



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 17, 2026 – 06:26 PM UTC

PDB ID : 1VH1 / pdb_00001vh1
Title : Crystal structure of CMP-KDO synthetase
Authors : Structural GenomiX
Deposited on : 2003-12-01
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

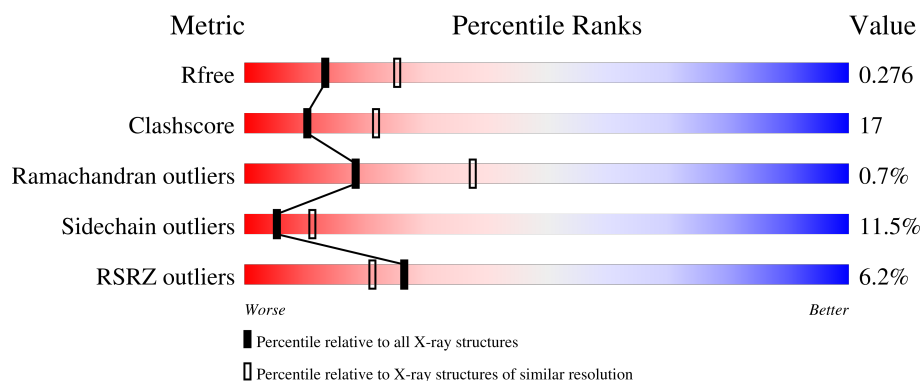
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	256	4% 61% 26% 5% 7%
1	B	256	6% 50% 27% 9% 12%
1	C	256	7% 63% 23% 5% 9%
1	D	256	4% 58% 30% 6% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7321 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 3-deoxy-manno-octulosonate cytidyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	239	Total	C	N	O	S	Se	0	0	0
			1826	1157	324	337	2	6			
1	B	224	Total	C	N	O	S	Se	0	0	0
			1729	1096	310	315	2	6			
1	C	233	Total	C	N	O	S	Se	0	0	0
			1782	1133	313	328	2	6			
1	D	241	Total	C	N	O	S	Se	0	0	0
			1828	1161	321	338	2	6			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	cloning artifact	UNP P04951
A	29	MSE	MET	modified residue	UNP P04951
A	67	MSE	MET	modified residue	UNP P04951
A	103	MSE	MET	modified residue	UNP P04951
A	123	MSE	MET	modified residue	UNP P04951
A	208	MSE	MET	modified residue	UNP P04951
A	247	MSE	MET	modified residue	UNP P04951
A	249	GLY	-	cloning artifact	UNP P04951
A	250	SER	-	cloning artifact	UNP P04951
A	251	HIS	-	cloning artifact	UNP P04951
A	252	HIS	-	cloning artifact	UNP P04951
A	253	HIS	-	cloning artifact	UNP P04951
A	254	HIS	-	cloning artifact	UNP P04951
A	255	HIS	-	cloning artifact	UNP P04951
A	256	HIS	-	cloning artifact	UNP P04951
B	1	MSE	-	cloning artifact	UNP P04951
B	29	MSE	MET	modified residue	UNP P04951
B	67	MSE	MET	modified residue	UNP P04951
B	103	MSE	MET	modified residue	UNP P04951
B	123	MSE	MET	modified residue	UNP P04951
B	208	MSE	MET	modified residue	UNP P04951

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Chain	Residue	Modelled	Actual	Comment	Reference
B	247	MSE	MET	modified residue	UNP P04951
B	249	GLY	-	cloning artifact	UNP P04951
B	250	SER	-	cloning artifact	UNP P04951
B	251	HIS	-	cloning artifact	UNP P04951
B	252	HIS	-	cloning artifact	UNP P04951
B	253	HIS	-	cloning artifact	UNP P04951
B	254	HIS	-	cloning artifact	UNP P04951
B	255	HIS	-	cloning artifact	UNP P04951
B	256	HIS	-	cloning artifact	UNP P04951
C	1	MSE	-	cloning artifact	UNP P04951
C	29	MSE	MET	modified residue	UNP P04951
C	67	MSE	MET	modified residue	UNP P04951
C	103	MSE	MET	modified residue	UNP P04951
C	123	MSE	MET	modified residue	UNP P04951
C	208	MSE	MET	modified residue	UNP P04951
C	247	MSE	MET	modified residue	UNP P04951
C	249	GLY	-	cloning artifact	UNP P04951
C	250	SER	-	cloning artifact	UNP P04951
C	251	HIS	-	cloning artifact	UNP P04951
C	252	HIS	-	cloning artifact	UNP P04951
C	253	HIS	-	cloning artifact	UNP P04951
C	254	HIS	-	cloning artifact	UNP P04951
C	255	HIS	-	cloning artifact	UNP P04951
C	256	HIS	-	cloning artifact	UNP P04951
D	1	MSE	-	cloning artifact	UNP P04951
D	29	MSE	MET	modified residue	UNP P04951
D	67	MSE	MET	modified residue	UNP P04951
D	103	MSE	MET	modified residue	UNP P04951
D	123	MSE	MET	modified residue	UNP P04951
D	208	MSE	MET	modified residue	UNP P04951
D	247	MSE	MET	modified residue	UNP P04951
D	249	GLY	-	cloning artifact	UNP P04951
D	250	SER	-	cloning artifact	UNP P04951
D	251	HIS	-	cloning artifact	UNP P04951
D	252	HIS	-	cloning artifact	UNP P04951
D	253	HIS	-	cloning artifact	UNP P04951
D	254	HIS	-	cloning artifact	UNP P04951
D	255	HIS	-	cloning artifact	UNP P04951
D	256	HIS	-	cloning artifact	UNP P04951

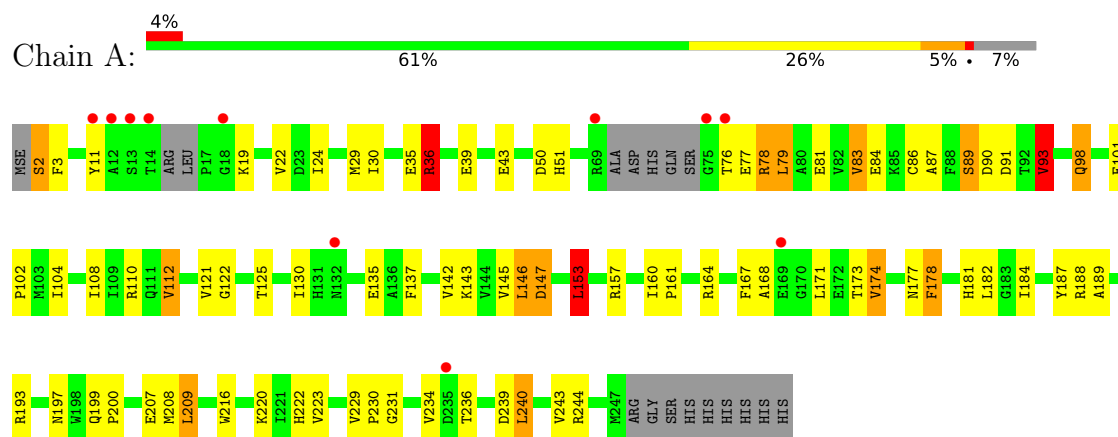
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	45	Total 45	O 45	0	0
2	B	34	Total 34	O 34	0	0
2	C	42	Total 42	O 42	0	0
2	D	35	Total 35	O 35	0	0

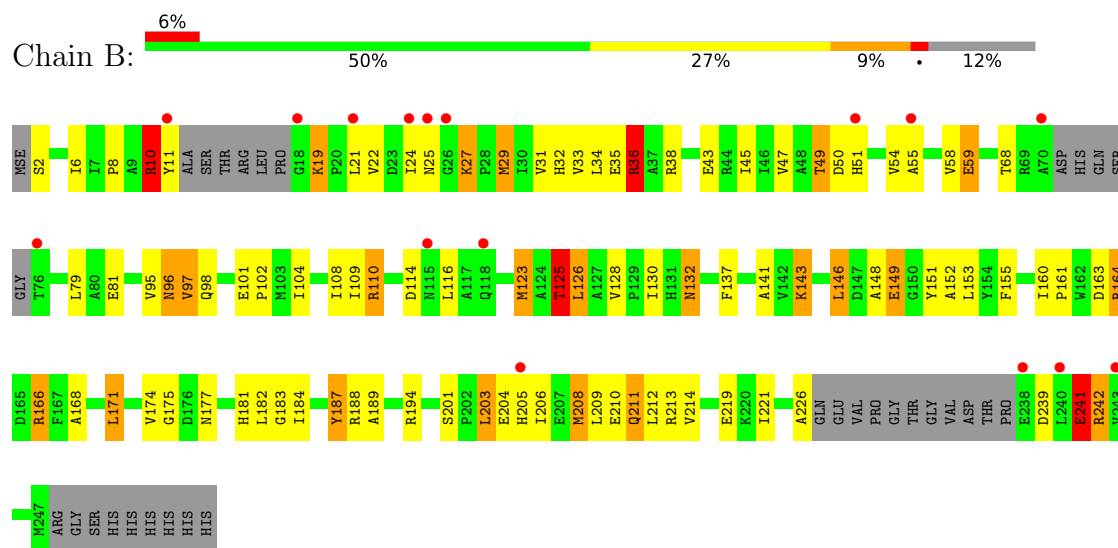
3 Residue-property plots

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.

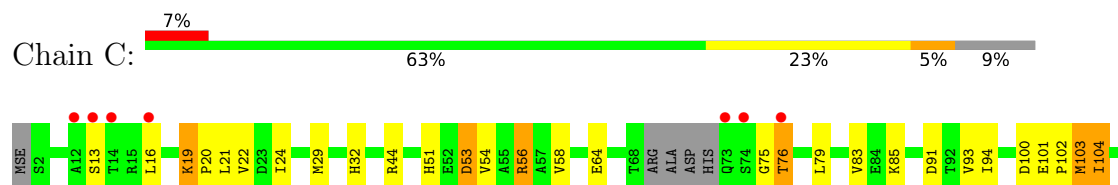
- Molecule 1: 3-deoxy-manno-octulosonate cytidyltransferase

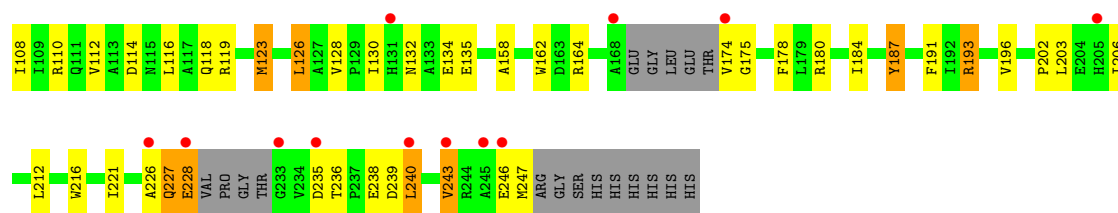


- Molecule 1: 3-deoxy-manno-octulosonate cytidyltransferase

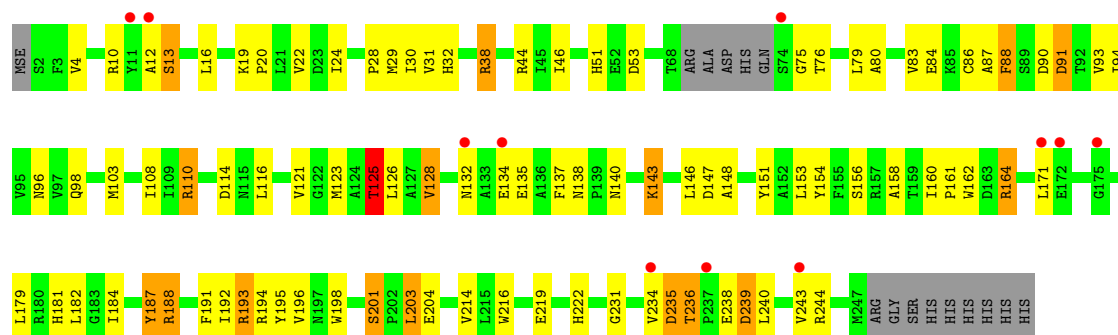


- Molecule 1: 3-deoxy-manno-octulosonate cytidyltransferase





● Molecule 1: 3-deoxy-manno-octulosonate cytidyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	51.59Å 130.81Å 159.08Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.92 – 2.60 19.92 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.92-2.60) 99.7 (19.92-2.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.88 (at 2.59Å)	Xtriage
Refinement program	REFMAC 4.0	Depositor
R, R_{free}	0.240 , 0.302 0.220 , 0.276	Depositor DCC
R_{free} test set	1718 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.304	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 61.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7321	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% 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	0.78	0/1856	1.43	16/2517 (0.6%)
1	B	0.79	0/1755	1.39	11/2374 (0.5%)
1	C	0.79	0/1810	1.41	9/2453 (0.4%)
1	D	0.79	0/1859	1.46	21/2525 (0.8%)
All	All	0.79	0/7280	1.43	57/9869 (0.6%)

There are no bond length outliers.

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	38	ARG	CD-NE-CZ	11.71	140.79	124.40
1	C	193	ARG	CD-NE-CZ	10.12	138.58	124.40
1	A	78	ARG	CD-NE-CZ	9.48	137.67	124.40
1	A	178	PHE	CA-CB-CG	-7.65	106.15	113.80
1	B	210	GLU	CA-C-N	7.35	130.86	120.28
1	B	210	GLU	C-N-CA	7.35	130.86	120.28
1	D	91	ASP	CA-CB-CG	-7.33	105.27	112.60
1	C	187	TYR	CA-CB-CG	7.00	126.49	113.90
1	B	36	ARG	CD-NE-CZ	6.93	134.10	124.40
1	A	36	ARG	CB-CG-CD	6.50	126.26	111.30
1	D	114	ASP	CA-CB-CG	6.49	119.09	112.60
1	B	241	GLU	N-CA-C	6.47	120.07	109.85
1	A	231	GLY	N-CA-C	-6.45	105.23	112.33
1	A	147	ASP	CA-CB-CG	6.34	118.94	112.60
1	C	238	GLU	CA-C-N	6.24	128.64	120.28
1	C	238	GLU	C-N-CA	6.24	128.64	120.28
1	B	155	PHE	CA-CB-CG	6.17	119.97	113.80
1	C	110	ARG	CD-NE-CZ	6.15	133.00	124.40
1	D	188	ARG	NE-CZ-NH1	-6.08	115.42	121.50
1	B	19	LYS	N-CA-C	6.08	121.90	113.45
1	D	164	ARG	N-CA-C	6.06	117.88	111.28
1	D	110	ARG	CA-CB-CG	6.00	126.09	114.10
1	A	36	ARG	CD-NE-CZ	-5.90	116.14	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	32	HIS	CA-CB-CG	5.89	119.69	113.80
1	D	244	ARG	CD-NE-CZ	5.88	132.64	124.40
1	A	77	GLU	N-CA-C	-5.79	105.11	111.82
1	D	147	ASP	CA-CB-CG	5.78	118.38	112.60
1	D	235	ASP	N-CA-C	-5.78	107.47	114.75
1	D	88	PHE	CA-CB-CG	5.70	119.50	113.80
1	D	90	ASP	N-CA-C	5.65	117.89	111.11
1	A	93	VAL	N-CA-CB	5.64	116.68	110.53
1	A	112	VAL	N-CA-CB	5.64	117.15	110.55
1	B	177	ASN	CA-CB-CG	-5.60	107.00	112.60
1	A	98	GLN	N-CA-C	5.59	118.34	109.96
1	C	53	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	19	LYS	N-CA-C	5.46	121.89	109.81
1	B	125	THR	N-CA-CB	5.46	119.83	110.65
1	D	239	ASP	CA-CB-CG	5.37	117.97	112.60
1	D	203	LEU	CA-C-N	5.31	128.79	120.82
1	D	203	LEU	C-N-CA	5.31	128.79	120.82
1	D	193	ARG	CA-CB-CG	5.30	124.70	114.10
1	B	10	ARG	NE-CZ-NH1	-5.21	116.29	121.50
1	D	164	ARG	CA-CB-CG	5.20	124.50	114.10
1	C	246	GLU	N-CA-C	-5.19	108.21	114.75
1	B	168	ALA	N-CA-C	-5.18	105.72	111.36
1	A	36	ARG	CA-CB-CG	5.16	124.41	114.10
1	B	132	ASN	CA-CB-CG	5.13	117.73	112.60
1	A	11	TYR	N-CA-C	-5.12	108.78	114.62
1	A	153	LEU	N-CA-C	-5.11	105.34	112.45
1	D	204	GLU	CA-CB-CG	5.10	124.29	114.10
1	A	229	VAL	CA-C-N	5.08	125.32	119.83
1	A	229	VAL	C-N-CA	5.08	125.32	119.83
1	D	231	GLY	N-CA-C	-5.06	105.61	112.14
1	C	91	ASP	CA-CB-CG	-5.05	107.55	112.60
1	D	110	ARG	CB-CG-CD	5.04	122.88	111.30
1	D	125	THR	N-CA-CB	5.02	119.70	111.31
1	C	56	ARG	CD-NE-CZ	-5.01	117.39	124.40

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	1826	0	1785	48	0
1	B	1729	0	1693	81	0
1	C	1782	0	1741	55	0
1	D	1828	0	1786	65	0
2	A	45	0	0	2	0
2	B	34	0	0	2	0
2	C	42	0	0	3	0
2	D	35	0	0	5	0
All	All	7321	0	7005	241	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 17.

All (241) 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:C:103:MSE:HG3	1:C:247:MSE:HE2	1.46	0.97
1:B:49:THR:HG21	1:B:54:VAL:HB	1.54	0.89
1:D:236:THR:HG22	1:D:239:ASP:H	1.37	0.88
1:B:125:THR:HG21	1:B:181:HIS:HE1	1.40	0.87
1:A:29:MSE:HG3	1:A:102:PRO:HG3	1.57	0.86
1:B:209:LEU:HD22	1:B:211:GLN:HE21	1.36	0.86
1:C:102:PRO:HG2	1:C:247:MSE:HE1	1.55	0.84
1:D:125:THR:HG21	1:D:181:HIS:HE1	1.44	0.83
1:C:243:VAL:HG13	1:C:247:MSE:HE3	1.61	0.82
1:B:123:MSE:HE3	1:B:221:ILE:HG12	1.61	0.80
1:B:108:ILE:HD12	1:B:126:LEU:HD22	1.61	0.80
1:B:36:ARG:HH11	1:B:36:ARG:HG2	1.50	0.77
1:B:209:LEU:HD22	1:B:211:GLN:NE2	1.99	0.76
1:C:93:VAL:HG13	1:C:116:LEU:HD23	1.66	0.76
1:B:110:ARG:HH11	1:B:110:ARG:HB3	1.50	0.74
1:B:8:PRO:HG3	1:B:96:ASN:HD21	1.52	0.73
1:D:236:THR:CG2	1:D:239:ASP:H	2.01	0.73
1:B:125:THR:HG21	1:B:181:HIS:CE1	2.25	0.72
1:B:123:MSE:HE2	1:B:214:VAL:HG21	1.71	0.72
1:D:79:LEU:HD22	1:D:96:ASN:HD22	1.55	0.71
1:A:220:LYS:HD3	2:A:257:HOH:O	1.92	0.70
1:D:236:THR:HG22	1:D:239:ASP:N	2.07	0.69
1:B:126:LEU:HD11	1:B:226:ALA:HB2	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:ARG:HG3	1:A:104:ILE:O	1.92	0.68
1:B:35:GLU:HB2	1:B:36:ARG:NH1	2.08	0.67
1:B:109:ILE:HA	1:B:184:ILE:HD11	1.76	0.67
1:D:132:ASN:OD1	1:D:135:GLU:HB2	1.94	0.67
1:C:19:LYS:HB2	1:C:20:PRO:CD	2.25	0.67
1:D:79:LEU:HD22	1:D:96:ASN:ND2	2.10	0.66
1:B:203:LEU:HD13	1:B:212:LEU:HD13	1.77	0.66
1:B:205:HIS:HA	1:B:208:MSE:HE3	1.78	0.66
1:B:125:THR:HG22	1:B:184:ILE:O	1.95	0.65
1:D:236:THR:HG23	1:D:238:GLU:H	1.62	0.65
1:A:24:ILE:HD13	1:A:243:VAL:HG11	1.78	0.65
1:C:19:LYS:HB2	1:C:20:PRO:HD3	1.79	0.65
1:A:240:LEU:HD13	1:A:244:ARG:NH2	2.12	0.65
1:B:104:ILE:HD11	1:B:108:ILE:HD11	1.78	0.65
1:B:208:MSE:CE	1:B:208:MSE:HA	2.26	0.65
1:B:114:ASP:HB3	2:B:268:HOH:O	1.97	0.64
1:C:174:VAL:HG22	1:C:175:GLY:H	1.60	0.64
1:A:208:MSE:HG3	1:B:164:ARG:NH2	2.13	0.64
1:A:240:LEU:HD13	1:A:244:ARG:HH21	1.62	0.64
1:A:137:PHE:CD1	1:A:171:LEU:HD13	2.33	0.64
1:A:147:ASP:HB3	1:A:153:LEU:HD13	1.80	0.63
1:B:55:ALA:O	1:B:59:GLU:HB2	1.99	0.63
1:C:13:SER:HB3	1:C:16:LEU:O	1.99	0.62
1:A:50:ASP:OD1	1:A:51:HIS:ND1	2.33	0.62
1:C:21:LEU:HD11	1:C:53:ASP:HB2	1.80	0.62
1:D:125:THR:HG21	1:D:181:HIS:CE1	2.31	0.61
1:B:49:THR:HG21	1:B:54:VAL:CB	2.30	0.61
1:B:32:HIS:O	1:B:36:ARG:NH1	2.34	0.60
1:C:132:ASN:HD21	1:C:134:GLU:HB3	1.66	0.60
1:A:121:VAL:HG22	1:A:122:GLY:H	1.67	0.60
1:B:242:ARG:HH11	1:B:242:ARG:HB3	1.65	0.60
1:C:103:MSE:CG	1:C:247:MSE:HE2	2.27	0.60
1:B:96:ASN:O	1:B:97:VAL:HB	2.00	0.60
1:A:35:GLU:O	1:A:39:GLU:HG3	2.02	0.60
1:B:24:ILE:HB	1:B:32:HIS:HE1	1.66	0.59
1:A:182:LEU:HD13	1:A:230:PRO:HG2	1.84	0.59
1:D:187:TYR:CD2	1:D:192:ILE:HD11	2.38	0.59
1:B:31:VAL:O	1:B:35:GLU:HG3	2.03	0.58
1:B:19:LYS:HA	1:B:22:VAL:HG23	1.86	0.58
1:B:95:VAL:HG12	1:B:97:VAL:HG23	1.84	0.58
1:C:44:ARG:NH2	1:C:64:GLU:OE2	2.28	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:137:PHE:CE2	1:D:171:LEU:HD23	2.38	0.58
1:A:208:MSE:HG3	1:B:164:ARG:HH21	1.67	0.58
1:B:10:ARG:O	1:B:11:TYR:HB2	2.04	0.58
1:D:154:TYR:CE1	1:D:156:SER:HB2	2.38	0.58
1:D:188:ARG:NH1	2:D:259:HOH:O	2.36	0.58
1:C:128:VAL:HG12	1:C:226:ALA:O	2.04	0.58
1:D:128:VAL:HG23	1:D:182:LEU:HD11	1.86	0.58
1:D:192:ILE:O	1:D:196:VAL:HG13	2.03	0.58
1:A:234:VAL:CG2	1:A:243:VAL:HG21	2.34	0.57
1:B:24:ILE:HB	1:B:32:HIS:CE1	2.39	0.57
1:D:29:MSE:HE1	1:D:234:VAL:HG11	1.87	0.57
1:C:112:VAL:HG22	1:C:126:LEU:HD23	1.87	0.56
1:A:234:VAL:HG22	1:A:243:VAL:HG21	1.87	0.56
1:B:35:GLU:HB2	1:B:36:ARG:HH12	1.68	0.56
1:B:38:ARG:HA	1:B:45:ILE:HD11	1.87	0.56
1:C:21:LEU:CD1	1:C:53:ASP:HB2	2.35	0.56
1:B:125:THR:CG2	1:B:181:HIS:HE1	2.17	0.56
1:B:239:ASP:O	1:B:241:GLU:HG3	2.06	0.56
1:B:34:LEU:HD21	1:B:38:ARG:HH21	1.71	0.56
1:A:193:ARG:O	1:A:197:ASN:HB2	2.06	0.56
1:D:46:ILE:HD12	1:D:88:PHE:HZ	1.70	0.55
1:B:137:PHE:CE2	1:B:171:LEU:HG	2.41	0.55
1:B:201:SER:O	1:B:204:GLU:HG2	2.07	0.55
1:C:93:VAL:HG13	1:C:116:LEU:CD2	2.36	0.54
1:A:108:ILE:HD13	1:A:230:PRO:HG3	1.89	0.54
1:B:10:ARG:O	1:B:11:TYR:CB	2.55	0.54
1:C:51:HIS:HB3	1:C:53:ASP:OD1	2.07	0.54
1:D:236:THR:HG23	1:D:238:GLU:N	2.22	0.54
1:D:121:VAL:HG21	1:D:151:TYR:HE2	1.72	0.54
1:A:130:ILE:HG23	1:A:135:GLU:OE2	2.08	0.53
1:B:194:ARG:NH2	1:B:219:GLU:OE2	2.42	0.53
1:C:54:VAL:O	1:C:58:VAL:HG23	2.08	0.53
1:D:91:ASP:HB2	2:D:259:HOH:O	2.09	0.53
1:C:226:ALA:O	1:C:228:GLU:HG2	2.08	0.53
1:B:33:VAL:HG22	1:B:102:PRO:HA	1.91	0.53
1:C:132:ASN:ND2	1:C:134:GLU:HB3	2.24	0.53
1:D:13:SER:HB3	1:D:16:LEU:O	2.09	0.53
1:B:123:MSE:HG3	1:B:187:TYR:CD1	2.44	0.52
1:A:98:GLN:HB2	1:A:101:GLU:OE2	2.09	0.52
1:B:203:LEU:HD13	1:B:212:LEU:HB3	1.92	0.52
1:C:76:THR:HG22	2:C:263:HOH:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:VAL:CG1	1:C:240:LEU:HD11	2.41	0.51
1:D:108:ILE:HB	1:D:126:LEU:CD1	2.41	0.51
1:C:162:TRP:HB2	1:D:158:ALA:HB2	1.93	0.51
1:B:34:LEU:HD21	1:B:38:ARG:NH2	2.26	0.51
1:C:101:GLU:O	1:C:104:ILE:HG22	2.10	0.51
1:B:98:GLN:NE2	1:B:183:GLY:HA3	2.26	0.50
1:B:130:ILE:HG22	1:B:132:ASN:H	1.74	0.50
1:B:141:ALA:O	1:B:143:LYS:HE2	2.11	0.50
1:C:130:ILE:HG23	1:C:135:GLU:OE2	2.10	0.50
1:B:208:MSE:HE3	1:B:208:MSE:HA	1.92	0.50
1:B:34:LEU:HD12	1:B:45:ILE:HG21	1.94	0.50
1:B:123:MSE:CE	1:B:214:VAL:HG21	2.40	0.50
1:D:214:VAL:HG13	1:D:219:GLU:HB2	1.94	0.50
1:B:47:VAL:HG11	1:B:58:VAL:HG21	1.94	0.50
1:A:89:SER:HB3	1:A:91:ASP:OD2	2.12	0.50
1:B:19:LYS:HB2	1:B:29:MSE:CE	2.42	0.50
1:C:79:LEU:O	1:C:83:VAL:HG23	2.12	0.50
1:B:146:LEU:HD12	1:B:152:ALA:HA	1.93	0.50
1:B:123:MSE:HE3	1:B:221:ILE:CG1	2.38	0.49
1:B:242:ARG:HB3	1:B:242:ARG:NH1	2.26	0.49
1:C:51:HIS:HA	2:C:272:HOH:O	2.12	0.49
1:C:112:VAL:CG2	1:C:126:LEU:HD23	2.43	0.49
1:D:80:ALA:HB2	1:D:196:VAL:HG11	1.94	0.49
1:D:98:GLN:HG2	2:D:276:HOH:O	2.12	0.49
1:B:2:SER:HA	1:B:43:GLU:OE2	2.12	0.49
1:D:160:ILE:HA	1:D:161:PRO:C	2.36	0.49
1:D:198:TRP:HH2	1:D:219:GLU:HG3	1.77	0.49
1:B:104:ILE:CD1	1:B:108:ILE:HD11	2.43	0.49
1:A:177:ASN:ND2	1:B:206:ILE:HD13	2.28	0.48
1:A:160:ILE:HA	1:A:161:PRO:C	2.38	0.48
1:C:203:LEU:HG	1:C:212:LEU:HD13	1.95	0.48
1:A:89:SER:O	1:A:189:ALA:HB3	2.13	0.48
1:D:22:VAL:HG11	1:D:240:LEU:CD1	2.44	0.48
1:D:28:PRO:HG2	1:D:31:VAL:CG2	2.43	0.48
1:D:201:SER:HB2	1:D:216:TRP:CE3	2.50	0.47
1:B:203:LEU:CD1	1:B:212:LEU:HD13	2.42	0.47
1:C:130:ILE:HD12	1:C:178:PHE:HB3	1.95	0.47
1:C:236:THR:O	1:C:239:ASP:HB2	2.15	0.47
1:D:143:LYS:HE2	1:D:143:LYS:N	2.30	0.47
1:A:81:GLU:O	1:A:84:GLU:HB3	2.15	0.47
1:C:103:MSE:HG3	1:C:247:MSE:CE	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ASP:O	1:C:118:GLN:HG3	2.15	0.47
1:D:125:THR:HG22	1:D:184:ILE:O	2.14	0.47
1:B:110:ARG:HH11	1:B:110:ARG:CB	2.22	0.47
1:D:4:VAL:HG22	1:D:44:ARG:HB3	1.97	0.47
1:A:36:ARG:HH11	1:A:36:ARG:HD2	1.54	0.46
1:C:202:PRO:O	1:C:206:ILE:HD12	2.15	0.46
1:D:28:PRO:HG2	1:D:31:VAL:HG23	1.97	0.46
1:A:145:VAL:HG22	1:A:161:PRO:HD3	1.96	0.46
1:A:146:LEU:HD11	1:A:223:VAL:HB	1.98	0.46
1:B:36:ARG:HG2	1:B:36:ARG:NH1	2.19	0.46
1:A:216:TRP:CE2	1:B:148:ALA:HB2	2.50	0.46
1:C:226:ALA:HB1	1:C:228:GLU:OE1	2.15	0.46
1:D:19:LYS:NZ	1:D:235:ASP:HB3	2.30	0.45
1:C:19:LYS:N	1:C:20:PRO:HD2	2.31	0.45
1:C:164:ARG:NH2	1:D:140:ASN:OD1	2.43	0.45
1:C:13:SER:OG	1:C:235:ASP:OD2	2.26	0.45
1:A:90:ASP:O	1:A:188:ARG:HB3	2.17	0.45
1:A:36:ARG:HH21	1:A:39:GLU:CD	2.24	0.45
1:B:104:ILE:CG1	1:B:108:ILE:HD11	2.47	0.45
1:A:157:ARG:HH11	1:A:157:ARG:HD2	1.59	0.44
1:A:207:GLU:O	1:A:208:MSE:HB2	2.17	0.44
1:C:24:ILE:O	1:C:32:HIS:HE1	2.00	0.44
1:D:123:MSE:HG2	1:D:187:TYR:HD1	1.82	0.44
1:C:24:ILE:O	1:C:32:HIS:CE1	2.71	0.44
1:D:236:THR:HG22	1:D:239:ASP:CB	2.47	0.44
1:C:22:VAL:HG11	1:C:240:LEU:HD11	1.99	0.44
1:C:102:PRO:CG	1:C:247:MSE:HE1	2.37	0.44
1:B:36:ARG:HA	1:B:36:ARG:HD3	1.77	0.44
1:A:24:ILE:HD13	1:A:243:VAL:CG1	2.45	0.44
1:D:29:MSE:HE1	1:D:234:VAL:CG1	2.47	0.44
1:D:132:ASN:OD1	1:D:135:GLU:N	2.43	0.44
1:D:195:TYR:C	1:D:195:TYR:CD2	2.95	0.44
1:A:3:PHE:HB2	1:A:93:VAL:HG22	2.00	0.44
1:B:49:THR:HG22	1:B:50:ASP:H	1.82	0.43
1:B:126:LEU:HD23	1:B:182:LEU:HD12	2.00	0.43
1:C:103:MSE:SE	1:C:243:VAL:HG22	2.68	0.43
1:B:24:ILE:HD12	1:B:29:MSE:HA	1.99	0.43
1:C:19:LYS:NZ	1:C:100:ASP:OD1	2.51	0.43
1:C:19:LYS:CB	1:C:20:PRO:CD	2.92	0.43
1:B:204:GLU:OE1	1:B:213:ARG:HB2	2.18	0.43
1:D:51:HIS:HB3	1:D:53:ASP:OD1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:THR:O	1:A:239:ASP:N	2.49	0.43
1:C:130:ILE:HG12	1:C:180:ARG:HB2	2.00	0.43
1:A:125:THR:OG1	1:A:181:HIS:HE1	2.02	0.43
1:B:160:ILE:HA	1:B:161:PRO:C	2.43	0.43
1:D:143:LYS:HA	1:D:179:LEU:O	2.19	0.43
1:C:158:ALA:HB2	1:D:162:TRP:HB2	2.00	0.43
1:D:134:GLU:O	1:D:138:ASN:HB2	2.18	0.43
1:D:83:VAL:HG21	1:D:192:ILE:HG21	2.01	0.43
1:B:6:ILE:HG21	1:B:79:LEU:HG	2.01	0.42
1:B:164:ARG:HG2	2:B:284:HOH:O	2.19	0.42
1:A:2:SER:HB3	1:A:43:GLU:OE2	2.20	0.42
1:B:149:GLU:HB3	1:B:151:TYR:HD1	1.84	0.42
1:D:12:ALA:O	1:D:13:SER:HB2	2.19	0.42
1:D:154:TYR:HE2	1:D:203:LEU:HD21	1.84	0.42
1:A:145:VAL:HG23	1:A:160:ILE:HG13	2.01	0.42
1:B:27:LYS:HB2	1:B:32:HIS:CE1	2.55	0.42
1:D:123:MSE:HE2	1:D:187:TYR:CD1	2.55	0.42
1:D:93:VAL:HG22	1:D:116:LEU:HD12	2.02	0.42
1:C:216:TRP:CE2	1:D:148:ALA:HB2	2.54	0.42
1:D:103:MSE:HE2	1:D:243:VAL:HG22	2.01	0.42
1:D:194:ARG:O	1:D:195:TYR:C	2.62	0.42
1:B:242:ARG:H	1:B:242:ARG:HD2	1.85	0.42
1:D:10:ARG:O	1:D:20:PRO:HD3	2.20	0.42
1:B:27:LYS:HZ3	1:B:27:LYS:HG3	1.72	0.42
1:B:203:LEU:HD13	1:B:212:LEU:CD1	2.47	0.42
1:D:191:PHE:HZ	1:D:214:VAL:HG22	1.85	0.42
1:C:123:MSE:HE2	1:C:221:ILE:CD1	2.50	0.42
1:A:199:GLN:HG2	1:A:200:PRO:HD2	2.02	0.41
1:D:19:LYS:HZ1	1:D:235:ASP:HB3	1.86	0.41
1:A:121:VAL:HG22	1:A:122:GLY:N	2.33	0.41
1:D:19:LYS:N	1:D:20:PRO:HD2	2.35	0.41
1:D:24:ILE:HD11	1:D:29:MSE:HE2	2.02	0.41
1:D:30:ILE:HD12	1:D:30:ILE:HA	1.86	0.41
1:D:86:CYS:O	1:D:87:ALA:C	2.63	0.41
1:A:104:ILE:HD11	1:A:184:ILE:HD12	2.03	0.41
1:B:68:THR:HA	1:B:81:GLU:OE2	2.21	0.41
1:B:188:ARG:O	1:B:189:ALA:C	2.64	0.41
1:C:243:VAL:HG13	1:C:247:MSE:CE	2.40	0.41
1:A:174:VAL:HG22	1:A:178:PHE:CE1	2.56	0.41
1:D:236:THR:HG22	1:D:239:ASP:CG	2.46	0.41
1:A:79:LEU:O	1:A:83:VAL:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:CYS:O	1:A:87:ALA:C	2.63	0.40
1:C:116:LEU:O	1:C:119:ARG:O	2.38	0.40
1:A:222:HIS:HD2	2:A:283:HOH:O	2.05	0.40
1:D:123:MSE:HE2	1:D:187:TYR:CE1	2.56	0.40
1:C:19:LYS:HB3	1:C:29:MSE:CE	2.51	0.40
1:C:75:GLY:HA2	2:C:279:HOH:O	2.22	0.40
1:C:108:ILE:HD13	1:C:108:ILE:HG21	1.90	0.40
1:D:222:HIS:HD2	2:D:267:HOH:O	2.04	0.40
1:A:142:VAL:HG21	1:A:209:LEU:HD11	2.03	0.40
1:A:167:PHE:O	1:A:168:ALA:C	2.62	0.40
1:B:163:ASP:OD2	1:B:166:ARG:HD2	2.22	0.40
1:C:123:MSE:HG3	1:C:191:PHE:CE2	2.56	0.40
1:D:80:ALA:HB3	2:D:278:HOH:O	2.21	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	233/256 (91%)	225 (97%)	8 (3%)	0	100	100
1	B	216/256 (84%)	202 (94%)	11 (5%)	3 (1%)	9	19
1	C	225/256 (88%)	215 (96%)	9 (4%)	1 (0%)	30	51
1	D	237/256 (93%)	230 (97%)	5 (2%)	2 (1%)	16	34
All	All	911/1024 (89%)	872 (96%)	33 (4%)	6 (1%)	18	38

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	227	GLN
1	D	13	SER

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Mol	Chain	Res	Type
1	B	96	ASN
1	B	97	VAL
1	D	75	GLY
1	B	175	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	185/203 (91%)	164 (89%)	21 (11%)	5	11
1	B	174/203 (86%)	144 (83%)	30 (17%)	2	3
1	C	180/203 (89%)	163 (91%)	17 (9%)	8	18
1	D	185/203 (91%)	170 (92%)	15 (8%)	11	24
All	All	724/812 (89%)	641 (88%)	83 (12%)	5	11

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	SER
1	A	22	VAL
1	A	30	ILE
1	A	36	ARG
1	A	76	THR
1	A	78	ARG
1	A	79	LEU
1	A	83	VAL
1	A	89	SER
1	A	93	VAL
1	A	110	ARG
1	A	112	VAL
1	A	143	LYS
1	A	146	LEU
1	A	153	LEU
1	A	164	ARG
1	A	173	THR

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Mol	Chain	Res	Type
1	A	174	VAL
1	A	187	TYR
1	A	209	LEU
1	A	240	LEU
1	B	10	ARG
1	B	21	LEU
1	B	25	ASN
1	B	27	LYS
1	B	29	MSE
1	B	36	ARG
1	B	49	THR
1	B	51	HIS
1	B	59	GLU
1	B	101	GLU
1	B	110	ARG
1	B	116	LEU
1	B	123	MSE
1	B	125	THR
1	B	126	LEU
1	B	128	VAL
1	B	143	LYS
1	B	146	LEU
1	B	149	GLU
1	B	153	LEU
1	B	164	ARG
1	B	166	ARG
1	B	171	LEU
1	B	174	VAL
1	B	187	TYR
1	B	203	LEU
1	B	208	MSE
1	B	211	GLN
1	B	241	GLU
1	B	242	ARG
1	C	19	LYS
1	C	56	ARG
1	C	76	THR
1	C	85	LYS
1	C	94	ILE
1	C	103	MSE
1	C	104	ILE
1	C	123	MSE

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Mol	Chain	Res	Type
1	C	126	LEU
1	C	184	ILE
1	C	187	TYR
1	C	193	ARG
1	C	196	VAL
1	C	227	GLN
1	C	228	GLU
1	C	240	LEU
1	C	243	VAL
1	D	38	ARG
1	D	76	THR
1	D	84	GLU
1	D	94	ILE
1	D	110	ARG
1	D	125	THR
1	D	128	VAL
1	D	143	LYS
1	D	146	LEU
1	D	153	LEU
1	D	164	ARG
1	D	187	TYR
1	D	193	ARG
1	D	201	SER
1	D	236	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	GLN
1	A	181	HIS
1	A	222	HIS
1	A	227	GLN
1	B	96	ASN
1	B	98	GLN
1	B	111	GLN
1	B	115	ASN
1	B	131	HIS
1	B	181	HIS
1	B	211	GLN
1	B	222	HIS
1	C	32	HIS
1	C	96	ASN

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Mol	Chain	Res	Type
1	C	98	GLN
1	C	111	GLN
1	C	120	GLN
1	C	222	HIS
1	D	96	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	233/256 (91%)	0.29	11 (4%)	36 30	51, 64, 94, 120	0
1	B	218/256 (85%)	0.56	16 (7%)	21 17	49, 68, 101, 124	0
1	C	227/256 (88%)	0.34	19 (8%)	17 13	49, 63, 95, 104	0
1	D	235/256 (91%)	0.36	11 (4%)	36 30	50, 68, 99, 111	0
All	All	913/1024 (89%)	0.39	57 (6%)	26 21	49, 66, 98, 124	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	ALA	4.4
1	C	73	GLN	4.2
1	B	18	GLY	4.1
1	B	238	GLU	4.1
1	C	245	ALA	3.9
1	B	70	ALA	3.6
1	C	174	VAL	3.6
1	B	26	GLY	3.5
1	D	171	LEU	3.5
1	A	14	THR	3.3
1	C	226	ALA	3.3
1	B	51	HIS	3.3
1	D	132	ASN	3.2
1	C	74	SER	3.2
1	C	233	GLY	3.1
1	C	228	GLU	3.1
1	C	13	SER	3.0
1	D	12	ALA	3.0
1	A	11	TYR	2.9
1	A	75	GLY	2.8
1	B	24	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	76	THR	2.8
1	B	240	LEU	2.6
1	A	13	SER	2.6
1	A	235	ASP	2.6
1	A	169	GLU	2.6
1	B	21	LEU	2.5
1	A	76	THR	2.5
1	D	74	SER	2.5
1	D	172	GLU	2.5
1	D	11	TYR	2.5
1	B	205	HIS	2.4
1	C	14	THR	2.4
1	C	16	LEU	2.4
1	B	25	ASN	2.4
1	D	234	VAL	2.3
1	D	237	PRO	2.3
1	A	18	GLY	2.3
1	D	175	GLY	2.3
1	C	205	HIS	2.3
1	D	134	GLU	2.2
1	C	235	ASP	2.2
1	B	118	GLN	2.2
1	C	246	GLU	2.2
1	C	243	VAL	2.2
1	C	168	ALA	2.2
1	D	243	VAL	2.2
1	A	69	ARG	2.1
1	C	131	HIS	2.1
1	C	12	ALA	2.1
1	C	76	THR	2.1
1	B	11	TYR	2.1
1	B	243	VAL	2.1
1	B	55	ALA	2.0
1	C	240	LEU	2.0
1	A	132	ASN	2.0
1	B	115	ASN	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 [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.