Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 04:35 PM EST

PDB ID	:	4FYF
Title	:	Structural basis for substrate recognition by a novel Legionella phosphoinositide phosphatase
Authors	:	Hsu, F.S.; Zhu, W.; Brennan, L.; Tao, L.; Luo, Z.Q.; Mao, Y.
Deposited on	:	2012-07-04
Resolution	:	2.42 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 (i) 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 (i)) were used in the production of this report:

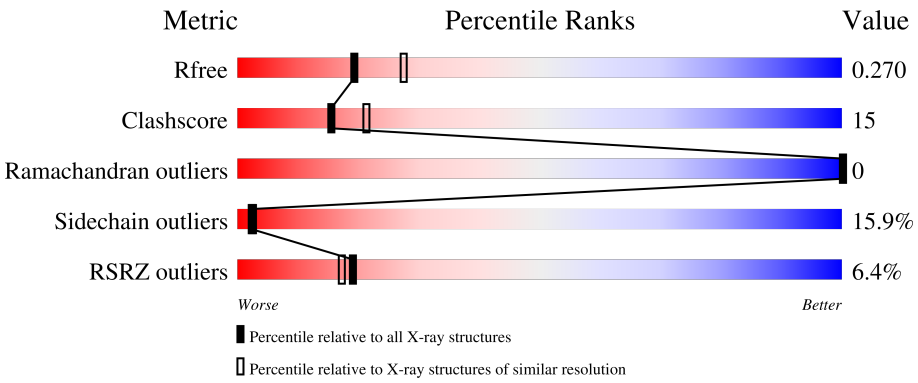
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

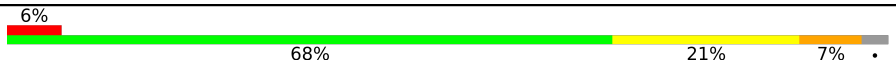
The reported resolution of this entry is 2.42 Å.

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	4647 (2.44-2.40)
Clashscore	141614	5161 (2.44-2.40)
Ramachandran outliers	138981	5073 (2.44-2.40)
Sidechain outliers	138945	5074 (2.44-2.40)
RSRZ outliers	127900	4543 (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 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 <=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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	801	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5984 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.

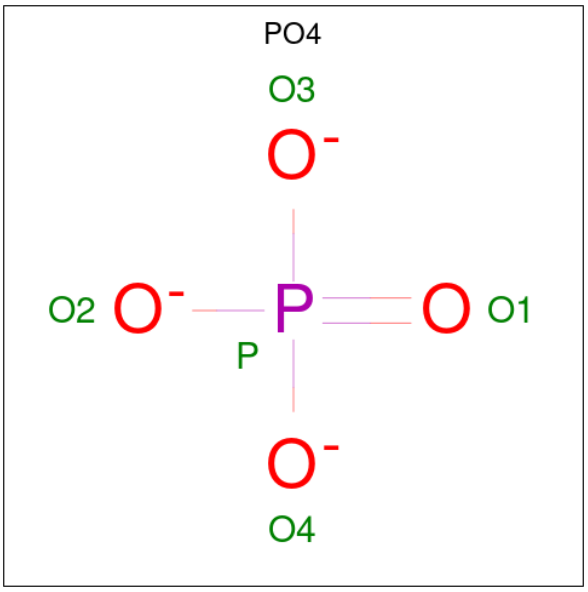
- Molecule 1 is a protein called SidF, inhibitor of growth family, member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	739	5907	3671	1057	1161	18	0	3	0

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
			Total	O	P		
2	A	1	5	4	1	0	0

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
3	A	3	3	3	0	0

- Molecule 4 is water.

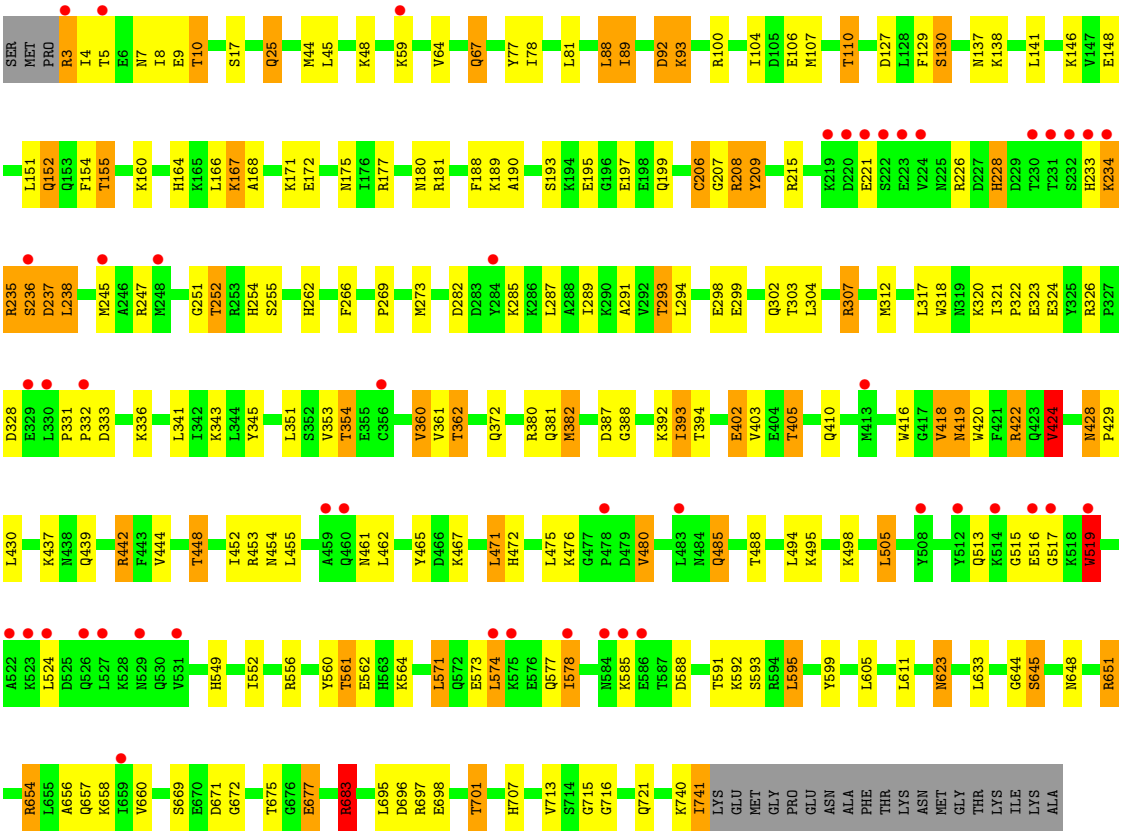
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	69	69	69	0	0

3 Residue-property plots (i)

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: SidF, inhibitor of growth family, member 3

Chain A: 6% 68% 21% 7%



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	71.83Å 115.71Å 125.11Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.18 – 2.42 47.18 – 2.42	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.18-2.42) 98.3 (47.18-2.42)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.85 (at 2.42Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.211 , 0.270 0.212 , 0.270	Depositor DCC
R_{free} test set	1992 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	48.4	Xtriage
Anisotropy	0.522	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5984	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% 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, 0.333 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: PO4, HG

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	0.83	5/6020 (0.1%)	1.02	28/8111 (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 (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	SER	CB-OG	-7.51	1.32	1.42
1	A	677	GLU	CD-OE1	5.21	1.31	1.25
1	A	519	TRP	CD2-CE2	5.16	1.47	1.41
1	A	318	TRP	CD2-CE2	5.11	1.47	1.41
1	A	416	TRP	CD2-CE2	5.02	1.47	1.41

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	422	ARG	NE-CZ-NH2	-17.31	111.65	120.30
1	A	422	ARG	NE-CZ-NH1	11.49	126.05	120.30
1	A	654	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	A	307	ARG	NE-CZ-NH2	-11.17	114.72	120.30
1	A	307	ARG	NE-CZ-NH1	9.47	125.03	120.30
1	A	683	ARG	NE-CZ-NH1	8.76	124.68	120.30
1	A	453	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	A	671	ASP	CB-CG-OD1	-7.34	111.69	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	424	VAL	CG1-CB-CG2	7.06	122.19	110.90
1	A	623	ASN	C-N-CA	-6.94	104.34	121.70
1	A	207	GLY	N-CA-C	-6.84	96.00	113.10
1	A	654	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	307	ARG	CG-CD-NE	-6.75	97.62	111.80
1	A	422	ARG	CG-CD-NE	-6.66	97.82	111.80
1	A	92	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	422	ARG	CD-NE-CZ	5.96	131.94	123.60
1	A	177	ARG	NE-CZ-NH2	-5.72	117.44	120.30
1	A	67	GLN	CA-CB-CG	5.63	125.80	113.40
1	A	651	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	A	654	ARG	CB-CG-CD	5.39	125.62	111.60
1	A	405	THR	CB-CA-C	-5.33	97.22	111.60
1	A	654	ARG	CD-NE-CZ	5.21	130.90	123.60
1	A	418	VAL	CG1-CB-CG2	5.20	119.22	110.90
1	A	307	ARG	CD-NE-CZ	5.17	130.83	123.60
1	A	17	SER	CB-CA-C	-5.15	100.31	110.10
1	A	360	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	A	623	ASN	O-C-N	-5.05	114.62	122.70
1	A	683	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	5907	0	5795	173	0
2	A	5	0	0	2	0
3	A	3	0	0	0	0
4	A	69	0	0	4	0
All	All	5984	0	5795	173	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 15.

All (173) 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:208:ARG:NH2	1:A:394:THR:HG22	1.45	1.29
1:A:235:ARG:O	1:A:235:ARG:HD2	1.55	1.07
1:A:235:ARG:HD2	1:A:235:ARG:C	1.71	1.06
1:A:208:ARG:NH2	1:A:394:THR:CG2	2.26	0.98
1:A:208:ARG:HH22	1:A:394:THR:CG2	1.77	0.97
1:A:394:THR:HG23	1:A:402:GLU:HG3	1.46	0.97
1:A:516:GLU:HA	1:A:519:TRP:HE3	1.31	0.95
1:A:516:GLU:HA	1:A:519:TRP:CE3	2.03	0.93
1:A:208:ARG:HH22	1:A:394:THR:HG22	1.18	0.91
1:A:252:THR:CG2	1:A:262:HIS:NE2	2.34	0.91
1:A:252:THR:HG23	1:A:262:HIS:NE2	1.86	0.90
1:A:151:LEU:O	1:A:155:THR:HG23	1.71	0.88
1:A:238:LEU:HD22	1:A:238:LEU:H	1.38	0.88
1:A:208:ARG:HH21	1:A:394:THR:HG22	1.37	0.88
1:A:235:ARG:C	1:A:235:ARG:CD	2.42	0.86
1:A:362:THR:HG21	1:A:419:ASN:HD21	1.40	0.84
1:A:208:ARG:O	1:A:299:GLU:OE1	1.95	0.83
1:A:424:VAL:HG13	1:A:428:ASN:HB3	1.59	0.82
1:A:362:THR:HG21	1:A:419:ASN:ND2	1.95	0.82
1:A:394:THR:CG2	1:A:402:GLU:HG3	2.09	0.81
1:A:302:GLN:HE21	1:A:394:THR:H	1.29	0.81
1:A:574:LEU:O	1:A:578:ILE:HB	1.81	0.81
1:A:77:TYR:OH	1:A:155:THR:HG21	1.81	0.80
1:A:428:ASN:HD22	1:A:430:LEU:H	1.30	0.80
1:A:428:ASN:ND2	1:A:430:LEU:H	1.81	0.78
1:A:444:VAL:O	1:A:448:THR:CG2	2.32	0.78
1:A:7:ASN:HD22	1:A:10:THR:HG23	1.50	0.76
1:A:561:THR:HA	1:A:564:LYS:HE2	1.68	0.75
1:A:127:ASP:H	1:A:137:ASN:HD21	1.33	0.74
1:A:444:VAL:O	1:A:448:THR:HG22	1.89	0.72
1:A:235:ARG:HD3	1:A:236:SER:O	1.89	0.72
1:A:235:ARG:CD	1:A:236:SER:O	2.38	0.71
1:A:188:PHE:CD2	1:A:698:GLU:HG2	2.26	0.71
1:A:494:LEU:HD13	1:A:498:LYS:HE3	1.73	0.71
1:A:291:ALA:HB2	1:A:505:LEU:CD2	2.20	0.71
1:A:93:LYS:HD2	1:A:93:LYS:O	1.89	0.71
1:A:354:THR:HB	1:A:410:GLN:HB3	1.73	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:O	1:A:110:THR:HG22	1.91	0.70
1:A:237:ASP:OD2	1:A:285:LYS:HE2	1.91	0.70
1:A:591:THR:O	1:A:595:LEU:HD22	1.92	0.69
1:A:25:GLN:HE21	1:A:25:GLN:H	1.41	0.69
1:A:197:GLU:HG2	1:A:254:HIS:HA	1.74	0.68
1:A:656:ALA:O	1:A:660:VAL:HG23	1.94	0.68
1:A:291:ALA:HB2	1:A:505:LEU:HD22	1.73	0.68
1:A:234:LYS:HD2	1:A:234:LYS:H	1.59	0.67
1:A:382:MET:HA	1:A:382:MET:HE2	1.77	0.67
1:A:93:LYS:HD2	1:A:93:LYS:C	2.14	0.67
1:A:372:GLN:NE2	1:A:651:ARG:HH12	1.93	0.67
1:A:465:TYR:HD1	1:A:577:GLN:NE2	1.94	0.66
1:A:7:ASN:HD22	1:A:10:THR:H	1.44	0.66
1:A:465:TYR:HD1	1:A:577:GLN:HE21	1.45	0.65
1:A:516:GLU:HG2	1:A:517:GLY:H	1.62	0.65
1:A:235:ARG:CZ	1:A:237:ASP:HA	2.27	0.65
1:A:428:ASN:HD22	1:A:428:ASN:C	2.01	0.64
1:A:419:ASN:HD22	1:A:419:ASN:C	2.01	0.64
1:A:190:ALA:H	1:A:199:GLN:HE21	1.45	0.63
1:A:578:ILE:CD1	1:A:595:LEU:HG	2.28	0.63
1:A:382:MET:HA	1:A:382:MET:CE	2.29	0.63
1:A:7:ASN:HD21	1:A:9:GLU:HB3	1.63	0.62
1:A:302:GLN:NE2	1:A:394:THR:H	1.95	0.62
1:A:382:MET:N	1:A:382:MET:HE3	2.15	0.62
1:A:238:LEU:HD22	1:A:238:LEU:N	2.12	0.62
1:A:442:ARG:HG2	1:A:549:HIS:CD2	2.35	0.62
1:A:59[B]:LYS:CB	1:A:59[B]:LYS:NZ	2.63	0.62
1:A:428:ASN:HD22	1:A:429:PRO:N	1.98	0.62
1:A:571:LEU:HD22	1:A:599:TYR:CE2	2.35	0.62
1:A:362:THR:CG2	1:A:419:ASN:ND2	2.63	0.61
1:A:93:LYS:O	1:A:93:LYS:CD	2.48	0.61
1:A:444:VAL:O	1:A:448:THR:HG23	2.00	0.61
1:A:226:ARG:HH22	1:A:394:THR:HG21	1.65	0.61
1:A:362:THR:HG22	4:A:925:HOH:O	2.00	0.61
1:A:683:ARG:HD3	1:A:696:ASP:OD2	2.01	0.60
1:A:152:GLN:HE22	1:A:741:ILE:HB	1.65	0.60
1:A:93:LYS:C	1:A:93:LYS:CD	2.69	0.60
1:A:428:ASN:HD21	1:A:430:LEU:HG	1.66	0.60
1:A:560:TYR:CE2	1:A:564:LYS:HD3	2.37	0.59
1:A:578:ILE:HD12	1:A:595:LEU:HG	1.85	0.58
1:A:152:GLN:NE2	1:A:741:ILE:HB	2.19	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:LYS:HD2	1:A:234:LYS:N	2.18	0.57
1:A:235:ARG:NE	1:A:237:ASP:HA	2.20	0.57
1:A:3:ARG:HH11	1:A:3:ARG:HB3	1.68	0.57
1:A:461:ASN:O	1:A:462:LEU:HD22	2.05	0.57
1:A:485:GLN:HE21	1:A:485:GLN:HA	1.69	0.57
1:A:233:HIS:CE1	1:A:234:LYS:O	2.57	0.56
1:A:209:TYR:O	1:A:226:ARG:NH1	2.36	0.56
1:A:669:SER:HB2	1:A:672:GLY:H	1.70	0.56
1:A:238:LEU:H	1:A:238:LEU:CD2	2.15	0.55
1:A:252:THR:HG22	1:A:262:HIS:NE2	2.20	0.55
1:A:237:ASP:OD1	1:A:237:ASP:N	2.38	0.55
1:A:362:THR:H	1:A:372:GLN:NE2	2.05	0.55
1:A:516:GLU:CA	1:A:519:TRP:CE3	2.86	0.54
1:A:167:LYS:HG3	1:A:168:ALA:N	2.23	0.54
1:A:291:ALA:CB	1:A:505:LEU:HD22	2.38	0.53
1:A:701:THR:HG21	4:A:920:HOH:O	2.08	0.53
1:A:317:LEU:O	1:A:321:ILE:HG13	2.09	0.52
1:A:59[B]:LYS:CB	1:A:59[B]:LYS:HZ2	2.22	0.52
1:A:234:LYS:H	1:A:234:LYS:CD	2.22	0.52
1:A:394:THR:HG23	1:A:402:GLU:CG	2.31	0.52
1:A:78:ILE:HD12	1:A:154:PHE:CD2	2.44	0.51
1:A:92:ASP:OD2	1:A:164:HIS:HE1	1.94	0.51
1:A:480:VAL:CG2	1:A:552:ILE:HG12	2.42	0.50
1:A:382:MET:CE	1:A:382:MET:CA	2.90	0.50
1:A:106:GLU:O	1:A:110:THR:CG2	2.58	0.49
1:A:167:LYS:HZ2	1:A:167:LYS:HB2	1.77	0.49
1:A:129:PHE:CD1	1:A:697:ARG:HG2	2.47	0.49
1:A:89:ILE:HG22	1:A:100:ARG:NH1	2.27	0.49
1:A:402:GLU:HG2	1:A:403:VAL:N	2.27	0.49
1:A:3:ARG:HH21	1:A:206:CYS:HB3	1.78	0.49
1:A:251:GLY:HA2	1:A:262:HIS:CD2	2.48	0.48
1:A:208:ARG:HH22	1:A:394:THR:HG21	1.71	0.48
1:A:7:ASN:ND2	1:A:10:THR:H	2.08	0.48
1:A:7:ASN:HD22	1:A:10:THR:CG2	2.23	0.47
1:A:25:GLN:H	1:A:25:GLN:NE2	2.08	0.47
1:A:107:MET:HA	1:A:110:THR:HG23	1.95	0.47
1:A:380:ARG:HG3	1:A:439:GLN:HG2	1.96	0.47
1:A:7:ASN:ND2	1:A:10:THR:HG23	2.25	0.47
1:A:100:ARG:O	1:A:104:ILE:HG12	2.14	0.47
1:A:215:ARG:HD3	1:A:221:GLU:OE2	2.14	0.47
1:A:467:LYS:HD2	1:A:573:GLU:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:O	1:A:235:ARG:CD	2.43	0.47
1:A:578:ILE:HD11	1:A:595:LEU:HG	1.95	0.47
1:A:151:LEU:O	1:A:155:THR:CG2	2.55	0.47
1:A:228:HIS:HE1	1:A:299:GLU:OE1	1.98	0.47
1:A:419:ASN:ND2	1:A:419:ASN:C	2.67	0.46
1:A:701:THR:HG22	4:A:948:HOH:O	2.15	0.46
1:A:234:LYS:O	1:A:234:LYS:HG2	2.16	0.46
1:A:707:HIS:CD2	1:A:716:GLY:H	2.34	0.46
1:A:88:LEU:HD13	1:A:172:GLU:HG2	1.98	0.46
1:A:289:ILE:O	1:A:293:THR:HG22	2.16	0.45
1:A:592:LYS:HE3	1:A:592:LYS:HB2	1.77	0.45
1:A:516:GLU:CG	1:A:517:GLY:H	2.27	0.45
1:A:516:GLU:CG	1:A:517:GLY:N	2.80	0.45
1:A:189:LYS:HE3	1:A:193:SER:OG	2.17	0.44
1:A:324:GLU:H	1:A:324:GLU:HG2	1.29	0.44
1:A:247:ARG:CZ	1:A:307:ARG:HG3	2.47	0.44
1:A:654:ARG:HH21	1:A:657:GLN:HE22	1.66	0.44
1:A:7:ASN:HB3	1:A:10:THR:HG23	2.00	0.44
1:A:675:THR:OG1	1:A:677:GLU:HG3	2.17	0.44
1:A:312:MET:HE1	1:A:345:TYR:CE2	2.53	0.43
1:A:465:TYR:HA	1:A:577:GLN:HE22	1.83	0.43
1:A:362:THR:H	1:A:372:GLN:HE21	1.66	0.43
1:A:3:ARG:HB3	1:A:3:ARG:NH1	2.32	0.43
1:A:452:ILE:HD12	1:A:476:LYS:HA	2.01	0.42
1:A:471:LEU:HD22	1:A:475:LEU:HG	1.99	0.42
1:A:480:VAL:HG21	1:A:552:ILE:HG12	2.01	0.42
1:A:644:GLY:HA2	1:A:648:ASN:OD1	2.18	0.42
1:A:321:ILE:O	1:A:322:PRO:C	2.58	0.42
1:A:422:ARG:HH22	1:A:721:GLN:HE21	1.67	0.42
1:A:571:LEU:CD2	1:A:599:TYR:CE2	3.01	0.42
1:A:323:GLU:HA	1:A:326:ARG:HD2	2.02	0.42
1:A:424:VAL:CG1	1:A:428:ASN:HB3	2.39	0.42
1:A:465:TYR:CD1	1:A:577:GLN:NE2	2.80	0.42
1:A:515:GLY:O	1:A:519:TRP:N	2.52	0.42
1:A:645:SER:HB2	2:A:801:PO4:P	2.59	0.42
1:A:387:ASP:OD1	1:A:387:ASP:C	2.57	0.42
1:A:645:SER:HB2	2:A:801:PO4:O2	2.20	0.42
1:A:302:GLN:HA	1:A:393:ILE:HG12	2.01	0.42
1:A:88:LEU:HD12	1:A:88:LEU:HA	1.74	0.41
1:A:44:MET:HE3	1:A:44:MET:HB3	1.82	0.41
1:A:381:GLN:C	1:A:382:MET:HE3	2.41	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PHE:CE2	1:A:304:LEU:CD2	3.04	0.41
1:A:78:ILE:HG23	1:A:154:PHE:CZ	2.56	0.41
1:A:362:THR:CG2	1:A:419:ASN:HD21	2.20	0.41
1:A:388:GLY:O	1:A:495:LYS:HD3	2.21	0.41
1:A:331:PRO:HA	1:A:332:PRO:HD3	1.93	0.41
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.99	0.41
1:A:420:TRP:HD1	1:A:721:GLN:HE22	1.68	0.41
1:A:654:ARG:HD3	4:A:929:HOH:O	2.20	0.41
1:A:148:GLU:O	1:A:152:GLN:HG2	2.21	0.40
1:A:333:ASP:HB3	1:A:336:LYS:HB3	2.03	0.40
1:A:387:ASP:OD1	1:A:388:GLY:N	2.54	0.40
1:A:78:ILE:HD11	1:A:151:LEU:CD2	2.51	0.40
1:A:245:MET:SD	1:A:269:PRO:HD3	2.61	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	740/761 (97%)	711 (96%)	29 (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	639/654 (98%)	538 (84%)	101 (16%)	2 2

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	ARG
1	A	4	ILE
1	A	5	THR
1	A	8	ILE
1	A	10	THR
1	A	25	GLN
1	A	45	LEU
1	A	48	LYS
1	A	64	VAL
1	A	67	GLN
1	A	81	LEU
1	A	88	LEU
1	A	89	ILE
1	A	93	LYS
1	A	110	THR
1	A	130	SER
1	A	138	LYS
1	A	146	LYS
1	A	152	GLN
1	A	155	THR
1	A	160	LYS
1	A	166	LEU
1	A	167	LYS
1	A	171	LYS
1	A	175	ASN
1	A	180	ASN
1	A	181	ARG
1	A	195	GLU
1	A	206	CYS
1	A	208	ARG
1	A	209	TYR
1	A	228	HIS
1	A	234	LYS
1	A	235	ARG
1	A	236	SER
1	A	237	ASP
1	A	238	LEU
1	A	252	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	255	SER
1	A	273	MET
1	A	282	ASP
1	A	287	LEU
1	A	293	THR
1	A	294	LEU
1	A	298	GLU
1	A	303	THR
1	A	320	LYS
1	A	328	ASP
1	A	341	LEU
1	A	343	LYS
1	A	351	LEU
1	A	353	VAL
1	A	354	THR
1	A	360	VAL
1	A	361	VAL
1	A	362	THR
1	A	382	MET
1	A	392	LYS
1	A	393	ILE
1	A	402	GLU
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	442	ARG
1	A	448	THR
1	A	454	ASN
1	A	455	LEU
1	A	471	LEU
1	A	472	HIS
1	A	480	VAL
1	A	485	GLN
1	A	488	THR
1	A	505	LEU
1	A	513	GLN
1	A	519	TRP
1	A	524	LEU
1	A	556	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	561	THR
1	A	562	GLU
1	A	571	LEU
1	A	574	LEU
1	A	578	ILE
1	A	585	LYS
1	A	588	ASP
1	A	593	SER
1	A	595	LEU
1	A	605	LEU
1	A	611	LEU
1	A	623	ASN
1	A	633	LEU
1	A	645	SER
1	A	658	LYS
1	A	683	ARG
1	A	695	LEU
1	A	701	THR
1	A	713	VAL
1	A	740	LYS
1	A	741	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	25	GLN
1	A	26	ASN
1	A	28	HIS
1	A	137	ASN
1	A	152	GLN
1	A	164	HIS
1	A	180	ASN
1	A	199	GLN
1	A	228	HIS
1	A	302	GLN
1	A	365	GLN
1	A	372	GLN
1	A	375	GLN
1	A	381	GLN
1	A	419	ASN
1	A	428	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	484	ASN
1	A	485	GLN
1	A	513	GLN
1	A	550	ASN
1	A	577	GLN
1	A	609	GLN
1	A	622	ASN
1	A	623	ASN
1	A	657	GLN
1	A	681	HIS
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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	PO4	A	801	-	4,4,4	2.00	1 (25%)	6,6,6	0.98	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	PO4	P-O3	-2.55	1.46	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	PO4	2	0

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	739/761 (97%)	0.28	47 (6%) 19 17	27, 53, 101, 148	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	459	ALA	7.8
1	A	330	LEU	5.9
1	A	460	GLN	4.3
1	A	231	THR	3.7
1	A	222	SER	3.7
1	A	356	CYS	3.5
1	A	508	TYR	3.4
1	A	220	ASP	3.4
1	A	3	ARG	3.4
1	A	233	HIS	3.4
1	A	236	SER	3.3
1	A	519	TRP	3.3
1	A	526	GLN	3.3
1	A	586	GLU	3.2
1	A	531	VAL	3.2
1	A	574	LEU	3.2
1	A	517	GLY	3.1
1	A	232	SER	3.0
1	A	584	ASN	3.0
1	A	329	GLU	2.9
1	A	578	ILE	2.9
1	A	248	MET	2.9
1	A	219	LYS	2.8
1	A	230	THR	2.8
1	A	585	LYS	2.8
1	A	512	TYR	2.7
1	A	234	LYS	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	523	LYS	2.6
1	A	332	PRO	2.6
1	A	524	LEU	2.5
1	A	478	PRO	2.5
1	A	516	GLU	2.4
1	A	575	LYS	2.4
1	A	59[A]	LYS	2.4
1	A	284	TYR	2.4
1	A	413	MET	2.3
1	A	5	THR	2.3
1	A	527	LEU	2.3
1	A	221	GLU	2.3
1	A	659	ILE	2.2
1	A	224	VAL	2.1
1	A	514	LYS	2.1
1	A	483	LEU	2.1
1	A	223	GLU	2.1
1	A	522	ALA	2.0
1	A	529	ASN	2.0
1	A	245	MET	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(Å^2)	Q<0.9
3	HG	A	804	1/1	0.94	0.32	132,132,132,132	1
3	HG	A	803	1/1	0.95	0.38	132,132,132,132	1
3	HG	A	802	1/1	0.96	0.37	132,132,132,132	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	PO4	A	801	5/5	0.99	0.19	38,48,51,55	0

6.5 Other polymers (i)

There are no such residues in this entry.