



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 05:29 AM UTC

PDB ID : 1ZOW / pdb_00001zow
Title : Crystal Structure of S. aureus FabH, beta-ketoacyl carrier protein synthase III
Authors : Qiu, X.; Choudhry, A.E.; Janson, C.A.; Grooms, M.; Daines, R.A.; Lonsdale, J.T.; Khandekar, S.S.
Deposited on : 2005-05-15
Resolution : 2.00 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

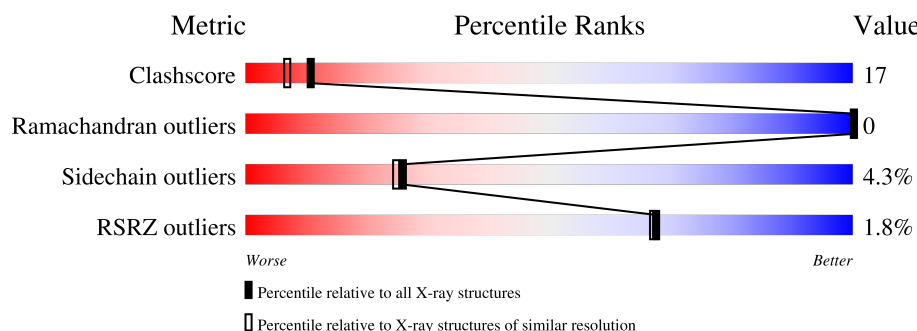
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	313	2% 67% 30% .
1	B	313	2% 71% 25% .
1	C	313	2% 66% 31% .
1	D	313	% 71% 26% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 10293 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-oxoacyl-[acyl-carrier-protein] synthase III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	3	0
			2377	1494	396	471	16			
1	B	312	Total	C	N	O	S	0	2	0
			2370	1487	395	471	17			
1	C	312	Total	C	N	O	S	0	4	0
			2379	1495	395	471	18			
1	D	312	Total	C	N	O	S	0	3	0
			2375	1489	398	471	17			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	60	VAL	LEU	SEE REMARK 999	UNP Q8NXE2
A	171	GLU	ASP	SEE REMARK 999	UNP Q8NXE2
A	287	LEU	ILE	SEE REMARK 999	UNP Q8NXE2
B	60	VAL	LEU	SEE REMARK 999	UNP Q8NXE2
B	171	GLU	ASP	SEE REMARK 999	UNP Q8NXE2
B	287	LEU	ILE	SEE REMARK 999	UNP Q8NXE2
C	60	VAL	LEU	SEE REMARK 999	UNP Q8NXE2
C	171	GLU	ASP	SEE REMARK 999	UNP Q8NXE2
C	287	LEU	ILE	SEE REMARK 999	UNP Q8NXE2
D	60	VAL	LEU	SEE REMARK 999	UNP Q8NXE2
D	171	GLU	ASP	SEE REMARK 999	UNP Q8NXE2
D	287	LEU	ILE	SEE REMARK 999	UNP Q8NXE2

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	218	Total	O	0	0
			218	218		
2	B	202	Total	O	0	0
			202	202		

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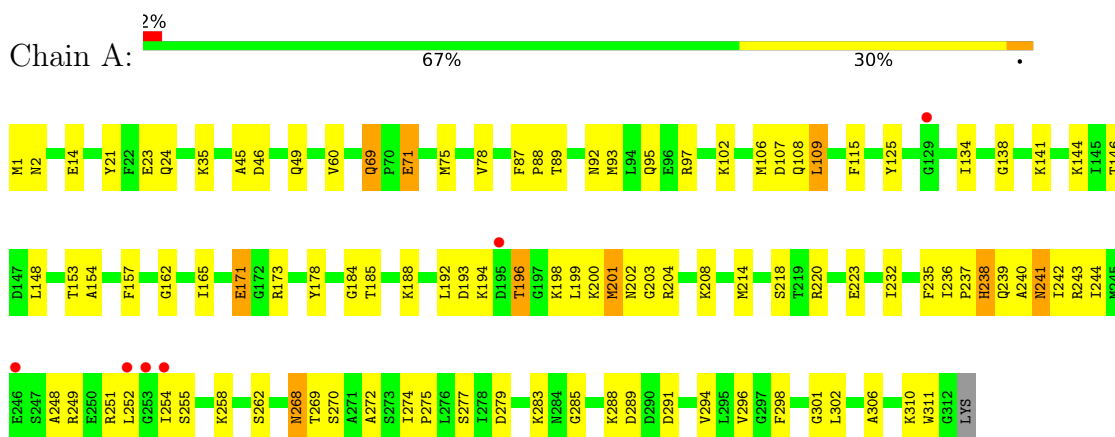
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	164	Total 164	O 164	0	0
2	D	208	Total 208	O 208	0	0

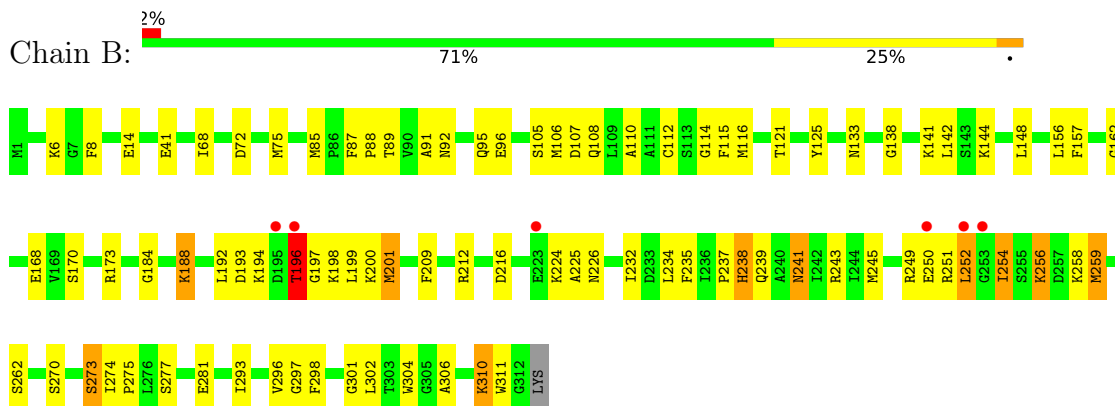
3 Residue-property plots

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.

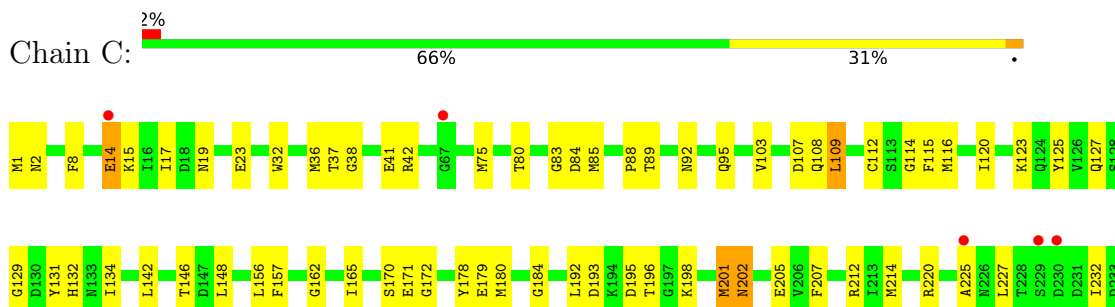
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase III

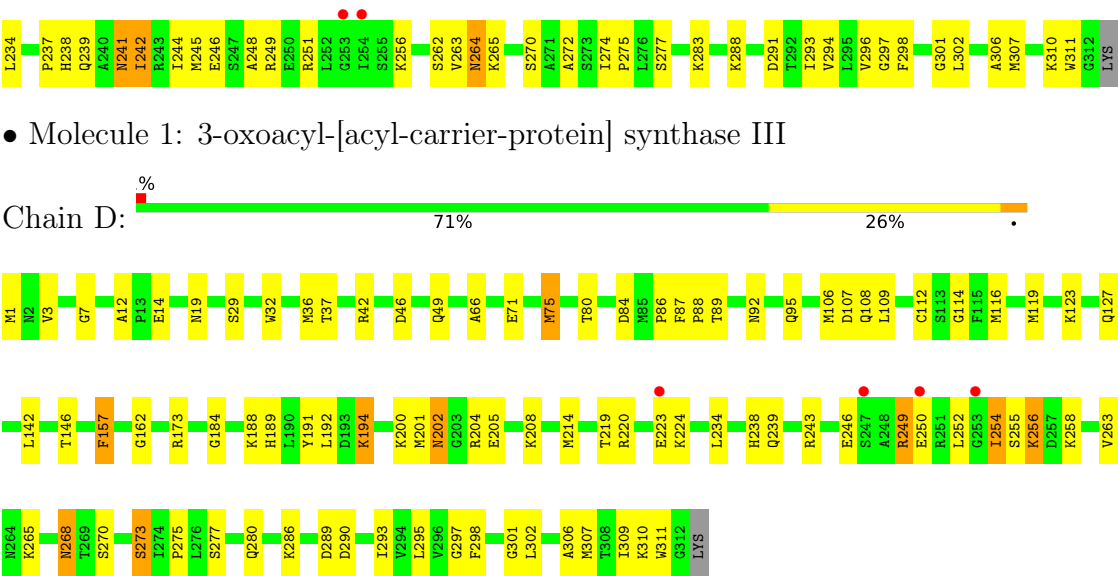


• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase III



• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase III





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.90Å 93.60Å 110.00Å 90.00° 93.90° 90.00°	Depositor
Resolution (Å)	20.00 – 2.00 20.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.00) 89.4 (20.00-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.87 (at 2.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.256 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	18.3	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	10293	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% 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	0.65	0/2429	1.03	9/3272 (0.3%)
1	B	0.68	1/2416 (0.0%)	1.01	13/3255 (0.4%)
1	C	0.61	1/2436 (0.0%)	0.99	9/3281 (0.3%)
1	D	0.66	1/2427 (0.0%)	1.01	9/3269 (0.3%)
All	All	0.65	3/9708 (0.0%)	1.01	40/13077 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	259	MET	SD-CE	-6.89	1.62	1.79
1	C	274	ILE	CA-CB	5.41	1.57	1.53
1	D	75	MET	SD-CE	-5.36	1.66	1.79

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	238	HIS	N-CA-C	-7.76	98.98	110.23
1	A	14	GLU	N-CA-C	7.34	118.97	110.97
1	B	196	THR	N-CA-C	-7.19	105.13	114.04
1	C	157	PHE	N-CA-C	7.11	121.61	110.17
1	B	14	GLU	N-CA-C	6.83	118.37	111.07
1	C	311	TRP	N-CA-C	6.72	119.48	110.35
1	A	311	TRP	N-CA-C	6.64	120.11	110.28
1	C	165	ILE	N-CA-C	-6.60	98.93	108.17
1	C	242	ILE	N-CA-C	6.60	117.35	110.62
1	B	273	SER	N-CA-C	6.58	118.45	111.28
1	D	157	PHE	N-CA-C	6.56	120.52	109.76
1	D	311	TRP	N-CA-C	6.39	119.49	110.23
1	D	14	GLU	N-CA-C	6.15	119.25	111.69
1	D	12	ALA	N-CA-C	-6.10	100.93	110.14
1	A	157	PHE	N-CA-C	6.07	119.71	109.76
1	D	114	GLY	N-CA-C	6.07	120.01	112.73
1	D	201	MET	N-CA-C	5.95	119.17	109.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ILE	N-CA-C	-5.85	99.31	107.80
1	A	238	HIS	N-CA-C	-5.84	101.39	110.10
1	B	238	HIS	N-CA-C	-5.83	101.67	110.24
1	B	114	GLY	N-CA-C	5.80	119.91	112.83
1	D	273	SER	N-CA-C	5.72	117.21	110.97
1	B	256	LYS	N-CA-C	5.69	118.25	111.71
1	B	194	LYS	N-CA-C	5.61	117.86	111.02
1	B	157	PHE	N-CA-C	5.59	119.17	110.17
1	B	201	MET	N-CA-C	5.48	118.38	109.06
1	B	110	ALA	N-CA-C	-5.45	105.58	113.21
1	C	38	GLY	N-CA-C	-5.37	107.91	115.32
1	B	310	LYS	N-CA-C	-5.36	99.03	108.20
1	A	201	MET	N-CA-C	5.34	117.50	109.23
1	D	29	SER	N-CA-C	-5.33	100.63	108.79
1	A	138	GLY	N-CA-C	-5.32	100.58	113.18
1	B	138	GLY	N-CA-C	-5.30	100.62	113.18
1	A	203	GLY	N-CA-C	5.25	119.00	112.64
1	C	103	VAL	N-CA-C	5.24	116.13	110.21
1	C	114	GLY	N-CA-C	5.21	119.19	112.83
1	C	201	MET	N-CA-C	5.18	117.87	109.06
1	B	311	TRP	N-CA-C	5.11	117.84	110.28
1	A	291	ASP	N-CA-C	-5.05	103.37	110.50
1	D	37	THR	N-CA-C	5.05	120.98	114.56

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	2377	0	2361	85	0
1	B	2370	0	2352	75	0
1	C	2379	0	2362	95	0
1	D	2375	0	2357	84	0
2	A	218	0	0	14	0
2	B	202	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	164	0	0	8	0
2	D	208	0	0	3	0
All	All	10293	0	9432	316	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 (316) 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:D:249:ARG:HH11	1:D:249:ARG:HB3	1.13	1.09
1:D:254:ILE:HD11	1:D:258:LYS:HD2	1.34	1.08
1:C:212:ARG:HA	1:C:251:ARG:HH21	1.28	0.97
1:B:237:PRO:HG3	1:B:259:MET:HE2	1.43	0.95
1:C:212:ARG:HA	1:C:251:ARG:NH2	1.82	0.94
1:A:184:GLY:H	1:B:95:GLN:NE2	1.67	0.93
1:C:179:GLU:O	1:C:180[B]:MET:HE2	1.68	0.93
1:D:249:ARG:HB3	1:D:249:ARG:NH1	1.84	0.93
1:D:254:ILE:HD13	1:D:255:SER:N	1.89	0.88
1:C:120:ILE:CD1	1:C:180[B]:MET:HE3	2.04	0.88
1:C:184:GLY:H	1:D:95:GLN:NE2	1.71	0.87
1:D:116[B]:MET:HE1	1:D:306:ALA:HA	1.59	0.84
1:D:254:ILE:HD13	1:D:255:SER:H	1.41	0.83
1:B:234:LEU:HB2	1:B:293:ILE:HG22	1.59	0.82
1:B:241:ASN:HD22	1:B:243:ARG:H	1.28	0.81
1:C:120:ILE:HD11	1:C:180[B]:MET:HE3	1.62	0.80
1:D:123:LYS:HE2	1:D:127:GLN:NE2	1.98	0.78
1:A:196:THR:HG21	2:A:512:HOH:O	1.84	0.77
1:A:102:LYS:HE2	1:B:304:TRP:HH2	1.49	0.77
1:D:142:LEU:O	1:D:146:THR:HG23	1.85	0.76
1:A:23:GLU:HG3	2:A:327:HOH:O	1.86	0.74
1:C:193:ASP:HB3	1:C:196:THR:HG22	1.69	0.74
1:C:109:LEU:HD21	1:D:109:LEU:HD12	1.68	0.73
1:B:241:ASN:ND2	1:B:243:ARG:H	1.86	0.73
1:C:123:LYS:HE2	1:C:127:GLN:OE1	1.89	0.73
1:C:239:GLN:NE2	1:C:262:SER:H	1.86	0.73
1:A:184:GLY:H	1:B:95:GLN:HE21	1.35	0.72
1:A:241:ASN:ND2	1:A:243:ARG:H	1.88	0.70
1:C:202:ASN:HD22	1:C:205:GLU:H	1.37	0.70
1:A:268:ASN:C	1:A:268:ASN:HD22	2.00	0.70
1:A:241:ASN:HD22	1:A:243:ARG:H	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:95:GLN:NE2	1:D:184:GLY:H	1.89	0.69
1:C:116[B]:MET:HE1	1:C:297:GLY:N	2.07	0.69
1:C:202:ASN:ND2	1:C:205:GLU:H	1.89	0.69
1:C:272:ALA:O	1:C:275:PRO:HD2	1.91	0.69
1:B:6:LYS:HE2	1:B:133:ASN:ND2	2.08	0.69
1:D:80:THR:O	1:D:109:LEU:HD23	1.92	0.69
1:A:69:GLN:NE2	2:A:488:HOH:O	2.25	0.68
1:B:238:HIS:HD2	1:B:273:SER:OG	1.76	0.68
1:C:184:GLY:H	1:D:95:GLN:HE21	1.39	0.68
1:C:109:LEU:HD21	1:D:109:LEU:CD1	2.23	0.68
1:B:249:ARG:NH2	1:B:256:LYS:HD2	2.09	0.67
1:C:116[B]:MET:HE1	1:C:297:GLY:H	1.59	0.67
1:A:69:GLN:HB3	1:A:71:GLU:HG2	1.75	0.67
1:C:85:MET:HG2	1:D:194:LYS:HG3	1.76	0.67
1:A:75:MET:HE1	1:A:125:TYR:CE2	2.29	0.67
1:D:46:ASP:H	1:D:49:GLN:HE21	1.42	0.66
1:B:239:GLN:NE2	1:B:262:SER:H	1.93	0.66
1:A:241:ASN:HD22	1:A:243:ARG:N	1.93	0.65
1:C:75:MET:HB3	1:C:134:ILE:HG12	1.78	0.65
1:D:204:ARG:HH22	1:D:243[A]:ARG:HH22	1.43	0.65
1:B:235:PHE:CD1	1:B:259:MET:HE3	2.31	0.65
1:D:254:ILE:CD1	1:D:258:LYS:HB2	2.26	0.65
1:D:219:THR:O	1:D:223:GLU:HG3	1.96	0.65
1:B:235:PHE:CE1	1:B:259:MET:HE3	2.31	0.65
1:A:248:ALA:O	1:A:252:LEU:HG	1.97	0.65
1:C:202:ASN:ND2	1:C:205:GLU:HG2	2.10	0.64
1:C:120:ILE:HD13	1:C:178:TYR:CD2	2.32	0.64
1:D:254:ILE:HD11	1:D:258:LYS:CD	2.19	0.64
1:A:235[B]:PHE:CD2	1:A:254:ILE:HD13	2.33	0.63
1:C:80:THR:O	1:C:109:LEU:HD13	1.98	0.63
1:B:224:LYS:HE3	2:B:374:HOH:O	1.98	0.63
1:A:283[A]:LYS:HE3	1:C:17:ILE:HD13	1.80	0.62
1:B:112:CYS:HB2	1:B:298:PHE:O	2.00	0.62
1:C:214:MET:CE	1:C:296:VAL:HG13	2.29	0.62
1:D:254:ILE:CD1	1:D:258:LYS:HD2	2.21	0.62
1:C:112:CYS:SG	2:C:413:HOH:O	2.56	0.62
1:B:193:ASP:HB3	1:B:196:THR:HG22	1.81	0.62
1:A:102:LYS:HE2	1:B:304:TRP:CH2	2.33	0.62
1:A:268:ASN:ND2	1:A:270:SER:H	1.98	0.61
1:A:45:ALA:HB3	1:A:141:LYS:HE3	1.83	0.61
1:A:46:ASP:H	1:A:49:GLN:HE21	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLN:NE2	1:D:108:GLN:NE2	2.49	0.61
1:D:89:THR:H	1:D:92:ASN:ND2	1.98	0.61
1:B:196:THR:HG22	1:B:198:LYS:H	1.65	0.61
1:A:115:PHE:CE1	1:A:275:PRO:HG3	2.35	0.60
1:C:116[A]:MET:SD	1:C:307:MET:HE3	2.41	0.60
1:C:225:ALA:O	1:C:227:LEU:HD13	2.02	0.60
1:C:108:GLN:HE21	1:D:108:GLN:NE2	2.00	0.60
1:D:112:CYS:HB2	1:D:298:PHE:O	2.01	0.60
1:D:246:GLU:OE2	1:D:249:ARG:NH1	2.35	0.59
1:B:115:PHE:CE2	1:B:275:PRO:HG3	2.37	0.59
1:A:193:ASP:HB3	1:A:196:THR:HG22	1.84	0.59
1:A:235[B]:PHE:CE2	1:A:254:ILE:HD13	2.37	0.59
1:B:241:ASN:HD22	1:B:243:ARG:N	1.99	0.59
1:D:214:MET:HE3	1:D:297:GLY:HA2	1.84	0.59
1:C:2:ASN:ND2	2:C:396:HOH:O	2.34	0.59
1:C:75:MET:HE1	1:C:125:TYR:CE2	2.37	0.59
1:A:218:SER:HG	1:A:235[A]:PHE:HE2	1.51	0.59
1:A:239:GLN:NE2	1:A:262:SER:H	2.01	0.59
1:C:196:THR:HG23	1:C:198:LYS:H	1.69	0.58
1:D:84:ASP:HB2	2:D:325:HOH:O	2.02	0.58
1:D:268:ASN:HD22	1:D:270:SER:H	1.49	0.58
1:D:202:ASN:C	1:D:202:ASN:HD22	2.12	0.58
1:C:108:GLN:NE2	1:D:108:GLN:HE21	2.02	0.58
1:C:264:ASN:H	1:C:264:ASN:HD22	1.51	0.58
1:B:232:ILE:HB	1:B:254:ILE:HD11	1.84	0.57
1:C:196:THR:HG21	2:C:448:HOH:O	2.04	0.57
1:A:2:ASN:ND2	1:A:171:GLU:HA	2.19	0.57
1:C:272:ALA:C	1:C:275:PRO:HD2	2.29	0.57
1:D:204:ARG:HA	1:D:204:ARG:NE	2.20	0.57
1:B:196:THR:CG2	1:B:198:LYS:H	2.16	0.57
1:D:7:GLY:HA3	1:D:66:ALA:HB2	1.87	0.57
1:C:156:LEU:CD1	1:C:201:MET:HE1	2.35	0.56
1:D:307:MET:HE2	1:D:309:ILE:HD11	1.87	0.56
1:B:249:ARG:HD3	1:B:254:ILE:O	2.06	0.56
1:A:238:HIS:CE1	1:A:240:ALA:HB2	2.40	0.56
1:C:14:GLU:HG2	1:C:15:LYS:N	2.17	0.56
1:D:123:LYS:O	1:D:127:GLN:HG3	2.06	0.56
1:D:254:ILE:HD11	1:D:258:LYS:HB2	1.88	0.56
1:A:185:THR:O	1:A:188:LYS:HE2	2.05	0.56
1:A:214:MET:HE3	1:A:237:PRO:HB3	1.88	0.56
1:D:249:ARG:HH11	1:D:249:ARG:CB	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:ASN:ND2	1:D:270:SER:H	2.05	0.55
1:A:268:ASN:HD22	1:A:270:SER:H	1.54	0.55
1:B:216:ASP:OD2	1:B:251:ARG:NH2	2.39	0.55
1:D:254:ILE:HD12	1:D:258:LYS:HB2	1.87	0.55
1:B:89:THR:H	1:B:92:ASN:ND2	2.05	0.54
1:C:112:CYS:HB2	1:C:298:PHE:O	2.07	0.54
1:C:120:ILE:HD12	1:C:180[B]:MET:HE3	1.89	0.54
1:C:109:LEU:N	1:C:109:LEU:HD22	2.23	0.54
1:A:35:LYS:HG2	2:A:480:HOH:O	2.08	0.54
1:D:256:LYS:HB2	1:D:256:LYS:NZ	2.22	0.53
1:C:19:ASN:ND2	1:C:42:ARG:HH22	2.07	0.53
1:D:249:ARG:HG2	1:D:254:ILE:HG22	1.89	0.53
1:D:268:ASN:HD22	1:D:268:ASN:C	2.17	0.53
1:B:170:SER:OG	1:B:173:ARG:HD2	2.10	0.52
1:C:129:GLY:HA2	2:C:435:HOH:O	2.08	0.52
1:D:162:GLY:HA3	1:D:275:PRO:CB	2.40	0.52
1:B:91:ALA:HB1	1:B:105:SER:HB2	1.92	0.52
1:C:88:PRO:HD3	1:D:191:TYR:CB	2.40	0.52
1:A:146:THR:CG2	1:A:154:ALA:HA	2.39	0.52
1:A:148:LEU:HD12	2:A:476:HOH:O	2.10	0.52
1:B:193:ASP:OD1	1:B:196:THR:HB	2.10	0.52
1:B:254:ILE:HG23	1:B:258:LYS:HE3	1.91	0.52
1:A:223:GLU:HG3	2:A:514:HOH:O	2.10	0.52
1:D:200:LYS:HE2	2:D:519:HOH:O	2.10	0.52
1:A:283[A]:LYS:HE3	1:C:17:ILE:CD1	2.40	0.51
1:A:196:THR:CG2	1:A:198:LYS:H	2.24	0.51
1:A:208:LYS:HG2	2:A:413:HOH:O	2.10	0.51
1:B:89:THR:H	1:B:92:ASN:HD22	1.58	0.51
1:B:245:MET:O	1:B:259:MET:HE1	2.11	0.51
1:C:32:TRP:O	1:C:36:MET:HG2	2.11	0.51
1:D:220:ARG:O	1:D:224:LYS:HG3	2.11	0.51
1:A:95:GLN:NE2	1:B:184:GLY:H	2.09	0.51
1:D:238:HIS:HD2	1:D:273:SER:CB	2.24	0.51
1:C:88:PRO:HD3	1:D:191:TYR:HB3	1.93	0.51
1:D:162:GLY:HA3	1:D:275:PRO:HB2	1.91	0.51
1:A:296:VAL:HG23	1:A:306:ALA:HB2	1.92	0.50
1:A:202:ASN:HB2	2:A:396:HOH:O	2.09	0.50
1:C:142:LEU:HD11	1:C:270:SER:HB2	1.94	0.50
1:B:96:GLU:CD	2:B:470:HOH:O	2.55	0.50
1:A:21:TYR:O	1:A:24:GLN:HG2	2.12	0.50
1:C:2:ASN:ND2	1:C:172:GLY:H	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:192:LEU:HD11	1:B:197:GLY:HA2	1.94	0.50
1:A:146:THR:HG21	1:A:154:ALA:HA	1.93	0.50
1:C:120:ILE:HD12	1:C:180[B]:MET:SD	2.51	0.50
1:D:116[B]:MET:HE3	1:D:295:LEU:HB2	1.94	0.50
1:D:254:ILE:CD1	1:D:255:SER:N	2.70	0.49
1:B:173:ARG:HA	1:B:310:LYS:HB3	1.93	0.49
1:B:141:LYS:HD3	1:B:144:LYS:HD3	1.94	0.49
1:D:289:ASP:O	1:D:290:ASP:HB2	2.12	0.49
1:D:89:THR:H	1:D:92:ASN:HD22	1.60	0.49
1:A:279:ASP:O	1:A:283[B]:LYS:HD3	2.12	0.49
1:C:23:GLU:HG3	2:C:355:HOH:O	2.11	0.49
1:D:19:ASN:HD22	1:D:42:ARG:HH12	1.59	0.49
1:D:142:LEU:HD11	1:D:270:SER:HB2	1.94	0.49
1:B:116[A]:MET:HE1	1:B:297:GLY:N	2.27	0.49
1:A:268:ASN:C	1:A:268:ASN:ND2	2.69	0.49
1:B:116[A]:MET:HE1	1:B:297:GLY:CA	2.42	0.49
1:C:214:MET:HE1	1:C:237:PRO:HB2	1.95	0.49
1:A:89:THR:H	1:A:92:ASN:ND2	2.11	0.49
1:B:168:GLU:HB2	2:B:475:HOH:O	2.13	0.49
1:C:172:GLY:O	1:C:310:LYS:HD3	2.13	0.49
1:C:249:ARG:CZ	1:C:256:LYS:HG2	2.43	0.49
1:C:242:ILE:O	1:C:246:GLU:HG2	2.13	0.48
1:A:194:LYS:HG3	1:B:85:MET:HG2	1.96	0.48
1:B:68:ILE:HB	1:B:72:ASP:OD2	2.13	0.48
1:A:89:THR:HB	1:A:107:ASP:CG	2.39	0.48
1:C:89:THR:HB	1:C:107:ASP:CG	2.39	0.48
1:A:162:GLY:HA3	1:A:275:PRO:HB2	1.96	0.48
1:C:262:SER:HA	1:C:264:ASN:ND2	2.29	0.48
1:A:196:THR:HG22	1:A:198:LYS:H	1.78	0.47
1:D:89:THR:HB	1:D:107:ASP:CG	2.39	0.47
1:A:241:ASN:ND2	1:A:243:ARG:HB2	2.30	0.47
1:D:238:HIS:HD2	1:D:273:SER:HB3	1.80	0.47
1:B:142:LEU:HD11	1:B:270:SER:HB2	1.96	0.47
1:C:109:LEU:N	1:C:109:LEU:CD2	2.77	0.47
1:D:208:LYS:HB3	2:D:435:HOH:O	2.13	0.47
1:D:239:GLN:HB3	1:D:263:VAL:HB	1.94	0.47
1:B:212:ARG:HG2	1:B:212:ARG:HH11	1.80	0.47
1:C:288:LYS:HG2	1:C:291:ASP:OD2	2.14	0.47
1:B:249:ARG:HH21	1:B:256:LYS:HB3	1.79	0.47
1:A:199:LEU:HD23	1:A:199:LEU:C	2.40	0.47
1:C:162:GLY:HA3	1:C:275:PRO:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:232:ILE:HD12	1:C:294:VAL:HG23	1.97	0.47
1:D:192:LEU:C	1:D:192:LEU:HD13	2.40	0.46
1:A:141:LYS:HD3	1:A:144:LYS:CD	2.46	0.46
1:C:108:GLN:C	1:C:109:LEU:HD22	2.41	0.46
1:A:255:SER:CB	2:A:520:HOH:O	2.63	0.46
1:B:310:LYS:HE2	1:B:310:LYS:HB2	1.69	0.46
1:A:251:ARG:O	1:A:251:ARG:HG3	2.16	0.46
1:D:249:ARG:HG2	1:D:254:ILE:CG2	2.46	0.46
1:C:214:MET:HE3	1:C:296:VAL:HG13	1.98	0.46
1:C:241:ASN:OD1	1:C:244:ILE:HG13	2.16	0.46
1:A:204:ARG:O	1:A:208:LYS:HG3	2.15	0.46
1:A:218:SER:OG	1:A:235[A]:PHE:HE2	1.98	0.46
1:D:46:ASP:H	1:D:49:GLN:NE2	2.12	0.46
1:A:1:MET:N	2:A:466:HOH:O	2.35	0.45
1:A:108:GLN:C	1:A:109:LEU:HD23	2.41	0.45
1:A:214:MET:HB2	1:A:298:PHE:CE2	2.51	0.45
1:A:75:MET:HB3	1:A:134:ILE:HG12	1.98	0.45
1:A:93:MET:HE1	2:A:485:HOH:O	2.15	0.45
1:C:19:ASN:ND2	1:C:42:ARG:HH12	2.14	0.45
1:C:89:THR:H	1:C:92:ASN:ND2	2.14	0.45
1:A:78:VAL:HB	1:A:107:ASP:OD1	2.16	0.45
1:D:19:ASN:ND2	1:D:42:ARG:HH12	2.14	0.45
1:A:194:LYS:HE3	1:A:194:LYS:HB2	1.77	0.45
1:B:75:MET:HE1	1:B:125:TYR:CE2	2.51	0.45
1:B:234:LEU:HB2	1:B:293:ILE:CG2	2.40	0.45
1:C:196:THR:HG23	1:C:198:LYS:N	2.30	0.45
1:C:41:GLU:HG2	1:C:265:LYS:HA	1.99	0.45
1:B:89:THR:HB	1:B:107:ASP:CG	2.42	0.45
1:B:209:PHE:CG	1:B:302:LEU:HD13	2.52	0.45
1:C:37:THR:HG21	1:C:156:LEU:HD23	1.99	0.45
1:C:283:LYS:NZ	2:C:422:HOH:O	2.50	0.45
1:B:199:LEU:C	1:B:199:LEU:HD23	2.41	0.44
1:D:246:GLU:OE2	1:D:249:ARG:CZ	2.66	0.44
1:A:178:TYR:CD1	1:A:178:TYR:C	2.95	0.44
1:D:234:LEU:HB2	1:D:293:ILE:HG22	1.98	0.44
1:A:153:THR:HG22	1:A:201:MET:CE	2.47	0.44
1:A:200:LYS:HB3	1:A:200:LYS:HE3	1.63	0.44
1:B:209:PHE:HE1	1:B:298:PHE:HB2	1.82	0.44
1:C:8:PHE:CD1	1:C:8:PHE:C	2.96	0.44
1:C:239:GLN:HE22	1:C:262:SER:H	1.64	0.44
1:C:132:HIS:HE1	2:C:437:HOH:O	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:274:ILE:N	1:B:275:PRO:CD	2.81	0.44
1:B:301:GLY:N	1:B:302:LEU:HA	2.31	0.44
1:D:301:GLY:N	1:D:302:LEU:HA	2.33	0.44
1:A:272:ALA:O	1:A:275:PRO:HD2	2.17	0.43
1:D:265:LYS:NZ	1:D:280:GLN:HE21	2.16	0.43
1:B:249:ARG:NH2	1:B:256:LYS:HB3	2.33	0.43
1:A:192:LEU:C	1:A:192:LEU:HD13	2.43	0.43
1:D:246:GLU:OE2	1:D:249:ARG:HD3	2.19	0.43
1:C:115:PHE:HD2	1:C:116[A]:MET:CE	2.30	0.43
1:D:256:LYS:HB2	1:D:256:LYS:HZ3	1.83	0.43
1:B:8:PHE:CD2	1:B:8:PHE:C	2.96	0.43
1:B:162:GLY:HA3	1:B:275:PRO:CB	2.49	0.43
1:D:142:LEU:HD13	1:D:157:PHE:CD1	2.53	0.43
1:B:225:ALA:O	1:B:226:ASN:HB2	2.18	0.43
1:B:250:GLU:C	1:B:252:LEU:N	2.77	0.43
1:D:194:LYS:CB	1:D:194:LYS:NZ	2.82	0.43
1:B:6:LYS:NZ	1:B:133:ASN:HD21	2.17	0.42
1:A:241:ASN:HB3	1:A:244:ILE:HB	2.00	0.42
1:B:156:LEU:CD1	1:B:201:MET:HE1	2.49	0.42
1:C:301:GLY:N	1:C:302:LEU:HA	2.33	0.42
1:B:6:LYS:HE2	1:B:133:ASN:HD21	1.82	0.42
1:C:83:GLY:O	1:C:84:ASP:C	2.62	0.42
1:C:192:LEU:HD22	1:D:86:PRO:CG	2.50	0.42
1:A:285:GLY:O	1:A:288:LYS:HE2	2.19	0.42
1:D:188:LYS:HE3	1:D:189:HIS:CE1	2.54	0.42
1:A:301:GLY:HA2	1:B:92:ASN:ND2	2.35	0.42
1:C:146:THR:O	1:C:148:LEU:HD22	2.20	0.42
1:D:87:PHE:HA	1:D:88:PRO:C	2.45	0.42
1:A:173:ARG:HA	1:A:310:LYS:HB3	2.01	0.42
1:B:281:GLU:HA	1:B:281:GLU:OE2	2.19	0.42
1:B:108:GLN:HE22	1:B:121:THR:HG21	1.84	0.42
1:C:120:ILE:HD12	1:C:180[B]:MET:CE	2.50	0.42
1:C:180[A]:MET:HE1	1:D:75:MET:HE1	2.02	0.42
1:D:32:TRP:O	1:D:36:MET:HG2	2.20	0.42
1:C:180[B]:MET:CE	1:C:306:ALA:H	2.33	0.42
1:B:87:PHE:HA	1:B:88:PRO:C	2.45	0.41
1:C:262:SER:HA	1:C:264:ASN:HD21	1.84	0.41
1:D:173:ARG:HA	1:D:310:LYS:HB3	2.02	0.41
1:A:301:GLY:N	1:A:302:LEU:HA	2.34	0.41
1:D:119:MET:HE3	1:D:307:MET:SD	2.60	0.41
1:D:202:ASN:ND2	1:D:205:GLU:H	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ILE:HD12	1:A:294:VAL:HG23	2.01	0.41
1:B:96:GLU:HG3	2:B:470:HOH:O	2.19	0.41
1:B:235:PHE:HD1	1:B:259:MET:HE3	1.83	0.41
1:C:1:MET:N	2:C:412:HOH:O	2.52	0.41
1:D:249:ARG:HH12	1:D:250:GLU:HG3	1.85	0.41
1:A:268:ASN:HD22	1:A:269:THR:N	2.18	0.41
1:C:125:TYR:HD2	1:C:131:TYR:CE2	2.37	0.41
1:C:234:LEU:HB2	1:C:293:ILE:HG22	2.02	0.41
1:A:288:LYS:O	1:A:289:ASP:C	2.64	0.41
1:B:162:GLY:HA3	1:B:275:PRO:HB2	2.03	0.41
1:B:188:LYS:HB2	2:B:382:HOH:O	2.19	0.41
1:B:241:ASN:HD22	1:B:241:ASN:C	2.29	0.41
1:C:95:GLN:HE21	1:D:184:GLY:H	1.67	0.41
1:A:87:PHE:HA	1:A:88:PRO:C	2.45	0.41
1:A:241:ASN:HD22	1:A:241:ASN:C	2.29	0.41
1:C:193:ASP:OD1	1:C:196:THR:HG22	2.20	0.41
1:C:239:GLN:HB3	1:C:263:VAL:HB	2.03	0.41
1:C:245:MET:HE1	1:C:263:VAL:CG1	2.50	0.41
1:A:255:SER:HB2	2:A:520:HOH:O	2.20	0.41
1:B:254:ILE:HG23	1:B:258:LYS:HB2	2.03	0.41
1:A:214:MET:HE3	1:A:237:PRO:CB	2.50	0.40
1:B:6:LYS:CE	1:B:133:ASN:HD21	2.34	0.40
1:B:209:PHE:CE1	1:B:298:PHE:HB2	2.56	0.40
1:C:248:ALA:O	1:C:251:ARG:HB3	2.21	0.40
1:D:1:MET:HG3	1:D:3:VAL:HG23	2.02	0.40
1:A:97:ARG:HD2	2:A:424:HOH:O	2.20	0.40
1:A:235[B]:PHE:CE2	1:A:254:ILE:CD1	3.03	0.40
1:C:162:GLY:HA3	1:C:275:PRO:HB2	2.02	0.40
1:C:201:MET:HE2	1:C:201:MET:HB3	1.91	0.40
1:A:274:ILE:HB	1:A:275:PRO:HD3	2.02	0.40
1:B:200:LYS:HE2	1:B:200:LYS:HB3	1.85	0.40
1:D:116[B]:MET:CE	1:D:306:ALA:HA	2.39	0.40
1:D:290:ASP:OD1	1:D:310:LYS:NZ	2.54	0.40
1:A:60:VAL:CG2	2:A:330:HOH:O	2.69	0.40
1:A:249:ARG:HG3	1:A:254:ILE:HG22	2.04	0.40
1:C:75:MET:HE1	1:C:125:TYR:CD2	2.56	0.40
1:C:207:PHE:CD1	1:C:244:ILE:HG12	2.56	0.40
1:A:251:ARG:HE	1:A:251:ARG:HB2	1.69	0.40
1:B:296:VAL:HG23	1:B:306:ALA:HB2	2.03	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	313/313 (100%)	302 (96%)	11 (4%)	0	100	100
1	B	312/313 (100%)	301 (96%)	11 (4%)	0	100	100
1	C	314/313 (100%)	299 (95%)	15 (5%)	0	100	100
1	D	313/313 (100%)	304 (97%)	9 (3%)	0	100	100
All	All	1252/1252 (100%)	1206 (96%)	46 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	254/252 (101%)	240 (94%)	14 (6%)	19	17
1	B	253/252 (100%)	243 (96%)	10 (4%)	28	27
1	C	255/252 (101%)	245 (96%)	10 (4%)	28	28
1	D	254/252 (101%)	242 (95%)	12 (5%)	23	22
All	All	1016/1008 (101%)	970 (96%)	46 (4%)	26	23

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	69	GLN
1	A	71	GLU

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Mol	Chain	Res	Type
1	A	106[A]	MET
1	A	106[B]	MET
1	A	109	LEU
1	A	171	GLU
1	A	196	THR
1	A	220	ARG
1	A	236	ILE
1	A	241	ASN
1	A	242	ILE
1	A	258	LYS
1	A	268	ASN
1	A	277	SER
1	B	41	GLU
1	B	106[A]	MET
1	B	106[B]	MET
1	B	148	LEU
1	B	188	LYS
1	B	196	THR
1	B	241	ASN
1	B	252	LEU
1	B	254	ILE
1	B	277	SER
1	C	14	GLU
1	C	109	LEU
1	C	170	SER
1	C	171	GLU
1	C	195	ASP
1	C	202	ASN
1	C	220	ARG
1	C	241	ASN
1	C	264	ASN
1	C	277	SER
1	D	71	GLU
1	D	106[A]	MET
1	D	106[B]	MET
1	D	194	LYS
1	D	202	ASN
1	D	249	ARG
1	D	252	LEU
1	D	254	ILE
1	D	256	LYS
1	D	268	ASN

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Mol	Chain	Res	Type
1	D	277	SER
1	D	286	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	49	GLN
1	A	69	GLN
1	A	92	ASN
1	A	95	GLN
1	A	226	ASN
1	A	238	HIS
1	A	239	GLN
1	A	241	ASN
1	A	268	ASN
1	B	49	GLN
1	B	92	ASN
1	B	95	GLN
1	B	108	GLN
1	B	133	ASN
1	B	189	HIS
1	B	238	HIS
1	B	239	GLN
1	B	241	ASN
1	C	2	ASN
1	C	19	ASN
1	C	49	GLN
1	C	92	ASN
1	C	95	GLN
1	C	108	GLN
1	C	132	HIS
1	C	202	ASN
1	C	239	GLN
1	C	264	ASN
1	D	19	ASN
1	D	24	GLN
1	D	49	GLN
1	D	92	ASN
1	D	95	GLN
1	D	108	GLN
1	D	124	GLN

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Mol	Chain	Res	Type
1	D	127	GLN
1	D	202	ASN
1	D	238	HIS
1	D	268	ASN
1	D	280	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	312/313 (99%)	0.19	6 (1%) 66 66	13, 22, 36, 46	3 (0%)
1	B	312/313 (99%)	0.13	6 (1%) 66 66	11, 20, 38, 47	2 (0%)
1	C	312/313 (99%)	0.34	7 (2%) 62 61	13, 24, 40, 51	4 (1%)
1	D	312/313 (99%)	0.13	4 (1%) 75 74	10, 20, 36, 40	3 (0%)
All	All	1248/1252 (99%)	0.20	23 (1%) 67 67	10, 22, 37, 51	12 (0%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	253	GLY	4.7
1	B	195	ASP	3.9
1	C	253	GLY	3.1
1	C	225	ALA	2.9
1	B	223	GLU	2.7
1	B	250	GLU	2.6
1	A	129	GLY	2.6
1	C	254	ILE	2.5
1	A	195	ASP	2.4
1	B	253	GLY	2.3
1	C	230	ASP	2.3
1	C	14	GLU	2.3
1	D	223	GLU	2.3
1	D	250	GLU	2.3
1	B	196	THR	2.3
1	D	247	SER	2.2
1	B	252	LEU	2.2
1	C	67	GLY	2.2
1	A	246	GLU	2.2
1	A	254	ILE	2.1
1	D	253	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	229	SER	2.1
1	A	252	LEU	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.