



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:25 AM UTC

PDB ID : 2HYB / pdb_00002hyb
Title : Crystal Structure of Hexameric DsrEFH
Authors : Shin, D.H.; Connie, H.; Schulte, A.; Dahl, C.; Kim, R.; Kim, S.H.; Berkeley
Structural Genomics Center (BSGC)
Deposited on : 2006-08-04
Resolution : 2.50 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

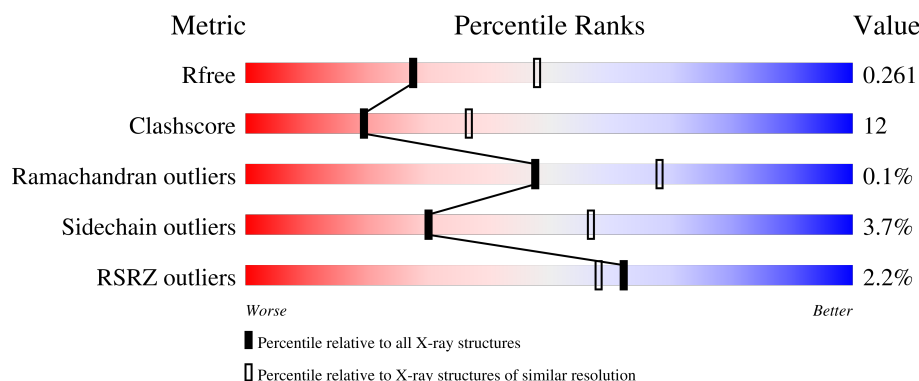
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	130	 75% 22% •
1	D	130	 77% 21% •
1	G	130	 75% 23% •
1	J	130	 73% 25% •
1	M	130	 69% 26% 5%

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Mol	Chain	Length	Quality of chain
1	P	130	75% 22% .
2	B	136	5% 65% 32% .
2	E	136	7% 60% 35% ..
2	H	136	6% 73% 22% ..
2	K	136	73% 23% ..
2	N	136	5% 68% 26% ..
2	Q	136	6% 71% 25% ..
3	C	102	80% 15% ...
3	F	102	75% 20% 5% .
3	I	102	78% 16% 5% .
3	L	102	2% 75% 23% ...
3	O	102	75% 22% ..
3	R	102	70% 25% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17611 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 Putative sulfurtransferase dsrE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1029	644	188	194	3			
1	D	130	Total	C	N	O	S	0	0	0
			1029	644	188	194	3			
1	G	130	Total	C	N	O	S	0	0	0
			1029	644	188	194	3			
1	J	130	Total	C	N	O	S	0	0	0
			1029	644	188	194	3			
1	M	130	Total	C	N	O	S	0	0	0
			1029	644	188	194	3			
1	P	130	Total	C	N	O	S	0	0	0
			1029	644	188	194	3			

- Molecule 2 is a protein called Intracellular sulfur oxidation protein dsrF.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	132	Total	C	N	O	S	0	0	0
			1065	676	170	214	5			
2	E	132	Total	C	N	O	S	0	0	0
			1065	676	170	214	5			
2	H	132	Total	C	N	O	S	0	0	0
			1065	676	170	214	5			
2	K	132	Total	C	N	O	S	0	0	0
			1065	676	170	214	5			
2	N	132	Total	C	N	O	S	0	0	0
			1065	676	170	214	5			
2	Q	132	Total	C	N	O	S	0	0	0
			1065	676	170	214	5			

- Molecule 3 is a protein called DsrH.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	101	Total	C	N	O	S	0	0	0
			771	493	125	151	2			
3	F	101	Total	C	N	O	S	0	0	0
			772	493	125	152	2			
3	I	101	Total	C	N	O	S	0	0	0
			771	493	125	151	2			
3	L	101	Total	C	N	O	S	0	0	0
			772	493	125	152	2			
3	O	101	Total	C	N	O	S	0	0	0
			771	493	125	151	2			
3	R	101	Total	C	N	O	S	0	0	0
			772	493	125	152	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total	O	0	0
			21	21		
4	B	17	Total	O	0	0
			17	17		
4	C	15	Total	O	0	0
			15	15		
4	D	23	Total	O	0	0
			23	23		
4	E	29	Total	O	0	0
			29	29		
4	F	20	Total	O	0	0
			20	20		
4	G	29	Total	O	0	0
			29	29		
4	H	11	Total	O	0	0
			11	11		
4	I	25	Total	O	0	0
			25	25		
4	J	28	Total	O	0	0
			28	28		
4	K	33	Total	O	0	0
			33	33		
4	L	22	Total	O	0	0
			22	22		
4	M	21	Total	O	0	0
			21	21		
4	N	18	Total	O	0	0
			18	18		

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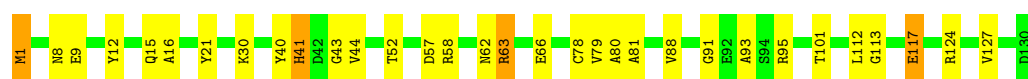
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	O	22	Total 22	O 22	0	0
4	P	32	Total 32	O 32	0	0
4	Q	30	Total 30	O 30	0	0
4	R	22	Total 22	O 22	0	0

3 Residue-property plots [i](#)

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.

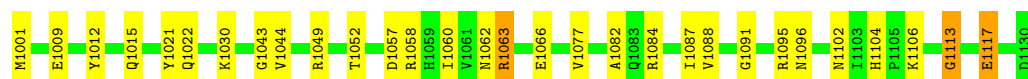
- Molecule 1: Putative sulfurtransferase dsrE

Chain A: 



- Molecule 1: Putative sulfurtransferase dsrE

Chain D: 



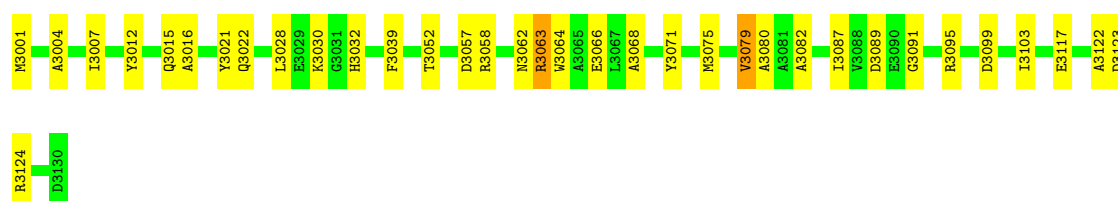
- Molecule 1: Putative sulfurtransferase dsrE

Chain G: 



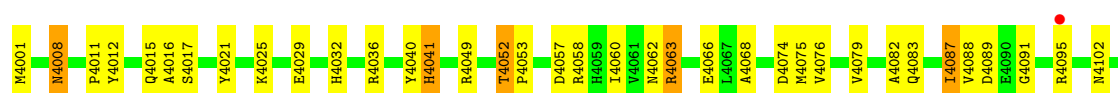
- Molecule 1: Putative sulfurtransferase dsrE

Chain J: 



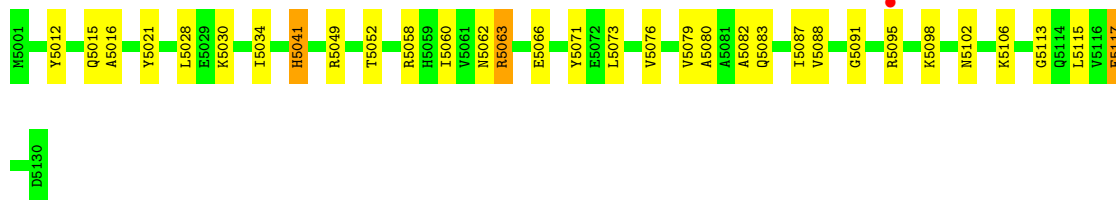
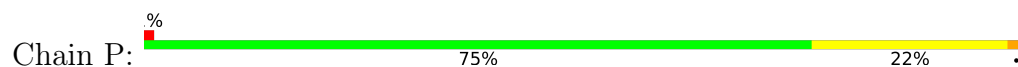
- Molecule 1: Putative sulfurtransferase dsrE

Chain M: 

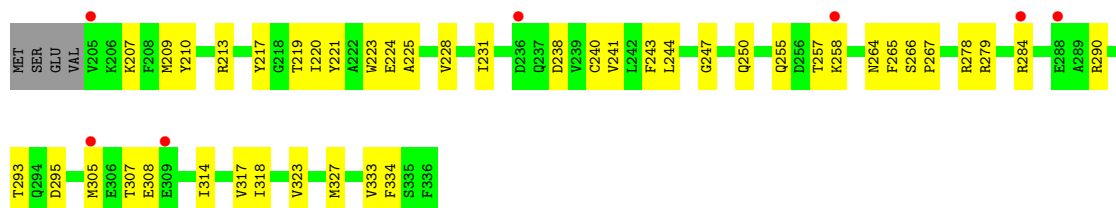




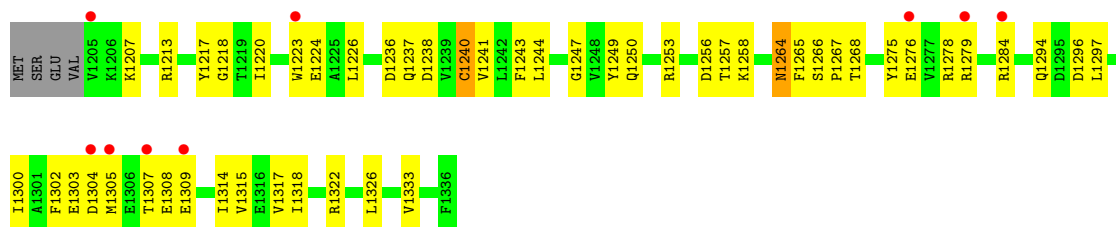
- Molecule 1: Putative sulfurtransferase dsrE



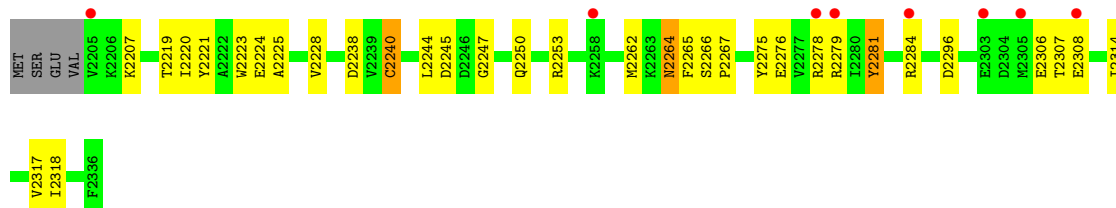
- Molecule 2: Intracellular sulfur oxidation protein dsrF



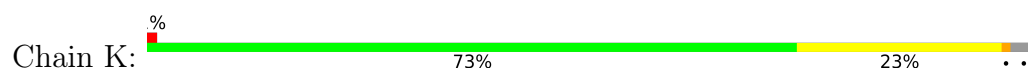
- Molecule 2: Intracellular sulfur oxidation protein dsrF



- Molecule 2: Intracellular sulfur oxidation protein dsrF



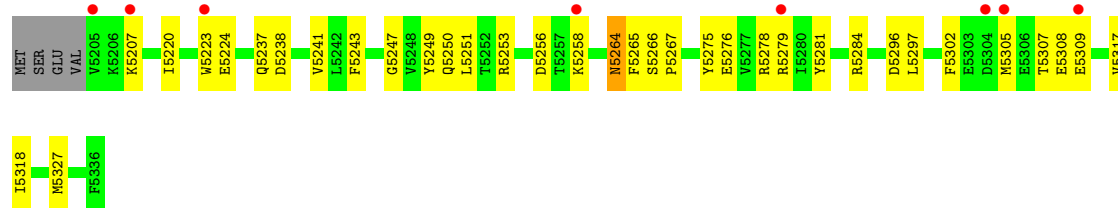
- Molecule 2: Intracellular sulfur oxidation protein dsrF



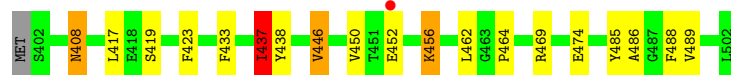
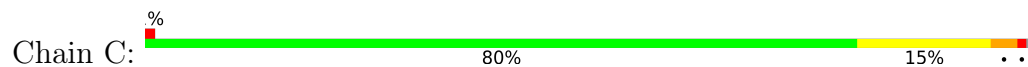
• Molecule 2: Intracellular sulfur oxidation protein dsrF



• Molecule 2: Intracellular sulfur oxidation protein dsrF



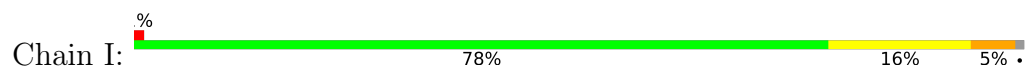
• Molecule 3: DsrH



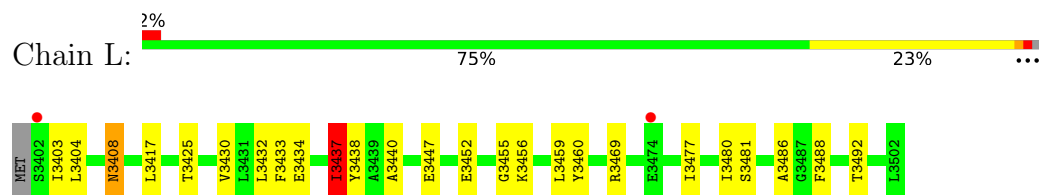
• Molecule 3: DsrH



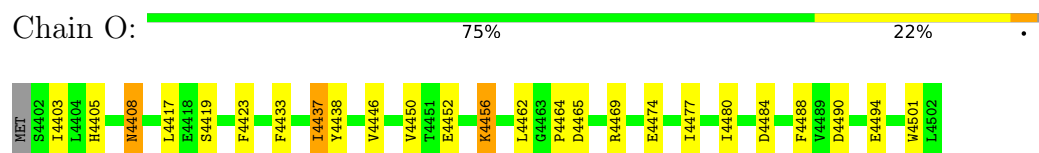
• Molecule 3: DsrH



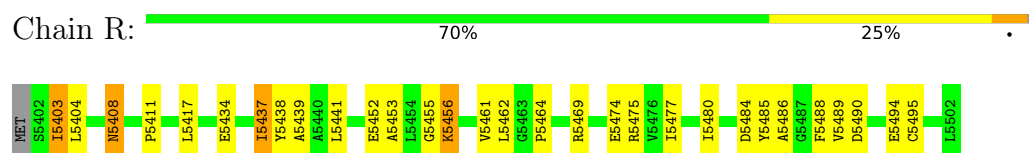
● Molecule 3: DsrH



● Molecule 3: DsrH



● Molecule 3: DsrH



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	56.61Å 183.11Å 107.83Å 90.00° 99.57° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	92.7 (19.98-2.50) 92.6 (19.98-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.262 0.205 , 0.261	Depositor DCC
R_{free} test set	7338 reflections (10.11%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17611	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 23.61 % 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 4.5041e-03. 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	0/1050	0.98	5/1419 (0.4%)
1	D	0.44	0/1050	1.03	5/1419 (0.4%)
1	G	0.45	0/1050	1.04	8/1419 (0.6%)
1	J	0.48	0/1050	0.95	3/1419 (0.2%)
1	M	0.46	0/1050	1.03	7/1419 (0.5%)
1	P	0.48	0/1050	1.04	7/1419 (0.5%)
2	B	0.48	0/1083	0.87	1/1464 (0.1%)
2	E	0.46	0/1083	0.88	2/1464 (0.1%)
2	H	0.44	0/1083	0.86	1/1464 (0.1%)
2	K	0.50	0/1083	0.88	1/1464 (0.1%)
2	N	0.47	0/1083	0.89	2/1464 (0.1%)
2	Q	0.49	1/1083 (0.1%)	0.87	1/1464 (0.1%)
3	C	0.47	0/784	1.00	2/1064 (0.2%)
3	F	0.42	0/785	0.95	1/1064 (0.1%)
3	I	0.48	0/784	0.99	2/1064 (0.2%)
3	L	0.46	0/785	0.99	4/1064 (0.4%)
3	O	0.45	0/784	0.95	0/1064
3	R	0.46	0/785	0.98	2/1064 (0.2%)
All	All	0.46	1/17505 (0.0%)	0.95	54/23682 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	5309	GLU	N-CA	5.42	1.52	1.46

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	5052	THR	CA-C-N	12.05	128.34	119.66
1	P	5052	THR	C-N-CA	12.05	128.34	119.66
1	G	2052	THR	CA-C-N	11.08	127.64	119.66
1	G	2052	THR	C-N-CA	11.08	127.64	119.66
1	M	4052	THR	CA-C-N	10.11	126.94	119.66
1	M	4052	THR	C-N-CA	10.11	126.94	119.66
1	D	1052	THR	CA-C-N	9.75	126.78	119.66
1	D	1052	THR	C-N-CA	9.75	126.78	119.66
1	P	5088	VAL	N-CA-C	7.34	118.39	108.11
1	M	4060	ILE	N-CA-C	7.14	118.75	110.62
1	A	41	HIS	CB-CA-C	-6.93	107.54	115.79
1	D	1088	VAL	N-CA-C	6.58	117.32	108.11
2	E	1218	GLY	N-CA-C	-6.26	105.21	112.73
2	K	3239	VAL	N-CA-C	6.21	117.96	108.71
1	P	5041	HIS	CB-CA-C	-6.21	108.40	115.79
2	Q	5237	GLN	N-CA-C	-6.17	101.07	110.14
3	C	446	VAL	N-CA-C	6.14	117.38	111.91
1	A	88	VAL	N-CA-C	6.04	116.81	108.12
3	R	5441	LEU	N-CA-C	5.91	118.83	109.96
1	G	2104	HIS	N-CA-C	-5.88	102.64	109.93
1	G	2104	HIS	CA-C-N	5.64	125.31	119.56
1	G	2104	HIS	C-N-CA	5.64	125.31	119.56
1	J	3052	THR	CA-C-N	5.62	126.17	120.38
1	J	3052	THR	C-N-CA	5.62	126.17	120.38
1	P	5060	ILE	N-CA-C	5.56	116.20	110.36
3	I	2450	VAL	N-CA-C	-5.54	105.32	110.53
1	A	52	THR	CA-C-N	5.53	126.08	120.38
1	A	52	THR	C-N-CA	5.53	126.08	120.38
1	G	2088	VAL	N-CA-C	5.47	116.36	108.48
2	E	1237	GLN	N-CA-C	-5.45	101.24	109.85
3	L	3425	THR	N-CA-C	5.43	118.13	110.14
1	A	127	VAL	N-CA-C	5.42	115.90	107.99
1	D	1060	ILE	N-CA-C	5.41	116.04	110.36
1	J	3079	VAL	N-CA-C	5.41	116.13	110.62
3	R	5403	ILE	N-CA-C	5.38	115.71	108.17
3	L	3488	PHE	N-CA-C	-5.38	105.31	111.07
2	B	225	ALA	N-CA-C	-5.38	105.33	111.14
3	L	3403	ILE	N-CA-C	5.35	115.66	108.17
1	M	4088	VAL	N-CA-C	5.34	115.96	108.17
3	I	2448	SER	N-CA-C	5.33	117.51	111.11
2	N	4316	GLU	N-CA-C	5.25	117.28	108.73
1	G	2041	HIS	CB-CA-C	-5.23	108.99	115.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	5115	LEU	N-CA-C	-5.23	105.23	111.03
3	L	3437	ILE	N-CA-C	5.21	115.94	110.62
3	C	437	ILE	N-CA-C	5.20	116.54	110.62
1	P	5076	VAL	N-CA-C	5.18	116.04	108.53
1	G	2008	ASN	N-CA-C	5.12	119.62	113.17
3	F	1488	PHE	N-CA-C	-5.10	105.61	111.07
1	M	4087	ILE	N-CA-C	-5.09	101.08	108.36
2	N	4281	TYR	N-CA-C	5.04	117.97	109.95
2	H	2281	TYR	N-CA-C	5.04	117.95	110.14
1	M	4041	HIS	CB-CA-C	-5.04	109.24	115.89
1	M	4008	ASN	N-CA-C	5.02	119.09	112.92
1	D	1113	GLY	N-CA-C	-5.00	109.17	114.67

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	1249	TYR	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	1029	0	992	23	0
1	D	1029	0	989	20	0
1	G	1029	0	989	20	0
1	J	1029	0	989	30	0
1	M	1029	0	989	30	0
1	P	1029	0	989	22	0
2	B	1065	0	1021	33	0
2	E	1065	0	1021	34	0
2	H	1065	0	1021	26	0
2	K	1065	0	1021	23	0
2	N	1065	0	1021	37	0
2	Q	1065	0	1021	26	0
3	C	771	0	771	15	0
3	F	772	0	771	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	I	771	0	771	13	0
3	L	772	0	771	14	0
3	O	771	0	771	22	0
3	R	772	0	771	20	0
4	A	21	0	0	2	0
4	B	17	0	0	1	0
4	C	15	0	0	0	0
4	D	23	0	0	3	0
4	E	29	0	0	1	0
4	F	20	0	0	2	0
4	G	29	0	0	1	0
4	H	11	0	0	1	0
4	I	25	0	0	2	0
4	J	28	0	0	1	0
4	K	33	0	0	2	0
4	L	22	0	0	0	0
4	M	21	0	0	3	0
4	N	18	0	0	5	0
4	O	22	0	0	1	0
4	P	32	0	0	1	0
4	Q	30	0	0	1	0
4	R	22	0	0	1	0
All	All	17611	0	16689	393	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 12.

All (393) 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:M:4091:GLY:O	1:M:4095:ARG:HG3	1.74	0.87
1:J:3091:GLY:O	1:J:3095:ARG:HG3	1.76	0.85
1:G:2062:ASN:O	1:G:2066:GLU:HG3	1.80	0.82
2:H:2253:ARG:HG2	2:H:2296:ASP:O	1.79	0.82
3:C:408:ASN:HD22	3:C:408:ASN:H	1.30	0.80
1:M:4112:LEU:HD21	2:N:4228:VAL:HG22	1.63	0.79
2:H:2278:ARG:O	2:H:2314:ILE:HD12	1.83	0.78
3:O:4408:ASN:HD22	3:O:4408:ASN:H	1.32	0.78
3:L:3438:TYR:CZ	3:L:3469:ARG:HD3	2.17	0.78
1:J:3082:ALA:HB1	1:J:3087:ILE:HB	1.66	0.76
1:J:3001:MET:HE2	1:J:3123:ASP:HB3	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4068:ALA:HB2	1:M:4075:MET:HE2	1.68	0.75
2:E:1220:ILE:HG12	2:E:1224:GLU:HG3	1.69	0.75
2:B:220:ILE:HG12	2:B:224:GLU:HG3	1.69	0.74
3:C:438:TYR:CZ	3:C:469:ARG:HD3	2.22	0.74
1:G:2091:GLY:O	1:G:2095:ARG:HG3	1.87	0.74
2:E:1264:ASN:C	2:E:1264:ASN:HD22	1.96	0.73
1:D:1091:GLY:O	1:D:1095:ARG:HG3	1.90	0.72
2:Q:5264:ASN:ND2	2:Q:5266:SER:H	1.87	0.72
2:Q:5220:ILE:HG12	2:Q:5224:GLU:HG3	1.71	0.72
1:A:57:ASP:HB3	4:A:6262:HOH:O	1.89	0.71
1:J:3001:MET:HE1	1:J:3124:ARG:NH1	2.05	0.71
1:J:3001:MET:HE1	1:J:3124:ARG:HH12	1.54	0.70
1:D:1113:GLY:O	1:D:1117:GLU:HB2	1.92	0.69
3:F:1472:SER:HB2	4:F:6123:HOH:O	1.91	0.69
3:O:4462:LEU:HG	3:O:4464:PRO:HD2	1.73	0.69
3:O:4438:TYR:CZ	3:O:4469:ARG:HD3	2.28	0.68
1:A:1:MET:HE1	1:A:124:ARG:HH12	1.58	0.68
3:C:462:LEU:HG	3:C:464:PRO:HD2	1.76	0.68
2:K:3264:ASN:ND2	2:K:3266:SER:H	1.91	0.68
2:E:1253:ARG:HG2	2:E:1296:ASP:O	1.94	0.68
3:O:4484:ASP:HB2	4:O:6379:HOH:O	1.95	0.66
2:B:323:VAL:HG12	2:B:327:MET:HE3	1.77	0.66
1:P:5091:GLY:O	1:P:5095:ARG:HG3	1.94	0.66
2:E:1236:ASP:HB3	4:E:6217:HOH:O	1.96	0.66
3:I:2408:ASN:H	3:I:2408:ASN:HD22	1.41	0.66
2:Q:5207:LYS:HD2	2:Q:5238:ASP:O	1.96	0.66
3:F:1408:ASN:H	3:F:1408:ASN:HD22	1.45	0.65
3:L:3408:ASN:HD22	3:L:3408:ASN:H	1.43	0.65
2:E:1207:LYS:HD2	2:E:1238:ASP:O	1.96	0.65
2:B:264:ASN:C	2:B:264:ASN:HD22	2.02	0.64
1:A:91:GLY:O	1:A:95:ARG:HG3	1.97	0.64
2:H:2264:ASN:ND2	2:H:2266:SER:H	1.95	0.64
2:B:278:ARG:O	2:B:314:ILE:HD12	1.97	0.64
2:H:2207:LYS:HD2	2:H:2238:ASP:O	1.98	0.63
1:M:4058:ARG:HG3	1:M:4063:ARG:NH2	2.14	0.62
1:A:21:TYR:CZ	1:A:63:ARG:HD2	2.33	0.62
2:E:1264:ASN:ND2	2:E:1266:SER:H	1.98	0.62
1:A:1:MET:HE1	1:A:124:ARG:NH1	2.14	0.62
3:F:1433:PHE:HA	3:F:1437:ILE:CD1	2.30	0.62
2:B:323:VAL:CG1	2:B:327:MET:HE3	2.30	0.61
2:K:3207:LYS:HD2	2:K:3238:ASP:O	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:3001:MET:HE2	1:J:3123:ASP:CB	2.30	0.60
2:K:3264:ASN:C	2:K:3264:ASN:HD22	2.09	0.60
1:J:3057:ASP:HB3	4:J:6188:HOH:O	2.00	0.60
1:M:4062:ASN:O	1:M:4066:GLU:HG3	2.02	0.60
3:R:5438:TYR:CZ	3:R:5469:ARG:HD3	2.37	0.60
3:O:4408:ASN:HD22	3:O:4408:ASN:N	1.98	0.60
3:I:2472:SER:OG	3:I:2474:GLU:HG2	2.02	0.59
2:Q:5284:ARG:HB3	2:Q:5317:VAL:CG1	2.32	0.59
1:D:1082:ALA:HB1	1:D:1087:ILE:HB	1.85	0.58
1:D:1062:ASN:O	1:D:1066:GLU:HG3	2.04	0.58
2:E:1275:TYR:O	2:E:1276:GLU:HB2	2.04	0.58
2:Q:5264:ASN:C	2:Q:5264:ASN:HD22	2.11	0.58
1:P:5062:ASN:O	1:P:5066:GLU:HG3	2.04	0.57
2:H:2264:ASN:HD22	2:H:2265:PHE:N	2.03	0.57
1:D:1044:VAL:HG12	1:D:1077:VAL:HG13	1.87	0.57
2:Q:5207:LYS:HE2	4:Q:6164:HOH:O	2.05	0.57
1:G:2058:ARG:HG3	1:G:2063:ARG:NH2	2.20	0.57
1:J:3089:ASP:HB3	1:J:3103:ILE:HG21	1.86	0.56
2:E:1318:ILE:HD12	2:E:1322:ARG:HG3	1.87	0.56
2:H:2244:LEU:HD12	2:H:2245:ASP:H	1.70	0.56
2:N:4264:ASN:C	2:N:4264:ASN:HD22	2.14	0.56
2:K:3220:ILE:HG12	2:K:3224:GLU:HG3	1.87	0.56
3:F:1462:LEU:HG	3:F:1464:PRO:HD2	1.88	0.56
1:M:4112:LEU:HD21	2:N:4228:VAL:CG2	2.35	0.56
3:R:5490:ASP:O	3:R:5494:GLU:HG3	2.05	0.56
2:N:4266:SER:OG	2:N:4267:PRO:HD3	2.06	0.55
1:M:4068:ALA:CB	1:M:4075:MET:HE2	2.36	0.55
2:N:4244:LEU:HD12	2:N:4245:ASP:H	1.70	0.55
2:K:3213:ARG:HA	2:K:3244:LEU:O	2.07	0.55
3:R:5408:ASN:HD22	3:R:5408:ASN:H	1.54	0.55
1:D:1058:ARG:HG3	1:D:1063:ARG:NH2	2.21	0.55
2:H:2262:MET:HE3	1:J:3058:ARG:NH2	2.22	0.55
2:H:2264:ASN:HD22	2:H:2264:ASN:C	2.15	0.55
2:Q:5253:ARG:HG2	2:Q:5296:ASP:O	2.07	0.55
2:B:264:ASN:ND2	2:B:266:SER:H	2.04	0.55
1:P:5082:ALA:HB1	1:P:5087:ILE:HB	1.87	0.55
1:A:62:ASN:O	1:A:66:GLU:HG3	2.07	0.54
1:M:4008:ASN:HB3	1:M:4041:HIS:HD2	1.72	0.54
3:F:1438:TYR:CZ	3:F:1469:ARG:HD3	2.43	0.54
1:D:1057:ASP:HB3	4:D:6320:HOH:O	2.07	0.54
2:E:1264:ASN:C	2:E:1264:ASN:ND2	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:2462:LEU:HG	3:I:2464:PRO:HD2	1.90	0.54
2:K:3307:THR:O	2:K:3308:GLU:HB3	2.08	0.54
3:C:408:ASN:HD22	3:C:408:ASN:N	1.99	0.53
1:J:3058:ARG:HG3	1:J:3063:ARG:NH2	2.23	0.53
3:O:4438:TYR:OH	3:O:4469:ARG:HD3	2.08	0.53
2:E:1284:ARG:HB3	2:E:1317:VAL:CG1	2.39	0.53
3:F:1490:ASP:O	3:F:1494:GLU:HG3	2.07	0.53
1:D:1030:LYS:HE3	3:F:1486:ALA:O	2.08	0.53
2:E:1264:ASN:HD22	2:E:1265:PHE:N	2.06	0.53
3:I:2433:PHE:HA	3:I:2437:ILE:HD13	1.90	0.53
2:K:3264:ASN:ND2	2:K:3264:ASN:C	2.67	0.53
3:O:4433:PHE:HA	3:O:4437:ILE:HD13	1.89	0.53
1:G:2104:HIS:CE1	1:G:2106:LYS:HB2	2.43	0.53
1:G:2113:GLY:O	1:G:2117:GLU:HB2	2.08	0.53
3:I:2462:LEU:HD23	3:I:2465:ASP:OD2	2.09	0.53
1:J:3030:LYS:HE2	3:L:3486:ALA:HB1	1.90	0.53
3:R:5462:LEU:HG	3:R:5464:PRO:HD2	1.91	0.53
3:C:446:VAL:O	3:C:450:VAL:HG23	2.09	0.53
3:F:1437:ILE:HG23	3:F:1466:LEU:HD23	1.90	0.53
1:J:3062:ASN:O	1:J:3066:GLU:HG3	2.09	0.52
2:E:1307:THR:O	2:E:1308:GLU:HB3	2.09	0.52
2:H:2306:GLU:HB2	4:H:6265:HOH:O	2.09	0.52
2:H:2262:MET:HE3	1:J:3058:ARG:HH22	1.75	0.52
2:N:4213:ARG:HA	2:N:4244:LEU:O	2.09	0.52
2:N:4305:MET:O	2:N:4305:MET:HE3	2.10	0.52
3:L:3432:LEU:HD12	3:L:3440:ALA:HB2	1.92	0.51
1:M:4049:ARG:HG2	1:M:4102:ASN:O	2.10	0.51
1:P:5049:ARG:HG2	1:P:5102:ASN:O	2.10	0.51
1:A:79:VAL:HG13	1:A:80:ALA:N	2.24	0.51
3:L:3438:TYR:OH	3:L:3469:ARG:HD3	2.09	0.51
2:Q:5264:ASN:HD22	2:Q:5266:SER:H	1.56	0.51
1:P:5058:ARG:HG3	1:P:5063:ARG:NH2	2.25	0.51
2:Q:5284:ARG:HG2	2:Q:5318:ILE:O	2.11	0.51
2:B:305:MET:HE3	2:B:305:MET:O	2.11	0.51
1:G:2079:VAL:HG13	1:G:2080:ALA:N	2.25	0.51
1:M:4079:VAL:O	1:M:4083:GLN:HG3	2.11	0.51
2:K:3264:ASN:HD22	2:K:3265:PHE:N	2.08	0.50
2:B:220:ILE:HB	1:D:1012:TYR:O	2.12	0.50
2:N:4220:ILE:HG12	2:N:4224:GLU:HG3	1.93	0.50
1:J:3099:ASP:CB	1:P:5095:ARG:HH22	2.24	0.50
2:N:4284:ARG:HB3	2:N:4317:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1015:GLN:CD	3:F:1434:GLU:HG2	2.36	0.50
2:H:2220:ILE:HB	1:J:3012:TYR:O	2.11	0.50
2:Q:5256:ASP:OD2	2:Q:5258:LYS:HG2	2.11	0.50
2:Q:5305:MET:HE3	2:Q:5305:MET:O	2.12	0.50
2:B:266:SER:OG	2:B:267:PRO:HD3	2.12	0.50
1:D:1022:GLN:NE2	1:D:1022:GLN:HA	2.27	0.50
2:E:1256:ASP:OD2	2:E:1258:LYS:HG2	2.12	0.50
2:N:4264:ASN:ND2	2:N:4266:SER:H	2.10	0.50
3:F:1433:PHE:HA	3:F:1437:ILE:HD13	1.93	0.49
3:O:4438:TYR:CD2	2:Q:5249:TYR:CZ	3.00	0.49
1:P:5079:VAL:O	1:P:5083:GLN:HG3	2.12	0.49
2:N:4284:ARG:HG2	2:N:4318:ILE:O	2.13	0.49
3:I:2446:VAL:O	3:I:2450:VAL:HG23	2.12	0.49
2:K:3266:SER:N	2:K:3267:PRO:CD	2.75	0.49
2:B:264:ASN:HD22	2:B:265:PHE:N	2.10	0.49
3:O:4408:ASN:H	3:O:4408:ASN:ND2	2.05	0.49
2:E:1303:GLU:O	2:E:1303:GLU:HG3	2.13	0.49
2:K:3212:ASN:HB3	2:K:3250:GLN:HE22	1.78	0.49
1:M:4015:GLN:O	1:M:4016:ALA:C	2.56	0.49
2:H:2284:ARG:HG2	2:H:2318:ILE:O	2.13	0.48
1:J:3021:TYR:CZ	1:J:3063:ARG:HD2	2.48	0.48
2:Q:5264:ASN:HD22	2:Q:5265:PHE:N	2.10	0.48
1:D:1015:GLN:OE1	3:F:1434:GLU:HG2	2.12	0.48
1:J:3099:ASP:CG	1:P:5095:ARG:HH22	2.21	0.48
1:G:2012:TYR:O	2:K:3220:ILE:HB	2.14	0.48
2:K:3279:ARG:HG3	4:K:6015:HOH:O	2.14	0.48
1:A:21:TYR:CE2	1:A:63:ARG:HD2	2.48	0.48
1:D:1021:TYR:CZ	1:D:1063:ARG:HD2	2.48	0.48
1:G:2104:HIS:CG	1:G:2105:PRO:HD2	2.48	0.48
1:M:4011:PRO:HB2	1:M:4012:TYR:CD1	2.48	0.48
3:F:1408:ASN:HD22	3:F:1408:ASN:N	2.08	0.48
1:A:58:ARG:HG3	1:A:63:ARG:NH2	2.29	0.48
1:M:4041:HIS:ND1	2:N:4224:GLU:OE1	2.43	0.48
2:Q:5278:ARG:HD3	2:Q:5302:PHE:CE1	2.49	0.48
2:E:1305:MET:HE3	2:E:1305:MET:O	2.13	0.48
2:H:2219:THR:HB	2:H:2221:TYR:CD1	2.49	0.48
2:Q:5307:THR:O	2:Q:5308:GLU:HB3	2.12	0.48
3:R:5453:ALA:C	3:R:5455:GLY:N	2.71	0.48
1:A:112:LEU:HD21	2:B:228:VAL:HG22	1.95	0.48
3:O:4433:PHE:HA	3:O:4437:ILE:CD1	2.44	0.48
2:B:207:LYS:HD2	2:B:238:ASP:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1278:ARG:HD3	2:E:1302:PHE:CE1	2.49	0.47
3:F:1501:TRP:HA	4:F:6063:HOH:O	2.13	0.47
1:G:2104:HIS:ND1	1:G:2106:LYS:HB2	2.28	0.47
2:H:2264:ASN:ND2	2:H:2264:ASN:C	2.72	0.47
2:B:209:MET:HB3	2:B:333:VAL:HG22	1.96	0.47
2:H:2266:SER:N	2:H:2267:PRO:CD	2.77	0.47
2:Q:5251:LEU:O	2:Q:5297:LEU:HA	2.14	0.47
2:H:2275:TYR:O	2:H:2276:GLU:HB2	2.13	0.47
2:B:210:TYR:CE1	2:B:334:PHE:CD2	3.03	0.47
2:Q:5264:ASN:HD21	2:Q:5266:SER:CB	2.28	0.47
1:A:8:ASN:HB3	1:A:41:HIS:CD2	2.49	0.47
2:B:255:GLN:HG2	3:F:1468:ALA:O	2.15	0.47
2:E:1217:TYR:CE2	2:E:1257:THR:HG21	2.48	0.47
3:L:3404:LEU:HD23	3:L:3492:THR:HG22	1.97	0.47
1:M:4021:TYR:CZ	1:M:4063:ARG:HD2	2.49	0.47
2:N:4222:ALA:HB3	4:N:6364:HOH:O	2.15	0.47
2:Q:5266:SER:N	2:Q:5267:PRO:CD	2.76	0.47
2:B:247:GLY:O	2:B:250:GLN:HB2	2.15	0.47
1:J:3015:GLN:O	1:J:3016:ALA:C	2.57	0.47
2:B:207:LYS:NZ	2:B:240:CYS:HB3	2.30	0.47
3:R:5485:TYR:O	3:R:5489:VAL:HG23	2.13	0.47
2:Q:5264:ASN:ND2	2:Q:5264:ASN:C	2.72	0.47
2:B:290:ARG:HH11	2:B:290:ARG:HG3	1.79	0.46
2:N:4304:ASP:HB3	2:N:4309:GLU:CG	2.45	0.46
1:J:3001:MET:N	1:J:3032:HIS:HD1	2.13	0.46
1:M:4008:ASN:HB3	1:M:4041:HIS:CD2	2.49	0.46
1:A:16:ALA:HB3	4:A:6181:HOH:O	2.14	0.46
2:H:2247:GLY:O	2:H:2250:GLN:HB2	2.16	0.46
1:P:5030:LYS:HE3	3:R:5486:ALA:O	2.16	0.46
3:I:2488:PHE:HD2	3:I:2488:PHE:O	1.99	0.46
1:M:4040:TYR:CZ	2:N:4224:GLU:HB3	2.50	0.46
2:B:279:ARG:HA	2:B:279:ARG:HD3	1.85	0.46
3:C:488:PHE:HD2	3:C:488:PHE:O	1.99	0.46
1:G:2021:TYR:HA	1:G:2064:TRP:CH2	2.51	0.46
3:O:4456:LYS:H	3:O:4456:LYS:HD3	1.80	0.46
2:Q:5241:VAL:HG12	2:Q:5243:PHE:CE1	2.51	0.46
1:D:1104:HIS:CE1	1:D:1106:LYS:HB2	2.51	0.46
2:H:2220:ILE:HD13	2:H:2224:GLU:CD	2.41	0.46
3:L:3469:ARG:HG3	3:L:3469:ARG:HH11	1.82	0.46
3:R:5408:ASN:HD22	3:R:5408:ASN:N	2.14	0.45
1:M:4082:ALA:HB1	1:M:4087:ILE:HB	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:4264:ASN:C	2:N:4264:ASN:ND2	2.75	0.45
2:N:4279:ARG:HB3	2:N:4281:TYR:CE1	2.51	0.45
1:J:3079:VAL:HG13	1:J:3080:ALA:N	2.30	0.45
2:B:257:THR:OG1	2:B:264:ASN:HB2	2.17	0.45
3:C:488:PHE:C	3:C:488:PHE:CD2	2.94	0.45
1:M:4113:GLY:O	1:M:4117:GLU:HB2	2.16	0.45
1:P:5028:LEU:HD13	1:P:5071:TYR:CD1	2.52	0.45
1:A:113:GLY:O	1:A:117:GLU:HB2	2.17	0.45
2:H:2284:ARG:HB3	2:H:2317:VAL:CG1	2.47	0.45
2:B:284:ARG:HB3	2:B:317:VAL:CG1	2.47	0.45
3:C:408:ASN:H	3:C:408:ASN:ND2	2.08	0.45
1:J:3028:LEU:HD13	1:J:3071:TYR:CD1	2.52	0.45
2:B:284:ARG:HG2	2:B:318:ILE:O	2.18	0.44
2:B:241:VAL:HG12	2:B:243:PHE:CE1	2.53	0.44
2:E:1247:GLY:O	2:E:1250:GLN:HB2	2.17	0.44
1:G:2021:TYR:CZ	1:G:2063:ARG:HD2	2.52	0.44
1:P:5015:GLN:O	1:P:5016:ALA:C	2.60	0.44
2:Q:5275:TYR:O	2:Q:5276:GLU:HB2	2.16	0.44
1:G:2082:ALA:HB1	1:G:2087:ILE:HB	2.00	0.44
3:I:2449:GLN:HG2	4:I:6097:HOH:O	2.17	0.44
2:B:217:TYR:CE2	2:B:257:THR:HG21	2.53	0.44
1:J:3068:ALA:HB2	1:J:3075:MET:HE2	1.98	0.44
3:L:3433:PHE:HA	3:L:3437:ILE:HD13	2.00	0.44
2:N:4253:ARG:HG2	2:N:4296:ASP:O	2.17	0.44
1:P:5113:GLY:O	1:P:5117:GLU:HB2	2.18	0.44
1:A:44:VAL:HG11	1:A:81:ALA:HB3	2.00	0.44
2:Q:5279:ARG:HA	2:Q:5279:ARG:HD3	1.85	0.44
1:G:2106:LYS:HA	1:G:2106:LYS:HD3	1.83	0.44
1:M:4040:TYR:OH	2:N:4224:GLU:HB3	2.18	0.44
1:D:1049:ARG:HG2	1:D:1102:ASN:O	2.18	0.44
1:G:2044:VAL:HG12	1:G:2077:VAL:HG13	1.99	0.44
2:H:2262:MET:HG2	1:J:3058:ARG:CZ	2.46	0.44
2:N:4264:ASN:HD22	2:N:4265:PHE:N	2.15	0.44
2:N:4266:SER:N	2:N:4267:PRO:CD	2.80	0.44
1:P:5028:LEU:HG	1:P:5034:ILE:HD12	2.00	0.44
2:E:1304:ASP:HB3	2:E:1309:GLU:HG2	1.99	0.43
2:K:3305:MET:HE3	2:K:3305:MET:O	2.18	0.43
3:O:4403:ILE:HG21	3:O:4405:HIS:CE1	2.54	0.43
2:H:2307:THR:O	2:H:2308:GLU:HB3	2.18	0.43
3:O:4490:ASP:O	3:O:4494:GLU:HG3	2.17	0.43
1:P:5079:VAL:HG13	1:P:5080:ALA:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1300:ILE:O	2:E:1314:ILE:HG12	2.19	0.43
1:G:2089:ASP:HB3	1:G:2103:ILE:HG21	2.00	0.43
1:J:3030:LYS:HE3	3:L:3486:ALA:O	2.19	0.43
2:K:3253:ARG:HG2	2:K:3296:ASP:O	2.19	0.43
2:N:4284:ARG:NE	4:N:6018:HOH:O	2.51	0.43
3:R:5404:LEU:HB2	3:R:5495:CYS:SG	2.58	0.43
1:G:2024:ALA:HB1	1:G:2034:ILE:CD1	2.49	0.43
2:H:2245:ASP:C	2:H:2247:GLY:H	2.26	0.43
2:E:1266:SER:N	2:E:1267:PRO:CD	2.82	0.43
1:G:2012:TYR:HB3	2:K:3220:ILE:HD12	2.01	0.43
1:M:4041:HIS:CE1	2:N:4224:GLU:HB2	2.54	0.43
2:N:4241:VAL:HG12	2:N:4243:PHE:CE1	2.54	0.43
2:N:4304:ASP:HB3	2:N:4309:GLU:HG2	2.00	0.43
2:K:3226:LEU:HD21	2:K:3268:THR:HB	2.00	0.43
3:F:1476:VAL:CG1	3:F:1477:ILE:N	2.82	0.43
1:M:4089:ASP:CG	1:M:4109:ILE:HD12	2.44	0.43
2:E:1253:ARG:HD2	2:E:1297:LEU:O	2.19	0.43
2:K:3302:PHE:CD1	2:K:3302:PHE:C	2.96	0.43
3:R:5437:ILE:HG22	3:R:5438:TYR:N	2.33	0.43
1:A:41:HIS:C	1:A:43:GLY:N	2.75	0.43
3:I:2456:LYS:H	3:I:2456:LYS:HD3	1.84	0.43
1:J:3064:TRP:HB3	1:J:3075:MET:HE1	2.00	0.43
2:K:3219:THR:HB	2:K:3221:TYR:CD1	2.54	0.43
1:M:4025:LYS:HG2	1:M:4029:GLU:OE2	2.19	0.43
2:N:4278:ARG:O	2:N:4314:ILE:HD12	2.18	0.43
3:O:4488:PHE:HD2	3:O:4488:PHE:O	2.02	0.43
3:R:5453:ALA:C	3:R:5455:GLY:H	2.26	0.43
1:A:8:ASN:HB3	1:A:41:HIS:HD2	1.84	0.42
1:A:9:GLU:O	1:A:43:GLY:HA2	2.19	0.42
2:B:307:THR:O	2:B:308:GLU:HB3	2.18	0.42
2:E:1264:ASN:HD22	2:E:1266:SER:H	1.65	0.42
2:E:1284:ARG:HB3	2:E:1317:VAL:HG12	2.01	0.42
1:J:3007:ILE:HD12	1:J:3039:PHE:CE2	2.54	0.42
1:M:4016:ALA:N	4:M:6371:HOH:O	2.45	0.42
3:O:4446:VAL:O	3:O:4450:VAL:HG23	2.19	0.42
3:C:456:LYS:HD3	3:C:456:LYS:H	1.85	0.42
2:E:1213:ARG:HA	2:E:1244:LEU:O	2.20	0.42
2:E:1241:VAL:HG12	2:E:1243:PHE:CE1	2.54	0.42
2:K:3209:MET:HB3	2:K:3333:VAL:HG22	2.02	0.42
2:K:3249:TYR:CE1	2:K:3290:ARG:HD3	2.55	0.42
3:L:3477:ILE:HB	3:L:3480:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:4419:SER:HB3	3:O:4501:TRP:CZ3	2.54	0.42
2:Q:5327:MET:O	3:R:5403:ILE:HD11	2.19	0.42
2:E:1294:GLN:NE2	2:E:1315:VAL:O	2.47	0.42
3:I:2452:GLU:CG	4:I:6020:HOH:O	2.67	0.42
1:P:5015:GLN:CD	3:R:5434:GLU:HG2	2.45	0.42
2:B:266:SER:N	2:B:267:PRO:CD	2.82	0.42
3:L:3460:TYR:CD2	3:L:3481:SER:HB2	2.54	0.42
1:A:15:GLN:O	1:A:16:ALA:C	2.62	0.42
1:A:78:CYS:HB3	1:A:81:ALA:HB3	2.02	0.42
2:E:1304:ASP:HB3	2:E:1309:GLU:CG	2.50	0.42
2:E:1333:VAL:HG11	3:F:1499:GLN:HG3	2.02	0.42
1:G:2066:GLU:O	1:G:2069:GLU:HB3	2.20	0.42
2:H:2279:ARG:HB3	2:H:2281:TYR:CE1	2.55	0.42
3:I:2419:SER:HB3	3:I:2501:TRP:CZ3	2.55	0.42
2:K:3214:LYS:N	4:K:6303:HOH:O	2.53	0.42
1:M:4017:SER:HB2	4:M:6031:HOH:O	2.19	0.42
2:Q:5247:GLY:O	2:Q:5250:GLN:HB2	2.19	0.42
3:C:485:TYR:O	3:C:489:VAL:HG23	2.19	0.42
3:F:1488:PHE:C	3:F:1488:PHE:CD2	2.98	0.42
2:N:4288:GLU:HA	4:N:6412:HOH:O	2.18	0.42
3:R:5484:ASP:HB2	4:R:6353:HOH:O	2.20	0.42
1:A:12:TYR:CD1	1:D:1084:ARG:HG2	2.54	0.42
1:M:4036:ARG:NE	1:M:4074:ASP:OD2	2.40	0.42
1:D:1009:GLU:O	1:D:1043:GLY:HA2	2.20	0.42
2:N:4220:ILE:HB	1:P:5012:TYR:O	2.19	0.42
3:O:4469:ARG:HH11	3:O:4469:ARG:HG3	1.85	0.42
3:R:5411:PRO:HG3	3:R:5439:ALA:HB2	2.02	0.42
3:R:5488:PHE:C	3:R:5488:PHE:CD2	2.97	0.42
3:C:419:SER:O	3:C:423:PHE:HD1	2.03	0.41
1:J:3004:ALA:HB2	1:J:3122:ALA:CB	2.50	0.41
3:L:3447:GLU:HG3	3:L:3477:ILE:HD11	2.02	0.41
2:N:4290:ARG:HG3	2:N:4290:ARG:HH11	1.85	0.41
1:P:5021:TYR:CZ	1:P:5063:ARG:HD2	2.55	0.41
1:P:5098:LYS:HA	1:P:5098:LYS:HE2	2.02	0.41
3:R:5437:ILE:HG13	3:R:5461:VAL:CG2	2.50	0.41
2:H:2224:GLU:O	2:H:2228:VAL:HG23	2.19	0.41
1:J:3015:GLN:CD	3:L:3434:GLU:HG2	2.45	0.41
1:J:3099:ASP:OD2	1:P:5095:ARG:NH2	2.53	0.41
3:C:433:PHE:HA	3:C:437:ILE:CD1	2.51	0.41
3:L:3430:VAL:HB	3:L:3459:LEU:CD2	2.50	0.41
1:M:4052:THR:N	1:M:4053:PRO:HD3	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:4462:LEU:HD23	3:O:4465:ASP:OD2	2.20	0.41
3:O:4477:ILE:HB	3:O:4480:ILE:HD12	2.01	0.41
3:O:4408:ASN:N	3:O:4408:ASN:ND2	2.67	0.41
1:A:30:LYS:HE2	3:C:486:ALA:HB1	2.02	0.41
1:A:40:TYR:CZ	2:B:224:GLU:HB3	2.55	0.41
3:I:2438:TYR:CZ	3:I:2469:ARG:HD3	2.55	0.41
1:M:4001:MET:N	1:M:4032:HIS:HD1	2.18	0.41
3:O:4419:SER:O	3:O:4423:PHE:HD1	2.04	0.41
2:B:293:THR:C	2:B:295:ASP:N	2.79	0.41
2:E:1226:LEU:HD21	2:E:1268:THR:HB	2.02	0.41
2:K:3284:ARG:HG2	2:K:3318:ILE:O	2.20	0.41
2:N:4207:LYS:NZ	2:N:4240:CYS:HB3	2.36	0.41
2:N:4219:THR:HB	2:N:4221:TYR:CD1	2.56	0.41
2:N:4236:ASP:HB3	4:N:6141:HOH:O	2.19	0.41
2:N:4296:ASP:OD2	3:R:5475:ARG:NH2	2.51	0.41
3:R:5477:ILE:HB	3:R:5480:ILE:HD12	2.03	0.41
1:D:1021:TYR:CE2	1:D:1063:ARG:HD2	2.56	0.41
1:D:1063:ARG:NH2	4:D:6086:HOH:O	2.53	0.41
1:M:4036:ARG:HD3	1:M:4076:VAL:HG21	2.01	0.41
1:A:93:ALA:HB2	1:A:101:THR:HG22	2.02	0.41
2:B:213:ARG:HA	2:B:244:LEU:O	2.21	0.41
2:E:1322:ARG:NH2	2:E:1326:LEU:HD21	2.36	0.41
3:F:1404:LEU:HB2	3:F:1495:CYS:SG	2.61	0.41
1:P:5106:LYS:HA	1:P:5106:LYS:HD3	1.85	0.41
3:C:488:PHE:HD2	3:C:488:PHE:C	2.28	0.41
3:F:1456:LYS:HD3	3:F:1456:LYS:H	1.84	0.41
1:G:2063:ARG:NH2	4:G:6069:HOH:O	2.54	0.41
1:P:5073:LEU:HA	4:P:6180:HOH:O	2.21	0.41
2:B:258:LYS:NZ	4:B:6260:HOH:O	2.54	0.41
1:M:4041:HIS:HE1	2:N:4224:GLU:HB2	1.86	0.41
2:B:264:ASN:HD22	2:B:266:SER:H	1.67	0.40
1:D:1096:ASN:ND2	4:D:6401:HOH:O	2.54	0.40
1:G:2075:MET:HE3	1:G:2107:PHE:CE2	2.56	0.40
2:N:4247:GLY:O	2:N:4250:GLN:HB2	2.21	0.40
3:O:4488:PHE:C	3:O:4488:PHE:CD2	2.99	0.40
3:R:5456:LYS:H	3:R:5456:LYS:HD3	1.86	0.40
2:B:219:THR:HB	2:B:221:TYR:CD1	2.56	0.40
3:F:1417:LEU:HD22	3:F:1417:LEU:O	2.21	0.40
1:M:4057:ASP:HB3	4:M:6284:HOH:O	2.21	0.40
1:P:5041:HIS:CE1	2:Q:5224:GLU:HB2	2.56	0.40
2:Q:5279:ARG:HD2	2:Q:5281:TYR:OH	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:438:TYR:OH	3:C:469:ARG:HD3	2.21	0.40
2:E:1279:ARG:HA	2:E:1279:ARG:HD3	1.78	0.40
2:H:2207:LYS:NZ	2:H:2240:CYS:HB3	2.36	0.40
2:H:2221:TYR:O	2:H:2225:ALA:HB2	2.21	0.40
1:J:3022:GLN:HA	1:J:3022:GLN:NE2	2.37	0.40
2:B:231:ILE:HD13	2:B:231:ILE:HA	1.90	0.40
2:E:1207:LYS:NZ	2:E:1240:CYS:HB3	2.37	0.40
3:F:1476:VAL:HG12	3:F:1477:ILE:N	2.37	0.40
3:I:2488:PHE:C	3:I:2488:PHE:CD2	3.00	0.40
2:K:3240:CYS:HB2	2:K:3279:ARG:CB	2.51	0.40
2:N:4315:VAL:HB	4:N:6146:HOH:O	2.21	0.40
2:E:1258:LYS:HA	2:E:1258:LYS:HD3	1.87	0.40
2:N:4279:ARG:HD2	2:N:4281:TYR:OH	2.22	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	128/130 (98%)	120 (94%)	8 (6%)	0	100	100
1	D	128/130 (98%)	121 (94%)	7 (6%)	0	100	100
1	G	128/130 (98%)	123 (96%)	5 (4%)	0	100	100
1	J	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
1	M	128/130 (98%)	122 (95%)	6 (5%)	0	100	100
1	P	128/130 (98%)	123 (96%)	5 (4%)	0	100	100
2	B	130/136 (96%)	120 (92%)	10 (8%)	0	100	100
2	E	130/136 (96%)	119 (92%)	11 (8%)	0	100	100
2	H	130/136 (96%)	120 (92%)	10 (8%)	0	100	100
2	K	130/136 (96%)	125 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	N	130/136 (96%)	123 (95%)	5 (4%)	2 (2%)	8	16
2	Q	130/136 (96%)	123 (95%)	7 (5%)	0	100	100
3	C	99/102 (97%)	96 (97%)	3 (3%)	0	100	100
3	F	99/102 (97%)	95 (96%)	4 (4%)	0	100	100
3	I	99/102 (97%)	95 (96%)	4 (4%)	0	100	100
3	L	99/102 (97%)	95 (96%)	3 (3%)	1 (1%)	12	24
3	O	99/102 (97%)	97 (98%)	2 (2%)	0	100	100
3	R	99/102 (97%)	94 (95%)	5 (5%)	0	100	100
All	All	2142/2208 (97%)	2033 (95%)	106 (5%)	3 (0%)	48	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	3455	GLY
2	N	4236	ASP
2	N	4217	TYR

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	105/105 (100%)	102 (97%)	3 (3%)	37	65
1	D	105/105 (100%)	102 (97%)	3 (3%)	37	65
1	G	105/105 (100%)	101 (96%)	4 (4%)	29	56
1	J	105/105 (100%)	103 (98%)	2 (2%)	50	76
1	M	105/105 (100%)	103 (98%)	2 (2%)	50	76
1	P	105/105 (100%)	103 (98%)	2 (2%)	50	76
2	B	115/119 (97%)	114 (99%)	1 (1%)	70	87
2	E	115/119 (97%)	112 (97%)	3 (3%)	40	68
2	H	115/119 (97%)	112 (97%)	3 (3%)	40	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	K	115/119 (97%)	112 (97%)	3 (3%)	40	68
2	N	115/119 (97%)	111 (96%)	4 (4%)	32	58
2	Q	115/119 (97%)	113 (98%)	2 (2%)	53	78
3	C	84/85 (99%)	78 (93%)	6 (7%)	13	29
3	F	84/85 (99%)	78 (93%)	6 (7%)	13	29
3	I	84/85 (99%)	78 (93%)	6 (7%)	13	29
3	L	84/85 (99%)	79 (94%)	5 (6%)	17	36
3	O	84/85 (99%)	78 (93%)	6 (7%)	13	29
3	R	84/85 (99%)	78 (93%)	6 (7%)	13	29
All	All	1824/1854 (98%)	1757 (96%)	67 (4%)	30	57

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	63	ARG
1	A	117	GLU
2	B	223	TRP
3	C	408	ASN
3	C	417	LEU
3	C	437	ILE
3	C	452	GLU
3	C	456	LYS
3	C	474	GLU
1	D	1001	MET
1	D	1063	ARG
1	D	1117	GLU
2	E	1223	TRP
2	E	1240	CYS
2	E	1264	ASN
3	F	1408	ASN
3	F	1417	LEU
3	F	1437	ILE
3	F	1452	GLU
3	F	1456	LYS
3	F	1502	LEU
1	G	2001	MET
1	G	2063	ARG
1	G	2084	ARG

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Mol	Chain	Res	Type
1	G	2117	GLU
2	H	2223	TRP
2	H	2240	CYS
2	H	2264	ASN
3	I	2408	ASN
3	I	2414	ARG
3	I	2417	LEU
3	I	2437	ILE
3	I	2452	GLU
3	I	2456	LYS
1	J	3063	ARG
1	J	3117	GLU
2	K	3205	VAL
2	K	3240	CYS
2	K	3264	ASN
3	L	3408	ASN
3	L	3417	LEU
3	L	3437	ILE
3	L	3452	GLU
3	L	3456	LYS
1	M	4063	ARG
1	M	4117	GLU
2	N	4205	VAL
2	N	4223	TRP
2	N	4240	CYS
2	N	4264	ASN
3	O	4408	ASN
3	O	4417	LEU
3	O	4437	ILE
3	O	4452	GLU
3	O	4456	LYS
3	O	4474	GLU
1	P	5063	ARG
1	P	5117	GLU
2	Q	5223	TRP
2	Q	5264	ASN
3	R	5408	ASN
3	R	5417	LEU
3	R	5437	ILE
3	R	5452	GLU
3	R	5456	LYS
3	R	5474	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	8	ASN
1	A	14	HIS
1	A	22	GLN
1	A	45	ASN
1	A	83	GLN
1	A	96	ASN
2	B	250	GLN
2	B	264	ASN
2	B	328	ASN
3	C	408	ASN
3	C	449	GLN
1	D	1014	HIS
1	D	1022	GLN
1	D	1045	ASN
1	D	1055	GLN
1	D	1062	ASN
1	D	1070	GLN
1	D	1083	GLN
1	D	1096	ASN
2	E	1250	GLN
2	E	1264	ASN
3	F	1408	ASN
1	G	2006	GLN
1	G	2008	ASN
1	G	2014	HIS
1	G	2022	GLN
1	G	2032	HIS
1	G	2083	GLN
1	G	2096	ASN
2	H	2250	GLN
2	H	2264	ASN
3	I	2408	ASN
1	J	3006	GLN
1	J	3008	ASN
1	J	3014	HIS
1	J	3022	GLN
1	J	3045	ASN
1	J	3083	GLN
1	J	3096	ASN
2	K	3212	ASN

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Mol	Chain	Res	Type
2	K	3250	GLN
2	K	3264	ASN
3	L	3408	ASN
1	M	4022	GLN
1	M	4045	ASN
1	M	4083	GLN
1	M	4096	ASN
2	N	4250	GLN
2	N	4264	ASN
2	N	4328	ASN
3	O	4408	ASN
3	O	4449	GLN
1	P	5006	GLN
1	P	5014	HIS
1	P	5022	GLN
1	P	5045	ASN
1	P	5083	GLN
1	P	5096	ASN
2	Q	5212	ASN
2	Q	5264	ASN
3	R	5408	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	130/130 (100%)	-0.27	0 100 100	9, 30, 60, 90	0
1	D	130/130 (100%)	-0.38	0 100 100	15, 27, 47, 78	0
1	G	130/130 (100%)	-0.34	0 100 100	15, 28, 46, 84	0
1	J	130/130 (100%)	-0.36	0 100 100	16, 28, 51, 75	0
1	M	130/130 (100%)	-0.32	1 (0%) 82 80	14, 29, 56, 83	0
1	P	130/130 (100%)	-0.44	1 (0%) 82 80	14, 26, 55, 76	0
2	B	132/136 (97%)	0.39	7 (5%) 32 28	19, 40, 105, 165	0
2	E	132/136 (97%)	0.09	9 (6%) 23 20	16, 31, 103, 154	0
2	H	132/136 (97%)	0.31	8 (6%) 27 23	23, 40, 101, 184	0
2	K	132/136 (97%)	-0.03	2 (1%) 72 68	15, 30, 85, 188	0
2	N	132/136 (97%)	0.30	7 (5%) 32 28	16, 39, 114, 167	0
2	Q	132/136 (97%)	0.05	8 (6%) 27 23	14, 30, 96, 184	0
3	C	101/102 (99%)	-0.17	1 (0%) 79 76	16, 29, 58, 78	0
3	F	101/102 (99%)	-0.02	0 100 100	19, 33, 62, 84	0
3	I	101/102 (99%)	-0.20	1 (0%) 79 76	10, 30, 62, 99	0
3	L	101/102 (99%)	0.07	2 (1%) 65 61	21, 34, 61, 104	0
3	O	101/102 (99%)	-0.29	0 100 100	17, 29, 51, 78	0
3	R	101/102 (99%)	-0.15	0 100 100	15, 30, 61, 82	0
All	All	2178/2208 (98%)	-0.09	47 (2%) 62 58	9, 31, 72, 188	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	K	3305	MET	4.4
2	E	1279	ARG	4.4
2	E	1305	MET	4.2

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Mol	Chain	Res	Type	RSRZ
2	Q	5305	MET	4.2
3	L	3474	GLU	3.8
2	H	2258	LYS	3.8
2	H	2305	MET	3.8
2	Q	5279	ARG	3.8
2	B	305	MET	3.7
3	L	3402	SER	3.3
2	N	4305	MET	3.1
2	B	309	GLU	2.9
3	C	452	GLU	2.9
3	I	2452	GLU	2.9
2	N	4236	ASP	2.8
2	E	1205	VAL	2.6
2	E	1309	GLU	2.6
2	N	4309	GLU	2.6
2	N	4284	ARG	2.6
2	H	2308	GLU	2.6
2	Q	5309	GLU	2.6
2	E	1307	THR	2.6
2	B	236	ASP	2.5
2	H	2205	VAL	2.5
2	E	1276	GLU	2.5
2	B	284	ARG	2.5
2	H	2279	ARG	2.5
2	Q	5258	LYS	2.4
1	P	5095	ARG	2.4
2	E	1223	TRP	2.4
2	H	2284	ARG	2.3
2	E	1304	ASP	2.3
2	Q	5205	VAL	2.3
2	N	4303	GLU	2.2
2	Q	5207	LYS	2.2
2	B	288	GLU	2.2
2	E	1284	ARG	2.2
2	N	4276	GLU	2.2
2	Q	5223	TRP	2.2
2	Q	5304	ASP	2.1
1	M	4095	ARG	2.1
2	B	258	LYS	2.1
2	H	2303	GLU	2.1
2	N	4307	THR	2.1
2	K	3284	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	205	VAL	2.0
2	H	2278	ARG	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.