



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 01:40 PM BST

PDB ID : 6PMP
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.13
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

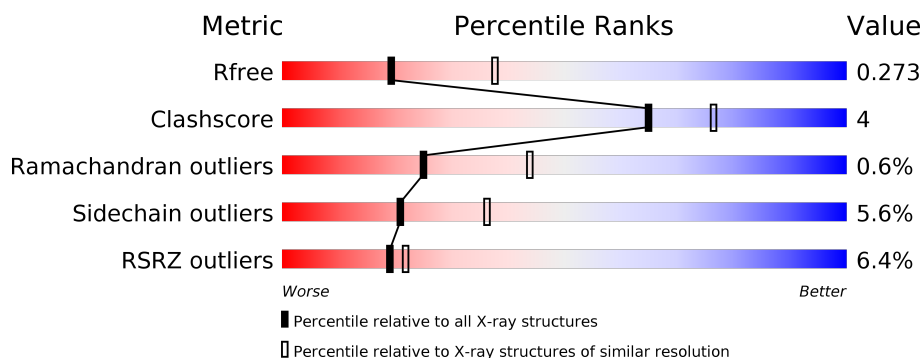
1 Overall quality at a glance

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}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (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 on 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	<div> <div>4%</div> <div> <div></div> <div>63%</div> <div>11%</div> <div>•</div> <div>26%</div> </div> </div>
1	B	818	<div> <div>3%</div> <div> <div></div> <div>62%</div> <div>12%</div> <div>•</div> <div>25%</div> </div> </div>
1	C	818	<div> <div>5%</div> <div> <div></div> <div>63%</div> <div>11%</div> <div>•</div> <div>25%</div> </div> </div>
1	D	818	<div> <div>6%</div> <div> <div></div> <div>63%</div> <div>11%</div> <div>•</div> <div>26%</div> </div> </div>

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 (three-letter code: CA) (formula: Ca).

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

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

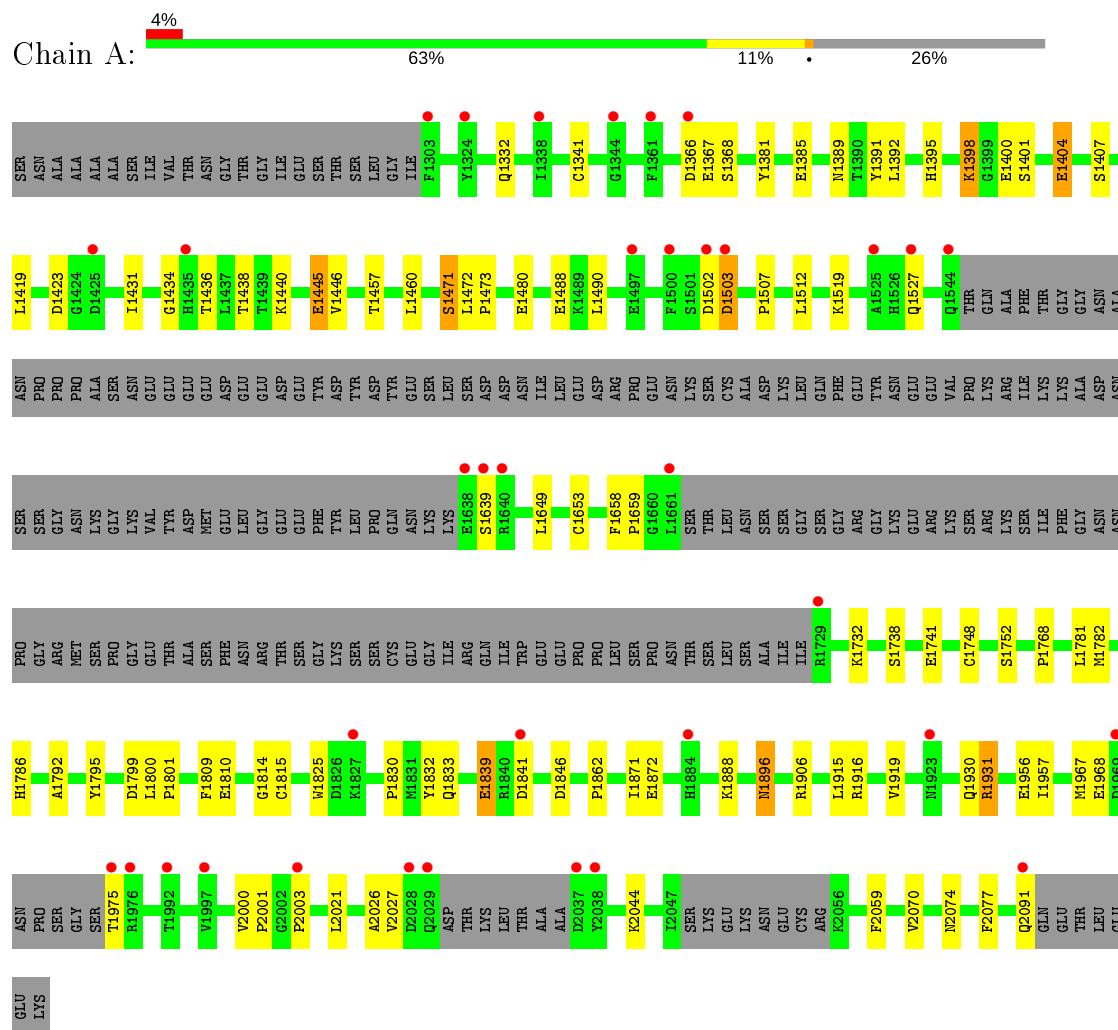
- Molecule 3 is water.

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

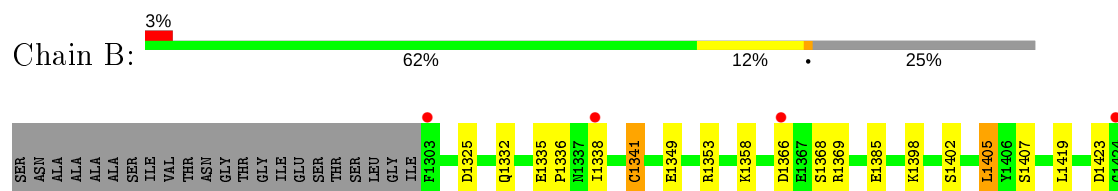
3 Residue-property plots

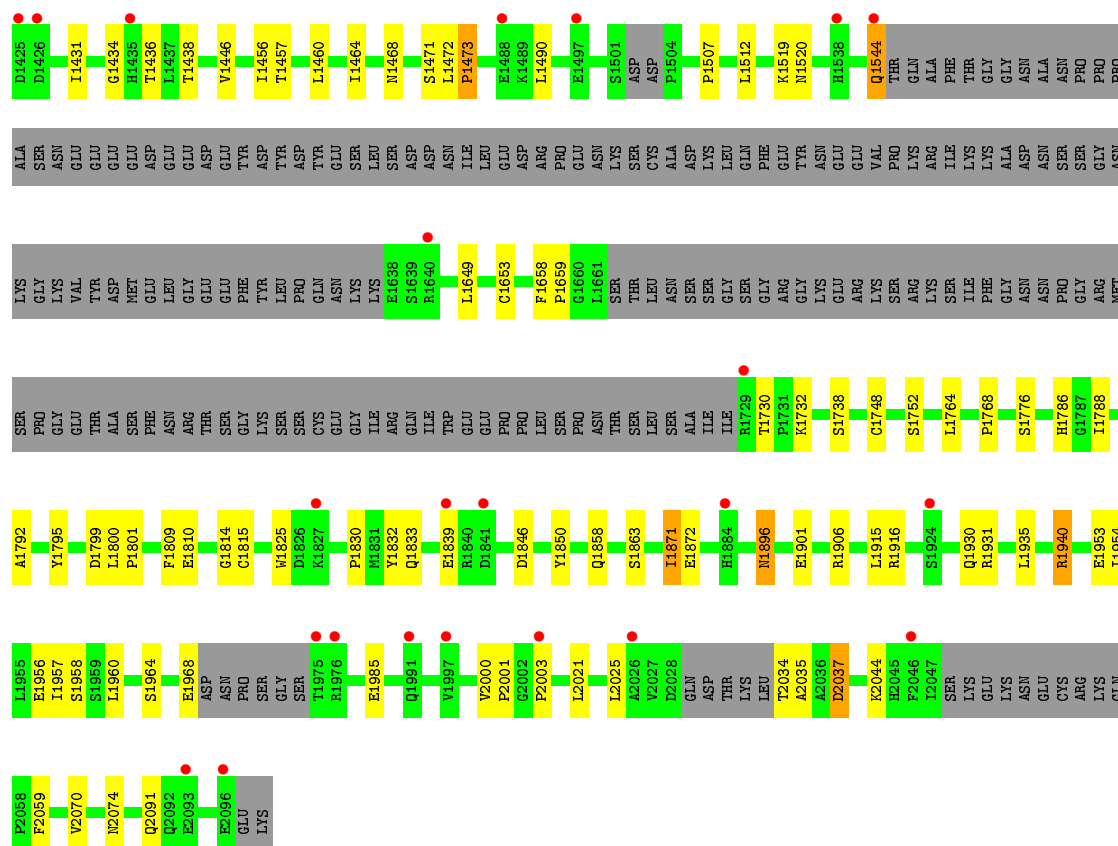
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

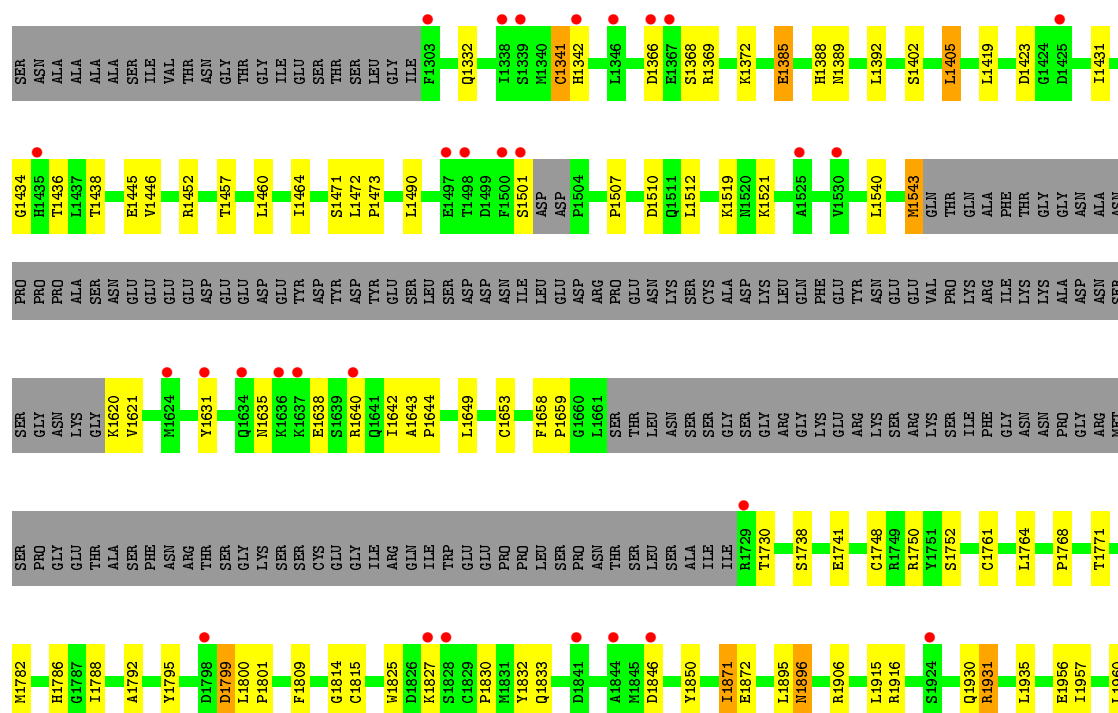


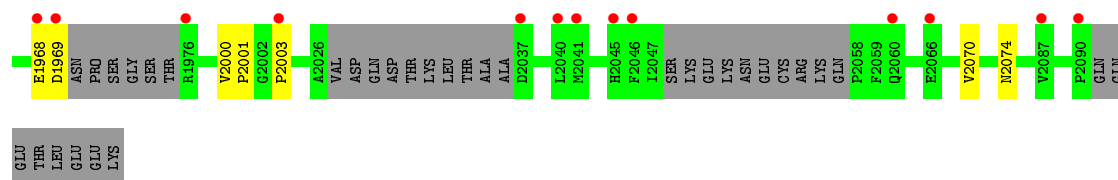
- Molecule 1: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase epsilon-1



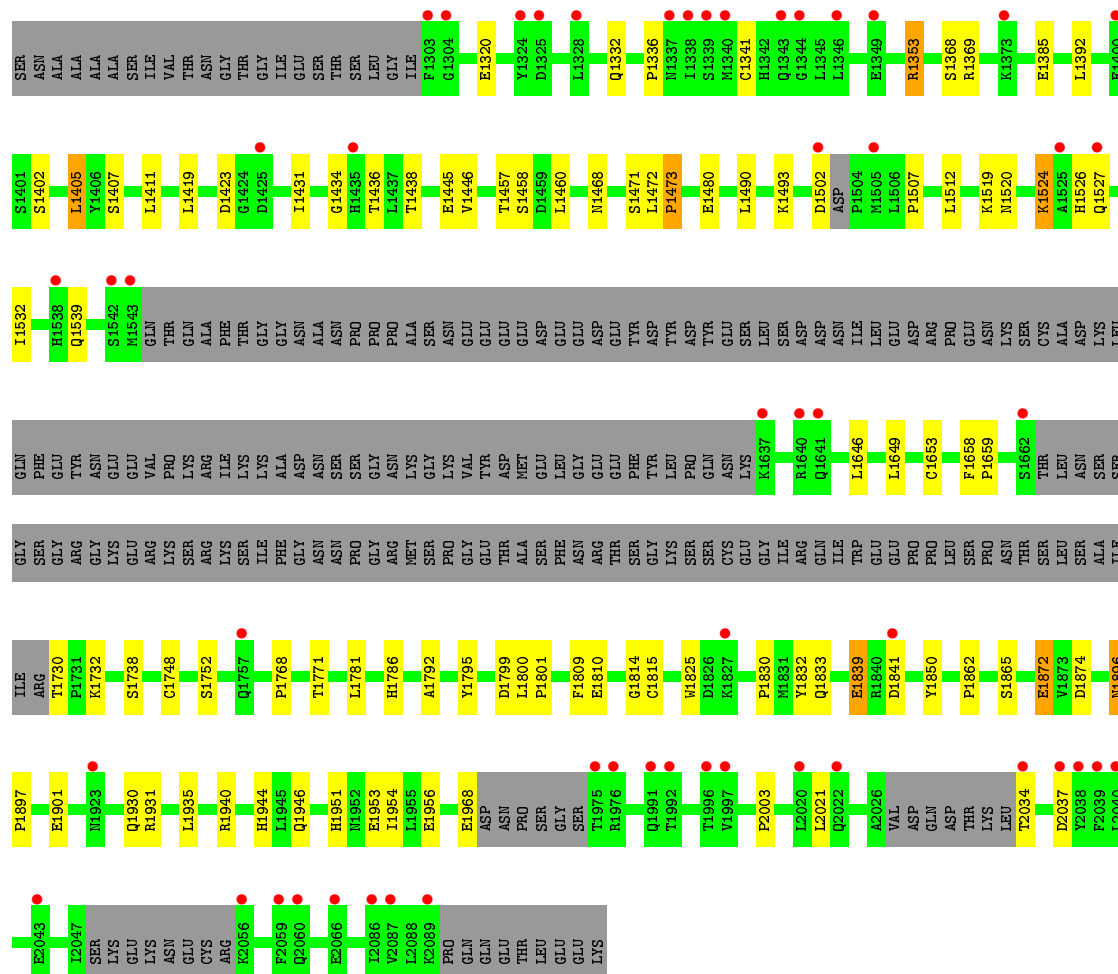


- Molecule 1: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase epsilon-1





- 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 19.99 – 2.73	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-2.73) 99.5 (19.99-2.73)	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	4196 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)	0.30 , 17.0	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	0.92	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 ⓘ

5.1 Standard geometry ⓘ

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	0.84	12/5008 (0.2%)	0.94	3/6773 (0.0%)
1	B	0.81	6/5012 (0.1%)	0.93	1/6777 (0.0%)
1	C	0.80	5/5084 (0.1%)	0.93	3/6870 (0.0%)
1	D	0.81	9/4962 (0.2%)	0.93	0/6707
All	All	0.81	32/20066 (0.2%)	0.93	7/27127 (0.0%)

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1872	GLU	CD-OE2	8.79	1.35	1.25
1	B	1956	GLU	CD-OE2	8.08	1.34	1.25
1	D	1901	GLU	CD-OE2	8.00	1.34	1.25
1	A	1810	GLU	CD-OE2	7.98	1.34	1.25
1	D	1810	GLU	CD-OE2	7.48	1.33	1.25
1	A	1810	GLU	CD-OE1	7.33	1.33	1.25
1	D	1956	GLU	CD-OE2	7.21	1.33	1.25
1	A	1956	GLU	CD-OE1	7.07	1.33	1.25
1	A	1480	GLU	CD-OE2	7.03	1.33	1.25
1	A	1480	GLU	CD-OE1	6.88	1.33	1.25
1	A	1872	GLU	CD-OE2	6.80	1.33	1.25
1	D	1872	GLU	CD-OE2	6.79	1.33	1.25
1	C	1385	GLU	CD-OE2	6.57	1.32	1.25
1	A	1956	GLU	CD-OE2	6.47	1.32	1.25
1	D	1953	GLU	CD-OE1	6.42	1.32	1.25
1	C	1445	GLU	CD-OE2	6.41	1.32	1.25
1	C	1872	GLU	CD-OE2	6.39	1.32	1.25
1	D	1480	GLU	CD-OE2	6.10	1.32	1.25
1	C	1956	GLU	CD-OE1	6.08	1.32	1.25
1	B	1953	GLU	CD-OE2	5.99	1.32	1.25
1	A	1404	GLU	CD-OE1	5.96	1.32	1.25
1	D	1810	GLU	CD-OE1	5.77	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1388	HIS	C-O	5.76	1.34	1.23
1	B	1810	GLU	CD-OE2	5.58	1.31	1.25
1	B	1953	GLU	CD-OE1	5.57	1.31	1.25
1	A	1400	GLU	CD-OE2	5.42	1.31	1.25
1	A	1445	GLU	CD-OE2	5.41	1.31	1.25
1	B	1901	GLU	CD-OE2	5.41	1.31	1.25
1	A	1404	GLU	CD-OE2	5.40	1.31	1.25
1	D	1320	GLU	CD-OE2	5.27	1.31	1.25
1	A	1488	GLU	CD-OE2	5.24	1.31	1.25
1	D	1445	GLU	CD-OE2	5.09	1.31	1.25

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1916	ARG	NE-CZ-NH2	-7.95	116.32	120.30
1	C	1916	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	1916	ARG	NE-CZ-NH2	-6.69	116.96	120.30
1	C	1931	ARG	CG-CD-NE	-5.75	99.72	111.80
1	A	1488	GLU	CB-CA-C	5.20	120.79	110.40
1	C	1799	ASP	CB-CA-C	5.17	120.74	110.40
1	A	1381	TYR	CB-CG-CD1	5.15	124.09	121.00

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	4897	0	4870	41	0
1	B	4902	0	4883	43	0
1	C	4970	0	4950	42	0
1	D	4853	0	4840	41	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	161	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 (161) 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
1:B:1809:PHE:O	1:B:1814:GLY:HA2	2.01	0.60
1:A:1896:ASN:HD22	1:A:1896:ASN:N	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:H	1:A:1896:ASN:HD22	1.51	0.59
1:B:1800:LEU:N	1:B:1801:PRO:CD	2.66	0.57
1:D:1896:ASN:H	1:D:1896:ASN:HD22	1.52	0.57
1:B:1896:ASN:HD22	1:B:1896:ASN:N	2.03	0.57
1:C:1640:ARG:CZ	1:C:1640:ARG:HB3	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:H	1:C:1896:ASN:HD22	1.54	0.54
1:D:1524:LYS:CE	1:D:1524:LYS:H	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:1832:TYR:CD2	1:B:1833:GLN:HG3	2.46	0.51
1:C:1419:LEU:N	1:C:1419:LEU:HD12	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:D:1392:LEU:HD21	1:D:1438:THR:HG21	1.96	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:A:1332:GLN:HA	1:A:1341:CYS:SG	2.55	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:1402:SER:HB3	1:B:1405:LEU:HD12	1.99	0.44
1:A:2021:LEU:HA	1:A:2021:LEU:HD23	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:B:1544:GLN:CD	1:B:1544:GLN:C	2.77	0.44
1:D:1419:LEU:CD1	1:D:1419:LEU:N	2.81	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:CD1	1:B:1419:LEU:N	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: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:HA	1:A:1781:LEU:HD23	1.89	0.43
1:A:1931:ARG:HA	3:A:2213:HOH:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:1503:ASP:N	1:A:1503:ASP:OD1	2.52	0.42
1:A:1799:ASP:CG	1:A:1801:PRO:HD2	2.39	0.42
1:B:1871:ILE:HD11	1:B:1960:LEU:HD22	2.01	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:B:2000:VAL:O	1:B:2001:PRO:C	2.57	0.42
1:C:1764:LEU:HD23	1:C:1788:ILE:HG12	2.02	0.42
1:D:1423:ASP:OD2	1:D:1471:SER:OG	2.37	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:C:1968:GLU:O	1:C:1969:ASP:C	2.58	0.42
1:D:1839:GLU:OE2	1:D:1841:ASP:HB3	2.20	0.42
1:D:1896:ASN:ND2	1:D:1896:ASN:N	2.67	0.42
1:A:2070:VAL:HG12	1:A:2074:ASN:ND2	2.34	0.42
1:C:1799:ASP:CG	1:C:1801:PRO:HD2	2.39	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:D:1781:LEU:HA	1:D:1781:LEU:HD23	1.92	0.41
1:B:1335:GLU:HA	1:B:1335:GLU:OE1	2.20	0.41
1:C:2000:VAL:O	1:C:2001:PRO:C	2.59	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:B:1799:ASP:CG	1:B:1801:PRO:HD2	2.40	0.41
1:A:2070:VAL:O	1:A:2074:ASN:ND2	2.53	0.41
1:D:1799:ASP:CG	1:D:1801:PRO:HD2	2.41	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:2000:VAL:O	1:A:2001:PRO:C	2.59	0.40
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
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%)	19	36
1	B	597/818 (73%)	570 (96%)	24 (4%)	3 (0%)	29	48
1	C	603/818 (74%)	573 (95%)	26 (4%)	4 (1%)	22	40
1	D	591/818 (72%)	564 (95%)	24 (4%)	3 (0%)	29	48
All	All	2388/3272 (73%)	2277 (95%)	96 (4%)	15 (1%)	25	44

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

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Mol	Chain	Res	Type
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
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%)	521 (95%)	30 (5%)	22	38
1	B	550/730 (75%)	514 (94%)	36 (6%)	17	30
1	C	558/730 (76%)	530 (95%)	28 (5%)	24	42
1	D	545/730 (75%)	516 (95%)	29 (5%)	22	39
All	All	2204/2920 (76%)	2081 (94%)	123 (6%)	21	36

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1366	ASP
1	A	1367	GLU
1	A	1368	SER
1	A	1398	LYS
1	A	1407	SER
1	A	1438	THR
1	A	1440	LYS
1	A	1457	THR
1	A	1502	ASP
1	A	1503	ASP
1	A	1527	GLN
1	A	1639	SER

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Mol	Chain	Res	Type
1	A	1732	LYS
1	A	1738	SER
1	A	1741	GLU
1	A	1752	SER
1	A	1782	MET
1	A	1839	GLU
1	A	1846	ASP
1	A	1862	PRO
1	A	1888	LYS
1	A	1896	ASN
1	A	1906	ARG
1	A	1915	LEU
1	A	1930	GLN
1	A	1931	ARG
1	A	1957	ILE
1	A	1968	GLU
1	A	1975	THR
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	1438	THR
1	B	1457	THR
1	B	1473	PRO
1	B	1544	GLN
1	B	1730	THR
1	B	1732	LYS
1	B	1738	SER
1	B	1752	SER
1	B	1776	SER
1	B	1839	GLU
1	B	1846	ASP
1	B	1871	ILE
1	B	1896	ASN
1	B	1906	ARG

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Mol	Chain	Res	Type
1	B	1915	LEU
1	B	1930	GLN
1	B	1931	ARG
1	B	1940	ARG
1	B	1954	ILE
1	B	1957	ILE
1	B	1968	GLU
1	B	1985	GLU
1	B	2021	LEU
1	B	2034	THR
1	B	2037	ASP
1	B	2091	GLN
1	C	1341	CYS
1	C	1342	HIS
1	C	1366	ASP
1	C	1368	SER
1	C	1369	ARG
1	C	1405	LEU
1	C	1457	THR
1	C	1501	SER
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	1750	ARG
1	C	1752	SER
1	C	1761	CYS
1	C	1771	THR
1	C	1782	MET
1	C	1827	LYS
1	C	1846	ASP
1	C	1871	ILE
1	C	1896	ASN
1	C	1906	ARG
1	C	1930	GLN
1	C	1931	ARG
1	C	1957	ILE
1	D	1353	ARG
1	D	1368	SER

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Mol	Chain	Res	Type
1	D	1369	ARG
1	D	1405	LEU
1	D	1407	SER
1	D	1457	THR
1	D	1458	SER
1	D	1473	PRO
1	D	1493	LYS
1	D	1502	ASP
1	D	1524	LYS
1	D	1527	GLN
1	D	1539	GLN
1	D	1730	THR
1	D	1732	LYS
1	D	1738	SER
1	D	1752	SER
1	D	1771	THR
1	D	1839	GLU
1	D	1862	PRO
1	D	1896	ASN
1	D	1930	GLN
1	D	1931	ARG
1	D	1940	ARG
1	D	1954	ILE
1	D	1968	GLU
1	D	2021	LEU
1	D	2034	THR
1	D	2037	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1388	HIS
1	A	1395	HIS
1	A	1408	GLN
1	A	1794	ASN
1	A	1805	ASN
1	A	1896	ASN
1	A	1908	HIS
1	A	1930	GLN
1	A	2022	GLN
1	A	2074	ASN
1	B	1343	GLN

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Mol	Chain	Res	Type
1	B	1468	ASN
1	B	1520	ASN
1	B	1526	HIS
1	B	1805	ASN
1	B	1896	ASN
1	B	1930	GLN
1	B	2074	ASN
1	B	2091	GLN
1	C	1408	GLN
1	C	1468	ASN
1	C	1526	HIS
1	C	1641	GLN
1	C	1805	ASN
1	C	1896	ASN
1	C	2012	ASN
1	C	2022	GLN
1	C	2071	GLN
1	C	2074	ASN
1	D	1408	GLN
1	D	1468	ASN
1	D	1520	ASN
1	D	1526	HIS
1	D	1805	ASN
1	D	1896	ASN
1	D	1930	GLN
1	D	1944	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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	609/818 (74%)	0.23	35 (5%)	23	26	37, 51, 87, 115	0
1	B	611/818 (74%)	0.25	27 (4%)	34	37	37, 58, 93, 125	0
1	C	617/818 (75%)	0.39	42 (6%)	17	19	41, 64, 103, 129	0
1	D	605/818 (73%)	0.44	53 (8%)	10	10	41, 63, 121, 167	0
All	All	2442/3272 (74%)	0.33	157 (6%)	19	22	37, 59, 101, 167	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1339	SER	7.0
1	C	1303	PHE	6.8
1	B	1303	PHE	5.6
1	B	1841	ASP	5.4
1	A	1435	HIS	5.3
1	C	2090	PRO	4.6
1	A	1640	ARG	4.4
1	D	1975	THR	4.4
1	B	1975	THR	4.4
1	D	1525	ALA	4.4
1	B	1425	ASP	4.3
1	D	1303	PHE	4.3
1	B	1976	ARG	4.2
1	D	2038	TYR	4.2
1	C	1497	GLU	4.2
1	A	1525	ALA	4.2
1	A	1841	ASP	4.2
1	D	1338	ILE	4.1
1	D	1841	ASP	4.1
1	C	1501	SER	4.1
1	B	1488	GLU	4.1

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Mol	Chain	Res	Type	RSRZ
1	C	1827	LYS	4.1
1	D	1425	ASP	4.0
1	D	2022	GLN	3.9
1	D	1435	HIS	3.9
1	C	1969	ASP	3.9
1	A	1502	ASP	3.8
1	D	1640	ARG	3.7
1	B	1497	GLU	3.7
1	B	1729	ARG	3.7
1	A	1503	ASP	3.6
1	C	1631	TYR	3.6
1	B	2096	GLU	3.5
1	A	1544	GLN	3.5
1	B	1640	ARG	3.5
1	B	2093	GLU	3.4
1	C	2040	LEU	3.4
1	A	1500	PHE	3.4
1	C	1637	LYS	3.3
1	A	1303	PHE	3.3
1	C	1342	HIS	3.3
1	D	2086	ILE	3.3
1	D	1637	LYS	3.3
1	B	1338	ILE	3.2
1	D	1340	MET	3.2
1	A	1729	ARG	3.2
1	C	1729	ARG	3.2
1	D	1992	THR	3.2
1	D	1662	SER	3.1
1	B	1435	HIS	3.1
1	A	2091	GLN	3.1
1	C	1640	ARG	3.1
1	C	1425	ASP	3.0
1	C	1500	PHE	3.0
1	C	1798	ASP	3.0
1	A	1366	ASP	2.9
1	A	1975	THR	2.9
1	C	2037	ASP	2.9
1	C	1338	ILE	2.9
1	D	1346	LEU	2.8
1	B	1424	GLY	2.8
1	D	2066	GLU	2.8
1	B	1839	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	2043	GLU	2.7
1	A	1997	VAL	2.7
1	C	1841	ASP	2.7
1	D	1502	ASP	2.7
1	D	1349	GLU	2.7
1	A	1661	LEU	2.7
1	A	1923	ASN	2.7
1	D	1344	GLY	2.7
1	C	1636	LYS	2.6
1	A	1969	ASP	2.6
1	C	1634	GLN	2.6
1	D	1527	GLN	2.6
1	D	2037	ASP	2.6
1	C	1846	ASP	2.6
1	A	1639	SER	2.6
1	D	1304	GLY	2.6
1	A	2037	ASP	2.5
1	D	2040	LEU	2.5
1	D	1542	SER	2.5
1	D	1343	GLN	2.5
1	D	1641	GLN	2.5
1	A	1338	ILE	2.5
1	A	1344	GLY	2.5
1	C	1976	ARG	2.5
1	B	1544	GLN	2.5
1	D	1400	GLU	2.5
1	C	1530	VAL	2.5
1	C	2087	VAL	2.5
1	B	2026	ALA	2.5
1	C	1924	SER	2.5
1	B	1366	ASP	2.5
1	D	2039	PHE	2.4
1	A	2028	ASP	2.4
1	C	2066	GLU	2.4
1	D	1328	LEU	2.4
1	B	2046	PHE	2.4
1	C	2046	PHE	2.4
1	D	2059	PHE	2.4
1	B	1924	SER	2.4
1	D	2087	VAL	2.4
1	C	1968	GLU	2.4
1	C	2041	MET	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	1991	GLN	2.3
1	D	1505	MET	2.3
1	A	1324	TYR	2.3
1	A	1497	GLU	2.3
1	A	1527	GLN	2.3
1	D	1325	ASP	2.3
1	D	2056	LYS	2.3
1	A	1884	HIS	2.3
1	C	1828	SER	2.3
1	D	1538	HIS	2.3
1	A	1976	ARG	2.3
1	B	1426	ASP	2.3
1	D	1997	VAL	2.2
1	C	2003	PRO	2.2
1	A	1827	LYS	2.2
1	B	1997	VAL	2.2
1	D	2089	LYS	2.2
1	D	1324	TYR	2.2
1	A	1638	GLU	2.2
1	B	1827	LYS	2.2
1	A	2029	GLN	2.2
1	C	2060	GLN	2.2
1	D	1373	LYS	2.2
1	B	1991	GLN	2.2
1	A	1425	ASP	2.2
1	C	1366	ASP	2.2
1	D	1543	MET	2.2
1	D	1337	ASN	2.2
1	B	1884	HIS	2.2
1	C	1498	THR	2.2
1	D	1923	ASN	2.1
1	A	2003	PRO	2.1
1	C	1346	LEU	2.1
1	C	1435	HIS	2.1
1	C	1525	ALA	2.1
1	C	1844	ALA	2.1
1	A	1361	PHE	2.1
1	D	1976	ARG	2.1
1	D	2034	THR	2.1
1	C	2045	HIS	2.1
1	D	2060	GLN	2.1
1	D	2020	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1992	THR	2.1
1	A	2038	TYR	2.1
1	D	1827	LYS	2.1
1	C	1339	SER	2.1
1	C	1367	GLU	2.1
1	D	1757	GLN	2.0
1	C	1624	MET	2.0
1	B	1538	HIS	2.0
1	B	2003	PRO	2.0
1	D	1996	THR	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 monosaccharides 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(\AA^2)	Q<0.9
2	CA	D	2100	1/1	0.63	0.30	132,132,132,132	0
2	CA	A	2100	1/1	0.83	0.20	83,83,83,83	0
2	CA	C	2100	1/1	0.87	0.30	115,115,115,115	0
2	CA	B	2100	1/1	0.88	0.17	103,103,103,103	0

6.5 Other polymers [i](#)

There are no such residues in this entry.