



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:05 PM UTC

PDB ID : 3NYW / pdb_00003nyw
Title : Crystal Structure of a betaketoacyl-[ACP] reductase (FabG) from Bacteroides thetaiotaomicron
Authors : Satyanarayana, L.; Burley, S.K.; Swaminathan, S.; New York SGX Research Center for Structural Genomics (NYSGXRC)
Deposited on : 2010-07-15
Resolution : 2.16 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

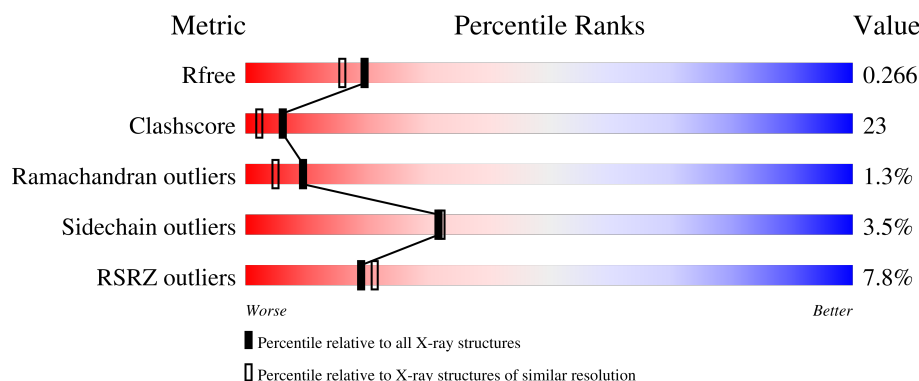
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.16 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	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (2.16-2.16)

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	250	
1	B	250	
1	C	250	
1	D	250	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7143 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 oxidoreductase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	232	Total	C	N	O	S	Se	0	0	0
			1779	1131	298	338	4	8			
1	B	220	Total	C	N	O	S	Se	0	0	0
			1694	1079	285	318	4	8			
1	C	228	Total	C	N	O	S	Se	0	0	0
			1755	1119	293	331	4	8			
1	D	213	Total	C	N	O	S	Se	0	0	0
			1646	1048	278	309	4	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MSE	-	expression tag	UNP Q8A562
A	0	SER	-	expression tag	UNP Q8A562
A	1	LEU	-	expression tag	UNP Q8A562
A	241	GLU	-	expression tag	UNP Q8A562
A	242	GLY	-	expression tag	UNP Q8A562
A	243	HIS	-	expression tag	UNP Q8A562
A	244	HIS	-	expression tag	UNP Q8A562
A	245	HIS	-	expression tag	UNP Q8A562
A	246	HIS	-	expression tag	UNP Q8A562
A	247	HIS	-	expression tag	UNP Q8A562
A	248	HIS	-	expression tag	UNP Q8A562
B	-1	MSE	-	expression tag	UNP Q8A562
B	0	SER	-	expression tag	UNP Q8A562
B	1	LEU	-	expression tag	UNP Q8A562
B	241	GLU	-	expression tag	UNP Q8A562
B	242	GLY	-	expression tag	UNP Q8A562
B	243	HIS	-	expression tag	UNP Q8A562
B	244	HIS	-	expression tag	UNP Q8A562
B	245	HIS	-	expression tag	UNP Q8A562
B	246	HIS	-	expression tag	UNP Q8A562
B	247	HIS	-	expression tag	UNP Q8A562

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Chain	Residue	Modelled	Actual	Comment	Reference
B	248	HIS	-	expression tag	UNP Q8A562
C	-1	MSE	-	expression tag	UNP Q8A562
C	0	SER	-	expression tag	UNP Q8A562
C	1	LEU	-	expression tag	UNP Q8A562
C	241	GLU	-	expression tag	UNP Q8A562
C	242	GLY	-	expression tag	UNP Q8A562
C	243	HIS	-	expression tag	UNP Q8A562
C	244	HIS	-	expression tag	UNP Q8A562
C	245	HIS	-	expression tag	UNP Q8A562
C	246	HIS	-	expression tag	UNP Q8A562
C	247	HIS	-	expression tag	UNP Q8A562
C	248	HIS	-	expression tag	UNP Q8A562
D	-1	MSE	-	expression tag	UNP Q8A562
D	0	SER	-	expression tag	UNP Q8A562
D	1	LEU	-	expression tag	UNP Q8A562
D	241	GLU	-	expression tag	UNP Q8A562
D	242	GLY	-	expression tag	UNP Q8A562
D	243	HIS	-	expression tag	UNP Q8A562
D	244	HIS	-	expression tag	UNP Q8A562
D	245	HIS	-	expression tag	UNP Q8A562
D	246	HIS	-	expression tag	UNP Q8A562
D	247	HIS	-	expression tag	UNP Q8A562
D	248	HIS	-	expression tag	UNP Q8A562

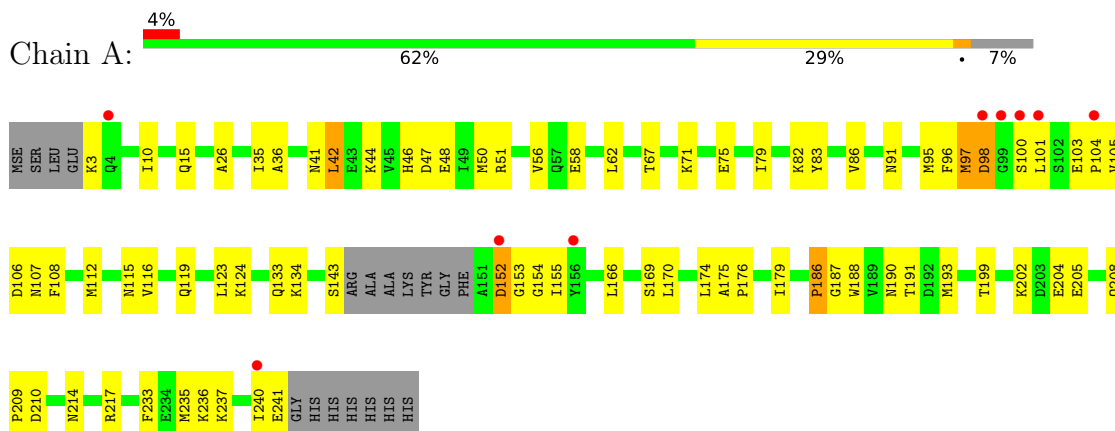
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	104	Total O 104 104	0	0
2	B	48	Total O 48 48	0	0
2	C	88	Total O 88 88	0	0
2	D	29	Total O 29 29	0	0

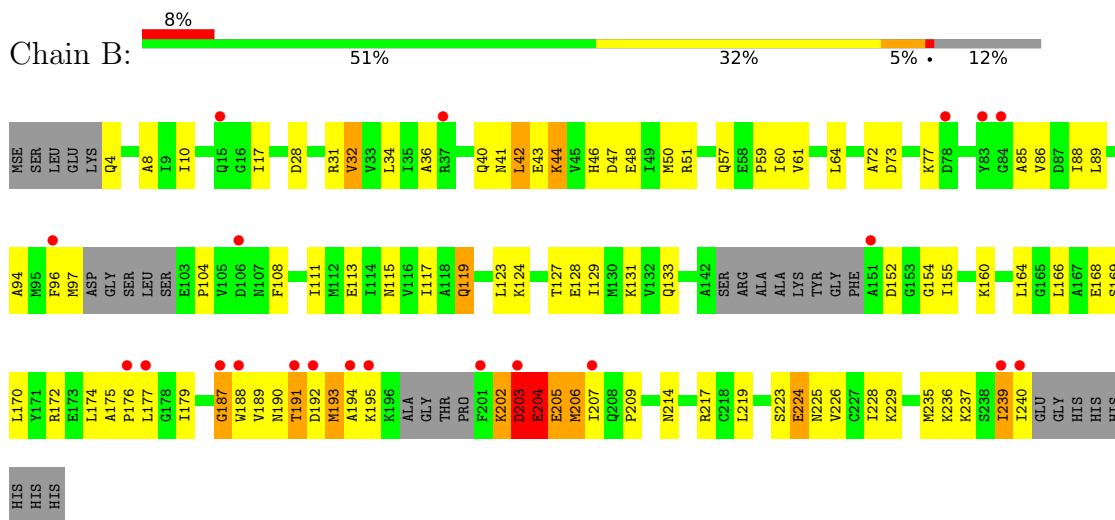
3 Residue-property plots

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.

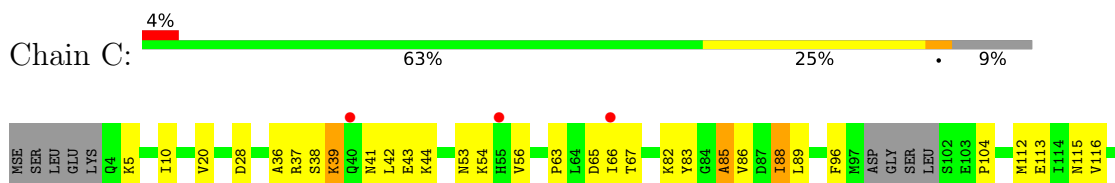
• Molecule 1: Putative oxidoreductase

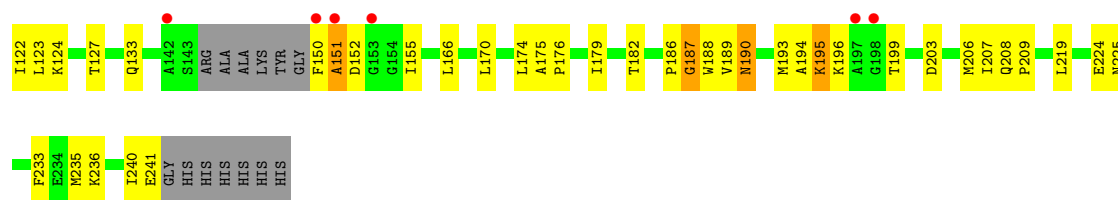


• Molecule 1: Putative oxidoreductase

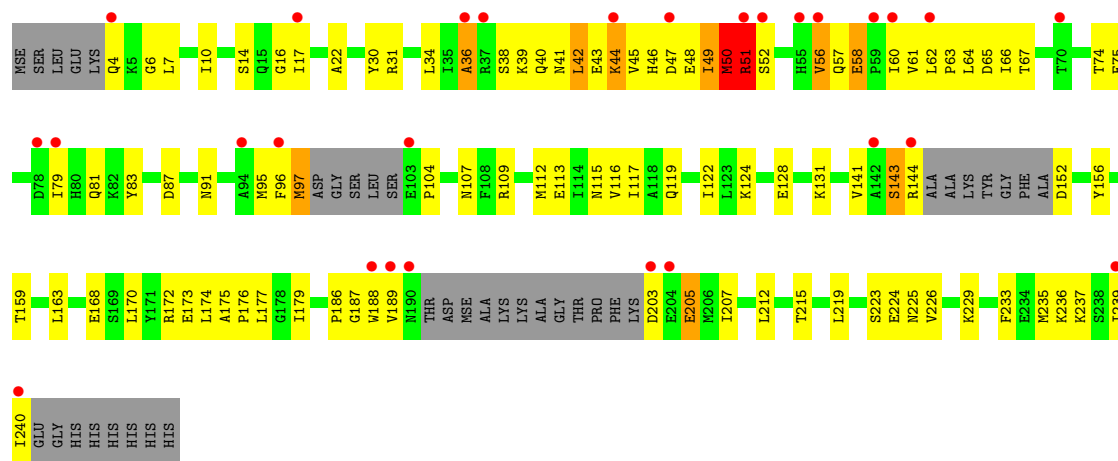


• Molecule 1: Putative oxidoreductase





● Molecule 1: Putative oxidoreductase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	59.88Å 105.72Å 78.83Å 90.00° 98.31° 90.00°	Depositor
Resolution (Å)	45.83 – 2.16 45.83 – 2.16	Depositor EDS
% Data completeness (in resolution range)	92.8 (45.83-2.16) 95.6 (45.83-2.16)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.05Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.236 , 0.263 0.234 , 0.266	Depositor DCC
R_{free} test set	4429 reflections (3.73%)	wwPDB-VP
Wilson B-factor (Å ²)	34.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 35.4	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	0.94	EDS
Total number of atoms	7143	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.04% 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	0.51	0/1793	1.01	5/2406 (0.2%)
1	B	0.41	0/1704	0.96	9/2283 (0.4%)
1	C	0.49	0/1769	0.99	7/2373 (0.3%)
1	D	0.43	0/1657	1.00	6/2223 (0.3%)
All	All	0.46	0/6923	0.99	27/9285 (0.3%)

There are no bond length outliers.

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	50	MSE	CB-CG-SE	-8.74	86.48	112.70
1	D	205	GLU	N-CA-C	-7.80	103.34	113.17
1	D	83	TYR	N-CA-C	7.42	122.05	112.92
1	A	153	GLY	N-CA-C	-7.36	105.06	115.43
1	B	187	GLY	N-CA-C	-6.97	102.79	112.13
1	A	97	MSE	N-CA-C	6.48	117.67	108.54
1	B	203	ASP	N-CA-C	6.21	119.37	108.56
1	D	39	LYS	N-CA-C	-6.01	98.01	110.80
1	C	85	ALA	N-CA-C	6.00	118.69	110.24
1	C	224	GLU	N-CA-C	5.98	119.40	111.75
1	A	187	GLY	N-CA-C	-5.96	101.26	112.64
1	B	195	LYS	N-CA-C	-5.94	98.14	110.80
1	B	206	MSE	N-CA-C	-5.72	101.11	109.63
1	A	67	THR	N-CA-C	-5.69	106.30	113.18
1	C	88	ILE	N-CA-C	5.66	117.98	108.81
1	C	116	VAL	N-CA-C	5.56	116.34	111.56
1	B	85	ALA	N-CA-C	5.49	117.81	110.35
1	D	116	VAL	N-CA-C	5.49	116.28	111.56
1	B	191	THR	N-CA-C	-5.39	101.33	109.85
1	C	187	GLY	N-CA-C	-5.33	102.47	112.64
1	C	38	SER	N-CA-C	5.30	116.89	108.67
1	B	57	GLN	N-CA-C	-5.25	102.52	110.28
1	B	32	VAL	N-CA-C	5.24	116.83	108.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	42	LEU	N-CA-C	-5.21	105.68	111.36
1	C	190	ASN	N-CA-C	5.19	117.55	108.52
1	D	51	ARG	N-CA-C	-5.14	99.84	110.80
1	B	239	ILE	N-CA-C	-5.06	98.82	109.34

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	1779	0	1841	67	0
1	B	1694	0	1758	101	0
1	C	1755	0	1813	75	0
1	D	1646	0	1705	101	0
2	A	104	0	0	8	0
2	B	48	0	0	12	0
2	C	88	0	0	9	0
2	D	29	0	0	8	0
All	All	7143	0	7117	315	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 23.

All (315) 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:A:190:ASN:HD22	1:A:208:GLN:HE22	1.09	0.96
1:A:86:VAL:H	1:A:133:GLN:HE22	1.11	0.93
1:C:124:LYS:HE2	1:D:104:PRO:HG2	1.50	0.92
1:B:96:PHE:H	1:B:115:ASN:HD21	1.17	0.92
1:B:192:ASP:C	1:B:194:ALA:H	1.76	0.91
1:B:97:MSE:HE3	1:B:111:ILE:HD13	1.52	0.91
1:C:104:PRO:HG3	1:D:124:LYS:NZ	1.86	0.91
1:D:91:ASN:ND2	1:D:119:GLN:HE22	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:131:LYS:HD3	1:D:177:LEU:HD23	1.53	0.90
1:C:96:PHE:H	1:C:115:ASN:HD21	1.15	0.90
1:B:86:VAL:H	1:B:133:GLN:HE22	1.19	0.89
1:B:94:ALA:HB2	1:B:193:MSE:HE1	1.56	0.86
1:C:43:GLU:HG3	2:C:327:HOH:O	1.75	0.85
1:D:56:VAL:HG12	1:D:58:GLU:H	1.42	0.85
1:B:152:ASP:HB3	2:B:285:HOH:O	1.76	0.84
1:D:17:ILE:HD13	1:D:141:VAL:HG11	1.59	0.83
1:C:41:ASN:HA	1:C:44:LYS:HD3	1.59	0.82
1:A:240:ILE:HG12	1:C:176:PRO:HB3	1.62	0.82
1:B:97:MSE:HE1	1:B:155:ILE:HG22	1.62	0.80
1:B:206:MSE:HA	1:B:235:MSE:HE3	1.65	0.79
1:D:205:GLU:O	1:D:235:MSE:HE3	1.82	0.78
1:C:104:PRO:HG3	1:D:124:LYS:HZ2	1.46	0.78
1:C:86:VAL:H	1:C:133:GLN:HE22	1.28	0.78
1:B:94:ALA:CB	1:B:193:MSE:HE1	2.15	0.77
1:B:175:ALA:HB3	1:B:176:PRO:HD3	1.65	0.77
1:D:50:MSE:HE1	1:D:58:GLU:HB2	1.67	0.76
1:B:127:THR:O	1:B:131:LYS:HG2	1.84	0.76
1:B:108:PHE:CD1	1:B:155:ILE:HG23	2.21	0.76
1:A:96:PHE:H	1:A:115:ASN:HD21	1.33	0.76
1:A:176:PRO:HB3	1:C:240:ILE:HG12	1.67	0.75
1:D:96:PHE:O	1:D:97:MSE:HG3	1.87	0.75
1:A:44:LYS:O	1:A:48:GLU:HG3	1.86	0.75
1:D:31:ARG:HE	1:D:60:ILE:HD11	1.50	0.75
1:B:188:TRP:O	1:B:206:MSE:HB3	1.87	0.74
1:B:193:MSE:HB2	2:B:284:HOH:O	1.86	0.74
1:D:66:ILE:HB	1:D:122:ILE:HD11	1.70	0.72
1:D:50:MSE:CE	1:D:58:GLU:HB2	2.19	0.72
1:D:223:SER:HB2	1:D:226:VAL:HG23	1.71	0.72
1:A:240:ILE:HD11	1:C:176:PRO:HA	1.71	0.72
1:B:108:PHE:HD1	1:B:155:ILE:HG23	1.55	0.71
1:B:193:MSE:O	1:B:193:MSE:HG2	1.90	0.71
1:D:224:GLU:HB3	2:D:286:HOH:O	1.88	0.71
1:D:36:ALA:HB3	1:D:42:LEU:HD21	1.73	0.70
1:B:239:ILE:O	1:B:240:ILE:O	2.09	0.70
1:A:41:ASN:HA	2:A:304:HOH:O	1.93	0.69
1:B:202:LYS:HD2	1:B:202:LYS:N	2.08	0.69
1:D:17:ILE:CD1	1:D:141:VAL:HG11	2.22	0.69
1:A:236:LYS:HE2	1:C:225:ASN:ND2	2.08	0.68
1:B:97:MSE:CE	1:B:111:ILE:HD13	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLY:H	1:B:207:ILE:CD1	2.06	0.68
1:D:96:PHE:CE1	1:D:97:MSE:HE3	2.28	0.68
1:D:175:ALA:HB3	1:D:176:PRO:HD3	1.77	0.67
1:A:190:ASN:HD22	1:A:208:GLN:NE2	1.89	0.67
1:B:160:LYS:O	1:B:164:LEU:HD13	1.94	0.67
1:C:96:PHE:H	1:C:115:ASN:ND2	1.91	0.67
1:B:192:ASP:O	1:B:194:ALA:N	2.28	0.66
1:D:38:SER:HB2	1:D:41:ASN:HB2	1.78	0.66
1:B:46:HIS:ND1	1:B:59:PRO:HG2	2.11	0.66
1:D:96:PHE:HE1	1:D:97:MSE:HE3	1.59	0.66
1:D:124:LYS:HD3	2:D:271:HOH:O	1.96	0.65
1:C:112:MSE:HE2	1:D:112:MSE:SE	2.47	0.65
1:A:202:LYS:HB2	1:A:205:GLU:HG3	1.79	0.65
1:A:190:ASN:ND2	1:A:208:GLN:HE22	1.90	0.65
1:C:39:LYS:HD3	1:C:63:PRO:CG	2.28	0.64
1:B:44:LYS:O	1:B:48:GLU:HG3	1.96	0.64
1:D:143:SER:O	1:D:144:ARG:HG2	1.96	0.64
1:A:205:GLU:O	1:A:235:MSE:HE3	1.97	0.64
1:D:112:MSE:HE1	1:D:159:THR:HA	1.80	0.64
1:D:240:ILE:HA	2:D:269:HOH:O	1.98	0.64
1:D:38:SER:C	1:D:40:GLN:H	2.05	0.63
1:B:34:LEU:HB3	1:B:42:LEU:HD12	1.80	0.63
1:B:189:VAL:HG22	1:B:207:ILE:HB	1.81	0.63
1:B:168:GLU:HG2	1:B:172:ARG:HH12	1.64	0.63
1:B:225:ASN:HB2	2:B:292:HOH:O	1.97	0.63
1:D:172:ARG:NH1	1:D:172:ARG:HB2	2.14	0.62
1:C:104:PRO:HG3	1:D:124:LYS:HZ1	1.60	0.62
1:A:97:MSE:HE1	1:A:155:ILE:HG22	1.81	0.62
1:B:168:GLU:CG	1:B:172:ARG:HH12	2.12	0.62
1:C:39:LYS:HD3	1:C:63:PRO:HG2	1.81	0.62
1:B:187:GLY:H	1:B:207:ILE:HD12	1.64	0.62
1:D:205:GLU:HG3	1:D:237:LYS:HE2	1.80	0.62
1:D:207:ILE:HD13	1:D:233:PHE:HB3	1.82	0.61
1:C:190:ASN:HD22	1:C:208:GLN:HE22	1.47	0.61
1:A:95:MSE:HE2	2:A:255:HOH:O	1.99	0.61
1:D:124:LYS:O	1:D:128:GLU:HG3	2.00	0.61
1:C:113:GLU:OE1	1:D:109:ARG:NH1	2.33	0.61
1:D:14:SER:HB3	1:D:42:LEU:HD13	1.82	0.61
1:B:190:ASN:OD1	1:B:204:GLU:HG3	2.01	0.61
1:B:31:ARG:HD3	1:B:60:ILE:HD11	1.83	0.60
1:C:150:PHE:O	1:C:151:ALA:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:LEU:HB3	1:B:61:VAL:HG13	1.83	0.60
1:B:223:SER:HB3	2:B:292:HOH:O	2.02	0.60
1:D:172:ARG:HB2	1:D:172:ARG:HH11	1.66	0.59
1:C:5:LYS:HE3	1:C:28:ASP:O	2.03	0.59
1:A:174:LEU:HB3	1:A:179:ILE:HB	1.85	0.58
1:A:86:VAL:H	1:A:133:GLN:NE2	1.91	0.58
1:A:35:ILE:HG12	1:A:62:LEU:HD23	1.85	0.58
1:A:47:ASP:O	1:A:51:ARG:HG3	2.04	0.58
1:B:189:VAL:HA	1:B:207:ILE:O	2.03	0.58
1:A:154:GLY:HA3	1:B:166:LEU:HD12	1.85	0.58
1:B:203:ASP:O	1:B:205:GLU:N	2.37	0.58
1:B:193:MSE:O	1:B:193:MSE:CG	2.52	0.58
1:D:62:LEU:HD12	1:D:79:ILE:HG13	1.85	0.58
1:D:96:PHE:C	1:D:97:MSE:HG3	2.28	0.58
1:A:97:MSE:O	1:A:98:ASP:HB2	2.04	0.58
1:A:143:SER:HB3	2:A:255:HOH:O	2.04	0.58
1:D:239:ILE:HG22	1:D:240:ILE:HG12	1.86	0.58
1:A:44:LYS:NZ	2:A:304:HOH:O	2.35	0.57
1:A:91:ASN:HB3	1:A:119:GLN:HE22	1.69	0.57
1:D:4:GLN:HA	1:D:30:TYR:CZ	2.39	0.57
1:C:186:PRO:HA	1:C:233:PHE:HB2	1.87	0.57
1:D:188:TRP:HB2	1:D:235:MSE:SE	2.56	0.56
1:B:192:ASP:C	1:B:194:ALA:N	2.47	0.56
1:B:36:ALA:HB3	1:B:42:LEU:HD21	1.86	0.56
1:D:38:SER:C	1:D:40:GLN:N	2.62	0.56
1:B:96:PHE:N	1:B:115:ASN:HD21	1.95	0.56
1:B:97:MSE:HE1	1:B:155:ILE:CG2	2.36	0.56
1:B:202:LYS:NZ	1:B:202:LYS:HB3	2.22	0.55
1:D:7:LEU:HD23	1:D:31:ARG:HB3	1.88	0.55
1:D:96:PHE:C	1:D:97:MSE:CG	2.79	0.55
1:D:7:LEU:CD2	1:D:31:ARG:HD3	2.36	0.55
1:D:4:GLN:HA	1:D:30:TYR:CE1	2.42	0.55
1:D:57:GLN:O	1:D:58:GLU:HB3	2.06	0.55
1:B:174:LEU:HB3	1:B:179:ILE:HB	1.89	0.55
1:A:154:GLY:HA2	1:B:169:SER:OG	2.07	0.55
1:B:193:MSE:C	2:B:286:HOH:O	2.50	0.55
2:A:275:HOH:O	1:B:124:LYS:HE3	2.06	0.55
1:B:189:VAL:HG13	1:B:207:ILE:O	2.07	0.55
1:B:17:ILE:HG13	1:B:191:THR:HG21	1.89	0.54
1:B:209:PRO:HD2	2:B:295:HOH:O	2.06	0.54
1:D:152:ASP:N	2:D:265:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:GLN:O	1:B:43:GLU:HB2	2.08	0.54
1:D:66:ILE:CB	1:D:122:ILE:HD11	2.36	0.54
1:C:20:VAL:HG11	1:C:209:PRO:HB2	1.90	0.54
1:C:123:LEU:O	1:C:127:THR:HG23	2.07	0.54
1:C:151:ALA:O	1:C:152:ASP:OD1	2.26	0.54
1:D:48:GLU:O	1:D:49:ILE:C	2.50	0.54
1:B:203:ASP:C	1:B:205:GLU:H	2.15	0.54
1:D:215:THR:O	1:D:219:LEU:HG	2.08	0.54
1:B:226:VAL:HG22	1:D:207:ILE:HG12	1.90	0.54
1:C:124:LYS:HE2	1:D:104:PRO:CG	2.32	0.54
1:C:187:GLY:H	1:C:207:ILE:CD1	2.20	0.54
1:C:225:ASN:HB2	2:C:285:HOH:O	2.08	0.54
1:D:47:ASP:O	1:D:51:ARG:HB2	2.07	0.54
1:B:193:MSE:HB3	2:B:286:HOH:O	2.08	0.54
1:C:113:GLU:HB2	2:C:311:HOH:O	2.07	0.54
1:A:82:LYS:HD2	1:A:83:TYR:CE2	2.42	0.53
1:B:193:MSE:CB	2:B:284:HOH:O	2.52	0.53
1:B:205:GLU:HG2	1:D:225:ASN:ND2	2.23	0.53
1:B:28:ASP:OD2	1:B:217:ARG:NE	2.39	0.53
1:C:209:PRO:HG2	2:C:270:HOH:O	2.08	0.53
1:A:166:LEU:HD12	1:B:154:GLY:HA3	1.90	0.53
1:C:53:ASN:HB3	1:C:56:VAL:HG13	1.90	0.53
1:A:91:ASN:CB	1:A:119:GLN:HE22	2.21	0.53
1:A:101:LEU:HB2	1:A:107:ASN:OD1	2.09	0.53
1:A:186:PRO:HA	1:A:233:PHE:HB2	1.91	0.52
1:C:240:ILE:HG22	1:C:241:GLU:N	2.24	0.52
1:C:113:GLU:CD	1:D:109:ARG:NH1	2.67	0.52
1:D:43:GLU:HG2	2:D:268:HOH:O	2.10	0.52
1:A:191:THR:HG22	1:A:209:PRO:HG3	1.90	0.52
1:C:193:MSE:SE	1:C:196:LYS:HD3	2.59	0.52
1:D:40:GLN:N	2:D:268:HOH:O	2.43	0.52
1:A:15:GLN:NE2	1:A:193:MSE:SE	2.93	0.51
1:D:189:VAL:HG23	1:D:207:ILE:O	2.10	0.51
1:D:34:LEU:HB3	1:D:42:LEU:HD12	1.91	0.51
1:D:36:ALA:O	1:D:64:LEU:O	2.29	0.51
1:B:129:ILE:O	1:B:133:GLN:HG3	2.11	0.51
1:A:71:LYS:HD3	2:A:308:HOH:O	2.10	0.51
1:B:205:GLU:HG2	1:D:225:ASN:HD21	1.76	0.51
1:D:91:ASN:CG	1:D:119:GLN:HE22	2.18	0.51
1:C:65:ASP:OD2	1:C:67:THR:HB	2.11	0.50
1:A:3:LYS:O	1:A:3:LYS:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:MSE:HE2	1:A:58:GLU:HG3	1.92	0.50
1:C:182:THR:HG21	1:C:219:LEU:HD11	1.93	0.50
1:A:105:VAL:HG23	2:A:275:HOH:O	2.11	0.50
1:B:168:GLU:HG2	1:B:172:ARG:HH22	1.77	0.50
1:C:43:GLU:CG	2:C:327:HOH:O	2.47	0.50
1:A:124:LYS:HE3	1:B:104:PRO:HB2	1.93	0.49
1:A:97:MSE:HE1	1:A:155:ILE:CG2	2.43	0.49
1:D:207:ILE:HD13	1:D:233:PHE:CB	2.41	0.49
1:C:189:VAL:O	1:C:194:ALA:HB2	2.13	0.49
1:D:75:GLU:O	1:D:79:ILE:HG12	2.13	0.49
1:C:112:MSE:CE	1:D:112:MSE:SE	3.10	0.49
1:C:152:ASP:OD1	1:C:152:ASP:C	2.56	0.49
1:A:79:ILE:HG23	1:A:83:TYR:HD2	1.77	0.49
1:A:112:MSE:SE	1:A:116:VAL:HG21	2.63	0.49
1:D:237:LYS:HD2	1:D:237:LYS:N	2.28	0.49
1:A:10:ILE:HD12	1:A:10:ILE:N	2.28	0.49
1:C:151:ALA:HA	1:D:173:GLU:OE1	2.13	0.49
1:D:44:LYS:HA	1:D:44:LYS:HE2	1.93	0.49
1:B:46:HIS:O	1:B:50:MSE:HG2	2.13	0.48
1:B:64:LEU:HD21	1:B:72:ALA:HA	1.95	0.48
1:D:186:PRO:HA	1:D:233:PHE:HB2	1.95	0.48
1:A:214:ASN:ND2	1:A:217:ARG:HH11	2.12	0.48
1:C:195:LYS:HG3	1:C:196:LYS:N	2.29	0.48
1:B:187:GLY:H	1:B:207:ILE:HD11	1.78	0.48
1:C:66:ILE:HG22	1:C:122:ILE:HD11	1.95	0.48
1:A:103:GLU:HB2	1:A:106:ASP:OD2	2.13	0.48
1:B:88:ILE:HG22	1:B:89:LEU:N	2.29	0.48
1:D:10:ILE:CD1	1:D:22:ALA:HA	2.44	0.48
1:A:26:ALA:O	1:A:56:VAL:HG23	2.14	0.47
1:A:108:PHE:CD1	1:A:155:ILE:HG23	2.49	0.47
1:B:8:ALA:HB3	1:B:32:VAL:HG12	1.96	0.47
1:A:97:MSE:HE2	1:A:152:ASP:OD2	2.13	0.47
1:C:39:LYS:HD3	1:C:63:PRO:HG3	1.97	0.47
1:D:46:HIS:HE1	1:D:58:GLU:HG3	1.79	0.47
1:D:143:SER:O	1:D:144:ARG:CG	2.61	0.47
1:A:71:LYS:O	1:A:75:GLU:HG2	2.14	0.47
1:D:56:VAL:CG1	1:D:58:GLU:H	2.22	0.47
1:C:54:LYS:HG3	2:C:322:HOH:O	2.15	0.47
1:C:187:GLY:H	1:C:207:ILE:HD12	1.80	0.47
1:D:31:ARG:NE	1:D:60:ILE:HD11	2.26	0.46
1:B:8:ALA:O	1:B:10:ILE:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ASN:HA	1:B:217:ARG:HG3	1.97	0.46
1:D:6:GLY:HA3	1:D:87:ASP:OD2	2.16	0.46
1:D:124:LYS:CD	2:D:271:HOH:O	2.61	0.46
1:C:150:PHE:N	1:C:150:PHE:CD2	2.84	0.46
1:C:199:THR:N	2:C:309:HOH:O	2.48	0.46
1:B:127:THR:CG2	1:B:131:LYS:HE3	2.46	0.46
1:D:143:SER:O	1:D:144:ARG:CB	2.64	0.46
1:A:97:MSE:O	1:A:98:ASP:CB	2.63	0.46
1:B:177:LEU:N	1:B:177:LEU:HD12	2.31	0.46
1:B:40:GLN:HG3	1:B:41:ASN:N	2.30	0.46
1:C:82:LYS:HD3	1:C:83:TYR:CE2	2.51	0.46
1:C:150:PHE:O	1:C:151:ALA:CB	2.64	0.46
1:C:174:LEU:HB3	1:C:179:ILE:HB	1.97	0.46
1:C:175:ALA:HB3	1:C:176:PRO:CD	2.46	0.46
1:D:95:MSE:HG3	1:D:115:ASN:OD1	2.16	0.46
1:D:42:LEU:O	1:D:45:VAL:N	2.48	0.46
1:A:169:SER:OG	1:B:154:GLY:HA2	2.15	0.45
1:C:188:TRP:H	1:C:235:MSE:HE2	1.80	0.45
1:D:112:MSE:CE	1:D:159:THR:HA	2.45	0.45
1:B:203:ASP:C	1:B:205:GLU:N	2.73	0.45
1:B:187:GLY:N	1:B:207:ILE:HD12	2.31	0.45
1:D:65:ASP:OD1	1:D:67:THR:HB	2.16	0.45
1:D:95:MSE:HE3	1:D:156:TYR:HE1	1.82	0.45
1:D:43:GLU:O	1:D:46:HIS:HB3	2.16	0.45
1:D:66:ILE:CG2	1:D:122:ILE:HD11	2.47	0.45
1:B:131:LYS:HD3	1:B:177:LEU:HD23	1.99	0.45
1:A:108:PHE:CD2	1:B:117:ILE:HD13	2.52	0.45
1:B:73:ASP:OD1	1:B:77:LYS:NZ	2.49	0.45
1:C:36:ALA:HB3	1:C:42:LEU:HD21	1.99	0.45
1:D:38:SER:HB3	1:D:41:ASN:H	1.81	0.44
1:A:36:ALA:HB3	1:A:42:LEU:HD21	1.99	0.44
1:C:199:THR:HG23	1:C:199:THR:O	2.16	0.44
1:B:4:GLN:HA	2:B:307:HOH:O	2.17	0.44
1:C:236:LYS:NZ	2:C:287:HOH:O	2.50	0.44
1:B:47:ASP:O	1:B:51:ARG:HG2	2.18	0.44
1:D:115:ASN:O	1:D:163:LEU:HD21	2.18	0.44
1:A:236:LYS:HE2	1:C:225:ASN:HD22	1.78	0.44
1:B:119:GLN:NE2	2:B:255:HOH:O	2.51	0.44
1:C:187:GLY:N	1:C:207:ILE:HD12	2.32	0.44
1:B:168:GLU:HG2	1:B:172:ARG:NH1	2.32	0.44
1:C:65:ASP:CG	1:C:67:THR:HB	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:ILE:HG22	1:C:89:LEU:N	2.33	0.44
1:C:85:ALA:HA	1:C:133:GLN:NE2	2.33	0.43
1:A:202:LYS:HB3	1:A:204:GLU:OE2	2.18	0.43
1:B:43:GLU:O	1:B:46:HIS:HB3	2.18	0.43
1:A:35:ILE:CG1	1:A:62:LEU:HD23	2.47	0.43
1:C:10:ILE:HD12	1:C:10:ILE:N	2.32	0.43
1:C:151:ALA:O	1:C:152:ASP:CG	2.61	0.43
1:B:119:GLN:HE21	1:B:119:GLN:HB2	1.60	0.43
1:D:237:LYS:HD2	1:D:237:LYS:H	1.83	0.43
1:A:205:GLU:HG2	1:A:237:LYS:HE3	1.99	0.43
1:A:240:ILE:HG12	1:C:176:PRO:CB	2.42	0.43
1:B:219:LEU:CD2	1:B:228:ILE:HD12	2.49	0.43
1:B:168:GLU:HG3	1:B:229:LYS:HE2	2.01	0.43
1:C:39:LYS:HB2	1:C:63:PRO:CG	2.48	0.43
1:D:36:ALA:HB3	1:D:42:LEU:CD2	2.46	0.43
1:D:174:LEU:HB3	1:D:179:ILE:HB	2.00	0.43
1:B:191:THR:OG1	2:B:286:HOH:O	2.21	0.42
1:D:17:ILE:HD12	1:D:212:LEU:CD1	2.49	0.42
1:B:235:MSE:C	1:B:237:LYS:N	2.76	0.42
1:A:82:LYS:HD2	1:A:83:TYR:CZ	2.54	0.42
1:A:188:TRP:CZ3	1:A:199:THR:HB	2.54	0.42
1:A:210:ASP:HB2	2:A:344:HOH:O	2.18	0.42
1:B:113:GLU:HA	1:B:117:ILE:HB	2.01	0.42
1:A:133:GLN:O	1:A:134:LYS:HB2	2.19	0.42
1:B:236:LYS:HE3	1:D:225:ASN:OD1	2.19	0.42
1:C:182:THR:HG21	1:C:219:LEU:CD1	2.49	0.42
1:A:123:LEU:HD13	1:A:170:LEU:CD1	2.50	0.42
1:B:188:TRP:HB3	1:B:206:MSE:SE	2.69	0.42
1:A:108:PHE:HD1	1:A:155:ILE:HG23	1.83	0.42
1:C:112:MSE:CE	1:D:112:MSE:HG3	2.49	0.42
1:D:7:LEU:HD21	1:D:31:ARG:HD3	2.00	0.42
1:C:152:ASP:OD1	1:C:155:ILE:N	2.53	0.42
1:D:62:LEU:C	1:D:62:LEU:HD23	2.45	0.42
1:D:113:GLU:HA	1:D:117:ILE:CG1	2.50	0.42
1:A:26:ALA:O	1:A:56:VAL:CG2	2.68	0.42
1:A:175:ALA:N	1:A:176:PRO:HD2	2.35	0.41
1:B:202:LYS:HB3	1:B:202:LYS:HZ2	1.84	0.41
1:B:205:GLU:CB	2:B:253:HOH:O	2.67	0.41
1:B:123:LEU:HD13	1:B:170:LEU:CD1	2.50	0.41
1:B:202:LYS:N	1:B:202:LYS:CD	2.77	0.41
1:C:113:GLU:OE2	1:D:109:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:ASP:HA	1:C:206:MSE:CE	2.51	0.41
1:D:168:GLU:OE2	1:D:229:LYS:HD3	2.21	0.41
1:C:37:ARG:HH12	1:C:65:ASP:CG	2.29	0.41
1:D:7:LEU:HA	1:D:31:ARG:O	2.20	0.41
1:D:61:VAL:HG12	1:D:63:PRO:HD3	2.02	0.41
1:A:46:HIS:ND1	1:A:46:HIS:C	2.79	0.41
1:C:170:LEU:HD23	1:C:170:LEU:HA	1.94	0.41
1:C:195:LYS:HD2	1:C:195:LYS:C	2.45	0.41
1:A:103:GLU:HA	1:A:104:PRO:HD3	1.95	0.41
1:B:128:GLU:O	1:B:131:LYS:HB2	2.21	0.41
1:B:190:ASN:HB2	1:B:206:MSE:HE3	2.03	0.41
1:B:225:ASN:OD1	1:D:236:LYS:HE2	2.21	0.41
1:C:96:PHE:N	1:C:115:ASN:HD21	1.98	0.41
1:A:104:PRO:HA	1:A:107:ASN:HD22	1.86	0.40
1:B:97:MSE:HE3	1:B:111:ILE:CD1	2.38	0.40
1:C:39:LYS:O	1:C:43:GLU:HG2	2.22	0.40
1:D:42:LEU:HB2	2:D:268:HOH:O	2.21	0.40
1:C:43:GLU:CD	2:C:327:HOH:O	2.64	0.40
1:B:214:ASN:O	1:B:217:ARG:HB2	2.21	0.40
1:B:224:GLU:H	1:B:224:GLU:HG3	1.53	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	228/250 (91%)	219 (96%)	8 (4%)	1 (0%)	30	26
1	B	212/250 (85%)	201 (95%)	9 (4%)	2 (1%)	14	9
1	C	222/250 (89%)	213 (96%)	8 (4%)	1 (0%)	24	20
1	D	205/250 (82%)	187 (91%)	11 (5%)	7 (3%)	3	0
All	All	867/1000 (87%)	820 (95%)	36 (4%)	11 (1%)	9	5

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	GLU
1	D	51	ARG
1	A	98	ASP
1	B	193	MSE
1	D	16	GLY
1	D	36	ALA
1	C	151	ALA
1	D	58	GLU
1	D	143	SER
1	D	49	ILE
1	D	187	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	195/200 (98%)	191 (98%)	4 (2%)	47	52
1	B	185/200 (92%)	177 (96%)	8 (4%)	26	24
1	C	192/200 (96%)	189 (98%)	3 (2%)	55	61
1	D	181/200 (90%)	170 (94%)	11 (6%)	17	12
All	All	753/800 (94%)	727 (96%)	26 (4%)	32	32

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	100	SER
1	A	152	ASP
1	A	186	PRO
1	A	241	GLU
1	B	42	LEU
1	B	44	LYS
1	B	119	GLN
1	B	202	LYS
1	B	203	ASP

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Mol	Chain	Res	Type
1	B	204	GLU
1	B	205	GLU
1	B	224	GLU
1	C	39	LYS
1	C	166	LEU
1	C	195	LYS
1	D	42	LEU
1	D	44	LYS
1	D	50	MSE
1	D	52	SER
1	D	56	VAL
1	D	74	THR
1	D	81	GLN
1	D	97	MSE
1	D	107	ASN
1	D	170	LEU
1	D	203	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	15	GLN
1	A	40	GLN
1	A	41	ASN
1	A	91	ASN
1	A	115	ASN
1	A	119	GLN
1	A	133	GLN
1	A	140	ASN
1	A	190	ASN
1	A	208	GLN
1	A	214	ASN
1	A	221	ASN
1	B	41	ASN
1	B	115	ASN
1	B	119	GLN
1	B	133	GLN
1	B	190	ASN
1	B	208	GLN
1	B	221	ASN
1	C	4	GLN

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Mol	Chain	Res	Type
1	C	115	ASN
1	C	133	GLN
1	C	135	ASN
1	C	190	ASN
1	C	208	GLN
1	C	225	ASN
1	D	4	GLN
1	D	41	ASN
1	D	91	ASN
1	D	107	ASN
1	D	119	GLN
1	D	140	ASN
1	D	208	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	224/250 (89%)	0.27	9 (4%) 42 47	20, 34, 59, 78	0
1	B	212/250 (84%)	0.83	21 (9%) 13 14	32, 49, 62, 69	0
1	C	220/250 (88%)	0.31	9 (4%) 41 46	19, 32, 58, 70	0
1	D	206/250 (82%)	1.02	28 (13%) 7 7	32, 50, 67, 73	0
All	All	862/1000 (86%)	0.60	67 (7%) 19 21	19, 42, 64, 78	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	151	ALA	5.3
1	D	189	VAL	4.7
1	C	153	GLY	4.6
1	A	99	GLY	4.3
1	B	240	ILE	4.2
1	D	4	GLN	4.1
1	B	194	ALA	3.8
1	B	192	ASP	3.8
1	D	203	ASP	3.3
1	D	17	ILE	3.3
1	A	156	TYR	3.2
1	D	56	VAL	3.2
1	D	96	PHE	3.2
1	B	203	ASP	3.2
1	B	106	ASP	3.1
1	C	150	PHE	3.1
1	A	100	SER	3.0
1	B	177	LEU	3.0
1	D	142	ALA	2.9
1	A	98	ASP	2.9
1	B	201	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	60	ILE	2.8
1	A	101	LEU	2.8
1	B	78	ASP	2.7
1	A	240	ILE	2.7
1	B	96	PHE	2.7
1	D	52	SER	2.7
1	D	239	ILE	2.7
1	D	240	ILE	2.6
1	B	15	GLN	2.6
1	B	151	ALA	2.6
1	B	188	TRP	2.6
1	A	104	PRO	2.6
1	D	188	TRP	2.6
1	D	36	ALA	2.5
1	A	152	ASP	2.5
1	B	191	THR	2.5
1	D	51	ARG	2.5
1	C	66	ILE	2.4
1	B	176	PRO	2.4
1	D	94	ALA	2.4
1	A	4	GLN	2.3
1	B	84	GLY	2.3
1	C	55	HIS	2.3
1	D	59	PRO	2.3
1	D	190	ASN	2.3
1	D	103	GLU	2.3
1	B	37	ARG	2.3
1	C	198	GLY	2.3
1	C	40	GLN	2.2
1	D	144	ARG	2.2
1	D	79	ILE	2.2
1	C	142	ALA	2.2
1	D	55	HIS	2.2
1	D	37	ARG	2.2
1	D	70	THR	2.2
1	B	187	GLY	2.1
1	B	239	ILE	2.1
1	B	195	LYS	2.1
1	D	62	LEU	2.1
1	D	44	LYS	2.1
1	C	197	ALA	2.1
1	D	78	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	83	TYR	2.0
1	B	207	ILE	2.0
1	D	204	GLU	2.0
1	D	47	ASP	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.