



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:03 AM UTC

PDB ID : 2FLO / pdb_00002flo
Title : Crystal structure of exopolyphosphatase (PPX) from E. coli O157:H7
Authors : Rangarajan, E.S.; Cygler, M.; Matte, A.; Montreal-Kingston Bacterial Structural Genomics Initiative (BSGI)
Deposited on : 2006-01-06
Resolution : 2.20 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)
Xtrriage (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

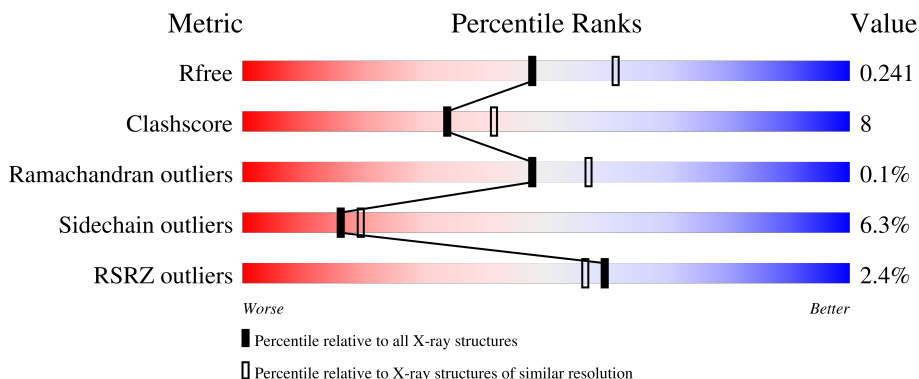
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION



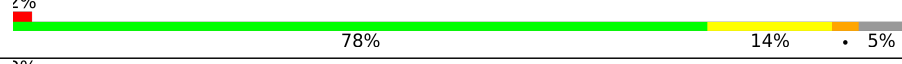

The reported resolution of this entry is 2.20 Å.

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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	524	 2% 76% 16% • 5%
1	B	524	 3% 79% 13% • 6%
1	C	524	 2% 78% 14% • 5%
1	D	524	 2% 76% 17% • 5%

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 16478 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 Exopolyphosphatase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	496	3964	2511	714	718	4	17	0	1	0
1	B	495	3955	2506	712	716	4	17	0	1	0
1	C	496	3965	2511	714	718	5	17	0	2	0
1	D	496	3964	2511	714	718	4	17	0	1	0

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MSE	-	cloning artifact	UNP P0AFL8
A	-9	GLY	-	cloning artifact	UNP P0AFL8
A	-8	SER	-	cloning artifact	UNP P0AFL8
A	-7	SER	-	cloning artifact	UNP P0AFL8
A	-6	HIS	-	expression tag	UNP P0AFL8
A	-5	HIS	-	expression tag	UNP P0AFL8
A	-4	HIS	-	expression tag	UNP P0AFL8
A	-3	HIS	-	expression tag	UNP P0AFL8
A	-2	HIS	-	expression tag	UNP P0AFL8
A	-1	HIS	-	expression tag	UNP P0AFL8
A	0	GLY	-	cloning artifact	UNP P0AFL8
A	1	SER	-	cloning artifact	UNP P0AFL8
A	25	MSE	MET	modified residue	UNP P0AFL8
A	35	MSE	MET	modified residue	UNP P0AFL8
A	56	MSE	MET	modified residue	UNP P0AFL8
A	62	MSE	MET	modified residue	UNP P0AFL8
A	127	MSE	MET	modified residue	UNP P0AFL8
A	167	MSE	MET	modified residue	UNP P0AFL8
A	192	MSE	MET	modified residue	UNP P0AFL8
A	214	MSE	MET	modified residue	UNP P0AFL8
A	228	MSE	MET	modified residue	UNP P0AFL8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	230	MSE	MET	modified residue	UNP P0AFL8
A	305	MSE	MET	modified residue	UNP P0AFL8
A	341	MSE	MET	modified residue	UNP P0AFL8
A	343	MSE	MET	modified residue	UNP P0AFL8
A	368	MSE	MET	modified residue	UNP P0AFL8
A	404	MSE	MET	modified residue	UNP P0AFL8
A	405	MSE	MET	modified residue	UNP P0AFL8
B	-10	MSE	-	cloning artifact	UNP P0AFL8
B	-9	GLY	-	cloning artifact	UNP P0AFL8
B	-8	SER	-	cloning artifact	UNP P0AFL8
B	-7	SER	-	cloning artifact	UNP P0AFL8
B	-6	HIS	-	expression tag	UNP P0AFL8
B	-5	HIS	-	expression tag	UNP P0AFL8
B	-4	HIS	-	expression tag	UNP P0AFL8
B	-3	HIS	-	expression tag	UNP P0AFL8
B	-2	HIS	-	expression tag	UNP P0AFL8
B	-1	HIS	-	expression tag	UNP P0AFL8
B	0	GLY	-	cloning artifact	UNP P0AFL8
B	1	SER	-	cloning artifact	UNP P0AFL8
B	25	MSE	MET	modified residue	UNP P0AFL8
B	35	MSE	MET	modified residue	UNP P0AFL8
B	56	MSE	MET	modified residue	UNP P0AFL8
B	62	MSE	MET	modified residue	UNP P0AFL8
B	127	MSE	MET	modified residue	UNP P0AFL8
B	167	MSE	MET	modified residue	UNP P0AFL8
B	192	MSE	MET	modified residue	UNP P0AFL8
B	214	MSE	MET	modified residue	UNP P0AFL8
B	228	MSE	MET	modified residue	UNP P0AFL8
B	230	MSE	MET	modified residue	UNP P0AFL8
B	305	MSE	MET	modified residue	UNP P0AFL8
B	341	MSE	MET	modified residue	UNP P0AFL8
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C	-8	SER	-	cloning artifact	UNP P0AFL8
C	-7	SER	-	cloning artifact	UNP P0AFL8
C	-6	HIS	-	expression tag	UNP P0AFL8
C	-5	HIS	-	expression tag	UNP P0AFL8
C	-4	HIS	-	expression tag	UNP P0AFL8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP P0AFL8
C	-2	HIS	-	expression tag	UNP P0AFL8
C	-1	HIS	-	expression tag	UNP P0AFL8
C	0	GLY	-	cloning artifact	UNP P0AFL8
C	1	SER	-	cloning artifact	UNP P0AFL8
C	25	MSE	MET	modified residue	UNP P0AFL8
C	35	MSE	MET	modified residue	UNP P0AFL8
C	56	MSE	MET	modified residue	UNP P0AFL8
C	62	MSE	MET	modified residue	UNP P0AFL8
C	127	MSE	MET	modified residue	UNP P0AFL8
C	167	MSE	MET	modified residue	UNP P0AFL8
C	192	MSE	MET	modified residue	UNP P0AFL8
C	214	MSE	MET	modified residue	UNP P0AFL8
C	228	MSE	MET	modified residue	UNP P0AFL8
C	230	MSE	MET	modified residue	UNP P0AFL8
C	305	MSE	MET	modified residue	UNP P0AFL8
C	341	MSE	MET	modified residue	UNP P0AFL8
C	343	MSE	MET	modified residue	UNP P0AFL8
C	368	MSE	MET	modified residue	UNP P0AFL8
C	404	MSE	MET	modified residue	UNP P0AFL8
C	405	MSE	MET	modified residue	UNP P0AFL8
D	-10	MSE	-	cloning artifact	UNP P0AFL8
D	-9	GLY	-	cloning artifact	UNP P0AFL8
D	-8	SER	-	cloning artifact	UNP P0AFL8
D	-7	SER	-	cloning artifact	UNP P0AFL8
D	-6	HIS	-	expression tag	UNP P0AFL8
D	-5	HIS	-	expression tag	UNP P0AFL8
D	-4	HIS	-	expression tag	UNP P0AFL8
D	-3	HIS	-	expression tag	UNP P0AFL8
D	-2	HIS	-	expression tag	UNP P0AFL8
D	-1	HIS	-	expression tag	UNP P0AFL8
D	0	GLY	-	cloning artifact	UNP P0AFL8
D	1	SER	-	cloning artifact	UNP P0AFL8
D	25	MSE	MET	modified residue	UNP P0AFL8
D	35	MSE	MET	modified residue	UNP P0AFL8
D	56	MSE	MET	modified residue	UNP P0AFL8
D	62	MSE	MET	modified residue	UNP P0AFL8
D	127	MSE	MET	modified residue	UNP P0AFL8
D	167	MSE	MET	modified residue	UNP P0AFL8
D	192	MSE	MET	modified residue	UNP P0AFL8
D	214	MSE	MET	modified residue	UNP P0AFL8
D	228	MSE	MET	modified residue	UNP P0AFL8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	230	MSE	MET	modified residue	UNP P0AFL8
D	305	MSE	MET	modified residue	UNP P0AFL8
D	341	MSE	MET	modified residue	UNP P0AFL8
D	343	MSE	MET	modified residue	UNP P0AFL8
D	368	MSE	MET	modified residue	UNP P0AFL8
D	404	MSE	MET	modified residue	UNP P0AFL8
D	405	MSE	MET	modified residue	UNP P0AFL8

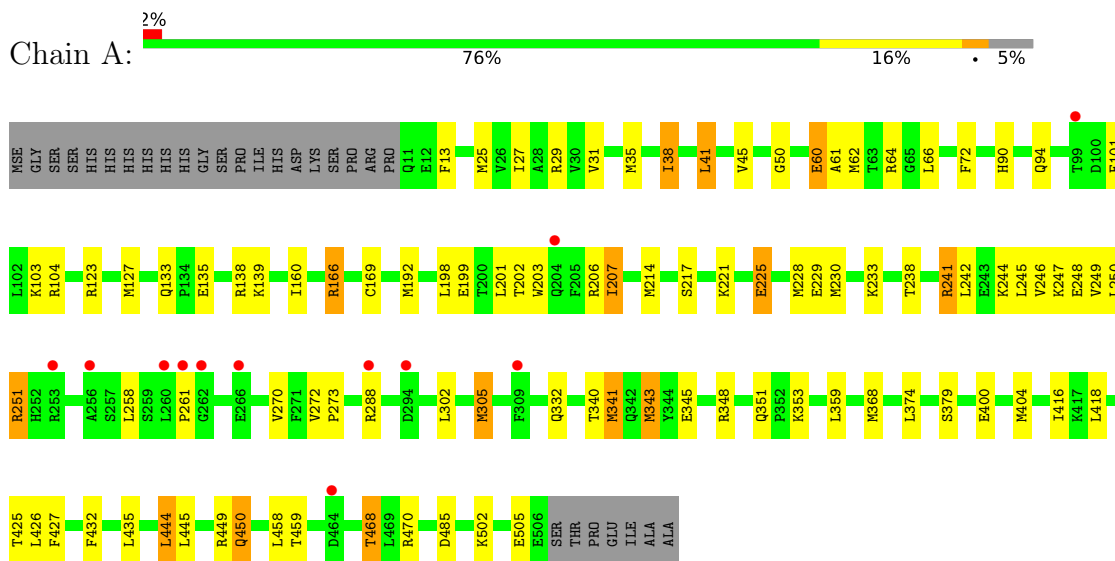
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	142	Total 142	O 142	0	0
2	B	167	Total 167	O 167	0	0
2	C	166	Total 166	O 166	0	0
2	D	155	Total 155	O 155	0	0

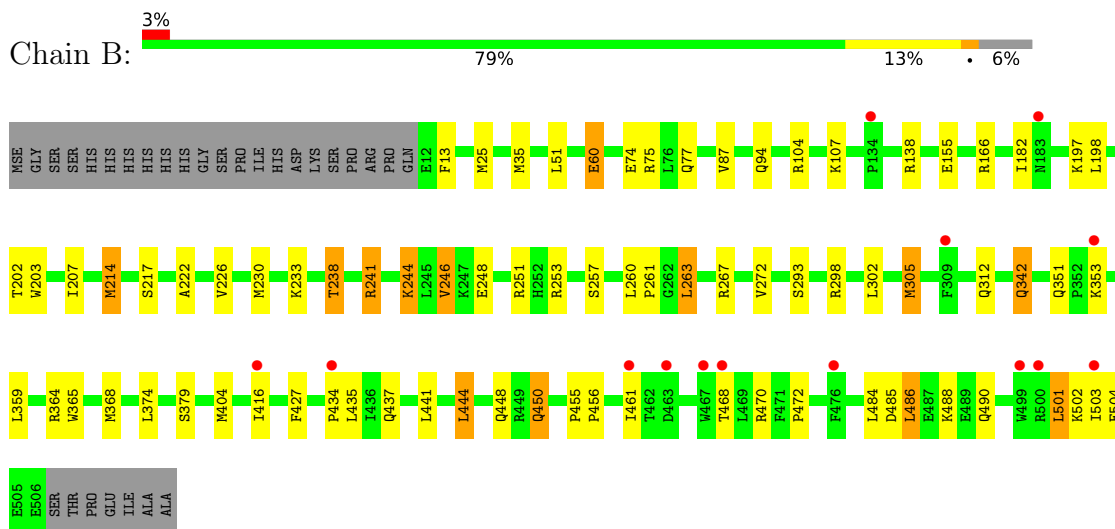
3 Residue-property plots [i](#)

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.

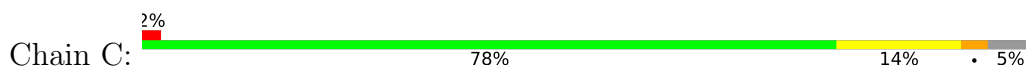
- Molecule 1: Exopolyphosphatase

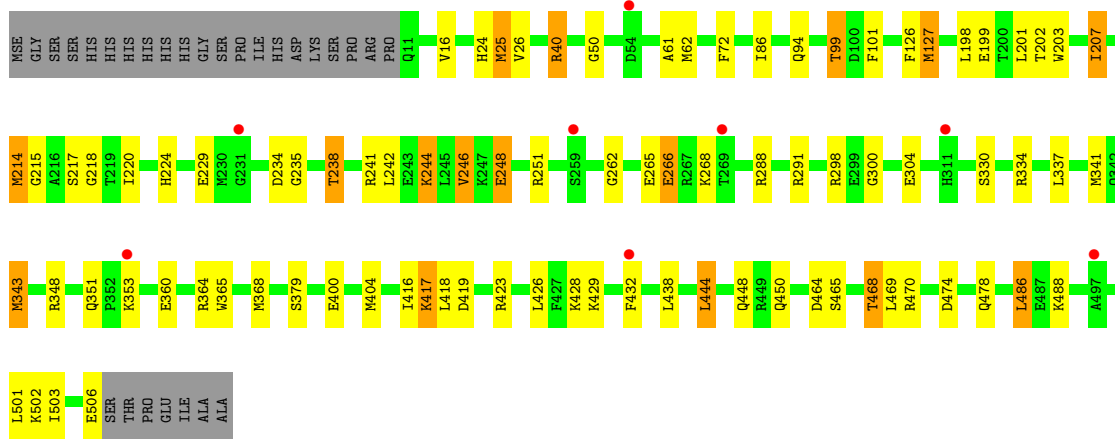


- Molecule 1: Exopolyphosphatase

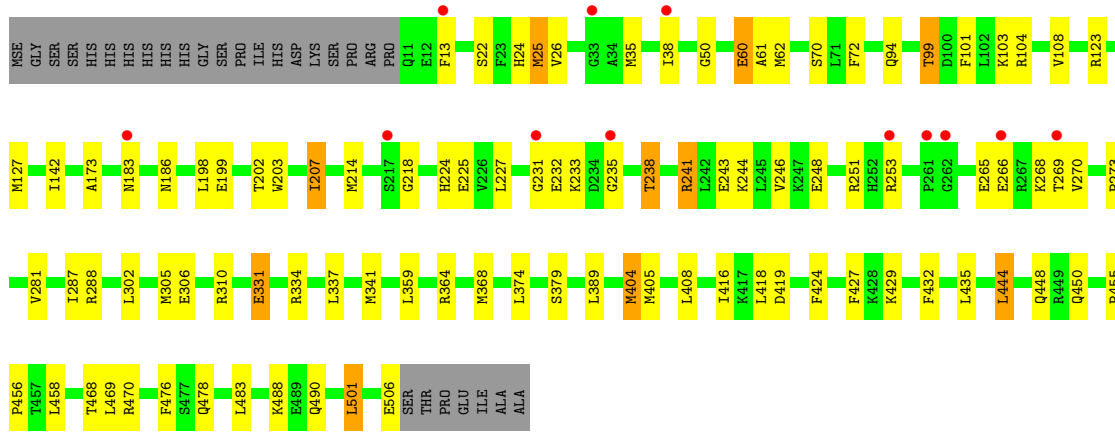
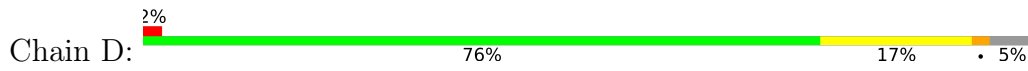


- Molecule 1: Exopolyphosphatase





● Molecule 1: Exopolyphosphatase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.55Å 132.14Å 107.85Å 90.00° 105.10° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.20) 97.9 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.05Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.202 , 0.247 0.199 , 0.241	Depositor DCC
R_{free} test set	6490 reflections (3.95%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtrriage
Anisotropy	0.275	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16478	wwPDB-VP
Average B, all atoms (Å ²)	35.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.70	3/4031 (0.1%)	0.87	1/5417 (0.0%)
1	B	0.69	2/4022 (0.0%)	0.88	2/5405 (0.0%)
1	C	0.74	3/4037 (0.1%)	0.87	0/5425
1	D	0.69	1/4031 (0.0%)	0.90	1/5417 (0.0%)
All	All	0.70	9/16121 (0.1%)	0.88	4/21664 (0.0%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	127	MSE	SE-CE	-9.28	1.67	1.95
1	A	305	MSE	SE-CE	-8.15	1.71	1.95
1	D	25	MSE	SE-CE	-7.78	1.72	1.95
1	A	343	MSE	SE-CE	-7.24	1.73	1.95
1	C	25	MSE	SE-CE	-6.99	1.74	1.95
1	A	341	MSE	SE-CE	-6.11	1.77	1.95
1	B	305	MSE	SE-CE	-5.73	1.78	1.95
1	C	404	MSE	SE-CE	-5.24	1.79	1.95
1	B	272	VAL	CA-C	5.12	1.57	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	218	GLY	N-CA-C	6.52	120.06	112.50
1	B	87	VAL	N-CA-C	5.59	116.64	108.53
1	A	160	ILE	N-CA-C	-5.36	107.38	111.62
1	B	246	VAL	N-CA-CB	5.09	117.47	110.54

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	3964	0	3993	65	0
1	B	3955	0	3985	62	0
1	C	3965	0	3994	64	0
1	D	3964	0	3993	71	0
2	A	142	0	0	2	0
2	B	167	0	0	5	0
2	C	166	0	0	1	0
2	D	155	0	0	6	0
All	All	16478	0	15965	244	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 8.

All (244) 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:368[A]:MSE:HG2	2:D:629:HOH:O	1.42	1.19
1:D:302:LEU:HA	1:D:305:MSE:HE2	1.23	1.16
1:A:302:LEU:HA	1:A:305:MSE:HE2	1.31	1.11
1:B:368[A]:MSE:HG2	2:B:642:HOH:O	1.50	1.10
1:A:444:LEU:HD21	1:A:485:ASP:HB3	1.20	1.10
1:C:126:PHE:CD2	1:C:127:MSE:HE2	1.87	1.08
1:D:302:LEU:HD23	1:D:305:MSE:HE1	1.36	1.03
1:C:126:PHE:HD2	1:C:127:MSE:HE2	1.21	1.00
1:C:300:GLY:O	1:C:304:GLU:HG2	1.60	1.00
1:A:302:LEU:HD23	1:A:305:MSE:HE1	1.44	0.98
1:B:302:LEU:HA	1:B:305:MSE:HE2	1.48	0.95
1:A:444:LEU:CD2	1:A:485:ASP:HB3	1.98	0.92
1:A:62:MSE:HE3	1:A:101:PHE:HA	1.54	0.90
1:C:126:PHE:CD2	1:C:127:MSE:CE	2.56	0.88
1:D:337:LEU:HD12	1:D:341:MSE:HE3	1.56	0.87
1:B:230:MSE:HE3	1:B:261:PRO:HD2	1.55	0.86
1:D:224:HIS:CE1	1:D:235:GLY:HA3	2.12	0.84
1:C:126:PHE:HD2	1:C:127:MSE:CE	1.91	0.84
1:B:365:TRP:HD1	1:B:368[B]:MSE:HE3	1.43	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:441:LEU:HA	1:B:444:LEU:HD12	1.57	0.84
1:B:444:LEU:HD23	1:B:485:ASP:HB3	1.59	0.83
1:D:62:MSE:HE3	1:D:101:PHE:HA	1.57	0.83
1:B:238:THR:HG22	1:B:241:ARG:H	1.42	0.83
1:C:99:THR:HG22	2:C:635:HOH:O	1.77	0.82
1:D:337:LEU:HD12	1:D:341:MSE:CE	2.10	0.82
1:D:302:LEU:HD23	1:D:305:MSE:CE	2.09	0.81
1:A:198:LEU:O	1:A:202:THR:HG23	1.81	0.80
1:B:456:PRO:HD2	1:B:472:PRO:HG2	1.64	0.79
1:A:302:LEU:HD23	1:A:305:MSE:CE	2.11	0.79
1:A:343:MSE:HE2	1:A:458:LEU:HD21	1.65	0.79
1:C:238:THR:HB	1:C:241:ARG:HG3	1.66	0.78
1:D:337:LEU:CD1	1:D:341:MSE:HE3	2.13	0.78
1:C:234:ASP:OD1	1:C:241:ARG:NH2	2.17	0.78
1:C:40:ARG:HG3	1:C:40:ARG:HH11	1.50	0.77
1:A:302:LEU:HA	1:A:305:MSE:CE	2.15	0.76
1:A:221:LYS:O	1:A:225:GLU:HG2	1.86	0.76
1:B:342:GLN:HG2	2:B:606:HOH:O	1.85	0.75
1:A:203:TRP:CE2	1:B:450:GLN:HG3	2.21	0.74
1:B:441:LEU:HA	1:B:444:LEU:CD1	2.18	0.74
1:D:302:LEU:HA	1:D:305:MSE:CE	2.13	0.73
1:A:238:THR:OG1	1:A:241:ARG:HG3	1.88	0.73
1:D:25:MSE:HE2	1:D:72:PHE:CG	2.24	0.73
1:A:343:MSE:CE	1:A:458:LEU:HD21	2.21	0.71
1:B:302:LEU:HD23	1:B:305:MSE:HE1	1.74	0.69
1:C:444:LEU:HD21	1:C:486:LEU:HD13	1.74	0.69
1:C:244:LYS:HE3	1:C:244:LYS:HA	1.76	0.68
1:D:341:MSE:HG2	1:D:364:ARG:HH11	1.57	0.68
1:C:62:MSE:HE3	1:C:101:PHE:HA	1.74	0.68
1:A:450:GLN:HG3	1:B:203:TRP:CE2	2.28	0.67
1:C:365:TRP:HD1	1:C:368[B]:MSE:CE	2.08	0.67
1:B:104:ARG:HD2	2:B:607:HOH:O	1.93	0.67
1:B:230:MSE:HE1	1:B:248:GLU:HG2	1.77	0.67
1:C:448:GLN:HG2	1:D:199:GLU:HB2	1.77	0.66
1:D:198:LEU:O	1:D:202:THR:HG23	1.96	0.65
1:B:244:LYS:HE3	1:B:244:LYS:HA	1.79	0.65
1:C:126:PHE:CE2	1:C:127:MSE:CE	2.80	0.65
1:B:182:ILE:O	1:B:253:ARG:NH2	2.29	0.65
1:A:228:MSE:HE2	1:A:233:LYS:O	1.97	0.64
1:C:400:GLU:HB2	1:C:426:LEU:HD22	1.79	0.64
1:D:389:LEU:HD22	1:D:405:MSE:HE3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:138:ARG:HA	1:B:155:GLU:HB3	1.81	0.63
1:C:126:PHE:CE2	1:C:127:MSE:HE1	2.34	0.63
1:C:341:MSE:HE1	1:C:360:GLU:HG3	1.80	0.63
1:B:13:PHE:HD1	1:B:305:MSE:CE	2.12	0.62
1:B:198:LEU:O	1:B:202:THR:HG23	1.99	0.61
1:D:25:MSE:HE2	1:D:72:PHE:CD1	2.35	0.61
1:B:302:LEU:HD23	1:B:305:MSE:CE	2.31	0.61
1:D:25:MSE:CE	1:D:72:PHE:CD1	2.84	0.61
1:C:199:GLU:HB2	1:D:448:GLN:HG2	1.82	0.60
1:D:62:MSE:HE3	1:D:101:PHE:CA	2.28	0.60
1:C:224:HIS:CE1	1:C:235:GLY:HA3	2.37	0.60
1:C:365:TRP:HD1	1:C:368[B]:MSE:HE3	1.65	0.60
1:D:24:HIS:HB3	2:D:613:HOH:O	2.02	0.60
1:B:13:PHE:CD1	1:B:305:MSE:HE3	2.36	0.59
1:D:404:MSE:HE1	1:D:408:LEU:HD11	1.83	0.59
1:A:400:GLU:HB2	1:A:426:LEU:HD22	1.85	0.59
1:D:243:GLU:HA	1:D:246:VAL:HG12	1.83	0.59
1:C:126:PHE:HE2	1:C:127:MSE:HE1	1.68	0.59
1:C:450:GLN:HG2	1:D:203:TRP:CD2	2.39	0.58
1:A:166:ARG:HG2	2:A:517:HOH:O	2.04	0.58
1:A:345:GLU:OE1	1:A:348:ARG:NH2	2.38	0.56
1:B:434:PRO:HA	1:B:437:GLN:OE1	2.06	0.56
1:A:340:THR:HG22	1:A:341:MSE:HE2	1.88	0.56
1:C:50:GLY:HA3	1:C:61:ALA:HB2	1.87	0.56
1:D:203:TRP:CZ2	1:D:207:ILE:HG13	2.41	0.56
1:A:13:PHE:CD1	1:A:305:MSE:HE3	2.41	0.56
1:C:343:MSE:HE1	1:C:469:LEU:CD2	2.36	0.56
1:C:214:MSE:HE3	1:C:291:ARG:HB2	1.89	0.55
1:C:242:LEU:O	1:C:246:VAL:HG13	2.07	0.55
1:D:238:THR:HB	1:D:241:ARG:HG3	1.89	0.55
1:D:266:GLU:O	1:D:269:THR:HG22	2.07	0.55
1:A:90:HIS:CE1	1:A:94:GLN:HG3	2.42	0.55
1:A:62:MSE:HE3	1:A:101:PHE:CA	2.34	0.55
1:D:183:ASN:HB2	1:D:186:ASN:HB2	1.89	0.55
1:C:343:MSE:HE1	1:C:469:LEU:HD22	1.89	0.54
1:C:203:TRP:CE2	1:D:450:GLN:HG3	2.43	0.54
1:A:50:GLY:HA3	1:A:61:ALA:HB2	1.91	0.53
1:A:207:ILE:HD11	1:C:330:SER:HB3	1.90	0.53
1:A:206:ARG:O	1:C:334:ARG:HD3	2.07	0.53
1:B:13:PHE:HD1	1:B:305:MSE:HE3	1.73	0.53
1:B:364:ARG:O	1:B:368[A]:MSE:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:248:GLU:O	1:B:251:ARG:HG2	2.08	0.53
1:C:343:MSE:HB2	1:C:438:LEU:HD22	1.91	0.53
1:B:468:THR:HG22	1:B:502:LYS:HB2	1.89	0.53
1:C:198:LEU:O	1:C:202:THR:HG23	2.08	0.53
1:D:238:THR:HG22	1:D:241:ARG:H	1.73	0.53
1:D:183:ASN:HB3	1:D:186:ASN:H	1.74	0.52
1:B:260:LEU:HB2	1:B:263:LEU:HD22	1.90	0.52
1:B:444:LEU:HD23	1:B:485:ASP:CB	2.35	0.52
1:C:40:ARG:HG3	1:C:40:ARG:NH1	2.21	0.52
1:A:169:CYS:HB2	1:A:270:VAL:HB	1.91	0.52
1:A:199:GLU:HB2	1:B:448:GLN:HG2	1.91	0.52
1:D:224:HIS:ND1	1:D:235:GLY:HA3	2.25	0.52
1:A:45:VAL:O	1:A:64:ARG:HD2	2.09	0.52
1:C:248:GLU:O	1:C:251:ARG:HG2	2.10	0.51
1:C:26:VAL:HG23	1:C:298:ARG:HD2	1.92	0.51
1:A:13:PHE:HD1	1:A:305:MSE:HE3	1.75	0.51
1:A:229:GLU:HB3	1:A:261:PRO:HB2	1.91	0.51
1:A:450:GLN:HG2	1:B:203:TRP:CD2	2.46	0.51
1:A:450:GLN:CG	1:B:203:TRP:CD2	2.94	0.51
1:B:13:PHE:CD1	1:B:305:MSE:CE	2.93	0.50
1:B:298:ARG:HG2	2:B:618:HOH:O	2.11	0.50
1:D:490:GLN:HG2	1:D:501:LEU:HB3	1.93	0.50
1:D:458:LEU:HD11	1:D:469:LEU:HD22	1.93	0.50
1:C:238:THR:HG22	1:C:241:ARG:H	1.77	0.50
1:D:50:GLY:HA3	1:D:61:ALA:HB2	1.93	0.50
1:A:368[A]:MSE:HG3	2:A:584:HOH:O	2.11	0.50
1:D:62:MSE:HE2	1:D:104:ARG:HD2	1.94	0.50
1:B:238:THR:CG2	1:B:241:ARG:HG3	2.41	0.50
1:B:13:PHE:HD1	1:B:305:MSE:HE1	1.78	0.49
1:D:331:GLU:HG2	2:D:574:HOH:O	2.12	0.49
1:D:470:ARG:HD3	1:D:506:GLU:HG3	1.94	0.49
1:B:404:MSE:HG3	1:B:427:PHE:CD2	2.47	0.49
1:C:203:TRP:CE2	1:C:207:ILE:HG13	2.47	0.49
1:A:343:MSE:HE1	1:A:445:LEU:HD11	1.94	0.49
1:B:25:MSE:HE1	1:B:75:ARG:HG2	1.95	0.49
1:B:222:ALA:HB2	1:B:267:ARG:HD3	1.94	0.49
1:C:343:MSE:HB2	1:C:438:LEU:CD2	2.42	0.49
1:B:51:LEU:HD21	1:B:94:GLN:HG2	1.95	0.49
1:B:490:GLN:HG2	1:B:501:LEU:HB3	1.95	0.49
1:A:450:GLN:CG	1:B:203:TRP:CE2	2.96	0.48
1:B:238:THR:HG22	1:B:241:ARG:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368[A]:MSE:CG	2:D:629:HOH:O	2.24	0.48
1:A:468:THR:HB	1:A:502:LYS:HB2	1.96	0.48
1:B:359:LEU:HB3	1:B:435:LEU:HD11	1.95	0.48
1:B:365:TRP:CD1	1:B:368[B]:MSE:HE3	2.35	0.48
1:A:123:ARG:O	1:A:127:MSE:HG2	2.13	0.48
1:B:226:VAL:HG21	1:B:263:LEU:HD13	1.95	0.48
1:C:266:GLU:CD	1:C:266:GLU:H	2.20	0.48
1:A:450:GLN:HG3	1:B:203:TRP:CZ2	2.49	0.48
1:C:501:LEU:HG	1:C:503:ILE:CD1	2.45	0.47
1:A:62:MSE:CE	1:A:101:PHE:HA	2.34	0.47
1:A:13:PHE:HD1	1:A:305:MSE:CE	2.27	0.47
1:B:226:VAL:CG2	1:B:263:LEU:HD13	2.44	0.47
1:D:306:GLU:OE2	1:D:310:ARG:HD3	2.15	0.47
1:A:133:GLN:HE22	1:A:214:MSE:SE	2.47	0.47
1:A:288:ARG:HA	1:A:288:ARG:NE	2.30	0.47
1:B:470:ARG:NH2	1:B:504:GLU:OE2	2.39	0.47
1:D:265:GLU:HA	1:D:268:LYS:HD2	1.97	0.47
1:A:359:LEU:HB3	1:A:435:LEU:HD11	1.97	0.47
1:D:123:ARG:O	1:D:127:MSE:HG2	2.14	0.47
1:B:455:PRO:HA	1:B:456:PRO:HD3	1.82	0.46
1:D:173:ALA:HB2	1:D:273:PRO:HG3	1.97	0.46
1:C:429:LYS:HE3	1:C:432:PHE:HZ	1.80	0.46
1:B:444:LEU:HD21	1:B:486:LEU:HD13	1.97	0.46
1:C:470:ARG:HD3	1:C:506:GLU:HG3	1.98	0.46
1:D:359:LEU:HB3	1:D:435:LEU:HD11	1.97	0.46
1:A:103:LYS:HE3	1:A:425:THR:HG22	1.98	0.46
1:A:66:LEU:HD11	1:A:104:ARG:HD2	1.98	0.46
1:A:230:MSE:HE2	1:A:248:GLU:HG2	1.98	0.46
1:D:337:LEU:HD11	1:D:341:MSE:HE3	1.97	0.46
1:A:459:THR:HB	1:A:470:ARG:HB3	1.98	0.45
1:C:365:TRP:HD1	1:C:368[B]:MSE:HE1	1.81	0.45
1:C:429:LYS:HE3	1:C:432:PHE:CZ	2.51	0.45
1:C:229:GLU:HG3	1:C:262:GLY:HA3	1.99	0.45
1:C:337:LEU:O	1:C:341:MSE:HG2	2.17	0.45
1:A:468:THR:HA	1:A:502:LYS:O	2.17	0.45
1:D:341:MSE:HG2	1:D:364:ARG:NH1	2.27	0.45
1:B:214:MSE:HE2	1:B:293:SER:HB2	1.99	0.44
1:D:142:ILE:HD11	1:D:287:ILE:HD13	1.98	0.44
1:A:246:VAL:O	1:A:250:LEU:HG	2.17	0.44
1:D:94:GLN:HG3	2:D:561:HOH:O	2.17	0.44
1:D:455:PRO:HA	1:D:456:PRO:HD2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:450:GLN:HG2	1:D:203:TRP:CE2	2.52	0.44
1:C:24:HIS:HB2	1:C:298:ARG:HD3	2.00	0.44
1:C:470:ARG:CD	1:C:506:GLU:HG3	2.47	0.43
1:A:41:LEU:HD11	1:A:72:PHE:CE1	2.53	0.43
1:C:203:TRP:CE2	1:D:450:GLN:CG	3.01	0.43
1:B:461:ILE:HB	1:B:468:THR:OG1	2.18	0.43
1:C:450:GLN:CG	1:D:203:TRP:CE2	3.01	0.43
1:A:247:LYS:HB2	1:A:247:LYS:HE3	1.85	0.43
1:A:90:HIS:NE2	1:A:94:GLN:HG3	2.34	0.43
1:B:77:GLN:HA	2:B:597:HOH:O	2.19	0.43
1:D:269:THR:HG23	1:D:270:VAL:HG13	2.00	0.43
1:B:74:GLU:O	1:B:77:GLN:HG2	2.19	0.43
1:D:470:ARG:CD	1:D:506:GLU:HG3	2.49	0.43
1:D:444:LEU:C	1:D:444:LEU:HD23	2.44	0.42
1:C:417:LYS:HD2	1:C:419:ASP:HB2	2.01	0.42
1:A:272:VAL:N	1:A:273:PRO:HD2	2.34	0.42
1:C:468:THR:HB	1:C:502:LYS:HB2	2.01	0.42
1:D:62:MSE:CE	1:D:101:PHE:HA	2.40	0.42
1:A:432:PHE:HA	1:A:435:LEU:HG	2.01	0.42
1:D:26:VAL:HG13	1:D:302:LEU:HD11	2.02	0.42
1:D:231:GLY:O	1:D:233:LYS:HD2	2.20	0.42
1:D:243:GLU:HA	1:D:246:VAL:CG1	2.49	0.42
1:B:260:LEU:HD12	1:B:260:LEU:H	1.85	0.42
1:C:16:VAL:HB	1:C:86:ILE:HG12	2.01	0.42
1:D:429:LYS:HA	1:D:432:PHE:CE2	2.55	0.42
1:A:248:GLU:O	1:A:251:ARG:HG3	2.20	0.42
1:B:166:ARG:O	1:B:197:LYS:HE3	2.20	0.42
1:C:288:ARG:HA	1:C:288:ARG:HD3	1.66	0.42
1:D:22:SER:HB2	1:D:24:HIS:NE2	2.35	0.42
1:A:192:MSE:HB3	1:B:484:LEU:HD11	2.01	0.41
1:C:265:GLU:HA	1:C:268:LYS:HD3	2.01	0.41
1:A:25:MSE:SE	1:A:27:ILE:HD11	2.70	0.41
1:A:38:ILE:HD13	1:A:38:ILE:HA	1.69	0.41
1:C:429:LYS:HA	1:C:432:PHE:CE2	2.55	0.41
1:D:227:LEU:HD22	1:D:232:GLU:HG3	2.02	0.41
1:A:60:GLU:CD	1:A:60:GLU:H	2.27	0.41
1:B:305:MSE:HE3	1:B:305:MSE:HB2	1.87	0.41
1:D:13:PHE:HE1	1:D:35:MSE:SE	2.54	0.41
1:D:404:MSE:HG2	1:D:424:PHE:CE1	2.56	0.41
1:A:332:GLN:OE1	1:A:449:ARG:HA	2.21	0.41
1:B:35:MSE:HE3	1:B:35:MSE:HB3	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:GLU:H	1:B:60:GLU:CD	2.28	0.41
1:C:25:MSE:HE1	1:C:72:PHE:HB3	2.02	0.41
1:C:215:GLY:HA3	1:C:220:ILE:HD13	2.03	0.41
1:C:217:SER:HB2	1:C:218:GLY:H	1.76	0.41
1:D:13:PHE:CE1	1:D:35:MSE:SE	3.24	0.41
1:D:142:ILE:HD13	1:D:281:VAL:HG11	2.02	0.41
1:D:288:ARG:HA	1:D:288:ARG:HD3	1.80	0.41
1:A:245:LEU:O	1:A:249:VAL:HG13	2.21	0.41
1:A:404:MSE:HG3	1:A:427:PHE:CD2	2.56	0.41
1:A:133:GLN:OE1	1:A:139:LYS:HE2	2.21	0.40
1:A:203:TRP:CD2	1:B:450:GLN:CG	3.04	0.40
1:C:62:MSE:CE	1:C:101:PHE:HA	2.48	0.40
1:D:99:THR:HG22	2:D:531:HOH:O	2.21	0.40
1:A:233:LYS:H	1:A:233:LYS:HD2	1.85	0.40
1:C:365:TRP:CD1	1:C:368[B]:MSE:HE1	2.57	0.40
1:D:60:GLU:H	1:D:60:GLU:HG2	1.57	0.40
1:D:404:MSE:HG3	1:D:427:PHE:CD2	2.55	0.40
1:D:476:PHE:CD1	1:D:483:LEU:HB2	2.57	0.40
1:C:464:ASP:HB3	1:C:465:SER:H	1.68	0.40
1:D:70:SER:HB3	1:D:108:VAL:HB	2.03	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	495/524 (94%)	479 (97%)	16 (3%)	0	100 100
1	B	494/524 (94%)	483 (98%)	10 (2%)	1 (0%)	43 51
1	C	496/524 (95%)	479 (97%)	17 (3%)	0	100 100
1	D	495/524 (94%)	481 (97%)	14 (3%)	0	100 100
All	All	1980/2096 (94%)	1922 (97%)	57 (3%)	1 (0%)	48 57

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	217	SER

5.3.2 Protein sidechains [i](#)

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	423/429 (99%)	395 (93%)	28 (7%)	15	18
1	B	422/429 (98%)	398 (94%)	24 (6%)	18	23
1	C	424/429 (99%)	396 (93%)	28 (7%)	15	18
1	D	423/429 (99%)	397 (94%)	26 (6%)	17	20
All	All	1692/1716 (99%)	1586 (94%)	106 (6%)	16	19

All (106) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ARG
1	A	31	VAL
1	A	35	MSE
1	A	38	ILE
1	A	41	LEU
1	A	60	GLU
1	A	135	GLU
1	A	138	ARG
1	A	166	ARG
1	A	201	LEU
1	A	207	ILE
1	A	217	SER
1	A	225	GLU
1	A	241	ARG
1	A	242	LEU
1	A	244	LYS
1	A	251	ARG
1	A	258	LEU
1	A	351	GLN

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Mol	Chain	Res	Type
1	A	353	LYS
1	A	374	LEU
1	A	379	SER
1	A	416	ILE
1	A	418	LEU
1	A	444	LEU
1	A	450	GLN
1	A	468	THR
1	A	505	GLU
1	B	60	GLU
1	B	107	LYS
1	B	207	ILE
1	B	214	MSE
1	B	233	LYS
1	B	238	THR
1	B	241	ARG
1	B	244	LYS
1	B	246	VAL
1	B	257	SER
1	B	263	LEU
1	B	312	GLN
1	B	342	GLN
1	B	351	GLN
1	B	353	LYS
1	B	374	LEU
1	B	379	SER
1	B	416	ILE
1	B	444	LEU
1	B	450	GLN
1	B	486	LEU
1	B	488	LYS
1	B	501	LEU
1	B	503	ILE
1	C	40	ARG
1	C	94	GLN
1	C	99	THR
1	C	201	LEU
1	C	207	ILE
1	C	214	MSE
1	C	238	THR
1	C	244	LYS
1	C	246	VAL

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Mol	Chain	Res	Type
1	C	248	GLU
1	C	266	GLU
1	C	343	MSE
1	C	348	ARG
1	C	351	GLN
1	C	353	LYS
1	C	364	ARG
1	C	379	SER
1	C	416	ILE
1	C	417	LYS
1	C	418	LEU
1	C	423	ARG
1	C	428	LYS
1	C	444	LEU
1	C	468	THR
1	C	474	ASP
1	C	478	GLN
1	C	486	LEU
1	C	488	LYS
1	D	38	ILE
1	D	60	GLU
1	D	99	THR
1	D	103	LYS
1	D	207	ILE
1	D	214	MSE
1	D	225	GLU
1	D	238	THR
1	D	241	ARG
1	D	244	LYS
1	D	248	GLU
1	D	251	ARG
1	D	253	ARG
1	D	331	GLU
1	D	334	ARG
1	D	374	LEU
1	D	379	SER
1	D	404	MSE
1	D	416	ILE
1	D	418	LEU
1	D	419	ASP
1	D	444	LEU
1	D	468	THR

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Mol	Chain	Res	Type
1	D	478	GLN
1	D	488	LYS
1	D	501	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	46	HIS
1	A	133	GLN
1	A	375	ASN
1	A	391	ASN
1	A	446	ASN
1	A	448	GLN
1	B	21	ASN
1	B	375	ASN
1	B	431	GLN
1	B	490	GLN
1	C	46	HIS
1	C	252	HIS
1	C	324	ASN
1	C	356	HIS
1	C	375	ASN
1	D	43	GLN
1	D	94	GLN
1	D	342	GLN
1	D	351	GLN
1	D	358	GLN
1	D	391	ASN
1	D	401	GLN
1	D	448	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	480/524 (91%)	0.17	12 (2%) 58 55	18, 34, 54, 67	0
1	B	479/524 (91%)	0.14	14 (2%) 53 50	18, 32, 56, 62	0
1	C	480/524 (91%)	0.02	8 (1%) 69 66	16, 30, 52, 66	1 (0%)
1	D	480/524 (91%)	0.20	12 (2%) 58 55	18, 35, 56, 66	0
All	All	1919/2096 (91%)	0.13	46 (2%) 59 56	16, 33, 55, 67	1 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	183	ASN	3.2
1	D	253	ARG	3.2
1	B	134	PRO	3.1
1	A	294	ASP	3.0
1	B	499	TRP	2.9
1	D	38	ILE	2.9
1	B	183	ASN	2.8
1	B	416	ILE	2.7
1	B	500	ARG	2.7
1	A	464	ASP	2.6
1	D	266	GLU	2.5
1	D	261	PRO	2.5
1	A	253	ARG	2.5
1	B	503	ILE	2.5
1	A	262	GLY	2.5
1	D	235	GLY	2.5
1	C	269	THR	2.5
1	D	13	PHE	2.5
1	B	434	PRO	2.5
1	A	266	GLU	2.4
1	A	260	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	99	THR	2.4
1	A	288	ARG	2.4
1	A	261	PRO	2.3
1	B	353	LYS	2.3
1	C	259	SER	2.3
1	D	217	SER	2.3
1	C	432	PHE	2.3
1	B	467	TRP	2.3
1	D	33	GLY	2.3
1	C	497	ALA	2.3
1	B	461	ILE	2.3
1	B	476	PHE	2.2
1	D	231	GLY	2.2
1	B	463	ASP	2.2
1	C	54	ASP	2.1
1	C	311	HIS	2.1
1	C	231	GLY	2.1
1	D	262	GLY	2.1
1	B	468	THR	2.1
1	D	269	THR	2.1
1	A	256	ALA	2.1
1	C	353	LYS	2.0
1	A	204	GLN	2.0
1	A	309	PHE	2.0
1	B	309	PHE	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.