Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:43 PM GMT

PDB ID	:	4FYE
Title	:	Crystal structure of a Legionella phosphoinositide phosphatase, SidF
Authors	:	Hsu, F.S.; Zhu, W.; Brennan, L.; Tao, L.; Luo, Z.Q.; Mao, Y.
Deposited on	:	2012-07-04
Resolution	:	2.41 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

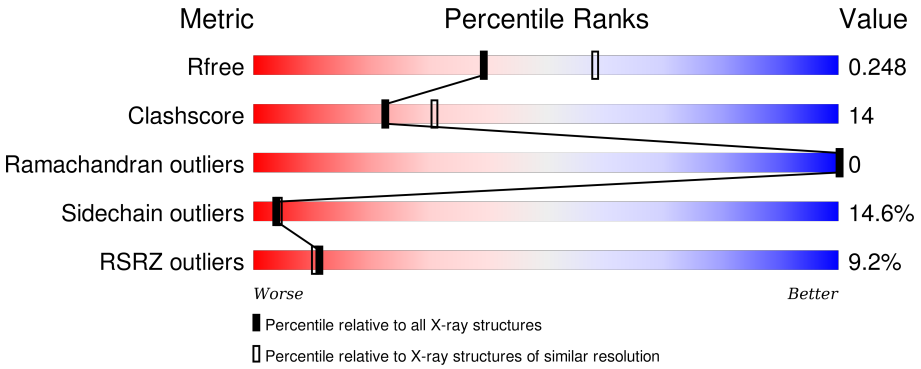
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.41 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	3386 (2.44-2.40)
Clashscore	102246	3897 (2.44-2.40)
Ramachandran outliers	100387	3837 (2.44-2.40)
Sidechain outliers	100360	3838 (2.44-2.40)
RSRZ outliers	91569	3396 (2.44-2.40)

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 <=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	761	9% 66% 22% 6% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5821 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.

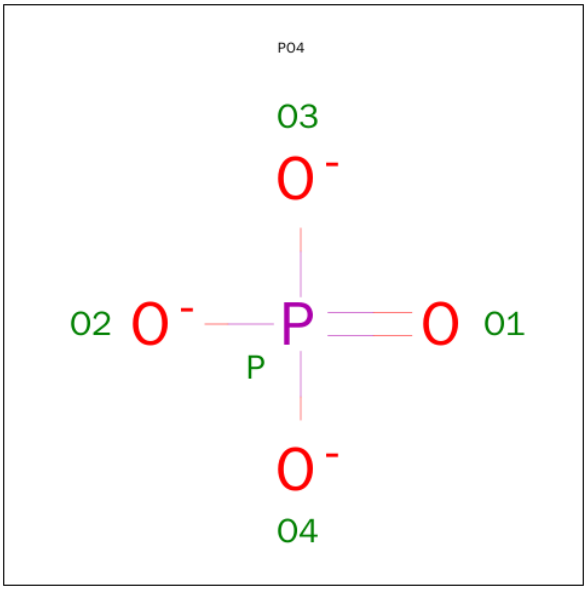
- Molecule 1 is a protein called SidF, inhibitor of growth family, member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	725	Total	C	N	O	S	0	1	0
			5778	3598	1028	1134	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q5ZSD5
A	645	SER	CYS	ENGINEERED MUTATION	UNP Q5ZSD5

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is water.

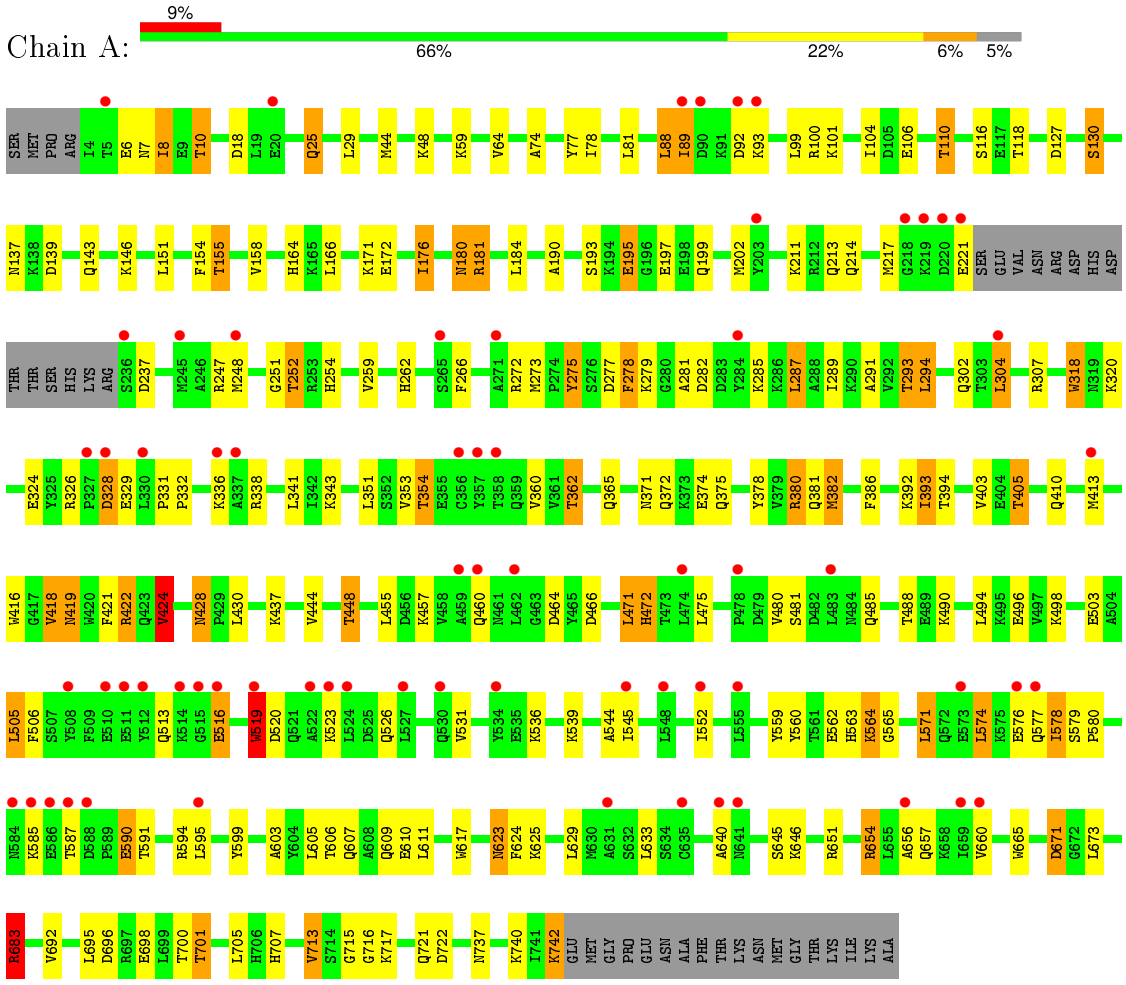
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	38	Total O 38 38	0	0

3 Residue-property plots (i)

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: SidF, inhibitor of growth family, member 3

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	72.18Å 115.96Å 124.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	84.77 – 2.41 47.08 – 2.41	Depositor EDS
% Data completeness (in resolution range)	98.6 (84.77-2.41) 98.7 (47.08-2.41)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.10 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.210 , 0.256 0.205 , 0.248	Depositor DCC
R_{free} test set	2021 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	54.4	Xtriage
Anisotropy	0.590	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 40330 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5821	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.90	7/5883 (0.1%)	1.06	23/7926 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	SER	CB-OG	-6.57	1.33	1.42
1	A	617	TRP	CD2-CE2	6.09	1.48	1.41
1	A	665	TRP	CD2-CE2	5.33	1.47	1.41
1	A	624	PHE	N-CA	5.18	1.56	1.46
1	A	416	TRP	CD2-CE2	5.18	1.47	1.41
1	A	519	TRP	CD2-CE2	5.16	1.47	1.41
1	A	318	TRP	CD2-CE2	5.06	1.47	1.41

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	307	ARG	NE-CZ-NH2	-17.99	111.31	120.30
1	A	422	ARG	NE-CZ-NH2	-17.87	111.36	120.30
1	A	422	ARG	NE-CZ-NH1	11.75	126.18	120.30
1	A	307	ARG	NE-CZ-NH1	10.87	125.73	120.30
1	A	623	ASN	C-N-CA	-8.89	99.47	121.70
1	A	654	ARG	NE-CZ-NH1	8.46	124.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	683	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	424	VAL	CG1-CB-CG2	6.92	121.97	110.90
1	A	338	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	422	ARG	CG-CD-NE	-6.71	97.71	111.80
1	A	623	ASN	O-C-N	-6.69	112.00	122.70
1	A	338	ARG	NE-CZ-NH2	-6.58	117.01	120.30
1	A	405	THR	CB-CA-C	-6.44	94.22	111.60
1	A	307	ARG	CG-CD-NE	-6.00	99.20	111.80
1	A	713	VAL	CG1-CB-CG2	5.93	120.39	110.90
1	A	645	SER	N-CA-C	-5.89	95.08	111.00
1	A	418	VAL	CG1-CB-CG2	5.73	120.06	110.90
1	A	304	LEU	CB-CG-CD2	5.54	120.42	111.00
1	A	307	ARG	CD-NE-CZ	5.46	131.25	123.60
1	A	424	VAL	N-CA-CB	-5.46	99.49	111.50
1	A	654	ARG	CB-CG-CD	5.37	125.57	111.60
1	A	130	SER	N-CA-CB	-5.32	102.52	110.50
1	A	671	ASP	CB-CG-OD1	-5.05	113.75	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	715	GLY	Peptide

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	5778	0	5671	157	0
2	A	5	0	0	0	0
3	A	38	0	0	0	0
All	All	5821	0	5671	157	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 14.

All (157) 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:252:THR:HG23	1:A:262:HIS:NE2	1.58	1.16
1:A:380:ARG:HH11	1:A:380:ARG:HG3	1.14	1.09
1:A:381:GLN:HG2	1:A:382:MET:HE3	1.35	1.09
1:A:740:LYS:O	1:A:742:LYS:HD2	1.52	1.07
1:A:381:GLN:HG2	1:A:382:MET:CE	1.86	1.05
1:A:181:ARG:HH11	1:A:181:ARG:HG2	1.20	1.04
1:A:151:LEU:O	1:A:155:THR:HG23	1.62	0.99
1:A:195:GLU:H	1:A:195:GLU:CD	1.71	0.93
1:A:362:THR:HG21	1:A:419:ASN:HD21	1.35	0.91
1:A:444:VAL:O	1:A:448:THR:HG22	1.73	0.88
1:A:252:THR:CG2	1:A:262:HIS:NE2	2.36	0.88
1:A:656:ALA:O	1:A:660:VAL:HG23	1.75	0.87
1:A:380:ARG:NH1	1:A:380:ARG:HG3	1.79	0.87
1:A:559:TYR:O	1:A:563:HIS:HD2	1.58	0.86
1:A:380:ARG:CG	1:A:380:ARG:HH11	1.88	0.86
1:A:25:GLN:HE21	1:A:25:GLN:H	1.20	0.86
1:A:127:ASP:H	1:A:137:ASN:HD21	1.20	0.84
1:A:424:VAL:HG13	1:A:428:ASN:HB3	1.61	0.83
1:A:444:VAL:O	1:A:448:THR:CG2	2.25	0.83
1:A:362:THR:HG21	1:A:419:ASN:ND2	1.99	0.77
1:A:181:ARG:HH11	1:A:181:ARG:CG	1.96	0.77
1:A:740:LYS:O	1:A:742:LYS:CD	2.33	0.75
1:A:419:ASN:C	1:A:419:ASN:HD22	1.86	0.75
1:A:428:ASN:HD22	1:A:430:LEU:H	1.33	0.74
1:A:100:ARG:O	1:A:104:ILE:HG12	1.88	0.73
1:A:304:LEU:HD13	1:A:640:ALA:HB3	1.71	0.71
1:A:278:PHE:CZ	1:A:374:GLU:HG2	2.26	0.71
1:A:559:TYR:O	1:A:563:HIS:CD2	2.42	0.70
1:A:354:THR:HB	1:A:410:GLN:HB2	1.72	0.69
1:A:381:GLN:HG2	1:A:382:MET:HE1	1.74	0.69
1:A:336:LYS:O	1:A:336:LYS:HD2	1.92	0.69
1:A:106:GLU:O	1:A:110:THR:HG23	1.92	0.69
1:A:275:TYR:O	1:A:278:PHE:HB2	1.93	0.68
1:A:74:ALA:O	1:A:78:ILE:HG12	1.94	0.68
1:A:89:ILE:HD11	1:A:101:LYS:HG2	1.77	0.67
1:A:190:ALA:H	1:A:199:GLN:HE21	1.43	0.67
1:A:275:TYR:CB	1:A:646:LYS:HE2	2.25	0.66
1:A:372:GLN:NE2	1:A:651:ARG:HH12	1.94	0.66
1:A:654:ARG:HH21	1:A:657:GLN:HE22	1.43	0.65
1:A:7:ASN:HD22	1:A:10:THR:H	1.44	0.65
1:A:490:LYS:HE3	1:A:544:ALA:HB3	1.80	0.64
1:A:428:ASN:ND2	1:A:430:LEU:H	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:C	1:A:419:ASN:ND2	2.53	0.61
1:A:195:GLU:N	1:A:195:GLU:CD	2.48	0.61
1:A:707:HIS:CD2	1:A:716:GLY:H	2.18	0.61
1:A:77:TYR:OH	1:A:155:THR:HG21	2.00	0.60
1:A:304:LEU:HD13	1:A:640:ALA:CB	2.30	0.60
1:A:275:TYR:CD2	1:A:646:LYS:HE2	2.37	0.60
1:A:378:TYR:O	1:A:382:MET:HG2	2.01	0.60
1:A:172:GLU:O	1:A:176:ILE:HG23	2.02	0.60
1:A:591:THR:O	1:A:595:LEU:HD13	2.01	0.59
1:A:591:THR:HA	1:A:594:ARG:HD2	1.85	0.59
1:A:444:VAL:O	1:A:448:THR:HG23	2.01	0.58
1:A:99:LEU:HD23	1:A:99:LEU:O	2.03	0.58
1:A:251:GLY:HA2	1:A:262:HIS:CD2	2.38	0.58
1:A:275:TYR:HD2	1:A:646:LYS:HE2	1.67	0.58
1:A:671:ASP:HB3	1:A:673:LEU:HG	1.86	0.58
1:A:419:ASN:ND2	1:A:421:PHE:H	2.03	0.57
1:A:579:SER:N	1:A:580:PRO:HD2	2.20	0.57
1:A:519:TRP:HD1	1:A:519:TRP:O	1.87	0.57
1:A:380:ARG:HB2	1:A:413:MET:SD	2.45	0.56
1:A:273:MET:CE	1:A:378:TYR:HB2	2.35	0.56
1:A:181:ARG:HG2	1:A:181:ARG:NH1	1.97	0.56
1:A:594:ARG:HG3	1:A:594:ARG:HH11	1.71	0.56
1:A:48:LYS:HD2	1:A:180:ASN:HD21	1.69	0.56
1:A:480:VAL:HG21	1:A:552:ILE:HG12	1.86	0.56
1:A:362:THR:CG2	1:A:419:ASN:ND2	2.69	0.55
1:A:6:GLU:HG2	1:A:44:MET:HE1	1.87	0.55
1:A:564:LYS:HG2	1:A:565:GLY:N	2.21	0.54
1:A:7:ASN:HB3	1:A:10:THR:HG23	1.89	0.54
1:A:480:VAL:CG2	1:A:552:ILE:HG12	2.37	0.54
1:A:302:GLN:HE21	1:A:394:THR:H	1.56	0.54
1:A:291:ALA:HB2	1:A:505:LEU:HD22	1.89	0.54
1:A:127:ASP:H	1:A:137:ASN:ND2	1.99	0.54
1:A:213:GLN:O	1:A:217:MET:HG3	2.08	0.54
1:A:48:LYS:CD	1:A:180:ASN:HD21	2.22	0.53
1:A:698:GLU:O	1:A:701:THR:HG23	2.10	0.52
1:A:211:LYS:HD3	1:A:221:GLU:HB3	1.92	0.52
1:A:683:ARG:HD3	1:A:696:ASP:OD2	2.10	0.52
1:A:717:LYS:HE3	1:A:737:ASN:OD1	2.10	0.52
1:A:362:THR:H	1:A:372:GLN:NE2	2.09	0.51
1:A:25:GLN:HE21	1:A:25:GLN:N	1.99	0.51
1:A:275:TYR:CD1	1:A:275:TYR:N	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:LEU:C	1:A:99:LEU:HD23	2.31	0.50
1:A:371:ASN:O	1:A:375:GLN:HG3	2.12	0.50
1:A:294:LEU:HD13	1:A:506:PHE:CZ	2.47	0.50
1:A:381:GLN:CG	1:A:382:MET:HE3	2.25	0.50
1:A:372:GLN:HE22	1:A:651:ARG:HH12	1.59	0.50
1:A:154:PHE:O	1:A:158:VAL:HG23	2.12	0.49
1:A:392:LYS:O	1:A:393:ILE:HD12	2.13	0.49
1:A:278:PHE:HZ	1:A:374:GLU:HG2	1.73	0.49
1:A:519:TRP:CD1	1:A:519:TRP:O	2.66	0.49
1:A:275:TYR:HB3	1:A:646:LYS:HE2	1.94	0.49
1:A:574:LEU:HD22	1:A:578:ILE:HG12	1.94	0.49
1:A:382:MET:HA	1:A:382:MET:HE2	1.93	0.48
1:A:428:ASN:C	1:A:428:ASN:HD22	2.17	0.48
1:A:88:LEU:HG	1:A:164:HIS:CD2	2.48	0.48
1:A:382:MET:HE3	1:A:382:MET:N	2.29	0.48
1:A:422:ARG:HH22	1:A:721:GLN:HE21	1.62	0.48
1:A:485:GLN:HA	1:A:485:GLN:HE21	1.80	0.47
1:A:266:PHE:CE2	1:A:304:LEU:HD22	2.49	0.47
1:A:625:LYS:O	1:A:629:LEU:HG	2.14	0.47
1:A:574:LEU:CD2	1:A:578:ILE:HG12	2.45	0.47
1:A:578:ILE:HD12	1:A:595:LEU:HD23	1.97	0.47
1:A:424:VAL:CG1	1:A:428:ASN:HB3	2.40	0.46
1:A:291:ALA:HB2	1:A:505:LEU:CD2	2.46	0.46
1:A:722:ASP:OD1	1:A:722:ASP:C	2.54	0.46
1:A:275:TYR:HB2	1:A:646:LYS:NZ	2.30	0.46
1:A:485:GLN:NE2	1:A:485:GLN:HA	2.30	0.46
1:A:281:ALA:HB1	1:A:285:LYS:HG2	1.98	0.46
1:A:494:LEU:HD13	1:A:498:LYS:HE3	1.98	0.46
1:A:289:ILE:O	1:A:293:THR:HG23	2.16	0.46
1:A:471:LEU:HD12	1:A:574:LEU:HD12	1.98	0.46
1:A:471:LEU:HD22	1:A:475:LEU:HG	1.98	0.45
1:A:560:TYR:OH	1:A:610:GLU:HB2	2.17	0.45
1:A:7:ASN:HD22	1:A:10:THR:HG23	1.81	0.45
1:A:118:THR:HG22	1:A:118:THR:O	2.15	0.45
1:A:193:SER:HB3	1:A:199:GLN:HE22	1.82	0.45
1:A:282:ASP:OD1	1:A:282:ASP:N	2.48	0.45
1:A:273:MET:HB3	1:A:293:THR:CG2	2.46	0.44
1:A:237:ASP:HB2	1:A:277:ASP:OD1	2.18	0.44
1:A:742:LYS:HE2	1:A:742:LYS:HB3	1.31	0.44
1:A:606:THR:HA	1:A:609:GLN:HE21	1.83	0.44
1:A:8:ILE:HG13	1:A:247:ARG:NH2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:LEU:HD22	1:A:599:TYR:CE2	2.53	0.44
1:A:571:LEU:CD2	1:A:599:TYR:CE2	3.01	0.44
1:A:100:ARG:O	1:A:104:ILE:CG1	2.64	0.43
1:A:279:LYS:HG3	1:A:279:LYS:O	2.18	0.43
1:A:590:GLU:HG3	1:A:594:ARG:HH12	1.83	0.43
1:A:328:ASP:OD1	1:A:328:ASP:N	2.51	0.43
1:A:275:TYR:HD2	1:A:646:LYS:CG	2.32	0.43
1:A:705:LEU:HA	1:A:705:LEU:HD23	1.76	0.43
1:A:472:HIS:C	1:A:472:HIS:HD1	2.21	0.43
1:A:181:ARG:CG	1:A:181:ARG:NH1	2.66	0.43
1:A:248:MET:HE3	1:A:660:VAL:HG22	2.00	0.43
1:A:127:ASP:OD2	1:A:130:SER:HB2	2.19	0.42
1:A:318:TRP:CZ2	1:A:326:ARG:HD3	2.54	0.42
1:A:362:THR:HG23	1:A:365:GLN:HE21	1.84	0.42
1:A:294:LEU:HD22	1:A:386:PHE:CE2	2.54	0.42
1:A:579:SER:N	1:A:580:PRO:CD	2.81	0.42
1:A:291:ALA:CB	1:A:505:LEU:HD22	2.49	0.42
1:A:275:TYR:HB2	1:A:646:LYS:HE2	1.99	0.42
1:A:184:LEU:O	1:A:202:MET:HA	2.20	0.42
1:A:490:LYS:HD2	1:A:545:ILE:HG13	2.02	0.42
1:A:343:LYS:HG3	1:A:403:VAL:HG11	2.01	0.42
1:A:331:PRO:HA	1:A:332:PRO:HD3	1.93	0.41
1:A:197:GLU:HG2	1:A:254:HIS:HA	2.03	0.41
1:A:294:LEU:HD22	1:A:386:PHE:HE2	1.86	0.41
1:A:422:ARG:NH2	1:A:721:GLN:HG3	2.36	0.41
1:A:629:LEU:HA	1:A:629:LEU:HD23	1.84	0.41
1:A:539:LYS:HA	1:A:539:LYS:HD3	1.89	0.41
1:A:671:ASP:HB3	1:A:673:LEU:CG	2.51	0.40
1:A:139:ASP:O	1:A:143:GLN:HG2	2.21	0.40
1:A:599:TYR:CD1	1:A:599:TYR:C	2.95	0.40
1:A:603:ALA:O	1:A:607:GLN:HG2	2.21	0.40
1:A:516:GLU:N	1:A:516:GLU:OE2	2.55	0.40
1:A:287:LEU:HD11	1:A:531:VAL:HG11	2.04	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	722/761 (95%)	691 (96%)	31 (4%)	0	100 100

There are no Ramachandran outliers to report.

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	623/654 (95%)	532 (85%)	91 (15%)	4 4

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	10	THR
1	A	18	ASP
1	A	25	GLN
1	A	29	LEU
1	A	59	LYS
1	A	64	VAL
1	A	81	LEU
1	A	88	LEU
1	A	89	ILE
1	A	92	ASP
1	A	93	LYS
1	A	110	THR

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Mol	Chain	Res	Type
1	A	116	SER
1	A	146	LYS
1	A	155	THR
1	A	166	LEU
1	A	171	LYS
1	A	176	ILE
1	A	180	ASN
1	A	181	ARG
1	A	195	GLU
1	A	214	GLN
1	A	252	THR
1	A	259	VAL
1	A	272	ARG
1	A	275	TYR
1	A	278	PHE
1	A	287	LEU
1	A	293	THR
1	A	294	LEU
1	A	320	LYS
1	A	324	GLU
1	A	328	ASP
1	A	329	GLU
1	A	341	LEU
1	A	351	LEU
1	A	353	VAL
1	A	354	THR
1	A	360	VAL
1	A	362	THR
1	A	380	ARG
1	A	382	MET
1	A	393	ILE
1	A	405	THR
1	A	418	VAL
1	A	419	ASN
1	A	424	VAL
1	A	428	ASN
1	A	437	LYS
1	A	448	THR
1	A	455	LEU
1	A	457	LYS
1	A	460	GLN
1	A	464	ASP

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Mol	Chain	Res	Type
1	A	466	ASP
1	A	471	LEU
1	A	472	HIS
1	A	481	SER
1	A	488	THR
1	A	496	GLU
1	A	503	GLU
1	A	505	LEU
1	A	513	GLN
1	A	516	GLU
1	A	519	TRP
1	A	520	ASP
1	A	523	LYS
1	A	526	GLN
1	A	536	LYS
1	A	562	GLU
1	A	564	LYS
1	A	571	LEU
1	A	574	LEU
1	A	576	GLU
1	A	577	GLN
1	A	578	ILE
1	A	585	LYS
1	A	587	THR
1	A	590	GLU
1	A	605	LEU
1	A	611	LEU
1	A	623	ASN
1	A	633	LEU
1	A	683	ARG
1	A	692	VAL
1	A	695	LEU
1	A	700	THR
1	A	701	THR
1	A	713	VAL
1	A	742	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	25	GLN

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Mol	Chain	Res	Type
1	A	26	ASN
1	A	28	HIS
1	A	137	ASN
1	A	164	HIS
1	A	175	ASN
1	A	180	ASN
1	A	199	GLN
1	A	214	GLN
1	A	302	GLN
1	A	348	HIS
1	A	365	GLN
1	A	372	GLN
1	A	419	ASN
1	A	428	ASN
1	A	460	GLN
1	A	485	GLN
1	A	486	GLN
1	A	513	GLN
1	A	541	GLN
1	A	550	ASN
1	A	563	HIS
1	A	583	GLN
1	A	584	ASN
1	A	609	GLN
1	A	615	ASN
1	A	622	ASN
1	A	623	ASN
1	A	657	GLN
1	A	691	ASN
1	A	703	GLN
1	A	721	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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	PO4	A	801	-	4,4,4	0.25	0	6,6,6	0.25	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PO4	A	801	-	-	0/0/0/0	0/0/0/0

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

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, 95^{th} 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	725/761 (95%)	0.45	67 (9%)	11	10	35, 62, 109, 167	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	221	GLU	9.1
1	A	220	ASP	7.9
1	A	519	TRP	6.2
1	A	330	LEU	5.8
1	A	236	SER	5.7
1	A	523	LYS	5.2
1	A	586	GLU	4.6
1	A	462	LEU	4.6
1	A	527	LEU	4.3
1	A	524	LEU	4.3
1	A	585	LYS	4.2
1	A	219	LYS	4.2
1	A	635	CYS	3.9
1	A	584	ASN	3.8
1	A	218	GLY	3.7
1	A	478	PRO	3.4
1	A	356	CYS	3.4
1	A	508	TYR	3.3
1	A	460	GLN	3.2
1	A	573	GLU	3.2
1	A	577	GLN	3.1
1	A	512	TYR	3.0
1	A	357	TYR	2.9
1	A	284	TYR	2.9
1	A	587	THR	2.8
1	A	656	ALA	2.8
1	A	545	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	327	PRO	2.8
1	A	588	ASP	2.8
1	A	515	GLY	2.7
1	A	89	ILE	2.7
1	A	248	MET	2.6
1	A	474	LEU	2.6
1	A	576	GLU	2.6
1	A	483	LEU	2.6
1	A	265	SER	2.5
1	A	534	TYR	2.5
1	A	328	ASP	2.4
1	A	511	GLU	2.4
1	A	595	LEU	2.4
1	A	659	ILE	2.4
1	A	522	ALA	2.4
1	A	413	MET	2.4
1	A	641	ASN	2.3
1	A	245	MET	2.3
1	A	358	THR	2.3
1	A	631	ALA	2.3
1	A	530	GLN	2.3
1	A	516	GLU	2.2
1	A	552	ILE	2.2
1	A	93	LYS	2.2
1	A	20	GLU	2.2
1	A	640	ALA	2.2
1	A	203	TYR	2.1
1	A	337	ALA	2.1
1	A	555	LEU	2.1
1	A	304	LEU	2.1
1	A	90	ASP	2.1
1	A	510	GLU	2.1
1	A	514	LYS	2.1
1	A	5	THR	2.1
1	A	271	ALA	2.1
1	A	660	VAL	2.1
1	A	92	ASP	2.1
1	A	336	LYS	2.0
1	A	459	ALA	2.0
1	A	548	LEU	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	PO4	A	801	5/5	0.97	0.14	-2.76	58,62,78,83	0

6.5 Other polymers (i)

There are no such residues in this entry.