:HA	1.80	0.47
1:B:240:ILE:HG13	1:B:241:ASP:N	2.30	0.47
1:B:534:GLN:O	1:B:537:GLN:HB2	2.14	0.47
1:D:426:LEU:HB3	1:D:428:ASP:OD2	2.14	0.47
1:C:163:SER:C	1:C:330:PRO:HG2	2.34	0.47
1:B:383:GLU:HG2	2:F:753:MSE:CB	2.44	0.47
1:B:171:GLN:O	1:B:175:LYS:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:374:LEU:HD13	1:B:378:LEU:HG	1.96	0.47
1:D:529:PHE:N	1:D:530:PRO:HD3	2.29	0.47
1:C:397:VAL:C	1:C:399:MSE:H	2.18	0.47
1:C:393:LEU:HD23	1:C:393:LEU:O	2.14	0.47
1:C:214:GLU:H	1:C:214:GLU:CD	2.17	0.47
1:C:130:CYS:HB2	1:C:305:TYR:CZ	2.50	0.47
1:B:109:GLN:C	1:B:111:SER:H	2.17	0.47
1:B:459:ILE:H	1:B:459:ILE:HG13	1.44	0.47
1:A:158:HIS:NE2	1:A:289:GLU:HB2	2.29	0.47
1:C:255:GLU:HA	1:C:277:ILE:HG22	1.97	0.47
1:C:354:LYS:O	1:C:358:ARG:HB2	2.15	0.47
1:D:44:ILE:HD13	1:D:57:PHE:HD1	1.79	0.47
1:D:319:LEU:HD12	1:D:345:PHE:CZ	2.50	0.47
1:B:385:LEU:HD22	1:B:389:ASP:HB2	1.97	0.47
1:B:192:ASP:OD2	1:B:257:THR:OG1	2.21	0.47
1:B:465:LYS:HD3	1:B:466:HIS:CE1	2.50	0.47
1:C:407:VAL:HG22	1:C:454:PHE:HE1	1.80	0.47
1:D:257:THR:HG22	1:D:258:ILE:N	2.30	0.47
1:B:397:VAL:O	1:B:461:HIS:NE2	2.45	0.46
1:D:1:MSE:HA	1:D:62:ARG:O	2.15	0.46
1:A:335:MSE:HE2	1:A:363:VAL:CG1	2.44	0.46
1:D:133:ARG:O	1:D:137:VAL:HG23	2.14	0.46
1:C:379:GLN:O	1:C:383:GLU:HG3	2.14	0.46
1:D:116:ASP:O	1:D:120:LEU:HB3	2.16	0.46
1:B:56:ASN:O	1:B:60:ILE:HB	2.14	0.46
1:B:8:ARG:HD3	1:B:90:TYR:OH	2.15	0.46
1:D:2:LEU:CD1	1:D:62:ARG:HE	2.28	0.46
1:D:127:GLN:HB3	1:D:170:SER:O	2.15	0.46
1:C:187:ILE:HD13	1:C:246:LEU:HB3	1.97	0.46
1:C:302:LEU:CD1	1:C:319:LEU:HD21	2.45	0.46
1:D:110:PHE:HA	1:D:110:PHE:HD1	1.57	0.46
1:A:347:LYS:O	1:A:347:LYS:HD3	2.15	0.46
1:C:478:SER:O	1:C:482:GLN:HG2	2.15	0.46
1:D:399:MSE:HG3	1:D:410:TRP:CZ2	2.51	0.46
1:D:461:HIS:O	1:D:464:LEU:N	2.48	0.46
1:A:249:PHE:HE2	1:A:261:ALA:HB2	1.81	0.46
1:C:378:LEU:HD23	1:C:378:LEU:HA	1.70	0.46
1:D:355:LEU:HD21	1:D:363:VAL:HB	1.97	0.46
1:B:128:MSE:CG	1:B:167:VAL:HG22	2.39	0.46
1:C:301:PHE:HE1	1:C:305:TYR:HE2	1.63	0.46
1:B:32:GLY:C	1:B:34:ASN:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:187:ILE:CD1	1:D:246:LEU:HB3	2.45	0.46
1:B:475:ASN:O	1:B:479:ILE:HG13	2.16	0.46
1:A:131:TYR:C	1:A:131:TYR:CD1	2.89	0.46
1:B:26:ALA:HB2	1:B:74:PHE:CZ	2.49	0.46
1:D:227:THR:HB	1:D:229:VAL:HG12	1.97	0.46
1:B:434:LEU:HD22	1:B:444:LEU:CD2	2.46	0.46
1:D:144:LEU:HB2	1:D:179:LEU:HD21	1.98	0.46
1:A:92:ASP:C	1:A:94:ALA:H	2.19	0.46
1:A:471:GLN:HG3	1:D:471:GLN:HE21	1.80	0.46
1:A:21:PHE:CE1	1:A:75:PHE:HE1	2.34	0.46
1:C:449:MSE:HE3	1:C:450:PRO:HA	1.97	0.46
1:C:342:PRO:O	1:C:343:LYS:HB3	2.16	0.46
1:C:160:ARG:HB3	1:C:163:SER:HB3	1.97	0.46
1:D:527:GLU:C	1:D:530:PRO:HD3	2.36	0.46
1:C:19:HIS:HD2	1:D:1:MSE:SE	2.48	0.46
1:C:319:LEU:HD12	1:C:345:PHE:CZ	2.50	0.46
1:D:207:ILE:HD11	1:D:249:PHE:HE1	1.80	0.46
1:A:21:PHE:CD1	1:A:75:PHE:HE1	2.34	0.46
1:A:22:GLU:HG3	1:A:24:ARG:H	1.81	0.46
1:C:21:PHE:CD1	1:C:75:PHE:CE1	3.04	0.46
1:C:219:ASN:O	1:C:221:PRO:HD3	2.16	0.46
1:D:118:LYS:HD3	1:D:180:ILE:HG22	1.98	0.46
1:C:165:LYS:HE3	1:C:272:THR:O	2.16	0.46
1:B:173:LEU:HD23	1:B:179:LEU:HD23	1.98	0.46
1:B:126:LYS:O	1:B:126:LYS:HE2	2.16	0.46
1:D:399:MSE:HE3	1:D:410:TRP:CG	2.51	0.46
1:B:49:THR:HG22	1:B:51:LEU:H	1.80	0.46
1:C:216:ASP:N	1:C:218:LEU:HD23	2.31	0.46
1:D:187:ILE:HD13	1:D:246:LEU:HD23	1.97	0.46
1:D:135:TYR:O	1:D:139:ARG:HG3	2.16	0.46
1:C:218:LEU:HG	1:C:219:ASN:N	2.32	0.45
1:B:109:GLN:C	1:B:111:SER:N	2.69	0.45
1:D:334:MSE:HA	1:D:334:MSE:HE3	1.98	0.45
1:B:26:ALA:HA	1:B:74:PHE:CE1	2.51	0.45
1:D:100:LEU:HD12	1:D:100:LEU:HA	1.83	0.45
1:A:99:ASP:C	1:A:101:LEU:H	2.19	0.45
1:D:399:MSE:HE3	1:D:410:TRP:CD1	2.50	0.45
1:B:160:ARG:O	1:B:165:LYS:NZ	2.48	0.45
1:A:257:THR:HG22	1:A:258:ILE:N	2.30	0.45
1:A:79:ASN:HD22	1:B:36:PHE:N	2.14	0.45
1:B:274:ASP:OD2	1:B:440:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:32:GLY:C	1:D:34:ASN:H	2.20	0.45
1:B:226:VAL:HG11	1:B:234:MSE:CE	2.46	0.45
1:D:197:PRO:HD2	1:D:198:LYS:HE2	1.97	0.45
1:C:141:ILE:HD12	1:C:175:LYS:HZ2	1.81	0.45
1:B:393:LEU:HB2	1:B:437:LEU:HD11	1.97	0.45
1:A:390:ARG:HB2	1:A:390:ARG:HE	1.10	0.45
1:C:318:VAL:HG13	1:C:349:ALA:HB2	1.97	0.45
1:B:408:LYS:HD2	1:B:408:LYS:HA	1.66	0.45
1:C:35:ILE:O	1:C:64:GLN:HB3	2.16	0.45
1:A:397:VAL:HG21	1:A:468:VAL:HG21	1.98	0.45
1:D:414:ILE:HG21	1:D:430:VAL:HG13	1.99	0.45
1:C:37:THR:H	1:C:40:HIS:HB2	1.81	0.45
1:A:17:LEU:HD23	1:A:21:PHE:CD2	2.51	0.45
1:A:437:LEU:HA	1:A:437:LEU:HD22	1.70	0.45
1:B:23:PRO:HG2	1:B:53:ARG:O	2.15	0.45
1:B:49:THR:HG22	1:B:50:ARG:H	1.82	0.45
1:C:477:ILE:HD13	1:C:544:LYS:HG3	1.98	0.45
1:B:385:LEU:HD22	1:B:389:ASP:CB	2.47	0.45
1:A:163:SER:O	1:A:330:PRO:HG2	2.17	0.45
1:D:331:ALA:HB2	4:D:602:ATP:H5'1	1.98	0.45
1:D:255:GLU:HB3	1:D:277:ILE:HG22	1.97	0.45
1:D:319:LEU:HD12	1:D:345:PHE:HE1	1.80	0.45
1:D:247:PHE:HE2	1:D:266:LEU:HD22	1.81	0.45
1:D:259:ARG:O	1:D:263:GLU:HG3	2.16	0.45
1:C:111:SER:C	1:C:113:GLN:H	2.20	0.45
1:A:405:ILE:HG12	1:A:410:TRP:CZ3	2.51	0.45
1:B:30:LEU:HA	1:B:30:LEU:HD23	1.75	0.45
1:D:192:ASP:OD2	1:D:257:THR:OG1	2.21	0.45
1:C:333:LEU:O	1:C:336:PHE:HB2	2.16	0.45
1:B:367:THR:HG23	1:B:369:TYR:HB3	1.99	0.45
1:C:38:GLU:O	1:C:38:GLU:CG	2.65	0.45
1:C:359:GLY:N	1:C:466:HIS:NE2	2.65	0.45
1:B:394:ALA:O	1:B:397:VAL:HG23	2.17	0.45
1:C:67:GLU:HG2	1:C:69:GLY:N	2.29	0.45
1:A:25:ASP:HB3	1:A:78:ASN:ND2	2.32	0.45
1:D:387:ASP:HA	1:D:390:ARG:HH21	1.81	0.45
1:C:382:VAL:HA	1:C:385:LEU:HD12	1.98	0.45
1:B:189:TRP:CZ3	1:B:248:VAL:HG11	2.52	0.45
1:B:252:VAL:CG2	1:B:257:THR:HG21	2.47	0.45
1:B:255:GLU:CB	1:B:277:ILE:HG22	2.46	0.45
1:D:143:LYS:O	1:D:147:MSE:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:463:PHE:O	1:D:467:VAL:HB	2.17	0.45
1:D:329:ASN:HA	1:D:330:PRO:HD2	1.70	0.45
1:D:491:ASN:HD21	1:D:531:LYS:HE3	1.82	0.44
1:A:235:ILE:O	1:A:239:LEU:HB2	2.18	0.44
1:C:331:ALA:HB2	4:C:602:ATP:H5'1	1.99	0.44
1:A:467:VAL:O	2:E:751:ASN:HB2	2.16	0.44
1:C:258:ILE:CG2	1:C:280:ALA:HB3	2.47	0.44
1:C:240:ILE:HG13	1:C:241:ASP:OD1	2.18	0.44
1:B:253:VAL:HG11	1:B:380:ARG:HD3	1.99	0.44
1:B:405:ILE:HA	1:B:406:PRO:HD3	1.59	0.44
1:B:434:LEU:HD22	1:B:444:LEU:HD23	1.99	0.44
1:A:461:HIS:O	1:A:464:LEU:N	2.50	0.44
1:C:302:LEU:HD13	1:C:319:LEU:HD21	1.98	0.44
1:D:469:ASP:HB2	2:H:749:MSE:HA	1.99	0.44
1:A:99:ASP:C	1:A:101:LEU:N	2.70	0.44
1:C:204:PHE:C	1:C:231:LEU:HD21	2.37	0.44
1:C:484:LEU:HD21	1:C:533:MSE:HG2	1.98	0.44
1:B:397:VAL:HG22	1:B:464:LEU:HB3	1.97	0.44
1:C:33:LYS:NZ	1:C:73:ASP:OD2	2.50	0.44
1:B:410:TRP:CZ3	1:B:454:PHE:HB2	2.52	0.44
1:D:252:VAL:CG2	1:D:257:THR:HG21	2.47	0.44
1:A:408:LYS:HD2	1:A:408:LYS:HA	1.83	0.44
1:D:527:GLU:HA	1:D:530:PRO:HG3	1.99	0.44
1:B:429:GLU:O	1:B:429:GLU:HG3	2.18	0.44
1:A:140:VAL:HG12	1:A:144:LEU:HD12	1.99	0.44
1:D:395:PHE:C	1:D:397:VAL:H	2.21	0.44
1:A:397:VAL:HG22	1:A:464:LEU:CB	2.48	0.44
1:B:307:MSE:HA	1:B:308:PRO:HD3	1.79	0.44
1:D:335:MSE:SE	1:D:373:SER:HA	2.68	0.44
1:D:399:MSE:CE	1:D:410:TRP:HA	2.48	0.44
1:A:168:ILE:HD13	1:A:168:ILE:HG21	1.74	0.44
1:B:147:MSE:O	1:B:150:LEU:HB2	2.18	0.44
1:A:247:PHE:CD2	1:A:266:LEU:HD13	2.53	0.44
1:B:44:ILE:O	1:B:53:ARG:HG2	2.18	0.44
1:A:79:ASN:ND2	1:B:36:PHE:O	2.51	0.44
1:C:158:HIS:CE1	1:C:289:GLU:HB2	2.53	0.44
1:A:212:LYS:HA	1:A:212:LYS:HE2	2.00	0.44
1:D:2:LEU:HD12	1:D:7:CYS:SG	2.58	0.44
1:D:27:LEU:HD22	1:D:41:SER:HA	2.00	0.44
1:A:79:ASN:ND2	1:B:36:PHE:N	2.65	0.44
1:D:17:LEU:HD23	1:D:21:PHE:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:322:THR:OG1	1:D:348:MSE:SE	2.86	0.44
1:D:534:GLN:O	1:D:537:GLN:HB2	2.17	0.44
1:D:393:LEU:HD21	1:D:464:LEU:HD21	2.00	0.43
1:D:148:CYS:HB3	1:D:183:ASN:HB3	2.00	0.43
1:A:120:LEU:HD13	1:B:265:ARG:HB2	1.99	0.43
1:C:190:LEU:HD23	1:C:190:LEU:HA	1.61	0.43
1:C:136:HIS:HB3	1:C:168:ILE:HD13	1.99	0.43
1:C:75:PHE:HB3	1:C:83:LEU:HB2	1.99	0.43
1:C:126:LYS:O	1:C:126:LYS:HE2	2.18	0.43
2:H:750:PHE:O	2:H:751:ASN:ND2	2.23	0.43
1:A:521:GLU:C	1:A:523:VAL:H	2.21	0.43
1:D:434:LEU:HD22	1:D:444:LEU:HD21	2.00	0.43
1:D:207:ILE:O	1:D:210:MSE:HB2	2.17	0.43
1:D:166:SER:HA	1:D:271:THR:HG21	2.01	0.43
1:A:160:ARG:HG2	1:A:161:ALA:N	2.28	0.43
1:D:284:THR:O	1:D:285:CYS:C	2.57	0.43
1:A:469:ASP:HB2	2:E:749:MSE:HA	1.99	0.43
1:C:46:LYS:HG3	1:C:46:LYS:H	1.66	0.43
1:A:405:ILE:HA	1:A:406:PRO:HD3	1.69	0.43
1:C:329:ASN:HA	1:C:330:PRO:HD2	1.84	0.43
1:D:315:GLU:HA	1:D:318:VAL:HG23	1.99	0.43
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.82	0.43
1:D:482:GLN:OE1	1:D:482:GLN:N	2.51	0.43
1:D:4:GLU:O	1:D:8:ARG:HG3	2.18	0.43
1:B:386:SER:OG	1:B:388:GLU:OE1	2.36	0.43
1:D:21:PHE:HD2	1:D:54:ILE:HG12	1.84	0.43
1:D:472:THR:HG21	2:H:749:MSE:HE2	2.00	0.43
1:C:326:SER:O	1:C:327:SER:C	2.55	0.43
2:G:750:PHE:HB2	2:G:753:MSE:HE2	2.00	0.43
1:C:178:GLN:O	1:C:182:ILE:HB	2.19	0.43
1:B:382:VAL:O	1:B:385:LEU:HB2	2.18	0.43
1:D:157:LEU:HD11	1:D:168:ILE:CG2	2.48	0.43
1:D:301:PHE:O	1:D:304:ALA:HB3	2.18	0.43
1:C:111:SER:HB3	1:C:113:GLN:HG2	2.00	0.43
1:D:349:ALA:HA	1:D:352:ASN:HB2	2.01	0.43
1:D:207:ILE:HG22	1:D:208:LEU:N	2.33	0.43
1:A:36:PHE:HE2	1:A:44:ILE:HD12	1.82	0.43
1:B:393:LEU:HD21	1:B:464:LEU:HD21	2.01	0.43
1:D:250:ASP:OD1	1:D:271:THR:OG1	2.27	0.43
1:D:283:GLN:C	1:D:285:CYS:N	2.71	0.43
1:B:295:ILE:HG23	1:B:323:ILE:HG21	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:CYS:SG	1:B:348:MSE:HG2	2.58	0.43
1:D:126:LYS:HB3	1:D:126:LYS:HE2	1.74	0.43
1:D:257:THR:HG22	1:D:258:ILE:HD12	2.01	0.43
1:B:160:ARG:HG3	1:B:441:GLY:O	2.17	0.43
1:C:248:VAL:HG22	1:C:269:LEU:HB3	2.00	0.43
1:B:190:LEU:HA	1:B:190:LEU:HD23	1.81	0.43
1:B:207:ILE:HG22	1:B:208:LEU:N	2.34	0.43
1:D:460:ILE:HA	1:D:460:ILE:HD12	1.77	0.43
1:D:315:GLU:HB3	1:D:345:PHE:CD2	2.53	0.43
1:C:408:LYS:HE2	1:C:427:ASP:HB2	2.01	0.43
1:C:157:LEU:HD23	1:C:288:ILE:O	2.19	0.43
1:D:405:ILE:HG12	1:D:410:TRP:CE3	2.53	0.43
1:B:329:ASN:HA	1:B:330:PRO:HD2	1.84	0.43
1:D:527:GLU:N	1:D:527:GLU:OE1	2.51	0.43
1:A:40:HIS:CD2	1:A:64:GLN:NE2	2.87	0.43
1:C:459:ILE:H	1:C:459:ILE:HG13	1.32	0.43
1:D:255:GLU:O	1:D:259:ARG:HG3	2.19	0.43
1:C:111:SER:O	1:C:113:GLN:N	2.51	0.43
1:C:258:ILE:HG22	1:C:280:ALA:HB3	2.01	0.43
1:A:307:MSE:HE1	1:A:348:MSE:HG3	2.01	0.43
1:B:477:ILE:HD13	1:B:544:LYS:HG3	2.00	0.43
1:C:485:LEU:HD12	1:C:486:GLU:H	1.83	0.43
1:A:24:ARG:HE	1:A:53:ARG:NH1	2.17	0.42
1:C:364:GLU:CB	1:C:373:SER:HB3	2.48	0.42
1:A:455:LYS:HG2	1:A:456:ILE:N	2.33	0.42
1:A:133:ARG:HH12	1:A:290:VAL:HG12	1.83	0.42
1:A:157:LEU:HD22	1:A:290:VAL:HG22	2.00	0.42
1:A:72:ILE:HG21	1:A:88:GLU:CG	2.42	0.42
1:A:449:MSE:HE3	1:A:449:MSE:HB2	1.76	0.42
1:A:136:HIS:O	1:A:139:ARG:N	2.53	0.42
1:C:354:LYS:HE2	1:D:429:GLU:OE1	2.19	0.42
1:C:273:ARG:NH2	1:C:377:ALA:HB1	2.34	0.42
1:C:393:LEU:HB2	1:C:437:LEU:HD11	2.01	0.42
1:B:46:LYS:O	1:B:47:MSE:SE	2.87	0.42
1:A:543:LEU:HA	1:A:543:LEU:HD23	1.77	0.42
1:A:435:LYS:HZ3	1:A:446:GLY:HA3	1.83	0.42
1:B:308:PRO:CG	1:B:343:LYS:HD3	2.49	0.42
1:B:34:ASN:O	1:B:35:ILE:HG13	2.19	0.42
1:C:334:MSE:HE3	1:C:334:MSE:HA	2.00	0.42
1:D:139:ARG:HH21	1:D:143:LYS:HE3	1.83	0.42
1:D:438:SER:O	1:D:442:ALA:HA	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:VAL:HG12	1:A:168:ILE:N	2.34	0.42
1:B:157:LEU:HD22	1:B:290:VAL:HG22	2.01	0.42
1:C:465:LYS:HB3	1:C:466:HIS:ND1	2.35	0.42
1:D:529:PHE:HB3	1:D:532:PHE:CE1	2.55	0.42
1:D:530:PRO:HD2	1:D:531:LYS:HG3	2.00	0.42
1:C:237:ASN:HD22	1:C:237:ASN:HA	1.67	0.42
1:D:318:VAL:O	1:D:321:LYS:HB3	2.19	0.42
1:B:158:HIS:ND1	1:B:158:HIS:O	2.52	0.42
1:D:301:PHE:HE1	1:D:305:TYR:HE1	1.65	0.42
1:B:347:LYS:HD3	1:B:347:LYS:O	2.19	0.42
1:A:482:GLN:C	1:A:484:LEU:H	2.21	0.42
1:B:331:ALA:HB2	4:B:602:ATP:H5'1	2.00	0.42
1:C:325:LEU:HD12	1:C:352:ASN:OD1	2.20	0.42
1:C:72:ILE:HD11	1:C:87:LEU:HB2	2.01	0.42
1:D:105:VAL:HG22	1:D:110:PHE:CE2	2.55	0.42
1:C:113:GLN:HG2	1:C:113:GLN:H	1.66	0.42
1:C:38:GLU:O	1:C:38:GLU:HG2	2.20	0.42
1:A:124:VAL:HA	1:A:125:PRO:HD3	1.67	0.42
1:A:21:PHE:CG	1:A:22:GLU:N	2.87	0.42
1:D:39:ASP:O	1:D:43:LEU:HD13	2.20	0.42
1:C:92:ASP:OD1	1:C:96:ASN:ND2	2.48	0.42
1:D:141:ILE:HD12	1:D:175:LYS:CE	2.48	0.42
1:D:49:THR:HG22	1:D:50:ARG:N	2.35	0.42
1:B:154:PHE:HE2	1:B:262:GLN:HG3	1.84	0.42
1:D:100:LEU:HB3	1:D:101:LEU:H	1.65	0.42
1:D:136:HIS:O	1:D:140:VAL:HG23	2.20	0.42
1:B:525:ARG:HD3	1:B:525:ARG:HA	1.84	0.42
1:A:302:LEU:HD13	1:A:319:LEU:HD11	2.01	0.42
1:B:332:THR:HG23	1:B:374:LEU:HB2	2.00	0.42
1:C:525:ARG:HA	1:C:526:PRO:HD3	1.54	0.42
1:C:60:ILE:HG23	1:C:64:GLN:HG3	2.01	0.42
1:C:395:PHE:O	1:C:398:VAL:HG22	2.20	0.42
1:B:122:GLY:HA3	1:B:187:ILE:HG23	2.02	0.42
1:D:104:VAL:HG12	1:D:105:VAL:HG23	2.01	0.42
1:A:525:ARG:HA	1:A:526:PRO:HD3	1.73	0.42
1:D:408:LYS:HD2	1:D:408:LYS:HA	1.76	0.42
1:C:4:GLU:OE2	1:C:267:ARG:NH2	2.53	0.42
1:C:2:LEU:HG	1:C:62:ARG:HA	2.02	0.42
1:D:302:LEU:HB3	1:D:307:MSE:HB3	2.01	0.42
1:A:235:ILE:HD13	1:A:235:ILE:HG21	1.78	0.42
1:D:398:VAL:HG11	1:D:476:GLY:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:PHE:O	1:A:231:LEU:HD21	2.20	0.42
1:C:134:GLU:O	1:C:135:TYR:C	2.58	0.42
1:A:326:SER:C	1:A:459:ILE:HG12	2.39	0.42
1:C:72:ILE:C	1:C:74:PHE:H	2.23	0.42
1:B:537:GLN:O	1:B:538:LYS:C	2.56	0.42
1:C:192:ASP:O	1:C:193:SER:HB2	2.19	0.42
1:D:121:LEU:HD23	1:D:121:LEU:HA	1.64	0.42
1:A:142:LYS:HE2	1:A:146:GLU:OE2	2.20	0.42
1:A:24:ARG:HH21	1:A:53:ARG:NH1	2.18	0.42
1:C:21:PHE:CG	1:C:22:GLU:N	2.88	0.42
2:E:752:PHE:N	2:E:752:PHE:CD1	2.88	0.42
1:A:117:ARG:HH21	1:A:120:LEU:CD2	2.29	0.42
1:B:2:LEU:HD12	1:B:7:CYS:SG	2.59	0.42
1:C:405:ILE:O	1:C:405:ILE:HG12	2.20	0.42
1:C:319:LEU:HA	1:C:348:MSE:HE1	2.02	0.42
1:A:135:TYR:CZ	1:A:139:ARG:HD2	2.55	0.42
1:A:479:ILE:HG23	1:A:483:ARG:HH22	1.84	0.42
1:A:19:HIS:O	1:B:1:MSE:HG3	2.20	0.41
1:A:182:ILE:N	1:A:182:ILE:HD12	2.35	0.41
1:D:27:LEU:CD1	1:D:45:SER:HB3	2.51	0.41
1:A:435:LYS:HD3	1:A:435:LYS:HA	1.90	0.41
1:D:168:ILE:HA	1:D:171:GLN:HE21	1.85	0.41
1:B:313:GLU:O	1:B:316:GLU:HG3	2.20	0.41
1:A:240:ILE:HG13	1:A:241:ASP:N	2.35	0.41
1:A:63:ARG:HE	1:A:240:ILE:CD1	2.12	0.41
1:B:160:ARG:HG2	1:B:161:ALA:N	2.31	0.41
1:D:235:ILE:HD13	1:D:235:ILE:HG21	1.73	0.41
1:B:393:LEU:HD23	1:B:393:LEU:O	2.20	0.41
1:C:8:ARG:NH1	1:C:185:ASP:OD1	2.52	0.41
1:C:74:PHE:C	1:C:74:PHE:CD2	2.92	0.41
1:D:127:GLN:HB2	1:D:171:GLN:HA	2.01	0.41
1:C:385:LEU:HD22	1:C:389:ASP:HB3	2.02	0.41
1:D:325:LEU:HA	1:D:325:LEU:HD23	1.80	0.41
1:D:335:MSE:CE	1:D:373:SER:HB2	2.49	0.41
1:B:167:VAL:HG12	1:B:168:ILE:N	2.35	0.41
1:D:237:ASN:C	1:D:239:LEU:N	2.74	0.41
1:A:35:ILE:O	1:A:64:GLN:HB3	2.20	0.41
1:D:481:GLU:HA	1:D:484:LEU:HG	2.02	0.41
1:C:397:VAL:O	1:C:399:MSE:N	2.50	0.41
1:D:2:LEU:HD23	1:D:2:LEU:N	2.35	0.41
1:C:434:LEU:HD22	1:C:444:LEU:HD23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:GLU:OE2	1:B:53:ARG:HD2	2.20	0.41
1:C:405:ILE:HA	1:C:406:PRO:HD3	1.78	0.41
1:B:194:GLY:O	1:B:254:GLN:HG3	2.21	0.41
1:A:91:ILE:O	1:A:95:ILE:HG13	2.20	0.41
1:D:366:ILE:H	1:D:366:ILE:CD1	2.16	0.41
1:D:385:LEU:HD11	1:D:393:LEU:HD12	2.01	0.41
1:D:434:LEU:HD22	1:D:444:LEU:CD2	2.50	0.41
1:A:371:TYR:CD2	1:A:377:ALA:HB2	2.55	0.41
1:B:395:PHE:O	1:B:397:VAL:N	2.54	0.41
1:B:405:ILE:HD13	1:B:405:ILE:HG21	1.69	0.41
1:A:388:GLU:O	1:A:391:SER:HB3	2.20	0.41
1:A:327:SER:N	1:A:459:ILE:HG12	2.36	0.41
1:D:247:PHE:CD2	1:D:266:LEU:HB3	2.55	0.41
1:D:242:ARG:HD2	1:D:242:ARG:HH11	1.65	0.41
1:A:157:LEU:HD22	1:A:290:VAL:CG2	2.50	0.41
1:B:330:PRO:HB3	4:B:602:ATP:N3	2.35	0.41
1:D:190:LEU:HD12	1:D:207:ILE:HG13	2.01	0.41
1:B:92:ASP:O	1:B:96:ASN:HB2	2.21	0.41
1:A:385:LEU:O	1:A:390:ARG:NH2	2.53	0.41
1:C:34:ASN:O	1:C:35:ILE:HG13	2.21	0.41
1:D:443:LEU:HA	1:D:460:ILE:HG12	2.02	0.41
1:A:332:THR:O	1:A:336:PHE:HB2	2.20	0.41
1:D:157:LEU:HD22	1:D:290:VAL:CG2	2.50	0.41
1:B:487:ILE:HA	1:B:490:ASN:OD1	2.20	0.41
1:A:38:GLU:O	1:A:42:GLU:HB2	2.20	0.41
1:C:426:LEU:HB3	1:C:428:ASP:OD1	2.20	0.41
1:B:218:LEU:HG	1:B:219:ASN:N	2.36	0.41
1:D:397:VAL:C	1:D:399:MSE:H	2.23	0.41
1:B:368:PRO:HB2	4:B:602:ATP:O2'	2.21	0.41
1:A:72:ILE:HD11	1:A:87:LEU:CB	2.47	0.41
1:B:397:VAL:O	1:B:399:MSE:N	2.54	0.41
1:C:8:ARG:HG2	1:C:8:ARG:NH1	2.29	0.41
1:B:295:ILE:O	1:B:299:TYR:HD1	2.03	0.41
1:A:459:ILE:HG13	1:A:459:ILE:H	1.46	0.41
1:D:104:VAL:HB	1:D:105:VAL:H	1.63	0.41
1:A:188:VAL:HB	1:A:247:PHE:CD1	2.55	0.41
1:A:189:TRP:CD1	1:A:189:TRP:C	2.94	0.41
1:B:250:ASP:HA	1:B:271:THR:OG1	2.20	0.41
1:A:478:SER:HB3	1:D:548:CYS:SG	2.60	0.41
1:C:116:ASP:OD1	1:C:116:ASP:N	2.54	0.41
1:A:203:LEU:HA	1:A:203:LEU:HD23	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:ILE:O	1:D:210:MSE:N	2.54	0.41
1:A:303:GLU:HA	1:A:309:MSE:HE1	2.03	0.41
1:C:525:ARG:HD3	1:C:535:LEU:HD13	2.03	0.41
1:A:395:PHE:C	1:A:397:VAL:H	2.23	0.41
1:D:252:VAL:HG22	1:D:257:THR:HG21	2.02	0.41
1:C:371:TYR:CD2	1:C:377:ALA:HB2	2.56	0.41
1:C:426:LEU:HA	1:C:426:LEU:HD23	1.73	0.41
1:B:113:GLN:O	1:B:117:ARG:N	2.53	0.41
1:C:139:ARG:HD2	1:C:288:ILE:HG23	2.03	0.41
1:D:444:LEU:HB3	1:D:445:SER:H	1.66	0.41
1:A:165:LYS:HG3	1:A:165:LYS:H	1.58	0.41
1:B:437:LEU:HA	1:B:437:LEU:HD23	1.81	0.41
1:C:335:MSE:HE2	1:C:363:VAL:HG13	2.03	0.41
1:A:413:VAL:HG23	1:A:414:ILE:HD12	2.03	0.41
1:C:456:ILE:HG12	1:C:457:ASP:O	2.21	0.41
1:D:43:LEU:HD12	1:D:43:LEU:HA	1.90	0.41
1:C:461:HIS:C	1:C:463:PHE:N	2.74	0.41
1:B:207:ILE:O	1:B:210:MSE:N	2.54	0.41
1:B:188:VAL:HB	1:B:247:PHE:HD1	1.84	0.41
1:D:443:LEU:HD23	1:D:460:ILE:HD11	2.02	0.41
1:B:135:TYR:CZ	1:B:139:ARG:HD2	2.56	0.41
1:A:237:ASN:C	1:A:239:LEU:H	2.24	0.41
1:B:211:LEU:HD11	1:B:239:LEU:HD23	2.03	0.41
1:A:2:LEU:HG	1:A:62:ARG:HA	2.03	0.41
1:D:122:GLY:HA3	1:D:187:ILE:HG23	2.02	0.41
1:B:481:GLU:O	1:B:484:LEU:HG	2.20	0.41
1:A:379:GLN:NE2	2:E:754:GLY:N	2.69	0.41
1:C:206:ASP:OD2	1:D:229:VAL:HG11	2.21	0.41
1:A:471:GLN:HG3	1:D:471:GLN:NE2	2.35	0.41
1:C:408:LYS:HA	1:C:408:LYS:HD2	1.74	0.41
1:A:429:GLU:OE2	1:A:433:ARG:NH1	2.54	0.41
1:D:165:LYS:H	1:D:165:LYS:HG3	1.56	0.41
1:A:72:ILE:HD12	1:A:72:ILE:HG23	1.85	0.41
1:C:189:TRP:CD1	1:C:189:TRP:C	2.95	0.41
1:A:389:ASP:HB3	1:A:437:LEU:CD2	2.46	0.41
1:A:393:LEU:C	1:A:393:LEU:HD23	2.41	0.41
1:A:394:ALA:O	1:A:397:VAL:HG23	2.20	0.41
1:A:465:LYS:HB3	1:A:466:HIS:H	1.81	0.41
1:C:197:PRO:HD2	1:C:198:LYS:CE	2.51	0.41
1:A:78:ASN:OD1	1:B:37:THR:HG21	2.21	0.41
1:D:483:ARG:HA	1:D:486:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:CB	1:D:265:ARG:HH12	2.34	0.41
1:C:1:MSE:HE2	1:C:1:MSE:HB3	1.64	0.41
1:D:67:GLU:OE1	1:D:67:GLU:N	2.54	0.41
1:D:153:PHE:CE1	1:D:267:ARG:HB3	2.56	0.41
1:D:335:MSE:HE3	1:D:373:SER:HB2	2.03	0.40
1:C:465:LYS:HB3	1:C:466:HIS:H	1.80	0.40
1:D:39:ASP:N	1:D:39:ASP:OD1	2.52	0.40
1:D:44:ILE:HG12	1:D:56:ASN:HB3	2.03	0.40
1:B:207:ILE:HD11	1:B:249:PHE:HE1	1.85	0.40
1:C:237:ASN:C	1:C:239:LEU:H	2.23	0.40
1:A:395:PHE:CD2	1:A:415:PRO:HD3	2.56	0.40
1:C:349:ALA:O	1:C:352:ASN:HB2	2.20	0.40
1:C:469:ASP:N	2:G:749:MSE:O	2.46	0.40
1:C:416:VAL:HG12	1:C:429:GLU:HG2	2.02	0.40
1:C:274:ASP:C	1:C:274:ASP:OD1	2.60	0.40
2:H:749:MSE:O	2:H:750:PHE:HB2	2.22	0.40
1:B:180:ILE:HD12	1:B:187:ILE:HB	2.03	0.40
1:C:158:HIS:ND1	1:C:158:HIS:O	2.54	0.40
1:C:158:HIS:CD2	1:C:275:VAL:HG13	2.55	0.40
1:A:142:LYS:O	1:A:146:GLU:HG3	2.20	0.40
1:B:273:ARG:NH2	1:B:380:ARG:HH21	2.20	0.40
1:C:327:SER:OG	1:C:458:HIS:HB2	2.21	0.40
1:A:398:VAL:HG11	1:A:476:GLY:HA3	2.03	0.40
1:B:155:LEU:HA	1:B:155:LEU:HD23	1.77	0.40
1:B:521:GLU:HG3	1:B:523:VAL:H	1.86	0.40
1:B:186:SER:OG	1:B:245:THR:HG23	2.22	0.40
1:A:296:ASP:O	1:A:299:TYR:HB2	2.21	0.40
1:A:485:LEU:HD12	1:A:486:GLU:OE2	2.21	0.40
1:D:524:ILE:HD12	1:D:525:ARG:H	1.86	0.40
1:A:111:SER:O	1:A:113:GLN:N	2.54	0.40
1:C:139:ARG:HD2	1:C:288:ILE:CG2	2.52	0.40
1:D:395:PHE:C	1:D:397:VAL:N	2.74	0.40
1:D:400:PRO:HG3	1:D:533:MSE:HE1	2.04	0.40
1:A:157:LEU:HA	1:A:288:ILE:O	2.22	0.40
1:D:137:VAL:HG13	1:D:172:ALA:HB2	2.02	0.40
1:B:200:THR:O	1:B:200:THR:HG22	2.20	0.40
1:D:61:TYR:HE2	1:D:68:LEU:HD22	1.85	0.40
1:B:372:LYS:H	1:B:376:MSE:HE2	1.87	0.40
1:D:406:PRO:CA	1:D:453:THR:HG22	2.47	0.40
1:A:447:LYS:HE2	1:A:449:MSE:O	2.21	0.40
1:B:234:MSE:O	1:B:237:ASN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:752:PHE:HB3	2:H:753:MSE:C	2.42	0.40
1:C:117:ARG:HH12	1:D:240:ILE:HA	1.86	0.40
1:C:388:GLU:H	1:C:388:GLU:CD	2.24	0.40
1:C:382:VAL:O	1:C:385:LEU:HB2	2.22	0.40
1:B:217:LEU:HA	1:B:217:LEU:HD23	1.89	0.40
1:C:390:ARG:HB2	1:C:390:ARG:HE	1.56	0.40
1:A:439:LYS:HD2	1:A:439:LYS:HA	1.75	0.40
1:D:204:PHE:CD1	1:D:204:PHE:N	2.88	0.40
1:A:313:GLU:O	1:A:316:GLU:HG3	2.21	0.40
1:D:474:ALA:HB2	1:D:547:ALA:CB	2.51	0.40
1:B:20:ASP:O	1:B:21:PHE:HB2	2.22	0.40
1:D:484:LEU:HD13	1:D:531:LYS:O	2.22	0.40
1:B:322:THR:OG1	1:B:348:MSE:SE	2.90	0.40
1:B:39:ASP:O	1:B:43:LEU:HD22	2.22	0.40
1:C:72:ILE:CD1	1:C:87:LEU:HB2	2.52	0.40
1:B:187:ILE:HD12	1:B:246:LEU:O	2.21	0.40
1:A:349:ALA:HA	1:A:352:ASN:HB2	2.04	0.40
1:D:521:GLU:C	1:D:523:VAL:H	2.24	0.40
1:D:539:PHE:CZ	1:D:543:LEU:HD22	2.55	0.40

All (1) 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:C:2:LEU:O	1:D:113:GLN:NE2[4_555]	2.19	0.01

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	504/549 (92%)	404 (80%)	77 (15%)	23 (5%)	3 23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	505/549 (92%)	407 (81%)	73 (14%)	25 (5%)	3	21
1	C	504/549 (92%)	404 (80%)	76 (15%)	24 (5%)	3	22
1	D	505/549 (92%)	405 (80%)	77 (15%)	23 (5%)	3	23
2	E	4/8 (50%)	1 (25%)	2 (50%)	1 (25%)	0	0
2	F	3/8 (38%)	1 (33%)	1 (33%)	1 (33%)	0	0
2	G	3/8 (38%)	1 (33%)	0	2 (67%)	0	0
2	H	4/8 (50%)	1 (25%)	2 (50%)	1 (25%)	0	0
All	All	2032/2228 (91%)	1624 (80%)	308 (15%)	100 (5%)	3	22

All (100) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	327	SER
1	A	341	GLU
1	A	398	VAL
1	A	445	SER
1	A	486	GLU
2	E	751	ASN
1	B	109	GLN
1	B	127	GLN
1	B	284	THR
1	B	327	SER
1	B	341	GLU
1	B	398	VAL
1	B	445	SER
2	F	751	ASN
1	C	127	GLN
1	C	284	THR
1	C	327	SER
1	C	341	GLU
1	C	398	VAL
1	C	445	SER
2	G	751	ASN
1	D	35	ILE
1	D	127	GLN
1	D	284	THR
1	D	327	SER
1	D	341	GLU
1	D	398	VAL
1	D	445	SER

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Mol	Chain	Res	Type
2	H	750	PHE
1	A	112	ARG
1	A	244	ASN
1	A	396	ALA
1	A	465	LYS
1	A	522	THR
1	B	244	ASN
1	B	396	ALA
1	B	465	LYS
1	C	112	ARG
1	C	244	ASN
1	C	396	ALA
1	C	465	LYS
1	C	522	THR
2	G	752	PHE
1	D	104	VAL
1	D	244	ASN
1	D	396	ALA
1	D	465	LYS
1	D	522	THR
1	A	2	LEU
1	A	73	ASP
1	A	160	ARG
1	A	208	LEU
1	A	238	ALA
1	B	2	LEU
1	B	104	VAL
1	B	208	LEU
1	B	522	THR
1	C	2	LEU
1	C	73	ASP
1	C	208	LEU
1	C	238	ALA
1	D	160	ARG
1	D	208	LEU
1	D	238	ALA
1	A	284	THR
1	B	35	ILE
1	B	160	ARG
1	B	176	SER
1	C	160	ARG
1	C	485	LEU

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Mol	Chain	Res	Type
1	C	486	GLU
1	D	52	GLU
1	D	111	SER
1	A	484	LEU
1	A	485	LEU
1	B	257	THR
1	B	328	GLY
1	C	484	LEU
1	D	34	ASN
1	D	257	THR
1	B	102	ARG
1	B	134	GLU
1	B	354	LYS
1	C	108	PRO
1	C	358	ARG
1	D	102	ARG
1	D	358	ARG
1	B	106	ILE
1	B	311	VAL
1	D	311	VAL
1	A	70	PRO
1	A	108	PRO
1	A	328	GLY
1	B	70	PRO
1	C	70	PRO
1	C	311	VAL
1	A	311	VAL
1	C	35	ILE
1	A	35	ILE
1	D	328	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain 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 sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	462/483 (96%)	386 (84%)	76 (16%)	3 13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	464/483 (96%)	387 (83%)	77 (17%)	3	13
1	C	462/483 (96%)	375 (81%)	87 (19%)	2	10
1	D	464/483 (96%)	372 (80%)	92 (20%)	1	8
2	E	5/5 (100%)	3 (60%)	2 (40%)	0	0
2	F	5/5 (100%)	4 (80%)	1 (20%)	1	8
2	G	5/5 (100%)	4 (80%)	1 (20%)	1	8
2	H	6/5 (120%)	3 (50%)	3 (50%)	0	0
All	All	1873/1952 (96%)	1534 (82%)	339 (18%)	2	11

All (339) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	4	GLU
1	A	15	THR
1	A	17	LEU
1	A	46	LYS
1	A	52	GLU
1	A	67	GLU
1	A	68	LEU
1	A	77	TYR
1	A	95	ILE
1	A	113	GLN
1	A	115	LEU
1	A	126	LYS
1	A	128	MSE
1	A	130	CYS
1	A	131	TYR
1	A	148	CYS
1	A	155	LEU
1	A	157	LEU
1	A	174	SER
1	A	179	LEU
1	A	180	ILE
1	A	185	ASP
1	A	189	TRP
1	A	198	LYS
1	A	203	LEU
1	A	217	LEU
1	A	218	LEU

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Mol	Chain	Res	Type
1	A	220	PHE
1	A	223	VAL
1	A	227	THR
1	A	233	ARG
1	A	239	LEU
1	A	241	ASP
1	A	253	VAL
1	A	255	GLU
1	A	262	GLN
1	A	269	LEU
1	A	272	THR
1	A	277	ILE
1	A	283	GLN
1	A	284	THR
1	A	286	GLU
1	A	296	ASP
1	A	316	GLU
1	A	332	THR
1	A	334	MSE
1	A	336	PHE
1	A	337	PHE
1	A	355	LEU
1	A	363	VAL
1	A	364	GLU
1	A	369	TYR
1	A	374	LEU
1	A	381	CYS
1	A	387	ASP
1	A	399	MSE
1	A	404	ASP
1	A	405	ILE
1	A	408	LYS
1	A	409	LEU
1	A	410	TRP
1	A	437	LEU
1	A	444	LEU
1	A	449	MSE
1	A	451	VAL
1	A	452	LEU
1	A	457	ASP
1	A	459	ILE
1	A	460	ILE

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Mol	Chain	Res	Type
1	A	466	HIS
1	A	467	VAL
1	A	485	LEU
1	A	525	ARG
1	A	533	MSE
1	A	539	PHE
2	E	749	MSE
2	E	750	PHE
1	B	1	MSE
1	B	4	GLU
1	B	15	THR
1	B	17	LEU
1	B	41	SER
1	B	46	LYS
1	B	52	GLU
1	B	64	GLN
1	B	67	GLU
1	B	68	LEU
1	B	77	TYR
1	B	97	GLU
1	B	99	ASP
1	B	104	VAL
1	B	109	GLN
1	B	112	ARG
1	B	116	ASP
1	B	117	ARG
1	B	126	LYS
1	B	128	MSE
1	B	130	CYS
1	B	131	TYR
1	B	148	CYS
1	B	155	LEU
1	B	157	LEU
1	B	160	ARG
1	B	174	SER
1	B	179	LEU
1	B	180	ILE
1	B	185	ASP
1	B	189	TRP
1	B	198	LYS
1	B	203	LEU
1	B	217	LEU

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Mol	Chain	Res	Type
1	B	218	LEU
1	B	220	PHE
1	B	223	VAL
1	B	227	THR
1	B	233	ARG
1	B	239	LEU
1	B	241	ASP
1	B	253	VAL
1	B	255	GLU
1	B	262	GLN
1	B	269	LEU
1	B	272	THR
1	B	284	THR
1	B	296	ASP
1	B	316	GLU
1	B	329	ASN
1	B	332	THR
1	B	336	PHE
1	B	355	LEU
1	B	363	VAL
1	B	364	GLU
1	B	366	ILE
1	B	369	TYR
1	B	381	CYS
1	B	382	VAL
1	B	387	ASP
1	B	404	ASP
1	B	405	ILE
1	B	408	LYS
1	B	409	LEU
1	B	410	TRP
1	B	437	LEU
1	B	444	LEU
1	B	451	VAL
1	B	452	LEU
1	B	457	ASP
1	B	459	ILE
1	B	462	MSE
1	B	466	HIS
1	B	467	VAL
1	B	480	LEU
1	B	539	PHE

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Mol	Chain	Res	Type
1	B	540	TYR
2	F	750	PHE
1	C	1	MSE
1	C	11	SER
1	C	15	THR
1	C	17	LEU
1	C	43	LEU
1	C	45	SER
1	C	46	LYS
1	C	47	MSE
1	C	51	LEU
1	C	52	GLU
1	C	67	GLU
1	C	68	LEU
1	C	77	TYR
1	C	78	ASN
1	C	79	ASN
1	C	82	HIS
1	C	99	ASP
1	C	109	GLN
1	C	111	SER
1	C	113	GLN
1	C	115	LEU
1	C	117	ARG
1	C	126	LYS
1	C	131	TYR
1	C	139	ARG
1	C	148	CYS
1	C	155	LEU
1	C	157	LEU
1	C	167	VAL
1	C	174	SER
1	C	176	SER
1	C	179	LEU
1	C	180	ILE
1	C	185	ASP
1	C	189	TRP
1	C	198	LYS
1	C	203	LEU
1	C	217	LEU
1	C	218	LEU
1	C	220	PHE

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Mol	Chain	Res	Type
1	C	223	VAL
1	C	227	THR
1	C	233	ARG
1	C	237	ASN
1	C	239	LEU
1	C	241	ASP
1	C	253	VAL
1	C	255	GLU
1	C	269	LEU
1	C	284	THR
1	C	286	GLU
1	C	296	ASP
1	C	316	GLU
1	C	319	LEU
1	C	326	SER
1	C	332	THR
1	C	336	PHE
1	C	345	PHE
1	C	355	LEU
1	C	360	LEU
1	C	363	VAL
1	C	366	ILE
1	C	369	TYR
1	C	381	CYS
1	C	387	ASP
1	C	404	ASP
1	C	405	ILE
1	C	408	LYS
1	C	409	LEU
1	C	410	TRP
1	C	416	VAL
1	C	437	LEU
1	C	444	LEU
1	C	451	VAL
1	C	452	LEU
1	C	456	ILE
1	C	457	ASP
1	C	459	ILE
1	C	466	HIS
1	C	467	VAL
1	C	485	LEU
1	C	486	GLU

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Mol	Chain	Res	Type
1	C	524	ILE
1	C	525	ARG
1	C	533	MSE
1	C	539	PHE
1	C	543	LEU
2	G	753	MSE
1	D	1	MSE
1	D	2	LEU
1	D	3	CYS
1	D	12	THR
1	D	17	LEU
1	D	35	ILE
1	D	36	PHE
1	D	39	ASP
1	D	43	LEU
1	D	46	LYS
1	D	51	LEU
1	D	52	GLU
1	D	57	PHE
1	D	64	GLN
1	D	68	LEU
1	D	71	LEU
1	D	77	TYR
1	D	82	HIS
1	D	93	PHE
1	D	99	ASP
1	D	100	LEU
1	D	110	PHE
1	D	116	ASP
1	D	117	ARG
1	D	126	LYS
1	D	128	MSE
1	D	130	CYS
1	D	131	TYR
1	D	148	CYS
1	D	155	LEU
1	D	157	LEU
1	D	167	VAL
1	D	174	SER
1	D	176	SER
1	D	179	LEU
1	D	180	ILE

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Mol	Chain	Res	Type
1	D	185	ASP
1	D	189	TRP
1	D	198	LYS
1	D	203	LEU
1	D	212	LYS
1	D	217	LEU
1	D	218	LEU
1	D	220	PHE
1	D	223	VAL
1	D	224	GLU
1	D	227	THR
1	D	233	ARG
1	D	239	LEU
1	D	241	ASP
1	D	253	VAL
1	D	255	GLU
1	D	262	GLN
1	D	269	LEU
1	D	284	THR
1	D	286	GLU
1	D	296	ASP
1	D	316	GLU
1	D	319	LEU
1	D	332	THR
1	D	334	MSE
1	D	336	PHE
1	D	337	PHE
1	D	338	LYS
1	D	345	PHE
1	D	355	LEU
1	D	363	VAL
1	D	366	ILE
1	D	369	TYR
1	D	381	CYS
1	D	382	VAL
1	D	387	ASP
1	D	388	GLU
1	D	404	ASP
1	D	405	ILE
1	D	408	LYS
1	D	409	LEU
1	D	410	TRP

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Mol	Chain	Res	Type
1	D	439	LYS
1	D	444	LEU
1	D	451	VAL
1	D	452	LEU
1	D	457	ASP
1	D	459	ILE
1	D	466	HIS
1	D	467	VAL
1	D	482	GLN
1	D	491	ASN
1	D	525	ARG
1	D	538	LYS
1	D	539	PHE
1	D	540	TYR
2	H	750	PHE
2	H	751	ASN
2	H	753	MSE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	78	ASN
1	A	79	ASN
1	A	379	GLN
1	B	475	ASN
1	C	64	GLN
1	C	80	GLN
1	D	262	GLN
1	D	458	HIS
1	D	471	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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$
4	ATP	A	602	3	24,33,33	1.30	1 (4%)	31,52,52	2.26	11 (35%)
4	ATP	B	602	3	24,33,33	1.25	3 (12%)	31,52,52	2.43	8 (25%)
4	ATP	C	602	3	24,33,33	1.31	2 (8%)	31,52,52	2.00	4 (12%)
4	ATP	D	602	3	24,33,33	1.68	4 (16%)	31,52,52	2.40	10 (32%)

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
4	ATP	A	602	3	-	0/18/38/38	0/3/3/3
4	ATP	B	602	3	-	0/18/38/38	0/3/3/3
4	ATP	C	602	3	-	0/18/38/38	0/3/3/3
4	ATP	D	602	3	-	0/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	ATP	C5-N7	-2.39	1.31	1.39
4	C	602	ATP	C4-N3	2.07	1.38	1.35
4	B	602	ATP	O4'-C1'	2.15	1.43	1.41
4	D	602	ATP	C2-N3	2.60	1.36	1.32
4	D	602	ATP	O4'-C1'	3.27	1.45	1.41
4	D	602	ATP	C4-N3	3.40	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	602	ATP	C5-C4	3.76	1.49	1.40
4	A	602	ATP	C5-C4	3.86	1.49	1.40
4	C	602	ATP	C5-C4	4.48	1.50	1.40
4	D	602	ATP	C5-C4	5.22	1.52	1.40

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	602	ATP	N3-C2-N1	-8.85	122.12	128.89
4	C	602	ATP	N3-C2-N1	-8.60	122.31	128.89
4	A	602	ATP	N3-C2-N1	-7.67	123.02	128.89
4	B	602	ATP	N3-C2-N1	-5.89	124.38	128.89
4	B	602	ATP	C2'-C1'-N9	-5.35	106.11	114.29
4	A	602	ATP	PA-O3A-PB	-4.27	120.74	132.73
4	B	602	ATP	PA-O3A-PB	-3.49	122.94	132.73
4	D	602	ATP	C4-C5-N7	-3.37	106.38	109.48
4	A	602	ATP	C4-C5-N7	-3.19	106.55	109.48
4	D	602	ATP	O2'-C2'-C3'	-3.05	101.92	111.83
4	D	602	ATP	C2'-C3'-C4'	-2.90	96.66	102.61
4	A	602	ATP	O3A-PA-O5'	-2.56	96.13	102.94
4	A	602	ATP	PB-O3B-PG	-2.38	124.68	132.67
4	D	602	ATP	O5'-PA-O1A	-2.37	100.43	109.62
4	A	602	ATP	O5'-C5'-C4'	-2.35	100.47	109.12
4	A	602	ATP	C2'-C1'-N9	-2.15	111.00	114.29
4	A	602	ATP	O3G-PG-O1G	2.05	117.19	110.58
4	D	602	ATP	O3G-PG-O2G	2.07	115.24	107.38
4	C	602	ATP	O2A-PA-O3A	2.27	115.40	105.09
4	A	602	ATP	C2-N1-C6	2.29	122.87	118.77
4	D	602	ATP	C2-N1-C6	2.37	123.01	118.77
4	C	602	ATP	O2G-PG-O1G	2.48	118.55	110.58
4	C	602	ATP	C2-N1-C6	2.56	123.34	118.77
4	D	602	ATP	C1'-N9-C4	2.69	131.00	126.94
4	A	602	ATP	O2G-PG-O1G	2.73	119.38	110.58
4	B	602	ATP	C2-N1-C6	2.89	123.93	118.77
4	A	602	ATP	C4'-O4'-C1'	3.07	113.10	109.72
4	D	602	ATP	O2A-PA-O3A	3.13	119.28	105.09
4	B	602	ATP	O4'-C1'-N9	3.98	116.44	108.10
4	B	602	ATP	O2G-PG-O1G	3.99	123.41	110.58
4	B	602	ATP	C1'-N9-C4	4.41	133.59	126.94
4	D	602	ATP	O4'-C1'-N9	4.43	117.37	108.10
4	B	602	ATP	N6-C6-N1	5.21	130.38	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	ATP	4	0
4	B	602	ATP	5	0
4	C	602	ATP	1	0
4	D	602	ATP	1	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	493/549 (89%)	0.28	20 (4%) 41 27	45, 102, 177, 252	0
1	B	494/549 (89%)	0.53	48 (9%) 10 6	48, 98, 237, 286	0
1	C	493/549 (89%)	0.37	37 (7%) 17 9	62, 111, 177, 275	0
1	D	494/549 (89%)	0.67	65 (13%) 4 3	53, 111, 245, 281	0
2	E	4/8 (50%)	0.41	0 100 100	81, 86, 86, 95	0
2	F	3/8 (37%)	0.33	0 100 100	74, 74, 78, 89	0
2	G	3/8 (37%)	0.57	0 100 100	91, 91, 106, 110	0
2	H	4/8 (50%)	0.89	1 (25%) 1 1	92, 108, 116, 126	0
All	All	1988/2228 (89%)	0.46	171 (8%) 13 7	45, 106, 214, 286	0

All (171) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	61	TYR	9.5
1	B	68	LEU	9.4
1	D	69	GLY	8.9
1	D	68	LEU	7.8
1	B	72	ILE	7.7
1	B	106	ILE	7.6
1	B	105	VAL	7.1
1	B	69	GLY	6.9
1	D	67	GLU	6.1
1	D	72	ILE	6.0
1	C	105	VAL	5.8
1	B	61	TYR	5.7
1	D	101	LEU	5.7
1	C	66	SER	5.5
1	D	70	PRO	5.4
1	C	27	LEU	5.3

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Mol	Chain	Res	Type	RSRZ
1	D	106	ILE	5.1
1	D	310	PRO	4.7
1	B	489	ASN	4.6
1	B	75	PHE	4.5
1	B	101	LEU	4.5
1	D	491	ASN	4.4
1	A	314	LYS	4.3
1	A	105	VAL	4.3
1	B	77	TYR	4.2
1	D	105	VAL	4.0
1	B	95	ILE	4.0
1	D	89	ASP	3.9
1	B	67	GLU	3.9
1	D	523	VAL	3.9
1	D	489	ASN	3.8
1	D	85	ASP	3.8
1	D	410	TRP	3.8
1	B	70	PRO	3.8
1	A	539	PHE	3.8
1	D	65	ALA	3.8
1	B	78	ASN	3.8
1	B	84	ALA	3.8
1	A	66	SER	3.7
1	D	521	GLU	3.7
1	D	522	THR	3.7
1	C	314	LYS	3.6
1	D	341	GLU	3.6
1	B	103	PRO	3.6
1	C	345	PHE	3.6
1	D	178	GLN	3.6
1	B	528	ASP	3.5
1	B	451	VAL	3.5
1	D	524	ILE	3.5
1	A	45	SER	3.4
1	D	25	ASP	3.4
1	D	6	GLU	3.4
1	D	37	THR	3.4
1	A	27	LEU	3.4
1	B	488	GLY	3.4
1	B	56	ASN	3.3
1	D	347	LYS	3.3
1	D	51	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	70	PRO	3.3
1	D	96	ASN	3.2
1	D	225	HIS	3.2
1	B	310	PRO	3.2
1	D	76	ASN	3.2
1	D	33	LYS	3.2
1	C	28	THR	3.1
1	D	175	LYS	3.1
1	D	84	ALA	3.1
1	B	98	PRO	3.1
1	D	71	LEU	3.1
1	D	34	ASN	3.1
1	D	222	SER	3.0
1	C	16	ARG	3.0
1	B	225	HIS	3.0
1	B	85	ASP	3.0
1	B	80	GLN	3.0
1	C	528	ASP	3.0
1	B	51	LEU	3.0
1	B	71	LEU	3.0
1	B	487	ILE	3.0
1	B	89	ASP	2.9
1	B	524	ILE	2.9
1	B	523	VAL	2.9
1	D	79	ASN	2.9
1	A	452	LEU	2.9
1	C	522	THR	2.9
1	C	398	VAL	2.9
1	D	179	LEU	2.9
1	B	6	GLU	2.9
1	B	521	GLU	2.9
1	D	90	TYR	2.9
1	B	491	ASN	2.9
1	A	64	GLN	2.9
1	A	110	PHE	2.9
1	D	488	GLY	2.9
1	B	44	ILE	2.8
1	D	100	LEU	2.8
1	B	79	ASN	2.8
1	C	303	GLU	2.8
1	D	490	ASN	2.8
1	D	95	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	H	748	PRO	2.8
1	A	32	GLY	2.8
1	D	224	GLU	2.8
1	D	487	ILE	2.7
1	B	88	GLU	2.7
1	C	26	ALA	2.7
1	B	311	VAL	2.7
1	C	110	PHE	2.7
1	C	20	ASP	2.7
1	A	19	HIS	2.6
1	C	174	SER	2.6
1	C	45	SER	2.6
1	C	108	PRO	2.6
1	D	486	GLU	2.6
1	B	90	TYR	2.6
1	A	313	GLU	2.5
1	C	32	GLY	2.5
1	D	145	ASP	2.5
1	B	96	ASN	2.5
1	C	175	LYS	2.5
1	C	293	LEU	2.5
1	D	60	ILE	2.5
1	D	153	PHE	2.4
1	C	106	ILE	2.4
1	C	109	GLN	2.4
1	D	44	ILE	2.4
1	D	107	ALA	2.4
1	B	116	ASP	2.4
1	A	89	ASP	2.3
1	B	299	TYR	2.3
1	D	104	VAL	2.3
1	D	57	PHE	2.3
1	D	223	VAL	2.3
1	B	57	PHE	2.3
1	B	525	ARG	2.3
1	B	100	LEU	2.3
1	D	181	GLY	2.2
1	D	527	GLU	2.2
1	D	525	ARG	2.2
1	C	107	ALA	2.2
1	C	447	LYS	2.2
1	C	532	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	521	GLU	2.2
1	C	283	GLN	2.2
1	D	176	SER	2.2
1	C	410	TRP	2.2
1	A	454	PHE	2.2
1	C	33	LYS	2.2
1	C	471	GLN	2.2
1	A	284	THR	2.2
1	C	539	PHE	2.1
1	A	102	ARG	2.1
1	A	107	ALA	2.1
1	A	109	GLN	2.1
1	D	451	VAL	2.1
1	C	92	ASP	2.1
1	C	484	LEU	2.1
1	C	284	THR	2.1
1	C	535	LEU	2.1
1	B	29	TYR	2.1
1	A	528	ASP	2.1
1	B	15	THR	2.1
1	C	46	LYS	2.1
1	D	152	SER	2.0
1	D	32	GLY	2.0
1	D	13	ALA	2.0
1	D	301	PHE	2.0
1	B	107	ALA	2.0
1	D	412	CYS	2.0
1	D	173	LEU	2.0
1	C	34	ASN	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(Å ²)	Q<0.9
3	MG	A	601	1/1	0.92	0.30	2.82	41,41,41,41	0
3	MG	D	601	1/1	0.86	0.31	2.40	62,62,62,62	0
4	ATP	C	602	31/31	0.89	0.25	0.16	58,73,92,93	0
4	ATP	B	602	31/31	0.90	0.23	0.00	53,65,76,82	0
4	ATP	A	602	31/31	0.93	0.21	-0.21	53,63,80,84	0
4	ATP	D	602	31/31	0.89	0.22	-0.33	55,73,87,88	0
3	MG	B	601	1/1	0.90	0.34	-	51,51,51,51	0
3	MG	C	601	1/1	0.91	0.51	-	62,62,62,62	0

6.5 Other polymers [i](#)

There are no such residues in this entry.