



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:07 AM GMT

PDB ID : 2FLO
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

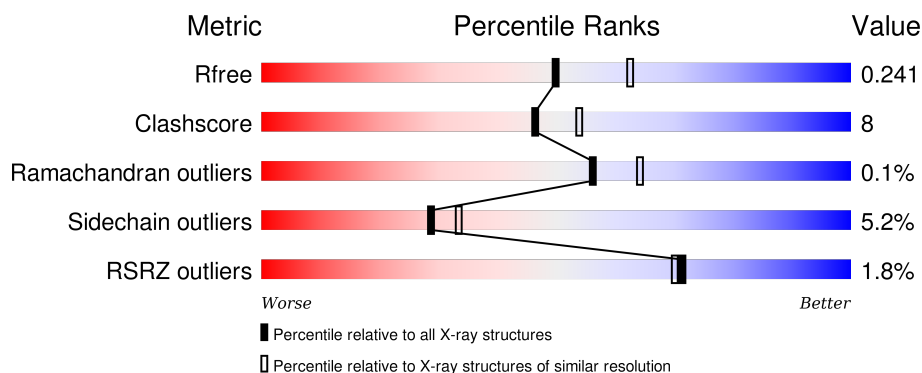
1 Overall quality at a glance

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}	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>3%</div> <div>76%</div> <div>17%</div> <div>• 5%</div> </div>
1	B	524	<div> <div>%</div> <div>81%</div> <div>12%</div> <div>• 6%</div> </div>
1	C	524	<div> <div>%</div> <div>79%</div> <div>13%</div> <div>• 5%</div> </div>
1	D	524	<div> <div>2%</div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div>

2 Entry composition

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
1	A	496	Total	C	N	O	S	Se	0	1	0
			3964	2511	714	718	4	17			
1	B	495	Total	C	N	O	S	Se	0	1	0
			3955	2506	712	716	4	17			
1	C	496	Total	C	N	O	S	Se	0	2	0
			3965	2511	714	718	5	17			
1	D	496	Total	C	N	O	S	Se	0	1	0
			3964	2511	714	718	4	17			

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
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B	230	MSE	MET	MODIFIED RESIDUE	UNP P0AFL8
B	305	MSE	MET	MODIFIED RESIDUE	UNP P0AFL8
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B	368	MSE	MET	MODIFIED RESIDUE	UNP P0AFL8
B	404	MSE	MET	MODIFIED RESIDUE	UNP P0AFL8
B	405	MSE	MET	MODIFIED RESIDUE	UNP P0AFL8
C	-10	MSE	-	CLONING ARTIFACT	UNP P0AFL8
C	-9	GLY	-	CLONING ARTIFACT	UNP P0AFL8
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

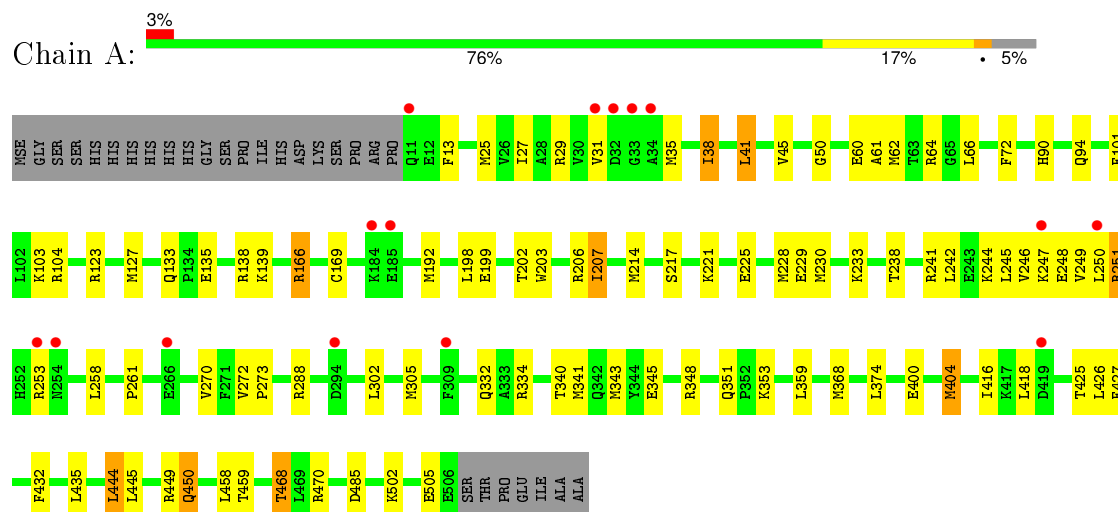
- Molecule 2 is water.

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

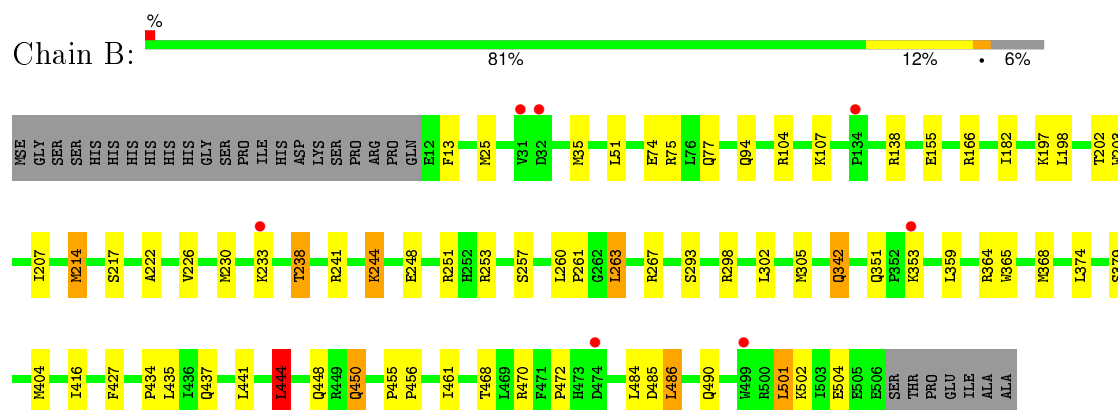
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

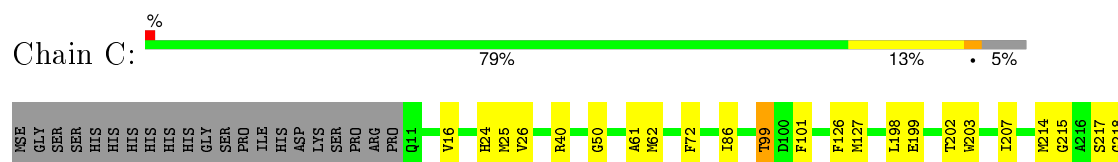
• Molecule 1: Exopolyphosphatase

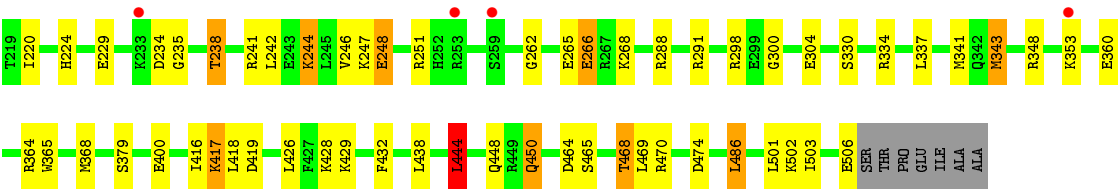


• Molecule 1: Exopolyphosphatase

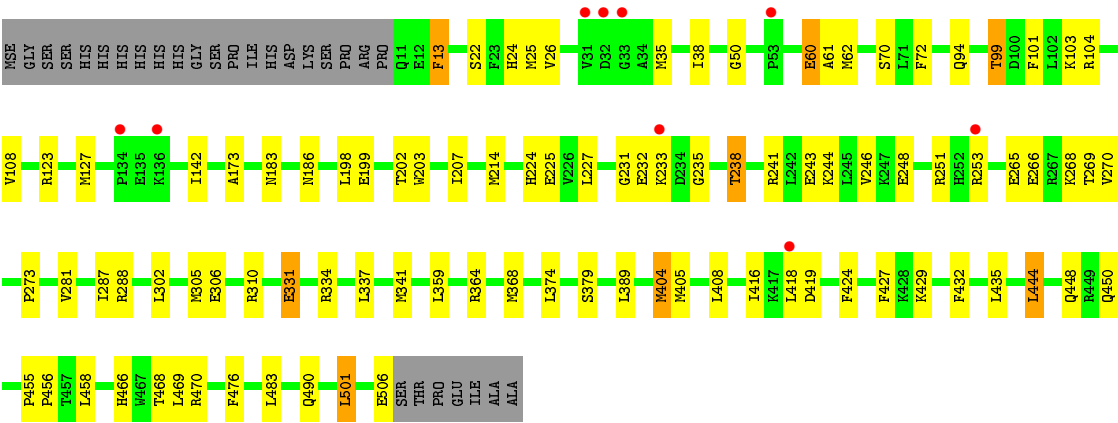
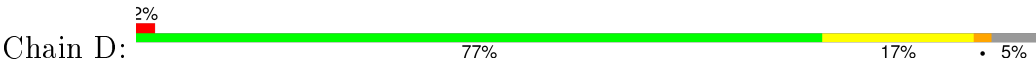


• Molecule 1: Exopolyphosphatase





• 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 34.84 – 2.04	Depositor EDS
% Data completeness (in resolution range)	98.0 (50.00-2.20) 87.5 (34.84-2.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 2.05Å)	Xtriage
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 (5.33%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 143740 reflections	Xtriage
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

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.36% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.55	0/4031	0.64	1/5417 (0.0%)
1	B	0.56	0/4022	0.64	1/5405 (0.0%)
1	C	0.59	0/4037	0.64	1/5425 (0.0%)
1	D	0.55	0/4031	0.63	1/5417 (0.0%)
All	All	0.56	0/16121	0.64	4/21664 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	444	LEU	CA-CB-CG	7.01	131.41	115.30
1	C	444	LEU	CA-CB-CG	5.81	128.67	115.30
1	A	444	LEU	CA-CB-CG	5.49	127.94	115.30
1	D	444	LEU	CA-CB-CG	5.10	127.04	115.30

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	3964	0	3993	64	0
1	B	3955	0	3985	61	0
1	C	3965	0	3994	64	0
1	D	3964	0	3993	70	0
2	A	142	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	241	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (241) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:341:MSE:HG2	1:D:364:ARG:HH11	1.57	0.68
1:C:244:LYS:HA	1:C:244:LYS:HE3	1.76	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:C:126:PHE:CE2	1:C:127:MSE:CE	2.80	0.65
1:B:244:LYS:HA	1:B:244:LYS:HE3	1.79	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
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:138:ARG:HA	1:B:155:GLU:HB3	1.81	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:365:TRP:HD1	1:C:368[B]:MSE:HE3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:HIS:CE1	1:C:235:GLY:HA3	2.37	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:D:243:GLU:HA	1:D:246:VAL:HG12	1.83	0.59
1:A:400:GLU:HB2	1:A:426:LEU:HD22	1.85	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:D:203:TRP:CZ2	1:D:207:ILE:HG13	2.41	0.56
1:C:50:GLY:HA3	1:C:61:ALA:HB2	1.87	0.56
1:A:340:THR:HG22	1:A:341:MSE:HE2	1.88	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: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:C:242:LEU:O	1:C:246:VAL:HG13	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
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:D:238:THR:HG22	1:D:241:ARG:H	1.73	0.53
1:C:198:LEU:O	1:C:202:THR:HG23	2.08	0.53
1:D:183:ASN:HB3	1:D:186:ASN:H	1.74	0.52
1:B:444:LEU:HD23	1:B:485:ASP:CB	2.35	0.52
1:B:260:LEU:HB2	1:B:263:LEU:HD22	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:450:GLN:HG2	1:B:203:TRP:CD2	2.46	0.51
1:A:229:GLU:HB3	1:A:261:PRO:HB2	1.91	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:D:62:MSE:HE2	1:D:104:ARG:HD2	1.94	0.50
1:A:368[A]:MSE:HG3	2:A:584:HOH:O	2.11	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:C:203:TRP:CE2	1:C:207:ILE:HG13	2.47	0.49
1:B:404:MSE:HG3	1:B:427:PHE:CD2	2.47	0.49
1:A:343:MSE:HE1	1:A:445:LEU:HD11	1.94	0.49
1:B:222:ALA:HB2	1:B:267:ARG:HD3	1.94	0.49
1:B:25:MSE:HE1	1:B:75:ARG:HG2	1.95	0.49
1:C:343:MSE:HB2	1:C:438:LEU:CD2	2.42	0.49
1:B:490:GLN:HG2	1:B:501:LEU:HB3	1.95	0.49
1:B:51:LEU:HD21	1:B:94:GLN:HG2	1.95	0.49
1:B:238:THR:HG22	1:B:241:ARG:HG3	1.95	0.48
1:A:450:GLN:CG	1:B:203:TRP:CE2	2.96	0.48
1:D:368[A]:MSE:CG	2:D:629:HOH:O	2.24	0.48
1:B:365:TRP:CD1	1:B:368[B]:MSE:HE3	2.35	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:226:VAL:HG21	1:B:263:LEU:HD13	1.95	0.48
1:A:123:ARG:O	1:A:127:MSE:HG2	2.13	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:306:GLU:OE2	1:D:310:ARG:HD3	2.15	0.47
1:A:288:ARG:NE	1:A:288:ARG:HA	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:133:GLN:HE22	1:A:214:MSE:SE	2.47	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:C:365:TRP:HD1	1:C:368[B]:MSE:HE1	1.81	0.45
1:A:459:THR:HB	1:A:470:ARG:HB3	1.98	0.45
1:C:429:LYS:HE3	1:C:432:PHE:CZ	2.51	0.45
1:C:337:LEU:O	1:C:341:MSE:HG2	2.17	0.45
1:C:229:GLU:HG3	1:C:262:GLY:HA3	1.99	0.45
1:D:341:MSE:HG2	1:D:364:ARG:NH1	2.27	0.45
1:A:468:THR:HA	1:A:502:LYS:O	2.17	0.45
1:D:142:ILE:HD11	1:D:287:ILE:HD13	1.98	0.44
1:B:214:MSE:HE2	1:B:293:SER:HB2	1.99	0.44
1:D:455:PRO:HA	1:D:456:PRO:HD2	1.82	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: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:C:266:GLU:H	1:C:266:GLU:CD	2.20	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:ARG:CD	1:D:506:GLU:HG3	2.49	0.43
1:B:74:GLU:O	1:B:77:GLN:HG2	2.19	0.43
1:C:417:LYS:HD2	1:C:419:ASP:HB2	2.01	0.42
1:D:62:MSE:CE	1:D:101:PHE:HA	2.40	0.42
1:C:468:THR:HB	1:C:502:LYS:HB2	2.01	0.42
1:A:272:VAL:N	1:A:273:PRO:HD2	2.34	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:243:GLU:HA	1:D:246:VAL:CG1	2.49	0.42
1:D:231:GLY:O	1:D:233:LYS:HD2	2.20	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:D:22:SER:HB2	1:D:24:HIS:NE2	2.35	0.42
1:A:248:GLU:O	1:A:251:ARG:HG3	2.20	0.42
1:C:288:ARG:HA	1:C:288:ARG:HD3	1.66	0.42
1:B:166:ARG:O	1:B:197:LYS:HE3	2.20	0.42
1:C:265:GLU:HA	1:C:268:LYS:HD3	2.01	0.41
1:A:192:MSE:HB3	1:B:484:LEU:HD11	2.01	0.41
1:C:429:LYS:HA	1:C:432:PHE:CE2	2.55	0.41
1:A:38:ILE:HA	1:A:38:ILE:HD13	1.69	0.41
1:A:25:MSE:SE	1:A:27:ILE:HD11	2.70	0.41
1:D:227:LEU:HD22	1:D:232:GLU:HG3	2.02	0.41
1:B:305:MSE:HE3	1:B:305:MSE:HB2	1.87	0.41
1:D:404:MSE:HG2	1:D:424:PHE:CE1	2.56	0.41
1:D:13:PHE:HE1	1:D:35:MSE:SE	2.54	0.41
1:D:142:ILE:HD13	1:D:281:VAL:HG11	2.02	0.41
1:D:13:PHE:CE1	1:D:35:MSE:SE	3.24	0.41
1:A:332:GLN:OE1	1:A:449:ARG:HA	2.21	0.41
1:C:217:SER:HB2	1:C:218:GLY:H	1.76	0.41
1:C:215:GLY:HA3	1:C:220:ILE:HD13	2.03	0.41
1:C:25:MSE:HE1	1:C:72:PHE:HB3	2.02	0.41
1:D:288:ARG:HD3	1:D:288:ARG:HA	1.80	0.41
1:B:35:MSE:HE3	1:B:35:MSE:HB3	1.90	0.41
1:A:404:MSE:HG3	1:A:427:PHE:CD2	2.56	0.41
1:A:245:LEU:O	1:A:249:VAL:HG13	2.21	0.41
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:A:133:GLN:OE1	1:A:139:LYS:HE2	2.21	0.40
1:D:99:THR:HG22	2:D:531:HOH:O	2.21	0.40
1:C:365:TRP:CD1	1:C:368[B]:MSE:HE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LYS:H	1:A:233:LYS:HD2	1.85	0.40
1:D:404:MSE:HG3	1:D:427:PHE:CD2	2.55	0.40
1:D:60:GLU:H	1:D:60:GLU:HG2	1.57	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%)	52	59
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%)	56	64

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%)	397 (94%)	26 (6%)	23	26
1	B	422/429 (98%)	404 (96%)	18 (4%)	35	43
1	C	424/429 (99%)	404 (95%)	20 (5%)	32	39
1	D	423/429 (99%)	399 (94%)	24 (6%)	25	29
All	All	1692/1716 (99%)	1604 (95%)	88 (5%)	29	33

All (88) 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	207	ILE
1	A	217	SER
1	A	242	LEU
1	A	244	LYS
1	A	251	ARG
1	A	253	ARG
1	A	258	LEU
1	A	334	ARG
1	A	351	GLN
1	A	353	LYS
1	A	374	LEU
1	A	404	MSE
1	A	416	ILE
1	A	418	LEU
1	A	450	GLN
1	A	468	THR
1	A	505	GLU
1	B	107	LYS
1	B	207	ILE
1	B	214	MSE
1	B	233	LYS
1	B	238	THR

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Mol	Chain	Res	Type
1	B	244	LYS
1	B	257	SER
1	B	263	LEU
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	501	LEU
1	C	99	THR
1	C	238	THR
1	C	244	LYS
1	C	247	LYS
1	C	248	GLU
1	C	266	GLU
1	C	343	MSE
1	C	348	ARG
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	428	LYS
1	C	444	LEU
1	C	450	GLN
1	C	468	THR
1	C	474	ASP
1	C	486	LEU
1	D	13	PHE
1	D	38	ILE
1	D	60	GLU
1	D	99	THR
1	D	103	LYS
1	D	214	MSE
1	D	225	GLU
1	D	238	THR
1	D	244	LYS

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Mol	Chain	Res	Type
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	466	HIS
1	D	468	THR
1	D	501	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	351	GLN
1	B	382	HIS
1	C	90	HIS
1	C	174	GLN
1	C	356	HIS
1	C	399	GLN
1	D	351	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	-0.18	15 (3%) 52 51	18, 34, 54, 67	0
1	B	479/524 (91%)	-0.24	7 (1%) 76 75	18, 32, 56, 62	0
1	C	480/524 (91%)	-0.31	4 (0%) 87 87	16, 30, 52, 66	0
1	D	480/524 (91%)	-0.09	9 (1%) 70 68	18, 35, 56, 66	0
All	All	1919/2096 (91%)	-0.21	35 (1%) 71 70	16, 33, 55, 67	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	32	ASP	4.6
1	D	233	LYS	4.4
1	D	134	PRO	4.4
1	D	31	VAL	4.3
1	B	134	PRO	4.2
1	A	253	ARG	4.0
1	D	253	ARG	3.5
1	A	247	LYS	3.4
1	A	31	VAL	3.2
1	A	309	PHE	3.2
1	C	353	LYS	3.2
1	A	32	ASP	2.9
1	A	294	ASP	2.9
1	A	184	LYS	2.9
1	A	33	GLY	2.9
1	D	53	PRO	2.9
1	A	11	GLN	2.9
1	A	419	ASP	2.9
1	B	32	ASP	2.8
1	B	233	LYS	2.7
1	D	33	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	31	VAL	2.6
1	B	353	LYS	2.6
1	C	233	LYS	2.6
1	B	474	ASP	2.4
1	C	259	SER	2.3
1	D	136	LYS	2.3
1	B	499	TRP	2.3
1	C	253	ARG	2.2
1	A	254	ASN	2.2
1	A	34	ALA	2.2
1	A	185	GLU	2.2
1	A	266	GLU	2.1
1	A	250	LEU	2.0
1	D	418	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.