



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 13, 2024 – 10:18 am BST

PDB ID : 4BEP
Title : Crystal structure of the Legionella pneumophila FIC domain-containing effector AnkX protein (apo-form)
Authors : Campanacci, V.; Mukherjee, S.; Roy, C.R.; Cherfils, J.
Deposited on : 2013-03-12
Resolution : 3.14 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

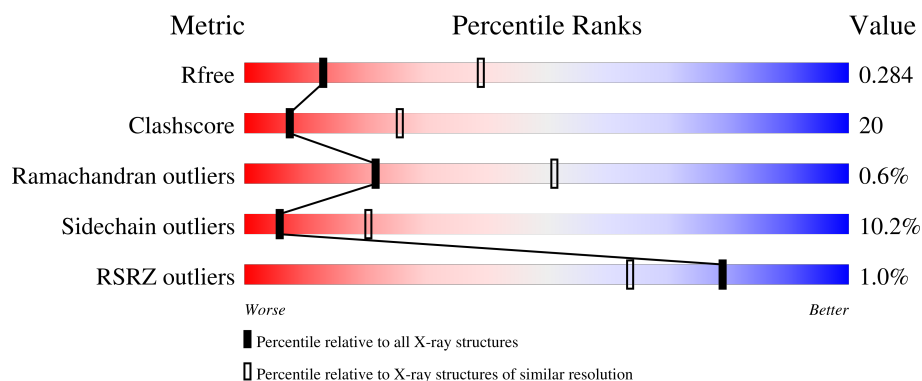
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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}	164625	2149 (3.18-3.10)
Clashscore	180529	2290 (3.18-3.10)
Ramachandran outliers	177936	2178 (3.18-3.10)
Sidechain outliers	177891	2178 (3.18-3.10)
RSRZ outliers	164620	2149 (3.18-3.10)

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	512	
1	B	512	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7531 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 PHOSPHOCHOLINE TRANSFERASE ANKX.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	478	Total	C	N	O	S	Se	0	0	0
			3814	2443	636	719	6	10			
1	B	464	Total	C	N	O	S	Se	0	0	0
			3695	2368	617	694	6	10			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-27	MSE	-	expression tag	UNP Q5ZXN6
A	-26	SER	-	expression tag	UNP Q5ZXN6
A	-25	TYR	-	expression tag	UNP Q5ZXN6
A	-24	TYR	-	expression tag	UNP Q5ZXN6
A	-23	HIS	-	expression tag	UNP Q5ZXN6
A	-22	HIS	-	expression tag	UNP Q5ZXN6
A	-21	HIS	-	expression tag	UNP Q5ZXN6
A	-20	HIS	-	expression tag	UNP Q5ZXN6
A	-19	HIS	-	expression tag	UNP Q5ZXN6
A	-18	HIS	-	expression tag	UNP Q5ZXN6
A	-17	LEU	-	expression tag	UNP Q5ZXN6
A	-16	GLU	-	expression tag	UNP Q5ZXN6
A	-15	SER	-	expression tag	UNP Q5ZXN6
A	-14	THR	-	expression tag	UNP Q5ZXN6
A	-13	SER	-	expression tag	UNP Q5ZXN6
A	-12	LEU	-	expression tag	UNP Q5ZXN6
A	-11	TYR	-	expression tag	UNP Q5ZXN6
A	-10	LYS	-	expression tag	UNP Q5ZXN6
A	-9	LYS	-	expression tag	UNP Q5ZXN6
A	-8	ALA	-	expression tag	UNP Q5ZXN6
A	-7	GLY	-	expression tag	UNP Q5ZXN6
A	-6	LEU	-	expression tag	UNP Q5ZXN6
A	-5	GLU	-	expression tag	UNP Q5ZXN6
A	-4	ASN	-	expression tag	UNP Q5ZXN6
A	-3	LEU	-	expression tag	UNP Q5ZXN6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	TYR	-	expression tag	UNP Q5ZXN6
A	-1	PHE	-	expression tag	UNP Q5ZXN6
A	0	GLN	-	expression tag	UNP Q5ZXN6
A	1	GLY	-	expression tag	UNP Q5ZXN6
A	247	PRO	LEU	engineered mutation	UNP Q5ZXN6
B	-27	MSE	-	expression tag	UNP Q5ZXN6
B	-26	SER	-	expression tag	UNP Q5ZXN6
B	-25	TYR	-	expression tag	UNP Q5ZXN6
B	-24	TYR	-	expression tag	UNP Q5ZXN6
B	-23	HIS	-	expression tag	UNP Q5ZXN6
B	-22	HIS	-	expression tag	UNP Q5ZXN6
B	-21	HIS	-	expression tag	UNP Q5ZXN6
B	-20	HIS	-	expression tag	UNP Q5ZXN6
B	-19	HIS	-	expression tag	UNP Q5ZXN6
B	-18	HIS	-	expression tag	UNP Q5ZXN6
B	-17	LEU	-	expression tag	UNP Q5ZXN6
B	-16	GLU	-	expression tag	UNP Q5ZXN6
B	-15	SER	-	expression tag	UNP Q5ZXN6
B	-14	THR	-	expression tag	UNP Q5ZXN6
B	-13	SER	-	expression tag	UNP Q5ZXN6
B	-12	LEU	-	expression tag	UNP Q5ZXN6
B	-11	TYR	-	expression tag	UNP Q5ZXN6
B	-10	LYS	-	expression tag	UNP Q5ZXN6
B	-9	LYS	-	expression tag	UNP Q5ZXN6
B	-8	ALA	-	expression tag	UNP Q5ZXN6
B	-7	GLY	-	expression tag	UNP Q5ZXN6
B	-6	LEU	-	expression tag	UNP Q5ZXN6
B	-5	GLU	-	expression tag	UNP Q5ZXN6
B	-4	ASN	-	expression tag	UNP Q5ZXN6
B	-3	LEU	-	expression tag	UNP Q5ZXN6
B	-2	TYR	-	expression tag	UNP Q5ZXN6
B	-1	PHE	-	expression tag	UNP Q5ZXN6
B	0	GLN	-	expression tag	UNP Q5ZXN6
B	1	GLY	-	expression tag	UNP Q5ZXN6
B	247	PRO	LEU	engineered mutation	UNP Q5ZXN6

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



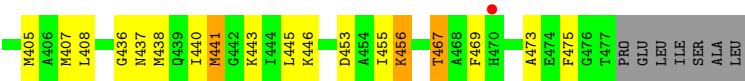
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	1	Total	O	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.27Å 91.63Å 239.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.00 – 3.14 44.00 – 3.14	Depositor EDS
% Data completeness (in resolution range)	98.8 (44.00-3.14) 98.8 (44.00-3.14)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.228 , 0.286 0.228 , 0.284	Depositor DCC
R_{free} test set	1130 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	79.5	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 80.1	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	0.92	EDS
Total number of atoms	7531	wwPDB-VP
Average B, all atoms (Å ²)	109.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% 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: SO4, MG

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	0.66	0/3891	0.80	5/5242 (0.1%)
1	B	0.51	0/3770	0.76	6/5078 (0.1%)
All	All	0.59	0/7661	0.78	11/10320 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	GLU	N-CA-C	-10.76	81.95	111.00
1	B	65	LYS	CB-CA-C	7.43	125.26	110.40
1	B	66	SER	N-CA-CB	-7.37	99.45	110.50
1	A	331	LEU	CB-CA-C	6.28	122.13	110.20
1	B	258	PHE	N-CA-C	6.02	127.26	111.00
1	A	69	GLU	N-CA-CB	5.92	121.25	110.60
1	A	80	ILE	CB-CA-C	-5.73	100.14	111.60
1	A	85	GLY	N-CA-C	-5.67	98.91	113.10
1	B	258	PHE	N-CA-CB	-5.62	100.48	110.60
1	B	261	PRO	CB-CA-C	-5.52	98.21	112.00
1	B	6	PRO	N-CA-C	5.51	126.43	112.10

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	3814	0	3788	178	0
1	B	3695	0	3659	126	0
2	A	15	0	0	0	0
3	A	1	0	0	0	0
4	A	5	0	0	0	0
4	B	1	0	0	0	0
All	All	7531	0	7447	300	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 20.

All (300) 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:A:81:HIS:HD2	1:A:231:PHE:CD1	1.45	1.31
1:A:81:HIS:CD2	1:A:231:PHE:CG	2.30	1.19
1:A:87:LYS:HA	1:A:96:PRO:HB3	1.22	1.14
1:A:81:HIS:HD2	1:A:231:PHE:CG	1.66	1.13
1:A:87:LYS:HA	1:A:96:PRO:CB	1.77	1.13
1:A:81:HIS:CD2	1:A:231:PHE:CD1	2.36	1.13
1:A:6:PRO:HG2	1:A:9:PRO:HG3	1.36	1.06
1:B:5:MSE:N	1:B:6:PRO:HD3	1.71	1.06
1:A:330:ASP:HB3	1:A:331:LEU:HA	1.08	1.04
1:B:63:VAL:HG13	1:B:70:PHE:CD2	1.95	1.00
1:A:330:ASP:HB3	1:A:331:LEU:CA	1.92	0.99
1:B:5:MSE:N	1:B:6:PRO:CD	2.27	0.98
1:A:87:LYS:HA	1:A:96:PRO:CG	1.95	0.96
1:A:93:GLU:HB3	1:A:103:GLU:OE2	1.64	0.96
1:A:95:ASN:HD22	1:A:98:GLU:HG3	1.31	0.95
1:B:8:LEU:HD11	1:B:11:LEU:HG	1.47	0.95
1:B:59:ILE:HD11	1:B:246:ILE:HD11	1.45	0.95
1:A:89:GLU:HB3	1:A:90:GLU:HA	1.51	0.92
1:A:330:ASP:CB	1:A:331:LEU:HA	2.00	0.91
1:A:87:LYS:CA	1:A:96:PRO:HB3	2.01	0.91
1:A:81:HIS:O	1:A:81:HIS:ND1	2.05	0.89
1:A:94:LYS:HG3	1:A:95:ASN:N	1.91	0.85
1:B:63:VAL:HG13	1:B:70:PHE:HD2	1.38	0.84
1:A:238:THR:HG23	1:A:239:PHE:CD2	2.14	0.82
1:A:95:ASN:HB2	1:A:98:GLU:HB2	1.61	0.82
1:A:330:ASP:HB3	1:A:331:LEU:HD22	1.62	0.82
1:A:330:ASP:CB	1:A:331:LEU:HD22	2.12	0.80
1:B:72:LEU:HD21	1:B:201:TYR:CD2	2.17	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LEU:O	1:B:356:GLY:N	2.16	0.79
1:B:59:ILE:CD1	1:B:246:ILE:HD11	2.12	0.79
1:B:82:LYS:HD3	1:B:82:LYS:O	1.83	0.78
1:B:141:GLY:HA3	1:B:144:GLY:O	1.83	0.77
1:B:9:PRO:HD2	1:B:249:MSE:O	1.84	0.77
1:A:94:LYS:HG3	1:A:95:ASN:H	1.46	0.77
1:B:68:GLU:N	1:B:69:GLU:O	2.17	0.77
1:A:91:LEU:HD23	1:A:92:GLN:HG2	1.66	0.76
1:A:91:LEU:CB	1:A:92:GLN:HA	2.16	0.75
1:A:68:GLU:OE1	1:A:69:GLU:N	2.20	0.75
1:A:76:LEU:HD12	1:A:76:LEU:O	1.87	0.74
1:A:95:ASN:O	1:A:97:GLY:N	2.21	0.73
1:B:350:GLN:OE1	1:B:350:GLN:HA	1.88	0.73
1:A:95:ASN:HB3	1:A:98:GLU:HG2	1.71	0.72
1:B:72:LEU:CD2	1:B:201:TYR:CD2	2.73	0.71
1:A:276:VAL:O	1:A:280:ILE:HG13	1.91	0.70
1:A:9:PRO:O	1:A:336:LEU:HD21	1.92	0.70
1:A:91:LEU:CD2	1:A:92:GLN:HG2	2.20	0.70
1:B:72:LEU:HD12	1:B:198:THR:HG23	1.74	0.69
1:B:353:LEU:O	1:B:354:HIS:C	2.28	0.69
1:A:95:ASN:HB2	1:A:98:GLU:CG	2.22	0.69
1:B:139:LYS:HG2	1:B:140:ALA:N	2.08	0.69
1:A:95:ASN:CB	1:A:98:GLU:CG	2.71	0.69
1:A:14:LEU:HB2	1:A:249:MSE:HE1	1.76	0.68
1:A:95:ASN:ND2	1:A:98:GLU:HG3	2.07	0.68
1:A:82:LYS:C	1:A:83:LYS:HD2	2.14	0.68
1:A:92:GLN:O	1:A:93:GLU:HG3	1.93	0.68
1:A:146:ARG:HD3	1:A:146:ARG:N	2.09	0.68
1:B:436:GLY:HA3	1:B:475:PHE:CE2	2.30	0.67
1:A:95:ASN:HB2	1:A:98:GLU:CB	2.23	0.67
1:B:36:ASN:C	1:B:301:TYR:CE1	2.69	0.67
1:A:44:ARG:C	1:A:45:GLU:HG3	2.16	0.66
1:A:235:ASN:O	1:A:238:THR:HG22	1.95	0.66
1:A:85:GLY:O	1:A:87:LYS:HG3	1.95	0.66
1:A:438:MSE:SE	1:B:441:MSE:HE2	2.45	0.66
1:A:82:LYS:O	1:A:83:LYS:HG3	1.96	0.66
1:A:95:ASN:CB	1:A:98:GLU:HG2	2.25	0.65
1:A:70:PHE:CD1	1:A:71:GLU:N	2.65	0.65
1:A:323:ILE:HA	1:A:326:MSE:SE	2.46	0.65
1:B:72:LEU:HD12	1:B:72:LEU:O	1.96	0.65
1:B:228:LEU:O	1:B:230:PRO:HD3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:C	1:B:8:LEU:HD12	2.18	0.64
1:B:70:PHE:CD1	1:B:71:GLU:N	2.66	0.64
1:A:81:HIS:HD2	1:A:231:PHE:CE1	2.10	0.64
1:B:72:LEU:O	1:B:198:THR:HG23	1.98	0.64
1:A:81:HIS:CD2	1:A:231:PHE:CD2	2.86	0.63
1:B:14:LEU:HB2	1:B:249:MSE:HE1	1.80	0.63
1:A:76:LEU:HD12	1:A:76:LEU:C	2.19	0.62
1:B:63:VAL:CG1	1:B:70:PHE:CD2	2.79	0.62
1:A:83:LYS:HD2	1:A:83:LYS:N	2.15	0.61
1:B:56:LEU:O	1:B:59:ILE:HG13	2.01	0.61
1:A:441:MSE:HE2	1:B:438:MSE:SE	2.51	0.61
1:B:37:GLY:N	1:B:301:TYR:CE1	2.68	0.61
1:A:76:LEU:O	1:A:79:ARG:HB3	1.99	0.61
1:B:55:SER:O	1:B:59:ILE:HG23	2.00	0.61
1:A:89:GLU:HB3	1:A:90:GLU:CA	2.29	0.61
1:A:6:PRO:CG	1:A:9:PRO:HG3	2.24	0.60
1:B:436:GLY:HA3	1:B:475:PHE:CZ	2.37	0.60
1:A:86:LYS:C	1:A:87:LYS:HG3	2.20	0.60
1:A:104:PRO:HB3	1:A:187:MSE:SE	2.52	0.60
1:A:263:VAL:HG11	1:A:388:PRO:HG3	1.83	0.59
1:B:225:TYR:O	1:B:228:LEU:O	2.20	0.59
1:B:344:LEU:C	1:B:346:SER:H	2.05	0.59
1:B:282:ASN:O	1:B:286:ILE:HG12	2.03	0.59
1:A:93:GLU:CB	1:A:103:GLU:OE2	2.45	0.59
1:A:282:ASN:O	1:A:286:ILE:HG12	2.03	0.59
1:A:88:VAL:HG12	1:A:89:GLU:N	2.17	0.58
1:A:405:MSE:SE	1:A:439:GLN:HE21	2.37	0.58
1:A:437:ASN:HB3	1:A:440:ILE:HG12	1.86	0.58
1:A:336:LEU:O	1:A:340:THR:HG23	2.04	0.57
1:B:58:SER:OG	1:B:83:LYS:NZ	2.32	0.57
1:B:370:LEU:HD11	1:B:407:MSE:SE	2.54	0.57
1:B:8:LEU:HD12	1:B:8:LEU:O	2.05	0.56
1:A:14:LEU:HB2	1:A:249:MSE:CE	2.35	0.56
1:A:81:HIS:CD2	1:A:231:PHE:CB	2.88	0.56
1:B:72:LEU:HD23	1:B:201:TYR:CE2	2.40	0.56
1:B:263:VAL:HG11	1:B:388:PRO:HG3	1.85	0.56
1:A:108:GLY:C	1:A:109:ILE:HG13	2.26	0.56
1:A:245:ASN:HD21	1:A:256:ALA:H	1.52	0.56
1:A:328:PHE:N	1:A:328:PHE:CD1	2.74	0.56
1:A:87:LYS:HA	1:A:96:PRO:HG3	1.87	0.55
1:A:281:PHE:CE1	1:A:285:GLU:HG3	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:PHE:CE1	1:A:72:LEU:HD12	2.42	0.55
1:A:370:LEU:HD11	1:A:407:MSE:SE	2.57	0.55
1:A:91:LEU:CG	1:A:92:GLN:HA	2.36	0.55
1:B:145:PRO:HB2	1:B:147:PHE:CE1	2.42	0.55
1:B:437:ASN:HB3	1:B:440:ILE:HG12	1.89	0.55
1:A:75:ASP:O	1:A:79:ARG:HB2	2.07	0.54
1:A:330:ASP:HB2	1:A:331:LEU:HD22	1.87	0.54
1:B:72:LEU:CD2	1:B:201:TYR:CE2	2.90	0.54
1:A:95:ASN:C	1:A:97:GLY:H	2.10	0.54
1:B:8:LEU:HD13	1:B:249:MSE:HB3	1.90	0.54
1:B:353:LEU:O	1:B:355:ARG:N	2.41	0.53
1:B:8:LEU:HB2	1:B:250:GLN:HA	1.90	0.53
1:A:249:MSE:HE3	1:A:255:PRO:HD3	1.91	0.53
1:A:99:LEU:HD12	1:A:231:PHE:CE1	2.44	0.53
1:A:87:LYS:CA	1:A:96:PRO:CB	2.68	0.53
1:A:83:LYS:N	1:A:83:LYS:CD	2.72	0.53
1:B:160:ILE:HG13	1:B:161:PRO:HD3	1.91	0.53
1:B:70:PHE:CE1	1:B:72:LEU:N	2.76	0.53
1:A:335:LYS:O	1:A:336:LEU:C	2.48	0.52
1:B:147:PHE:CD1	1:B:147:PHE:N	2.76	0.52
1:B:352:PRO:HG2	1:B:353:LEU:N	2.25	0.52
1:A:329:SER:O	1:A:330:ASP:HB2	2.09	0.52
1:A:61:LEU:HD13	1:A:323:ILE:HD11	1.90	0.52
1:A:332:ASN:C	1:A:334:GLU:H	2.12	0.52
1:B:36:ASN:C	1:B:301:TYR:HE1	2.12	0.52
1:A:235:ASN:C	1:A:238:THR:HG22	2.30	0.52
1:A:405:MSE:SE	1:A:440:ILE:HG22	2.60	0.52
1:A:91:LEU:HB3	1:A:92:GLN:HG3	1.90	0.52
1:B:96:PRO:HD3	1:B:232:ARG:HH21	1.73	0.52
1:A:10:GLY:HA3	1:A:249:MSE:HG2	1.92	0.52
1:A:328:PHE:N	1:A:328:PHE:HD1	2.08	0.52
1:B:301:TYR:HE2	1:B:303:SER:HB3	1.75	0.51
1:A:91:LEU:HB3	1:A:92:GLN:HA	1.90	0.51
1:A:160:ILE:HG13	1:A:161:PRO:HD3	1.91	0.51
1:B:304:SER:OG	1:B:307:GLU:HG2	2.10	0.51
1:B:9:PRO:HD2	1:B:10:GLY:H	1.75	0.51
1:B:14:LEU:HB2	1:B:249:MSE:CE	2.41	0.51
1:A:82:LYS:HG2	1:A:97:GLY:HA3	1.93	0.51
1:B:405:MSE:SE	1:B:440:ILE:HG22	2.60	0.51
1:A:220:LYS:O	1:A:224:MSE:HG3	2.11	0.51
1:A:334:GLU:O	1:A:338:LEU:HD23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:59:ILE:O	1:A:63:VAL:HG23	2.11	0.50
1:A:81:HIS:C	1:A:83:LYS:H	2.15	0.50
1:A:74:VAL:HG23	1:A:75:ASP:N	2.27	0.50
1:A:91:LEU:HD23	1:A:92:GLN:CG	2.38	0.49
1:B:261:PRO:C	1:B:263:VAL:H	2.14	0.49
1:A:133:ALA:HB2	1:A:186:VAL:HG23	1.93	0.49
1:A:217:ILE:O	1:A:221:HIS:HD2	1.95	0.49
1:A:235:ASN:HA	1:A:238:THR:CG2	2.43	0.49
1:B:70:PHE:CD1	1:B:70:PHE:C	2.86	0.49
1:B:81:HIS:O	1:B:84:CYS:N	2.44	0.49
1:A:81:HIS:NE2	1:A:231:PHE:HB3	2.28	0.49
1:B:352:PRO:HG2	1:B:353:LEU:H	1.78	0.49
1:A:88:VAL:CG1	1:A:89:GLU:N	2.76	0.49
1:B:348:ASN:CG	1:B:355:ARG:HH11	2.16	0.49
1:A:89:GLU:CB	1:A:90:GLU:HA	2.20	0.49
1:B:24:ARG:NH2	1:B:296:ILE:HG21	2.27	0.49
1:A:91:LEU:HB3	1:A:92:GLN:CG	2.43	0.48
1:A:238:THR:CG2	1:A:239:PHE:CD2	2.93	0.48
1:B:336:LEU:O	1:B:340:THR:HG23	2.12	0.48
1:A:70:PHE:CD1	1:A:70:PHE:C	2.87	0.48
1:A:139:LYS:HD2	1:A:146:ARG:HH21	1.77	0.48
1:B:72:LEU:HD21	1:B:201:TYR:CG	2.47	0.48
1:B:72:LEU:O	1:B:198:THR:CG2	2.59	0.48
1:B:70:PHE:CG	1:B:71:GLU:N	2.81	0.48
1:B:301:TYR:CE2	1:B:303:SER:HB3	2.48	0.48
1:A:332:ASN:HB3	1:A:335:LYS:HB3	1.95	0.48
1:B:59:ILE:O	1:B:63:VAL:HG23	2.14	0.48
1:A:237:ARG:HA	1:A:241:ASN:HD22	1.77	0.48
1:A:70:PHE:HE1	1:A:72:LEU:HA	1.78	0.48
1:B:133:ALA:HB2	1:B:186:VAL:HG23	1.94	0.48
1:A:405:MSE:HE2	1:A:443:LYS:NZ	2.28	0.48
1:B:63:VAL:HG13	1:B:70:PHE:CE2	2.46	0.48
1:A:58:SER:O	1:A:62:GLN:HG2	2.14	0.47
1:A:281:PHE:CD1	1:A:281:PHE:C	2.88	0.47
1:B:249:MSE:HE3	1:B:255:PRO:HD3	1.96	0.47
1:A:63:VAL:HG13	1:A:70:PHE:CD2	2.50	0.47
1:A:230:PRO:HD2	1:A:235:ASN:OD1	2.14	0.47
1:B:298:LEU:O	1:B:299:TYR:HB2	2.14	0.47
1:B:400:VAL:HG13	1:B:440:ILE:HD12	1.97	0.47
1:B:157:PRO:HA	1:B:160:ILE:HG23	1.96	0.47
1:A:83:LYS:HA	1:A:84:CYS:HA	1.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:MSE:HE2	1:B:443:LYS:NZ	2.29	0.47
1:A:330:ASP:OD1	1:A:333:PRO:HD3	2.15	0.46
1:A:94:LYS:CG	1:A:95:ASN:H	2.23	0.46
1:A:91:LEU:HB3	1:A:92:GLN:CA	2.46	0.46
1:A:87:LYS:NZ	1:A:87:LYS:CB	2.79	0.46
1:B:69:GLU:HG3	1:B:70:PHE:H	1.80	0.46
1:B:96:PRO:CD	1:B:232:ARG:HH21	2.29	0.46
1:B:9:PRO:HB2	1:B:331:LEU:HD11	1.97	0.46
1:A:157:PRO:HA	1:A:160:ILE:HG23	1.98	0.46
1:A:87:LYS:CA	1:A:96:PRO:CG	2.81	0.45
1:A:332:ASN:O	1:A:336:LEU:HB2	2.17	0.45
1:B:108:GLY:C	1:B:109:ILE:HG13	2.37	0.45
1:B:41:TYR:HA	1:B:44:ARG:NH1	2.31	0.45
1:A:94:LYS:CG	1:A:95:ASN:N	2.69	0.45
1:A:331:LEU:HA	1:A:331:LEU:HD22	1.90	0.45
1:B:400:VAL:HG13	1:B:440:ILE:CD1	2.47	0.45
1:B:147:PHE:N	1:B:147:PHE:HD1	2.14	0.45
1:B:436:GLY:CA	1:B:475:PHE:CE2	2.99	0.45
1:B:36:ASN:HA	1:B:301:TYR:HE1	1.82	0.45
1:A:70:PHE:HD1	1:A:71:GLU:N	2.12	0.45
1:A:228:LEU:HD12	1:A:228:LEU:O	2.16	0.45
1:B:467:THR:HG23	1:B:469:PHE:H	1.81	0.45
1:B:455:ILE:HD12	1:B:456:LYS:H	1.82	0.44
1:A:235:ASN:HA	1:A:238:THR:HG22	1.98	0.44
1:B:301:TYR:CE2	1:B:303:SER:CB	3.00	0.44
1:A:455:ILE:HD12	1:A:456:LYS:H	1.83	0.44
1:B:120:GLU:HG2	1:B:160:ILE:HD12	2.00	0.44
1:B:344:LEU:C	1:B:346:SER:N	2.70	0.44
1:B:351:TYR:O	1:B:351:TYR:CD2	2.70	0.44
1:A:70:PHE:CE1	1:A:71:GLU:O	2.71	0.44
1:A:10:GLY:HA3	1:A:249:MSE:HA	2.00	0.44
1:B:352:PRO:CG	1:B:353:LEU:N	2.80	0.44
1:B:69:GLU:HA	1:B:69:GLU:OE1	2.18	0.43
1:B:72:LEU:HD13	1:B:225:TYR:OH	2.18	0.43
1:B:142:PRO:O	1:B:143:PHE:CD1	2.70	0.43
1:B:147:PHE:HD1	1:B:147:PHE:H	1.66	0.43
1:A:281:PHE:CD1	1:A:281:PHE:O	2.71	0.43
1:A:332:ASN:C	1:A:334:GLU:N	2.72	0.43
1:A:89:GLU:CB	1:A:90:GLU:CA	2.93	0.43
1:A:81:HIS:C	1:A:83:LYS:N	2.72	0.43
1:A:120:GLU:HG2	1:A:160:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:VAL:HG13	1:A:440:ILE:HD12	2.00	0.43
1:A:400:VAL:HG13	1:A:440:ILE:CD1	2.49	0.43
1:B:12:TYR:CZ	1:B:333:PRO:HB3	2.53	0.43
1:A:29:GLY:HA2	1:A:32:TRP:CE2	2.53	0.43
1:A:68:GLU:OE1	1:A:69:GLU:HB3	2.19	0.43
1:A:81:HIS:CD2	1:A:231:PHE:HB3	2.54	0.43
1:B:301:TYR:HE2	1:B:303:SER:CB	2.31	0.43
1:A:109:ILE:HG21	1:A:266:LEU:HD22	2.01	0.43
1:A:163:LEU:O	1:A:167:ILE:HG13	2.18	0.43
1:A:330:ASP:CB	1:A:331:LEU:CA	2.70	0.43
1:B:59:ILE:CD1	1:B:246:ILE:CD1	2.92	0.43
1:A:249:MSE:HE3	1:A:255:PRO:CD	2.49	0.43
1:A:480:LEU:HD23	1:A:480:LEU:HA	1.88	0.43
1:B:145:PRO:O	1:B:147:PHE:CD1	2.72	0.43
1:A:72:LEU:HD22	1:A:201:TYR:CD2	2.54	0.42
1:A:73:SER:O	1:A:76:LEU:HB3	2.18	0.42
1:A:249:MSE:CE	1:A:255:PRO:HD3	2.49	0.42
1:B:256:ALA:HB3	1:B:258:PHE:CZ	2.54	0.42
1:A:61:LEU:HD22	1:A:319:SER:HB3	2.01	0.42
1:A:8:LEU:HD23	1:A:250:GLN:CA	2.49	0.42
1:A:149:LYS:HE3	1:A:149:LYS:HB2	1.80	0.42
1:A:245:ASN:ND2	1:A:256:ALA:H	2.17	0.42
1:A:383:GLU:OE2	1:A:423:TYR:OH	2.38	0.42
1:B:29:GLY:HA2	1:B:32:TRP:CE2	2.54	0.42
1:A:72:LEU:HD22	1:A:201:TYR:CE2	2.54	0.42
1:A:235:ASN:O	1:A:238:THR:CG2	2.67	0.42
1:B:263:VAL:O	1:B:267:TYR:HB2	2.18	0.42
1:A:405:MSE:HE2	1:A:443:LYS:HZ3	1.85	0.42
1:B:59:ILE:HG13	1:B:60:ALA:N	2.35	0.42
1:B:249:MSE:CE	1:B:255:PRO:HD3	2.49	0.42
1:B:348:ASN:ND2	1:B:355:ARG:NH1	2.68	0.42
1:A:10:GLY:HA3	1:A:249:MSE:CB	2.50	0.41
1:A:254:PRO:HD3	1:A:340:THR:HG21	2.02	0.41
1:B:35:GLU:OE1	1:B:44:ARG:NH2	2.53	0.41
1:B:70:PHE:O	1:B:71:GLU:HG2	2.20	0.41
1:A:437:ASN:C	1:A:437:ASN:HD22	2.24	0.41
1:B:192:VAL:HG12	1:B:196:LYS:HE2	2.02	0.41
1:A:181:HIS:O	1:A:182:PHE:CG	2.73	0.41
1:A:225:TYR:O	1:A:228:LEU:HB3	2.21	0.41
1:A:17:TYR:CE2	1:A:25:LEU:HD23	2.55	0.41
1:B:350:GLN:O	1:B:351:TYR:CD1	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:439:GLN:HG3	1:B:473:ALA:O	2.20	0.41
1:B:81:HIS:O	1:B:83:LYS:N	2.54	0.41
1:A:467:THR:HG23	1:A:469:PHE:H	1.86	0.41
1:B:9:PRO:CD	1:B:10:GLY:H	2.33	0.41
1:B:81:HIS:C	1:B:83:LYS:N	2.74	0.41
1:A:81:HIS:CD2	1:A:231:PHE:CE1	2.94	0.41
1:B:257:THR:OG1	1:B:283:THR:OG1	2.29	0.41
1:A:74:VAL:HG13	1:A:195:GLU:OE1	2.21	0.41
1:A:181:HIS:C	1:A:182:PHE:CD2	2.94	0.41
1:A:336:LEU:HD12	1:A:336:LEU:HA	1.94	0.41
1:B:8:LEU:C	1:B:8:LEU:CD1	2.89	0.41
1:B:36:ASN:CA	1:B:301:TYR:HE1	2.33	0.41
1:A:99:LEU:CD1	1:A:231:PHE:CE1	3.03	0.41
1:B:10:GLY:C	1:B:12:TYR:H	2.23	0.40
1:B:96:PRO:HD3	1:B:232:ARG:NH2	2.34	0.40
1:B:254:PRO:HD3	1:B:340:THR:HG21	2.03	0.40
1:A:86:LYS:HA	1:A:86:LYS:CE	2.51	0.40
1:A:181:HIS:O	1:A:182:PHE:CD2	2.73	0.40
1:A:81:HIS:HB2	1:A:231:PHE:CE2	2.57	0.40
1:B:8:LEU:CD1	1:B:11:LEU:H	2.34	0.40
1:B:17:TYR:CE2	1:B:25:LEU:HD23	2.57	0.40
1:B:405:MSE:HE1	1:B:408:LEU:HD23	2.03	0.40
1:A:235:ASN:CA	1:A:238:THR:HG22	2.51	0.40
1:A:467:THR:HG22	1:A:470:HIS:H	1.87	0.40
1:A:469:PHE:CE1	1:B:445:LEU:HD13	2.56	0.40
1:B:55:SER:O	1:B:59:ILE:HG12	2.22	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	476/512 (93%)	435 (91%)	37 (8%)	4 (1%)	16	45
1	B	460/512 (90%)	426 (93%)	32 (7%)	2 (0%)	30	60
All	All	936/1024 (91%)	861 (92%)	69 (7%)	6 (1%)	22	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	PRO
1	A	348	ASN
1	A	332	ASN
1	A	104	PRO
1	B	6	PRO
1	B	9	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	416/436 (95%)	373 (90%)	43 (10%)	6	20
1	B	401/436 (92%)	361 (90%)	40 (10%)	6	21
All	All	817/872 (94%)	734 (90%)	83 (10%)	6	20

All (83) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLU
1	A	33	SER
1	A	45	GLU
1	A	48	CYS
1	A	53	LEU
1	A	61	LEU
1	A	62	GLN
1	A	65	LYS
1	A	72	LEU
1	A	76	LEU

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Mol	Chain	Res	Type
1	A	81	HIS
1	A	83	LYS
1	A	86	LYS
1	A	87	LYS
1	A	91	LEU
1	A	93	GLU
1	A	99	LEU
1	A	126	VAL
1	A	186	VAL
1	A	196	LYS
1	A	211	LEU
1	A	215	LEU
1	A	229	HIS
1	A	240	VAL
1	A	288	GLU
1	A	305	LEU
1	A	315	LEU
1	A	328	PHE
1	A	331	LEU
1	A	334	GLU
1	A	340	THR
1	A	347	LEU
1	A	350	GLN
1	A	368	LEU
1	A	384	GLN
1	A	401	ILE
1	A	437	ASN
1	A	441	MSE
1	A	451	GLN
1	A	453	ASP
1	A	456	LYS
1	A	467	THR
1	A	482	SER
1	B	8	LEU
1	B	20	GLU
1	B	33	SER
1	B	53	LEU
1	B	61	LEU
1	B	66	SER
1	B	147	PHE
1	B	166	GLN
1	B	180	ASN

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Mol	Chain	Res	Type
1	B	186	VAL
1	B	196	LYS
1	B	211	LEU
1	B	215	LEU
1	B	223	ARG
1	B	229	HIS
1	B	240	VAL
1	B	257	THR
1	B	288	GLU
1	B	291	LYS
1	B	292	ARG
1	B	305	LEU
1	B	315	LEU
1	B	330	ASP
1	B	331	LEU
1	B	332	ASN
1	B	340	THR
1	B	342	LYS
1	B	347	LEU
1	B	350	GLN
1	B	368	LEU
1	B	374	ASN
1	B	375	GLU
1	B	380	GLN
1	B	384	GLN
1	B	401	ILE
1	B	441	MSE
1	B	446	LYS
1	B	453	ASP
1	B	456	LYS
1	B	467	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	95	ASN
1	A	199	GLN
1	A	221	HIS
1	A	241	ASN
1	A	245	ASN
1	A	289	GLN

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Mol	Chain	Res	Type
1	A	308	GLN
1	A	332	ASN
1	A	350	GLN
1	A	380	GLN
1	A	384	GLN
1	A	437	ASN
1	A	439	GLN
1	A	463	ASN
1	B	180	ASN
1	B	241	ASN
1	B	308	GLN
1	B	374	ASN
1	B	384	GLN
1	B	463	ASN

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](#)

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	1483	-	4,4,4	0.33	0	6,6,6	0.70	0
2	SO4	A	1485	-	4,4,4	0.34	0	6,6,6	0.19	0
2	SO4	A	1484	-	4,4,4	0.38	0	6,6,6	0.25	0

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	467/512 (91%)	-0.27	4 (0%) 81 66	39, 79, 151, 197	1 (0%)
1	B	453/512 (88%)	-0.01	5 (1%) 77 61	69, 133, 180, 209	1 (0%)
All	All	920/1024 (89%)	-0.14	9 (0%) 79 64	39, 106, 173, 209	2 (0%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	470	HIS	3.4
1	A	331	LEU	3.1
1	B	258	PHE	2.5
1	A	240	VAL	2.4
1	B	123	LEU	2.3
1	A	84	CYS	2.2
1	B	122	PHE	2.1
1	A	470	HIS	2.1
1	B	164	ALA	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	SO4	A	1484	5/5	0.78	0.15	132,133,139,139	0
2	SO4	A	1483	5/5	0.88	0.20	112,116,127,141	0
2	SO4	A	1485	5/5	0.89	0.14	117,119,129,140	0
3	MG	A	1486	1/1	0.93	0.12	39,39,39,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.