Full wwPDB X-ray Structure Validation Report (i)

Apr 20, 2016 – 05:47 AM EDT

PDB ID	:	5C16
Title	:	Myotubularin-related proetin 1
Authors	:	Lee, B.I.; Bong, S.M.
Deposited on	:	2015-06-13
Resolution	:	2.07 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:

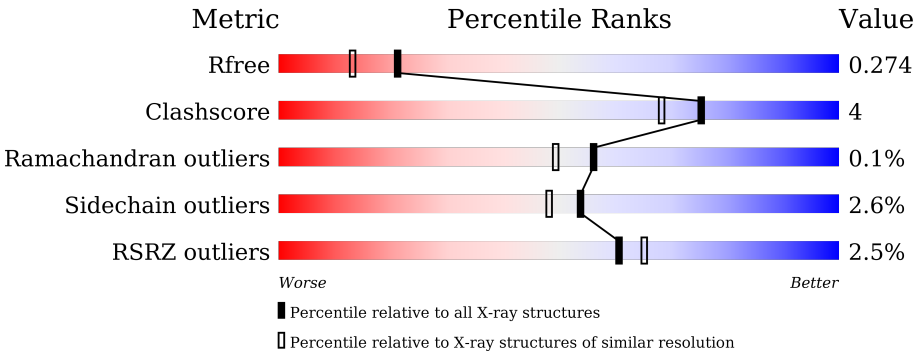
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027257
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20027257

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 2.07 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	1799 (2.08-2.04)
Clashscore	102246	1910 (2.08-2.04)
Ramachandran outliers	100387	1893 (2.08-2.04)
Sidechain outliers	100360	1893 (2.08-2.04)
RSRZ outliers	91569	1802 (2.08-2.04)

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	571	76% 9% 15%
1	B	571	74% 11% 15%
1	C	571	76% 9% 15%
1	D	571	75% 9% 15%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	702	-	-	-	X
2	PO4	B	702	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16506 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.

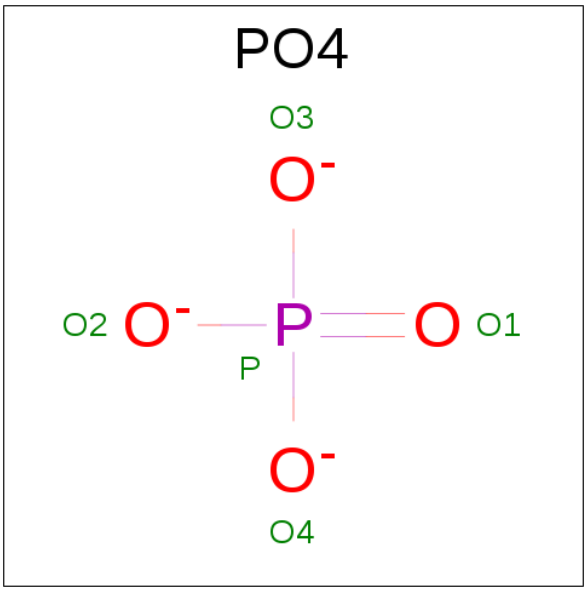
- Molecule 1 is a protein called Myotubularin-related protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3956	2555	662	721	18			
1	B	487	Total	C	N	O	S	0	0	0
			3956	2555	662	721	18			
1	C	487	Total	C	N	O	S	0	0	0
			3956	2555	662	721	18			
1	D	487	Total	C	N	O	S	0	0	0
			3956	2555	662	721	18			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	438	SER	CYS	engineered mutation	UNP Q13613
B	438	SER	CYS	engineered mutation	UNP Q13613
C	438	SER	CYS	engineered mutation	UNP Q13613
D	438	SER	CYS	engineered mutation	UNP Q13613

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



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

- Molecule 3 is water.

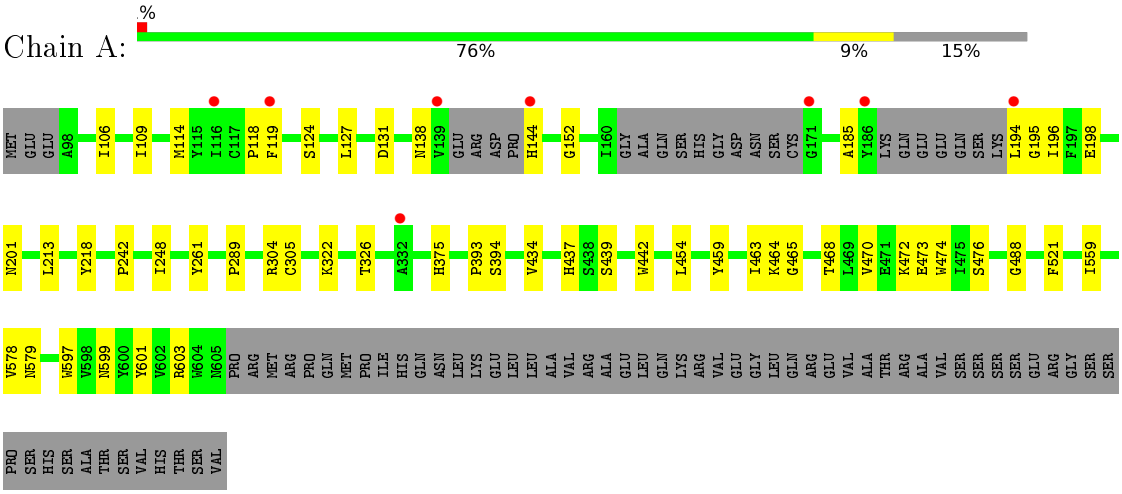
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	210	Total O 210 210	0	0
3	B	195	Total O 195 195	0	0
3	C	119	Total O 119 119	0	0
3	D	128	Total O 128 128	0	0

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.

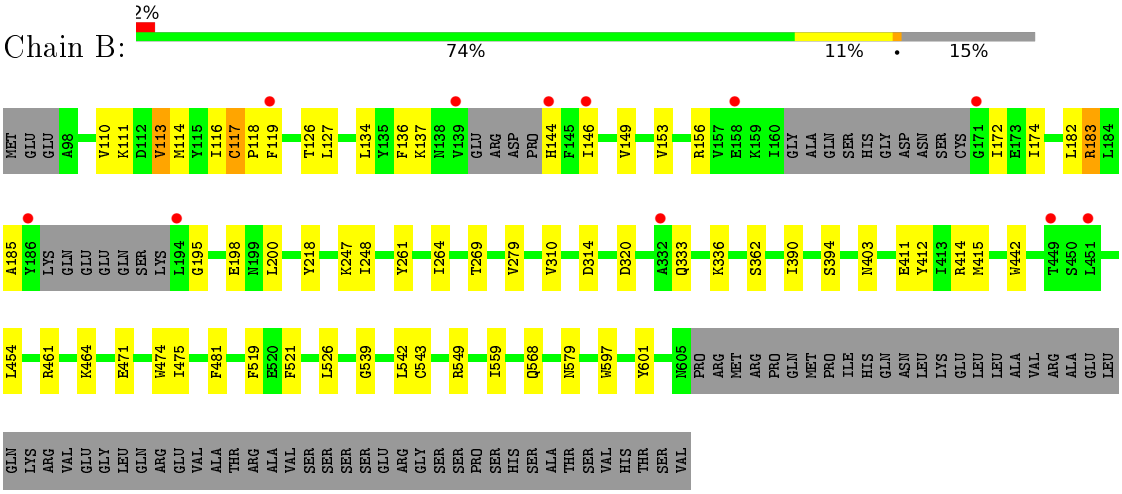
- Molecule 1: Myotubularin-related protein 1

Chain A:



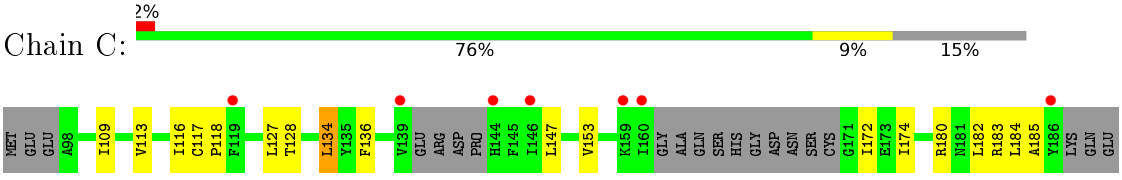
- Molecule 1: Myotubularin-related protein 1

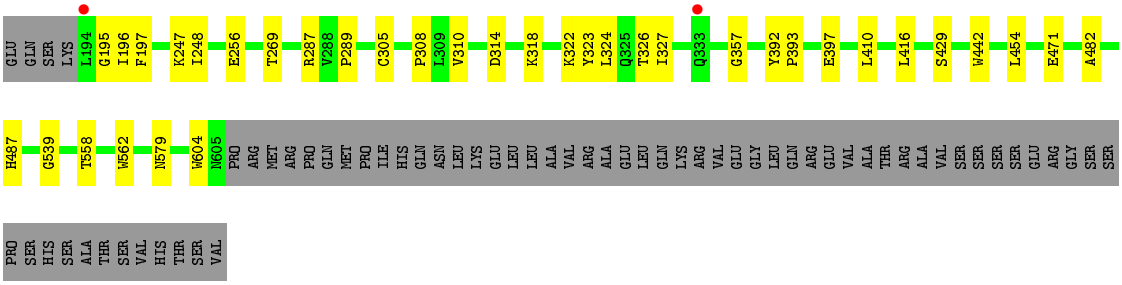
Chain B:



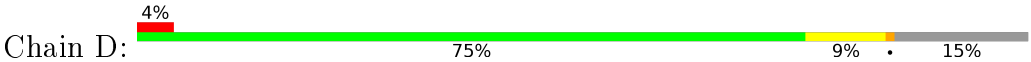
- Molecule 1: Myotubularin-related protein 1

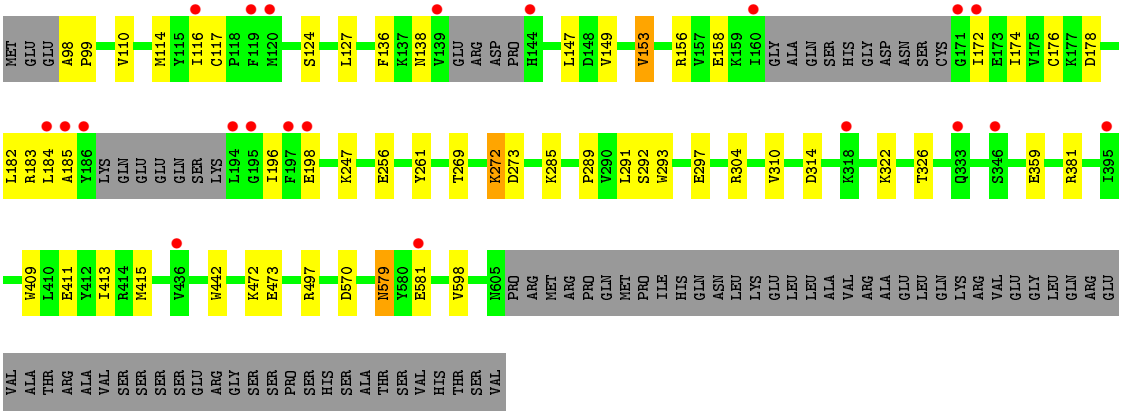
Chain C:





- Molecule 1: Myotubularin-related protein 1





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	67.22Å 96.59Å 97.58Å 87.60° 86.07° 77.33°	Depositor
Resolution (Å)	34.81 – 2.07 35.08 – 2.00	Depositor EDS
% Data completeness (in resolution range)	85.8 (34.81-2.07) 84.0 (35.08-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.96 (at 2.00Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.220 , 0.274 0.220 , 0.274	Depositor DCC
R_{free} test set	6204 reflections (4.97%)	DCC
Wilson B-factor (Å^2)	24.8	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	16506	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 96.61 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.5396e-10. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.46	0/4059	0.56	0/5503
1	B	0.43	0/4059	0.54	0/5503
1	C	0.37	0/4059	0.49	0/5503
1	D	0.39	0/4059	0.50	0/5503
All	All	0.41	0/16236	0.52	0/22012

There are no bond length outliers.

There are no bond angle outliers.

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	3956	0	3887	25	0
1	B	3956	0	3887	40	0
1	C	3956	0	3887	27	0
1	D	3956	0	3887	29	0
2	A	10	0	0	1	0
2	B	10	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	210	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	195	0	0	3	0
3	C	119	0	0	0	0
3	D	128	0	0	0	0
All	All	16506	0	15548	121	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 (121) 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:114:MET:HB2	1:A:185:ALA:HB3	1.59	0.85
1:B:116:ILE:HD13	1:B:183:ARG:HD3	1.68	0.76
1:C:172:ILE:HG22	1:C:184:LEU:HB2	1.66	0.76
1:D:172:ILE:HG22	1:D:184:LEU:HB2	1.69	0.73
1:C:113:VAL:HG21	1:C:127:LEU:HB2	1.70	0.73
1:A:242:PRO:HG3	1:A:248:ILE:HG12	1.70	0.73
1:D:114:MET:HB2	1:D:185:ALA:HB3	1.72	0.71
1:B:134:LEU:HD21	1:B:200:LEU:HD21	1.75	0.67
1:D:272:LYS:HE2	1:D:273:ASP:H	1.63	0.63
1:B:247:LYS:HB3	1:B:269:THR:HG22	1.79	0.63
1:A:152:GLY:O	3:A:801:HOH:O	2.16	0.63
1:A:579:ASN:ND2	3:A:804:HOH:O	2.33	0.62
1:B:411:GLU:HG3	1:B:415:MET:HE2	1.82	0.61
1:B:114:MET:HB2	1:B:185:ALA:HB3	1.83	0.58
1:D:127:LEU:HD23	1:D:196:ILE:HD12	1.84	0.58
1:D:310:VAL:HG12	1:D:314:ASP:HA	1.86	0.58
1:B:137:LYS:HG3	1:B:146:ILE:HG12	1.86	0.58
1:C:397:GLU:H	1:C:397:GLU:CD	2.06	0.57
1:B:411:GLU:OE2	1:B:414:ARG:NH2	2.33	0.57
1:A:106:ILE:HD13	1:A:109:ILE:HD11	1.87	0.56
1:D:247:LYS:HB3	1:D:269:THR:HG22	1.89	0.55
1:B:579:ASN:ND2	3:B:807:HOH:O	2.39	0.55
1:D:110:VAL:HG21	1:D:196:ILE:HD11	1.88	0.54
1:C:109:ILE:HG12	1:C:128:THR:HG23	1.89	0.54
1:D:289:PRO:HA	1:D:304:ARG:O	2.08	0.54
1:B:471:GLU:HA	1:B:475:ILE:HD12	1.90	0.54
1:C:310:VAL:HG12	1:C:314:ASP:HA	1.89	0.54
1:D:116:ILE:HG13	1:D:183:ARG:HD2	1.90	0.54
1:C:117:CYS:SG	1:C:118:PRO:HD2	2.47	0.53
1:B:390:ILE:HD13	1:B:403:ASN:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:CYS:SG	1:B:118:PRO:HD2	2.49	0.53
1:A:124:SER:O	1:A:138:ASN:ND2	2.33	0.52
1:B:110:VAL:O	1:B:127:LEU:N	2.37	0.52
1:B:461:ARG:HG2	1:B:519:PHE:CD2	2.44	0.52
1:D:411:GLU:HG3	1:D:415:MET:HE2	1.92	0.52
1:A:127:LEU:HD23	1:A:196:ILE:HD12	1.92	0.52
1:D:149:VAL:HG21	1:D:182:LEU:HD11	1.92	0.51
1:B:111:LYS:HA	1:B:126:THR:HA	1.92	0.51
1:C:247:LYS:HG2	1:C:269:THR:HA	1.92	0.51
1:B:195:GLY:HA3	1:B:198:GLU:OE1	2.12	0.50
1:A:218:TYR:CD2	1:A:559:ILE:HD12	2.48	0.49
1:A:118:PRO:HB3	1:A:393:PRO:HB3	1.94	0.49
1:B:174:ILE:HB	1:B:182:LEU:HB2	1.93	0.49
1:B:414:ARG:NH1	3:B:802:HOH:O	2.28	0.48
1:A:322:LYS:O	1:A:326:THR:HG23	2.13	0.48
1:D:272:LYS:HE2	1:D:273:ASP:N	2.28	0.48
1:D:579:ASN:OD1	1:D:579:ASN:N	2.37	0.48
1:C:174:ILE:HB	1:C:182:LEU:HB2	1.94	0.48
1:A:119:PHE:CZ	1:A:394:SER:HB3	2.49	0.48
1:B:119:PHE:CZ	1:B:394:SER:HB3	2.49	0.48
1:C:289:PRO:HB2	1:C:323:TYR:HE2	1.78	0.48
1:D:156:ARG:NH1	1:D:158:GLU:OE1	2.47	0.48
1:D:136:PHE:HB3	1:D:147:LEU:HB3	1.95	0.48
1:C:471:GLU:OE2	1:C:562:TRP:NE1	2.43	0.48
1:B:310:VAL:HG12	1:B:314:ASP:HA	1.96	0.48
1:B:474:TRP:HB3	1:B:481:PHE:HZ	1.78	0.48
1:B:539:GLY:HA2	1:B:542:LEU:HG	1.95	0.47
1:A:470:VAL:O	1:A:474:TRP:HB2	2.15	0.47
1:B:149:VAL:HG21	1:B:182:LEU:HD21	1.97	0.47
1:A:194:LEU:N	1:A:195:GLY:HA2	2.29	0.47
1:A:463:ILE:HG12	1:A:521:PHE:HB3	1.96	0.46
1:D:153:VAL:HG13	1:D:176:CYS:HB3	1.97	0.46
1:A:131:ASP:N	1:A:131:ASP:OD1	2.48	0.46
1:C:392:TYR:CG	1:C:393:PRO:HA	2.50	0.46
1:B:411:GLU:HG3	1:B:415:MET:CE	2.44	0.46
1:D:116:ILE:HD11	1:D:185:ALA:HB2	1.97	0.46
1:D:174:ILE:HB	1:D:182:LEU:HB2	1.97	0.46
1:A:213:LEU:HD21	1:A:488:GLY:HA3	1.98	0.46
1:B:134:LEU:HD23	1:B:134:LEU:HA	1.61	0.46
1:C:127:LEU:HD11	1:C:134:LEU:HG	1.97	0.46
1:D:359:GLU:N	1:D:359:GLU:OE1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:LYS:NZ	3:B:815:HOH:O	2.45	0.46
1:A:289:PRO:HA	1:A:304:ARG:O	2.16	0.45
1:D:124:SER:O	1:D:138:ASN:ND2	2.49	0.45
1:B:137:LYS:HE3	1:B:146:ILE:HD11	1.98	0.45
1:B:412:TYR:HA	1:B:415:MET:HE3	1.99	0.45
1:B:156:ARG:HE	1:B:156:ARG:HB2	1.56	0.45
1:A:599:ASN:O	1:A:603:ARG:HB2	2.17	0.44
1:D:411:GLU:HG3	1:D:415:MET:CE	2.47	0.44
1:D:472:LYS:NZ	1:D:473:GLU:OE2	2.47	0.44
1:C:482:ALA:HA	1:C:487:HIS:CD2	2.52	0.44
1:A:194:LEU:HB3	1:A:198:GLU:HB2	1.99	0.44
1:C:136:PHE:HB3	1:C:147:LEU:HB3	1.98	0.44
1:A:305:CYS:SG	1:A:437:HIS:HB3	2.58	0.44
1:C:172:ILE:HD11	1:C:197:PHE:HD1	1.83	0.44
1:D:291:LEU:HD12	1:D:292:SER:N	2.32	0.44
1:A:439:SER:OG	2:A:702:PO4:O4	2.22	0.43
1:B:521:PHE:HE1	1:B:526:LEU:HD11	1.83	0.43
1:D:381:ARG:HD3	1:D:497:ARG:O	2.19	0.43
1:A:464:LYS:O	1:A:468:THR:HG23	2.18	0.43
1:B:218:TYR:CD2	1:B:559:ILE:HD12	2.54	0.43
1:B:116:ILE:HB	1:B:183:ARG:HB3	2.00	0.42
1:D:98:ALA:HA	1:D:99:PRO:HD3	1.93	0.42
1:B:279:VAL:HG13	1:B:320:ASP:OD1	2.20	0.42
1:C:180:ARG:HB3	1:C:604:TRP:CD1	2.54	0.42
1:B:127:LEU:HD11	1:B:134:LEU:HD22	2.01	0.42
1:B:310:VAL:CG1	1:B:314:ASP:HA	2.50	0.42
1:B:113:VAL:HG12	1:B:136:PHE:HE2	1.85	0.42
1:B:116:ILE:HD11	1:B:185:ALA:HB2	2.01	0.42
1:C:116:ILE:HD11	1:C:185:ALA:HB2	2.02	0.42
1:C:289:PRO:HA	1:C:305:CYS:HB3	2.02	0.42
1:C:116:ILE:HG21	1:C:183:ARG:HH11	1.85	0.42
1:C:324:LEU:O	1:C:327:ILE:HB	2.20	0.42
1:D:322:LYS:O	1:D:326:THR:HG23	2.20	0.41
1:D:291:LEU:HD11	1:D:293:TRP:O	2.21	0.41
1:C:322:LYS:O	1:C:326:THR:HG23	2.21	0.41
1:A:472:LYS:NZ	1:A:473:GLU:OE2	2.38	0.41
1:B:134:LEU:HB2	1:B:149:VAL:HB	2.02	0.41
1:D:247:LYS:HG2	1:D:269:THR:HA	2.03	0.41
1:A:459:TYR:O	1:A:465:GLY:HA3	2.21	0.41
1:B:248:ILE:HG23	1:B:264:ILE:HG23	2.03	0.41
1:C:416:LEU:HD12	1:C:416:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:597:TRP:HB3	1:B:601:TYR:CE2	2.56	0.40
1:C:308:PRO:HD2	1:C:357:GLY:O	2.20	0.40
1:A:597:TRP:HB3	1:A:601:TYR:CE2	2.56	0.40
1:C:539:GLY:HA3	1:C:558:THR:OG1	2.22	0.40
1:B:543:CYS:HB2	1:B:549:ARG:HG3	2.02	0.40
1:C:410:LEU:HD23	1:C:410:LEU:HA	1.76	0.40
1:C:113:VAL:HG23	1:C:136:PHE:HE2	1.86	0.40
1:D:409:TRP:O	1:D:413:ILE:HG12	2.21	0.40
1:C:454:LEU:HD23	1:C:454:LEU:HA	1.87	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	479/571 (84%)	460 (96%)	19 (4%)	0	100	100
1	B	479/571 (84%)	465 (97%)	14 (3%)	0	100	100
1	C	479/571 (84%)	461 (96%)	17 (4%)	1 (0%)	52	43
1	D	479/571 (84%)	454 (95%)	24 (5%)	1 (0%)	52	43
All	All	1916/2284 (84%)	1840 (96%)	74 (4%)	2 (0%)	56	49

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	195	GLY
1	D	581	GLU

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	435/509 (86%)	426 (98%)	9 (2%)	61	57
1	B	435/509 (86%)	422 (97%)	13 (3%)	48	42
1	C	435/509 (86%)	425 (98%)	10 (2%)	58	53
1	D	435/509 (86%)	422 (97%)	13 (3%)	48	42
All	All	1740/2036 (86%)	1695 (97%)	45 (3%)	54	48

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	201	ASN
1	A	261	TYR
1	A	375	HIS
1	A	434	VAL
1	A	442	TRP
1	A	454	LEU
1	A	476	SER
1	A	578	VAL
1	B	113	VAL
1	B	117	CYS
1	B	144	HIS
1	B	153	VAL
1	B	172	ILE
1	B	183	ARG
1	B	261	TYR
1	B	333	GLN
1	B	336	LYS
1	B	362	SER
1	B	442	TRP
1	B	454	LEU
1	B	568	GLN
1	C	134	LEU
1	C	153	VAL

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Mol	Chain	Res	Type
1	C	196	ILE
1	C	248	ILE
1	C	256	GLU
1	C	287	ARG
1	C	318	LYS
1	C	429	SER
1	C	442	TRP
1	C	579	ASN
1	D	117	CYS
1	D	153	VAL
1	D	178	ASP
1	D	198	GLU
1	D	256	GLU
1	D	261	TYR
1	D	272	LYS
1	D	285	LYS
1	D	297	GLU
1	D	442	TRP
1	D	570	ASP
1	D	579	ASN
1	D	598	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	579	ASN
1	B	492	HIS
1	B	547	GLN
1	B	579	ASN
1	D	299	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are 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	701	-	4,4,4	0.72	0	6,6,6	0.25	0
2	PO4	A	702	-	4,4,4	0.60	0	6,6,6	0.24	0
2	PO4	B	701	-	4,4,4	0.76	0	6,6,6	0.25	0
2	PO4	B	702	-	4,4,4	0.59	0	6,6,6	0.25	0
2	PO4	C	701	-	4,4,4	0.78	0	6,6,6	0.24	0
2	PO4	D	701	-	4,4,4	0.78	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	701	-	-	0/0/0/0	0/0/0/0
2	PO4	A	702	-	-	0/0/0/0	0/0/0/0
2	PO4	B	701	-	-	0/0/0/0	0/0/0/0
2	PO4	B	702	-	-	0/0/0/0	0/0/0/0
2	PO4	C	701	-	-	0/0/0/0	0/0/0/0
2	PO4	D	701	-	-	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	702	PO4	1	0

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, 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	487/571 (85%)	-0.25	8 (1%) 74 78	11, 26, 60, 104	0
1	B	487/571 (85%)	-0.22	11 (2%) 64 67	13, 29, 65, 96	0
1	C	487/571 (85%)	-0.05	9 (1%) 71 74	17, 38, 76, 120	0
1	D	487/571 (85%)	-0.01	21 (4%) 39 43	17, 35, 70, 130	0
All	All	1948/2284 (85%)	-0.13	49 (2%) 61 65	11, 32, 69, 130	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	194	LEU	12.6
1	C	194	LEU	9.4
1	A	194	LEU	7.9
1	C	139	VAL	7.6
1	D	139	VAL	6.8
1	B	194	LEU	6.4
1	A	186	TYR	5.3
1	D	119	PHE	4.8
1	D	144	HIS	4.8
1	C	186	TYR	4.7
1	B	186	TYR	4.6
1	D	195	GLY	4.4
1	C	119	PHE	4.2
1	C	144	HIS	4.1
1	D	120	MET	3.9
1	A	139	VAL	3.8
1	A	171	GLY	3.7
1	D	186	TYR	3.7
1	D	172	ILE	3.5
1	B	144	HIS	3.4
1	D	116	ILE	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	171	GLY	3.0
1	C	146	ILE	2.8
1	D	198	GLU	2.8
1	D	160	ILE	2.8
1	B	139	VAL	2.7
1	D	395	ILE	2.7
1	D	185	ALA	2.7
1	B	146	ILE	2.7
1	B	332	ALA	2.6
1	A	119	PHE	2.6
1	A	144	HIS	2.5
1	A	332	ALA	2.5
1	B	119	PHE	2.5
1	A	116	ILE	2.4
1	D	184	LEU	2.4
1	D	197	PHE	2.4
1	D	318	LYS	2.4
1	C	160	ILE	2.3
1	B	158	GLU	2.3
1	B	171	GLY	2.2
1	D	581	GLU	2.1
1	C	333	GLN	2.1
1	B	449	THR	2.1
1	D	333	GLN	2.0
1	C	159	LYS	2.0
1	D	436	VAL	2.0
1	D	346	SER	2.0
1	B	451	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	702	5/5	0.96	0.18	4.62	71,75,81,82	0
2	PO4	B	702	5/5	0.96	0.14	2.24	61,63,65,69	0
2	PO4	A	701	5/5	0.98	0.13	0.76	21,21,26,29	0
2	PO4	D	701	5/5	0.99	0.11	-0.11	25,33,35,38	0
2	PO4	C	701	5/5	0.99	0.10	-0.35	24,33,37,45	0
2	PO4	B	701	5/5	0.99	0.08	-1.19	25,28,31,35	0

6.5 Other polymers (i)

There are no such residues in this entry.