



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 03:21 PM UTC

PDB ID : 4OFW / pdb_00004ofw
Title : Crystal Structure of Arabidopsis thaliana DJ-1d
Authors : Choi, D.; Kim, J.; Ryu, K.-S.; Park, C.
Deposited on : 2014-01-15
Resolution : 2.30 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
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

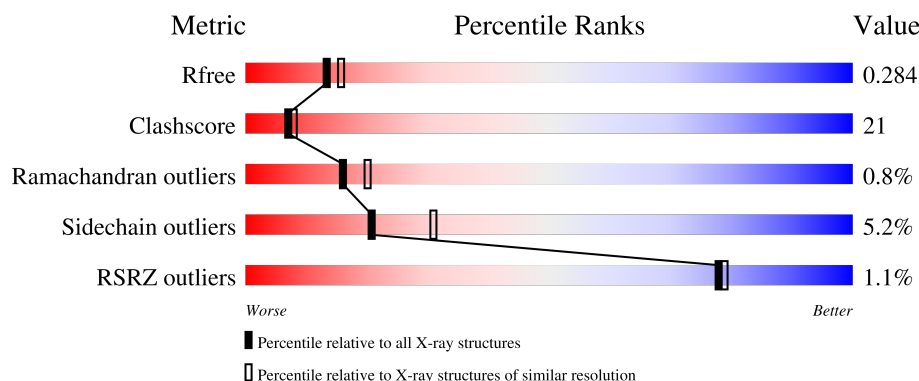
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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.



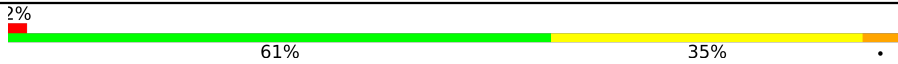
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	387	% 63% 31% 6%
1	B	387	% 64% 34% .
1	C	387	% 66% 29% 5%
1	D	387	% 58% 38% .
1	E	387	% 65% 32% .

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Mol	Chain	Length	Quality of chain
1	F	387	 A horizontal bar chart showing the quality of chain F. The bar is divided into four segments: a small red segment at the beginning labeled '2%', followed by a large green segment labeled '61%', then a yellow segment labeled '35%', and a very small orange segment at the end. A single dot is visible at the far right end of the bar.

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 18086 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 Protein DJ-1 homolog D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	B	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	C	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	D	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	E	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			
1	F	387	Total	C	N	O	S	0	0	0
			2924	1864	487	554	19			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	GLU	ASP	conflict	UNP Q9M8R4
A	389	HIS	-	expression tag	UNP Q9M8R4
B	238	GLU	ASP	conflict	UNP Q9M8R4
B	389	HIS	-	expression tag	UNP Q9M8R4
C	238	GLU	ASP	conflict	UNP Q9M8R4
C	389	HIS	-	expression tag	UNP Q9M8R4
D	238	GLU	ASP	conflict	UNP Q9M8R4
D	389	HIS	-	expression tag	UNP Q9M8R4
E	238	GLU	ASP	conflict	UNP Q9M8R4
E	389	HIS	-	expression tag	UNP Q9M8R4
F	238	GLU	ASP	conflict	UNP Q9M8R4
F	389	HIS	-	expression tag	UNP Q9M8R4

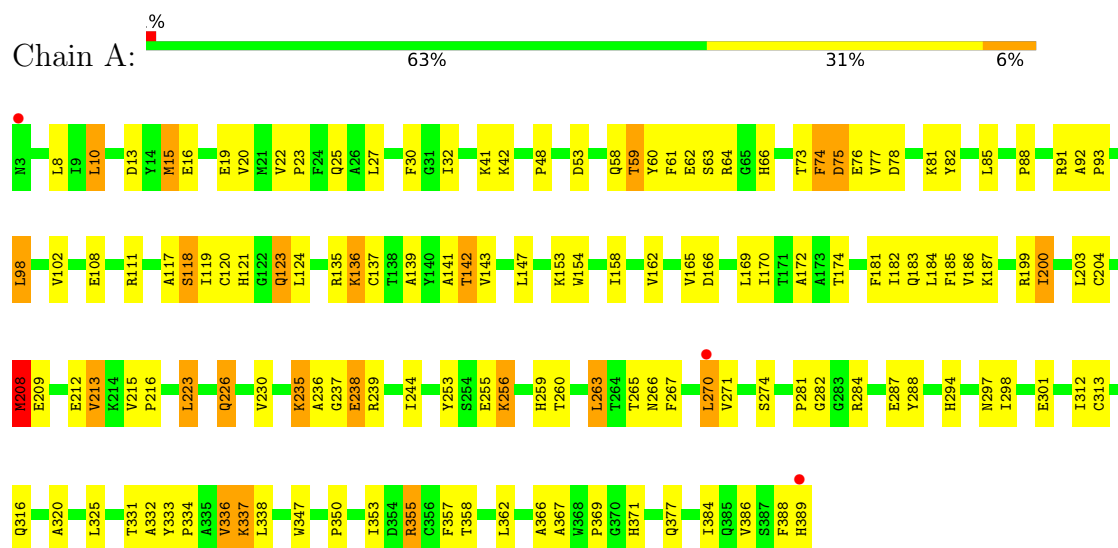
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	97	Total 97	O 97	0	0
2	B	81	Total 81	O 81	0	0
2	C	96	Total 96	O 96	0	0
2	D	100	Total 100	O 100	0	0
2	E	82	Total 82	O 82	0	0
2	F	86	Total 86	O 86	0	0

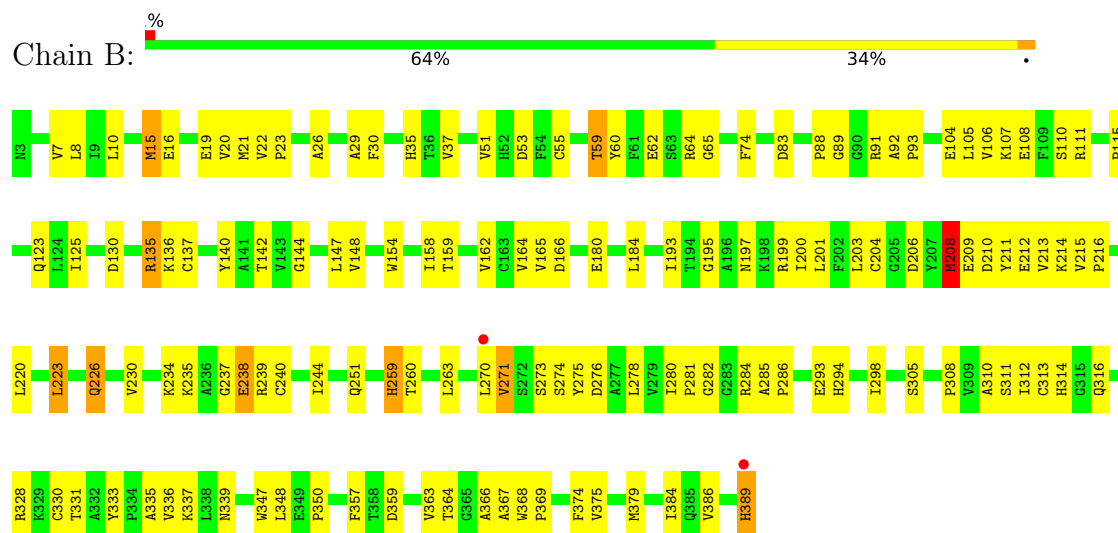
3 Residue-property plots

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: Protein DJ-1 homolog D

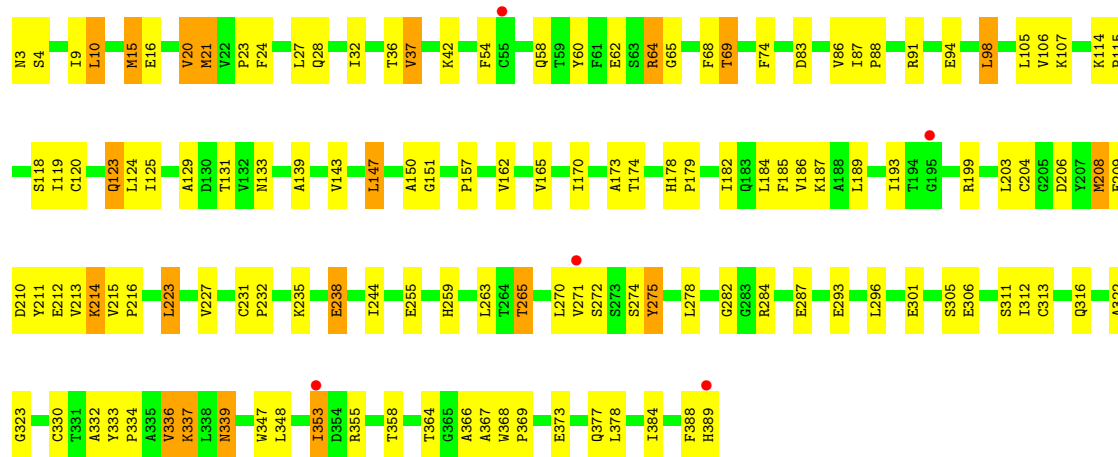


• Molecule 1: Protein DJ-1 homolog D

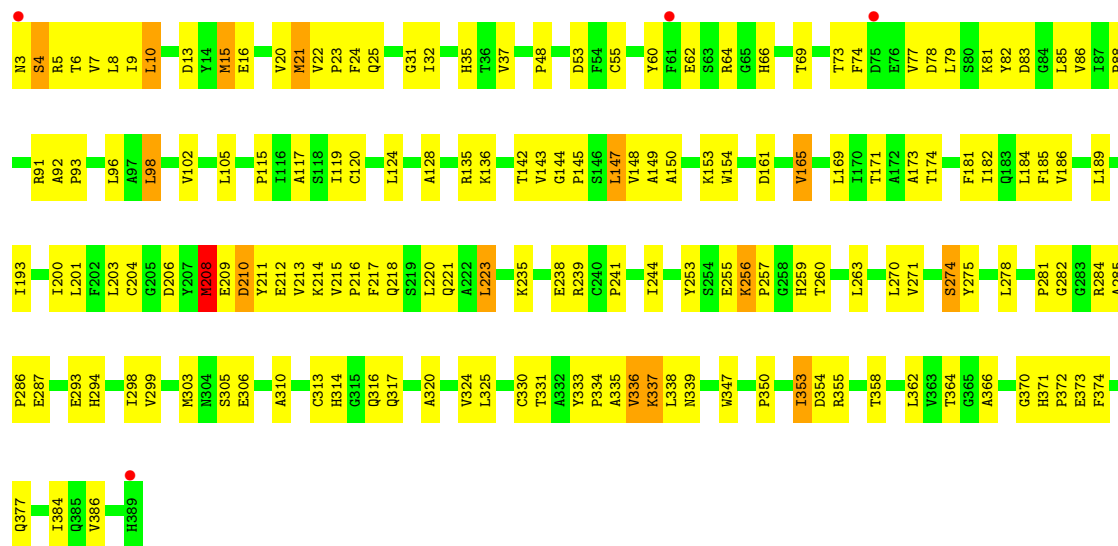


• Molecule 1: Protein DJ-1 homolog D

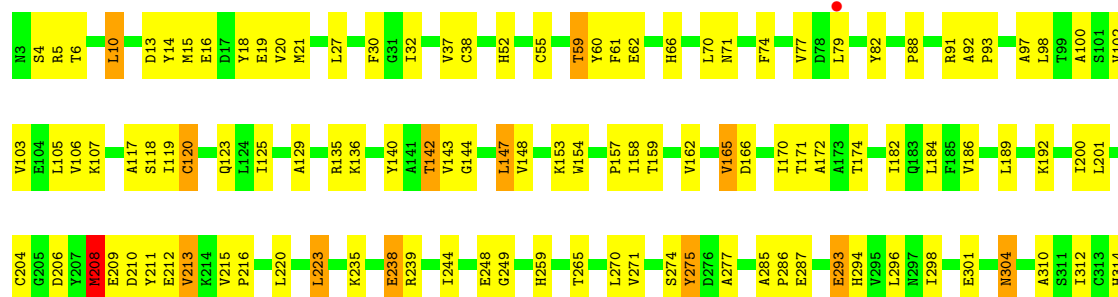




• Molecule 1: Protein DJ-1 homolog D

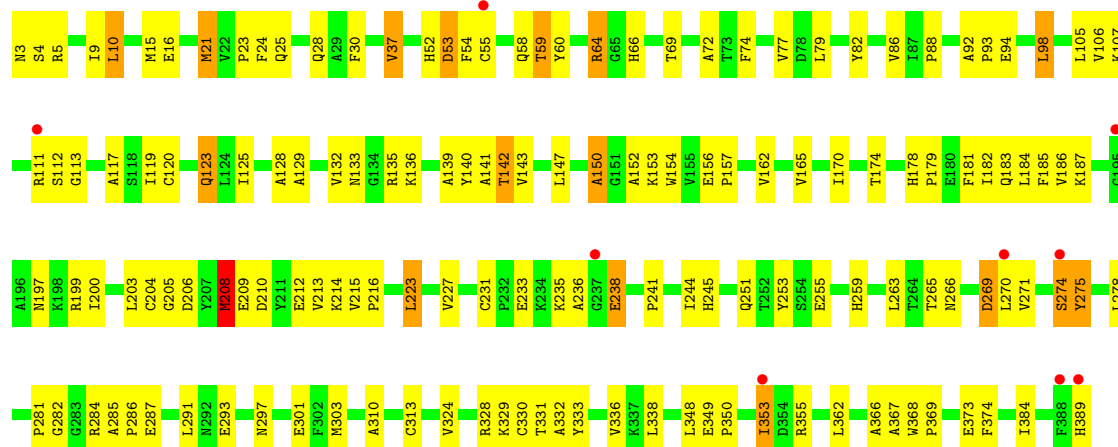


• Molecule 1: Protein DJ-1 homolog D





• Molecule 1: Protein DJ-1 homolog D



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.56Å 115.05Å 115.53Å 90.00° 91.51° 90.00°	Depositor
Resolution (Å)	50.00 – 2.30 50.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	95.9 (50.00-2.30) 95.8 (50.00-2.30)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.29Å)	Xtriage
Refinement program	CNS, REFMAC	Depositor
R, R_{free}	0.243 , 0.284 0.243 , 0.284	Depositor DCC
R_{free} test set	11742 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.0	Xtriage
Anisotropy	0.678	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 43.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.000 for -h,l,k 0.000 for -h,-l,-k 0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18086	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1795e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

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	0.45	0/2994	0.94	8/4075 (0.2%)
1	B	0.43	0/2994	0.96	5/4075 (0.1%)
1	C	0.46	0/2994	0.96	12/4075 (0.3%)
1	D	0.44	0/2994	0.95	11/4075 (0.3%)
1	E	0.43	0/2994	0.93	2/4075 (0.0%)
1	F	0.46	1/2994 (0.0%)	0.94	5/4075 (0.1%)
All	All	0.44	1/17964 (0.0%)	0.95	43/24450 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	21	MET	SD-CE	-5.31	1.66	1.79

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	337	LYS	N-CA-C	-7.08	103.61	111.82
1	A	208	MET	N-CA-C	-6.77	101.60	110.53
1	F	208	MET	N-CA-C	-6.74	100.51	110.48
1	B	208	MET	N-CA-C	-6.72	101.65	110.53
1	F	227	VAL	N-CA-C	6.72	117.97	108.36
1	B	15	MET	N-CA-C	-6.51	101.77	110.55
1	D	161	ASP	N-CA-C	6.47	120.91	112.89
1	D	337	LYS	N-CA-C	-6.44	104.68	112.54
1	D	208	MET	N-CA-C	-6.43	101.87	110.55
1	B	154	TRP	N-CA-C	6.42	119.59	109.96
1	C	208	MET	N-CA-C	-6.37	101.95	110.55
1	D	21	MET	N-CA-C	6.37	117.89	111.07
1	C	214	LYS	N-CA-C	6.36	117.87	111.07
1	D	15	MET	N-CA-C	-6.18	101.33	110.48
1	D	362	LEU	N-CA-C	6.07	118.62	108.73
1	A	15	MET	N-CA-C	-6.02	102.42	110.55
1	F	15	MET	N-CA-C	-5.95	101.68	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	150	ALA	N-CA-C	-5.83	106.03	113.02
1	A	136	LYS	N-CA-C	-5.82	102.29	110.50
1	D	214	LYS	N-CA-C	5.81	118.08	111.11
1	A	213	VAL	CB-CA-C	-5.78	106.80	111.71
1	D	48	PRO	N-CA-C	-5.70	102.86	111.41
1	C	114	LYS	CA-C-N	5.65	125.58	119.76
1	C	114	LYS	C-N-CA	5.65	125.58	119.76
1	E	208	MET	N-CA-C	-5.62	102.16	110.48
1	D	210	ASP	N-CA-C	5.59	118.91	111.75
1	A	226	GLN	N-CA-C	-5.53	100.16	108.96
1	A	154	TRP	N-CA-C	5.51	118.34	110.24
1	F	362	LEU	N-CA-C	5.51	117.71	108.73
1	D	24	PHE	N-CA-C	5.45	117.93	111.33
1	C	15	MET	N-CA-C	-5.42	103.23	110.55
1	D	154	TRP	N-CA-C	5.42	117.88	110.24
1	A	362	LEU	N-CA-C	5.35	117.24	108.52
1	B	305	SER	N-CA-C	-5.31	106.77	113.20
1	F	150	ALA	N-CA-C	-5.29	106.61	113.16
1	C	87	ILE	CA-C-N	5.25	125.22	120.03
1	C	87	ILE	C-N-CA	5.25	125.22	120.03
1	C	227	VAL	N-CA-C	5.15	115.54	108.12
1	C	20	VAL	CB-CA-C	-5.13	106.56	111.44
1	B	333	TYR	N-CA-C	-5.11	103.28	109.57
1	E	213	VAL	CB-CA-C	-5.11	106.59	111.44
1	C	337	LYS	N-CA-C	-5.06	105.89	111.71
1	C	378	LEU	N-CA-C	-5.05	105.86	111.36

There are no chirality outliers.

There are no planarity outliers.

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	2924	0	2872	136	0
1	B	2924	0	2872	124	0
1	C	2924	0	2872	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2924	0	2872	127	0
1	E	2924	0	2872	120	0
1	F	2924	0	2872	139	0
2	A	97	0	0	23	0
2	B	81	0	0	11	0
2	C	96	0	0	14	0
2	D	100	0	0	20	0
2	E	82	0	0	13	0
2	F	86	0	0	15	0
All	All	18086	0	17232	729	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 21.

All (729) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:21:MET:HE2	1:F:25:GLN:HG3	1.35	1.06
1:B:197:ASN:HA	2:B:468:HOH:O	1.59	1.00
1:F:133:ASN:HA	2:F:460:HOH:O	1.66	0.95
1:B:20:VAL:HB	2:B:455:HOH:O	1.66	0.94
1:F:353:ILE:HD12	1:F:353:ILE:H	1.28	0.94
1:D:7:VAL:HG23	2:D:486:HOH:O	1.70	0.91
1:B:59:THR:HG22	2:B:450:HOH:O	1.73	0.89
1:E:79:LEU:HD21	1:E:105:LEU:HG	1.56	0.87
1:E:287:GLU:OE1	1:F:142:THR:HG21	1.74	0.87
1:F:72:ALA:HB3	2:F:463:HOH:O	1.73	0.87
1:C:389:HIS:HB3	2:C:457:HOH:O	1.75	0.87
1:E:335:ALA:HA	1:F:98:LEU:HD13	1.58	0.85
1:A:30:PHE:HB2	2:A:434:HOH:O	1.76	0.84
1:D:239:ARG:HH21	1:D:260:THR:HG23	1.39	0.84
1:C:353:ILE:H	1:C:353:ILE:HD12	1.41	0.84
1:F:21:MET:HE2	1:F:25:GLN:CG	2.07	0.84
2:E:418:HOH:O	1:F:59:THR:HG21	1.77	0.83
1:B:15:MET:SD	1:B:20:VAL:HG21	2.20	0.82
1:B:37:VAL:HG21	1:B:74:PHE:HA	1.61	0.81
1:D:78:ASP:OD2	1:D:81:LYS:HD3	1.81	0.80
1:A:108:GLU:HA	1:A:111:ARG:NH1	1.97	0.80
1:A:16:GLU:OE2	1:A:259:HIS:HE1	1.64	0.80
1:B:210:ASP:OD2	1:B:259:HIS:HD2	1.66	0.79
1:B:55:CYS:HB3	2:B:445:HOH:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:VAL:HB	1:E:216:PRO:HD3	1.64	0.79
1:B:335:ALA:HA	1:C:98:LEU:HD13	1.65	0.78
1:D:21:MET:HG3	1:D:211:TYR:CZ	2.18	0.78
1:D:330:CYS:HB2	1:D:364:THR:HG21	1.64	0.77
1:E:37:VAL:HG21	1:E:74:PHE:HA	1.67	0.76
1:D:53:ASP:OD1	1:D:260:THR:HG22	1.86	0.76
1:B:215:VAL:HB	1:B:216:PRO:HD3	1.68	0.76
1:F:69:THR:HB	2:F:407:HOH:O	1.84	0.76
1:A:59:THR:HG21	2:C:413:HOH:O	1.84	0.75
1:F:150:ALA:O	2:F:460:HOH:O	2.03	0.75
1:A:142:THR:HG21	1:C:287:GLU:OE2	1.87	0.74
1:A:239:ARG:HH21	1:A:260:THR:HG23	1.51	0.74
1:A:61:PHE:HB3	2:A:454:HOH:O	1.88	0.74
1:D:235:LYS:H	1:D:238:GLU:HG3	1.52	0.74
1:E:210:ASP:OD2	1:E:259:HIS:HD2	1.71	0.73
1:C:179:PRO:HG2	2:C:414:HOH:O	1.86	0.73
1:F:16:GLU:OE2	1:F:259:HIS:HE1	1.71	0.73
1:D:79:LEU:HD12	1:D:79:LEU:H	1.53	0.73
1:A:32:ILE:HG13	2:A:434:HOH:O	1.88	0.73
1:A:22:VAL:HB	1:A:23:PRO:HD3	1.68	0.73
1:C:133:ASN:HA	1:C:151:GLY:O	1.88	0.72
1:D:203:LEU:HG	1:D:278:LEU:HD11	1.70	0.72
1:F:23:PRO:HD3	2:F:419:HOH:O	1.88	0.72
1:C:133:ASN:HB2	2:C:472:HOH:O	1.89	0.72
1:F:182:ILE:O	1:F:186:VAL:HG23	1.89	0.72
1:B:209:GLU:HB3	1:B:212:GLU:HB2	1.72	0.72
1:B:237:GLY:HA3	1:D:235:LYS:NZ	2.03	0.72
1:B:239:ARG:HH21	1:B:260:THR:HG23	1.52	0.72
1:B:235:LYS:O	1:B:238:GLU:HG2	1.89	0.72
1:E:248:GLU:HB3	2:E:464:HOH:O	1.90	0.71
1:A:208:MET:HE2	1:A:213:VAL:HG22	1.71	0.71
1:E:208:MET:HG3	1:E:213:VAL:HG21	1.71	0.71
1:A:136:LYS:HA	1:A:153:LYS:HB2	1.72	0.71
1:D:208:MET:HG3	1:D:213:VAL:HG21	1.72	0.71
1:A:19:GLU:HB2	2:A:483:HOH:O	1.90	0.71
1:D:235:LYS:H	1:D:238:GLU:CG	2.03	0.71
1:C:203:LEU:HG	1:C:278:LEU:HD11	1.73	0.70
1:A:88:PRO:HB3	2:A:483:HOH:O	1.92	0.70
1:E:37:VAL:CG2	1:E:74:PHE:HA	2.21	0.70
1:F:37:VAL:HG21	1:F:74:PHE:HA	1.72	0.70
1:F:204:CYS:HA	1:F:208:MET:HE1	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:165:VAL:HG22	1:E:184:LEU:HD13	1.74	0.70
1:F:265:THR:HG22	2:F:434:HOH:O	1.91	0.69
1:D:16:GLU:OE2	1:D:259:HIS:HE1	1.74	0.69
1:A:15:MET:SD	1:A:20:VAL:HG21	2.32	0.69
1:F:154:TRP:HE1	1:F:156:GLU:HG2	1.57	0.69
1:C:339:ASN:HD22	1:C:339:ASN:H	1.40	0.69
1:E:120:CYS:SG	2:E:478:HOH:O	2.49	0.69
1:A:183:GLN:HE21	1:A:187:LYS:HE3	1.58	0.69
1:D:119:ILE:HD11	1:D:174:THR:O	1.93	0.68
1:B:204:CYS:HA	1:B:208:MET:HE1	1.75	0.68
1:F:389:HIS:HB3	2:F:466:HOH:O	1.91	0.68
1:A:182:ILE:O	1:A:186:VAL:HG23	1.94	0.68
1:B:235:LYS:H	1:B:238:GLU:HG3	1.58	0.68
1:A:200:ILE:HD12	1:A:200:ILE:N	2.09	0.68
1:D:182:ILE:O	1:D:186:VAL:HG23	1.93	0.68
1:E:204:CYS:HA	1:E:208:MET:HE1	1.76	0.68
1:F:21:MET:HE1	1:F:24:PHE:HD2	1.58	0.68
1:A:282:GLY:HA3	1:A:313:CYS:HB3	1.76	0.67
1:B:158:ILE:HD12	1:B:159:THR:N	2.09	0.67
1:F:165:VAL:HG23	1:F:184:LEU:HD13	1.77	0.67
1:F:203:LEU:HG	1:F:278:LEU:HD11	1.77	0.67
1:D:313:CYS:SG	2:D:498:HOH:O	2.50	0.67
1:E:103:VAL:O	1:E:107:LYS:HG3	1.94	0.67
1:B:235:LYS:H	1:B:238:GLU:CG	2.07	0.67
1:A:256:LYS:HG2	2:A:402:HOH:O	1.95	0.67
1:E:30:PHE:CZ	1:E:223:LEU:HD13	2.30	0.66
1:D:253:TYR:O	1:E:91:ARG:NH2	2.28	0.66
1:F:235:LYS:H	1:F:238:GLU:HG3	1.61	0.66
1:B:165:VAL:CG2	1:B:184:LEU:HD13	2.25	0.66
1:B:282:GLY:HA3	1:B:313:CYS:HB3	1.78	0.66
1:C:182:ILE:O	1:C:186:VAL:HG23	1.96	0.66
1:A:53:ASP:OD1	1:A:260:THR:HG22	1.96	0.66
1:B:22:VAL:HB	1:B:23:PRO:HD3	1.78	0.66
1:D:218:GLN:HG2	2:D:463:HOH:O	1.95	0.65
1:E:182:ILE:O	1:E:186:VAL:HG23	1.97	0.65
1:A:119:ILE:HD11	1:A:174:THR:O	1.97	0.65
1:E:350:PRO:HB2	2:E:461:HOH:O	1.96	0.65
1:F:120:CYS:SG	2:F:479:HOH:O	2.53	0.65
1:F:213:VAL:HG13	1:F:214:LYS:N	2.11	0.65
1:F:208:MET:HE2	1:F:281:PRO:HB2	1.77	0.65
1:C:23:PRO:HD3	2:C:437:HOH:O	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:355:ARG:HB3	2:C:453:HOH:O	1.96	0.64
1:B:235:LYS:N	1:B:238:GLU:HG3	2.13	0.64
1:B:237:GLY:HA3	1:D:235:LYS:HZ2	1.59	0.64
1:A:62:GLU:OE1	1:A:91:ARG:HD3	1.98	0.64
1:D:3:ASN:O	1:D:4:SER:HB2	1.96	0.64
1:E:5:ARG:NH2	1:E:189:LEU:O	2.31	0.64
1:B:330:CYS:HB2	1:B:364:THR:HG21	1.79	0.64
1:C:37:VAL:HG22	1:C:74:PHE:N	2.13	0.64
1:D:320:ALA:HB2	1:D:325:LEU:HD12	1.77	0.64
1:D:355:ARG:HA	1:D:373:GLU:OE1	1.98	0.64
1:F:333:TYR:O	1:F:336:VAL:HG22	1.97	0.64
1:C:37:VAL:HG13	1:C:74:PHE:HD1	1.63	0.64
1:C:209:GLU:HB3	1:C:212:GLU:HB2	1.80	0.64
1:D:169:LEU:HG	2:D:457:HOH:O	1.98	0.64
1:F:21:MET:CE	1:F:24:PHE:HD2	2.11	0.64
1:A:120:CYS:SG	2:A:488:HOH:O	2.52	0.63
1:F:154:TRP:NE1	1:F:156:GLU:HG2	2.12	0.63
1:A:20:VAL:HG22	1:A:88:PRO:HB3	1.80	0.63
1:C:21:MET:HG3	1:C:211:TYR:CZ	2.33	0.63
1:C:330:CYS:HA	1:C:348:LEU:HD12	1.80	0.63
1:E:355:ARG:HD2	2:E:429:HOH:O	1.97	0.63
1:C:16:GLU:OE2	1:C:259:HIS:HE1	1.80	0.63
1:D:117:ALA:HB1	1:D:181:PHE:CZ	2.33	0.63
1:A:19:GLU:CB	2:A:483:HOH:O	2.43	0.63
1:A:284:ARG:NH1	1:B:60:TYR:O	2.24	0.63
1:F:204:CYS:HA	1:F:208:MET:CE	2.29	0.63
1:A:78:ASP:OD2	1:A:81:LYS:HD3	1.99	0.62
1:C:15:MET:SD	1:C:20:VAL:HG21	2.39	0.62
1:C:120:CYS:SG	2:C:490:HOH:O	2.46	0.62
1:C:305:SER:O	1:C:306:GLU:HB2	1.99	0.62
1:F:313:CYS:HA	1:F:366:ALA:O	1.99	0.62
1:F:21:MET:HE3	1:F:21:MET:HA	1.82	0.62
1:F:140:TYR:HD2	1:F:142:THR:HB	1.65	0.62
1:E:5:ARG:HH11	1:E:389:HIS:H	1.48	0.62
1:D:77:VAL:HG13	1:D:82:TYR:HE1	1.64	0.62
1:F:330:CYS:HA	1:F:348:LEU:HD12	1.80	0.62
1:A:333:TYR:CD1	1:A:334:PRO:HD2	2.35	0.61
1:F:353:ILE:H	1:F:353:ILE:CD1	2.04	0.61
1:A:74:PHE:O	1:A:76:GLU:N	2.34	0.61
1:B:209:GLU:O	1:B:213:VAL:HG23	2.00	0.61
1:E:15:MET:SD	1:E:20:VAL:HG21	2.41	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:VAL:HB	2:F:463:HOH:O	1.99	0.61
1:B:312:ILE:HD11	1:B:367:ALA:O	1.99	0.61
1:C:282:GLY:HA3	1:C:313:CYS:HB3	1.82	0.61
1:D:3:ASN:HB2	1:D:31:GLY:O	2.01	0.61
1:A:77:VAL:HB	2:A:440:HOH:O	2.01	0.61
1:A:208:MET:SD	1:A:213:VAL:HG21	2.41	0.61
1:A:60:TYR:O	1:C:284:ARG:NH1	2.34	0.61
1:C:170:ILE:HD13	1:C:185:PHE:HA	1.82	0.61
1:E:5:ARG:NH1	1:E:389:HIS:H	1.99	0.60
1:E:338:LEU:CD2	1:E:342:LEU:HD12	2.31	0.60
1:F:200:ILE:HD12	1:F:200:ILE:N	2.16	0.60
1:C:165:VAL:CG2	1:C:184:LEU:HD13	2.32	0.60
1:D:255:GLU:OE2	1:D:284:ARG:HD3	2.01	0.60
1:E:301:GLU:HA	1:E:304:ASN:ND2	2.16	0.60
1:A:124:LEU:CD2	1:A:143:VAL:HG13	2.32	0.60
1:B:331:THR:OG1	1:B:350:PRO:HG3	2.02	0.60
1:B:53:ASP:OD1	1:B:260:THR:HG22	2.02	0.60
1:A:77:VAL:HG13	1:A:82:TYR:HE1	1.66	0.59
1:C:9:ILE:HG12	1:C:86:VAL:HB	1.83	0.59
1:B:337:LYS:HE2	1:B:347:TRP:CD1	2.38	0.59
1:D:124:LEU:HD23	1:D:143:VAL:HG13	1.83	0.59
1:B:200:ILE:CD1	1:B:220:LEU:HD13	2.33	0.59
1:C:213:VAL:HG13	1:C:214:LYS:N	2.18	0.59
1:D:73:THR:HG22	1:D:74:PHE:O	2.02	0.59
1:D:358:THR:OG1	1:D:377:GLN:NE2	2.36	0.59
1:B:64:ARG:HD2	2:B:425:HOH:O	2.03	0.59
1:F:349:GLU:CD	1:F:350:PRO:HD2	2.28	0.59
1:B:313:CYS:HA	1:B:366:ALA:O	2.02	0.59
1:B:350:PRO:HB3	1:B:366:ALA:HB2	1.83	0.59
1:C:187:LYS:HG3	2:C:443:HOH:O	2.03	0.59
1:F:274:SER:O	1:F:275:TYR:HB2	2.03	0.59
1:B:30:PHE:CZ	1:B:223:LEU:HD13	2.37	0.59
1:B:226:GLN:HE21	1:B:226:GLN:HA	1.68	0.59
1:F:106:VAL:HG21	1:F:125:ILE:CG2	2.33	0.59
1:C:62:GLU:OE1	1:C:91:ARG:HD3	2.03	0.58
1:C:157:PRO:HA	1:C:162:VAL:HG21	1.85	0.58
1:C:235:LYS:H	1:C:238:GLU:HG3	1.69	0.58
1:A:265:THR:HG23	2:A:460:HOH:O	2.04	0.58
1:F:3:ASN:O	1:F:4:SER:HB2	2.03	0.58
1:A:77:VAL:HG13	1:A:82:TYR:CE1	2.38	0.58
1:D:22:VAL:HB	1:D:23:PRO:HD3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:VAL:HG21	1:B:184:LEU:HD13	1.86	0.57
1:F:165:VAL:CG2	1:F:184:LEU:HD13	2.35	0.57
1:B:209:GLU:HG3	1:B:212:GLU:H	1.70	0.57
1:C:106:VAL:HG21	1:C:125:ILE:CG2	2.34	0.57
1:D:91:ARG:NH2	1:F:253:TYR:O	2.37	0.57
1:B:285:ALA:HB3	1:B:286:PRO:HD3	1.85	0.57
1:A:209:GLU:HG3	1:A:212:GLU:H	1.69	0.57
1:D:209:GLU:O	1:D:213:VAL:HG23	2.05	0.57
1:B:204:CYS:HA	1:B:208:MET:CE	2.34	0.57
1:C:255:GLU:OE2	1:C:284:ARG:NH2	2.38	0.57
1:A:353:ILE:HG12	2:A:425:HOH:O	2.03	0.57
1:B:16:GLU:OE2	1:B:259:HIS:HE1	1.88	0.57
1:F:209:GLU:HG3	1:F:212:GLU:H	1.70	0.57
1:E:97:ALA:C	1:E:98:LEU:HD12	2.30	0.57
1:A:66:HIS:CD2	1:A:244:ILE:HG23	2.40	0.56
1:A:235:LYS:O	1:A:238:GLU:HG2	2.05	0.56
1:C:3:ASN:O	1:C:4:SER:HB2	2.05	0.56
1:B:208:MET:SD	1:B:213:VAL:HG21	2.45	0.56
1:F:123:GLN:OE1	1:F:123:GLN:N	2.39	0.56
1:B:193:ILE:HG12	1:B:386:VAL:HG22	1.87	0.56
1:A:117:ALA:HB1	1:A:181:PHE:CZ	2.41	0.56
1:E:10:LEU:HD11	1:E:102:VAL:HG13	1.87	0.56
1:E:4:SER:O	1:E:5:ARG:HD3	2.06	0.56
1:D:335:ALA:HA	1:E:98:LEU:HD22	1.87	0.56
1:D:210:ASP:OD2	1:D:259:HIS:HD2	1.88	0.56
1:E:326:LYS:HD3	1:E:344:GLY:HA3	1.88	0.56
1:B:235:LYS:N	1:B:238:GLU:CG	2.69	0.56
1:C:333:TYR:O	1:C:336:VAL:HG22	2.06	0.55
1:D:193:ILE:HG12	1:D:386:VAL:HG22	1.88	0.55
1:D:200:ILE:HD12	1:D:220:LEU:HD13	1.88	0.55
1:A:123:GLN:HG2	1:A:139:ALA:HB2	1.88	0.55
1:B:230:VAL:HG21	1:B:270:LEU:HD11	1.88	0.55
1:C:223:LEU:HG	1:C:384:ILE:HG21	1.89	0.55
1:D:239:ARG:NH2	1:D:260:THR:HG23	2.17	0.55
1:E:338:LEU:HD21	1:E:342:LEU:HD12	1.87	0.55
1:B:140:TYR:HD2	1:B:142:THR:HG22	1.71	0.55
1:B:367:ALA:HB3	1:B:369:PRO:HD2	1.89	0.55
1:D:165:VAL:HG22	1:D:184:LEU:HD13	1.88	0.55
1:D:208:MET:CG	1:D:213:VAL:HG21	2.37	0.55
1:D:217:PHE:O	1:D:221:GLN:HG3	2.06	0.55
1:F:37:VAL:CG2	1:F:74:PHE:HA	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:VAL:HG13	1:F:74:PHE:HD1	1.72	0.55
1:A:59:THR:HG22	1:A:60:TYR:H	1.72	0.55
1:E:147:LEU:HD23	1:E:154:TRP:CZ3	2.42	0.55
1:E:209:GLU:O	1:E:213:VAL:HG23	2.07	0.54
1:B:37:VAL:CG2	1:B:74:PHE:HA	2.35	0.54
1:B:184:LEU:HD23	2:B:442:HOH:O	2.07	0.54
1:B:294:HIS:O	1:B:298:ILE:HG13	2.07	0.54
1:B:280:ILE:HB	1:B:311:SER:HB2	1.89	0.54
1:E:206:ASP:OD2	1:F:58:GLN:HG3	2.07	0.54
1:E:235:LYS:H	1:E:238:GLU:CG	2.20	0.54
1:F:55:CYS:HB3	2:F:415:HOH:O	2.07	0.54
1:B:212:GLU:HG3	1:B:368:TRP:HB3	1.89	0.54
1:F:355:ARG:HG2	1:F:355:ARG:HH21	1.71	0.54
1:C:119:ILE:HD11	1:C:174:THR:O	2.07	0.54
1:E:338:LEU:HD12	1:F:128:ALA:HB2	1.88	0.54
1:A:10:LEU:O	1:A:88:PRO:HD2	2.08	0.54
1:F:64:ARG:HD3	2:F:437:HOH:O	2.08	0.54
1:A:119:ILE:HG13	1:A:172:ALA:HB3	1.89	0.54
1:F:213:VAL:HG13	1:F:214:LYS:H	1.73	0.54
1:D:16:GLU:O	1:D:20:VAL:HG23	2.08	0.54
1:F:233:GLU:HG3	1:F:233:GLU:O	2.07	0.54
1:C:210:ASP:OD2	1:C:259:HIS:HD2	1.90	0.53
1:D:148:VAL:C	1:D:150:ALA:H	2.15	0.53
1:D:212:GLU:HA	1:D:371:HIS:HE2	1.73	0.53
1:D:353:ILE:HD12	1:D:354:ASP:H	1.72	0.53
1:A:15:MET:CG	1:A:20:VAL:HG21	2.39	0.53
1:A:165:VAL:CG2	1:A:184:LEU:HD13	2.38	0.53
1:F:263:LEU:HD22	1:F:263:LEU:H	1.72	0.53
1:B:200:ILE:HD12	1:B:220:LEU:HD13	1.89	0.53
1:F:105:LEU:HD23	1:F:105:LEU:C	2.33	0.53
1:D:15:MET:HG3	1:D:20:VAL:HG21	1.89	0.53
1:F:235:LYS:N	1:F:238:GLU:HG3	2.22	0.53
1:E:19:GLU:O	1:E:88:PRO:HB3	2.09	0.53
1:D:201:LEU:HD22	1:D:270:LEU:HD21	1.90	0.53
1:E:52:HIS:HE1	1:E:62:GLU:OE1	1.91	0.53
1:B:62:GLU:OE2	1:B:91:ARG:NH1	2.42	0.53
1:D:62:GLU:OE2	1:D:91:ARG:NH1	2.42	0.53
1:D:200:ILE:CD1	1:D:220:LEU:HD13	2.39	0.53
1:D:287:GLU:OE1	1:E:142:THR:HG21	2.08	0.53
1:A:10:LEU:HD11	1:A:102:VAL:HG13	1.90	0.53
1:C:235:LYS:N	1:C:238:GLU:HG3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:VAL:HG13	1:C:274:SER:OG	2.09	0.53
1:A:25:GLN:NE2	1:A:371:HIS:ND1	2.55	0.53
1:E:293:GLU:OE1	1:E:293:GLU:HA	2.09	0.52
1:A:118:SER:HB3	1:A:123:GLN:OE1	2.09	0.52
1:D:8:LEU:O	1:D:85:LEU:HD12	2.09	0.52
1:C:69:THR:HG23	2:C:486:HOH:O	2.09	0.52
1:C:24:PHE:O	1:C:28:GLN:HG3	2.09	0.52
1:D:215:VAL:HB	1:D:216:PRO:HD3	1.91	0.52
1:F:255:GLU:OE2	1:F:284:ARG:HD3	2.09	0.52
1:B:240:CYS:SG	1:B:263:LEU:HD21	2.50	0.52
1:C:143:VAL:HG12	1:C:147:LEU:CD2	2.40	0.52
1:F:282:GLY:HA3	1:F:313:CYS:HB3	1.92	0.52
1:C:209:GLU:HG3	1:C:212:GLU:H	1.74	0.52
1:D:32:ILE:HG23	2:D:486:HOH:O	2.09	0.52
1:E:27:LEU:HD22	1:E:32:ILE:HD12	1.92	0.52
1:E:312:ILE:HD11	1:E:367:ALA:O	2.10	0.52
1:F:157:PRO:HA	1:F:162:VAL:HG21	1.91	0.52
1:F:143:VAL:HG12	1:F:143:VAL:O	2.10	0.52
1:E:140:TYR:HD2	1:E:142:THR:HB	1.75	0.52
1:E:301:GLU:HA	1:E:304:ASN:HD22	1.75	0.52
1:E:329:LYS:HG3	2:E:445:HOH:O	2.09	0.52
1:A:208:MET:HE2	1:A:213:VAL:CG2	2.40	0.52
1:C:312:ILE:HD11	1:C:367:ALA:O	2.10	0.52
1:E:285:ALA:HB3	1:E:286:PRO:HD3	1.92	0.51
1:F:329:LYS:O	1:F:330:CYS:HB3	2.09	0.51
1:A:235:LYS:H	1:A:238:GLU:CG	2.23	0.51
1:B:348:LEU:HD13	1:B:357:PHE:CD2	2.45	0.51
1:F:293:GLU:HA	1:F:293:GLU:OE1	2.08	0.51
1:A:25:GLN:HE21	1:A:215:VAL:HG21	1.75	0.51
1:A:73:THR:HG22	1:A:74:PHE:O	2.10	0.51
1:B:20:VAL:HG22	1:B:88:PRO:HG3	1.93	0.51
1:B:51:VAL:HG13	1:B:259:HIS:CD2	2.44	0.51
1:E:249:GLY:N	2:E:464:HOH:O	2.43	0.51
1:C:265:THR:HG23	2:C:419:HOH:O	2.11	0.51
1:E:37:VAL:CG2	1:E:74:PHE:CA	2.88	0.51
1:F:21:MET:CE	1:F:25:GLN:HG3	2.25	0.51
1:D:77:VAL:HB	2:D:470:HOH:O	2.11	0.51
1:D:208:MET:SD	1:D:213:VAL:HG21	2.51	0.51
1:A:74:PHE:O	1:A:75:ASP:C	2.54	0.51
1:A:98:LEU:HD21	1:C:337:LYS:HB3	1.93	0.51
1:D:353:ILE:HD12	1:D:354:ASP:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:123:GLN:N	1:E:123:GLN:OE1	2.43	0.51
1:B:37:VAL:CG2	1:B:74:PHE:CA	2.89	0.51
1:C:54:PHE:HB3	2:C:458:HOH:O	2.09	0.51
1:E:336:VAL:O	1:E:336:VAL:HG12	2.09	0.51
1:F:77:VAL:HG13	1:F:82:TYR:HE1	1.75	0.51
1:E:38:CYS:HB3	1:E:70:LEU:HD11	1.93	0.50
1:E:294:HIS:O	1:E:298:ILE:HG13	2.10	0.50
1:B:336:VAL:HG12	1:B:336:VAL:O	2.11	0.50
1:E:200:ILE:CD1	1:E:220:LEU:HD13	2.41	0.50
1:A:8:LEU:HB2	1:A:82:TYR:CD2	2.46	0.50
1:B:271:VAL:HG13	1:B:271:VAL:O	2.11	0.50
1:B:271:VAL:HG22	1:B:273:SER:HB2	1.93	0.50
1:C:368:TRP:N	1:C:369:PRO:CD	2.75	0.50
1:D:285:ALA:N	1:D:286:PRO:CD	2.74	0.50
1:A:235:LYS:H	1:A:238:GLU:HG3	1.77	0.50
1:A:332:ALA:CB	1:A:336:VAL:HG23	2.41	0.50
1:D:372:PRO:HD2	2:D:425:HOH:O	2.12	0.50
1:F:235:LYS:H	1:F:238:GLU:CG	2.22	0.50
1:B:91:ARG:NH2	2:B:453:HOH:O	2.44	0.50
1:C:215:VAL:HB	1:C:216:PRO:HD3	1.93	0.50
1:E:135:ARG:HD2	1:E:166:ASP:OD2	2.12	0.50
1:C:235:LYS:H	1:C:238:GLU:CG	2.23	0.50
1:F:197:ASN:HB2	2:F:404:HOH:O	2.12	0.50
1:A:313:CYS:HA	1:A:366:ALA:O	2.11	0.50
1:F:21:MET:HE1	1:F:24:PHE:CD2	2.44	0.50
1:B:123:GLN:N	1:B:123:GLN:OE1	2.45	0.50
1:C:353:ILE:H	1:C:353:ILE:CD1	2.08	0.50
1:E:204:CYS:HA	1:E:208:MET:CE	2.41	0.50
1:F:5:ARG:HH22	1:F:389:HIS:CD2	2.30	0.50
1:B:91:ARG:HG3	1:B:91:ARG:HH11	1.77	0.50
1:D:120:CYS:SG	2:D:493:HOH:O	2.55	0.50
1:D:204:CYS:SG	1:D:208:MET:HE1	2.52	0.50
1:A:135:ARG:HD2	1:A:166:ASP:OD2	2.12	0.49
1:B:389:HIS:HB2	2:B:461:HOH:O	2.10	0.49
1:C:332:ALA:HB1	1:C:336:VAL:CG2	2.42	0.49
1:E:16:GLU:HB3	1:E:19:GLU:HB2	1.94	0.49
1:F:106:VAL:HG21	1:F:125:ILE:HG22	1.92	0.49
1:A:88:PRO:CA	2:A:483:HOH:O	2.60	0.49
1:C:293:GLU:OE1	1:C:293:GLU:HA	2.12	0.49
1:A:16:GLU:OE2	1:A:259:HIS:CE1	2.56	0.49
1:E:77:VAL:HG13	1:E:82:TYR:HE1	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:270:LEU:HD13	1:C:271:VAL:N	2.27	0.49
1:E:61:PHE:HB3	2:E:459:HOH:O	2.11	0.49
1:A:367:ALA:HB3	1:A:369:PRO:HD2	1.95	0.49
1:D:256:LYS:HG2	2:D:407:HOH:O	2.13	0.49
1:C:199:ARG:HB2	1:C:275:TYR:HA	1.94	0.49
1:F:205:GLY:HA2	1:F:231:CYS:SG	2.53	0.49
1:C:83:ASP:O	1:C:115:PRO:HD2	2.12	0.49
1:E:355:ARG:HG3	1:E:356:CYS:N	2.28	0.49
1:F:269:ASP:N	1:F:269:ASP:OD2	2.45	0.49
1:C:274:SER:O	1:C:275:TYR:HB2	2.12	0.49
1:A:92:ALA:N	1:A:93:PRO:CD	2.76	0.49
1:B:314:HIS:HA	1:B:336:VAL:HG21	1.93	0.49
1:A:98:LEU:HD22	1:C:334:PRO:O	2.13	0.48
1:D:171:THR:HG23	2:D:457:HOH:O	2.13	0.48
1:D:256:LYS:HG3	1:D:257:PRO:HD2	1.94	0.48
1:E:351:ASP:N	2:E:461:HOH:O	2.46	0.48
1:F:154:TRP:HE1	1:F:156:GLU:CG	2.22	0.48
1:B:336:VAL:HA	1:B:339:ASN:HD22	1.78	0.48
1:C:178:HIS:N	1:C:179:PRO:HD2	2.28	0.48
1:D:32:ILE:CG2	2:D:486:HOH:O	2.60	0.48
1:E:337:LYS:HE2	1:E:347:TRP:CD1	2.48	0.48
1:A:8:LEU:O	1:A:85:LEU:HD12	2.13	0.48
1:A:15:MET:HG3	1:A:20:VAL:HG21	1.95	0.48
1:D:331:THR:OG1	1:D:350:PRO:HB3	2.13	0.48
1:F:212:GLU:OE1	1:F:313:CYS:HB2	2.13	0.48
1:A:58:GLN:HG3	1:C:206:ASP:OD2	2.13	0.48
1:B:16:GLU:HB3	1:B:19:GLU:HB2	1.94	0.48
1:D:66:HIS:CD2	1:D:244:ILE:HG23	2.48	0.48
1:C:353:ILE:HD12	1:C:353:ILE:N	2.20	0.48
1:D:55:CYS:HB3	2:D:442:HOH:O	2.13	0.48
1:D:64:ARG:NH1	2:D:429:HOH:O	2.45	0.48
1:E:157:PRO:HA	1:E:162:VAL:HG21	1.95	0.48
1:E:298:ILE:HG12	2:E:474:HOH:O	2.13	0.48
1:A:332:ALA:HB1	1:A:336:VAL:CG2	2.44	0.48
1:B:180:GLU:O	1:B:184:LEU:HG	2.14	0.48
1:D:271:VAL:HG13	1:D:274:SER:OG	2.14	0.48
1:F:206:ASP:OD1	1:F:241:PRO:HD2	2.13	0.48
1:E:274:SER:O	1:E:275:TYR:HB2	2.13	0.48
1:A:255:GLU:OE1	1:A:284:ARG:NH2	2.46	0.48
1:A:320:ALA:HB2	1:A:325:LEU:HD12	1.95	0.48
1:A:316:GLN:OE1	1:A:316:GLN:N	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:353:ILE:HD12	1:F:353:ILE:N	2.12	0.47
1:A:358:THR:OG1	1:A:377:GLN:NE2	2.48	0.47
1:D:92:ALA:N	1:D:93:PRO:CD	2.77	0.47
1:D:316:GLN:N	1:D:316:GLN:OE1	2.47	0.47
1:E:117:ALA:HA	1:E:170:ILE:O	2.14	0.47
1:E:18:TYR:OH	1:E:210:ASP:OD1	2.31	0.47
1:A:136:LYS:O	1:A:137:CYS:HB3	2.14	0.47
1:B:223:LEU:HD21	1:B:379:MET:HE3	1.96	0.47
1:C:37:VAL:CG2	1:C:74:PHE:N	2.78	0.47
1:C:119:ILE:HD11	1:C:174:THR:C	2.40	0.47
1:F:77:VAL:HG13	1:F:82:TYR:CE1	2.49	0.47
1:B:368:TRP:N	1:B:369:PRO:CD	2.78	0.47
1:C:339:ASN:HD22	1:C:339:ASN:N	2.09	0.47
1:D:201:LEU:HD21	1:D:270:LEU:HD11	1.96	0.47
1:A:117:ALA:HB1	1:A:181:PHE:CE1	2.50	0.47
1:B:280:ILE:HB	1:B:311:SER:CB	2.45	0.47
1:C:313:CYS:HA	1:C:366:ALA:O	2.15	0.47
1:D:64:ARG:NH2	2:D:446:HOH:O	2.48	0.47
1:D:223:LEU:HG	1:D:384:ILE:HG21	1.95	0.47
1:D:310:ALA:HB1	1:D:374:PHE:CZ	2.50	0.47
1:E:100:ALA:HB3	2:E:437:HOH:O	2.14	0.47
1:E:144:GLY:O	1:E:148:VAL:HG23	2.14	0.47
1:E:158:ILE:HG13	1:E:159:THR:HG23	1.96	0.47
1:A:25:GLN:NE2	1:A:215:VAL:HG21	2.30	0.47
1:B:37:VAL:HG21	1:B:74:PHE:CA	2.38	0.47
1:E:59:THR:HG22	1:E:60:TYR:H	1.80	0.47
1:E:140:TYR:CD2	1:E:142:THR:HB	2.50	0.47
1:F:123:GLN:HG2	1:F:139:ALA:HB2	1.95	0.47
1:A:208:MET:HG3	1:A:213:VAL:HG21	1.97	0.47
1:F:263:LEU:HD22	1:F:263:LEU:N	2.30	0.47
1:F:270:LEU:C	1:F:270:LEU:HD13	2.40	0.47
1:F:199:ARG:HB2	1:F:275:TYR:HA	1.97	0.46
1:B:83:ASP:O	1:B:115:PRO:HD2	2.15	0.46
1:C:143:VAL:HG12	1:C:147:LEU:HD22	1.97	0.46
1:D:7:VAL:HG12	1:D:8:LEU:N	2.31	0.46
1:D:299:VAL:O	1:D:303:MET:HG2	2.15	0.46
1:E:337:LYS:HB3	1:F:98:LEU:HD21	1.98	0.46
1:D:6:THR:HG22	1:D:82:TYR:CD2	2.50	0.46
1:B:62:GLU:OE1	1:B:91:ARG:NH1	2.48	0.46
1:B:106:VAL:HG21	1:B:125:ILE:CG2	2.45	0.46
1:D:313:CYS:HB3	2:D:498:HOH:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:71:ASN:OD1	1:E:71:ASN:C	2.58	0.46
1:E:338:LEU:HD23	1:E:338:LEU:C	2.40	0.46
1:A:200:ILE:N	1:A:200:ILE:CD1	2.78	0.46
1:B:226:GLN:HG2	2:B:441:HOH:O	2.15	0.46
1:C:185:PHE:CE2	1:C:189:LEU:HD11	2.49	0.46
1:D:153:LYS:HE2	2:D:482:HOH:O	2.15	0.46
1:E:235:LYS:H	1:E:238:GLU:HG2	1.81	0.46
1:A:119:ILE:HD11	1:A:174:THR:C	2.41	0.46
1:A:183:GLN:HE21	1:A:187:LYS:CE	2.27	0.46
1:B:201:LEU:HB2	1:B:275:TYR:CD2	2.50	0.46
1:C:355:ARG:HG3	1:C:373:GLU:OE1	2.15	0.46
1:D:124:LEU:CD2	1:D:143:VAL:HG13	2.45	0.46
1:A:238:GLU:HB2	1:A:263:LEU:HD23	1.97	0.46
1:E:62:GLU:OE2	1:E:91:ARG:NH1	2.48	0.46
1:B:107:LYS:O	1:B:110:SER:HB3	2.16	0.46
1:B:239:ARG:HE	1:B:260:THR:CG2	2.29	0.46
1:D:7:VAL:CG1	1:D:8:LEU:N	2.79	0.46
1:D:9:ILE:HG12	1:D:86:VAL:HB	1.98	0.46
1:F:245:HIS:CD2	1:F:255:GLU:HG3	2.51	0.46
1:A:271:VAL:HG13	1:A:271:VAL:O	2.15	0.46
1:C:263:LEU:N	1:C:263:LEU:HD22	2.30	0.46
1:E:270:LEU:HD13	1:E:271:VAL:N	2.31	0.46
1:F:37:VAL:CG2	1:F:74:PHE:CA	2.94	0.46
1:F:92:ALA:N	1:F:93:PRO:CD	2.79	0.46
1:C:105:LEU:HD23	1:C:105:LEU:C	2.41	0.45
1:C:271:VAL:HG13	1:C:271:VAL:O	2.16	0.45
1:E:200:ILE:HD13	1:E:220:LEU:HD13	1.98	0.45
1:A:123:GLN:OE1	1:A:123:GLN:N	2.49	0.45
1:B:137:CYS:HA	1:B:164:VAL:HG11	1.98	0.45
1:D:206:ASP:OD1	1:D:241:PRO:HD2	2.17	0.45
1:E:16:GLU:OE2	1:E:259:HIS:HE1	1.99	0.45
1:E:209:GLU:HG2	1:E:212:GLU:OE2	2.16	0.45
1:A:88:PRO:CB	2:A:483:HOH:O	2.56	0.45
1:B:259:HIS:CD2	1:B:259:HIS:H	2.35	0.45
1:E:6:THR:HG22	1:E:82:TYR:CD2	2.52	0.45
1:C:65:GLY:HA2	1:C:244:ILE:HD13	1.98	0.45
1:C:332:ALA:HB1	1:C:336:VAL:HG21	1.99	0.45
1:D:142:THR:HA	1:F:291:LEU:HD11	1.99	0.45
1:E:98:LEU:HD12	1:E:98:LEU:N	2.31	0.45
1:F:235:LYS:N	1:F:238:GLU:CG	2.80	0.45
1:B:21:MET:HE2	1:B:211:TYR:CE1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ARG:HD2	2:B:418:HOH:O	2.15	0.45
1:D:136:LYS:HA	1:D:153:LYS:HB2	1.97	0.45
1:D:337:LYS:HG3	1:D:347:TRP:CD2	2.52	0.45
1:D:370:GLY:HA2	2:D:425:HOH:O	2.17	0.45
1:F:10:LEU:O	1:F:88:PRO:HD2	2.16	0.45
1:F:213:VAL:CG1	1:F:214:LYS:N	2.77	0.45
1:D:204:CYS:HA	1:D:208:MET:HE1	1.99	0.45
1:F:236:ALA:N	1:F:266:ASN:OD1	2.49	0.45
1:B:284:ARG:NH1	1:C:60:TYR:O	2.43	0.45
1:B:285:ALA:N	1:B:286:PRO:CD	2.79	0.45
1:D:235:LYS:H	1:D:238:GLU:HG2	1.80	0.45
1:A:13:ASP:OD1	1:A:48:PRO:HD2	2.17	0.45
1:A:73:THR:C	1:A:74:PHE:O	2.58	0.45
1:C:123:GLN:HG2	1:C:139:ALA:HB2	1.99	0.45
1:D:10:LEU:HD11	1:D:102:VAL:HG13	1.98	0.45
1:D:79:LEU:H	1:D:79:LEU:CD1	2.24	0.45
1:A:204:CYS:HA	1:A:208:MET:HE1	1.99	0.45
1:C:165:VAL:HG23	1:C:184:LEU:HD13	1.99	0.45
1:C:296:LEU:HD22	1:C:322:ALA:HB2	1.98	0.45
1:D:8:LEU:HD12	1:D:35:HIS:O	2.16	0.45
1:E:314:HIS:HA	1:E:336:VAL:HG21	1.99	0.45
1:D:303:MET:HG3	1:D:324:VAL:HG11	1.97	0.45
1:F:367:ALA:HB3	1:F:369:PRO:HD2	1.99	0.45
1:A:208:MET:CG	1:A:213:VAL:HG21	2.48	0.44
1:C:10:LEU:O	1:C:88:PRO:HD2	2.16	0.44
1:C:311:SER:O	1:C:364:THR:HA	2.18	0.44
1:F:111:ARG:C	1:F:113:GLY:H	2.26	0.44
1:F:355:ARG:HG2	1:F:355:ARG:NH2	2.31	0.44
1:B:199:ARG:HD3	1:B:274:SER:O	2.17	0.44
1:C:16:GLU:O	1:C:20:VAL:HG23	2.18	0.44
1:C:367:ALA:HB3	1:C:369:PRO:HD2	1.99	0.44
1:D:13:ASP:OD2	1:F:251:GLN:HB2	2.17	0.44
1:D:143:VAL:HG12	1:D:147:LEU:HD22	1.99	0.44
1:E:367:ALA:HB3	1:E:369:PRO:HD2	1.99	0.44
1:F:223:LEU:HG	1:F:384:ILE:HG21	1.98	0.44
1:B:26:ALA:O	1:B:29:ALA:HB3	2.17	0.44
1:D:310:ALA:HB1	1:D:374:PHE:CE1	2.52	0.44
1:E:106:VAL:HG21	1:E:125:ILE:HG22	1.99	0.44
1:E:271:VAL:O	1:E:271:VAL:HG13	2.18	0.44
1:F:170:ILE:HD13	1:F:185:PHE:HA	1.99	0.44
1:A:23:PRO:HG2	2:A:449:HOH:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:VAL:HG12	1:A:388:PHE:CE1	2.52	0.44
1:B:30:PHE:N	1:B:30:PHE:CD2	2.85	0.44
1:B:206:ASP:OD2	1:C:58:GLN:HG3	2.18	0.44
1:F:136:LYS:HA	1:F:153:LYS:HB2	1.99	0.44
1:A:332:ALA:HB1	1:A:336:VAL:HG23	1.98	0.44
1:B:276:ASP:O	1:B:308:PRO:HD2	2.18	0.44
1:B:158:ILE:CD1	1:B:159:THR:HG23	2.48	0.44
1:C:223:LEU:HD12	1:C:223:LEU:HA	1.82	0.44
1:E:30:PHE:CE2	1:E:223:LEU:HD13	2.53	0.44
1:E:55:CYS:HB3	2:E:459:HOH:O	2.18	0.44
1:A:74:PHE:C	2:A:440:HOH:O	2.61	0.44
1:A:347:TRP:CZ2	1:A:350:PRO:HD3	2.52	0.44
1:B:135:ARG:NH2	1:B:166:ASP:O	2.51	0.44
1:C:235:LYS:N	1:C:238:GLU:CG	2.81	0.44
1:C:337:LYS:HA	1:C:347:TRP:CZ3	2.53	0.44
1:E:15:MET:HG3	1:E:20:VAL:HG21	1.99	0.44
1:A:271:VAL:HG13	1:A:274:SER:OG	2.18	0.44
1:B:136:LYS:O	1:B:137:CYS:HB3	2.17	0.44
1:B:200:ILE:HD13	1:B:220:LEU:HD13	1.98	0.44
1:C:213:VAL:HG13	1:C:214:LYS:H	1.80	0.44
1:D:333:TYR:CD1	1:D:334:PRO:HD2	2.52	0.44
1:E:105:LEU:C	1:E:105:LEU:HD23	2.43	0.44
1:E:310:ALA:HA	1:E:363:VAL:O	2.18	0.44
1:E:353:ILE:HA	2:E:461:HOH:O	2.17	0.44
1:F:66:HIS:CE1	1:F:244:ILE:HG23	2.52	0.44
1:A:27:LEU:O	2:A:434:HOH:O	2.21	0.44
1:B:130:ASP:O	1:B:130:ASP:CG	2.60	0.44
1:F:303:MET:HG3	1:F:324:VAL:HB	2.00	0.44
1:A:25:GLN:OE1	1:A:371:HIS:HB2	2.18	0.43
1:A:287:GLU:OE1	1:B:142:THR:HG21	2.18	0.43
1:B:328:ARG:NH1	1:B:359:ASP:O	2.51	0.43
1:E:201:LEU:HB2	1:E:275:TYR:CD2	2.53	0.43
1:A:297:ASN:O	1:A:301:GLU:HG3	2.18	0.43
1:C:330:CYS:CA	1:C:348:LEU:HD12	2.46	0.43
1:E:21:MET:HE2	1:E:211:TYR:CE1	2.53	0.43
1:E:165:VAL:CG2	1:E:184:LEU:HD13	2.46	0.43
1:B:214:LYS:HD3	2:B:405:HOH:O	2.18	0.43
1:C:204:CYS:HA	1:C:208:MET:HE1	2.00	0.43
1:D:117:ALA:HB1	1:D:181:PHE:CE1	2.53	0.43
1:D:282:GLY:HA3	1:D:313:CYS:HB3	2.00	0.43
1:D:320:ALA:CB	1:D:325:LEU:HD12	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:ALA:HB3	1:E:93:PRO:HD3	2.00	0.43
1:E:277:ALA:HB2	1:E:382:LEU:HD21	2.00	0.43
1:F:24:PHE:O	1:F:28:GLN:HG3	2.19	0.43
1:F:59:THR:HG22	1:F:60:TYR:CD1	2.52	0.43
1:F:66:HIS:CD2	1:F:244:ILE:HG23	2.53	0.43
1:A:59:THR:HG23	2:A:430:HOH:O	2.18	0.43
1:B:62:GLU:CD	1:B:91:ARG:NH1	2.77	0.43
1:B:204:CYS:CA	1:B:208:MET:HE1	2.45	0.43
1:C:204:CYS:SG	1:C:208:MET:HE1	2.58	0.43
1:C:255:GLU:CD	1:C:284:ARG:NH2	2.76	0.43
1:D:143:VAL:HG12	1:D:143:VAL:O	2.18	0.43
1:D:79:LEU:HD12	1:D:79:LEU:N	2.26	0.43
1:E:223:LEU:HD21	1:E:379:MET:HG2	2.00	0.43
1:F:213:VAL:CG1	1:F:214:LYS:H	2.31	0.43
1:C:339:ASN:N	1:C:339:ASN:ND2	2.66	0.43
1:D:25:GLN:NE2	1:D:371:HIS:ND1	2.65	0.43
1:E:66:HIS:CD2	1:E:244:ILE:HG23	2.54	0.43
1:E:285:ALA:N	1:E:286:PRO:CD	2.81	0.43
1:F:117:ALA:HA	1:F:170:ILE:O	2.18	0.43
1:F:154:TRP:HE1	1:F:156:GLU:CD	2.27	0.43
1:A:253:TYR:O	1:B:91:ARG:NH2	2.50	0.43
1:C:388:PHE:O	1:C:389:HIS:HB2	2.18	0.43
1:E:143:VAL:HG12	1:E:143:VAL:O	2.18	0.43
1:F:373:GLU:HG2	2:F:451:HOH:O	2.19	0.43
1:A:81:LYS:HE3	2:A:437:HOH:O	2.18	0.43
1:A:199:ARG:HA	1:A:226:GLN:O	2.19	0.43
1:A:223:LEU:HG	1:A:384:ILE:HG21	2.00	0.43
1:F:107:LYS:HE2	1:F:129:ALA:O	2.19	0.43
1:F:332:ALA:HB1	1:F:336:VAL:CG2	2.48	0.43
1:A:355:ARG:HG2	1:A:357:PHE:CZ	2.54	0.43
1:D:208:MET:HE2	1:D:281:PRO:CG	2.49	0.43
1:E:4:SER:C	1:E:5:ARG:HD3	2.43	0.43
1:E:136:LYS:HA	1:E:153:LYS:HB2	2.00	0.43
1:E:310:ALA:HB1	1:E:374:PHE:CZ	2.53	0.43
1:F:183:GLN:O	1:F:187:LYS:HG2	2.18	0.43
1:A:230:VAL:HG21	1:A:270:LEU:HD11	2.01	0.43
1:C:187:LYS:HZ3	1:C:193:ILE:H	1.65	0.43
1:E:328:ARG:NH1	1:E:359:ASP:O	2.52	0.43
1:A:235:LYS:N	1:A:238:GLU:HG3	2.34	0.42
1:A:265:THR:HG22	1:A:266:ASN:N	2.33	0.42
1:B:375:VAL:O	1:B:379:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:334:PRO:O	1:E:98:LEU:HD22	2.18	0.42
1:E:235:LYS:H	1:E:238:GLU:HG3	1.82	0.42
1:A:41:LYS:C	1:A:42:LYS:HD3	2.43	0.42
1:B:195:GLY:O	1:B:384:ILE:HG12	2.18	0.42
1:B:310:ALA:HA	1:B:363:VAL:O	2.19	0.42
1:B:337:LYS:HG3	1:B:347:TRP:CD2	2.54	0.42
1:F:52:HIS:O	1:F:53:ASP:HB3	2.19	0.42
1:F:132:VAL:CG2	1:F:152:ALA:HB2	2.49	0.42
1:F:297:ASN:O	1:F:301:GLU:HG3	2.19	0.42
1:B:335:ALA:HB1	1:C:94:GLU:HG2	2.01	0.42
1:D:128:ALA:HB2	1:F:338:LEU:HD13	2.00	0.42
1:D:314:HIS:HD2	1:D:317:GLN:NE2	2.17	0.42
1:A:170:ILE:HD12	1:A:185:PHE:HA	2.01	0.42
1:A:235:LYS:O	1:A:237:GLY:N	2.53	0.42
1:A:288:TYR:CD2	1:B:59:THR:HG23	2.54	0.42
1:A:333:TYR:O	1:A:336:VAL:HG22	2.19	0.42
1:C:123:GLN:OE1	1:C:123:GLN:N	2.51	0.42
1:A:23:PRO:O	1:A:27:LEU:HG	2.19	0.42
1:C:358:THR:OG1	1:C:377:GLN:NE2	2.52	0.42
1:D:60:TYR:O	1:F:284:ARG:NH1	2.26	0.42
1:D:294:HIS:O	1:D:298:ILE:HG13	2.19	0.42
1:F:9:ILE:HG12	1:F:86:VAL:HB	2.01	0.42
1:F:210:ASP:OD2	1:F:259:HIS:HD2	2.03	0.42
1:F:212:GLU:OE1	1:F:313:CYS:CB	2.68	0.42
1:F:331:THR:OG1	1:F:350:PRO:HB3	2.20	0.42
1:A:203:LEU:O	1:A:281:PRO:HD2	2.20	0.42
1:E:119:ILE:HG13	1:E:172:ALA:HB3	2.02	0.42
1:F:54:PHE:N	1:F:54:PHE:CD1	2.86	0.42
1:B:203:LEU:HG	1:B:278:LEU:HD11	2.02	0.42
1:C:124:LEU:CD2	1:C:143:VAL:HG13	2.50	0.42
1:C:231:CYS:O	1:C:232:PRO:C	2.62	0.42
1:D:336:VAL:HB	1:D:339:ASN:HD22	1.85	0.42
1:A:169:LEU:HG	2:A:442:HOH:O	2.20	0.42
1:F:328:ARG:HA	1:F:328:ARG:HD2	1.94	0.42
1:A:108:GLU:HA	1:A:111:ARG:HH12	1.80	0.42
1:A:124:LEU:HD21	1:A:143:VAL:HG13	2.01	0.42
1:A:312:ILE:HG12	1:A:313:CYS:N	2.33	0.42
1:B:37:VAL:CG2	1:B:74:PHE:N	2.82	0.42
1:D:3:ASN:O	1:D:4:SER:CB	2.65	0.42
1:D:5:ARG:HH21	1:D:5:ARG:HG2	1.84	0.42
1:E:106:VAL:HG21	1:E:125:ILE:CG2	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:165:VAL:HG22	1:F:170:ILE:HG12	2.02	0.42
1:A:42:LYS:HD3	1:A:42:LYS:N	2.33	0.41
1:A:235:LYS:C	1:A:237:GLY:H	2.28	0.41
1:A:337:LYS:HG3	1:A:347:TRP:CD2	2.55	0.41
1:B:8:LEU:HD12	1:B:35:HIS:O	2.20	0.41
1:E:13:ASP:O	1:E:14:TYR:HB2	2.20	0.41
1:A:204:CYS:SG	1:A:208:MET:HE1	2.60	0.41
1:A:215:VAL:HB	1:A:216:PRO:HD3	2.00	0.41
1:B:105:LEU:C	1:B:105:LEU:HD23	2.45	0.41
1:B:310:ALA:HB1	1:B:374:PHE:CE1	2.55	0.41
1:C:27:LEU:HD22	1:C:32:ILE:HD12	2.03	0.41
1:C:64:ARG:NH2	2:C:467:HOH:O	2.52	0.41
1:D:96:LEU:C	1:D:98:LEU:H	2.28	0.41
1:D:313:CYS:HA	1:D:366:ALA:O	2.21	0.41
1:F:271:VAL:O	1:F:271:VAL:HG13	2.20	0.41
1:C:64:ARG:HB2	2:C:420:HOH:O	2.19	0.41
1:E:159:THR:O	1:E:162:VAL:HG13	2.20	0.41
1:F:310:ALA:HB1	1:F:374:PHE:CZ	2.56	0.41
1:B:234:LYS:HB3	1:B:238:GLU:HG3	2.02	0.41
1:C:36:THR:HG21	1:C:68:PHE:CZ	2.55	0.41
1:C:106:VAL:HG21	1:C:125:ILE:HG21	2.01	0.41
1:C:124:LEU:HD23	1:C:143:VAL:HG13	2.03	0.41
1:E:335:ALA:CB	1:F:94:GLU:HG2	2.51	0.41
1:F:285:ALA:HB3	1:F:286:PRO:HD3	2.01	0.41
1:B:65:GLY:HA2	1:B:244:ILE:HD13	2.01	0.41
1:B:239:ARG:NH2	1:B:260:THR:HG23	2.28	0.41
1:D:235:LYS:N	1:D:238:GLU:HG3	2.27	0.41
1:E:30:PHE:N	1:E:30:PHE:CD2	2.88	0.41
1:E:107:LYS:HG2	1:E:129:ALA:HB1	2.02	0.41
1:E:119:ILE:HD11	1:E:174:THR:O	2.21	0.41
1:F:368:TRP:N	1:F:369:PRO:CD	2.83	0.41
1:A:120:CYS:HB3	1:A:121:HIS:H	1.66	0.41
1:A:267:PHE:O	1:A:270:LEU:HB2	2.21	0.41
1:C:120:CYS:HA	1:C:173:ALA:O	2.21	0.41
1:C:213:VAL:CG1	1:C:214:LYS:N	2.82	0.41
1:C:255:GLU:CD	1:C:284:ARG:HH22	2.27	0.41
1:F:271:VAL:HG13	1:F:274:SER:OG	2.21	0.41
1:B:7:VAL:HG12	1:B:8:LEU:N	2.36	0.41
1:B:144:GLY:O	1:B:148:VAL:HG23	2.20	0.41
1:D:10:LEU:O	1:D:88:PRO:HD2	2.21	0.41
1:A:88:PRO:HA	2:A:483:HOH:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:HIS:O	1:A:298:ILE:HG13	2.20	0.41
1:A:367:ALA:CB	1:A:369:PRO:HD2	2.51	0.41
1:D:144:GLY:O	1:D:145:PRO:C	2.63	0.41
1:B:108:GLU:HA	1:B:111:ARG:NH1	2.35	0.41
1:C:272:SER:HB3	1:C:301:GLU:OE1	2.21	0.41
1:C:323:GLY:HA2	2:C:403:HOH:O	2.21	0.41
1:C:332:ALA:CB	1:C:336:VAL:CG2	2.99	0.41
1:D:173:ALA:N	2:D:411:HOH:O	2.46	0.41
1:E:235:LYS:N	1:E:238:GLU:HG2	2.36	0.41
1:E:239:ARG:HG3	1:E:239:ARG:HH11	1.85	0.41
1:F:178:HIS:N	1:F:179:PRO:CD	2.84	0.41
1:C:129:ALA:O	1:C:131:THR:HG23	2.21	0.41
1:D:119:ILE:HD11	1:D:174:THR:C	2.46	0.41
1:A:32:ILE:CG1	2:A:434:HOH:O	2.57	0.40
1:A:331:THR:OG1	1:A:350:PRO:HB3	2.21	0.40
1:C:37:VAL:HG22	1:C:74:PHE:CA	2.51	0.40
1:D:91:ARG:HB3	2:D:421:HOH:O	2.21	0.40
1:F:30:PHE:CZ	1:F:223:LEU:HD13	2.57	0.40
1:F:37:VAL:CG2	1:F:74:PHE:N	2.84	0.40
1:F:119:ILE:HD11	1:F:174:THR:O	2.21	0.40
1:A:255:GLU:OE2	1:A:284:ARG:HD3	2.20	0.40
1:B:92:ALA:HB3	1:B:93:PRO:HD3	2.03	0.40
1:D:79:LEU:HD21	1:D:105:LEU:HG	2.02	0.40
1:E:118:SER:O	1:E:171:THR:HA	2.22	0.40
1:E:208:MET:HG3	1:E:213:VAL:CG2	2.45	0.40
1:E:335:ALA:HB1	1:F:94:GLU:HG2	2.03	0.40
1:F:37:VAL:CB	2:F:463:HOH:O	2.66	0.40
1:F:330:CYS:CA	1:F:348:LEU:HD12	2.48	0.40
1:A:20:VAL:HG22	1:A:88:PRO:CB	2.49	0.40
1:A:325:LEU:HB2	2:A:431:HOH:O	2.21	0.40
1:B:208:MET:HE2	1:B:281:PRO:HB2	2.03	0.40
1:C:388:PHE:HB3	1:C:389:HIS:H	1.76	0.40
1:D:185:PHE:O	1:D:189:LEU:HG	2.22	0.40
1:D:271:VAL:HG13	1:D:271:VAL:O	2.21	0.40
1:D:305:SER:O	1:D:306:GLU:HB2	2.21	0.40
1:F:120:CYS:HB3	2:F:479:HOH:O	2.20	0.40
1:F:133:ASN:C	1:F:135:ARG:H	2.30	0.40
1:B:367:ALA:CB	1:B:369:PRO:HD2	2.52	0.40
1:D:83:ASP:O	1:D:115:PRO:HD2	2.22	0.40
1:D:221:GLN:OE1	2:D:463:HOH:O	2.22	0.40
1:F:66:HIS:CE1	1:F:244:ILE:HG12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:236:ALA:O	1:F:263:LEU:O	2.39	0.40
1:A:62:GLU:HG2	1:A:63:SER:N	2.37	0.40
1:A:77:VAL:HG22	2:A:461:HOH:O	2.22	0.40
1:B:19:GLU:OE1	1:B:89:GLY:HA3	2.21	0.40
1:B:316:GLN:N	1:B:316:GLN:OE1	2.55	0.40
1:E:296:LEU:HA	1:E:296:LEU:HD23	1.87	0.40
1:F:117:ALA:HB1	1:F:181:PHE:CZ	2.56	0.40
1:F:215:VAL:HB	1:F:216:PRO:CD	2.52	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	385/387 (100%)	353 (92%)	27 (7%)	5 (1%)	9	10
1	B	385/387 (100%)	356 (92%)	27 (7%)	2 (0%)	24	31
1	C	385/387 (100%)	356 (92%)	28 (7%)	1 (0%)	36	46
1	D	385/387 (100%)	358 (93%)	24 (6%)	3 (1%)	16	20
1	E	385/387 (100%)	352 (91%)	31 (8%)	2 (0%)	24	31
1	F	385/387 (100%)	356 (92%)	24 (6%)	5 (1%)	9	10
All	All	2310/2322 (100%)	2131 (92%)	161 (7%)	18 (1%)	16	20

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	ASP
1	E	238	GLU
1	A	74	PHE
1	A	236	ALA

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Mol	Chain	Res	Type
1	D	275	TYR
1	B	238	GLU
1	C	275	TYR
1	F	112	SER
1	D	149	ALA
1	A	141	ALA
1	D	4	SER
1	E	275	TYR
1	F	53	ASP
1	F	79	LEU
1	F	141	ALA
1	F	275	TYR
1	B	271	VAL
1	A	336	VAL

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	313/313 (100%)	292 (93%)	21 (7%)	15	21
1	B	313/313 (100%)	300 (96%)	13 (4%)	26	40
1	C	313/313 (100%)	295 (94%)	18 (6%)	18	26
1	D	313/313 (100%)	297 (95%)	16 (5%)	21	32
1	E	313/313 (100%)	299 (96%)	14 (4%)	24	37
1	F	313/313 (100%)	298 (95%)	15 (5%)	23	35
All	All	1878/1878 (100%)	1781 (95%)	97 (5%)	21	31

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	LEU
1	A	59	THR
1	A	64	ARG
1	A	98	LEU

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Mol	Chain	Res	Type
1	A	118	SER
1	A	123	GLN
1	A	142	THR
1	A	147	LEU
1	A	158	ILE
1	A	162	VAL
1	A	200	ILE
1	A	208	MET
1	A	223	LEU
1	A	235	LYS
1	A	238	GLU
1	A	256	LYS
1	A	263	LEU
1	A	270	LEU
1	A	338	LEU
1	A	355	ARG
1	A	389	HIS
1	B	10	LEU
1	B	59	THR
1	B	104	GLU
1	B	135	ARG
1	B	147	LEU
1	B	162	VAL
1	B	208	MET
1	B	223	LEU
1	B	226	GLN
1	B	251	GLN
1	B	259	HIS
1	B	293	GLU
1	B	389	HIS
1	C	10	LEU
1	C	21	MET
1	C	37	VAL
1	C	42	LYS
1	C	64	ARG
1	C	69	THR
1	C	98	LEU
1	C	107	LYS
1	C	118	SER
1	C	123	GLN
1	C	147	LEU
1	C	223	LEU

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Mol	Chain	Res	Type
1	C	238	GLU
1	C	265	THR
1	C	316	GLN
1	C	336	VAL
1	C	339	ASN
1	C	353	ILE
1	D	10	LEU
1	D	37	VAL
1	D	69	THR
1	D	98	LEU
1	D	135	ARG
1	D	147	LEU
1	D	165	VAL
1	D	208	MET
1	D	223	LEU
1	D	256	LYS
1	D	263	LEU
1	D	274	SER
1	D	293	GLU
1	D	336	VAL
1	D	338	LEU
1	D	353	ILE
1	E	10	LEU
1	E	59	THR
1	E	120	CYS
1	E	142	THR
1	E	147	LEU
1	E	165	VAL
1	E	192	LYS
1	E	208	MET
1	E	223	LEU
1	E	265	THR
1	E	293	GLU
1	E	304	ASN
1	E	334	PRO
1	E	355	ARG
1	F	10	LEU
1	F	37	VAL
1	F	59	THR
1	F	64	ARG
1	F	98	LEU
1	F	123	GLN

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Mol	Chain	Res	Type
1	F	142	THR
1	F	147	LEU
1	F	208	MET
1	F	223	LEU
1	F	238	GLU
1	F	269	ASP
1	F	274	SER
1	F	287	GLU
1	F	353	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	28	GLN
1	A	58	GLN
1	A	183	GLN
1	A	197	ASN
1	A	221	GLN
1	A	251	GLN
1	A	259	HIS
1	A	339	ASN
1	A	377	GLN
1	A	385	GLN
1	A	389	HIS
1	B	28	GLN
1	B	133	ASN
1	B	226	GLN
1	B	251	GLN
1	B	259	HIS
1	B	317	GLN
1	B	339	ASN
1	B	385	GLN
1	C	28	GLN
1	C	52	HIS
1	C	58	GLN
1	C	133	ASN
1	C	226	GLN
1	C	251	GLN
1	C	259	HIS
1	C	317	GLN
1	C	339	ASN

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Mol	Chain	Res	Type
1	C	377	GLN
1	D	3	ASN
1	D	25	GLN
1	D	28	GLN
1	D	67	ASN
1	D	183	GLN
1	D	197	ASN
1	D	251	GLN
1	D	259	HIS
1	D	266	ASN
1	D	317	GLN
1	D	339	ASN
1	D	377	GLN
1	E	3	ASN
1	E	28	GLN
1	E	52	HIS
1	E	57	HIS
1	E	183	GLN
1	E	197	ASN
1	E	218	GLN
1	E	221	GLN
1	E	259	HIS
1	E	294	HIS
1	E	377	GLN
1	E	389	HIS
1	F	28	GLN
1	F	35	HIS
1	F	58	GLN
1	F	133	ASN
1	F	183	GLN
1	F	221	GLN
1	F	259	HIS
1	F	339	ASN
1	F	377	GLN
1	F	389	HIS

5.3.3 RNA ⓘ

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](#)

There are no ligands in this entry.

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	387/387 (100%)	0.12	3 (0%) 82 83	16, 30, 48, 69	0
1	B	387/387 (100%)	0.20	2 (0%) 87 87	14, 33, 49, 68	0
1	C	387/387 (100%)	0.06	5 (1%) 75 76	15, 28, 46, 68	0
1	D	387/387 (100%)	0.14	4 (1%) 79 80	18, 31, 49, 69	0
1	E	387/387 (100%)	0.07	3 (0%) 82 83	15, 31, 47, 68	0
1	F	387/387 (100%)	0.16	9 (2%) 61 63	14, 31, 48, 67	0
All	All	2322/2322 (100%)	0.12	26 (1%) 78 79	14, 31, 48, 69	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	3	ASN	3.4
1	E	350	PRO	3.3
1	A	389	HIS	3.2
1	F	353	ILE	3.0
1	B	389	HIS	2.9
1	F	389	HIS	2.8
1	E	79	LEU	2.8
1	C	389	HIS	2.7
1	E	389	HIS	2.6
1	C	55	CYS	2.6
1	C	195	GLY	2.6
1	C	353	ILE	2.6
1	F	195	GLY	2.5
1	D	389	HIS	2.5
1	F	237	GLY	2.4
1	F	388	PHE	2.4
1	B	270	LEU	2.4
1	D	61	PHE	2.3
1	D	3	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	270	LEU	2.2
1	F	55	CYS	2.1
1	F	274	SER	2.1
1	D	75	ASP	2.1
1	A	270	LEU	2.1
1	F	111	ARG	2.1
1	C	271	VAL	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.