



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 22, 2016 – 04:50 AM EDT

PDB ID : 5HZG
Title : The crystal structure of the strigolactone-induced AtD14-D3-ASK1 complex
Authors : Yao, R.F.; Ming, Z.H.; Yan, L.M.; Rao, Z.H.; Lou, Z.Y.; Xie, D.X.
Deposited on : 2016-02-02
Resolution : 3.30 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 : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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) : rb-20027939

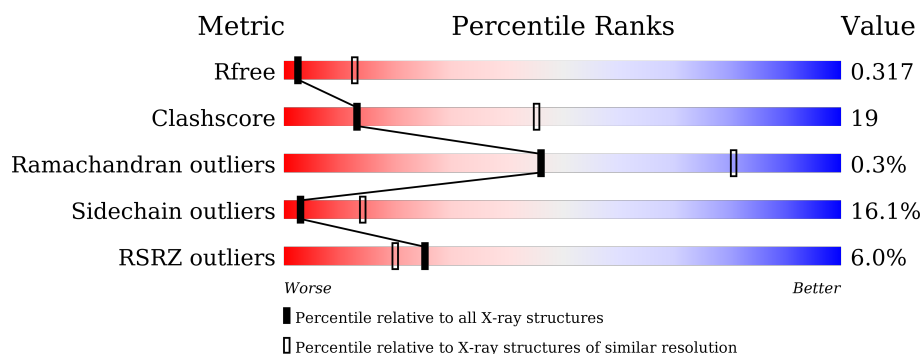
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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	267	<div> <div>0%</div> <div> <div>66%</div> <div>25%</div> <div>• •</div> </div> </div>
1	E	267	<div> <div>3%</div> <div> <div>70%</div> <div>22%</div> <div>5%</div> <div>•</div> </div> </div>
2	B	740	<div> <div>2%</div> <div> <div>50%</div> <div>24%</div> <div>8%</div> <div>•</div> <div>17%</div> </div> </div>
2	F	740	<div> <div>3%</div> <div> <div>49%</div> <div>24%</div> <div>9%</div> <div>•</div> <div>17%</div> </div> </div>
3	C	169	<div> <div>27%</div> <div> <div>56%</div> <div>17%</div> <div>• •</div> <div>23%</div> </div> </div>
3	G	169	<div> <div>19%</div> <div> <div>59%</div> <div>18%</div> <div>•</div> <div>22%</div> </div> </div>

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
4	6OM	A	301	-	X	X	X
4	6OM	E	301	-	X	X	X

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 15676 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 Strigolactone esterase D14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	257	Total	C	N	O	S	0	0	0
			2001	1285	341	369	6			
1	E	257	Total	C	N	O	S	0	0	0
			2001	1285	341	369	6			

- Molecule 2 is a protein called F-box/LRR-repeat MAX2 homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	615	Total	C	N	O	S	0	0	0
			4791	3055	842	862	32			
2	F	614	Total	C	N	O	S	0	0	0
			4782	3048	840	862	32			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-19	GLY	-	expression tag	UNP Q5VMP0
B	-18	ALA	-	expression tag	UNP Q5VMP0
B	-17	MET	-	expression tag	UNP Q5VMP0
B	-16	GLY	-	expression tag	UNP Q5VMP0
B	-15	SER	-	expression tag	UNP Q5VMP0
B	-14	GLY	-	expression tag	UNP Q5VMP0
B	-13	ILE	-	expression tag	UNP Q5VMP0
B	-12	GLN	-	expression tag	UNP Q5VMP0
B	-11	ARG	-	expression tag	UNP Q5VMP0
B	-10	PRO	-	expression tag	UNP Q5VMP0
B	-9	THR	-	expression tag	UNP Q5VMP0
B	-8	SER	-	expression tag	UNP Q5VMP0
B	-7	THR	-	expression tag	UNP Q5VMP0
B	-6	SER	-	expression tag	UNP Q5VMP0
B	-5	SER	-	expression tag	UNP Q5VMP0
B	-4	LEU	-	expression tag	UNP Q5VMP0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	VAL	-	expression tag	UNP Q5VMP0
B	-2	ALA	-	expression tag	UNP Q5VMP0
B	-1	ALA	-	expression tag	UNP Q5VMP0
B	0	ALA	-	expression tag	UNP Q5VMP0
F	-19	GLY	-	expression tag	UNP Q5VMP0
F	-18	ALA	-	expression tag	UNP Q5VMP0
F	-17	MET	-	expression tag	UNP Q5VMP0
F	-16	GLY	-	expression tag	UNP Q5VMP0
F	-15	SER	-	expression tag	UNP Q5VMP0
F	-14	GLY	-	expression tag	UNP Q5VMP0
F	-13	ILE	-	expression tag	UNP Q5VMP0
F	-12	GLN	-	expression tag	UNP Q5VMP0
F	-11	ARG	-	expression tag	UNP Q5VMP0
F	-10	PRO	-	expression tag	UNP Q5VMP0
F	-9	THR	-	expression tag	UNP Q5VMP0
F	-8	SER	-	expression tag	UNP Q5VMP0
F	-7	THR	-	expression tag	UNP Q5VMP0
F	-6	SER	-	expression tag	UNP Q5VMP0
F	-5	SER	-	expression tag	UNP Q5VMP0
F	-4	LEU	-	expression tag	UNP Q5VMP0
F	-3	VAL	-	expression tag	UNP Q5VMP0
F	-2	ALA	-	expression tag	UNP Q5VMP0
F	-1	ALA	-	expression tag	UNP Q5VMP0
F	0	ALA	-	expression tag	UNP Q5VMP0

- Molecule 3 is a protein called SKP1-like protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	130	Total	C	N	O	S	0	0	0
			1024	645	168	207	4			
3	G	132	Total	C	N	O	S	0	0	0
			1039	655	170	210	4			

There are 18 discrepancies between the modelled and reference sequences:

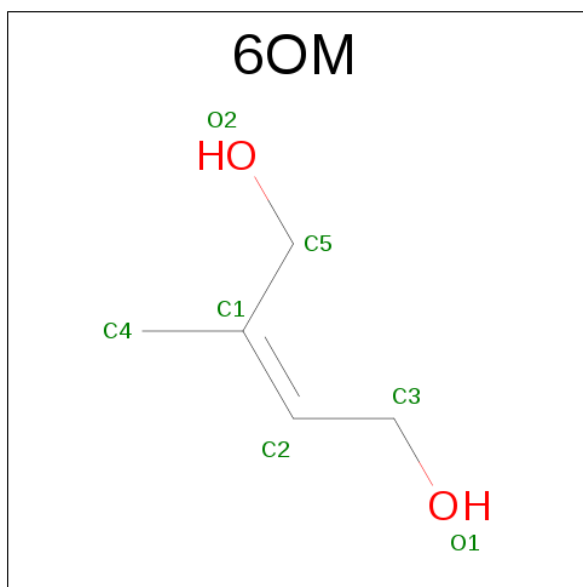
Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	MET	-	expression tag	UNP Q39255
C	-7	ASP	-	expression tag	UNP Q39255
C	-6	TYR	-	expression tag	UNP Q39255
C	-5	LYS	-	expression tag	UNP Q39255
C	-4	ASP	-	expression tag	UNP Q39255
C	-3	ASP	-	expression tag	UNP Q39255

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	ASP	-	expression tag	UNP Q39255
C	-1	ASP	-	expression tag	UNP Q39255
C	0	LYS	-	expression tag	UNP Q39255
G	-8	MET	-	expression tag	UNP Q39255
G	-7	ASP	-	expression tag	UNP Q39255
G	-6	TYR	-	expression tag	UNP Q39255
G	-5	LYS	-	expression tag	UNP Q39255
G	-4	ASP	-	expression tag	UNP Q39255
G	-3	ASP	-	expression tag	UNP Q39255
G	-2	ASP	-	expression tag	UNP Q39255
G	-1	ASP	-	expression tag	UNP Q39255
G	0	LYS	-	expression tag	UNP Q39255

- Molecule 4 is (2Z)-2-methylbut-2-ene-1,4-diol (three-letter code: 6OM) (formula: C₅H₁₀O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 5 2	0	0
4	E	1	Total C O 7 5 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0

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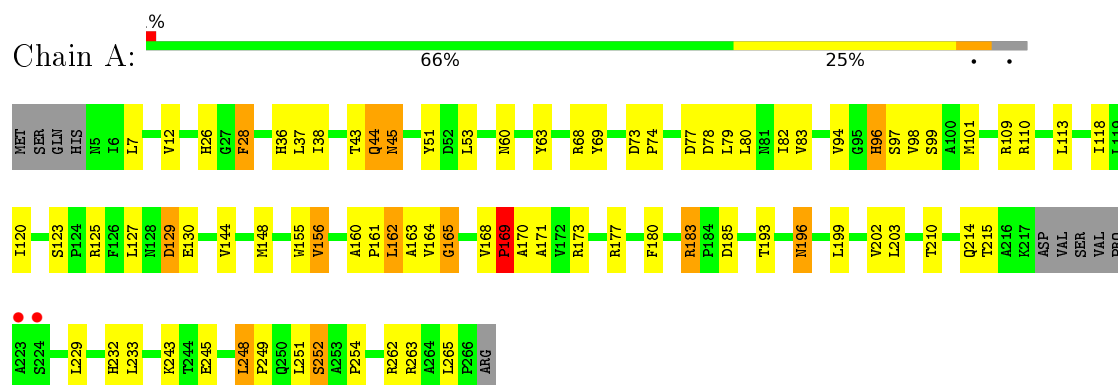
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total 5	O 5	0	0
5	E	2	Total 2	O 2	0	0
5	F	10	Total 10	O 10	0	0
5	G	4	Total 4	O 4	0	0

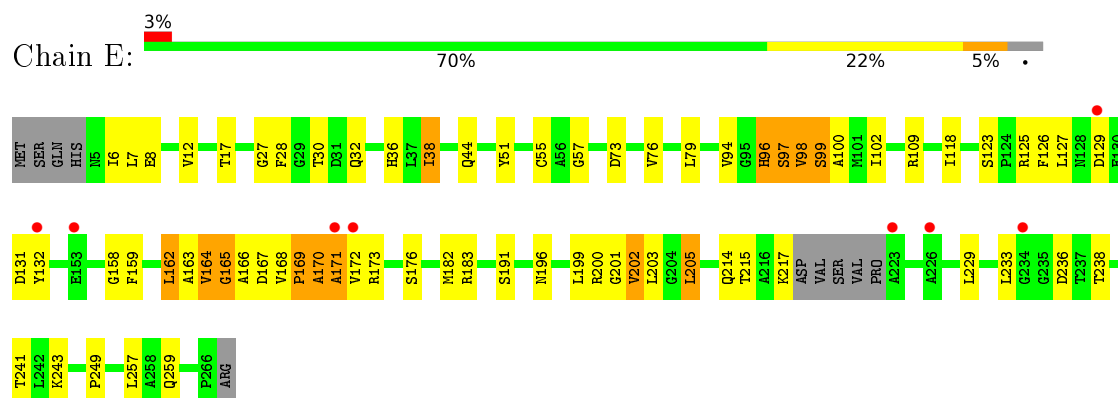
3 Residue-property plots

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.

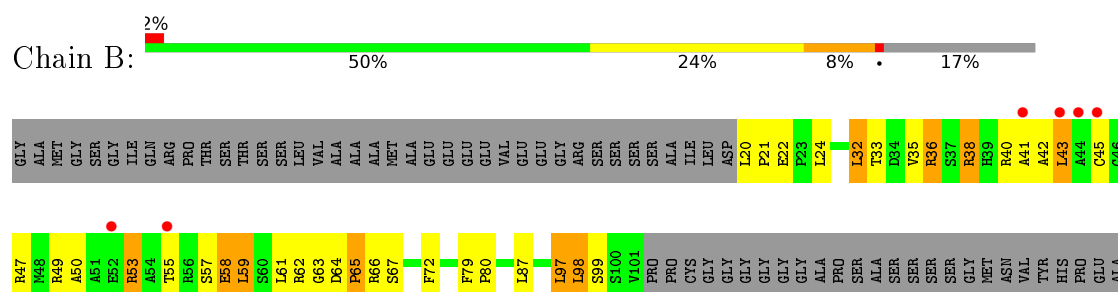
• Molecule 1: Strigolactone esterase D14

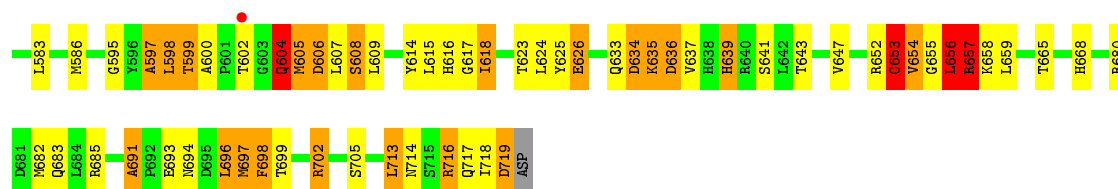


• Molecule 1: Strigolactone esterase D14

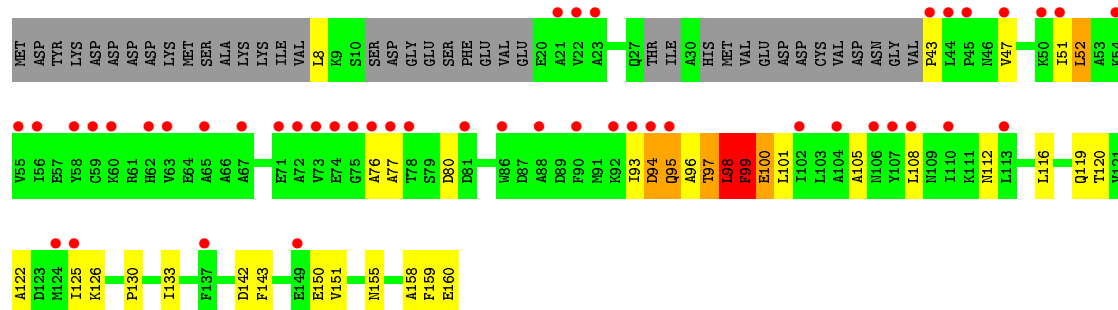


• Molecule 2: F-box/LRR-repeat MAX2 homolog

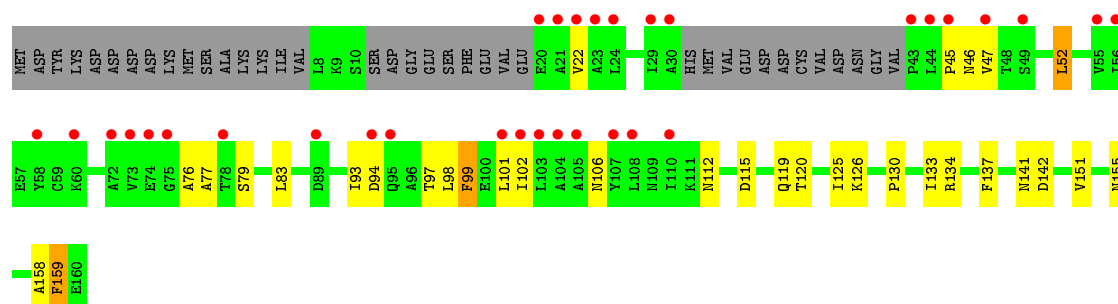




• Molecule 3: SKP1-like protein 1A



• Molecule 3: SKP1-like protein 1A



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.40Å 172.98Å 186.84Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.07 – 3.30 49.07 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.07-3.30) 99.5 (49.07-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.35 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0123	Depositor
R, R_{free}	0.246 , 0.316 0.256 , 0.317	Depositor DCC
R_{free} test set	2669 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 60.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	15676	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: 6OM

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	0.56	0/2046	1.05	8/2785 (0.3%)
1	E	0.56	0/2046	1.17	22/2785 (0.8%)
2	B	0.64	2/4904 (0.0%)	1.27	53/6669 (0.8%)
2	F	0.63	3/4892 (0.1%)	1.31	72/6650 (1.1%)
3	C	0.52	0/1036	0.99	8/1397 (0.6%)
3	G	0.53	0/1052	0.85	6/1421 (0.4%)
All	All	0.60	5/15976 (0.0%)	1.20	169/21707 (0.8%)

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	2
1	E	0	1
2	B	0	9
2	F	0	15
3	G	0	1
All	All	0	28

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	435	PRO	N-CD	13.99	1.67	1.47
2	B	186	PRO	N-CD	6.95	1.57	1.47
2	F	435	PRO	N-CD	6.95	1.57	1.47
2	F	568	PRO	N-CD	6.09	1.56	1.47
2	F	186	PRO	N-CD	5.12	1.55	1.47

All (169) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	597	ALA	CB-CA-C	-24.47	73.39	110.10
1	A	170	ALA	CB-CA-C	22.46	143.79	110.10
2	B	692	PRO	N-CA-CB	-18.29	81.35	103.30
2	F	656	LEU	CB-CA-C	-17.40	77.14	110.20
2	F	42	ALA	N-CA-C	16.11	154.50	111.00
2	F	42	ALA	C-N-CA	15.57	160.62	121.70
2	B	545	SER	N-CA-CB	15.41	133.61	110.50
2	B	692	PRO	N-CA-C	15.29	151.86	112.10
2	B	694	ASN	N-CA-C	14.99	151.48	111.00
1	E	170	ALA	N-CA-CB	-14.36	90.00	110.10
2	F	42	ALA	N-CA-CB	-14.01	90.49	110.10
2	B	693	GLU	CB-CA-C	-13.67	83.06	110.40
2	B	692	PRO	N-CD-CG	-13.19	83.42	103.20
2	B	694	ASN	N-CA-CB	-13.16	86.91	110.60
1	E	201	GLY	N-CA-C	13.11	145.88	113.10
2	B	371	SER	CB-CA-C	-12.92	85.55	110.10
2	F	47	ARG	N-CA-CB	-12.68	87.78	110.60
1	E	163	ALA	N-CA-CB	-12.60	92.46	110.10
2	F	402	ALA	N-CA-C	12.44	144.60	111.00
3	C	95	GLN	N-CA-C	12.44	144.59	111.00
1	E	169	PRO	CB-CA-C	-12.40	81.00	112.00
2	F	96	PRO	N-CA-C	12.39	144.30	112.10
2	B	405	ARG	CB-CA-C	12.37	135.14	110.40
2	F	657	ARG	N-CA-CB	-12.33	88.40	110.60
2	B	421	VAL	CB-CA-C	-12.14	88.33	111.40
2	B	238	ALA	N-CA-CB	11.68	126.44	110.10
2	B	544	ASP	CB-CA-C	-11.55	87.29	110.40
2	B	65	PRO	N-CA-C	11.26	141.38	112.10
3	C	94	ASP	N-CA-C	-11.11	80.99	111.00
1	A	169	PRO	CB-CA-C	-10.77	85.07	112.00
2	F	43	LEU	CB-CA-C	-10.61	90.04	110.20
2	B	691	ALA	CB-CA-C	-10.47	94.40	110.10
2	B	66	ARG	N-CA-CB	10.40	129.32	110.60
2	B	421	VAL	N-CA-C	10.40	139.08	111.00
2	B	372	TRP	N-CA-C	10.33	138.88	111.00
2	B	372	TRP	N-CA-CB	-10.30	92.06	110.60
1	E	159	PHE	N-CA-CB	10.14	128.85	110.60
2	B	544	ASP	N-CA-C	9.68	137.14	111.00
2	B	540	SER	N-CA-CB	9.61	124.91	110.50
1	A	170	ALA	N-CA-CB	9.35	123.19	110.10
1	E	171	ALA	N-CA-CB	-9.32	97.05	110.10
2	B	691	ALA	C-N-CD	-9.24	100.27	120.60
2	F	389	MET	N-CA-CB	-9.02	94.36	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	187	ASP	N-CA-C	9.02	135.35	111.00
2	F	187	ASP	CB-CA-C	-8.97	92.46	110.40
3	G	45	PRO	N-CA-C	8.97	135.42	112.10
1	E	163	ALA	N-CA-C	8.86	134.92	111.00
2	F	274	ASP	N-CA-C	-8.86	87.08	111.00
1	E	162	LEU	N-CA-C	8.80	134.77	111.00
2	F	604	GLN	CB-CA-C	-8.75	92.89	110.40
1	E	171	ALA	N-CA-C	-8.74	87.41	111.00
2	B	434	ARG	C-N-CD	-8.72	101.41	120.60
2	F	442	VAL	N-CA-C	-8.71	87.47	111.00
2	F	97	LEU	N-CA-CB	8.58	127.56	110.40
2	F	41	ALA	CB-CA-C	-8.56	97.26	110.10
2	F	653	CYS	N-CA-C	-8.54	87.95	111.00
1	E	96	HIS	CB-CA-C	8.45	127.30	110.40
1	A	170	ALA	N-CA-C	-8.44	88.21	111.00
2	B	389	MET	CB-CA-C	8.37	127.14	110.40
2	F	35	VAL	CB-CA-C	-8.35	95.53	111.40
2	B	237	LEU	CB-CA-C	-8.31	94.40	110.20
2	F	43	LEU	N-CA-C	-7.78	89.99	111.00
2	B	405	ARG	N-CA-C	-7.77	90.01	111.00
1	E	176	SER	CB-CA-C	-7.73	95.42	110.10
1	E	158	GLY	N-CA-C	-7.70	93.86	113.10
2	B	407	CYS	N-CA-C	-7.69	90.24	111.00
2	F	188	GLY	N-CA-C	-7.52	94.29	113.10
2	B	435	PRO	CA-N-CD	-7.48	101.03	111.50
3	G	46	ASN	N-CA-C	7.47	131.18	111.00
3	C	126	LYS	N-CA-CB	-7.44	97.20	110.60
2	F	328	LEU	CA-CB-CG	7.41	132.35	115.30
2	F	403	ILE	N-CA-C	-7.28	91.34	111.00
2	F	600	ALA	N-CA-CB	-7.06	100.22	110.10
2	B	434	ARG	N-CA-C	7.03	129.99	111.00
2	F	238	ALA	N-CA-C	-7.01	92.08	111.00
2	F	65	PRO	CB-CA-C	-6.81	94.97	112.00
2	F	433	LEU	CB-CA-C	-6.79	97.30	110.20
1	E	164	VAL	N-CA-C	6.78	129.30	111.00
1	A	171	ALA	N-CA-C	-6.72	92.86	111.00
1	E	97	SER	CB-CA-C	-6.69	97.38	110.10
2	B	186	PRO	CA-N-CD	-6.69	102.14	111.50
2	B	691	ALA	N-CA-C	6.67	129.00	111.00
2	F	434	ARG	N-CA-C	6.59	128.80	111.00
2	F	363	SER	N-CA-CB	6.51	120.26	110.50
3	G	46	ASN	N-CA-CB	-6.51	98.89	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	40	ARG	CB-CA-C	-6.50	97.39	110.40
2	F	33	THR	CB-CA-C	-6.49	94.09	111.60
1	A	165	GLY	N-CA-C	-6.47	96.92	113.10
1	E	170	ALA	CB-CA-C	6.47	119.80	110.10
1	E	97	SER	N-CA-C	6.47	128.46	111.00
2	F	537	PRO	CB-CA-C	-6.46	95.85	112.00
2	F	539	ILE	N-CA-C	6.45	128.41	111.00
2	B	388	TYR	N-CA-CB	6.39	122.10	110.60
1	E	164	VAL	N-CA-CB	-6.39	97.44	111.50
1	E	165	GLY	N-CA-C	-6.38	97.15	113.10
2	F	447	LEU	CA-CB-CG	-6.30	100.81	115.30
2	F	653	CYS	CB-CA-C	6.29	122.97	110.40
2	F	657	ARG	C-N-CA	-6.27	106.03	121.70
1	E	166	ALA	CB-CA-C	6.25	119.47	110.10
2	B	434	ARG	N-CA-CB	-6.23	99.39	110.60
2	F	567	ALA	CB-CA-C	6.23	119.44	110.10
2	F	458	SER	N-CA-CB	-6.19	101.21	110.50
2	F	454	LEU	CB-CG-CD1	6.18	121.52	111.00
3	G	22	VAL	CB-CA-C	6.16	123.09	111.40
2	F	434	ARG	N-CA-CB	-6.14	99.55	110.60
2	B	371	SER	N-CA-C	6.13	127.56	111.00
2	F	654	VAL	N-CA-C	-6.13	94.45	111.00
2	B	458	SER	N-CA-CB	-6.11	101.34	110.50
2	B	389	MET	N-CA-C	-6.08	94.57	111.00
2	B	458	SER	N-CA-C	6.04	127.30	111.00
2	F	311	ALA	CB-CA-C	-5.99	101.12	110.10
2	F	598	LEU	N-CA-C	5.98	127.14	111.00
2	B	63	GLY	N-CA-C	-5.96	98.21	113.10
2	B	65	PRO	CB-CA-C	-5.88	97.30	112.00
2	F	43	LEU	CA-CB-CG	5.88	128.82	115.30
2	F	81	ALA	CB-CA-C	-5.86	101.31	110.10
2	B	386	SER	N-CA-C	-5.83	95.25	111.00
3	C	126	LYS	N-CA-C	5.79	126.62	111.00
2	F	43	LEU	N-CA-CB	5.77	121.94	110.40
2	F	312	ALA	N-CA-CB	-5.77	102.03	110.10
2	F	605	MET	N-CA-CB	-5.76	100.23	110.60
2	F	599	THR	N-CA-C	5.75	126.53	111.00
2	B	559	ASP	N-CA-C	5.73	126.48	111.00
2	B	64	ASP	N-CA-CB	5.73	120.91	110.60
2	B	390	LYS	N-CA-CB	5.70	120.85	110.60
2	F	521	MET	N-CA-CB	-5.66	100.42	110.60
2	B	408	ARG	N-CA-C	-5.63	95.81	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	433	LEU	N-CA-C	5.62	126.19	111.00
1	A	156	VAL	N-CA-C	-5.61	95.84	111.00
1	E	98	VAL	CB-CA-C	-5.60	100.76	111.40
2	B	387	LEU	CB-CA-C	-5.60	99.56	110.20
2	F	35	VAL	N-CA-C	5.59	126.09	111.00
2	F	388	TYR	CB-CA-C	-5.59	99.22	110.40
2	F	458	SER	N-CA-C	5.58	126.08	111.00
2	B	422	THR	N-CA-C	-5.47	96.22	111.00
2	B	561	ARG	NE-CZ-NH1	5.46	123.03	120.30
2	B	464	ILE	CB-CA-C	-5.40	100.80	111.60
2	F	521	MET	N-CA-C	5.39	125.56	111.00
2	B	66	ARG	N-CA-C	-5.38	96.47	111.00
2	F	276	VAL	N-CA-C	-5.38	96.48	111.00
2	F	442	VAL	CB-CA-C	5.36	121.59	111.40
3	C	95	GLN	N-CA-CB	-5.36	100.95	110.60
2	F	386	SER	N-CA-C	-5.36	96.53	111.00
2	B	186	PRO	N-CA-C	5.33	125.95	112.10
2	F	362	GLY	N-CA-C	5.29	126.33	113.10
2	F	82	LEU	N-CA-C	-5.29	96.73	111.00
2	B	433	LEU	CB-CA-C	-5.28	100.17	110.20
2	F	39	HIS	CB-CA-C	-5.27	99.86	110.40
3	C	100	GLU	CB-CA-C	-5.22	99.96	110.40
2	F	275	CYS	CB-CA-C	-5.21	99.97	110.40
2	B	391	ASN	N-CA-CB	-5.21	101.22	110.60
2	F	276	VAL	CB-CA-C	5.21	121.30	111.40
3	G	94	ASP	CB-CG-OD2	5.21	122.99	118.30
2	F	636	ASP	N-CA-C	5.20	125.04	111.00
3	C	94	ASP	CB-CG-OD2	5.17	122.96	118.30
2	F	702	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	E	202	VAL	N-CA-C	-5.15	97.10	111.00
2	F	402	ALA	CB-CA-C	-5.13	102.40	110.10
2	F	519	TRP	N-CA-C	-5.13	97.14	111.00
2	B	61	LEU	CA-CB-CG	5.12	127.08	115.30
1	E	98	VAL	O-C-N	5.11	130.87	122.70
2	F	617	GLY	N-CA-C	5.09	125.84	113.10
3	C	98	LEU	N-CA-C	5.08	124.73	111.00
2	F	538	LEU	N-CA-CB	5.08	120.56	110.40
2	F	634	ASP	N-CA-C	-5.06	97.34	111.00
2	B	458	SER	C-N-CD	5.03	138.97	128.40
2	F	388	TYR	N-CA-C	5.03	124.58	111.00
1	A	263	ARG	NE-CZ-NH2	-5.01	117.80	120.30
3	G	99	PHE	CB-CG-CD1	5.00	124.30	120.80

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	155	TRP	Peptide
1	A	96	HIS	Peptide
2	B	186	PRO	Peptide
2	B	241	THR	Peptide
2	B	400	LEU	Peptide
2	B	431	PHE	Peptide
2	B	439	GLU	Peptide
2	B	451	ALA	Peptide
2	B	453	CYS	Peptide
2	B	544	ASP	Peptide
2	B	636	ASP	Peptide
1	E	200	ARG	Peptide
2	F	180	GLN	Peptide
2	F	241	THR	Peptide
2	F	339	VAL	Peptide
2	F	374	HIS	Peptide
2	F	377	GLY	Peptide
2	F	41	ALA	Peptide
2	F	42	ALA	Peptide
2	F	422	THR	Peptide
2	F	431	PHE	Peptide
2	F	439	GLU	Peptide
2	F	452	GLU	Peptide
2	F	538	LEU	Peptide
2	F	541	ALA	Peptide
2	F	543	LEU	Peptide
2	F	691	ALA	Peptide
3	G	98	LEU	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	2001	0	1972	45	0
1	E	2001	0	1972	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4791	0	4814	226	0
2	F	4782	0	4808	218	0
3	C	1024	0	1011	75	0
3	G	1039	0	1030	33	0
4	A	7	0	0	4	0
4	E	7	0	0	5	0
5	A	3	0	0	0	0
5	B	5	0	0	2	0
5	E	2	0	0	0	0
5	F	10	0	0	0	0
5	G	4	0	0	0	0
All	All	15676	0	15607	595	0

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 19.

All (595) 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)
2:F:92:PRO:HB2	2:F:95:HIS:CD2	1.26	1.61
2:B:389:MET:CE	2:B:392:CYS:HB2	1.32	1.59
1:E:170:ALA:CB	1:E:172:VAL:HB	1.36	1.52
2:B:389:MET:HE1	2:B:392:CYS:CA	1.36	1.52
2:B:389:MET:CE	2:B:392:CYS:CB	1.88	1.52
2:B:20:LEU:HD12	3:C:99:PHE:CE2	1.42	1.51
2:B:389:MET:HE1	2:B:392:CYS:N	1.24	1.46
2:B:270:PRO:CG	2:B:311:ALA:HB1	1.47	1.44
2:B:389:MET:CE	2:B:392:CYS:N	1.77	1.44
2:B:653:CYS:O	2:B:656:LEU:CD1	1.66	1.40
3:C:97:THR:CG2	3:C:100:GLU:H	1.36	1.36
1:E:170:ALA:HB3	1:E:172:VAL:CB	1.54	1.35
2:B:394:ASP:O	2:B:422:THR:HG21	1.23	1.35
2:B:389:MET:HE2	2:B:392:CYS:CB	1.46	1.33
2:B:20:LEU:CD1	3:C:99:PHE:HE2	1.42	1.32
2:B:36:ARG:NH2	2:B:657:ARG:NH1	1.77	1.28
1:E:170:ALA:HB1	1:E:172:VAL:CG2	1.62	1.28
2:B:653:CYS:CB	2:B:656:LEU:HD11	1.65	1.26
1:E:170:ALA:CB	1:E:172:VAL:CB	2.12	1.25
2:F:92:PRO:CB	2:F:95:HIS:CD2	2.17	1.25
2:B:433:LEU:O	2:B:433:LEU:HD23	1.35	1.22
2:B:389:MET:SD	2:B:392:CYS:HB2	1.78	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:49:ARG:HH12	3:G:125:ILE:HD13	1.04	1.18
2:F:43:LEU:HD22	3:G:155:ASN:OD1	1.39	1.18
2:B:653:CYS:O	2:B:656:LEU:HD12	1.45	1.15
1:A:28:PHE:HB2	4:A:301:6OM:C4	1.79	1.13
2:B:21:PRO:HD3	3:C:99:PHE:CE1	1.83	1.12
3:C:97:THR:CG2	3:C:100:GLU:N	2.12	1.12
2:B:20:LEU:HB2	3:C:99:PHE:CZ	1.85	1.11
2:F:388:TYR:O	2:F:388:TYR:CD1	2.02	1.11
2:B:653:CYS:HB3	2:B:656:LEU:HD11	1.32	1.09
2:B:389:MET:HE2	2:B:392:CYS:HB3	1.34	1.09
2:B:21:PRO:HD3	3:C:99:PHE:CZ	1.89	1.07
2:B:270:PRO:HG3	2:B:311:ALA:CB	1.85	1.06
3:C:97:THR:HG22	3:C:100:GLU:H	1.09	1.05
3:C:97:THR:HA	3:C:99:PHE:H	1.21	1.05
4:A:301:6OM:O1	4:A:301:6OM:C5	2.02	1.04
2:F:25:LEU:HD21	2:F:49:ARG:HE	1.17	1.03
2:B:653:CYS:O	2:B:656:LEU:HD13	1.54	1.03
2:F:92:PRO:HB2	2:F:95:HIS:NE2	1.72	1.02
1:A:169:PRO:HG2	1:A:169:PRO:O	1.57	1.01
2:F:47:ARG:HD2	3:G:142:ASP:OD2	1.59	1.01
2:F:25:LEU:HD11	2:F:49:ARG:HG2	1.04	1.01
4:E:301:6OM:O1	4:E:301:6OM:C5	2.02	1.00
2:B:394:ASP:O	2:B:422:THR:CG2	2.08	1.00
2:F:92:PRO:CB	2:F:95:HIS:HD2	1.62	1.00
3:C:96:ALA:CB	3:C:98:LEU:HB2	1.91	1.00
1:E:170:ALA:HB1	1:E:172:VAL:HG23	1.40	1.00
2:F:49:ARG:HH12	3:G:125:ILE:CD1	1.74	1.00
2:B:544:ASP:O	2:B:580:PHE:CE1	2.14	1.00
1:E:170:ALA:C	1:E:172:VAL:N	2.00	1.00
2:B:389:MET:CE	2:B:392:CYS:CA	2.11	0.99
2:F:25:LEU:HD11	2:F:49:ARG:CG	1.91	0.99
2:B:433:LEU:CD2	2:B:433:LEU:O	2.11	0.99
1:E:167:ASP:OD1	1:E:168:VAL:N	1.95	0.99
2:B:544:ASP:O	2:B:580:PHE:HE1	1.47	0.98
1:E:170:ALA:CB	1:E:172:VAL:CG2	2.39	0.98
2:B:389:MET:CE	2:B:392:CYS:H	1.67	0.98
1:A:98:VAL:N	4:A:301:6OM:O2	1.96	0.97
2:B:270:PRO:CG	2:B:311:ALA:CB	2.39	0.97
1:A:161:PRO:C	1:A:162:LEU:HD23	1.84	0.97
3:C:97:THR:HA	3:C:99:PHE:N	1.80	0.96
2:B:20:LEU:HB2	3:C:99:PHE:HZ	1.17	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:LEU:HD22	3:G:155:ASN:CG	1.86	0.96
2:F:43:LEU:CD2	3:G:155:ASN:OD1	2.14	0.95
2:B:403:ILE:O	2:B:403:ILE:HG22	1.63	0.95
2:F:449:HIS:O	2:F:452:GLU:HG3	1.68	0.94
2:B:421:VAL:HG12	2:B:421:VAL:O	1.63	0.94
2:F:96:PRO:O	2:F:158:THR:CG2	2.15	0.94
2:B:270:PRO:HG3	2:B:311:ALA:HB1	0.96	0.94
1:A:169:PRO:CG	1:A:169:PRO:O	2.03	0.94
1:E:170:ALA:C	1:E:172:VAL:H	1.61	0.93
2:F:25:LEU:CD2	2:F:49:ARG:HE	1.79	0.93
2:B:394:ASP:C	2:B:422:THR:HG21	1.89	0.93
3:C:97:THR:HG23	3:C:99:PHE:HB3	1.48	0.93
1:A:28:PHE:CD1	1:A:98:VAL:HG11	2.03	0.92
2:F:43:LEU:HA	2:F:50:ALA:CB	1.99	0.92
3:C:96:ALA:CA	3:C:98:LEU:HB2	1.98	0.92
1:A:164:VAL:HG11	2:B:608:SER:OG	1.70	0.92
2:F:49:ARG:NH1	3:G:125:ILE:HD13	1.82	0.91
3:C:97:THR:HG23	3:C:100:GLU:N	1.84	0.91
3:C:97:THR:HG23	3:C:99:PHE:CA	2.01	0.91
2:B:270:PRO:HG2	2:B:311:ALA:HB1	1.52	0.90
3:G:134:ARG:O	3:G:137:PHE:O	1.90	0.90
1:E:28:PHE:HB2	4:E:301:6OM:C4	2.02	0.90
2:B:380:VAL:O	2:B:380:VAL:HG12	1.72	0.89
2:B:389:MET:HE3	2:B:392:CYS:N	1.84	0.89
2:B:693:GLU:HG2	2:B:694:ASN:N	1.71	0.89
2:F:652:ARG:O	2:F:653:CYS:C	2.11	0.88
2:F:639:HIS:NE2	2:F:699:THR:HA	1.88	0.88
1:E:98:VAL:CG1	1:E:99:SER:N	2.37	0.88
2:B:653:CYS:HB2	2:B:656:LEU:HD11	1.53	0.88
3:C:97:THR:HG23	3:C:99:PHE:CB	2.04	0.88
3:C:98:LEU:O	3:C:101:LEU:N	2.07	0.87
2:F:96:PRO:O	2:F:158:THR:HG21	1.72	0.86
3:G:134:ARG:HH12	3:G:141:ASN:HD22	1.19	0.86
3:C:96:ALA:HB2	3:C:98:LEU:HB2	1.56	0.86
2:B:310:GLU:CB	2:B:311:ALA:HA	2.04	0.86
1:E:167:ASP:O	1:E:168:VAL:HG13	1.74	0.86
2:B:36:ARG:NH2	2:B:657:ARG:HH12	1.70	0.85
3:G:134:ARG:NH1	3:G:141:ASN:HD22	1.75	0.85
2:B:21:PRO:CD	3:C:99:PHE:CE1	2.59	0.85
3:C:125:ILE:O	3:C:125:ILE:CG2	2.23	0.85
2:B:36:ARG:NH2	2:B:657:ARG:HH11	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:366:GLY:HA2	2:F:391:ASN:HD21	1.42	0.84
3:C:125:ILE:O	3:C:125:ILE:HG22	1.74	0.84
2:B:21:PRO:CD	3:C:99:PHE:HE1	1.89	0.84
2:B:41:ALA:HB2	3:C:133:ILE:HD13	1.59	0.83
2:B:427:ARG:NH2	2:B:452:GLU:HB2	1.93	0.83
2:B:455:THR:O	2:B:459:PRO:HD3	1.77	0.83
3:C:96:ALA:HA	3:C:98:LEU:HB2	1.60	0.82
2:B:427:ARG:CZ	2:B:452:GLU:HB2	2.08	0.82
2:B:605:MET:CE	2:B:609:LEU:HD13	2.09	0.82
2:B:310:GLU:HB3	2:B:311:ALA:HA	1.59	0.82
2:F:388:TYR:HD1	2:F:388:TYR:O	1.59	0.82
2:B:653:CYS:C	2:B:656:LEU:CD1	2.46	0.82
2:F:25:LEU:HD21	2:F:49:ARG:NE	1.94	0.82
3:C:93:ILE:HG23	3:C:98:LEU:HD13	1.61	0.81
2:F:595:GLY:O	2:F:634:ASP:HA	1.78	0.81
2:B:693:GLU:CG	2:B:694:ASN:N	2.39	0.81
2:F:58:GLU:OE2	2:F:81:ALA:O	1.99	0.81
2:B:653:CYS:CB	2:B:656:LEU:CD1	2.55	0.81
1:E:98:VAL:HB	4:E:301:6OM:O2	1.81	0.80
2:B:421:VAL:CG1	2:B:421:VAL:O	2.27	0.80
1:E:98:VAL:HG13	1:E:99:SER:N	1.96	0.80
3:G:130:PRO:O	3:G:134:ARG:HG2	1.82	0.80
2:B:20:LEU:CD1	3:C:99:PHE:CE2	2.31	0.79
2:B:21:PRO:HD3	3:C:99:PHE:HE1	1.41	0.79
2:B:211:CYS:HB2	2:B:237:LEU:HG	1.63	0.79
2:F:697:MET:HE3	2:F:697:MET:H	1.47	0.79
2:B:55:THR:O	2:B:80:PRO:HD2	1.83	0.78
1:E:170:ALA:HB1	1:E:172:VAL:HG21	1.66	0.78
2:B:368:CYS:O	2:B:396:THR:HG21	1.84	0.77
2:F:597:ALA:HB2	2:F:634:ASP:OD2	1.83	0.77
2:F:29:LEU:HD11	2:F:49:ARG:HD3	1.66	0.77
2:F:604:GLN:O	2:F:604:GLN:NE2	2.18	0.77
2:B:406:GLY:O	2:B:407:CYS:C	2.24	0.76
2:F:639:HIS:CE1	2:F:699:THR:HA	2.19	0.76
2:F:99:SER:O	2:F:157:THR:OG1	2.02	0.76
2:B:581:PRO:O	2:B:623:THR:HG21	1.85	0.76
2:B:389:MET:HE1	2:B:392:CYS:CB	1.78	0.76
2:F:447:LEU:HD22	2:F:538:LEU:O	1.86	0.74
2:F:391:ASN:C	2:F:391:ASN:HD22	1.90	0.74
2:F:634:ASP:OD1	2:F:635:LYS:N	2.19	0.74
2:B:36:ARG:HH21	2:B:657:ARG:NH1	1.81	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:LEU:HD23	1:A:162:LEU:N	2.02	0.73
2:F:45:CYS:HB2	3:G:134:ARG:NH1	2.03	0.73
2:B:389:MET:HE1	2:B:392:CYS:HA	1.60	0.73
2:F:92:PRO:HB2	2:F:95:HIS:HD2	0.94	0.72
2:F:187:ASP:C	2:F:187:ASP:OD1	2.28	0.72
2:B:36:ARG:HH22	2:B:657:ARG:NH1	1.80	0.72
2:F:24:LEU:HD11	3:G:106:ASN:HD22	1.55	0.72
2:F:43:LEU:HA	2:F:50:ALA:HB1	1.70	0.72
2:B:597:ALA:HB2	2:B:634:ASP:HB2	1.70	0.72
3:C:98:LEU:CD2	3:C:101:LEU:HD13	2.18	0.72
2:F:187:ASP:O	2:F:215:ASP:OD1	2.08	0.72
2:F:43:LEU:HB3	3:G:151:VAL:HG12	1.70	0.71
2:B:653:CYS:O	2:B:656:LEU:HD11	1.88	0.71
2:B:20:LEU:CB	3:C:99:PHE:HZ	2.00	0.71
2:B:368:CYS:O	2:B:396:THR:CG2	2.39	0.71
2:F:28:ILE:HG21	2:F:49:ARG:NH2	2.06	0.71
3:C:98:LEU:HD22	3:C:101:LEU:HD13	1.71	0.71
2:F:388:TYR:O	2:F:388:TYR:CG	2.43	0.71
2:B:53:ARG:O	2:B:57:SER:O	2.08	0.70
2:F:25:LEU:CD1	2:F:49:ARG:HG2	2.00	0.70
2:B:525:LEU:HB2	2:B:549:LEU:HD11	1.73	0.70
2:B:21:PRO:CG	3:C:99:PHE:HE1	2.04	0.70
2:F:393:GLN:O	2:F:396:THR:OG1	2.06	0.70
2:B:230:LEU:O	2:B:258:ASN:O	2.09	0.70
2:B:605:MET:HE1	2:B:609:LEU:HD13	1.74	0.70
2:B:653:CYS:HB2	2:B:656:LEU:CD1	2.18	0.69
3:C:93:ILE:CG2	3:C:98:LEU:HD13	2.22	0.69
2:F:29:LEU:HD11	2:F:49:ARG:CZ	2.22	0.69
3:C:98:LEU:HD23	3:C:101:LEU:HD12	1.75	0.69
2:F:427:ARG:NH1	2:F:452:GLU:O	2.26	0.69
2:F:639:HIS:NE2	2:F:699:THR:HG22	2.07	0.69
2:B:412:LYS:HG3	2:B:415:ILE:HD12	1.73	0.68
2:B:371:SER:O	2:B:371:SER:OG	2.07	0.68
3:C:96:ALA:HA	3:C:97:THR:C	2.12	0.68
2:F:310:GLU:N	2:F:311:ALA:HA	2.08	0.68
1:A:83:VAL:HG11	1:A:113:LEU:HD21	1.74	0.68
3:C:94:ASP:O	3:C:95:GLN:HB2	1.92	0.68
2:F:652:ARG:O	2:F:654:VAL:N	2.26	0.68
2:F:697:MET:H	2:F:697:MET:CE	2.06	0.68
2:B:389:MET:HE2	2:B:392:CYS:HB2	1.18	0.68
2:F:400:LEU:HD13	2:F:403:ILE:HD11	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:ARG:CD	3:G:142:ASP:OD2	2.39	0.68
1:E:170:ALA:O	1:E:172:VAL:N	2.27	0.68
3:C:98:LEU:CD2	3:C:101:LEU:CD1	2.72	0.68
2:B:433:LEU:CG	2:B:433:LEU:O	2.37	0.67
3:C:97:THR:CG2	3:C:99:PHE:HB3	2.23	0.67
2:F:29:LEU:HD11	2:F:49:ARG:CD	2.24	0.67
2:B:567:ALA:O	2:B:570:THR:OG1	2.11	0.67
2:F:92:PRO:CB	2:F:95:HIS:NE2	2.44	0.67
3:G:134:ARG:HH12	3:G:141:ASN:ND2	1.91	0.67
2:B:389:MET:HE1	2:B:391:ASN:C	2.09	0.66
2:B:43:LEU:HD11	2:B:53:ARG:NH1	2.11	0.66
3:C:97:THR:HG22	3:C:100:GLU:N	1.94	0.66
2:B:420:LEU:HD23	2:B:421:VAL:HG23	1.78	0.66
2:F:92:PRO:CG	2:F:95:HIS:CD2	2.78	0.66
2:B:179:HIS:ND1	2:B:691:ALA:O	2.28	0.66
1:E:28:PHE:CD1	1:E:98:VAL:HG11	2.31	0.65
2:F:99:SER:HB2	2:F:101:VAL:HG23	1.78	0.65
2:B:21:PRO:HD3	3:C:99:PHE:HZ	1.56	0.65
2:F:447:LEU:CD2	2:F:538:LEU:O	2.45	0.65
2:F:428:ARG:HB2	2:F:454:LEU:HD23	1.79	0.65
2:B:376:ASP:HA	2:B:403:ILE:HD11	1.79	0.65
3:C:97:THR:HG23	3:C:99:PHE:C	2.16	0.65
3:C:97:THR:HG21	3:C:100:GLU:HG3	1.77	0.64
1:E:164:VAL:HG12	1:E:165:GLY:N	2.13	0.64
2:B:544:ASP:O	2:B:580:PHE:CZ	2.50	0.64
3:C:97:THR:HG23	3:C:99:PHE:N	2.12	0.64
2:F:411:ALA:HB2	2:F:437:LEU:HD13	1.77	0.64
2:F:29:LEU:HD11	2:F:49:ARG:NE	2.12	0.64
2:F:237:LEU:HD12	2:F:241:THR:HG21	1.79	0.64
2:F:346:MET:HB2	2:F:375:LEU:HD22	1.80	0.64
1:A:196:ASN:C	1:A:196:ASN:HD22	2.00	0.64
2:F:639:HIS:CD2	2:F:699:THR:HG22	2.32	0.64
2:F:275:CYS:HB3	2:F:276:VAL:O	1.97	0.64
2:F:42:ALA:C	2:F:44:ALA:H	1.93	0.63
1:E:167:ASP:O	1:E:168:VAL:CG1	2.46	0.63
1:E:96:HIS:O	1:E:100:ALA:N	2.32	0.63
2:F:98:LEU:HD22	2:F:132:ASN:HA	1.80	0.63
2:B:420:LEU:HD23	2:B:420:LEU:N	2.14	0.63
1:A:160:ALA:O	1:A:162:LEU:CD2	2.47	0.63
2:B:310:GLU:HB3	2:B:311:ALA:CA	2.29	0.63
3:C:96:ALA:HA	3:C:98:LEU:CB	2.28	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:GLY:O	2:B:408:ARG:N	2.32	0.62
2:B:36:ARG:CZ	2:B:657:ARG:NH1	2.60	0.62
2:B:424:ALA:HA	2:B:427:ARG:NH2	2.14	0.62
1:A:160:ALA:O	1:A:162:LEU:HD21	2.00	0.62
2:F:393:GLN:HG2	2:F:417:GLY:HA3	1.81	0.62
2:B:420:LEU:CD2	2:B:420:LEU:H	2.12	0.62
1:A:262:ARG:HA	1:A:265:LEU:HD12	1.81	0.62
1:E:203:LEU:O	1:E:233:LEU:HA	2.00	0.62
2:F:633:GLN:HG2	2:F:634:ASP:O	2.00	0.62
2:B:653:CYS:C	2:B:656:LEU:HD11	2.19	0.61
2:F:98:LEU:O	2:F:158:THR:HA	2.00	0.61
1:E:168:VAL:O	1:E:173:ARG:HB2	2.00	0.61
2:B:380:VAL:O	2:B:380:VAL:CG1	2.44	0.61
3:C:96:ALA:HA	3:C:98:LEU:N	2.16	0.61
2:F:29:LEU:CD1	2:F:49:ARG:CZ	2.78	0.61
3:C:98:LEU:HD23	3:C:101:LEU:CD1	2.29	0.61
2:B:394:ASP:CA	2:B:422:THR:HG21	2.29	0.60
2:F:187:ASP:OD1	2:F:188:GLY:N	2.35	0.60
2:F:311:ALA:HB2	2:F:338:ASN:O	2.00	0.60
2:B:269:ASN:HA	2:B:337:HIS:HD2	1.66	0.60
2:B:362:GLY:HA2	2:B:387:LEU:HD12	1.84	0.60
2:F:697:MET:HE3	2:F:697:MET:N	2.15	0.60
2:B:335:LEU:N	2:B:335:LEU:HD23	2.16	0.60
2:B:389:MET:CE	2:B:391:ASN:C	2.68	0.59
2:B:403:ILE:O	2:B:403:ILE:CG2	2.39	0.59
2:B:387:LEU:O	2:B:413:PHE:O	2.20	0.59
2:F:637:VAL:HG23	2:F:639:HIS:HB2	1.83	0.59
2:B:653:CYS:CA	2:B:656:LEU:HD11	2.31	0.59
2:B:20:LEU:HD12	3:C:99:PHE:HE2	0.53	0.58
2:F:43:LEU:CA	2:F:50:ALA:CB	2.77	0.58
2:F:604:GLN:O	2:F:604:GLN:CD	2.42	0.58
2:F:625:TYR:O	2:F:625:TYR:CD1	2.56	0.58
1:A:68:ARG:NH1	1:A:69:TYR:OH	2.36	0.58
2:B:401:ALA:CB	2:B:429:LEU:HD12	2.34	0.58
1:A:37:LEU:HD23	1:A:254:PRO:HG3	1.85	0.58
2:B:128:ILE:HD13	5:B:801:HOH:O	2.03	0.58
2:F:531:ALA:O	2:F:614:TYR:OH	2.21	0.58
2:F:293:VAL:HG22	2:F:330:ASP:CB	2.33	0.58
2:F:45:CYS:CB	3:G:134:ARG:CZ	2.81	0.57
2:B:389:MET:HE3	2:B:392:CYS:H	1.54	0.57
2:F:719:ASP:N	2:F:719:ASP:OD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:43:LEU:HD22	3:G:155:ASN:ND2	2.19	0.57
2:F:449:HIS:CD2	2:F:450:THR:N	2.73	0.57
1:A:248:LEU:HD23	1:A:251:LEU:HD12	1.85	0.57
2:B:220:LEU:O	2:B:227:THR:HG21	2.04	0.57
2:F:519:TRP:HE1	2:F:543:LEU:HB3	1.70	0.56
3:G:79:SER:HB2	3:G:83:LEU:HD12	1.85	0.56
3:C:93:ILE:HG23	3:C:98:LEU:CD1	2.34	0.56
2:F:46:GLY:O	2:F:50:ALA:CB	2.53	0.56
2:F:187:ASP:O	2:F:215:ASP:HA	2.04	0.56
2:F:595:GLY:HA3	2:F:607:LEU:HD21	1.88	0.56
2:B:595:GLY:HA3	2:B:607:LEU:HD21	1.88	0.56
2:F:96:PRO:O	2:F:158:THR:HG23	2.06	0.56
2:B:65:PRO:HB3	3:C:160:GLU:HB2	1.86	0.55
2:F:186:PRO:HG2	2:F:189:ALA:CB	2.35	0.55
2:B:55:THR:O	2:B:80:PRO:CD	2.54	0.55
2:F:343:ALA:HB3	2:F:344:PRO:CD	2.36	0.55
2:F:35:VAL:HG12	2:F:35:VAL:O	2.07	0.55
2:F:28:ILE:HG21	2:F:49:ARG:HH22	1.71	0.55
2:B:333:MET:HB3	2:B:335:LEU:HD21	1.89	0.55
2:B:445:CYS:HB3	2:B:449:HIS:CD2	2.41	0.55
2:F:683:GLN:HE21	2:F:685:ARG:HE	1.55	0.55
2:F:45:CYS:HB2	3:G:134:ARG:CZ	2.37	0.55
2:F:34:ASP:OD1	2:F:36:ARG:N	2.40	0.55
2:F:535:LEU:HD22	2:F:573:GLY:O	2.07	0.55
2:B:450:THR:HG22	2:B:519:TRP:CZ2	2.42	0.55
1:E:28:PHE:O	4:E:301:6OM:C2	2.55	0.55
2:B:423:SER:HB3	2:B:427:ARG:HH12	1.72	0.54
2:B:581:PRO:O	2:B:623:THR:CG2	2.54	0.54
2:F:38:ARG:NH1	2:F:58:GLU:HA	2.22	0.54
1:A:7:LEU:HA	1:A:12:VAL:HG13	1.89	0.54
1:E:170:ALA:HB3	1:E:172:VAL:HB	0.60	0.54
2:F:43:LEU:CA	2:F:50:ALA:HB2	2.38	0.54
1:E:169:PRO:O	1:E:170:ALA:C	2.46	0.54
2:B:212:TRP:HE3	2:B:215:ASP:OD1	1.91	0.54
2:B:36:ARG:HH21	2:B:657:ARG:HH12	1.48	0.54
1:E:98:VAL:HG12	1:E:99:SER:N	2.21	0.54
3:C:93:ILE:HD11	3:C:116:LEU:HD21	1.90	0.54
2:F:403:ILE:HG13	2:F:403:ILE:O	2.07	0.54
2:F:293:VAL:HG22	2:F:330:ASP:HB3	1.90	0.53
2:F:388:TYR:C	2:F:388:TYR:CD1	2.74	0.53
2:B:420:LEU:CD2	2:B:420:LEU:N	2.71	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:164:VAL:CG2	2:F:608:SER:HB2	2.37	0.53
3:C:93:ILE:HA	3:C:98:LEU:HD11	1.90	0.53
2:F:454:LEU:CD1	2:F:454:LEU:N	2.71	0.53
2:F:653:CYS:HB2	2:F:656:LEU:CD2	2.39	0.53
2:F:323:ALA:HA	2:F:352:ARG:HG2	1.89	0.53
2:B:420:LEU:HD23	2:B:420:LEU:H	1.73	0.53
2:B:401:ALA:HB2	2:B:429:LEU:HD12	1.89	0.53
2:B:586:MET:HB2	2:B:624:LEU:HD21	1.90	0.53
1:E:38:ILE:HD12	1:E:257:LEU:HD23	1.88	0.53
2:F:33:THR:O	2:F:59:LEU:HD13	2.08	0.53
2:B:658:LYS:HE3	3:C:159:PHE:CZ	2.43	0.53
2:B:536:SER:N	2:B:537:PRO:HD2	2.24	0.53
2:F:46:GLY:O	2:F:50:ALA:N	2.34	0.53
2:B:268:PHE:HE2	2:B:335:LEU:HD22	1.73	0.53
1:E:169:PRO:C	1:E:170:ALA:O	2.41	0.52
2:F:43:LEU:HA	2:F:50:ALA:CA	2.38	0.52
2:F:519:TRP:O	2:F:547:PRO:HD2	2.09	0.52
2:F:653:CYS:HB2	2:F:656:LEU:HD21	1.90	0.52
2:F:716:ARG:HB2	2:F:718:ILE:HD12	1.91	0.52
2:F:45:CYS:HB3	3:G:134:ARG:CZ	2.40	0.52
1:A:28:PHE:CE1	1:A:98:VAL:HG11	2.44	0.52
2:F:187:ASP:O	2:F:215:ASP:CG	2.47	0.52
2:B:258:ASN:HD22	2:B:290:ARG:HD3	1.74	0.52
2:F:66:ARG:O	2:F:68:PRO:HD3	2.10	0.52
1:A:177:ARG:HD3	2:B:606:ASP:HB3	1.92	0.52
3:C:97:THR:CG2	3:C:99:PHE:N	2.72	0.52
1:E:167:ASP:OD1	1:E:168:VAL:HG22	2.09	0.52
3:C:96:ALA:HB2	3:C:98:LEU:CB	2.37	0.51
2:B:349:LEU:HD21	2:B:356:ILE:HD13	1.92	0.51
2:F:293:VAL:HA	2:F:330:ASP:HB3	1.92	0.51
2:F:21:PRO:CB	2:F:24:LEU:HD12	2.41	0.51
2:F:217:VAL:HG21	2:F:248:GLU:HB3	1.91	0.51
2:B:42:ALA:HB2	2:B:49:ARG:CB	2.40	0.51
2:F:334:ASP:HA	2:F:362:GLY:HA3	1.92	0.51
2:F:34:ASP:C	2:F:34:ASP:OD1	2.48	0.51
2:B:42:ALA:HB2	2:B:49:ARG:HB3	1.93	0.51
2:B:269:ASN:HA	2:B:337:HIS:CD2	2.45	0.51
2:B:32:LEU:HD13	2:B:38:ARG:HG2	1.92	0.50
2:B:376:ASP:OD1	2:B:376:ASP:N	2.44	0.50
2:B:394:ASP:HA	2:B:422:THR:OG1	2.11	0.50
2:F:652:ARG:O	2:F:654:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:581:PRO:C	2:B:623:THR:HG21	2.32	0.50
2:F:29:LEU:CD1	2:F:49:ARG:NE	2.74	0.50
3:G:76:ALA:N	3:G:77:ALA:HB3	2.26	0.50
2:F:346:MET:HB2	2:F:375:LEU:CD2	2.41	0.50
2:F:346:MET:HG3	2:F:375:LEU:HD21	1.93	0.50
2:F:694:ASN:H	2:F:696:LEU:HB2	1.77	0.50
1:A:97:SER:OG	4:A:301:6OM:O1	2.29	0.50
2:B:412:LYS:O	2:B:438:LYS:HA	2.11	0.50
2:B:315:VAL:HG13	2:B:345:ALA:HB2	1.94	0.50
2:B:642:LEU:HB2	2:B:665:THR:CG2	2.42	0.50
3:C:94:ASP:O	3:C:95:GLN:CB	2.58	0.50
2:F:310:GLU:N	2:F:311:ALA:CA	2.73	0.50
2:F:42:ALA:C	2:F:44:ALA:N	2.56	0.50
2:B:334:ASP:OD1	2:B:387:LEU:CD1	2.60	0.49
1:E:36:HIS:HB2	2:F:698:PHE:CD1	2.47	0.49
2:F:45:CYS:CB	3:G:134:ARG:NH1	2.72	0.49
1:A:7:LEU:HA	1:A:12:VAL:CG1	2.42	0.49
2:B:182:PRO:HB2	2:B:185:LEU:HG	1.94	0.49
2:F:311:ALA:CB	2:F:338:ASN:O	2.61	0.49
2:F:43:LEU:HD23	3:G:151:VAL:HG12	1.94	0.49
2:F:696:LEU:O	2:F:696:LEU:HD13	2.13	0.49
1:E:170:ALA:CA	1:E:172:VAL:H	2.24	0.49
2:F:697:MET:N	2:F:697:MET:CE	2.73	0.49
2:F:680:ARG:O	2:F:713:LEU:HD11	2.13	0.49
3:C:93:ILE:CG2	3:C:98:LEU:CD1	2.89	0.49
1:A:36:HIS:CE1	1:A:37:LEU:HD13	2.48	0.49
2:F:626:GLU:HG2	2:F:658:LYS:HD2	1.94	0.49
2:F:92:PRO:CA	2:F:95:HIS:HD2	2.22	0.49
1:A:129:ASP:O	1:A:130:GLU:C	2.50	0.48
2:F:605:MET:SD	2:F:609:LEU:HD13	2.53	0.48
2:B:410:LEU:HG	2:B:411:ALA:N	2.28	0.48
1:E:7:LEU:HD22	1:E:12:VAL:HG21	1.95	0.48
2:F:237:LEU:HD12	2:F:241:THR:CG2	2.43	0.48
2:F:41:ALA:HB2	3:G:133:ILE:HD13	1.93	0.48
2:B:411:ALA:HB2	2:B:437:LEU:HD13	1.94	0.48
2:B:179:HIS:CE1	2:B:691:ALA:O	2.66	0.48
1:E:27:GLY:HA2	1:E:98:VAL:HG12	1.95	0.48
2:F:455:THR:O	2:F:459:PRO:HD3	2.13	0.48
2:F:49:ARG:O	2:F:53:ARG:N	2.43	0.48
2:F:55:THR:O	2:F:80:PRO:HD2	2.13	0.48
2:B:270:PRO:CD	2:B:311:ALA:CB	2.90	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:558:GLY:HA2	2:B:593:ALA:HA	1.95	0.48
2:F:179:HIS:CD2	2:F:691:ALA:HB3	2.49	0.48
2:F:393:GLN:HG2	2:F:417:GLY:CA	2.44	0.48
1:E:170:ALA:O	1:E:171:ALA:C	2.48	0.48
2:F:615:LEU:HD22	2:F:618:ILE:HD11	1.96	0.48
1:E:97:SER:OG	4:E:301:6OM:O1	2.31	0.48
2:F:391:ASN:ND2	2:F:391:ASN:C	2.64	0.48
2:F:643:THR:O	2:F:647:VAL:HG23	2.14	0.48
2:B:310:GLU:N	2:B:311:ALA:HB2	2.29	0.48
2:F:335:LEU:HD12	2:F:337:HIS:O	2.14	0.48
2:F:186:PRO:HG2	2:F:189:ALA:HB2	1.96	0.47
2:F:439:GLU:O	2:F:442:VAL:HG23	2.14	0.47
2:B:99:SER:HB2	2:B:157:THR:OG1	2.14	0.47
2:B:43:LEU:HB3	3:C:151:VAL:HG12	1.96	0.47
2:F:637:VAL:CG2	2:F:639:HIS:HB2	2.45	0.47
2:F:49:ARG:NH1	3:G:125:ILE:CD1	2.58	0.47
3:G:47:VAL:HB	3:G:52:LEU:HD12	1.96	0.47
2:F:28:ILE:CG2	2:F:49:ARG:NH2	2.76	0.47
1:A:73:ASP:N	1:A:74:PRO:HD2	2.29	0.47
2:B:334:ASP:OD1	2:B:387:LEU:HD13	2.13	0.47
2:B:45:CYS:O	3:C:143:PHE:CD1	2.68	0.47
1:E:131:ASP:HA	1:E:132:TYR:C	2.33	0.47
2:F:599:THR:O	2:F:599:THR:OG1	2.29	0.47
2:B:42:ALA:O	2:B:45:CYS:N	2.46	0.47
2:F:428:ARG:CA	2:F:454:LEU:HD23	2.44	0.47
2:F:24:LEU:HD13	3:G:102:ILE:HG22	1.97	0.47
2:B:97:LEU:O	2:B:98:LEU:HD12	2.15	0.47
2:B:357:LYS:O	2:B:381:CYS:HA	2.14	0.47
3:C:119:GLN:O	3:C:122:ALA:HB3	2.14	0.47
2:F:394:ASP:HB3	2:F:422:THR:HG21	1.97	0.47
1:A:160:ALA:CB	1:A:162:LEU:HD21	2.45	0.47
1:A:94:VAL:HG22	1:A:118:ILE:HD12	1.97	0.47
2:B:35:VAL:HA	2:B:38:ARG:HG3	1.95	0.47
2:F:46:GLY:O	2:F:50:ALA:HB2	2.14	0.47
2:B:584:ALA:HB1	2:B:625:TYR:HB3	1.97	0.47
2:B:574:LEU:HD23	2:B:618:ILE:HG23	1.96	0.47
3:C:99:PHE:O	3:C:99:PHE:HD1	1.98	0.47
2:F:292:THR:HA	2:F:328:LEU:HA	1.97	0.47
2:B:131:GLN:N	5:B:801:HOH:O	2.39	0.46
2:B:389:MET:HE2	2:B:392:CYS:H	1.71	0.46
2:F:361:LEU:HD13	2:F:367:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:134:ARG:NH1	3:G:141:ASN:ND2	2.54	0.46
2:F:181:ARG:HD3	2:F:212:TRP:CZ2	2.50	0.46
1:A:160:ALA:C	1:A:162:LEU:CD2	2.84	0.46
1:A:163:ALA:O	1:A:180:PHE:CE1	2.68	0.46
1:E:167:ASP:C	1:E:168:VAL:HG13	2.36	0.46
2:B:41:ALA:CB	3:C:133:ILE:HD13	2.39	0.46
2:F:428:ARG:CB	2:F:454:LEU:HD23	2.45	0.46
2:B:151:VAL:HG11	2:B:162:LEU:HD12	1.97	0.46
2:B:268:PHE:CD2	2:B:335:LEU:HD13	2.51	0.46
2:B:343:ALA:HB3	2:B:344:PRO:CD	2.45	0.46
2:F:346:MET:CB	2:F:375:LEU:HD22	2.44	0.46
2:B:237:LEU:HD23	2:B:241:THR:HG21	1.97	0.46
3:C:8:LEU:HD22	3:C:43:PRO:HD3	1.96	0.46
3:C:76:ALA:HA	3:C:77:ALA:HB3	1.97	0.46
2:F:236:GLY:O	2:F:238:ALA:O	2.34	0.46
2:B:361:LEU:O	2:B:387:LEU:HG	2.14	0.46
2:F:606:ASP:OD2	2:F:608:SER:OG	2.31	0.46
2:B:606:ASP:OD1	2:B:608:SER:OG	2.23	0.46
2:B:408:ARG:HG3	2:B:434:ARG:HB2	1.98	0.46
2:F:343:ALA:CB	2:F:374:HIS:CD2	2.99	0.46
2:F:186:PRO:HG2	2:F:189:ALA:HB3	1.97	0.45
2:F:43:LEU:HA	2:F:50:ALA:HA	1.98	0.45
1:E:164:VAL:HG22	2:F:608:SER:HB2	1.98	0.45
1:E:57:GLY:HA2	2:F:668:HIS:CD2	2.51	0.45
2:F:361:LEU:HD22	2:F:364:PHE:CD2	2.52	0.45
1:A:144:VAL:HG12	1:A:148:MET:CE	2.46	0.45
2:B:446:ARG:C	2:B:447:LEU:HD22	2.37	0.45
2:B:692:PRO:O	2:B:696:LEU:HD23	2.16	0.45
1:E:164:VAL:HG21	2:F:608:SER:HB2	1.97	0.45
1:A:96:HIS:HB2	1:A:120:ILE:HB	1.98	0.45
2:F:217:VAL:HG21	2:F:248:GLU:CB	2.47	0.45
2:F:697:MET:HA	2:F:697:MET:HE2	1.98	0.45
2:B:419:ASP:C	2:B:421:VAL:H	2.20	0.45
2:B:20:LEU:CB	3:C:99:PHE:CZ	2.76	0.45
2:B:656:LEU:HD12	2:B:656:LEU:H	1.81	0.45
1:A:101:MET:HG2	1:A:199:LEU:HD21	1.99	0.45
3:G:134:ARG:H	3:G:134:ARG:HG2	1.57	0.45
2:B:58:GLU:HG2	2:B:79:PHE:HB3	1.99	0.45
3:C:47:VAL:HG12	3:C:52:LEU:HB2	1.99	0.45
1:A:162:LEU:CD2	1:A:162:LEU:N	2.72	0.45
2:B:368:CYS:O	2:B:396:THR:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:42:ALA:HB1	2:B:50:ALA:N	2.31	0.45
2:B:653:CYS:C	2:B:656:LEU:HD12	2.23	0.45
1:A:173:ARG:O	1:A:177:ARG:N	2.50	0.44
2:F:21:PRO:HB2	2:F:24:LEU:HD12	1.98	0.44
2:B:20:LEU:HB2	3:C:99:PHE:CE2	2.47	0.44
2:B:238:ALA:O	2:B:239:ALA:HB3	2.17	0.44
2:F:436:THR:C	2:F:437:LEU:HD12	2.38	0.44
2:F:47:ARG:HA	2:F:50:ALA:HB3	2.00	0.44
2:B:436:THR:C	2:B:437:LEU:HD12	2.38	0.44
2:F:389:MET:HB2	2:F:415:ILE:HG12	1.99	0.44
2:F:605:MET:CE	2:F:609:LEU:HD13	2.47	0.44
2:F:696:LEU:HA	2:F:696:LEU:HD22	1.68	0.44
2:F:658:LYS:NZ	3:G:159:PHE:CZ	2.76	0.44
2:B:268:PHE:CE2	2:B:335:LEU:HD22	2.53	0.44
2:F:400:LEU:HD13	2:F:403:ILE:CD1	2.44	0.44
2:F:658:LYS:NZ	3:G:159:PHE:CE1	2.66	0.44
1:E:38:ILE:CD1	1:E:257:LEU:HD23	2.48	0.44
1:A:60:ASN:HB3	1:A:63:TYR:CD2	2.52	0.44
2:B:419:ASP:C	2:B:421:VAL:N	2.70	0.44
2:B:597:ALA:HB2	2:B:634:ASP:CB	2.45	0.44
2:B:670:MET:HE3	2:B:706:TRP:HA	2.00	0.44
3:C:105:ALA:O	3:C:108:LEU:O	2.36	0.44
2:B:372:TRP:N	2:B:372:TRP:CD1	2.68	0.43
2:B:389:MET:HB3	2:B:389:MET:HE2	1.85	0.43
2:B:609:LEU:HD23	2:B:609:LEU:O	2.18	0.43
1:E:55:CYS:O	1:E:182:MET:HG2	2.18	0.43
2:F:315:VAL:HG13	2:F:345:ALA:HB2	1.99	0.43
2:B:268:PHE:HD2	2:B:335:LEU:HD13	1.83	0.43
2:B:33:THR:HG22	2:B:59:LEU:HD11	2.00	0.43
2:B:580:PHE:HA	2:B:581:PRO:HD3	1.89	0.43
2:F:260:ARG:HA	2:F:291:LEU:HA	2.01	0.43
2:F:63:GLY:O	3:G:158:ALA:O	2.37	0.43
1:A:165:GLY:HA3	1:A:173:ARG:HD3	2.00	0.43
2:B:350:ALA:HB2	2:B:378:VAL:HA	2.00	0.43
2:B:618:ILE:HB	2:B:653:CYS:SG	2.59	0.43
2:F:185:LEU:C	2:F:187:ASP:H	2.22	0.43
2:F:389:MET:H	2:F:415:ILE:HG12	1.84	0.43
2:F:42:ALA:HB1	2:F:50:ALA:N	2.33	0.43
1:A:28:PHE:CG	1:A:98:VAL:HG11	2.52	0.43
3:C:52:LEU:O	3:C:52:LEU:HD23	2.19	0.43
2:F:206:LEU:HB2	2:F:209:PHE:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:559:ASP:HA	2:B:594:VAL:HG12	2.00	0.43
1:E:123:SER:HB3	1:E:126:PHE:CE1	2.53	0.43
2:F:653:CYS:CB	2:F:656:LEU:HD21	2.48	0.43
2:F:36:ARG:CZ	2:F:657:ARG:NH2	2.82	0.43
2:B:293:VAL:HG13	2:B:330:ASP:HB3	2.01	0.42
1:E:202:VAL:HA	1:E:205:LEU:HB2	2.01	0.42
2:F:152:TYR:OH	2:F:179:HIS:CD2	2.72	0.42
1:A:26:HIS:CE1	1:A:53:LEU:HG	2.54	0.42
2:B:152:TYR:CE1	2:B:176:VAL:HG12	2.55	0.42
2:B:310:GLU:O	2:B:338:ASN:N	2.53	0.42
3:C:47:VAL:HG13	3:C:51:ILE:HG22	2.01	0.42
1:E:169:PRO:O	1:E:170:ALA:O	2.38	0.42
2:F:410:LEU:HD11	2:F:412:LYS:NZ	2.34	0.42
2:F:654:VAL:CG1	2:F:655:GLY:N	2.82	0.42
2:B:131:GLN:HE21	2:B:135:ILE:HD11	1.84	0.42
2:B:410:LEU:HD21	2:B:412:LYS:CD	2.49	0.42
2:B:87:LEU:CD1	2:B:162:LEU:HD11	2.49	0.42
1:E:32:GLN:HG2	2:F:702:ARG:NH2	2.34	0.42
2:F:659:LEU:O	2:F:682:MET:HA	2.19	0.42
1:A:78:ASP:O	1:A:82:ILE:HG12	2.20	0.42
3:C:101:LEU:HD23	3:C:101:LEU:O	2.20	0.42
1:A:44:GLN:HG2	1:A:45:ASN:ND2	2.33	0.42
2:B:709:PHE:C	2:B:709:PHE:CD1	2.93	0.42
2:B:87:LEU:HD13	2:B:162:LEU:HD11	2.01	0.42
3:C:125:ILE:O	3:C:125:ILE:HG23	2.13	0.42
2:F:29:LEU:HD21	2:F:49:ARG:HD3	2.01	0.42
2:B:298:GLU:HB3	2:B:335:LEU:HA	2.02	0.42
1:E:76:VAL:HG22	1:E:102:ILE:HG23	2.00	0.42
1:A:249:PRO:O	1:A:252:SER:O	2.38	0.42
2:F:361:LEU:HD22	2:F:364:PHE:CG	2.55	0.42
2:B:449:HIS:O	2:B:449:HIS:ND1	2.53	0.41
1:E:94:VAL:HA	1:E:118:ILE:O	2.20	0.41
2:B:182:PRO:HG2	2:B:185:LEU:HD11	2.03	0.41
2:F:34:ASP:O	2:F:38:ARG:HB2	2.20	0.41
2:B:589:ASP:HA	2:B:630:TRP:HB2	2.02	0.41
2:F:152:TYR:CE1	2:F:154:ARG:HD3	2.56	0.41
2:F:220:LEU:HA	2:F:227:THR:HG21	2.01	0.41
2:F:59:LEU:HG	2:F:61:LEU:HG	2.03	0.41
1:A:203:LEU:HB3	1:A:233:LEU:HD23	2.02	0.41
2:B:355:ARG:O	2:B:357:LYS:HG2	2.21	0.41
2:B:634:ASP:O	2:B:635:LYS:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:98:VAL:HG12	1:E:99:SER:H	1.85	0.41
2:B:385:GLU:HG2	2:B:387:LEU:HD21	2.03	0.41
2:F:331:PHE:O	2:F:359:LEU:HA	2.20	0.41
2:B:397:ASP:HB3	2:B:426:ILE:HD11	2.02	0.41
2:B:392:CYS:HB3	2:B:415:ILE:HG21	2.02	0.41
2:B:454:LEU:HD12	2:B:454:LEU:H	1.86	0.41
2:B:565:ARG:O	2:B:566:PRO:C	2.59	0.41
2:B:394:ASP:HA	2:B:422:THR:HG21	2.00	0.41
2:B:43:LEU:HB2	3:C:155:ASN:HD21	1.85	0.41
2:B:47:ARG:NH2	3:C:142:ASP:O	2.54	0.41
2:F:625:TYR:CG	2:F:625:TYR:O	2.74	0.41
1:A:127:LEU:C	1:A:127:LEU:HD23	2.41	0.41
2:F:343:ALA:HB3	2:F:344:PRO:HD3	2.02	0.41
2:F:172:ARG:HG3	2:F:203:GLU:HB2	2.03	0.41
2:F:211:CYS:HB3	2:F:237:LEU:HD22	2.02	0.41
2:F:446:ARG:O	2:F:447:LEU:HB2	2.19	0.41
2:B:425:GLY:O	2:B:428:ARG:HB3	2.21	0.41
2:F:368:CYS:HA	2:F:374:HIS:HB3	2.03	0.41
2:F:616:HIS:CG	2:F:616:HIS:O	2.74	0.41
2:F:97:LEU:HD23	2:F:97:LEU:HA	1.97	0.41
1:A:183:ARG:NE	1:A:185:ASP:OD1	2.47	0.41
2:B:680:ARG:NH2	3:C:158:ALA:O	2.54	0.41
1:E:249:PRO:HB2	1:E:257:LEU:HD22	2.03	0.41
2:B:256:CYS:HB2	2:B:259:LEU:HD22	2.03	0.40
2:B:556:VAL:HG11	2:B:614:TYR:OH	2.21	0.40
3:C:130:PRO:HA	3:C:133:ILE:HD12	2.03	0.40
1:E:203:LEU:O	1:E:233:LEU:HD23	2.21	0.40
2:F:282:LEU:HD12	2:F:286:THR:HG23	2.02	0.40
2:F:98:LEU:HD22	2:F:132:ASN:CA	2.50	0.40
1:A:196:ASN:ND2	1:A:196:ASN:C	2.69	0.40
2:B:233:LEU:CD2	2:B:235:LEU:HD21	2.51	0.40
2:B:259:LEU:HA	2:B:259:LEU:HD12	1.95	0.40
2:F:343:ALA:CB	2:F:344:PRO:CD	2.99	0.40
2:B:567:ALA:O	2:B:568:PRO:C	2.59	0.40
2:B:693:GLU:O	2:B:693:GLU:HG2	1.94	0.40
1:A:160:ALA:C	1:A:162:LEU:HD23	2.42	0.40
2:B:424:ALA:HA	2:B:427:ARG:CZ	2.52	0.40
2:B:428:ARG:HB2	2:B:454:LEU:CD2	2.52	0.40
2:B:615:LEU:HD22	2:B:618:ILE:HD11	2.04	0.40
2:F:400:LEU:HB3	2:F:403:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

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	253/267 (95%)	224 (88%)	28 (11%)	1 (0%)	39	76
1	E	253/267 (95%)	221 (87%)	32 (13%)	0	100	100
2	B	607/740 (82%)	517 (85%)	89 (15%)	1 (0%)	52	85
2	F	604/740 (82%)	516 (85%)	86 (14%)	2 (0%)	46	81
3	C	123/169 (73%)	101 (82%)	20 (16%)	2 (2%)	12	48
3	G	126/169 (75%)	108 (86%)	18 (14%)	0	100	100
All	All	1966/2352 (84%)	1687 (86%)	273 (14%)	6 (0%)	46	81

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	169	PRO
3	C	98	LEU
2	F	598	LEU
3	C	99	PHE
2	F	65	PRO
2	B	458	SER

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	214/226 (95%)	183 (86%)	31 (14%)	4	18
1	E	214/226 (95%)	185 (86%)	29 (14%)	5	21

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	519/615 (84%)	420 (81%)	99 (19%)	2	8
2	F	519/615 (84%)	425 (82%)	94 (18%)	2	9
3	C	110/146 (75%)	103 (94%)	7 (6%)	22	60
3	G	112/146 (77%)	101 (90%)	11 (10%)	10	37
All	All	1688/1974 (86%)	1417 (84%)	271 (16%)	3	14

All (271) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	PHE
1	A	38	ILE
1	A	43	THR
1	A	44	GLN
1	A	45	ASN
1	A	51	TYR
1	A	77	ASP
1	A	79	LEU
1	A	80	LEU
1	A	99	SER
1	A	109	ARG
1	A	110	ARG
1	A	123	SER
1	A	125	ARG
1	A	129	ASP
1	A	156	VAL
1	A	162	LEU
1	A	168	VAL
1	A	183	ARG
1	A	193	THR
1	A	196	ASN
1	A	202	VAL
1	A	210	THR
1	A	214	GLN
1	A	215	THR
1	A	229	LEU
1	A	232	HIS
1	A	243	LYS
1	A	245	GLU
1	A	248	LEU
1	A	252	SER
2	B	22	GLU

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Mol	Chain	Res	Type
2	B	24	LEU
2	B	32	LEU
2	B	36	ARG
2	B	38	ARG
2	B	40	ARG
2	B	43	LEU
2	B	53	ARG
2	B	58	GLU
2	B	59	LEU
2	B	62	ARG
2	B	67	SER
2	B	72	PHE
2	B	97	LEU
2	B	98	LEU
2	B	128	ILE
2	B	138	ARG
2	B	143	PHE
2	B	147	THR
2	B	151	VAL
2	B	181	ARG
2	B	186	PRO
2	B	211	CYS
2	B	213	THR
2	B	214	GLU
2	B	230	LEU
2	B	237	LEU
2	B	245	LYS
2	B	249	LEU
2	B	266	CYS
2	B	271	ARG
2	B	275	CYS
2	B	283	SER
2	B	284	LEU
2	B	288	CYS
2	B	310	GLU
2	B	335	LEU
2	B	338	ASN
2	B	349	LEU
2	B	357	LYS
2	B	359	LEU
2	B	372	TRP
2	B	374	HIS

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Mol	Chain	Res	Type
2	B	375	LEU
2	B	376	ASP
2	B	385	GLU
2	B	389	MET
2	B	397	ASP
2	B	405	ARG
2	B	407	CYS
2	B	422	THR
2	B	423	SER
2	B	433	LEU
2	B	435	PRO
2	B	437	LEU
2	B	438	LYS
2	B	441	THR
2	B	443	LEU
2	B	446	ARG
2	B	447	LEU
2	B	450	THR
2	B	452	GLU
2	B	455	THR
2	B	464	ILE
2	B	465	GLU
2	B	534	LEU
2	B	536	SER
2	B	540	SER
2	B	543	LEU
2	B	548	VAL
2	B	552	ILE
2	B	553	SER
2	B	570	THR
2	B	582	VAL
2	B	586	MET
2	B	594	VAL
2	B	599	THR
2	B	602	THR
2	B	612	ARG
2	B	618	ILE
2	B	624	LEU
2	B	628	ASP
2	B	635	LYS
2	B	636	ASP
2	B	642	LEU

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Mol	Chain	Res	Type
2	B	652	ARG
2	B	657	ARG
2	B	659	LEU
2	B	664	THR
2	B	670	MET
2	B	693	GLU
2	B	695	ASP
2	B	696	LEU
2	B	697	MET
2	B	698	PHE
2	B	699	THR
2	B	701	MET
2	B	713	LEU
2	B	714	ASN
3	C	52	LEU
3	C	80	ASP
3	C	97	THR
3	C	99	PHE
3	C	112	ASN
3	C	120	THR
3	C	150	GLU
1	E	6	ILE
1	E	8	GLU
1	E	17	THR
1	E	30	THR
1	E	38	ILE
1	E	44	GLN
1	E	51	TYR
1	E	73	ASP
1	E	79	LEU
1	E	99	SER
1	E	109	ARG
1	E	125	ARG
1	E	127	LEU
1	E	129	ASP
1	E	162	LEU
1	E	183	ARG
1	E	191	SER
1	E	196	ASN
1	E	199	LEU
1	E	205	LEU
1	E	214	GLN

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Mol	Chain	Res	Type
1	E	215	THR
1	E	217	LYS
1	E	229	LEU
1	E	236	ASP
1	E	238	THR
1	E	241	THR
1	E	243	LYS
1	E	259	GLN
2	F	18	LEU
2	F	19	ASP
2	F	32	LEU
2	F	34	ASP
2	F	36	ARG
2	F	47	ARG
2	F	48	MET
2	F	53	ARG
2	F	58	GLU
2	F	61	LEU
2	F	64	ASP
2	F	72	PHE
2	F	78	ARG
2	F	99	SER
2	F	128	ILE
2	F	138	ARG
2	F	143	PHE
2	F	154	ARG
2	F	155	ASP
2	F	157	THR
2	F	158	THR
2	F	180	GLN
2	F	181	ARG
2	F	187	ASP
2	F	190	ASP
2	F	202	ARG
2	F	204	LEU
2	F	230	LEU
2	F	259	LEU
2	F	275	CYS
2	F	284	LEU
2	F	301	GLU
2	F	310	GLU
2	F	328	LEU

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Mol	Chain	Res	Type
2	F	333	MET
2	F	335	LEU
2	F	340	LEU
2	F	349	LEU
2	F	355	ARG
2	F	363	SER
2	F	368	CYS
2	F	374	HIS
2	F	380	VAL
2	F	384	LEU
2	F	387	LEU
2	F	389	MET
2	F	391	ASN
2	F	397	ASP
2	F	405	ARG
2	F	407	CYS
2	F	412	LYS
2	F	418	CYS
2	F	435	PRO
2	F	437	LEU
2	F	449	HIS
2	F	450	THR
2	F	454	LEU
2	F	461	ARG
2	F	465	GLU
2	F	518	SER
2	F	522	LEU
2	F	526	SER
2	F	530	SER
2	F	536	SER
2	F	540	SER
2	F	577	LEU
2	F	583	LEU
2	F	586	MET
2	F	602	THR
2	F	604	GLN
2	F	606	ASP
2	F	608	SER
2	F	618	ILE
2	F	623	THR
2	F	624	LEU
2	F	626	GLU

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Mol	Chain	Res	Type
2	F	635	LYS
2	F	636	ASP
2	F	639	HIS
2	F	641	SER
2	F	653	CYS
2	F	656	LEU
2	F	657	ARG
2	F	665	THR
2	F	693	GLU
2	F	696	LEU
2	F	697	MET
2	F	698	PHE
2	F	705	SER
2	F	713	LEU
2	F	714	ASN
2	F	716	ARG
2	F	717	GLN
2	F	719	ASP
3	G	52	LEU
3	G	93	ILE
3	G	97	THR
3	G	99	PHE
3	G	101	LEU
3	G	112	ASN
3	G	115	ASP
3	G	119	GLN
3	G	120	THR
3	G	126	LYS
3	G	159	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	44	GLN
1	A	45	ASN
1	A	96	HIS
1	A	196	ASN
1	A	256	GLN
2	B	131	GLN
2	B	167	GLN
2	B	179	HIS

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Mol	Chain	Res	Type
2	B	180	GLN
2	B	232	HIS
2	B	258	ASN
2	B	337	HIS
2	B	533	GLN
2	B	668	HIS
2	B	683	GLN
1	E	196	ASN
2	F	95	HIS
2	F	179	HIS
2	F	180	GLN
2	F	232	HIS
2	F	374	HIS
2	F	391	ASN
2	F	604	GLN
2	F	668	HIS
2	F	683	GLN
2	F	717	GLN
3	G	46	ASN
3	G	106	ASN
3	G	141	ASN

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](#)

2 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	$\# Z > 2$
4	6OM	A	301	1	5,6,6	3.67	5 (100%)	6,6,6	3.40	2 (33%)
4	6OM	E	301	-	5,6,6	3.66	5 (100%)	6,6,6	3.40	2 (33%)

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	6OM	A	301	1	-	1/5/5/5	0/0/0/0
4	6OM	E	301	-	-	1/5/5/5	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	6OM	C3-C2	-3.94	1.45	1.50
4	E	301	6OM	C3-C2	-3.91	1.45	1.50
4	E	301	6OM	C4-C1	-3.43	1.41	1.50
4	A	301	6OM	C4-C1	-3.42	1.41	1.50
4	E	301	6OM	O2-C5	-2.82	1.31	1.41
4	A	301	6OM	O2-C5	-2.81	1.31	1.41
4	A	301	6OM	O1-C3	-2.59	1.31	1.41
4	E	301	6OM	O1-C3	-2.59	1.31	1.41
4	E	301	6OM	C2-C1	5.03	1.45	1.32
4	A	301	6OM	C2-C1	5.04	1.45	1.32

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	6OM	C3-C2-C1	-7.62	115.22	126.61
4	E	301	6OM	C3-C2-C1	-7.60	115.25	126.61
4	E	301	6OM	O2-C5-C1	-2.60	106.12	111.76
4	A	301	6OM	O2-C5-C1	-2.58	106.15	111.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	301	6OM	O1-C3-C2-C1
4	A	301	6OM	O1-C3-C2-C1

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	301	6OM	4	0
4	E	301	6OM	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	257/267 (96%)	-0.12	2 (0%) 87 84	41, 65, 119, 148	0
1	E	257/267 (96%)	0.15	8 (3%) 52 46	53, 86, 155, 192	0
2	B	615/740 (83%)	0.06	12 (1%) 68 62	40, 78, 124, 159	0
2	F	614/740 (82%)	0.13	20 (3%) 50 43	41, 74, 126, 171	0
3	C	130/169 (76%)	1.64	46 (35%) 0 1	77, 152, 200, 232	0
3	G	132/169 (78%)	1.12	32 (24%) 1 1	77, 140, 182, 210	0
All	All	2005/2352 (85%)	0.24	120 (5%) 25 20	40, 80, 158, 232	0

All (120) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	73	VAL	10.5
3	G	73	VAL	7.9
3	C	90	PHE	7.2
3	C	76	ALA	6.5
3	C	77	ALA	6.4
3	C	62	HIS	5.8
3	G	74	GLU	5.6
3	G	78	THR	5.5
3	G	102	ILE	5.4
3	C	21	ALA	5.3
3	C	23	ALA	5.3
3	C	44	LEU	5.2
2	F	55	THR	5.2
2	F	45	CYS	5.2
3	C	59	CYS	5.2
1	E	223	ALA	5.1
3	G	75	GLY	5.1
2	B	43	LEU	5.0
3	C	58	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
3	G	44	LEU	4.8
3	C	22	VAL	4.6
2	B	45	CYS	4.5
3	C	55	VAL	4.5
2	F	28	ILE	4.5
2	B	52	GLU	4.2
3	G	22	VAL	4.2
1	A	223	ALA	4.1
2	F	49	ARG	4.1
2	F	56	ARG	4.1
2	F	29	LEU	3.9
3	C	63	VAL	3.9
2	B	539	ILE	3.9
3	C	108	LEU	3.8
3	G	103	LEU	3.8
3	G	104	ALA	3.7
3	G	72	ALA	3.6
3	G	23	ALA	3.6
1	E	129	ASP	3.6
2	F	43	LEU	3.5
3	C	107	TYR	3.5
1	E	171	ALA	3.5
3	C	124	MET	3.4
3	G	56	ILE	3.4
3	C	56	ILE	3.4
3	C	113	LEU	3.4
2	B	55	THR	3.4
3	C	94	ASP	3.3
2	F	191	LEU	3.3
3	C	60	LYS	3.3
2	B	44	ALA	3.3
3	C	51	ILE	3.2
2	F	539	ILE	3.2
3	G	110	ILE	3.2
1	E	172	VAL	3.1
3	C	72	ALA	3.1
2	F	52	GLU	3.1
2	B	441	THR	3.0
3	G	45	PRO	3.0
2	B	416	HIS	3.0
3	G	95	GLN	2.9
3	G	49	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	110	ILE	2.8
2	F	41	ALA	2.8
3	C	106	ASN	2.7
1	E	234	GLY	2.7
2	B	41	ALA	2.7
1	A	224	SER	2.7
3	C	102	ILE	2.7
3	C	67	ALA	2.7
3	G	29	ILE	2.6
3	C	43	PRO	2.6
3	C	78	THR	2.6
3	C	45	PRO	2.6
3	C	81	ASP	2.6
3	C	88	ALA	2.5
2	F	390	LYS	2.5
3	C	54	LYS	2.5
3	C	75	GLY	2.5
3	C	50	LYS	2.5
2	F	77	PHE	2.5
2	F	48	MET	2.4
3	G	108	LEU	2.4
3	G	107	TYR	2.4
3	G	24	LEU	2.4
3	G	43	PRO	2.4
2	B	393	GLN	2.4
3	G	20	GLU	2.4
3	C	125	ILE	2.4
3	C	74	GLU	2.4
3	G	94	ASP	2.4
1	E	132	TYR	2.3
3	G	89	ASP	2.3
3	G	60	LYS	2.3
2	F	59	LEU	2.3
3	G	101	LEU	2.3
1	E	226	ALA	2.3
2	F	532	GLY	2.3
3	G	30	ALA	2.3
3	C	47	VAL	2.3
3	C	93	ILE	2.2
3	C	92	LYS	2.2
2	F	441	THR	2.2
2	B	449	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	149	GLU	2.2
3	C	86	TRP	2.2
1	E	153	GLU	2.2
2	F	602	THR	2.2
3	C	95	GLN	2.1
3	G	47	VAL	2.1
3	G	55	VAL	2.1
3	C	71	GLU	2.1
3	C	137	PHE	2.1
3	C	65	ALA	2.1
3	G	58	TYR	2.1
3	C	104	ALA	2.1
2	F	538	LEU	2.1
3	G	105	ALA	2.0
2	B	427	ARG	2.0
2	F	374	HIS	2.0
3	G	21	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

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
4	6OM	A	301	7/7	0.75	0.36	3.44	50,51,55,55	0
4	6OM	E	301	7/7	0.80	0.42	2.23	50,51,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.