



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:30 AM UTC

PDB ID : 5HZG / pdb_00005hzg
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

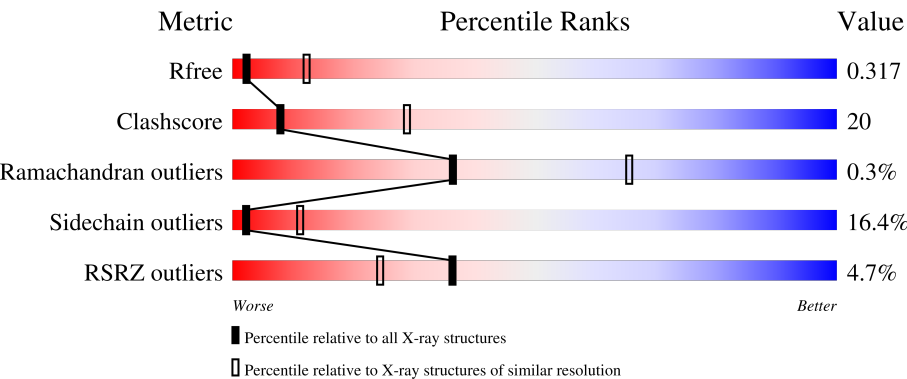
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	66%24%6% . .
1	E	267	3%70%20%7% .
2	B	740	4%47%25%8% . 17%
2	F	740	4%46%24%10% . 17%
3	C	169	9%54%16%7%23%

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Mol	Chain	Length	Quality of chain
3	G	169	

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	-
4	6OM	E	301	-	X	X	-

2 Entry composition

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:

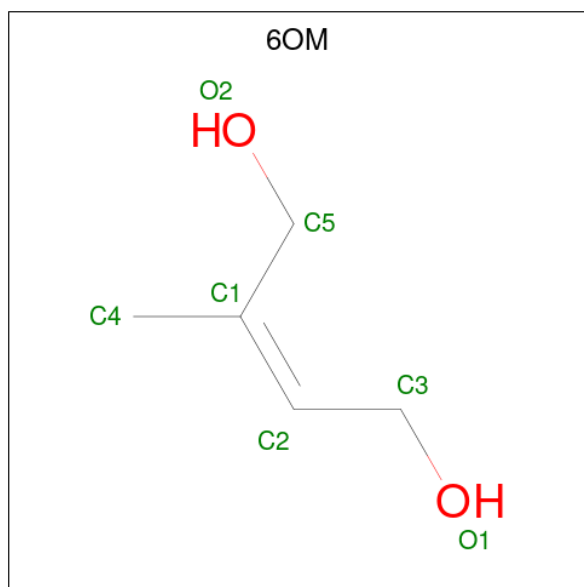
Chain	Residue	Modelled	Actual	Comment	Reference
C	-8	MET	-	expression tag	UNP Q39255
C	-7	ASP	-	expression tag	UNP Q39255
C	-6	TYR	-	expression tag	UNP Q39255
C	-5	LYS	-	expression tag	UNP Q39255
C	-4	ASP	-	expression tag	UNP Q39255
C	-3	ASP	-	expression tag	UNP Q39255

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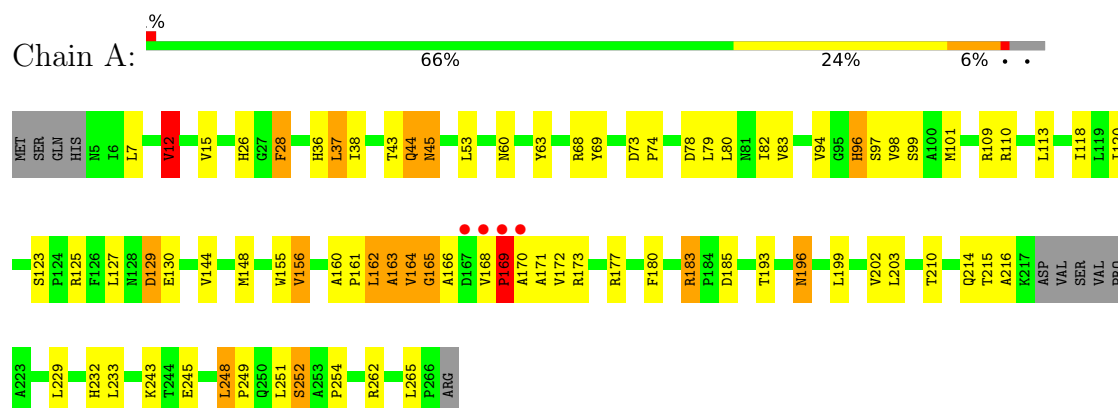
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	5	Total 5	O 5	0	0
5	E	2	Total 2	O 2	0	0
5	F	10	Total 10	O 10	0	0
5	G	4	Total 4	O 4	0	0

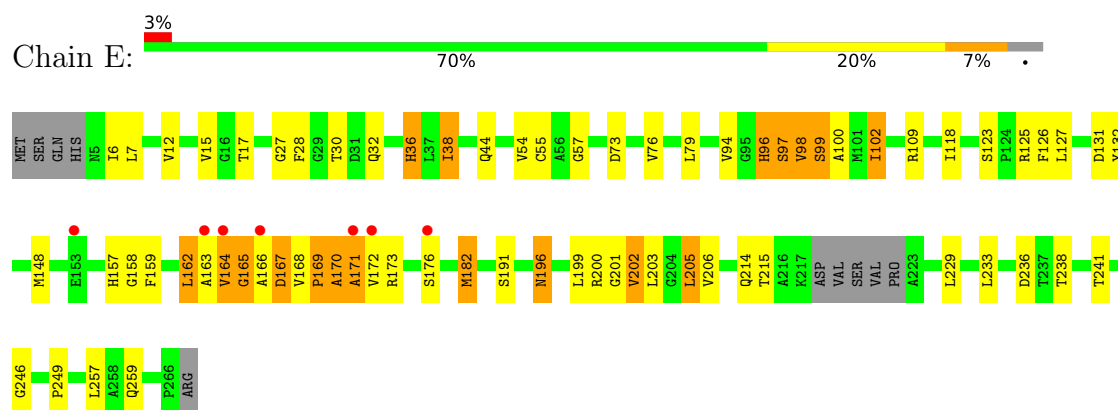
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

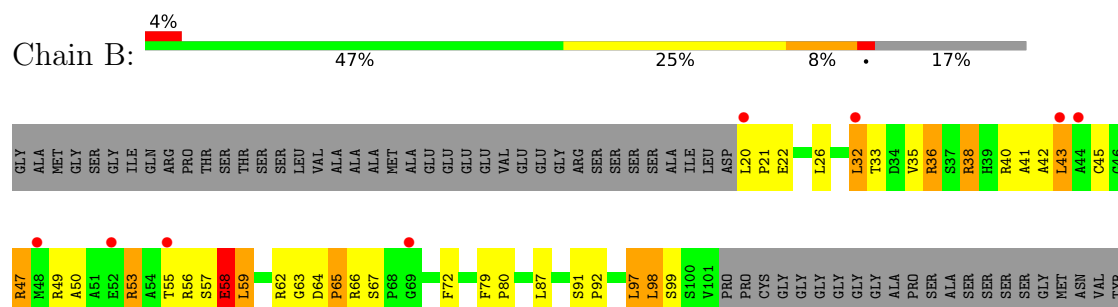
• Molecule 1: Strigolactone esterase D14

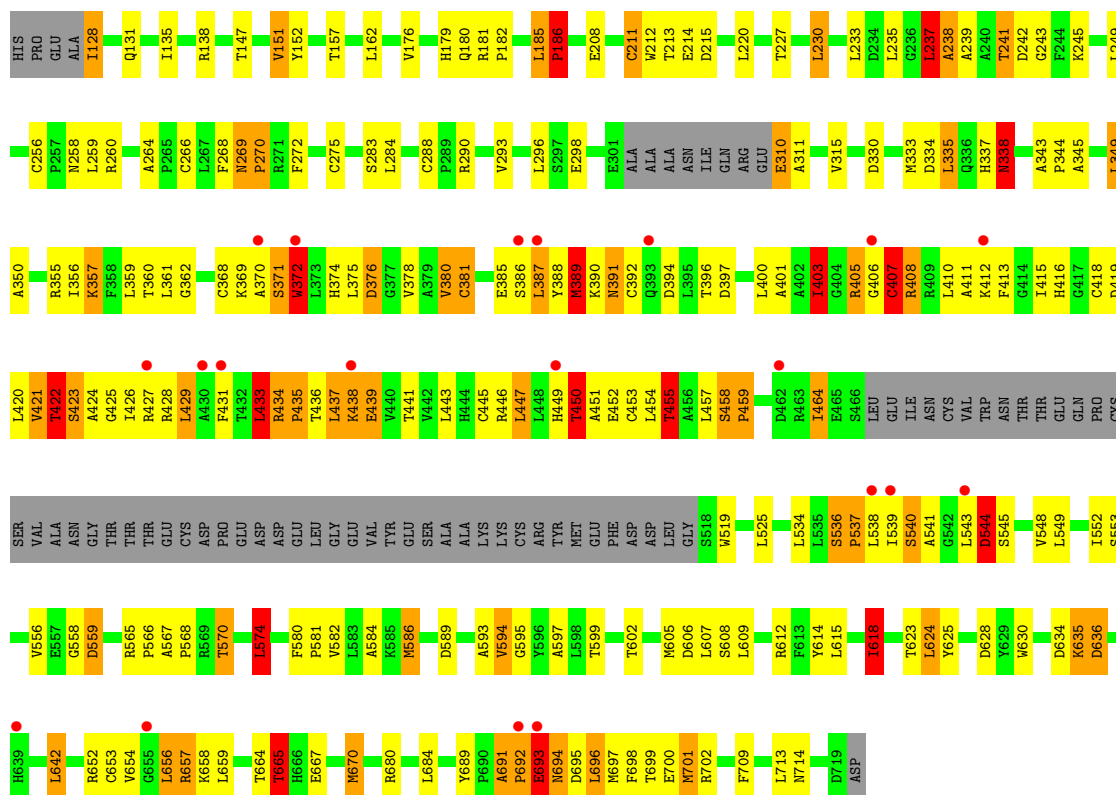


• Molecule 1: Strigolactone esterase D14

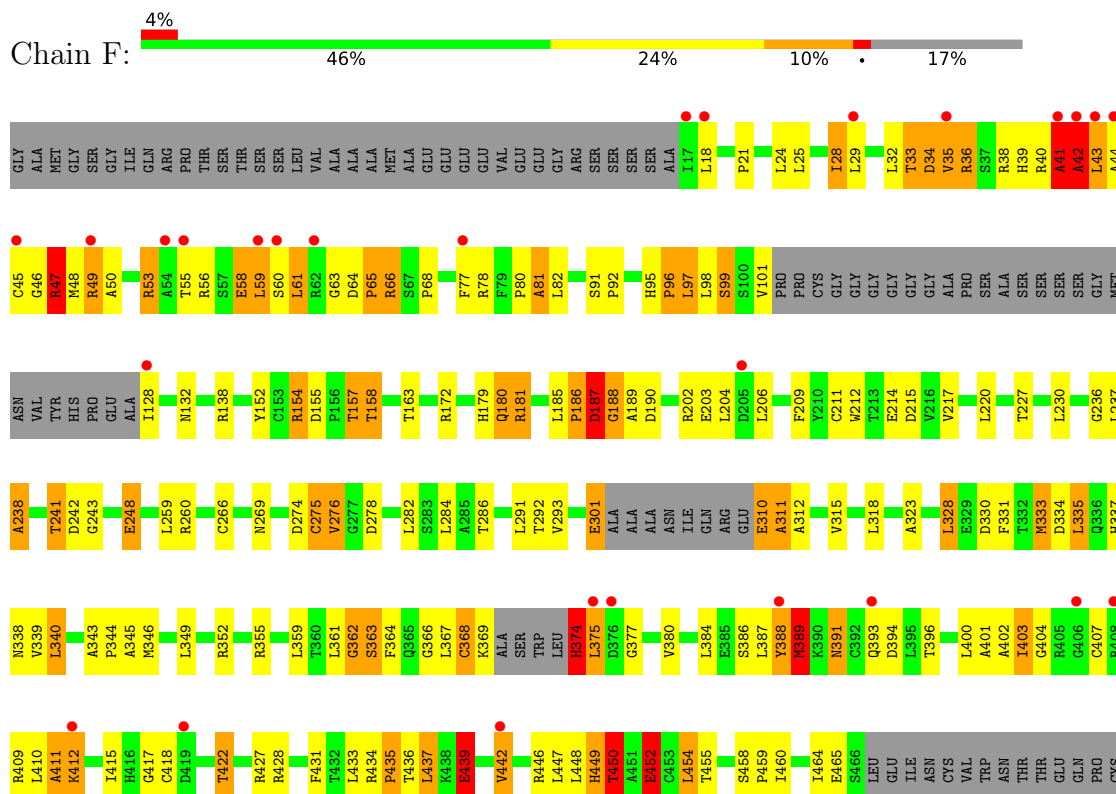


• Molecule 2: F-box/LRR-repeat MAX2 homolog





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



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 (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	81.2	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 83.5	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	0.89	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	0.78	1/2046 (0.0%)	1.32	16/2785 (0.6%)
1	E	0.77	0/2046	1.52	36/2785 (1.3%)
2	B	0.88	5/4904 (0.1%)	1.60	108/6669 (1.6%)
2	F	0.87	7/4892 (0.1%)	1.67	112/6650 (1.7%)
3	C	0.76	0/1036	1.43	12/1397 (0.9%)
3	G	0.76	0/1052	1.24	7/1421 (0.5%)
All	All	0.84	13/15976 (0.1%)	1.54	291/21707 (1.3%)

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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	435	PRO	N-CD	14.06	1.67	1.47
2	F	278	ASP	N-CA	7.53	1.55	1.46
2	B	186	PRO	N-CD	7.02	1.57	1.47
2	F	435	PRO	N-CD	7.02	1.57	1.47
2	F	43	LEU	CA-C	6.61	1.61	1.52
2	B	693	GLU	N-CA	6.20	1.53	1.46
2	F	568	PRO	N-CD	6.16	1.56	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	543	LEU	CA-C	5.75	1.59	1.52
2	B	458	SER	CA-C	5.32	1.59	1.52
1	A	166	ALA	CA-CB	5.26	1.59	1.52
2	B	338	ASN	N-CA	5.23	1.52	1.45
2	F	386	SER	CA-CB	5.22	1.59	1.53
2	F	186	PRO	N-CD	5.20	1.55	1.47

All (291) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	692	PRO	N-CA-C	26.10	151.86	114.80
3	C	95	GLN	N-CA-C	24.38	144.59	111.92
2	F	42	ALA	CA-C-N	23.89	160.62	120.72
2	F	42	ALA	C-N-CA	23.89	160.62	120.72
2	F	597	ALA	CB-CA-C	-22.28	73.39	111.05
2	F	656	LEU	CB-CA-C	-20.41	77.14	110.81
1	A	170	ALA	CB-CA-C	20.38	143.79	111.39
1	E	164	VAL	N-CA-C	19.05	129.30	110.82
1	E	201	GLY	N-CA-C	18.96	145.88	115.73
1	E	171	ALA	N-CA-C	-18.82	87.41	113.37
1	E	169	PRO	CB-CA-C	-18.52	81.00	111.56
2	F	43	LEU	N-CA-C	-18.48	89.99	112.54
2	F	539	ILE	N-CA-C	18.24	128.41	111.45
2	B	692	PRO	N-CA-CB	-17.78	81.35	102.33
3	G	45	PRO	N-CA-C	17.68	135.42	114.20
3	C	94	ASP	N-CA-C	-17.43	80.99	109.40
2	B	421	VAL	N-CA-C	17.40	139.08	113.16
2	B	371	SER	CB-CA-C	-17.38	85.55	109.71
1	E	162	LEU	N-CA-C	17.36	134.77	112.03
2	B	544	ASP	N-CA-C	16.56	137.14	114.12
1	A	169	PRO	CB-CA-C	-16.05	85.07	111.56
2	F	402	ALA	N-CA-C	15.87	144.60	110.80
3	G	46	ASN	N-CA-C	15.84	131.18	111.69
2	F	42	ALA	N-CA-C	15.53	154.50	111.00
2	F	96	PRO	N-CA-C	15.45	144.30	112.47
2	F	653	CYS	N-CA-C	-15.33	87.95	110.64
1	E	163	ALA	N-CA-C	15.15	134.92	108.56
2	F	47	ARG	N-CA-CB	-15.05	87.78	110.20
2	B	545	SER	N-CA-CB	14.98	133.61	110.84
2	B	405	ARG	CB-CA-C	14.94	135.14	111.39
2	B	408	ARG	N-CA-C	-14.76	95.81	114.56
1	A	170	ALA	N-CA-C	-14.73	88.21	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	694	ASN	N-CA-C	14.46	151.48	111.00
2	B	693	GLU	CB-CA-C	-14.34	83.06	111.17
2	F	657	ARG	N-CA-CB	-14.12	88.40	110.28
2	B	65	PRO	N-CA-C	14.03	141.38	112.47
2	F	442	VAL	N-CA-C	-13.89	87.47	107.75
2	B	694	ASN	N-CA-CB	-13.88	86.91	110.50
2	B	407	CYS	N-CA-C	-13.79	90.24	110.64
1	A	171	ALA	N-CA-C	-13.70	92.86	114.09
2	B	405	ARG	N-CA-C	-13.57	90.01	111.04
2	B	422	THR	N-CA-C	-13.44	96.22	112.89
1	E	163	ALA	N-CA-CB	-13.41	92.46	110.57
2	F	42	ALA	N-CA-CB	-13.27	90.49	110.40
2	B	692	PRO	N-CD-CG	-13.19	83.42	103.20
2	B	544	ASP	CB-CA-C	-13.15	87.29	109.38
1	E	170	ALA	N-CA-CB	-12.12	90.00	110.49
3	C	126	LYS	N-CA-C	11.92	126.62	111.24
2	F	238	ALA	N-CA-C	-11.78	92.08	109.63
2	B	371	SER	N-CA-C	11.74	127.56	110.42
2	B	237	LEU	CB-CA-C	-11.30	94.40	112.03
1	E	159	PHE	N-CA-CB	11.29	128.85	111.46
2	B	185	LEU	CA-C-N	11.06	133.67	119.84
2	B	185	LEU	C-N-CA	11.06	133.67	119.84
2	F	636	ASP	N-CA-C	11.03	125.04	112.57
2	F	187	ASP	N-CA-C	11.03	135.35	113.29
2	F	433	LEU	N-CA-C	10.97	126.19	108.63
2	B	372	TRP	N-CA-CB	-10.85	92.06	110.50
2	F	448	LEU	N-CA-C	-10.83	98.28	112.68
2	B	540	SER	N-CA-CB	10.77	124.91	110.59
2	F	657	ARG	N-CA-C	10.77	124.31	111.82
2	F	653	CYS	CB-CA-C	10.71	122.97	109.80
2	B	559	ASP	N-CA-C	10.68	126.48	111.52
2	F	657	ARG	CA-C-N	-10.68	106.03	122.81
2	F	657	ARG	C-N-CA	-10.68	106.03	122.81
2	B	390	LYS	N-CA-C	-10.68	99.28	114.12
2	F	521	MET	N-CA-C	10.63	125.56	112.59
1	A	15	VAL	N-CA-C	10.62	120.01	111.62
2	F	41	ALA	CB-CA-C	-10.37	97.26	112.09
2	F	634	ASP	N-CA-C	-10.22	97.34	110.53
2	B	66	ARG	N-CA-CB	10.21	129.32	111.55
2	F	389	MET	N-CA-CB	-10.13	94.36	110.87
2	F	65	PRO	CB-CA-C	-10.06	94.97	111.56
2	B	372	TRP	N-CA-C	9.96	138.88	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	56	ARG	N-CA-C	-9.93	99.72	112.93
2	F	274	ASP	N-CA-C	-9.87	87.08	107.70
2	B	429	LEU	N-CA-C	-9.79	100.88	113.12
2	F	35	VAL	N-CA-C	9.78	126.09	112.50
2	F	43	LEU	CB-CA-C	-9.70	90.04	110.31
2	B	421	VAL	CB-CA-C	-9.61	88.33	111.02
2	F	537	PRO	CB-CA-C	-9.52	95.85	111.56
2	F	276	VAL	N-CA-C	-9.47	96.48	109.55
2	F	604	GLN	CB-CA-C	-9.43	92.89	109.86
2	F	187	ASP	CB-CA-C	-9.37	92.46	110.35
2	F	654	VAL	N-CA-C	-9.35	94.45	108.85
1	A	170	ALA	N-CA-CB	9.22	123.19	110.10
2	B	389	MET	N-CA-C	-9.18	94.57	108.99
2	B	434	ARG	N-CA-C	9.13	129.99	109.81
1	E	164	VAL	N-CA-CB	-9.08	97.44	110.52
2	F	520	GLU	N-CA-C	-9.06	100.35	111.40
2	B	238	ALA	N-CA-CB	9.05	126.44	112.41
2	B	539	ILE	N-CA-C	8.89	121.85	112.96
1	E	167	ASP	N-CA-C	8.83	120.84	111.03
2	F	597	ALA	N-CA-C	8.80	123.37	108.23
2	B	386	SER	N-CA-C	-8.75	95.25	109.96
1	A	156	VAL	N-CA-C	-8.75	95.84	108.36
3	C	126	LYS	N-CA-CB	-8.75	97.20	110.07
2	B	691	ALA	N-CA-C	8.68	129.00	109.81
3	G	22	VAL	CB-CA-C	8.68	123.09	110.77
2	F	403	ILE	N-CA-C	-8.65	91.34	109.34
2	B	65	PRO	CB-CA-C	-8.64	97.30	111.56
2	F	434	ARG	N-CA-C	8.59	128.80	109.81
2	B	407	CYS	CB-CA-C	8.49	120.24	109.80
2	F	433	LEU	CB-CA-C	-8.49	97.30	110.88
2	B	416	HIS	N-CA-C	8.45	120.26	111.14
2	B	66	ARG	N-CA-C	-8.42	96.47	109.52
2	F	599	THR	N-CA-C	8.41	126.53	112.99
2	B	692	PRO	CB-CA-C	-8.30	99.56	110.27
1	E	97	SER	N-CA-C	8.29	128.46	110.80
2	F	43	LEU	CA-C-O	8.24	129.52	119.38
2	B	369	LYS	N-CA-C	8.24	123.90	112.04
2	F	439	GLU	N-CA-C	8.22	123.87	108.65
2	B	63	GLY	N-CA-C	-8.17	98.21	110.71
1	E	96	HIS	CB-CA-C	8.16	127.30	110.40
1	E	158	GLY	N-CA-C	-8.15	93.86	113.18
3	C	95	GLN	CB-CA-C	-8.12	100.58	111.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	176	SER	CB-CA-C	-8.11	95.42	110.01
2	B	389	MET	CB-CA-C	8.08	127.14	109.94
2	B	264	ALA	N-CA-C	8.05	115.46	108.22
2	B	388	TYR	N-CA-CB	8.04	122.10	110.37
2	B	691	ALA	CB-CA-C	-8.01	94.40	110.17
2	F	188	GLY	N-CA-C	-7.97	94.29	113.18
2	B	458	SER	N-CA-C	7.91	127.30	109.81
2	F	388	TYR	N-CA-C	7.91	124.58	107.49
1	E	157	HIS	N-CA-C	-7.84	100.42	110.53
2	B	435	PRO	CA-N-CD	-7.84	101.03	112.00
2	F	386	SER	N-CA-C	-7.83	96.53	108.67
2	F	598	LEU	N-CA-C	7.67	127.14	110.80
2	F	442	VAL	CB-CA-C	7.62	121.59	110.77
3	G	46	ASN	N-CA-CB	-7.59	98.89	110.20
2	B	538	LEU	N-CA-C	-7.41	103.84	113.17
2	F	388	TYR	CB-CA-C	-7.40	99.22	111.51
2	F	458	SER	N-CA-C	7.36	126.08	109.81
2	B	433	LEU	N-CA-C	7.35	121.77	108.17
1	E	96	HIS	N-CA-C	-7.34	101.06	110.53
3	C	95	GLN	N-CA-CB	-7.33	100.95	112.46
2	B	539	ILE	CB-CA-C	-7.29	104.65	111.06
2	B	381	CYS	N-CA-C	-7.25	98.94	109.59
2	B	390	LYS	N-CA-CB	7.23	120.85	110.88
2	B	540	SER	N-CA-C	-7.15	105.08	113.88
2	B	186	PRO	CA-N-CD	-7.04	102.14	112.00
2	B	450	THR	N-CA-C	-7.02	102.83	111.40
1	A	163	ALA	N-CA-C	7.01	121.44	107.62
2	F	276	VAL	CB-CA-C	7.01	121.30	111.63
2	F	59	LEU	N-CA-C	-6.97	105.19	113.21
2	F	43	LEU	N-CA-CB	6.96	121.94	110.39
3	G	23	ALA	N-CA-C	-6.95	103.14	112.94
2	F	49	ARG	N-CA-C	6.90	121.74	113.12
1	A	165	GLY	N-CA-C	-6.86	96.92	113.18
1	E	166	ALA	N-CA-C	6.85	120.73	112.38
2	B	338	ASN	N-CA-C	6.84	120.74	110.14
2	F	33	THR	CB-CA-C	-6.83	94.09	109.10
2	F	96	PRO	CB-CA-C	-6.82	100.30	111.56
2	F	538	LEU	N-CA-CB	6.82	120.56	110.33
1	E	176	SER	N-CA-C	6.82	121.61	113.16
2	B	433	LEU	CB-CA-C	-6.81	100.17	111.41
2	F	77	PHE	N-CA-C	-6.79	100.14	109.71
2	F	363	SER	N-CA-C	6.79	122.99	113.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	36	ARG	N-CA-C	-6.77	103.36	111.69
1	E	165	GLY	N-CA-C	-6.76	97.15	113.18
2	F	56	ARG	N-CA-C	-6.73	103.73	112.68
1	E	98	VAL	O-C-N	6.64	130.87	122.57
2	B	457	LEU	N-CA-C	-6.64	103.74	110.97
2	F	596	TYR	N-CA-C	6.60	120.25	109.76
2	F	242	ASP	N-CA-C	-6.59	101.38	110.35
2	F	521	MET	N-CA-CB	-6.56	100.42	110.92
1	E	97	SER	CB-CA-C	-6.55	97.38	110.42
1	E	171	ALA	N-CA-CB	-6.55	97.05	110.67
2	B	186	PRO	N-CA-C	6.54	125.95	112.47
2	B	269	ASN	CA-C-N	6.54	127.06	119.47
2	B	269	ASN	C-N-CA	6.54	127.06	119.47
2	F	40	ARG	CB-CA-C	-6.54	97.39	109.29
2	F	600	ALA	N-CA-C	6.52	124.22	109.81
2	F	97	LEU	N-CA-CB	6.50	127.56	111.30
1	A	156	VAL	N-CA-CB	6.50	118.79	110.99
2	F	519	TRP	N-CA-C	-6.47	97.14	108.20
2	F	81	ALA	CB-CA-C	-6.46	101.31	111.51
1	E	98	VAL	CB-CA-C	-6.42	100.76	111.29
2	B	464	ILE	CB-CA-C	-6.40	100.80	111.29
2	B	693	GLU	N-CA-C	-6.37	99.30	108.60
2	B	62	ARG	CB-CA-C	-6.37	101.94	110.79
2	F	82	LEU	N-CA-C	-6.36	96.73	107.99
2	B	537	PRO	N-CA-C	6.36	122.37	113.53
1	E	246	GLY	N-CA-C	6.35	118.58	111.85
3	C	125	ILE	N-CA-C	6.35	122.54	109.34
2	F	543	LEU	N-CA-C	6.29	119.11	110.24
2	B	537	PRO	CB-CA-C	-6.28	102.26	112.62
2	F	311	ALA	CB-CA-C	-6.25	101.12	110.50
2	F	694	ASN	CA-C-N	6.23	132.91	121.70
2	F	694	ASN	C-N-CA	6.23	132.91	121.70
1	E	170	ALA	N-CA-C	-6.22	97.55	110.80
2	F	604	GLN	N-CA-C	6.20	118.59	108.55
2	B	434	ARG	N-CA-CB	-6.17	99.39	110.37
2	B	391	ASN	N-CA-CB	-6.14	101.22	110.73
2	B	58	GLU	N-CA-C	-6.13	104.20	113.89
2	B	370	ALA	N-CA-C	-6.12	97.76	110.80
2	B	657	ARG	N-CA-C	-6.11	105.95	113.41
2	F	404	GLY	N-CA-C	-6.08	105.55	115.46
2	F	434	ARG	N-CA-CB	-6.08	99.55	110.37
1	E	159	PHE	N-CA-C	-6.05	99.76	108.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	450	THR	CB-CA-C	-6.05	99.44	110.63
2	F	605	MET	N-CA-CB	-6.04	100.23	110.50
2	B	691	ALA	C-N-CD	-6.03	100.27	125.00
2	B	455	THR	CB-CA-C	-6.02	101.01	110.94
2	B	387	LEU	CB-CA-C	-6.00	99.56	109.65
1	E	15	VAL	CB-CA-C	-5.97	104.80	110.65
2	F	66	ARG	N-CA-C	-5.94	100.38	109.41
2	F	691	ALA	CA-C-N	5.94	127.27	119.84
2	F	691	ALA	C-N-CA	5.94	127.27	119.84
2	F	35	VAL	CB-CA-C	-5.90	95.53	111.34
2	F	312	ALA	N-CA-CB	-5.89	102.03	110.57
1	E	202	VAL	N-CA-C	-5.88	97.10	109.34
2	F	637	VAL	N-CA-C	5.88	121.58	109.34
3	C	111	LYS	N-CA-C	5.85	117.35	110.97
2	F	542	GLY	N-CA-C	-5.84	102.48	112.30
3	G	95	GLN	N-CA-C	5.82	118.01	108.52
2	B	243	GLY	N-CA-C	5.82	120.04	112.25
2	F	340	LEU	N-CA-C	5.79	120.41	113.23
2	B	408	ARG	N-CA-CB	5.79	118.69	111.00
2	F	464	ILE	N-CA-C	5.77	115.84	107.88
2	B	434	ARG	C-N-CD	-5.75	101.41	125.00
2	F	312	ALA	N-CA-C	5.75	119.83	113.21
2	B	64	ASP	N-CA-CB	5.75	120.91	110.10
2	B	429	LEU	N-CA-CB	5.74	119.21	110.42
2	B	656	LEU	N-CA-CB	-5.73	101.09	110.43
2	B	665	THR	CB-CA-C	-5.71	100.00	110.62
2	B	416	HIS	CB-CA-C	-5.71	101.89	110.90
3	C	108	LEU	N-CA-C	-5.70	99.89	108.96
2	F	600	ALA	N-CA-CB	-5.70	100.22	110.37
2	B	403	ILE	CB-CA-C	-5.69	101.96	111.29
2	F	458	SER	CA-C-N	-5.66	113.73	120.13
2	F	458	SER	C-N-CA	-5.66	113.73	120.13
2	F	652	ARG	N-CA-C	5.61	118.24	111.40
1	E	164	VAL	CB-CA-C	-5.60	104.70	112.04
2	B	574	LEU	CA-C-N	5.59	127.78	120.28
2	B	574	LEU	C-N-CA	5.59	127.78	120.28
2	F	59	LEU	CB-CA-C	-5.59	100.82	110.72
2	F	362	GLY	N-CA-C	5.55	126.33	113.18
1	A	166	ALA	N-CA-C	-5.53	97.58	107.98
1	A	12	VAL	N-CA-C	-5.53	103.97	110.21
2	B	541	ALA	N-CA-C	-5.51	106.23	113.17
1	A	164	VAL	N-CA-C	5.50	120.79	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	270	PRO	CB-CA-C	-5.50	103.08	112.26
2	F	452	GLU	CB-CA-C	5.49	118.02	110.34
1	E	98	VAL	CA-C-N	-5.47	111.00	121.94
1	E	98	VAL	C-N-CA	-5.47	111.00	121.94
2	B	380	VAL	CB-CA-C	-5.44	102.36	111.29
2	B	64	ASP	CA-C-N	5.43	126.62	119.84
2	B	64	ASP	C-N-CA	5.43	126.62	119.84
2	F	411	ALA	N-CA-C	5.37	117.36	108.13
1	E	202	VAL	N-CA-CB	-5.35	102.40	111.23
3	C	100	GLU	CB-CA-C	-5.34	99.96	110.11
2	F	617	GLY	N-CA-C	5.34	125.84	113.18
1	A	129	ASP	CA-C-N	-5.33	112.60	120.38
1	A	129	ASP	C-N-CA	-5.33	112.60	120.38
3	C	127	GLY	N-CA-C	-5.31	107.38	115.66
2	B	242	ASP	N-CA-C	-5.30	102.76	110.24
2	B	684	LEU	N-CA-C	-5.29	100.10	108.73
2	F	65	PRO	N-CA-C	5.29	123.37	112.47
2	F	692	PRO	N-CA-C	5.29	123.37	112.47
2	B	237	LEU	N-CA-C	5.29	117.76	108.56
2	B	391	ASN	N-CA-C	5.25	119.65	112.88
2	F	269	ASN	CA-C-N	5.21	125.26	119.32
2	F	269	ASN	C-N-CA	5.21	125.26	119.32
1	E	15	VAL	N-CA-C	5.21	118.63	113.53
2	B	72	PHE	N-CA-C	-5.20	99.28	108.23
2	F	615	LEU	CB-CA-C	-5.19	101.84	110.81
2	B	421	VAL	O-C-N	5.17	128.28	122.18
2	B	618	ILE	N-CA-C	5.16	120.08	109.34
2	B	47	ARG	N-CA-C	5.16	117.30	111.11
2	F	39	HIS	CB-CA-C	-5.15	99.86	110.38
2	F	458	SER	N-CA-CB	-5.14	101.21	110.37
2	F	460	ILE	CB-CA-C	5.14	119.32	112.22
2	B	386	SER	CB-CA-C	5.13	118.00	109.53
2	B	435	PRO	N-CA-C	-5.12	101.92	112.47
3	C	110	ILE	CB-CA-C	-5.12	105.41	111.09
2	B	381	CYS	N-CA-CB	5.09	117.55	109.71
1	E	36	HIS	N-CA-C	5.09	118.96	112.34
3	G	44	LEU	N-CA-C	5.08	116.46	108.23
2	B	185	LEU	N-CA-C	-5.08	102.89	110.20
2	B	458	SER	N-CA-CB	-5.07	101.34	110.37
1	E	54	VAL	N-CA-C	5.07	117.39	111.05
2	F	186	PRO	CA-N-CD	-5.07	104.91	112.00
2	B	56	ARG	N-CA-CB	5.05	119.12	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	459	PRO	N-CA-CB	5.04	108.54	103.25
2	F	572	PHE	N-CA-C	-5.03	102.84	110.28
1	A	216	ALA	N-CA-C	5.02	116.42	110.19
2	B	418	CYS	N-CA-CB	-5.02	101.88	110.16
2	F	401	ALA	N-CA-C	-5.01	105.48	112.45
2	F	604	GLN	CA-C-N	5.01	130.71	121.70
2	F	604	GLN	C-N-CA	5.01	130.71	121.70

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	46	0
1	E	2001	0	1972	54	0
2	B	4791	0	4814	233	0
2	F	4782	0	4808	229	0
3	C	1024	0	1011	74	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	615	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 20.

All (615) 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
2:B:389:MET:HE1	2:B:392:CYS:CA	1.19	1.56
1:E:170:ALA:CB	1:E:172:VAL:HB	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:CB	1.42	1.47
2:B:389:MET:CE	2:B:392:CYS:N	1.77	1.45
2:B:270:PRO:CG	2:B:311:ALA:HB1	1.47	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
2:B:389:MET:HE1	2:B:392:CYS:N	1.37	1.35
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	2:B:433:LEU:O	1.35	1.22
2:B:389:MET:SD	2:B:392:CYS:HB2	1.78	1.21
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:21:PRO:HD3	3:C:99:PHE:CZ	1.89	1.07
2:B:389:MET:HE2	2:B:392:CYS:CB	1.82	1.06
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
2:B:389:MET:HE3	2:B:392:CYS:N	1.65	1.05
3:C:97:THR:HA	3:C:99:PHE:H	1.21	1.05
1:E:170:ALA:C	1:E:172:VAL:N	2.00	1.04
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:697:MET:HE3	2:F:697:MET:H	1.20	1.02
2:F:92:PRO:HB2	2:F:95:HIS:NE2	1.72	1.02
1:A:161:PRO:C	1:A:162:LEU:HD23	1.84	1.02
1:A:169:PRO:O	1:A:169:PRO:HG2	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:C5	4:E:301:6OM:O1	2.02	1.00
2:B:394:ASP:O	2:B:422:THR:CG2	2.08	1.00
2:F:43:LEU:HD22	3:G:155:ASN:CG	1.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:B:433:LEU:CD2	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:394:ASP:C	2:B:422:THR:HG21	1.89	0.97
2:B:270:PRO:CG	2:B:311:ALA:CB	2.39	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
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:O	1:A:169:PRO:CG	2.03	0.94
1:E:170:ALA:C	1:E:172:VAL:H	1.61	0.93
2:F:652:ARG:O	2:F:653:CYS:C	2.11	0.93
2:F:25:LEU:CD2	2:F:49:ARG:HE	1.79	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:B:389:MET:HE2	2:B:392:CYS:HB2	1.46	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:F:697:MET:HE3	2:F:697:MET:N	1.86	0.89
2:B:693:GLU:HG2	2:B:694:ASN:N	1.71	0.89
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:653:CYS:C	2:B:656:LEU:CD1	2.46	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:389:MET:HE1	2:B:392:CYS:HA	1.56	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
2:F:366:GLY:HA2	2:F:391:ASN:HD21	1.42	0.84
2:B:21:PRO:CD	3:C:99:PHE:HE1	1.89	0.84
3:C:125:ILE:O	3:C:125:ILE:HG22	1.74	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:O	2:F:388:TYR:HD1	1.59	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:406:GLY:O	2:B:407:CYS:C	2.24	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:O	2:B:421:VAL:CG1	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:F:391:ASN:C	2:F:391:ASN:HD22	1.90	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:B:55:THR:O	2:B:80:PRO:HD2	1.83	0.78
2:B:389:MET:HE2	2:B:392:CYS:HB3	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:187:ASP:OD1	2:F:187:ASP:C	2.28	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:F:99:SER:O	2:F:157:THR:OG1	2.02	0.76
2:F:639:HIS:CE1	2:F:699:THR:HA	2.19	0.76
2:B:581:PRO:O	2:B:623:THR:HG21	1.85	0.76
2:B:372:TRP:H	2:B:372:TRP:CD1	2.02	0.74
2:F:447:LEU:HD22	2:F:538:LEU:O	1.86	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
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:F:92:PRO:HB2	2:F:95:HIS:HD2	0.94	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
3:C:96:ALA:HA	3:C:97:THR:C	2.12	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:389:MET:HE3	2:B:391:ASN:C	2.15	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: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
1:A:196:ASN:C	1:A:196:ASN:HD22	2.00	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:97:THR:HG23	3:C:99:PHE:C	2.16	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
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
2:B:605:MET:HE3	2:B:609:LEU:HD13	1.75	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:47:ARG:CD	3:G:142:ASP:OD2	2.39	0.68
2:F:400:LEU:HD13	2:F:403:ILE:HD11	1.76	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:O	2:B:433:LEU:CG	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:F:42:ALA:C	2:F:44:ALA:H	1.93	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:653:CYS:C	2:B:656:LEU:HD11	2.19	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: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:29:LEU:HD11	2:F:49:ARG:NE	2.12	0.64
2:F:411:ALA:HB2	2:F:437:LEU:HD13	1.77	0.64
2:F:237:LEU:HD12	2:F:241:THR:HG21	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:346:MET:HB2	2:F:375:LEU:HD22	1.80	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
1:E:167:ASP:O	1:E:168:VAL:CG1	2.46	0.63
2:F:604:GLN:O	2:F:604:GLN:CD	2.42	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
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: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:311:ALA:HB2	2:F:338:ASN:O	2.00	0.60
2:F:318:LEU:HD21	2:F:333:MET:HE1	1.83	0.60
2:B:269:ASN:HA	2:B:337:HIS:HD2	1.66	0.60
2:F:187:ASP:OD1	2:F:188:GLY:N	2.35	0.60
2:B:362:GLY:HA2	2:B:387:LEU:HD12	1.84	0.60
2:B:670:MET:HE3	2:B:709:PHE:HB2	1.82	0.60
2:B:335:LEU:N	2:B:335:LEU:HD23	2.16	0.60
2:B:387:LEU:O	2:B:413:PHE:O	2.20	0.59
2:B:403:ILE:O	2:B:403:ILE:CG2	2.39	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
1:E:169:PRO:O	1:E:170:ALA:C	2.46	0.58
2:F:43:LEU:CA	2:F:50:ALA:CB	2.77	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:697:MET:H	2:F:697:MET:CE	2.06	0.58
2:B:401:ALA:CB	2:B:429:LEU:HD12	2.34	0.58
2:F:388:TYR:CD1	2:F:388:TYR:C	2.74	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:B:653:CYS:C	2:B:656:LEU:HD12	2.23	0.57
2:F:45:CYS:CB	3:G:134:ARG:CZ	2.81	0.57
1:E:169:PRO:C	1:E:170:ALA:O	2.41	0.57
2:F:43:LEU:HD22	3:G:155:ASN:ND2	2.19	0.57
2:F:719:ASP:OD1	2:F:719:ASP:N	2.35	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:187:ASP:O	2:F:215:ASP:CG	2.47	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:F:34:ASP:OD1	2:F:34:ASP:C	2.48	0.56
2:B:65:PRO:HB3	3:C:160:GLU:HB2	1.86	0.55
2:B:389:MET:CE	2:B:391:ASN:C	2.68	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:28:ILE:HG21	2:F:49:ARG:HH22	1.71	0.55
2:F:35:VAL:HG12	2:F:35:VAL:O	2.07	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:B:606:ASP:OD1	2:B:608:SER:OG	2.23	0.55
2:F:45:CYS:HB2	3:G:134:ARG:CZ	2.37	0.55
2:B:581:PRO:C	2:B:623:THR:HG21	2.32	0.55
2:F:34:ASP:OD1	2:F:36:ARG:N	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:574:LEU:HD11	2:F:586:MET:HE1	1.89	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
2:B:36:ARG:HH21	2:B:657:ARG:HH12	1.48	0.54
2:B:212:TRP:HE3	2:B:215:ASP:OD1	1.91	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:O	2:F:403:ILE:HG13	2.07	0.54
2:F:293:VAL:HG22	2:F:330:ASP:HB3	1.90	0.53
2:B:420:LEU:N	2:B:420:LEU:CD2	2.71	0.53
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:401:ALA:HB2	2:B:429:LEU:HD12	1.89	0.53
2:B:420:LEU:HD23	2:B:420:LEU:H	1.73	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:F:42:ALA:C	2:F:44:ALA:N	2.56	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:F:333:MET:HE3	2:F:364:PHE:HZ	1.74	0.53
2:B:268:PHE:HE2	2:B:335:LEU:HD22	1.73	0.53
1:E:170:ALA:O	1:E:171:ALA:C	2.48	0.53
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:B:258:ASN:HD22	2:B:290:ARG:HD3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:129:ASP:O	1:A:130:GLU:C	2.50	0.52
1:E:131:ASP:HA	1:E:132:TYR:C	2.33	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
1:A:160:ALA:C	1:A:162:LEU:CD2	2.84	0.51
1:E:167:ASP:C	1:E:168:VAL:HG13	2.36	0.51
2:F:334:ASP:HA	2:F:362:GLY:HA3	1.92	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:N	2:B:376:ASP:OD1	2.44	0.50
2:B:394:ASP:HA	2:B:422:THR:OG1	2.11	0.50
2:B:701:MET:HE3	2:B:702:ARG:C	2.36	0.50
2:F:652:ARG:O	2:F:654:VAL:HG23	2.12	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:605:MET:HE3	2:F:609:LEU:HD13	1.92	0.50
1:A:196:ASN:C	1:A:196:ASN:ND2	2.69	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:446:ARG:C	2:B:447:LEU:HD22	2.37	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
2:F:310:GLU:N	2:F:311:ALA:CA	2.73	0.50
2:B:334:ASP:OD1	2:B:387:LEU:CD1	2.60	0.49
2:B:419:ASP:C	2:B:421:VAL:H	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD13	2:F:696:LEU:O	2.13	0.49
1:E:170:ALA:CA	1:E:172:VAL:H	2.24	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
2:F:436:THR:C	2:F:437:LEU:HD12	2.38	0.49
1:A:36:HIS:CE1	1:A:37:LEU:HD13	2.48	0.49
2:F:92:PRO:CA	2:F:95:HIS:HD2	2.22	0.49
2:F:626:GLU:HG2	2:F:658:LYS:HD2	1.94	0.49
2:B:436:THR:C	2:B:437:LEU:HD12	2.38	0.49
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:41:ALA:HB2	3:G:133:ILE:HD13	1.93	0.48
2:F:237:LEU:HD12	2:F:241:THR:CG2	2.43	0.48
2:B:179:HIS:CE1	2:B:691:ALA:O	2.66	0.48
2:B:411:ALA:HB2	2:B:437:LEU:HD13	1.94	0.48
2:B:389:MET:HE2	2:B:392:CYS:H	1.68	0.48
1:E:27:GLY:HA2	1:E:98:VAL:HG12	1.95	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:F:455:THR:O	2:F:459:PRO:HD3	2.13	0.48
2:B:270:PRO:CD	2:B:311:ALA:CB	2.90	0.48
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
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: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:43:LEU:HB3	3:C:151:VAL:HG12	1.96	0.47
2:B:99:SER:HB2	2:B:157:THR:OG1	2.14	0.47
2:F:49:ARG:NH1	3:G:125:ILE:CD1	2.58	0.47
2:F:637:VAL:CG2	2:F:639:HIS:HB2	2.45	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:CYS:O	3:C:143:PHE:CD1	2.68	0.47
2:B:334:ASP:OD1	2:B:387:LEU:HD13	2.13	0.47
2:F:185:LEU:C	2:F:187:ASP:H	2.22	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:B:419:ASP:C	2:B:421:VAL:N	2.70	0.47
2:F:24:LEU:HD13	3:G:102:ILE:HG22	1.97	0.47
2:F:428:ARG:CA	2:F:454:LEU:HD23	2.44	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
2:F:695:ASP:HA	2:F:697:MET:HE1	1.95	0.47
1:A:94:VAL:HG22	1:A:118:ILE:HD12	1.97	0.47
1:A:160:ALA:CB	1:A:162:LEU:HD21	2.45	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:574:LEU:HD23	2:B:618:ILE:HG23	1.96	0.47
2:B:584:ALA:HB1	2:B:625:TYR:HB3	1.97	0.47
2:B:709:PHE:CD1	2:B:709:PHE:C	2.93	0.47
3:C:99:PHE:HD1	3:C:99:PHE:O	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:F:361:LEU:HD13	2:F:367:LEU:HD21	1.97	0.46
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:163:ALA:O	1:A:180:PHE:CE1	2.68	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
2:B:634:ASP:O	2:B:635:LYS:C	2.58	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:B:565:ARG:O	2:B:566:PRO:C	2.59	0.46
2:F:606:ASP:OD2	2:F:608:SER:OG	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:391:ASN:C	2:F:391:ASN:ND2	2.64	0.46
1:A:127:LEU:C	1:A:127:LEU:HD23	2.41	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
1:E:164:VAL:HG22	2:F:608:SER:HB2	1.98	0.45
2:F:43:LEU:HA	2:F:50:ALA:HA	1.98	0.45
2:F:186:PRO:HG2	2:F:189:ALA:HB3	1.97	0.45
2:F:697:MET:HE3	2:F:697:MET:CA	2.46	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: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:B:605:MET:HE3	2:B:609:LEU:CD1	2.43	0.45
2:F:217:VAL:HG21	2:F:248:GLU:CB	2.47	0.45
2:B:20:LEU:CB	3:C:99:PHE:CZ	2.76	0.45
2:B:567:ALA:O	2:B:568:PRO:C	2.59	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
1:A:160:ALA:C	1:A:162:LEU:HD23	2.42	0.45
1:E:196:ASN:HD22	1:E:196:ASN:C	2.24	0.45
2:F:91:SER:HA	2:F:92:PRO:C	2.42	0.45
3:G:134:ARG:HG2	3:G:134:ARG:H	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:N	1:A:162:LEU:CD2	2.72	0.45
2:B:42:ALA:HB1	2:B:50:ALA:N	2.31	0.45
2:B:368:CYS:O	2:B:396:THR:HG22	2.15	0.45
2:F:243:GLY:HA3	2:F:266:CYS:C	2.42	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:F:449:HIS:CD2	2:F:449:HIS:C	2.94	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:47:ARG:HA	2:F:50:ALA:HB3	2.00	0.44
2:F:446:ARG:C	2:F:447:LEU:HD12	2.41	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:658:LYS:NZ	3:G:159:PHE:CZ	2.76	0.44
2:F:696:LEU:HA	2:F:696:LEU:HD22	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:268:PHE:CE2	2:B:335:LEU:HD22	2.53	0.44
2:B:605:MET:HE1	2:B:609:LEU:HD13	1.98	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:597:ALA:HB2	2:B:634:ASP:CB	2.45	0.44
3:C:105:ALA:O	3:C:108:LEU:O	2.36	0.44
2:B:372:TRP:CD1	2:B:372:TRP:N	2.68	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:33:THR:HG22	2:B:59:LEU:HD11	2.00	0.43
2:B:268:PHE:HD2	2:B:335:LEU:HD13	1.83	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:160:ALA:C	1:A:162:LEU:HD21	2.42	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:B:389:MET:HE2	2:B:389:MET:HB3	1.61	0.43
2:F:58:GLU:C	2:F:60:SER:H	2.24	0.43
2:F:42:ALA:HB1	2:F:50:ALA:N	2.33	0.43
2:F:389:MET:H	2:F:415:ILE:HG12	1.84	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
2:B:559:ASP:HA	2:B:594:VAL:HG12	2.00	0.43
2:B:670:MET:HE3	2:B:709:PHE:CB	2.47	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:667:GLU:HA	2:B:670:MET:HE2	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:91:SER:HA	2:B:92:PRO:C	2.44	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: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:F:301:GLU:N	2:F:301:GLU:CD	2.78	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:B:689:TYR:CD1	2:B:689:TYR:C	2.98	0.41
2:F:59:LEU:HG	2:F:61:LEU:HG	2.03	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
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
1:E:98:VAL:HG12	1:E:99:SER:H	1.85	0.41
2:F:185:LEU:C	2:F:187:ASP:N	2.79	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:392:CYS:HB3	2:B:415:ILE:HG21	2.02	0.41
2:B:397:ASP:HB3	2:B:426:ILE:HD11	2.02	0.41
2:B:454:LEU:H	2:B:454:LEU:HD12	1.86	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:B:394:ASP:HA	2:B:422:THR:HG21	2.00	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:148:MET:HE3	1:E:148:MET:HB2	1.91	0.41
2:F:625:TYR:O	2:F:625:TYR:CG	2.74	0.41
2:F:343:ALA:HB3	2:F:344:PRO:HD3	2.02	0.41
2:B:270:PRO:C	2:B:272:PHE:H	2.28	0.41
2:B:425:GLY:O	2:B:428:ARG:HB3	2.21	0.41
2:F:97:LEU:HD23	2:F:97:LEU:HA	1.97	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:368:CYS:HA	2:F:374:HIS:HB3	2.03	0.41
2:F:446:ARG:O	2:F:447:LEU:HB2	2.19	0.41
2:F:616:HIS:O	2:F:616:HIS:CG	2.74	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:98:LEU:HD22	2:F:132:ASN:CA	2.50	0.40
2:F:282:LEU:HD12	2:F:286:THR:HG23	2.02	0.40
2:B:233:LEU:CD2	2:B:235:LEU:HD21	2.51	0.40
2:B:259:LEU:HD12	2:B:259:LEU:HA	1.95	0.40
2:F:343:ALA:CB	2:F:344:PRO:CD	2.99	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%)	30	60
1	E	253/267 (95%)	221 (87%)	32 (13%)	0	100	100
2	B	607/740 (82%)	517 (85%)	89 (15%)	1 (0%)	43	71
2	F	604/740 (82%)	516 (85%)	86 (14%)	2 (0%)	36	65
3	C	123/169 (73%)	101 (82%)	20 (16%)	2 (2%)	7	31
3	G	126/169 (75%)	108 (86%)	18 (14%)	0	100	100
All	All	1966/2352 (84%)	1687 (86%)	273 (14%)	6 (0%)	36	65

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%)	3	14
1	E	214/226 (95%)	188 (88%)	26 (12%)	5	20
2	B	519/615 (84%)	419 (81%)	100 (19%)	1	6
2	F	519/615 (84%)	420 (81%)	99 (19%)	1	7
3	C	110/146 (75%)	103 (94%)	7 (6%)	16	44
3	G	112/146 (77%)	99 (88%)	13 (12%)	5	21
All	All	1688/1974 (86%)	1412 (84%)	276 (16%)	2	11

All (276) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	28	PHE
1	A	37	LEU
1	A	38	ILE
1	A	43	THR
1	A	44	GLN
1	A	45	ASN
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	156	VAL
1	A	162	LEU
1	A	168	VAL
1	A	172	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
2	B	26	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	67	SER
2	B	97	LEU

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Mol	Chain	Res	Type
2	B	98	LEU
2	B	128	ILE
2	B	138	ARG
2	B	147	THR
2	B	151	VAL
2	B	180	GLN
2	B	181	ARG
2	B	186	PRO
2	B	208	GLU
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	260	ARG
2	B	266	CYS
2	B	275	CYS
2	B	283	SER
2	B	284	LEU
2	B	288	CYS
2	B	296	LEU
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	360	THR
2	B	372	TRP
2	B	374	HIS
2	B	375	LEU
2	B	376	ASP
2	B	389	MET
2	B	403	ILE
2	B	405	ARG
2	B	407	CYS
2	B	422	THR
2	B	423	SER
2	B	433	LEU
2	B	435	PRO

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Mol	Chain	Res	Type
2	B	437	LEU
2	B	438	LYS
2	B	439	GLU
2	B	441	THR
2	B	443	LEU
2	B	447	LEU
2	B	450	THR
2	B	455	THR
2	B	464	ILE
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	574	LEU
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
2	B	652	ARG
2	B	654	VAL
2	B	659	LEU
2	B	664	THR
2	B	665	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

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Mol	Chain	Res	Type
2	B	700	GLU
2	B	701	MET
2	B	713	LEU
2	B	714	ASN
3	C	52	LEU
3	C	93	ILE
3	C	97	THR
3	C	112	ASN
3	C	120	THR
3	C	150	GLU
3	C	160	GLU
1	E	6	ILE
1	E	17	THR
1	E	30	THR
1	E	38	ILE
1	E	44	GLN
1	E	73	ASP
1	E	79	LEU
1	E	99	SER
1	E	102	ILE
1	E	109	ARG
1	E	125	ARG
1	E	127	LEU
1	E	162	LEU
1	E	182	MET
1	E	191	SER
1	E	196	ASN
1	E	199	LEU
1	E	205	LEU
1	E	206	VAL
1	E	214	GLN
1	E	215	THR
1	E	229	LEU
1	E	236	ASP
1	E	238	THR
1	E	241	THR
1	E	259	GLN
2	F	18	LEU
2	F	28	ILE
2	F	32	LEU
2	F	34	ASP
2	F	47	ARG

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Mol	Chain	Res	Type
2	F	48	MET
2	F	53	ARG
2	F	58	GLU
2	F	61	LEU
2	F	64	ASP
2	F	78	ARG
2	F	99	SER
2	F	128	ILE
2	F	138	ARG
2	F	154	ARG
2	F	155	ASP
2	F	157	THR
2	F	158	THR
2	F	163	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	214	GLU
2	F	230	LEU
2	F	248	GLU
2	F	259	LEU
2	F	275	CYS
2	F	284	LEU
2	F	301	GLU
2	F	310	GLU
2	F	328	LEU
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	369	LYS
2	F	374	HIS
2	F	375	LEU
2	F	380	VAL
2	F	384	LEU
2	F	387	LEU

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Mol	Chain	Res	Type
2	F	389	MET
2	F	391	ASN
2	F	407	CYS
2	F	409	ARG
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	465	GLU
2	F	522	LEU
2	F	526	SER
2	F	530	SER
2	F	536	SER
2	F	568	PRO
2	F	577	LEU
2	F	582	VAL
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	612	ARG
2	F	618	ILE
2	F	623	THR
2	F	624	LEU
2	F	626	GLU
2	F	635	LYS
2	F	636	ASP
2	F	639	HIS
2	F	641	SER
2	F	652	ARG
2	F	653	CYS
2	F	654	VAL
2	F	656	LEU
2	F	657	ARG
2	F	665	THR
2	F	679	LEU
2	F	693	GLU

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Mol	Chain	Res	Type
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	718	ILE
2	F	719	ASP
3	G	52	LEU
3	G	71	GLU
3	G	93	ILE
3	G	97	THR
3	G	99	PHE
3	G	111	LYS
3	G	112	ASN
3	G	119	GLN
3	G	120	THR
3	G	126	LYS
3	G	135	THR
3	G	139	ILE
3	G	160	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	45	ASN
1	A	67	ASN
1	A	196	ASN
1	A	256	GLN
2	B	27	HIS
2	B	131	GLN
2	B	167	GLN
2	B	179	HIS
2	B	180	GLN
2	B	258	ASN
2	B	337	HIS
2	B	668	HIS
2	B	683	GLN
1	E	32	GLN

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Mol	Chain	Res	Type
1	E	151	ASN
1	E	196	ASN
1	E	214	GLN
2	F	39	HIS
2	F	95	HIS
2	F	179	HIS
2	F	180	GLN
2	F	374	HIS
2	F	391	ASN
2	F	444	HIS
2	F	604	GLN
2	F	633	GLN
2	F	638	HIS
2	F	668	HIS
2	F	683	GLN
2	F	717	GLN
3	G	46	ASN
3	G	106	ASN
3	G	141	ASN
3	G	156	GLN

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 oligosaccharides 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	E	301	-	6,6,6	3.41	5 (83%)	5,6,6	1.89	2 (40%)
4	6OM	A	301	-	6,6,6	3.41	5 (83%)	5,6,6	1.89	2 (40%)

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	E	301	-	-	3/5/5/5	-
4	6OM	A	301	-	-	3/5/5/5	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	301	6OM	C2-C1	5.53	1.45	1.33
4	E	301	6OM	C2-C1	5.53	1.45	1.33
4	E	301	6OM	C4-C1	-3.80	1.41	1.50
4	A	301	6OM	C4-C1	-3.78	1.41	1.50
4	E	301	6OM	O2-C5	-3.14	1.31	1.41
4	A	301	6OM	O2-C5	-3.13	1.31	1.41
4	A	301	6OM	O1-C3	-2.83	1.31	1.41
4	E	301	6OM	O1-C3	-2.82	1.31	1.41
4	A	301	6OM	C3-C2	-2.24	1.45	1.50
4	E	301	6OM	C3-C2	-2.23	1.45	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	301	6OM	C3-C2-C1	-3.36	115.22	126.38
4	E	301	6OM	C3-C2-C1	-3.35	115.25	126.38
4	E	301	6OM	O2-C5-C1	-2.19	106.12	112.22
4	A	301	6OM	O2-C5-C1	-2.18	106.15	112.22

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	6OM	C1-C2-C3-O1
4	E	301	6OM	C1-C2-C3-O1
4	A	301	6OM	C4-C1-C5-O2
4	E	301	6OM	C4-C1-C5-O2
4	A	301	6OM	C2-C1-C5-O2
4	E	301	6OM	C2-C1-C5-O2

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	301	6OM	5	0
4	A	301	6OM	4	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(Å²)	Q<0.9
1	A	257/267 (96%)	-0.13	4 (1%)	70	52	41, 65, 119, 148	0
1	E	257/267 (96%)	0.18	7 (2%)	56	37	53, 86, 155, 192	0
2	B	615/740 (83%)	0.20	28 (4%)	37	25	40, 78, 124, 159	0
2	F	614/740 (82%)	0.26	32 (5%)	33	22	41, 74, 126, 171	0
3	C	130/169 (76%)	0.71	15 (11%)	9	8	77, 152, 200, 232	0
3	G	132/169 (78%)	0.61	8 (6%)	27	18	77, 140, 182, 210	0
All	All	2005/2352 (85%)	0.23	94 (4%)	36	24	40, 80, 158, 232	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	45	CYS	7.1
2	F	49	ARG	6.2
2	F	375	LEU	5.9
2	F	538	LEU	5.9
2	B	43	LEU	5.3
2	F	43	LEU	5.2
2	B	449	HIS	5.1
2	B	539	ILE	4.3
2	F	59	LEU	4.1
2	F	44	ALA	4.1
2	F	393	GLN	4.1
2	B	427	ARG	4.0
2	F	55	THR	4.0
3	C	94	ASP	3.9
2	B	438	LYS	3.9
2	B	393	GLN	3.8
2	B	44	ALA	3.7
3	C	95	GLN	3.7
3	C	22	VAL	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	538	LEU	3.6
2	B	387	LEU	3.5
3	G	94	ASP	3.4
1	E	171	ALA	3.4
1	A	168	VAL	3.4
3	G	56	ILE	3.3
2	F	17	ILE	3.3
3	G	95	GLN	3.3
2	B	639	HIS	3.3
1	E	176	SER	3.2
2	B	543	LEU	3.2
1	A	170	ALA	3.2
2	B	430	ALA	3.1
2	F	406	GLY	3.1
2	F	60	SER	3.1
2	F	54	ALA	3.0
2	F	62	ARG	3.0
1	E	172	VAL	3.0
2	B	431	PHE	3.0
2	F	205	ASP	3.0
2	F	408	ARG	3.0
1	E	163	ALA	3.0
2	F	41	ALA	2.9
2	B	52	GLU	2.8
3	C	58	TYR	2.8
3	C	90	PHE	2.7
1	E	153	GLU	2.7
2	F	653	CYS	2.7
2	B	693	GLU	2.7
3	C	76	ALA	2.7
3	C	105	ALA	2.7
2	B	20	LEU	2.6
2	B	370	ALA	2.6
3	C	73	VAL	2.5
2	B	386	SER	2.5
3	C	93	ILE	2.5
3	C	108	LEU	2.5
3	G	156	GLN	2.4
2	F	442	VAL	2.4
2	B	412	LYS	2.4
2	F	658	LYS	2.4
2	F	77	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	543	LEU	2.3
3	C	142	ASP	2.3
3	C	125	ILE	2.3
3	C	23	ALA	2.3
2	F	412	LYS	2.3
2	F	388	TYR	2.3
3	G	22	VAL	2.3
2	B	55	THR	2.3
2	F	42	ALA	2.2
2	B	32	LEU	2.2
1	A	167	ASP	2.2
2	B	69	GLY	2.2
2	B	406	GLY	2.2
2	B	655	GLY	2.2
3	C	21	ALA	2.2
3	G	93	ILE	2.2
2	B	692	PRO	2.2
2	B	372	TRP	2.2
2	B	462	ASP	2.1
2	F	376	ASP	2.1
2	F	419	ASP	2.1
2	F	29	LEU	2.1
1	A	169	PRO	2.1
3	G	75	GLY	2.1
3	G	8	LEU	2.1
3	C	159	PHE	2.1
2	F	128	ILE	2.0
2	F	35	VAL	2.0
2	F	18	LEU	2.0
2	B	48	MET	2.0
1	E	166	ALA	2.0
1	E	164	VAL	2.0
2	F	539	ILE	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 oligosaccharides 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. 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	B-factors($\text{\AA}^2$)	Q<0.9
4	6OM	A	301	7/7	0.66	0.28	50,51,55,55	0
4	6OM	E	301	7/7	0.72	0.28	50,51,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.