



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:14 AM UTC

PDB ID : 6PMP / pdb_00006pmp
Title : Crystal structure of a fragment of rat phospholipase Cepsilon EF3-RA1
Authors : Rugema, N.Y.; Lyon, A.M.
Deposited on : 2019-07-02
Resolution : 2.73 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

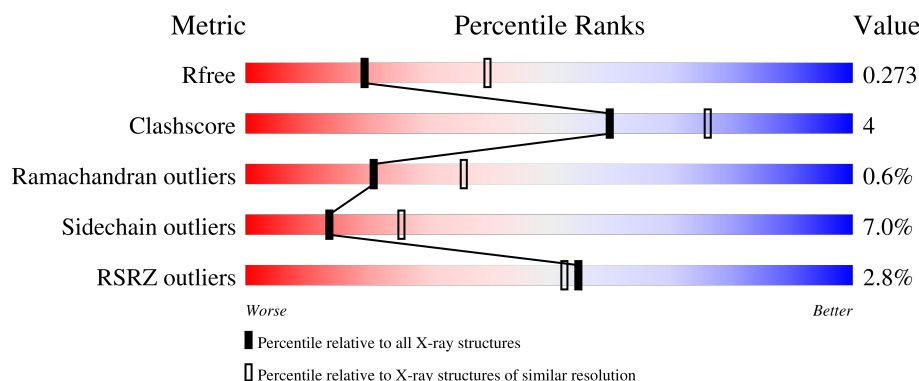
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.73 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	1819 (2.76-2.72)
Clashscore	190562	1866 (2.76-2.72)
Ramachandran outliers	187476	1830 (2.76-2.72)
Sidechain outliers	187428	1831 (2.76-2.72)
RSRZ outliers	180081	1819 (2.76-2.72)

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	818	 61% 12% • 26%
1	B	818	 60% 13% • 25%
1	C	818	 62% 12% • 25%
1	D	818	 61% 12% • 26%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19693 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 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase epsilon-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	609	Total	C	N	O	S	0	0	0
			4897	3121	844	901	31			
1	B	611	Total	C	N	O	S	0	0	0
			4902	3127	844	900	31			
1	C	617	Total	C	N	O	S	0	0	0
			4970	3176	852	910	32			
1	D	605	Total	C	N	O	S	0	0	0
			4853	3097	835	890	31			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1281	SER	-	expression tag	UNP Q99P84
A	1282	ASN	-	expression tag	UNP Q99P84
A	1283	ALA	-	expression tag	UNP Q99P84
B	1281	SER	-	expression tag	UNP Q99P84
B	1282	ASN	-	expression tag	UNP Q99P84
B	1283	ALA	-	expression tag	UNP Q99P84
C	1281	SER	-	expression tag	UNP Q99P84
C	1282	ASN	-	expression tag	UNP Q99P84
C	1283	ALA	-	expression tag	UNP Q99P84
D	1281	SER	-	expression tag	UNP Q99P84
D	1282	ASN	-	expression tag	UNP Q99P84
D	1283	ALA	-	expression tag	UNP Q99P84

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total 1	Ca 1	0	0
2	C	1	Total 1	Ca 1	0	0
2	D	1	Total 1	Ca 1	0	0

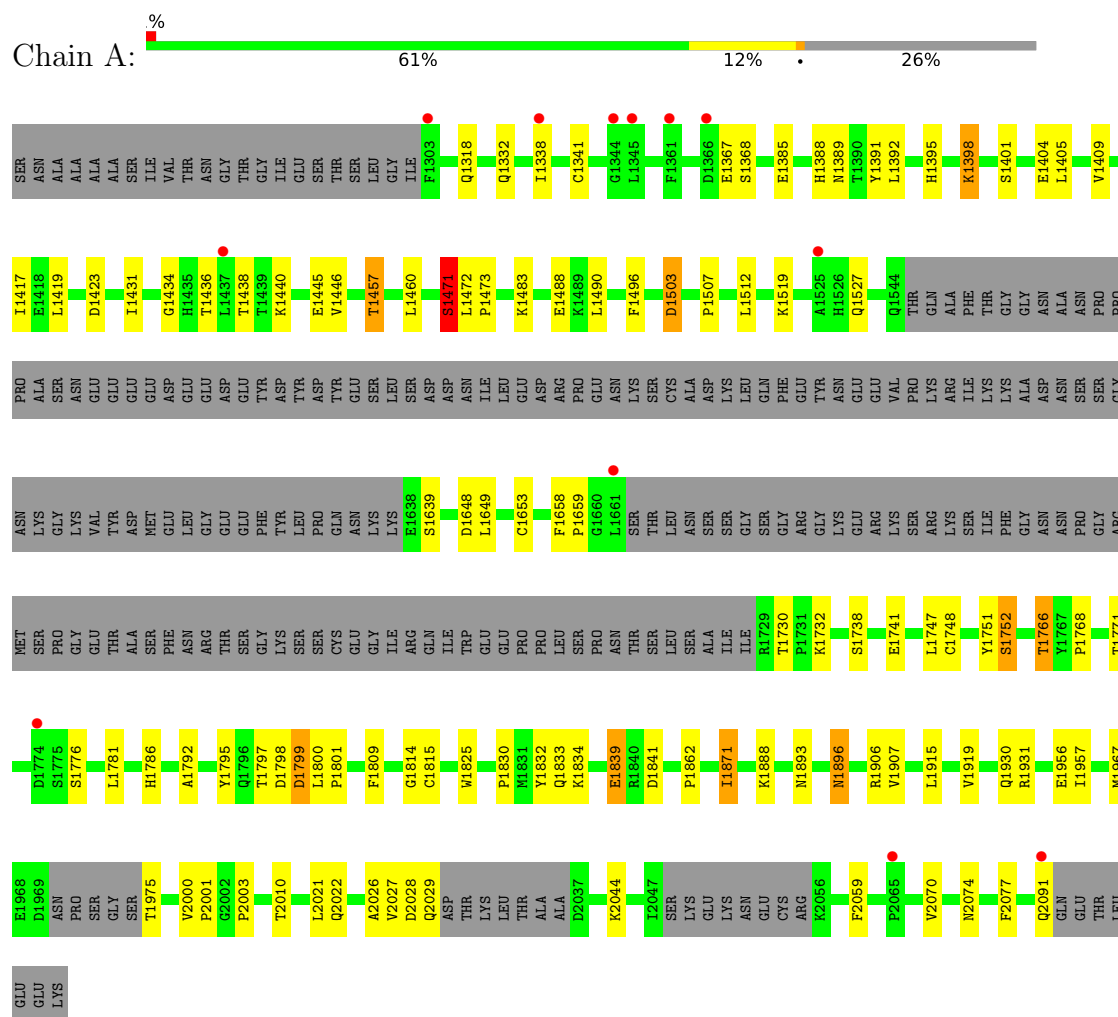
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	21	Total 21	O 21	0	0
3	B	17	Total 17	O 17	0	0
3	C	19	Total 19	O 19	0	0
3	D	10	Total 10	O 10	0	0

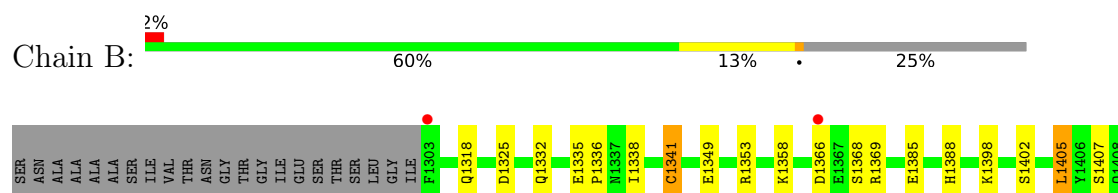
3 Residue-property plots

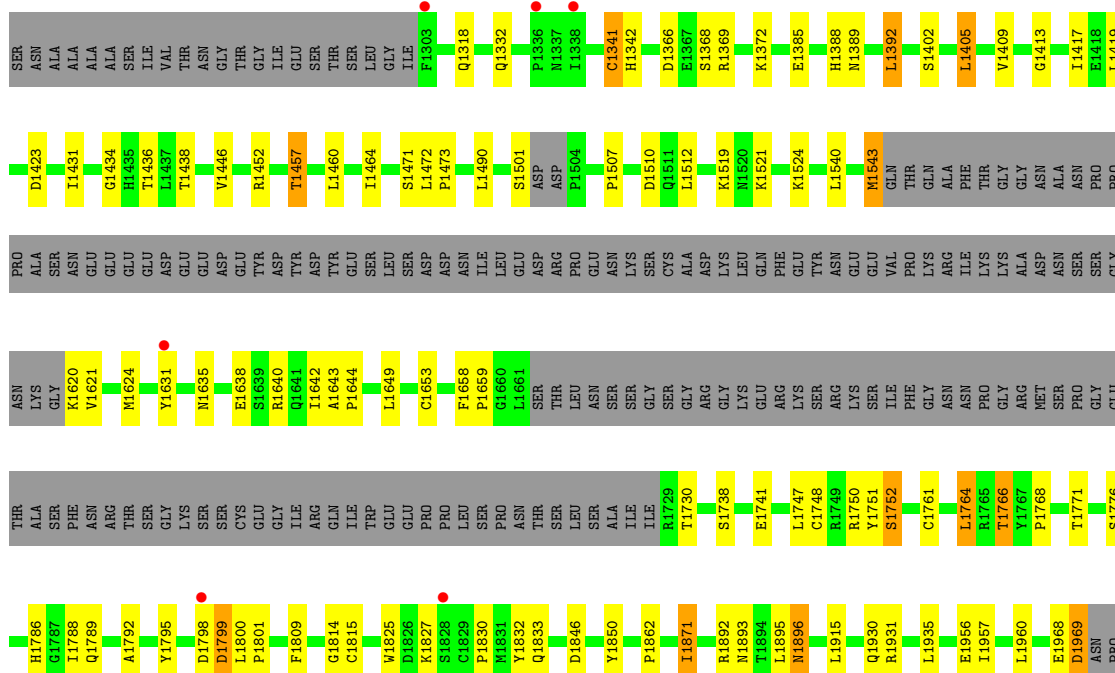
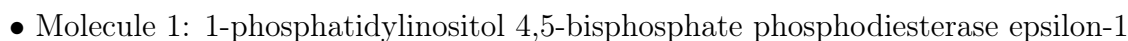
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

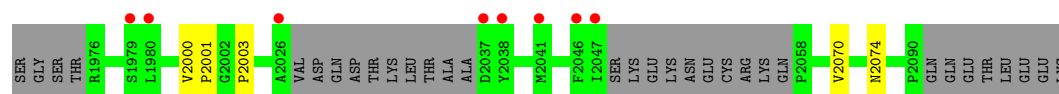
- Molecule 1: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase epsilon-1



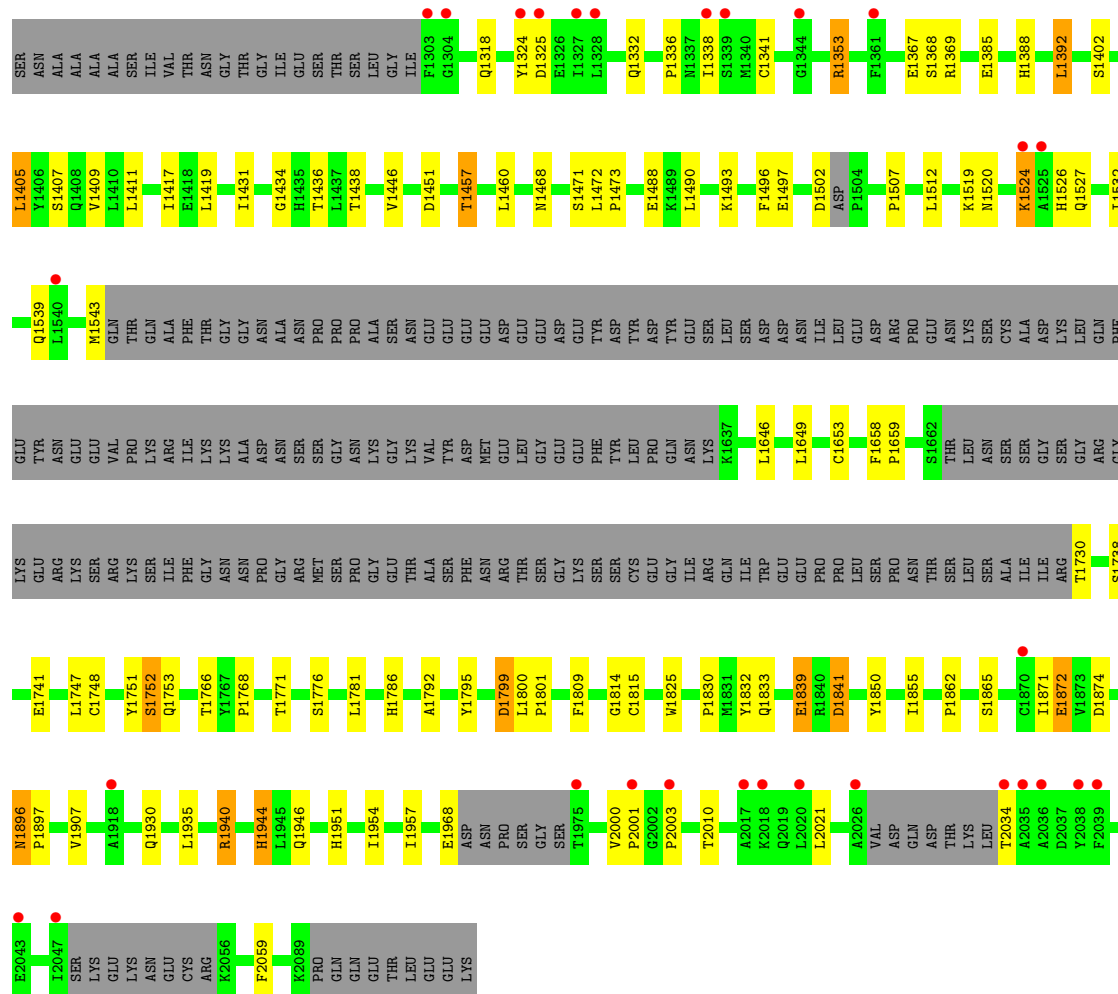
- Molecule 1: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase epsilon-1







- Molecule 1: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase epsilon-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.57Å 127.75Å 139.34Å 90.00° 101.12° 90.00°	Depositor
Resolution (Å)	20.00 – 2.73 20.00 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.73) 99.3 (20.00-2.73)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.75Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.234 , 0.273 0.236 , 0.273	Depositor DCC
R_{free} test set	4215 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	36.2	Xtriage
Anisotropy	1.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	19693	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.80% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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	1.13	1/5008 (0.0%)	1.47	13/6773 (0.2%)
1	B	1.12	5/5012 (0.1%)	1.47	9/6777 (0.1%)
1	C	1.12	5/5084 (0.1%)	1.47	11/6870 (0.2%)
1	D	1.12	4/4962 (0.1%)	1.48	16/6707 (0.2%)
All	All	1.12	15/20066 (0.1%)	1.47	49/27127 (0.2%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1388	HIS	C-O	8.46	1.34	1.24
1	B	1884	HIS	CE1-NE2	7.59	1.40	1.32
1	A	1388	HIS	C-O	6.49	1.31	1.24
1	B	1388	HIS	C-O	6.16	1.31	1.24
1	C	1789	GLN	C-O	6.16	1.31	1.23
1	D	1388	HIS	C-O	6.03	1.31	1.24
1	C	1764	LEU	C-O	5.80	1.30	1.23
1	B	1884	HIS	CG-ND1	5.45	1.44	1.38
1	C	1392	LEU	C-O	5.44	1.30	1.23
1	B	1803	HIS	CE1-NE2	5.38	1.38	1.32
1	D	1392	LEU	C-O	5.32	1.30	1.23
1	D	1944	HIS	CE1-NE2	5.29	1.37	1.32
1	C	1413	GLY	C-O	5.29	1.31	1.23
1	B	1872	GLU	CD-OE2	5.25	1.35	1.25
1	D	1855	ILE	C-O	-5.10	1.19	1.24

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1872	GLU	CB-CG-CD	8.43	126.93	112.60
1	B	1799	ASP	CA-CB-CG	8.01	120.61	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1799	ASP	CA-CB-CG	7.98	120.58	112.60
1	C	1799	ASP	CA-CB-CG	7.84	120.44	112.60
1	A	1799	ASP	CA-CB-CG	7.59	120.19	112.60
1	D	1325	ASP	CB-CA-C	-6.68	100.68	110.96
1	A	1457	THR	CA-CB-OG1	-6.60	99.70	109.60
1	C	1766	THR	CA-CB-OG1	-6.40	100.00	109.60
1	B	1457	THR	CA-CB-OG1	-6.38	100.03	109.60
1	D	1457	THR	CA-CB-OG1	-6.17	100.35	109.60
1	C	1956	GLU	CB-CG-CD	6.15	123.05	112.60
1	D	1325	ASP	CA-CB-CG	6.04	118.64	112.60
1	A	1488	GLU	CB-CG-CD	6.00	122.81	112.60
1	D	1488	GLU	CB-CG-CD	6.00	122.79	112.60
1	C	1457	THR	CA-CB-OG1	-5.85	100.82	109.60
1	D	1324	TYR	CA-C-N	5.76	128.26	120.65
1	D	1324	TYR	C-N-CA	5.76	128.26	120.65
1	B	1906	ARG	CB-CG-CD	5.69	124.38	111.30
1	A	1798	ASP	CB-CA-C	5.66	120.22	110.77
1	A	1488	GLU	CB-CA-C	5.62	120.79	110.11
1	C	1366	ASP	CA-CB-CG	5.62	118.22	112.60
1	C	1931	ARG	CG-CD-NE	-5.58	99.72	112.00
1	A	1496	PHE	CA-C-N	5.52	127.67	120.28
1	A	1496	PHE	C-N-CA	5.52	127.67	120.28
1	D	2059	PHE	CA-CB-CG	5.41	119.21	113.80
1	A	1893	ASN	CB-CA-C	5.38	118.10	111.43
1	A	1766	THR	CA-CB-OG1	-5.36	101.55	109.60
1	D	1318	GLN	N-CA-C	-5.34	106.94	113.50
1	D	1451	ASP	CA-CB-CG	5.32	117.92	112.60
1	B	1766	THR	CA-CB-OG1	-5.30	101.64	109.60
1	C	1798	ASP	CB-CA-C	5.30	119.62	110.77
1	B	1318	GLN	N-CA-C	-5.20	107.10	113.50
1	C	1318	GLN	N-CA-C	-5.20	107.11	113.50
1	D	1367	GLU	CB-CG-CD	5.18	121.41	112.60
1	D	1841	ASP	CA-CB-CG	5.15	117.75	112.60
1	C	1892	ARG	CB-CG-CD	5.15	123.14	111.30
1	A	1797	THR	CA-CB-OG1	-5.14	101.89	109.60
1	C	1969	ASP	CA-CB-CG	5.11	117.71	112.60
1	A	1648	ASP	CA-CB-CG	5.10	117.70	112.60
1	D	1496	PHE	CA-C-N	5.07	127.07	120.28
1	D	1496	PHE	C-N-CA	5.07	127.07	120.28
1	D	1940	ARG	CB-CA-C	5.05	118.84	109.54
1	B	2010	THR	CB-CA-C	5.05	118.08	109.80
1	B	1488	GLU	CB-CG-CD	5.04	121.16	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1730	THR	N-CA-CB	5.03	117.88	109.98
1	A	1318	GLN	N-CA-C	-5.01	107.21	113.38
1	C	1893	ASN	CB-CA-C	5.01	117.64	111.43
1	B	1782	MET	CA-C-N	5.01	127.25	120.44
1	B	1782	MET	C-N-CA	5.01	127.25	120.44

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	4897	0	4870	44	0
1	B	4902	0	4883	46	0
1	C	4970	0	4950	44	0
1	D	4853	0	4840	42	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	21	0	0	2	0
3	B	17	0	0	0	0
3	C	19	0	0	0	0
3	D	10	0	0	0	0
All	All	19693	0	19543	169	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 4.

All (169) 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:1468:ASN:HD22	1:D:1520:ASN:HD21	1.33	0.77
1:A:1809:PHE:O	1:A:1814:GLY:HA2	1.98	0.63
1:D:1809:PHE:O	1:D:1814:GLY:HA2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1809:PHE:O	1:B:1814:GLY:HA2	2.01	0.60
1:A:1896:ASN:N	1:A:1896:ASN:HD22	1.99	0.59
1:C:1809:PHE:O	1:C:1814:GLY:HA2	2.02	0.59
1:D:1832:TYR:CD2	1:D:1833:GLN:HG3	2.37	0.59
1:D:1896:ASN:N	1:D:1896:ASN:HD22	1.99	0.59
1:A:1896:ASN:HD22	1:A:1896:ASN:H	1.51	0.59
1:B:1800:LEU:N	1:B:1801:PRO:CD	2.66	0.57
1:D:1896:ASN:HD22	1:D:1896:ASN:H	1.52	0.57
1:B:1896:ASN:HD22	1:B:1896:ASN:N	2.03	0.57
1:C:1640:ARG:HB3	1:C:1640:ARG:CZ	2.34	0.56
1:B:1768:PRO:HD3	1:B:1792:ALA:O	2.06	0.56
1:D:1768:PRO:HD3	1:D:1792:ALA:O	2.06	0.56
1:C:1490:LEU:HD21	1:C:1649:LEU:HD22	1.88	0.56
1:A:1460:LEU:HD12	1:A:1815:CYS:SG	2.46	0.55
1:C:1896:ASN:HD22	1:C:1896:ASN:N	2.02	0.55
1:B:1460:LEU:HD12	1:B:1815:CYS:SG	2.46	0.55
1:C:1768:PRO:HD3	1:C:1792:ALA:O	2.07	0.55
1:C:1832:TYR:CD2	1:C:1833:GLN:HG3	2.43	0.55
1:C:1896:ASN:HD22	1:C:1896:ASN:H	1.54	0.54
1:D:1524:LYS:H	1:D:1524:LYS:CE	2.20	0.54
1:C:1748:CYS:HB3	1:C:1786:HIS:CE1	2.42	0.54
1:C:1385:GLU:HG2	1:C:1795:TYR:OH	2.08	0.53
1:D:1800:LEU:N	1:D:1801:PRO:CD	2.71	0.53
1:A:1490:LEU:HD21	1:A:1649:LEU:HD22	1.89	0.53
1:B:1544:GLN:CD	1:B:1544:GLN:C	2.77	0.53
1:D:1872:GLU:HG2	1:D:1874:ASP:OD1	2.09	0.53
1:B:1896:ASN:HD22	1:B:1896:ASN:H	1.55	0.52
1:A:1832:TYR:CD2	1:A:1833:GLN:HG3	2.43	0.52
1:B:1468:ASN:HB2	1:B:1520:ASN:HD21	1.75	0.52
1:A:1472:LEU:N	1:A:1473:PRO:HD2	2.25	0.52
1:A:1768:PRO:HD3	1:A:1792:ALA:O	2.10	0.52
1:D:1460:LEU:HD12	1:D:1815:CYS:SG	2.50	0.52
1:C:1800:LEU:N	1:C:1801:PRO:CD	2.73	0.52
1:D:1385:GLU:HG2	1:D:1795:TYR:OH	2.10	0.52
1:A:2001:PRO:HD2	1:C:1624:MET:HE2	1.92	0.51
1:B:1472:LEU:N	1:B:1473:PRO:HD2	2.25	0.51
1:D:1490:LEU:HD21	1:D:1649:LEU:HD22	1.91	0.51
1:A:1385:GLU:HG2	1:A:1795:TYR:OH	2.11	0.51
1:B:1490:LEU:HD21	1:B:1649:LEU:HD22	1.93	0.51
1:B:1748:CYS:HB3	1:B:1786:HIS:CE1	2.45	0.51
1:D:1472:LEU:N	1:D:1473:PRO:HD2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1832:TYR:CD2	1:B:1833:GLN:HG3	2.46	0.51
1:C:1419:LEU:HD12	1:C:1419:LEU:N	2.25	0.51
1:D:1336:PRO:HD3	1:D:1353:ARG:NH2	2.25	0.51
1:D:1748:CYS:HB3	1:D:1786:HIS:CE1	2.45	0.51
1:A:1800:LEU:N	1:A:1801:PRO:CD	2.74	0.50
1:C:1472:LEU:N	1:C:1473:PRO:HD2	2.26	0.50
1:B:1385:GLU:HG2	1:B:1795:TYR:OH	2.11	0.50
1:A:1748:CYS:HB3	1:A:1786:HIS:CE1	2.46	0.50
1:C:1392:LEU:HD21	1:C:1438:THR:HG21	1.94	0.50
1:C:1521:LYS:HD3	1:C:1642:ILE:HD11	1.94	0.50
1:B:1419:LEU:HD12	1:B:1419:LEU:N	2.27	0.49
1:D:1419:LEU:HD12	1:D:1419:LEU:N	2.28	0.49
1:B:2025:LEU:HD13	1:B:2035:ALA:HA	1.95	0.49
1:B:1431:ILE:HD12	1:B:1446:VAL:HG21	1.94	0.48
1:D:1460:LEU:CD1	1:D:1815:CYS:SG	3.02	0.48
1:B:2037:ASP:OD2	1:D:1951:HIS:NE2	2.47	0.47
1:C:1431:ILE:HD12	1:C:1446:VAL:HG21	1.96	0.47
1:A:1799:ASP:CG	1:A:1801:PRO:HD2	2.39	0.47
1:D:1392:LEU:HD21	1:D:1438:THR:HG21	1.96	0.47
1:B:2000:VAL:O	1:B:2001:PRO:C	2.57	0.47
1:B:1460:LEU:CD1	1:B:1815:CYS:SG	3.03	0.47
1:B:1507:PRO:HG2	1:B:1512:LEU:HD11	1.97	0.47
1:C:1968:GLU:O	1:C:1969:ASP:C	2.58	0.47
1:A:1332:GLN:HA	1:A:1341:CYS:SG	2.55	0.46
1:C:1799:ASP:CG	1:C:1801:PRO:HD2	2.39	0.46
1:A:1445:GLU:HG2	3:A:2216:HOH:O	2.13	0.46
1:D:1507:PRO:HG2	1:D:1512:LEU:HD11	1.97	0.46
1:A:1404:GLU:OE1	1:B:1863:SER:HA	2.16	0.46
1:C:1460:LEU:HD12	1:C:1815:CYS:SG	2.56	0.46
1:B:2044:LYS:HB2	1:B:2059:PHE:HB3	1.97	0.46
1:C:2000:VAL:O	1:C:2001:PRO:C	2.59	0.46
1:D:1799:ASP:CG	1:D:1801:PRO:HD2	2.41	0.46
1:B:1799:ASP:CG	1:B:1801:PRO:HD2	2.40	0.46
1:B:1871:ILE:CD1	1:B:1960:LEU:HD22	2.46	0.46
1:D:1332:GLN:HA	1:D:1341:CYS:SG	2.56	0.46
1:A:1507:PRO:HG2	1:A:1512:LEU:HD11	1.98	0.46
1:C:1423:ASP:OD2	1:C:1471:SER:OG	2.34	0.46
1:A:1460:LEU:CD1	1:A:1815:CYS:SG	3.04	0.46
1:D:1658:PHE:CD1	1:D:1659:PRO:HD2	2.51	0.45
1:A:1419:LEU:N	1:A:1419:LEU:HD12	2.31	0.45
1:B:1808:MET:HE2	1:B:1818:VAL:HG11	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2000:VAL:O	1:A:2001:PRO:C	2.59	0.45
1:A:2026:ALA:HB3	1:C:1621:VAL:HG23	1.99	0.45
1:B:1940:ARG:NH2	1:B:1964:SER:OG	2.50	0.45
1:C:1507:PRO:HG2	1:C:1512:LEU:HD11	1.98	0.45
1:D:1431:ILE:HD12	1:D:1446:VAL:HG21	1.99	0.45
1:C:1332:GLN:HA	1:C:1341:CYS:SG	2.57	0.45
1:C:1871:ILE:CD1	1:C:1960:LEU:HD22	2.46	0.45
1:D:1519:LYS:HG3	1:D:1653:CYS:HB3	1.99	0.45
1:D:1944:HIS:HE1	1:D:1946:GLN:OE1	2.00	0.44
1:A:1423:ASP:OD2	1:A:1471:SER:OG	2.34	0.44
1:A:1896:ASN:HB3	1:B:1456:ILE:HD12	1.99	0.44
1:D:2000:VAL:O	1:D:2001:PRO:C	2.59	0.44
1:B:1402:SER:HB3	1:B:1405:LEU:HD12	1.99	0.44
1:A:2021:LEU:HD23	1:A:2021:LEU:HA	1.86	0.44
1:C:1658:PHE:CD1	1:C:1659:PRO:HD2	2.51	0.44
1:A:1871:ILE:HD13	1:A:1919:VAL:HG22	1.99	0.44
1:D:1419:LEU:N	1:D:1419:LEU:CD1	2.81	0.44
1:D:1497:GLU:H	1:D:1497:GLU:CD	2.25	0.44
1:C:1402:SER:HB3	1:C:1405:LEU:HD12	1.99	0.43
1:C:1915:LEU:HD11	1:C:1935:LEU:HD12	2.00	0.43
1:B:1423:ASP:OD2	1:B:1471:SER:OG	2.36	0.43
1:B:1419:LEU:N	1:B:1419:LEU:CD1	2.81	0.43
1:B:1419:LEU:HD13	1:B:1464:ILE:HG23	1.99	0.43
1:B:1800:LEU:N	1:B:1801:PRO:HD3	2.33	0.43
1:C:2070:VAL:HG12	1:C:2074:ASN:ND2	2.34	0.43
1:C:1540:LEU:O	1:C:1543:MET:HB2	2.18	0.43
1:C:1372:LYS:HE2	1:C:1510:ASP:OD1	2.19	0.43
1:A:1419:LEU:N	1:A:1419:LEU:CD1	2.82	0.43
1:B:1751:TYR:O	1:B:1752:SER:C	2.62	0.43
1:B:1764:LEU:HD23	1:B:1788:ILE:HG12	2.00	0.43
1:D:1468:ASN:ND2	1:D:1646:LEU:HD21	2.34	0.43
1:B:1358:LYS:O	1:B:1358:LYS:HD3	2.18	0.43
1:B:1850:TYR:CZ	1:B:1935:LEU:HD21	2.53	0.43
1:B:1519:LYS:HG3	1:B:1653:CYS:HB3	2.01	0.43
1:D:1402:SER:HB3	1:D:1405:LEU:HD12	2.01	0.43
1:A:1391:TYR:O	1:A:1401:SER:HA	2.18	0.43
1:A:1434:GLY:O	1:A:1436:THR:HG23	2.19	0.43
1:A:1781:LEU:HD23	1:A:1781:LEU:HA	1.89	0.43
1:A:1931:ARG:HA	3:A:2213:HOH:O	2.19	0.43
1:B:1332:GLN:HA	1:B:1341:CYS:SG	2.59	0.43
1:B:1658:PHE:CD1	1:B:1659:PRO:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1389:ASN:HB3	1:C:1392:LEU:HD12	2.01	0.43
1:C:1871:ILE:HD11	1:C:1960:LEU:HD22	2.01	0.43
1:A:1751:TYR:O	1:A:1752:SER:C	2.61	0.42
1:A:1503:ASP:N	1:A:1503:ASP:OD1	2.52	0.42
1:B:1871:ILE:HD11	1:B:1960:LEU:HD22	2.01	0.42
1:D:1751:TYR:O	1:D:1752:SER:C	2.62	0.42
1:A:1431:ILE:HD12	1:A:1446:VAL:HG21	2.01	0.42
1:B:1434:GLY:O	1:B:1436:THR:HG23	2.19	0.42
1:C:1764:LEU:HD23	1:C:1788:ILE:HG12	2.02	0.42
1:C:1452:ARG:NH2	1:D:1865:SER:OG	2.53	0.42
1:A:1967:MET:HB2	1:A:2077:PHE:CD1	2.55	0.42
1:C:1895:LEU:HD22	1:D:1411:LEU:HD11	2.01	0.42
1:D:1526:HIS:CD2	1:D:1532:ILE:HG12	2.54	0.42
1:A:2070:VAL:HG12	1:A:2074:ASN:HD21	1.85	0.42
1:D:1839:GLU:OE2	1:D:1841:ASP:HB3	2.20	0.42
1:A:2070:VAL:HG12	1:A:2074:ASN:ND2	2.34	0.42
1:B:1468:ASN:HD21	1:B:1475:GLN:CD	2.27	0.42
1:D:1850:TYR:CZ	1:D:1935:LEU:HD21	2.54	0.42
1:C:1434:GLY:O	1:C:1436:THR:HG23	2.20	0.41
1:C:1751:TYR:O	1:C:1752:SER:C	2.63	0.41
1:D:1781:LEU:HD23	1:D:1781:LEU:HA	1.92	0.41
1:B:1335:GLU:OE1	1:B:1335:GLU:HA	2.20	0.41
1:D:1434:GLY:O	1:D:1436:THR:HG23	2.20	0.41
1:B:1336:PRO:HD3	1:B:1353:ARG:NH1	2.35	0.41
1:A:2070:VAL:O	1:A:2074:ASN:ND2	2.53	0.41
1:D:1896:ASN:N	1:D:1897:PRO:CD	2.84	0.41
1:A:1519:LYS:HG3	1:A:1653:CYS:HB3	2.03	0.41
1:C:2070:VAL:O	1:C:2074:ASN:ND2	2.54	0.41
1:A:2028:ASP:O	1:A:2029:GLN:C	2.63	0.41
1:A:2044:LYS:HB2	1:A:2059:PHE:HB3	2.02	0.41
1:A:1389:ASN:HB3	1:A:1392:LEU:HD12	2.02	0.41
1:C:1850:TYR:CZ	1:C:1935:LEU:HD21	2.56	0.41
1:A:1839:GLU:OE2	1:A:1841:ASP:HB3	2.20	0.41
1:A:1395:HIS:CD2	1:A:1398:LYS:HG3	2.56	0.41
1:A:1658:PHE:CD1	1:A:1659:PRO:HD2	2.55	0.41
1:C:1460:LEU:CD1	1:C:1815:CYS:SG	3.09	0.41
1:B:2070:VAL:O	1:B:2074:ASN:ND2	2.54	0.41
1:C:1519:LYS:HG3	1:C:1653:CYS:HB3	2.02	0.40
1:D:1468:ASN:HD21	1:D:1646:LEU:CD2	2.34	0.40
1:B:1858:GLN:O	1:B:1958:SER:HA	2.22	0.40
1:C:1419:LEU:HD13	1:C:1464:ILE:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1643:ALA:HA	1:C:1644:PRO:HD3	1.95	0.40
1:D:1468:ASN:ND2	1:D:1646:LEU:CD2	2.84	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	597/818 (73%)	570 (96%)	22 (4%)	5 (1%)	16	29
1	B	597/818 (73%)	570 (96%)	24 (4%)	3 (0%)	24	40
1	C	603/818 (74%)	573 (95%)	26 (4%)	4 (1%)	18	32
1	D	591/818 (72%)	564 (95%)	24 (4%)	3 (0%)	24	40
All	All	2388/3272 (73%)	2277 (95%)	96 (4%)	15 (1%)	21	36

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1825	TRP
1	C	1638	GLU
1	C	1825	TRP
1	D	1825	TRP
1	A	1825	TRP
1	A	1471	SER
1	A	2003	PRO
1	C	2003	PRO
1	A	1830	PRO
1	A	2027	VAL
1	B	1830	PRO
1	B	2003	PRO
1	C	1830	PRO

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Mol	Chain	Res	Type
1	D	2003	PRO
1	D	1830	PRO

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	551/730 (76%)	512 (93%)	39 (7%)	13	24
1	B	550/730 (75%)	504 (92%)	46 (8%)	10	18
1	C	558/730 (76%)	527 (94%)	31 (6%)	19	35
1	D	545/730 (75%)	507 (93%)	38 (7%)	14	26
All	All	2204/2920 (76%)	2050 (93%)	154 (7%)	14	26

All (154) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1338	ILE
1	A	1367	GLU
1	A	1368	SER
1	A	1398	LYS
1	A	1405	LEU
1	A	1409	VAL
1	A	1417	ILE
1	A	1438	THR
1	A	1440	LYS
1	A	1457	THR
1	A	1471	SER
1	A	1483	LYS
1	A	1503	ASP
1	A	1527	GLN
1	A	1639	SER
1	A	1732	LYS
1	A	1738	SER
1	A	1741	GLU
1	A	1747	LEU

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Mol	Chain	Res	Type
1	A	1752	SER
1	A	1766	THR
1	A	1771	THR
1	A	1776	SER
1	A	1834	LYS
1	A	1839	GLU
1	A	1862	PRO
1	A	1871	ILE
1	A	1888	LYS
1	A	1896	ASN
1	A	1906	ARG
1	A	1907	VAL
1	A	1915	LEU
1	A	1930	GLN
1	A	1956	GLU
1	A	1957	ILE
1	A	1975	THR
1	A	2010	THR
1	A	2022	GLN
1	A	2091	GLN
1	B	1325	ASP
1	B	1338	ILE
1	B	1341	CYS
1	B	1349	GLU
1	B	1366	ASP
1	B	1368	SER
1	B	1369	ARG
1	B	1398	LYS
1	B	1405	LEU
1	B	1407	SER
1	B	1409	VAL
1	B	1417	ILE
1	B	1425	ASP
1	B	1438	THR
1	B	1457	THR
1	B	1493	LYS
1	B	1544	GLN
1	B	1730	THR
1	B	1738	SER
1	B	1741	GLU
1	B	1747	LEU
1	B	1752	SER

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Mol	Chain	Res	Type
1	B	1766	THR
1	B	1776	SER
1	B	1839	GLU
1	B	1846	ASP
1	B	1871	ILE
1	B	1896	ASN
1	B	1906	ARG
1	B	1907	VAL
1	B	1915	LEU
1	B	1930	GLN
1	B	1940	ARG
1	B	1954	ILE
1	B	1957	ILE
1	B	1968	GLU
1	B	1985	GLU
1	B	2010	THR
1	B	2012	ASN
1	B	2016	LYS
1	B	2021	LEU
1	B	2034	THR
1	B	2071	GLN
1	B	2091	GLN
1	B	2094	THR
1	B	2096	GLU
1	C	1341	CYS
1	C	1342	HIS
1	C	1368	SER
1	C	1369	ARG
1	C	1405	LEU
1	C	1409	VAL
1	C	1417	ILE
1	C	1457	THR
1	C	1501	SER
1	C	1524	LYS
1	C	1543	MET
1	C	1620	LYS
1	C	1631	TYR
1	C	1635	ASN
1	C	1730	THR
1	C	1738	SER
1	C	1741	GLU
1	C	1747	LEU

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Mol	Chain	Res	Type
1	C	1750	ARG
1	C	1752	SER
1	C	1761	CYS
1	C	1766	THR
1	C	1771	THR
1	C	1776	SER
1	C	1827	LYS
1	C	1846	ASP
1	C	1862	PRO
1	C	1871	ILE
1	C	1896	ASN
1	C	1930	GLN
1	C	1957	ILE
1	D	1338	ILE
1	D	1353	ARG
1	D	1368	SER
1	D	1369	ARG
1	D	1405	LEU
1	D	1407	SER
1	D	1409	VAL
1	D	1417	ILE
1	D	1457	THR
1	D	1471	SER
1	D	1493	LYS
1	D	1502	ASP
1	D	1524	LYS
1	D	1527	GLN
1	D	1539	GLN
1	D	1543	MET
1	D	1730	THR
1	D	1738	SER
1	D	1741	GLU
1	D	1747	LEU
1	D	1752	SER
1	D	1753	GLN
1	D	1766	THR
1	D	1771	THR
1	D	1776	SER
1	D	1839	GLU
1	D	1862	PRO
1	D	1871	ILE
1	D	1896	ASN

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Mol	Chain	Res	Type
1	D	1907	VAL
1	D	1930	GLN
1	D	1940	ARG
1	D	1954	ILE
1	D	1957	ILE
1	D	1968	GLU
1	D	2010	THR
1	D	2021	LEU
1	D	2034	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1388	HIS
1	A	1395	HIS
1	A	1408	GLN
1	A	1412	GLN
1	A	1805	ASN
1	A	1833	GLN
1	A	1896	ASN
1	A	1902	GLN
1	A	1908	HIS
1	A	1930	GLN
1	A	1998	HIS
1	A	2022	GLN
1	A	2074	ASN
1	B	1342	HIS
1	B	1343	GLN
1	B	1468	ASN
1	B	1520	ASN
1	B	1526	HIS
1	B	1753	GLN
1	B	1805	ASN
1	B	1896	ASN
1	B	1902	GLN
1	B	1930	GLN
1	B	2074	ASN
1	B	2091	GLN
1	C	1332	GLN
1	C	1371	ASN
1	C	1376	GLN
1	C	1388	HIS

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Mol	Chain	Res	Type
1	C	1468	ASN
1	C	1526	HIS
1	C	1535	GLN
1	C	1641	GLN
1	C	1753	GLN
1	C	1758	HIS
1	C	1762	GLN
1	C	1805	ASN
1	C	1896	ASN
1	C	1902	GLN
1	C	1908	HIS
1	C	1930	GLN
1	C	1993	HIS
1	C	2012	ASN
1	C	2022	GLN
1	C	2071	GLN
1	C	2074	ASN
1	D	1332	GLN
1	D	1371	ASN
1	D	1388	HIS
1	D	1468	ASN
1	D	1526	HIS
1	D	1539	GLN
1	D	1641	GLN
1	D	1758	HIS
1	D	1762	GLN
1	D	1805	ASN
1	D	1896	ASN
1	D	1908	HIS
1	D	1930	GLN
1	D	1944	HIS
1	D	1998	HIS
1	D	2022	GLN
1	D	2074	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	609/818 (74%)	0.28	12 (1%) 65 62	37, 51, 87, 115	0
1	B	611/818 (74%)	0.37	14 (2%) 61 58	37, 58, 93, 125	0
1	C	617/818 (75%)	0.48	14 (2%) 61 58	41, 64, 103, 129	0
1	D	605/818 (73%)	0.59	29 (4%) 35 35	41, 63, 121, 167	0
All	All	2442/3272 (74%)	0.43	69 (2%) 55 52	37, 59, 101, 167	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1303	PHE	4.5
1	B	1303	PHE	4.4
1	D	1525	ALA	4.2
1	B	2028	ASP	4.0
1	B	1525	ALA	4.0
1	B	2095	LEU	3.9
1	D	2026	ALA	3.7
1	D	2035	ALA	3.6
1	C	2047	ILE	3.6
1	A	1344	GLY	3.6
1	C	1303	PHE	3.3
1	D	2003	PRO	3.2
1	D	2020	LEU	3.1
1	B	1524	LYS	3.0
1	D	2036	ALA	3.0
1	D	2039	PHE	2.9
1	A	1303	PHE	2.9
1	A	1525	ALA	2.8
1	D	1975	THR	2.8
1	C	2038	TYR	2.8
1	B	2047	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	1338	ILE	2.7
1	D	1304	GLY	2.7
1	D	1344	GLY	2.7
1	D	1327	ILE	2.7
1	D	2017	ALA	2.7
1	B	1529	PRO	2.7
1	C	1980	LEU	2.6
1	D	2038	TYR	2.6
1	C	1336	PRO	2.6
1	A	1338	ILE	2.5
1	D	1339	SER	2.5
1	D	1338	ILE	2.5
1	B	2003	PRO	2.5
1	D	2043	GLU	2.5
1	B	2058	PRO	2.4
1	D	2034	THR	2.4
1	B	1366	ASP	2.4
1	C	1631	TYR	2.4
1	D	2047	ILE	2.3
1	C	2041	MET	2.3
1	C	2026	ALA	2.3
1	D	1328	LEU	2.3
1	A	2091	GLN	2.3
1	B	2035	ALA	2.3
1	A	1366	ASP	2.3
1	D	2001	PRO	2.3
1	C	1798	ASP	2.2
1	B	1841	ASP	2.2
1	D	1361	PHE	2.2
1	B	1975	THR	2.2
1	A	2065	PRO	2.2
1	D	1324	TYR	2.2
1	C	2037	ASP	2.2
1	D	1325	ASP	2.2
1	D	1918	ALA	2.1
1	D	2018	LYS	2.1
1	A	1661	LEU	2.1
1	C	1979	SER	2.1
1	A	1437	LEU	2.1
1	B	2027	VAL	2.1
1	C	2046	PHE	2.1
1	D	1870	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1828	SER	2.1
1	A	1345	LEU	2.1
1	A	1361	PHE	2.1
1	D	1540	LEU	2.0
1	A	1774	ASP	2.0
1	D	1524	LYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	D	2100	1/1	0.56	0.19	132,132,132,132	0
2	CA	C	2100	1/1	0.89	0.12	115,115,115,115	0
2	CA	A	2100	1/1	0.92	0.12	83,83,83,83	0
2	CA	B	2100	1/1	0.96	0.08	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.