



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2026 – 04:12 PM JST

PDB ID : 22PO / pdb_000022po
Title : Class III Aminotransferase
Authors : Hwang, J.; Lee, J.H.; Do, H.
Deposited on : 2026-01-20
Resolution : 2.31 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:

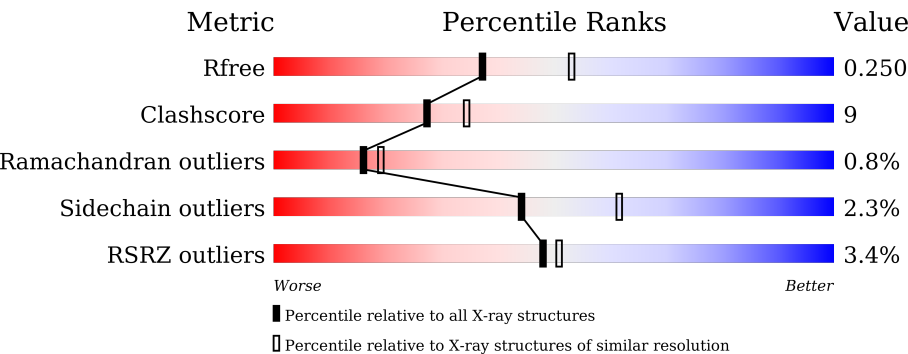
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.31 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	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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	450	4% 76% 15% • 8%
1	B	450	3% 74% 17% • 7%
1	C	450	3% 78% 13% •• 8%
1	D	450	3% 73% 19% • 7%
1	E	450	3% 76% 16% • 7%
1	F	450	2% 78% 14% 7%

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Mol	Chain	Length	Quality of chain
1	G	450	3% 78% 14% 8%
1	H	450	5% 68% 23% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 26450 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 Class III Aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	416	Total	C	N	O	S	0	0	0
			3200	2032	551	598	19			
1	B	419	Total	C	N	O	S	0	0	0
			3226	2050	554	603	19			
1	C	415	Total	C	N	O	S	0	0	0
			3192	2026	550	597	19			
1	D	418	Total	C	N	O	S	0	0	0
			3217	2044	552	602	19			
1	E	417	Total	C	N	O	S	0	0	0
			3207	2037	552	599	19			
1	F	417	Total	C	N	O	S	0	0	0
			3207	2037	552	599	19			
1	G	415	Total	C	N	O	S	0	0	0
			3192	2026	550	597	19			
1	H	417	Total	C	N	O	S	0	0	0
			3207	2037	552	599	19			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	126	Total	O	0	0
			126	126		
2	B	114	Total	O	0	0
			114	114		
2	C	150	Total	O	0	0
			150	150		
2	D	105	Total	O	0	0
			105	105		
2	E	87	Total	O	0	0
			87	87		
2	F	85	Total	O	0	0
			85	85		

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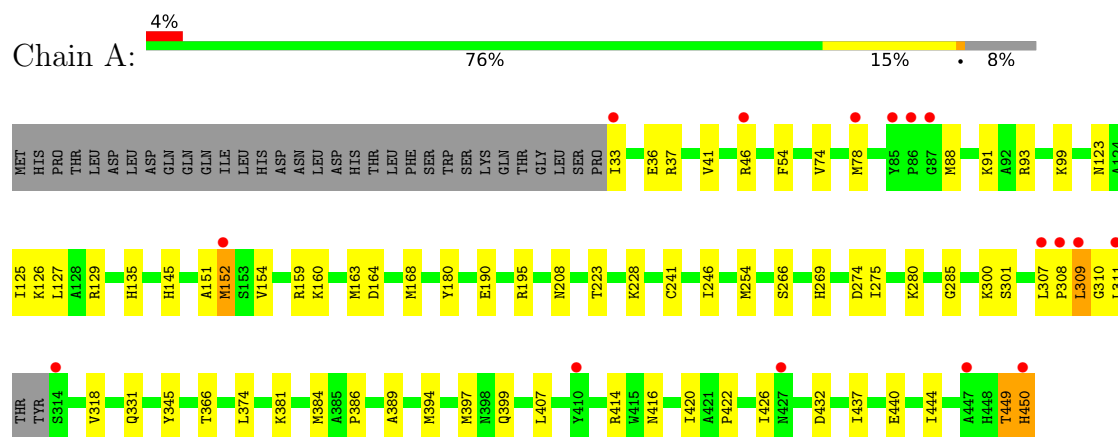
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	87	Total	O	0	0
			87	87		
2	H	48	Total	O	0	0
			48	48		

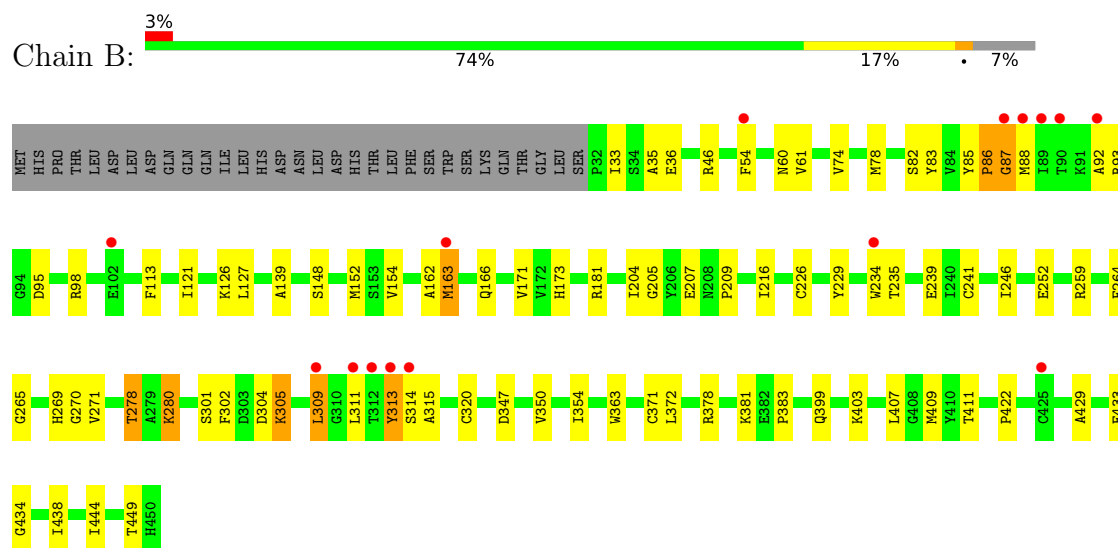
3 Residue-property plots

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.

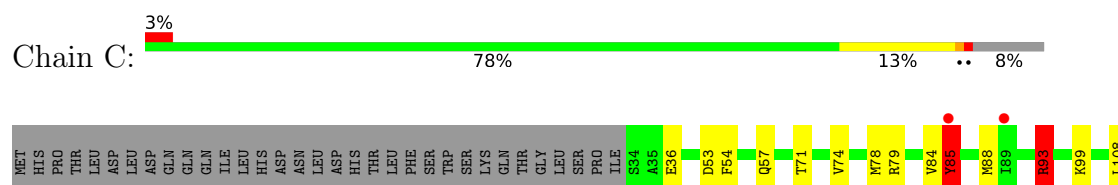
• Molecule 1: Class III Aminotransferase

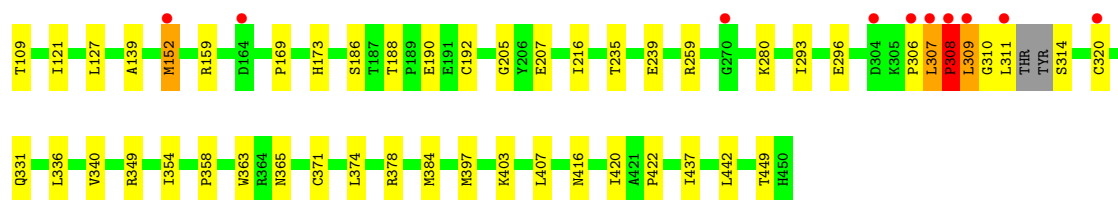


• Molecule 1: Class III Aminotransferase

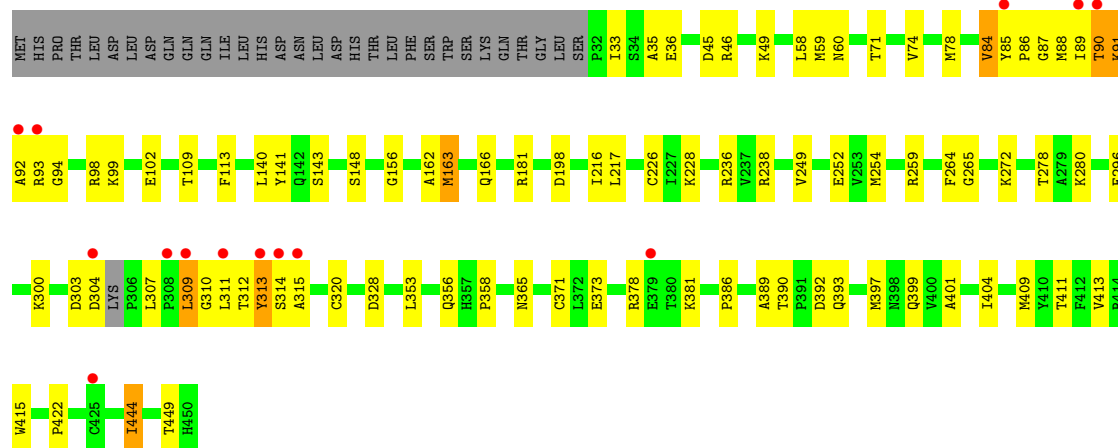
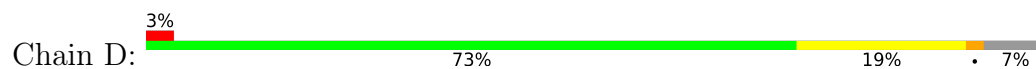


• Molecule 1: Class III Aminotransferase

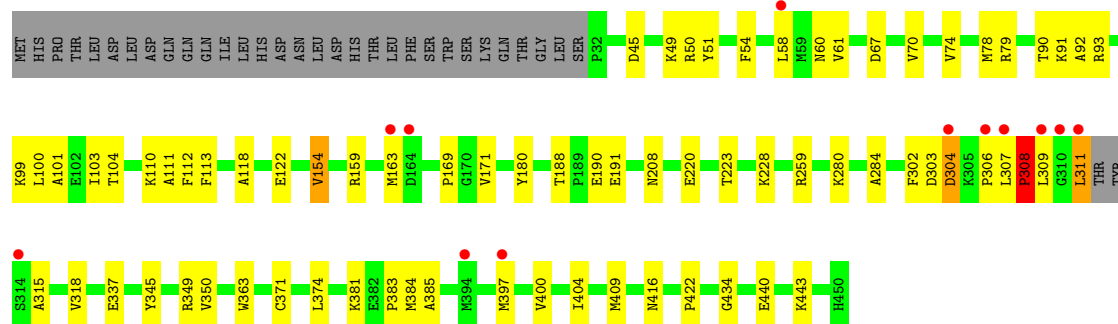
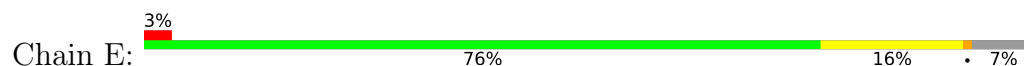




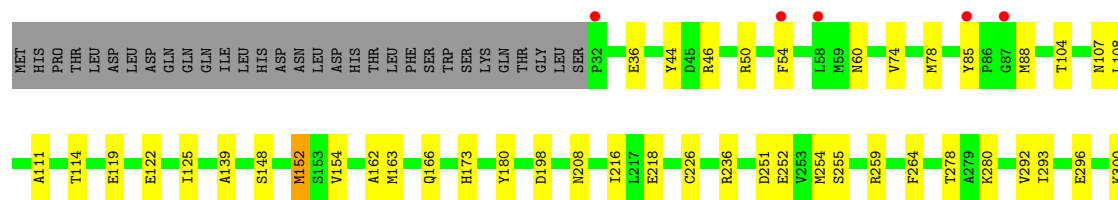
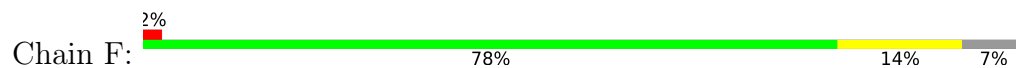
• Molecule 1: Class III Aminotransferase

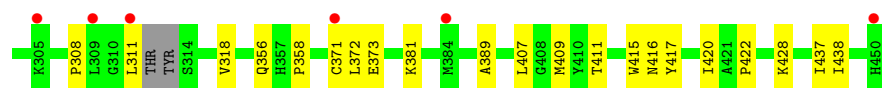


• Molecule 1: Class III Aminotransferase

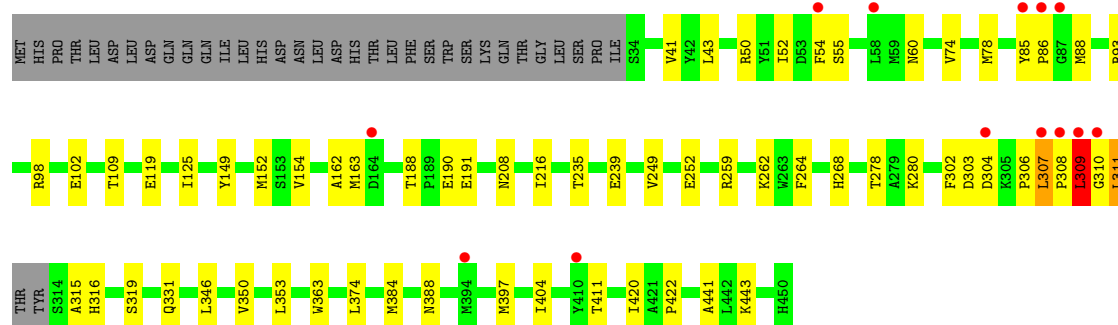
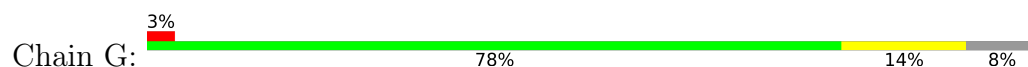


• Molecule 1: Class III Aminotransferase

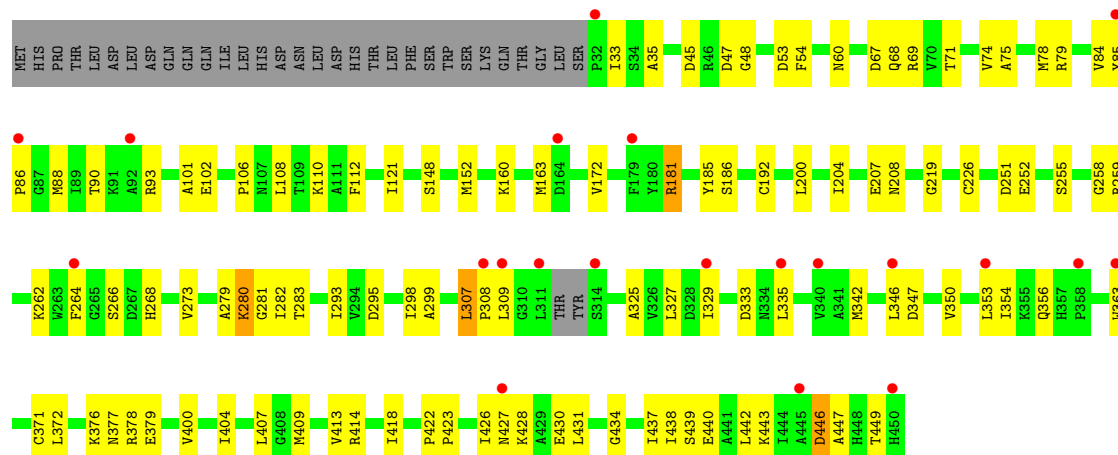




• Molecule 1: Class III Aminotransferase



• Molecule 1: Class III Aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	100.81Å 152.26Å 117.37Å 90.00° 104.60° 90.00°	Depositor
Resolution (Å)	33.56 – 2.31 33.56 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.1 (33.56-2.31) 99.1 (33.56-2.31)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.31Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.196 , 0.250 0.197 , 0.250	Depositor DCC
R_{free} test set	7440 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.051	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 39.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26450	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.72% 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

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	0.46	0/3271	0.69	0/4438
1	B	0.47	0/3300	0.73	2/4480 (0.0%)
1	C	0.48	0/3263	0.75	3/4427 (0.1%)
1	D	0.49	0/3290	0.75	3/4465 (0.1%)
1	E	0.46	0/3279	0.73	2/4449 (0.0%)
1	F	0.44	0/3279	0.67	0/4449
1	G	0.44	0/3263	0.66	1/4427 (0.0%)
1	H	0.45	0/3279	0.70	1/4449 (0.0%)
All	All	0.46	0/26224	0.71	12/35584 (0.0%)

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	C	0	2
1	E	0	1
1	H	0	2
All	All	0	7

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	308	PRO	N-CA-CB	-10.18	92.56	103.25
1	E	303	ASP	N-CA-C	-7.64	104.88	112.97
1	C	308	PRO	N-CA-CB	-7.18	95.71	103.25
1	G	308	PRO	CA-C-O	-6.05	114.73	121.32
1	B	207	GLU	N-CA-C	-5.83	102.14	110.59
1	D	87	GLY	N-CA-C	-5.78	107.60	114.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	446	ASP	N-CA-C	-5.45	105.50	111.82
1	D	310	GLY	N-CA-C	-5.39	107.58	114.37
1	D	313	TYR	N-CA-C	-5.30	106.88	113.19
1	C	85	TYR	CB-CA-C	5.17	118.04	109.56
1	B	313	TYR	N-CA-C	-5.15	106.26	112.54
1	C	308	PRO	N-CA-C	5.05	122.88	112.47

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	159	ARG	Sidechain
1	A	414	ARG	Sidechain
1	C	79	ARG	Sidechain
1	C	93	ARG	Sidechain
1	E	159	ARG	Sidechain
1	H	181	ARG	Sidechain
1	H	93	ARG	Sidechain

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	3200	0	3162	64	0
1	B	3226	0	3187	74	0
1	C	3192	0	3151	52	0
1	D	3217	0	3174	73	0
1	E	3207	0	3170	51	0
1	F	3207	0	3170	46	0
1	G	3192	0	3151	59	0
1	H	3207	0	3170	85	0
2	A	126	0	0	5	0
2	B	114	0	0	0	0
2	C	150	0	0	0	0
2	D	105	0	0	1	0
2	E	87	0	0	2	0
2	F	85	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	87	0	0	1	0
2	H	48	0	0	2	0
All	All	26450	0	25335	462	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 9.

All (462) 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:G:54:PHE:HE2	1:G:420:ILE:HG12	1.05	1.12
1:G:54:PHE:CE2	1:G:420:ILE:HG23	1.91	1.05
1:G:54:PHE:CE2	1:G:420:ILE:HG12	1.92	1.03
1:H:252:GLU:HG2	1:H:264:PHE:HD1	1.27	0.98
1:G:54:PHE:HE2	1:G:420:ILE:CG1	1.75	0.97
1:C:152:MET:HE1	1:D:309:LEU:HB3	1.46	0.97
1:H:110:LYS:HE3	1:H:299:ALA:HB1	1.48	0.96
1:H:54:PHE:CG	1:H:409:MET:HE2	2.04	0.92
1:H:354:ILE:CG2	1:H:378:ARG:HH22	1.82	0.90
1:G:54:PHE:CZ	1:G:420:ILE:HG23	2.09	0.88
1:H:354:ILE:HG23	1:H:378:ARG:HH22	1.38	0.87
1:B:54:PHE:CZ	1:B:434:GLY:HA3	2.09	0.86
1:H:413:VAL:HG22	1:H:418:ILE:HD13	1.55	0.86
1:G:374:LEU:HD12	1:G:397:MET:HE1	1.54	0.86
1:F:409:MET:HE1	1:F:438:ILE:HD11	1.59	0.84
1:H:252:GLU:HG2	1:H:264:PHE:CD1	2.13	0.84
1:B:252:GLU:HG2	1:B:264:PHE:HD1	1.43	0.83
1:B:315:ALA:HB3	1:B:320:CYS:SG	2.20	0.82
1:E:93:ARG:NH2	1:E:311:LEU:HB3	1.95	0.82
1:G:93:ARG:HD3	1:G:315:ALA:HB1	1.62	0.80
1:F:252:GLU:HG2	1:F:264:PHE:HD1	1.46	0.79
1:B:409:MET:HE1	1:B:438:ILE:HD11	1.63	0.79
1:C:374:LEU:HD12	1:C:397:MET:HE1	1.66	0.78
1:G:54:PHE:CE2	1:G:420:ILE:CG2	2.66	0.77
1:D:252:GLU:HG2	1:D:264:PHE:HD1	1.50	0.76
1:H:413:VAL:HG22	1:H:418:ILE:CD1	2.17	0.75
1:B:93:ARG:NH1	1:B:314:SER:HA	2.02	0.74
1:H:333:ASP:HB2	1:H:335:LEU:HD11	1.68	0.74
1:E:308:PRO:HG3	1:F:152:MET:HE1	1.69	0.73
1:A:308:PRO:HD2	1:B:163:MET:HE1	1.71	0.72
1:D:90:THR:C	1:D:92:ALA:H	1.98	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:309:LEU:O	1:A:311:LEU:CD2	2.38	0.72
1:A:309:LEU:O	1:A:311:LEU:HD22	1.90	0.72
1:B:252:GLU:HG2	1:B:264:PHE:CD1	2.24	0.71
1:C:93:ARG:HH22	1:C:311:LEU:HD13	1.55	0.71
1:A:308:PRO:O	1:A:309:LEU:HB2	1.89	0.70
1:B:259:ARG:NH2	1:B:422:PRO:O	2.24	0.70
1:B:399:GLN:HG3	1:B:444:ILE:HG21	1.73	0.70
1:C:93:ARG:HH12	1:C:311:LEU:HB2	1.56	0.70
1:C:354:ILE:HG23	1:C:378:ARG:HH22	1.57	0.70
1:A:228:LYS:NZ	1:A:366:THR:OG1	2.21	0.70
1:D:315:ALA:HB3	1:D:320:CYS:SG	2.31	0.70
1:D:296:GLU:HG2	1:D:300:LYS:HE2	1.75	0.69
1:H:434:GLY:HA2	1:H:437:ILE:HD12	1.74	0.69
1:E:90:THR:HG22	1:E:92:ALA:H	1.58	0.68
1:E:397:MET:HE3	1:E:416:ASN:HA	1.76	0.68
1:D:399:GLN:HG3	1:D:444:ILE:HG21	1.76	0.68
1:G:86:PRO:O	1:G:93:ARG:NH2	2.26	0.68
1:G:259:ARG:NH2	1:G:422:PRO:O	2.27	0.68
1:D:259:ARG:NH2	1:D:422:PRO:O	2.24	0.67
1:E:381:LYS:NZ	2:E:501:HOH:O	2.27	0.67
1:F:252:GLU:HG2	1:F:264:PHE:CD1	2.27	0.67
1:A:78:MET:HE1	1:B:74:VAL:HG11	1.77	0.67
1:B:95:ASP:OD1	1:B:98:ARG:NH1	2.28	0.67
1:A:374:LEU:HD12	1:A:397:MET:HE1	1.76	0.67
1:D:252:GLU:HG2	1:D:264:PHE:CD1	2.29	0.67
1:A:309:LEU:C	1:A:311:LEU:HD22	2.20	0.66
1:A:399:GLN:HG2	1:A:444:ILE:HG21	1.78	0.66
1:E:113:PHE:HB2	1:E:315:ALA:HB2	1.76	0.66
1:H:110:LYS:CE	1:H:299:ALA:HB1	2.24	0.66
1:C:188:THR:HG22	1:C:190:GLU:H	1.61	0.66
1:H:354:ILE:HG23	1:H:378:ARG:NH2	2.09	0.66
1:H:363:TRP:CD1	1:H:372:LEU:HD23	2.31	0.66
1:D:181:ARG:NH2	1:D:381:LYS:O	2.29	0.66
1:A:397:MET:HE3	1:A:416:ASN:HA	1.78	0.65
1:D:252:GLU:HB3	1:D:278:THR:CG2	2.27	0.65
1:B:229:TYR:CE2	1:B:234:TRP:HZ3	2.14	0.65
1:C:310:GLY:O	1:C:311:LEU:C	2.38	0.65
1:B:181:ARG:NH2	1:B:381:LYS:O	2.29	0.64
1:G:74:VAL:HB	1:H:78:MET:HE1	1.79	0.64
1:H:413:VAL:CG2	1:H:418:ILE:HD13	2.27	0.64
1:A:399:GLN:NE2	2:A:501:HOH:O	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:LEU:HB2	1:D:163:MET:HE1	1.78	0.64
1:E:78:MET:HE1	1:F:74:VAL:HG11	1.80	0.64
1:G:54:PHE:CE2	1:G:420:ILE:CG1	2.66	0.64
1:D:93:ARG:HD3	1:D:314:SER:HA	1.78	0.64
1:F:54:PHE:CE2	1:F:420:ILE:HG12	2.33	0.64
1:D:109:THR:HG21	1:D:296:GLU:HA	1.80	0.64
1:H:279:ALA:O	1:H:281:GLY:N	2.31	0.63
1:B:252:GLU:HB3	1:B:278:THR:HG23	1.79	0.63
1:D:93:ARG:CD	1:D:314:SER:HA	2.26	0.63
1:B:154:VAL:HA	1:B:171:VAL:HG11	1.79	0.63
1:H:54:PHE:CB	1:H:409:MET:HE2	2.28	0.63
1:H:407:LEU:HB2	1:H:437:ILE:HG23	1.79	0.63
1:A:310:GLY:C	1:A:311:LEU:HD22	2.25	0.62
1:D:358:PRO:HA	1:D:378:ARG:HH11	1.65	0.62
1:H:404:ILE:HG22	1:H:409:MET:HB3	1.81	0.62
1:C:88:MET:HE2	1:D:35:ALA:HB2	1.82	0.62
1:G:93:ARG:HH11	1:G:315:ALA:CB	2.12	0.61
1:C:397:MET:HE3	1:C:416:ASN:HA	1.82	0.61
1:D:84:VAL:HG13	1:D:88:MET:HB2	1.82	0.61
1:H:266:SER:OG	1:H:273:VAL:HG21	2.00	0.61
1:C:127:LEU:HD23	1:C:307:LEU:HD21	1.81	0.61
1:A:407:LEU:HD11	1:A:440:GLU:HG2	1.81	0.61
1:D:228:LYS:NZ	1:D:365:ASN:O	2.31	0.61
1:F:180:TYR:CE1	1:F:381:LYS:HE2	2.36	0.61
1:A:307:LEU:HD12	1:A:310:GLY:H	1.66	0.61
1:F:409:MET:HE3	1:F:411:THR:HB	1.82	0.60
1:C:354:ILE:HG23	1:C:378:ARG:NH2	2.15	0.60
1:E:400:VAL:O	1:E:404:ILE:HG13	2.01	0.60
1:F:226:CYS:HB2	1:F:371:CYS:HB3	1.83	0.60
1:H:400:VAL:O	1:H:404:ILE:HG13	2.01	0.60
1:A:36:GLU:OE1	1:A:46:ARG:HD3	2.01	0.60
1:C:358:PRO:HA	1:C:378:ARG:HH11	1.65	0.60
1:F:259:ARG:NH2	1:F:422:PRO:O	2.34	0.60
1:H:282:ILE:HG23	1:H:283:THR:HG23	1.82	0.60
1:D:36:GLU:HB2	1:D:46:ARG:HG3	1.82	0.60
1:F:252:GLU:HB3	1:F:278:THR:CG2	2.32	0.59
1:B:205:GLY:HA2	1:B:209:PRO:HG3	1.82	0.59
1:G:149:TYR:HA	1:G:152:MET:HE3	1.84	0.59
1:G:78:MET:HE1	1:H:74:VAL:HB	1.86	0.58
1:H:54:PHE:CD2	1:H:409:MET:HE2	2.38	0.58
1:A:33:ILE:HB	1:B:88:MET:HE3	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:101:ALA:O	1:E:104:THR:HG22	2.03	0.58
1:E:188:THR:HG22	1:E:191:GLU:H	1.68	0.58
1:A:41:VAL:HG11	1:A:426:ILE:HG13	1.86	0.58
1:G:350:VAL:HA	1:G:353:LEU:HB2	1.85	0.58
1:H:413:VAL:CG2	1:H:418:ILE:CD1	2.81	0.58
1:C:235:THR:O	1:C:239:GLU:HG3	2.04	0.57
1:A:88:MET:CE	1:B:35:ALA:HB2	2.34	0.57
1:A:126:LYS:HB2	1:A:307:LEU:HD22	1.86	0.57
1:D:216:ILE:HD13	1:D:249:VAL:HB	1.86	0.57
1:D:252:GLU:O	1:D:278:THR:HG22	2.04	0.57
1:G:54:PHE:CZ	1:G:420:ILE:CG2	2.85	0.57
1:G:74:VAL:HG12	1:G:78:MET:HE2	1.85	0.57
1:G:125:ILE:HD13	1:G:154:VAL:HG21	1.85	0.57
1:D:74:VAL:HG12	1:D:78:MET:HE2	1.86	0.57
1:B:86:PRO:HB3	1:B:314:SER:HB3	1.86	0.57
1:D:404:ILE:HG23	1:D:409:MET:HE2	1.87	0.57
1:C:54:PHE:CE2	1:C:420:ILE:HG23	2.39	0.57
1:D:92:ALA:O	1:D:320:CYS:HB3	2.04	0.57
1:H:219:GLY:HA3	1:H:252:GLU:OE2	2.05	0.57
1:B:302:PHE:HA	1:B:305:LYS:HG2	1.86	0.57
1:C:384:MET:HB3	1:C:397:MET:HE2	1.87	0.56
1:C:85:TYR:CE1	1:C:88:MET:HG3	2.40	0.56
1:C:384:MET:HG2	1:C:397:MET:HE2	1.88	0.56
1:A:88:MET:HE2	1:B:35:ALA:HB2	1.87	0.56
1:B:92:ALA:O	1:B:320:CYS:HB3	2.04	0.56
1:H:45:ASP:OD2	1:H:47:ASP:HB2	2.05	0.56
1:B:54:PHE:CE2	1:B:434:GLY:HA3	2.40	0.56
1:E:74:VAL:HG11	1:F:78:MET:HE1	1.87	0.56
1:G:119:GLU:HG2	1:G:309:LEU:HD11	1.88	0.56
1:E:112:PHE:HA	1:E:311:LEU:HA	1.87	0.56
1:G:78:MET:HB3	1:H:71:THR:HG22	1.86	0.56
1:H:252:GLU:OE2	1:H:255:SER:OG	2.23	0.56
1:G:252:GLU:O	1:G:278:THR:HG22	2.06	0.56
1:G:302:PHE:CE1	1:G:307:LEU:HD21	2.40	0.56
1:A:152:MET:HG2	1:A:160:LYS:HB3	1.88	0.55
1:A:384:MET:HG2	1:A:397:MET:HE2	1.89	0.55
1:G:163:MET:HE1	1:H:308:PRO:HB3	1.88	0.55
1:E:374:LEU:HD12	1:E:397:MET:HE1	1.87	0.55
1:B:269:HIS:O	1:B:271:VAL:N	2.38	0.55
1:F:162:ALA:HB3	1:F:163:MET:HE2	1.88	0.55
1:F:54:PHE:HE2	1:F:420:ILE:HG12	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:GLU:OE2	1:B:265:GLY:N	2.39	0.55
1:A:74:VAL:HG11	1:B:78:MET:HE1	1.89	0.55
1:H:350:VAL:O	1:H:354:ILE:HG13	2.05	0.55
1:H:353:LEU:HA	1:H:356:GLN:HB2	1.89	0.55
1:A:37:ARG:NH2	2:A:509:HOH:O	2.40	0.54
1:B:113:PHE:CB	1:B:315:ALA:HB2	2.37	0.54
1:C:74:VAL:HG12	1:C:78:MET:HE2	1.89	0.54
1:C:309:LEU:HD11	1:D:148:SER:HA	1.88	0.54
1:F:114:THR:HB	1:F:119:GLU:CD	2.33	0.54
1:H:363:TRP:HD1	1:H:372:LEU:HD23	1.72	0.54
1:A:78:MET:HE2	1:A:318:VAL:HG11	1.90	0.54
1:H:186:SER:OG	1:H:192:CYS:HB2	2.08	0.54
1:E:58:LEU:HB2	1:E:60:ASN:OD1	2.07	0.54
1:G:350:VAL:HG21	1:G:363:TRP:CD1	2.42	0.54
1:H:35:ALA:HA	1:H:45:ASP:HA	1.89	0.54
1:A:310:GLY:O	1:A:311:LEU:HD13	2.07	0.54
1:B:235:THR:O	1:B:239:GLU:HG3	2.08	0.54
1:D:303:ASP:O	1:D:304:ASP:C	2.50	0.54
1:E:93:ARG:HH21	1:E:311:LEU:C	2.15	0.54
1:G:188:THR:HG22	1:G:190:GLU:N	2.23	0.54
1:E:91:LYS:HG3	1:E:92:ALA:N	2.23	0.54
1:G:235:THR:O	1:G:239:GLU:HG3	2.07	0.54
1:G:302:PHE:C	1:G:304:ASP:H	2.16	0.54
1:H:347:ASP:OD1	1:H:363:TRP:HZ3	1.90	0.54
1:D:198:ASP:CG	1:D:236:ARG:HH22	2.15	0.53
1:B:152:MET:HE1	1:B:163:MET:HB3	1.90	0.53
1:E:54:PHE:CZ	1:E:434:GLY:HA3	2.42	0.53
1:F:44:TYR:CE2	1:F:50:ARG:HG3	2.43	0.53
1:D:113:PHE:CB	1:D:315:ALA:HB2	2.39	0.53
1:B:347:ASP:OD1	1:B:363:TRP:HZ3	1.91	0.53
1:B:347:ASP:OD1	1:B:363:TRP:CZ3	2.62	0.53
1:A:74:VAL:CG1	1:A:78:MET:HE3	2.38	0.52
1:A:123:ASN:OD1	1:A:309:LEU:HB3	2.08	0.52
1:H:74:VAL:HG12	1:H:78:MET:HE2	1.91	0.52
1:B:234:TRP:HD1	1:B:271:VAL:HG21	1.74	0.52
1:C:358:PRO:HA	1:C:378:ARG:NH1	2.24	0.52
1:D:93:ARG:HD3	1:D:313:TYR:O	2.08	0.52
1:E:440:GLU:O	1:E:443:LYS:HG2	2.10	0.52
1:G:384:MET:HG2	1:G:397:MET:HE2	1.90	0.52
1:C:109:THR:HG21	1:C:296:GLU:HA	1.91	0.52
1:F:85:TYR:CE2	1:F:88:MET:HG3	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:440:GLU:HA	1:H:443:LYS:HE2	1.92	0.52
1:H:258:GLY:HA2	1:H:262:LYS:O	2.10	0.52
1:A:384:MET:CG	1:A:397:MET:HE2	2.40	0.52
1:D:358:PRO:HA	1:D:378:ARG:NH1	2.24	0.52
1:E:49:LYS:HD3	1:E:50:ARG:N	2.25	0.52
1:H:372:LEU:HB2	1:H:418:ILE:HB	1.91	0.52
1:D:272:LYS:NZ	2:D:504:HOH:O	2.38	0.51
1:D:162:ALA:O	1:D:163:MET:HB2	2.11	0.51
1:E:54:PHE:CG	1:E:409:MET:HE2	2.45	0.51
1:E:169:PRO:HG2	1:F:166:GLN:NE2	2.26	0.51
1:H:112:PHE:CE1	1:H:307:LEU:HD21	2.46	0.51
1:F:252:GLU:HB3	1:F:278:THR:HG23	1.92	0.51
1:B:93:ARG:NH1	1:B:313:TYR:O	2.43	0.51
1:B:93:ARG:CZ	1:B:314:SER:HB2	2.41	0.51
1:B:229:TYR:CD2	1:B:234:TRP:HZ3	2.28	0.51
1:D:252:GLU:HB3	1:D:278:THR:HG22	1.93	0.51
1:G:252:GLU:HB2	1:G:278:THR:HG23	1.93	0.51
1:E:93:ARG:HH21	1:E:311:LEU:HB3	1.75	0.50
1:C:88:MET:CE	1:D:35:ALA:HB2	2.41	0.50
1:H:54:PHE:CD2	1:H:409:MET:CE	2.94	0.50
1:C:188:THR:HG22	1:C:190:GLU:N	2.27	0.50
1:D:386:PRO:HD2	1:D:389:ALA:HB2	1.92	0.50
1:C:71:THR:HG23	1:D:78:MET:HE3	1.94	0.50
1:D:226:CYS:HB2	1:D:371:CYS:HB3	1.92	0.50
1:E:49:LYS:HG3	1:E:51:TYR:CE2	2.47	0.50
1:D:390:THR:OG1	1:D:393:GLN:HG3	2.11	0.50
1:H:84:VAL:CG1	1:H:88:MET:HB2	2.42	0.50
1:A:195:ARG:HG2	1:H:185:TYR:CZ	2.46	0.50
1:B:121:ILE:HD12	1:B:216:ILE:HD11	1.93	0.50
1:H:342:MET:HE3	1:H:426:ILE:O	2.12	0.50
1:B:113:PHE:HB3	1:B:315:ALA:HB2	1.93	0.49
1:C:78:MET:HE3	1:D:71:THR:HG23	1.93	0.49
1:A:374:LEU:HB2	1:A:397:MET:HE1	1.93	0.49
1:D:93:ARG:NE	1:D:314:SER:HA	2.27	0.49
1:H:112:PHE:HE1	1:H:307:LEU:HD21	1.76	0.49
1:H:414:ARG:NH1	2:H:508:HOH:O	2.43	0.49
1:B:78:MET:HG2	1:B:82:SER:OG	2.11	0.49
1:C:121:ILE:HD12	1:C:216:ILE:HD11	1.94	0.49
1:D:238:ARG:NH1	1:D:272:LYS:O	2.40	0.49
1:D:401:ALA:HB2	1:D:413:VAL:HG21	1.94	0.49
1:C:308:PRO:HG2	1:D:163:MET:SD	2.52	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:VAL:CG1	1:D:88:MET:HB2	2.43	0.49
1:F:308:PRO:HG2	1:F:311:LEU:CD1	2.43	0.49
1:B:60:ASN:N	1:B:60:ASN:OD1	2.46	0.49
1:E:337:GLU:CD	1:E:337:GLU:H	2.20	0.49
1:G:98:ARG:O	1:G:102:GLU:HG3	2.12	0.49
1:A:285:GLY:O	1:B:83:TYR:HB2	2.13	0.49
1:F:104:THR:HG22	1:F:264:PHE:CE2	2.47	0.49
1:C:259:ARG:NH2	1:C:422:PRO:O	2.43	0.48
1:D:252:GLU:HB3	1:D:278:THR:HG23	1.94	0.48
1:H:325:ALA:O	1:H:329:ILE:HG13	2.14	0.48
1:B:61:VAL:HG23	1:B:61:VAL:O	2.13	0.48
1:B:126:LYS:NZ	1:B:309:LEU:O	2.46	0.48
1:E:93:ARG:HH22	1:E:311:LEU:HB3	1.75	0.48
1:H:110:LYS:HE3	1:H:299:ALA:CB	2.30	0.48
1:C:152:MET:HE1	1:D:309:LEU:CB	2.33	0.48
1:B:60:ASN:HB3	1:B:280:LYS:HG2	1.96	0.48
1:G:216:ILE:HD13	1:G:249:VAL:HB	1.95	0.48
1:G:163:MET:CE	1:H:308:PRO:HB3	2.44	0.48
1:A:135:HIS:HB2	1:B:166:GLN:NE2	2.29	0.47
1:E:345:TYR:CE1	1:E:349:ARG:HD3	2.49	0.47
1:F:252:GLU:OE2	1:F:255:SER:OG	2.26	0.47
1:B:234:TRP:HD1	1:B:271:VAL:CG2	2.27	0.47
1:G:85:TYR:CE1	1:G:88:MET:HG3	2.49	0.47
1:G:119:GLU:CD	1:G:309:LEU:HD21	2.38	0.47
1:A:386:PRO:HD2	1:A:389:ALA:HB2	1.96	0.47
1:G:262:LYS:HD2	1:G:268:HIS:CE1	2.49	0.47
1:A:126:LYS:CB	1:A:307:LEU:HD22	2.44	0.47
1:B:354:ILE:HG23	1:B:378:ARG:HH22	1.80	0.47
1:C:384:MET:HE2	1:C:384:MET:HB2	1.78	0.47
1:G:162:ALA:HB3	1:G:163:MET:SD	2.54	0.47
1:H:60:ASN:HB3	1:H:280:LYS:HG2	1.97	0.47
1:B:350:VAL:HG11	1:B:363:TRP:CG	2.49	0.47
1:C:139:ALA:O	1:C:173:HIS:HA	2.15	0.47
1:C:384:MET:CG	1:C:397:MET:HE2	2.45	0.47
1:A:274:ASP:O	1:A:275:ILE:HG13	2.16	0.46
1:G:309:LEU:O	1:G:310:GLY:C	2.58	0.46
1:H:342:MET:HE1	1:H:428:LYS:HG2	1.97	0.46
1:A:54:PHE:CE2	1:A:420:ILE:HG23	2.50	0.46
1:D:98:ARG:O	1:D:102:GLU:HG3	2.15	0.46
1:A:164:ASP:N	2:A:504:HOH:O	2.47	0.46
1:B:86:PRO:C	1:B:88:MET:H	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:74:VAL:CB	1:H:78:MET:HE1	2.46	0.46
1:G:188:THR:HG22	1:G:190:GLU:H	1.79	0.46
1:A:309:LEU:C	1:A:311:LEU:CD2	2.88	0.46
1:E:259:ARG:NH2	1:E:422:PRO:O	2.45	0.46
1:E:302:PHE:C	1:E:304:ASP:H	2.22	0.46
1:F:407:LEU:HB2	1:F:437:ILE:HG23	1.97	0.46
1:H:346:LEU:O	1:H:350:VAL:HG22	2.15	0.46
1:G:346:LEU:O	1:G:350:VAL:HG13	2.16	0.46
1:A:88:MET:HE3	1:B:33:ILE:CG2	2.46	0.46
1:E:188:THR:HG22	1:E:190:GLU:N	2.31	0.46
1:C:108:LEU:HB3	1:C:293:ILE:HG22	1.97	0.46
1:D:94:GLY:O	1:D:98:ARG:HG3	2.15	0.46
1:E:78:MET:CE	1:F:74:VAL:HG11	2.45	0.46
1:E:99:LYS:O	1:E:103:ILE:HG12	2.16	0.46
1:H:259:ARG:NH2	1:H:422:PRO:O	2.49	0.46
1:A:127:LEU:HG	1:A:307:LEU:HD21	1.98	0.46
1:D:58:LEU:C	1:D:59:MET:HE2	2.41	0.46
1:D:141:TYR:O	1:D:156:GLY:HA3	2.16	0.46
1:E:91:LYS:HB3	1:F:46:ARG:NH2	2.31	0.45
1:E:100:LEU:HD23	1:E:103:ILE:HD11	1.98	0.45
1:G:125:ILE:CD1	1:G:154:VAL:HG21	2.46	0.45
1:G:316:HIS:HB3	1:G:319:SER:HB2	1.99	0.45
1:H:75:ALA:O	1:H:79:ARG:HG3	2.16	0.45
1:G:93:ARG:NH1	1:G:315:ALA:CB	2.78	0.45
1:A:145:HIS:O	1:A:151:ALA:HB1	2.16	0.45
1:A:309:LEU:O	1:A:311:LEU:HD23	2.15	0.45
1:D:90:THR:O	1:D:92:ALA:N	2.45	0.45
1:F:54:PHE:CE2	1:F:420:ILE:HG23	2.52	0.45
1:C:85:TYR:CD1	1:C:88:MET:HG3	2.51	0.45
1:C:442:LEU:HD23	1:C:442:LEU:HA	1.85	0.45
1:E:91:LYS:HB3	1:F:46:ARG:HH21	1.81	0.45
1:A:78:MET:CE	1:B:74:VAL:HG11	2.45	0.45
1:A:266:SER:HA	1:A:269:HIS:CD2	2.52	0.45
1:A:394:MET:HA	2:A:563:HOH:O	2.16	0.45
1:E:93:ARG:HE	1:E:315:ALA:CB	2.30	0.45
1:F:356:GLN:O	1:F:358:PRO:HD3	2.17	0.45
1:E:61:VAL:HA	1:E:284:ALA:O	2.16	0.45
1:E:383:PRO:HB2	1:E:385:ALA:O	2.17	0.45
1:G:404:ILE:HG13	1:G:441:ALA:CB	2.46	0.45
1:H:262:LYS:HD2	1:H:268:HIS:NE2	2.32	0.45
1:E:220:GLU:OE2	1:E:228:LYS:HA	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:389:ALA:H	1:F:415:TRP:CD1	2.34	0.45
1:D:99:LYS:NZ	1:D:328:ASP:OD1	2.47	0.45
1:D:254:MET:HE3	1:D:254:MET:HB2	1.75	0.45
1:H:108:LEU:HB3	1:H:293:ILE:HG22	1.97	0.45
1:D:312:THR:C	1:D:314:SER:H	2.25	0.45
1:E:350:VAL:HG21	1:E:363:TRP:CE2	2.52	0.45
1:F:372:LEU:O	1:F:417:TYR:HA	2.17	0.45
1:B:252:GLU:HB3	1:B:278:THR:CG2	2.45	0.44
1:H:54:PHE:CZ	1:H:434:GLY:HA3	2.52	0.44
1:B:226:CYS:HB2	1:B:371:CYS:HB3	1.99	0.44
1:C:152:MET:CE	1:D:309:LEU:HB3	2.33	0.44
1:E:180:TYR:CE1	1:E:381:LYS:HE2	2.52	0.44
1:H:121:ILE:HD11	1:H:251:ASP:HB2	1.99	0.44
1:H:200:LEU:O	1:H:204:ILE:HG13	2.16	0.44
1:B:93:ARG:HH11	1:B:314:SER:HA	1.81	0.44
1:G:350:VAL:HG21	1:G:363:TRP:CG	2.52	0.44
1:H:53:ASP:O	1:H:423:PRO:HD3	2.17	0.44
1:H:427:ASN:N	1:H:430:GLU:OE1	2.43	0.44
1:D:252:GLU:OE2	1:D:265:GLY:N	2.51	0.44
1:E:45:ASP:CG	1:E:49:LYS:HB3	2.42	0.44
1:G:93:ARG:HD3	1:G:315:ALA:CB	2.40	0.44
1:A:93:ARG:NH2	1:A:311:LEU:O	2.43	0.44
1:G:54:PHE:CE2	1:G:420:ILE:CB	3.00	0.44
1:H:68:GLN:OE1	1:H:71:THR:HG21	2.18	0.44
1:C:374:LEU:HB2	1:C:397:MET:HE1	2.00	0.44
1:G:309:LEU:HD12	1:H:148:SER:HA	1.99	0.44
1:E:110:LYS:HD2	1:E:111:ALA:H	1.82	0.44
1:E:79:ARG:NH1	2:E:514:HOH:O	2.50	0.43
1:G:55:SER:HB3	1:G:411:THR:HA	2.00	0.43
1:A:78:MET:HE1	1:B:74:VAL:HG21	2.00	0.43
1:B:139:ALA:O	1:B:173:HIS:HA	2.18	0.43
1:E:384:MET:HG2	1:E:397:MET:HE2	2.01	0.43
1:A:407:LEU:HB2	1:A:437:ILE:HG23	2.00	0.43
1:D:392:ASP:OD2	1:D:392:ASP:N	2.51	0.43
1:F:74:VAL:HG13	1:F:318:VAL:CG1	2.49	0.43
1:A:99:LYS:NZ	1:A:331:GLN:OE1	2.40	0.43
1:B:241:CYS:HB3	1:B:246:ILE:O	2.18	0.43
1:B:162:ALA:O	1:B:163:MET:HB2	2.18	0.43
1:B:429:ALA:O	1:B:433:GLU:HG3	2.19	0.43
1:F:154:VAL:HG11	1:F:216:ILE:HD12	2.01	0.43
1:E:74:VAL:HG13	1:E:318:VAL:CG1	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:60:ASN:OD1	1:F:60:ASN:N	2.51	0.43
1:H:60:ASN:OD1	1:H:60:ASN:N	2.51	0.43
1:H:172:VAL:HG11	1:H:207:GLU:HG3	2.01	0.43
1:F:125:ILE:CD1	1:F:154:VAL:HG21	2.49	0.43
1:F:139:ALA:O	1:F:173:HIS:HA	2.19	0.43
1:F:296:GLU:O	1:F:300:LYS:HG2	2.18	0.43
1:C:169:PRO:HG2	1:D:166:GLN:OE1	2.19	0.43
1:H:48:GLY:O	2:H:501:HOH:O	2.21	0.43
1:B:36:GLU:HG3	1:B:46:ARG:NE	2.34	0.43
1:F:254:MET:HE3	1:F:254:MET:HB2	1.57	0.43
1:A:125:ILE:CD1	1:A:154:VAL:HG21	2.49	0.42
1:A:450:HIS:HA	2:A:600:HOH:O	2.18	0.42
1:C:407:LEU:HB2	1:C:437:ILE:HG23	2.00	0.42
1:G:311:LEU:HD23	1:G:311:LEU:HA	1.74	0.42
1:B:181:ARG:NH2	1:B:383:PRO:HG3	2.35	0.42
1:B:409:MET:HE2	1:B:411:THR:HG21	2.00	0.42
1:B:229:TYR:CE2	1:B:234:TRP:CZ3	3.02	0.42
1:D:409:MET:HE3	1:D:411:THR:HB	2.00	0.42
1:H:442:LEU:HD23	1:H:442:LEU:HA	1.82	0.42
1:C:349:ARG:HH11	1:C:349:ARG:HG2	1.84	0.42
1:H:152:MET:O	1:H:160:LYS:HE3	2.18	0.42
1:D:90:THR:C	1:D:92:ALA:N	2.65	0.42
1:H:377:ASN:OD1	1:H:379:GLU:HG2	2.18	0.42
1:H:438:ILE:O	1:H:442:LEU:HG	2.20	0.42
1:E:118:ALA:O	1:E:122:GLU:HG3	2.19	0.42
1:A:74:VAL:HG13	1:A:78:MET:HE3	2.02	0.42
1:A:129:ARG:HH22	1:A:168:MET:HE3	1.85	0.42
1:C:99:LYS:NZ	1:C:331:GLN:OE1	2.53	0.42
1:E:169:PRO:HG2	1:F:166:GLN:HE21	1.83	0.42
1:H:295:ASP:HB3	1:H:298:ILE:HD12	2.02	0.42
1:A:449:THR:O	1:A:450:HIS:C	2.62	0.42
1:C:159:ARG:HD2	1:D:309:LEU:HD13	2.00	0.42
1:C:384:MET:HB3	1:C:397:MET:CE	2.48	0.42
1:E:100:LEU:O	1:E:104:THR:HB	2.19	0.42
1:F:107:ASN:OD1	2:F:501:HOH:O	2.21	0.42
1:G:41:VAL:HG23	1:G:52:ILE:HD12	2.02	0.42
1:H:226:CYS:SG	1:H:371:CYS:HB2	2.60	0.42
1:F:373:GLU:HG3	1:F:416:ASN:ND2	2.35	0.42
1:G:264:PHE:HE1	1:G:278:THR:HG21	1.85	0.42
1:G:388:ASN:ND2	2:G:503:HOH:O	2.44	0.42
1:H:447:ALA:C	1:H:449:THR:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:TYR:CE1	1:A:381:LYS:HE2	2.55	0.42
1:B:85:TYR:O	1:B:87:GLY:N	2.53	0.42
1:B:309:LEU:HD23	1:B:309:LEU:HA	1.80	0.42
1:A:190:GLU:CD	1:A:190:GLU:H	2.28	0.41
1:B:403:LYS:O	1:B:407:LEU:HG	2.19	0.41
1:C:186:SER:OG	1:C:192:CYS:HB2	2.21	0.41
1:C:363:TRP:CE2	1:C:365:ASN:HB2	2.55	0.41
1:D:85:TYR:O	1:D:86:PRO:C	2.63	0.41
1:D:397:MET:HG3	1:D:415:TRP:O	2.20	0.41
1:F:198:ASP:OD1	1:F:236:ARG:NH2	2.53	0.41
1:F:218:GLU:HA	1:F:251:ASP:HB3	2.02	0.41
1:A:309:LEU:HD11	1:B:148:SER:HA	2.02	0.41
1:D:311:LEU:HA	1:D:311:LEU:HD23	1.62	0.41
1:A:74:VAL:CG1	1:B:78:MET:HE1	2.51	0.41
1:C:336:LEU:O	1:C:340:VAL:HG23	2.19	0.41
1:A:91:LYS:HB3	1:A:91:LYS:HE3	1.75	0.41
1:A:254:MET:HB2	1:A:254:MET:HE3	1.76	0.41
1:A:422:PRO:HB2	1:A:426:ILE:HD12	2.03	0.41
1:D:181:ARG:NH1	1:D:373:GLU:OE2	2.53	0.41
1:E:154:VAL:HA	1:E:171:VAL:HG11	2.02	0.41
1:H:426:ILE:HG12	1:H:431:LEU:HG	2.03	0.41
1:C:53:ASP:OD2	1:C:57:GLN:HG2	2.20	0.41
1:C:88:MET:HE3	1:D:33:ILE:HB	2.01	0.41
1:A:241:CYS:HB3	1:A:246:ILE:O	2.21	0.41
1:B:86:PRO:CB	1:B:314:SER:HB3	2.50	0.41
1:B:350:VAL:HG11	1:B:363:TRP:CD2	2.56	0.41
1:D:60:ASN:HB3	1:D:280:LYS:HD3	2.02	0.41
1:E:70:VAL:O	1:E:74:VAL:HG23	2.21	0.41
1:E:100:LEU:HD23	1:E:100:LEU:HA	1.91	0.41
1:F:428:LYS:HB3	1:F:428:LYS:NZ	2.35	0.41
1:G:306:PRO:C	1:G:307:LEU:HD13	2.46	0.41
1:H:426:ILE:HG13	1:H:430:GLU:HB2	2.02	0.41
1:D:45:ASP:OD2	1:D:49:LYS:HB3	2.21	0.41
1:D:358:PRO:O	1:D:378:ARG:HD2	2.21	0.41
1:H:85:TYR:CD1	1:H:86:PRO:HD2	2.56	0.41
1:B:152:MET:HE1	1:B:163:MET:CB	2.50	0.40
1:B:301:SER:O	1:B:305:LYS:HD3	2.21	0.40
1:H:354:ILE:CG2	1:H:378:ARG:NH2	2.66	0.40
1:C:205:GLY:O	1:C:207:GLU:O	2.39	0.40
1:D:91:LYS:HZ3	1:D:91:LYS:HG3	1.71	0.40
1:D:140:LEU:O	1:D:143:SER:OG	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:43:LEU:O	1:G:50:ARG:HA	2.21	0.40
1:G:188:THR:HB	1:G:191:GLU:HB2	2.04	0.40
1:G:307:LEU:HD22	1:G:307:LEU:N	2.37	0.40
1:A:345:TYR:OH	1:A:432:ASP:OD2	2.27	0.40
1:B:354:ILE:HG23	1:B:378:ARG:NH2	2.35	0.40
1:B:409:MET:HE3	1:B:411:THR:HB	2.03	0.40
1:C:93:ARG:HG2	1:C:320:CYS:SG	2.61	0.40
1:D:353:LEU:HD23	1:D:356:GLN:OE1	2.22	0.40
1:F:111:ALA:HA	1:F:292:VAL:O	2.22	0.40
1:H:54:PHE:HB2	1:H:409:MET:HE2	2.02	0.40
1:H:327:LEU:HD23	1:H:327:LEU:HA	1.86	0.40
1:B:363:TRP:CD1	1:B:372:LEU:HD23	2.56	0.40
1:F:108:LEU:HB3	1:F:293:ILE:HG22	2.04	0.40
1:G:443:LYS:HE2	1:G:443:LYS:HB3	1.78	0.40
1:H:67:ASP:OD1	1:H:69:ARG:HB2	2.21	0.40
1:H:353:LEU:CD2	1:H:439:SER:HB2	2.51	0.40
1:H:353:LEU:HD22	1:H:439:SER:HB2	2.04	0.40
1:H:442:LEU:O	1:H:446:ASP:N	2.54	0.40
1:C:403:LYS:HA	1:C:403:LYS:HD3	1.98	0.40
1:D:217:LEU:HD23	1:D:217:LEU:HA	1.93	0.40
1:F:122:GLU:OE2	1:F:148:SER:OG	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	412/450 (92%)	393 (95%)	16 (4%)	3 (1%)	18	22
1	B	417/450 (93%)	395 (95%)	17 (4%)	5 (1%)	10	11
1	C	411/450 (91%)	396 (96%)	12 (3%)	3 (1%)	18	22
1	D	414/450 (92%)	395 (95%)	19 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	413/450 (92%)	387 (94%)	21 (5%)	5 (1%)	10	11
1	F	413/450 (92%)	390 (94%)	21 (5%)	2 (0%)	24	30
1	G	411/450 (91%)	396 (96%)	11 (3%)	4 (1%)	12	14
1	H	413/450 (92%)	391 (95%)	18 (4%)	4 (1%)	12	14
All	All	3304/3600 (92%)	3143 (95%)	135 (4%)	26 (1%)	16	19

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	308	PRO
1	E	308	PRO
1	H	280	LYS
1	A	309	LEU
1	B	163	MET
1	B	270	GLY
1	E	306	PRO
1	H	102	GLU
1	C	280	LYS
1	C	306	PRO
1	A	208	ASN
1	B	280	LYS
1	E	67	ASP
1	E	208	ASN
1	F	208	ASN
1	F	280	LYS
1	G	280	LYS
1	G	303	ASP
1	G	309	LEU
1	H	101	ALA
1	A	280	LYS
1	E	280	LYS
1	G	208	ASN
1	H	208	ASN
1	B	86	PRO
1	B	87	GLY

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	330/363 (91%)	323 (98%)	7 (2%)	47	65
1	B	333/363 (92%)	325 (98%)	8 (2%)	43	60
1	C	329/363 (91%)	318 (97%)	11 (3%)	33	48
1	D	332/363 (92%)	323 (97%)	9 (3%)	39	56
1	E	331/363 (91%)	322 (97%)	9 (3%)	39	56
1	F	331/363 (91%)	329 (99%)	2 (1%)	78	88
1	G	329/363 (91%)	323 (98%)	6 (2%)	51	69
1	H	331/363 (91%)	323 (98%)	8 (2%)	43	60
All	All	2646/2904 (91%)	2586 (98%)	60 (2%)	44	62

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	152	MET
1	A	163	MET
1	A	223	THR
1	A	300	LYS
1	A	301	SER
1	A	449	THR
1	A	450	HIS
1	B	127	LEU
1	B	204	ILE
1	B	278	THR
1	B	304	ASP
1	B	305	LYS
1	B	309	LEU
1	B	311	LEU
1	B	449	THR
1	C	36	GLU
1	C	84	VAL
1	C	85	TYR
1	C	93	ARG
1	C	152	MET
1	C	307	LEU
1	C	308	PRO
1	C	309	LEU

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Mol	Chain	Res	Type
1	C	314	SER
1	C	371	CYS
1	C	449	THR
1	D	84	VAL
1	D	89	ILE
1	D	90	THR
1	D	91	LYS
1	D	163	MET
1	D	307	LEU
1	D	309	LEU
1	D	444	ILE
1	D	449	THR
1	E	154	VAL
1	E	163	MET
1	E	223	THR
1	E	304	ASP
1	E	307	LEU
1	E	308	PRO
1	E	309	LEU
1	E	311	LEU
1	E	371	CYS
1	F	36	GLU
1	F	152	MET
1	G	60	ASN
1	G	109	THR
1	G	307	LEU
1	G	309	LEU
1	G	311	LEU
1	G	331	GLN
1	H	33	ILE
1	H	90	THR
1	H	106	PRO
1	H	163	MET
1	H	181	ARG
1	H	307	LEU
1	H	309	LEU
1	H	376	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	HIS

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Mol	Chain	Res	Type
1	B	166	GLN
1	B	194	GLN
1	B	244	HIS
1	B	338	ASN
1	B	356	GLN
1	B	450	HIS
1	D	268	HIS
1	D	331	GLN
1	D	344	GLN
1	E	142	GLN
1	E	268	HIS
1	F	244	HIS
1	F	268	HIS
1	F	344	GLN
1	G	107	ASN
1	G	244	HIS
1	G	268	HIS
1	G	269	HIS
1	G	450	HIS
1	H	269	HIS
1	H	331	GLN
1	H	450	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	416/450 (92%)	-0.01	16 (3%)	44	47	26, 33, 56, 68	0
1	B	419/450 (93%)	-0.00	15 (3%)	46	49	23, 34, 58, 75	0
1	C	415/450 (92%)	-0.11	12 (2%)	53	56	23, 32, 54, 72	0
1	D	418/450 (92%)	0.04	14 (3%)	49	52	24, 36, 59, 72	0
1	E	417/450 (92%)	0.13	12 (2%)	53	56	26, 40, 62, 74	0
1	F	417/450 (92%)	0.11	11 (2%)	57	60	25, 39, 61, 71	0
1	G	415/450 (92%)	0.23	13 (3%)	51	54	27, 40, 63, 68	0
1	H	417/450 (92%)	0.73	21 (5%)	34	36	25, 51, 66, 76	0
All	All	3334/3600 (92%)	0.14	114 (3%)	48	51	23, 37, 62, 76	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	311	LEU	4.9
1	D	90	THR	4.8
1	G	58	LEU	4.7
1	A	450	HIS	4.1
1	D	313	TYR	4.1
1	C	311	LEU	4.0
1	D	92	ALA	4.0
1	D	309	LEU	4.0
1	F	85	TYR	3.8
1	B	314	SER	3.8
1	B	312	THR	3.5
1	G	54	PHE	3.5
1	F	87	GLY	3.4
1	H	85	TYR	3.3
1	E	307	LEU	3.2
1	C	309	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	89	ILE	3.2
1	F	309	LEU	3.1
1	F	311	LEU	3.1
1	G	85	TYR	3.1
1	A	311	LEU	3.1
1	E	309	LEU	3.1
1	D	89	ILE	3.1
1	H	363	TRP	3.0
1	B	313	TYR	3.0
1	B	309	LEU	2.9
1	D	311	LEU	2.9
1	B	54	PHE	2.9
1	D	93	ARG	2.9
1	D	425	CYS	2.9
1	C	304	ASP	2.9
1	A	307	LEU	2.8
1	E	164	ASP	2.8
1	A	309	LEU	2.8
1	H	164	ASP	2.8
1	B	87	GLY	2.8
1	G	87	GLY	2.8
1	E	58	LEU	2.8
1	G	309	LEU	2.8
1	F	58	LEU	2.8
1	H	92	ALA	2.8
1	E	314	SER	2.7
1	C	306	PRO	2.7
1	C	320	CYS	2.7
1	E	394	MET	2.7
1	B	92	ALA	2.7
1	D	315	ALA	2.7
1	E	310	GLY	2.6
1	A	86	PRO	2.6
1	G	308	PRO	2.6
1	H	340	VAL	2.6
1	H	314	SER	2.6
1	H	445	ALA	2.6
1	D	308	PRO	2.6
1	C	307	LEU	2.5
1	H	309	LEU	2.5
1	A	78	MET	2.5
1	B	88	MET	2.5

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Mol	Chain	Res	Type	RSRZ
1	H	450	HIS	2.5
1	H	32	PRO	2.5
1	B	425	CYS	2.4
1	H	353	LEU	2.4
1	A	152	MET	2.4
1	G	164	ASP	2.4
1	G	86	PRO	2.4
1	A	314	SER	2.4
1	D	85	TYR	2.4
1	A	33	ILE	2.4
1	A	46	ARG	2.4
1	A	87	GLY	2.4
1	G	310	GLY	2.4
1	E	163	MET	2.4
1	F	32	PRO	2.3
1	H	358	PRO	2.3
1	F	54	PHE	2.3
1	C	152	MET	2.3
1	F	450	HIS	2.3
1	D	304	ASP	2.3
1	A	85	TYR	2.3
1	H	264	PHE	2.2
1	E	304	ASP	2.2
1	H	308	PRO	2.2
1	D	379	GLU	2.2
1	F	305	LYS	2.2
1	H	311	LEU	2.2
1	C	270	GLY	2.2
1	H	179	PHE	2.2
1	F	384	MET	2.2
1	A	447	ALA	2.2
1	G	410	TYR	2.2
1	B	311	LEU	2.2
1	C	308	PRO	2.2
1	C	89	ILE	2.1
1	G	307	LEU	2.1
1	G	394	MET	2.1
1	A	308	PRO	2.1
1	B	163	MET	2.1
1	F	371	CYS	2.1
1	B	90	THR	2.1
1	A	410	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	306	PRO	2.1
1	B	234	TRP	2.1
1	E	397	MET	2.1
1	H	335	LEU	2.1
1	H	346	LEU	2.1
1	A	427	ASN	2.1
1	C	85	TYR	2.1
1	D	314	SER	2.0
1	H	427	ASN	2.0
1	H	329	ILE	2.0
1	B	102	GLU	2.0
1	C	164	ASP	2.0
1	G	304	ASP	2.0
1	H	86	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.