



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 06:09 AM UTC

PDB ID : 5C16 / pdb_00005c16
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

<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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

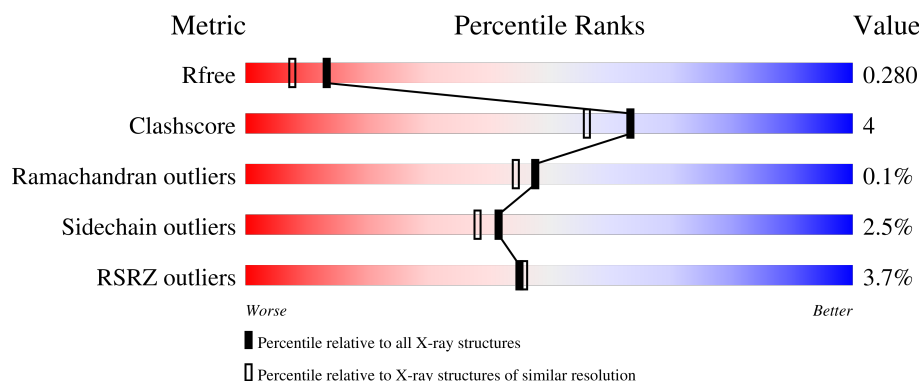
1 Overall quality at a glance

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}	180053	3774 (2.08-2.04)
Clashscore	190562	3883 (2.08-2.04)
Ramachandran outliers	187476	3860 (2.08-2.04)
Sidechain outliers	187428	3860 (2.08-2.04)
RSRZ outliers	180081	3775 (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 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	571	
1	B	571	
1	C	571	
1	D	571	

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 (CCD ID: PO4) (formula: O₄P).



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

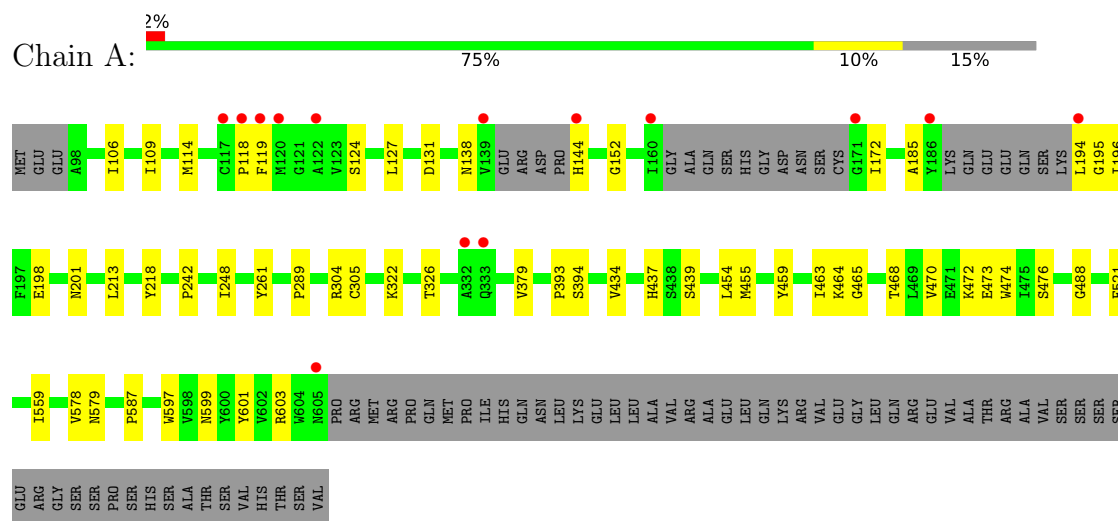
- Molecule 3 is water.

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

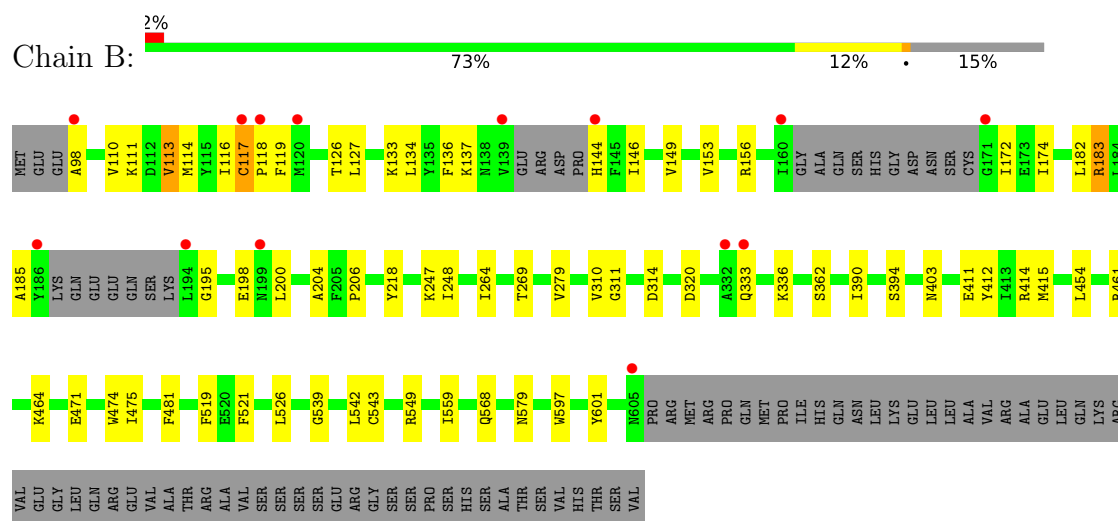
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

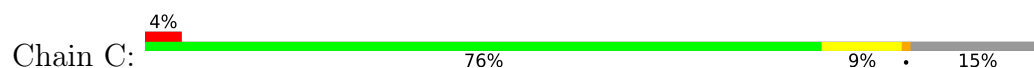
• Molecule 1: Myotubularin-related protein 1

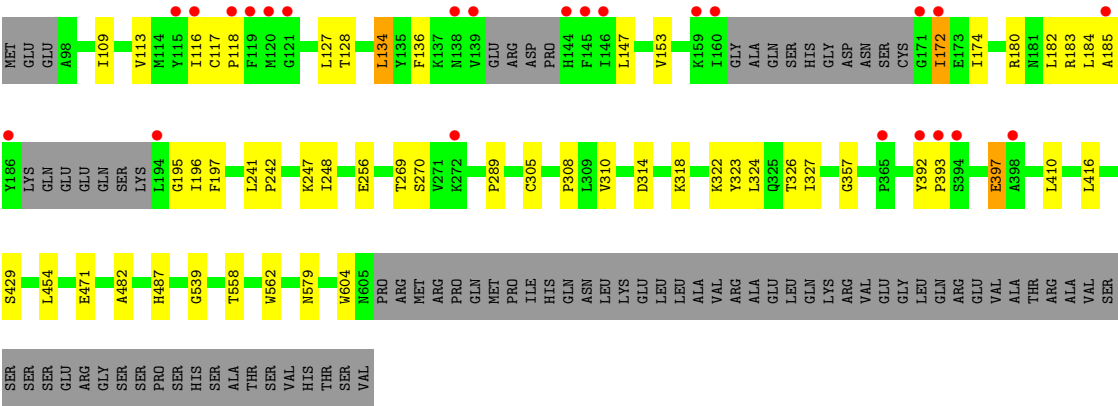


• Molecule 1: Myotubularin-related protein 1

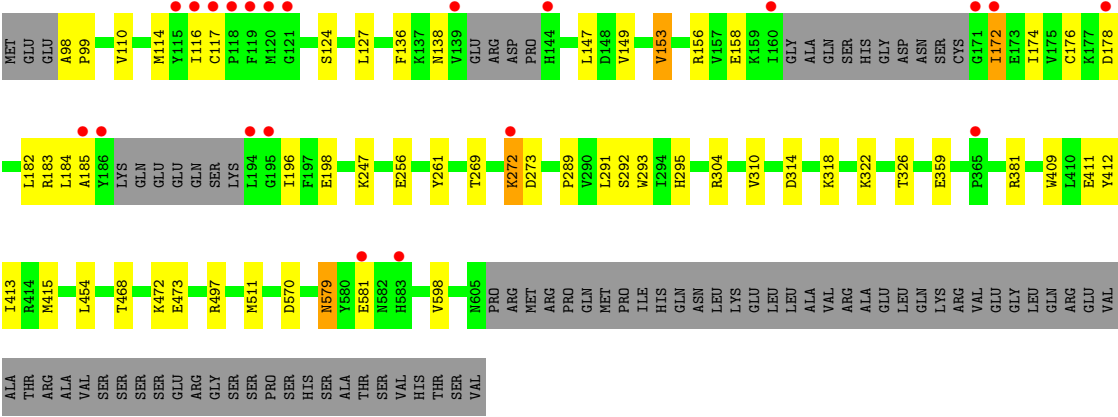
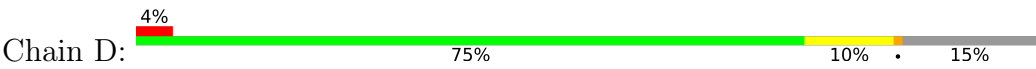


• Molecule 1: Myotubularin-related protein 1





• Molecule 1: Myotubularin-related protein 1



4 Data and refinement statistics

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 34.81 – 2.07	Depositor EDS
% Data completeness (in resolution range)	85.8 (34.81-2.07) 86.1 (34.81-2.07)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.96 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.220 , 0.274 0.228 , 0.280	Depositor DCC
R_{free} test set	6803 reflections (4.19%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 51.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	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.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.56	0/4059	0.82	0/5503
1	B	0.55	0/4059	0.80	5/5503 (0.1%)
1	C	0.46	0/4059	0.76	0/5503
1	D	0.47	0/4059	0.78	2/5503 (0.0%)
All	All	0.51	0/16236	0.79	7/22012 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ALA	CA-C-N	5.74	125.67	119.76
1	B	98	ALA	C-N-CA	5.74	125.67	119.76
1	B	311	GLY	CA-C-N	5.38	125.04	119.56
1	B	311	GLY	C-N-CA	5.38	125.04	119.56
1	D	295	HIS	CA-C-N	5.13	124.92	119.28
1	D	295	HIS	C-N-CA	5.13	124.92	119.28
1	B	133	LYS	N-CA-C	5.12	116.60	108.96

There are no chirality outliers.

There are no planarity outliers.

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	3956	0	3887	26	0
1	B	3956	0	3887	42	0
1	C	3956	0	3887	28	0
1	D	3956	0	3887	31	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
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	127	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 (127) 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:B:411:GLU:HG3	1:B:415:MET:HE2	1.77	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:D:454:LEU:HD23	1:D:511:MET:HE1	1.80	0.62
1:A:579:ASN:ND2	3:A:804:HOH:O	2.33	0.62
1:C:397:GLU:H	1:C:397:GLU:CD	2.06	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:D:411:GLU:HG3	1:D:415:MET:HE2	1.86	0.58
1:B:137:LYS:HG3	1:B:146:ILE:HG12	1.86	0.58
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:412:TYR:HA	1:B:415:MET:HE3	1.93	0.50
1:B:411:GLU:CD	1:B:414:ARG:HH21	2.20	0.50
1:B:195:GLY:HA3	1:B:198:GLU:OE1	2.12	0.50
1:A:472:LYS:NZ	1:A:473:GLU:OE2	2.38	0.49
1:A:118:PRO:HB3	1:A:393:PRO:HB3	1.94	0.49
1:A:218:TYR:CD2	1:A:559:ILE:HD12	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:N	1:A:195:GLY:HA2	2.29	0.47
1:D:472:LYS:NZ	1:D:473:GLU:OE2	2.47	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:OD1	1:A:131:ASP:N	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:OE1	1:D:359:GLU:N	2.47	0.46
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:134:LEU:HB2	1:B:149:VAL:HB	2.02	0.41
1:B:204:ALA:C	1:B:206:PRO:HD3	2.46	0.41
1:A:459:TYR:O	1:A:465:GLY:HA3	2.21	0.41
1:D:247:LYS:HG2	1:D:269:THR:HA	2.03	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
1:D:412:TYR:HA	1:D:415:MET:HE3	2.02	0.41
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:455:MET:HE2	1:A:587:PRO:CG	2.52	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:241:LEU:HA	1:C:242:PRO:C	2.46	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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	479/571 (84%)	461 (96%)	17 (4%)	1 (0%)	43	38
1	D	479/571 (84%)	454 (95%)	24 (5%)	1 (0%)	43	38
All	All	1916/2284 (84%)	1840 (96%)	74 (4%)	2 (0%)	48	44

All (2) Ramachandran outliers are listed below:

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

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	435/509 (86%)	426 (98%)	9 (2%)	47	45
1	B	435/509 (86%)	424 (98%)	11 (2%)	42	38
1	C	435/509 (86%)	424 (98%)	11 (2%)	42	38
1	D	435/509 (86%)	422 (97%)	13 (3%)	36	32
All	All	1740/2036 (86%)	1696 (98%)	44 (2%)	42	38

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	144	HIS
1	A	172	ILE
1	A	201	ASN
1	A	261	TYR
1	A	379	VAL
1	A	434	VAL
1	A	454	LEU
1	A	476	SER
1	A	578	VAL
1	B	113	VAL

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Mol	Chain	Res	Type
1	B	117	CYS
1	B	144	HIS
1	B	153	VAL
1	B	172	ILE
1	B	183	ARG
1	B	333	GLN
1	B	336	LYS
1	B	362	SER
1	B	454	LEU
1	B	568	GLN
1	C	134	LEU
1	C	153	VAL
1	C	172	ILE
1	C	196	ILE
1	C	248	ILE
1	C	256	GLU
1	C	270	SER
1	C	318	LYS
1	C	397	GLU
1	C	429	SER
1	C	579	ASN
1	D	117	CYS
1	D	153	VAL
1	D	172	ILE
1	D	178	ASP
1	D	198	GLU
1	D	256	GLU
1	D	261	TYR
1	D	272	LYS
1	D	318	LYS
1	D	468	THR
1	D	570	ASP
1	D	579	ASN
1	D	598	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	203	HIS
1	A	211	GLN
1	A	344	GLN
1	A	579	ASN

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Mol	Chain	Res	Type
1	B	299	GLN
1	B	325	GLN
1	B	344	GLN
1	B	366	ASN
1	B	491	ASN
1	B	492	HIS
1	B	547	GLN
1	B	548	GLN
1	B	579	ASN
1	C	201	ASN
1	C	203	HIS
1	C	568	GLN
1	D	203	HIS
1	D	209	ASN
1	D	211	GLN
1	D	299	GLN
1	D	447	GLN
1	D	503	GLN
1	D	568	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 oligosaccharides 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	702	-	4,4,4	0.87	0	6,6,6	0.65	0
2	PO4	B	701	-	4,4,4	0.99	0	6,6,6	0.68	0
2	PO4	C	701	-	4,4,4	1.10	0	6,6,6	0.64	0
2	PO4	D	701	-	4,4,4	1.04	0	6,6,6	0.78	0
2	PO4	A	701	-	4,4,4	0.95	0	6,6,6	0.75	0
2	PO4	B	702	-	4,4,4	0.88	0	6,6,6	0.72	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 [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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/571 (85%)	-0.09	14 (2%) 53 55	11, 26, 60, 104	0
1	B	487/571 (85%)	-0.05	14 (2%) 53 55	13, 29, 65, 96	0
1	C	487/571 (85%)	0.24	24 (4%) 35 35	17, 38, 76, 120	0
1	D	487/571 (85%)	0.20	21 (4%) 40 40	17, 35, 70, 130	0
All	All	1948/2284 (85%)	0.07	73 (3%) 45 46	11, 32, 69, 130	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	194	LEU	6.6
1	A	186	TYR	6.4
1	B	186	TYR	5.9
1	D	171	GLY	5.6
1	B	139	VAL	5.5
1	A	139	VAL	5.2
1	C	194	LEU	5.0
1	C	119	PHE	4.5
1	D	186	TYR	4.4
1	A	194	LEU	4.2
1	C	139	VAL	4.0
1	D	160	ILE	3.9
1	C	186	TYR	3.8
1	B	118	PRO	3.8
1	D	139	VAL	3.7
1	C	171	GLY	3.6
1	D	116	ILE	3.5
1	D	144	HIS	3.5
1	D	195	GLY	3.5
1	B	171	GLY	3.4
1	C	120	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	121	GLY	3.3
1	A	119	PHE	3.3
1	B	194	LEU	3.2
1	C	394	SER	3.2
1	A	144	HIS	3.2
1	C	185	ALA	3.1
1	C	272	LYS	3.1
1	C	365	PRO	3.1
1	C	160	ILE	3.0
1	B	605	ASN	3.0
1	C	118	PRO	2.9
1	D	119	PHE	2.9
1	D	120	MET	2.8
1	C	144	HIS	2.8
1	C	145	PHE	2.7
1	D	185	ALA	2.7
1	A	160	ILE	2.7
1	C	116	ILE	2.7
1	D	172	ILE	2.7
1	A	118	PRO	2.6
1	D	118	PRO	2.6
1	A	171	GLY	2.6
1	A	120	MET	2.6
1	B	120	MET	2.6
1	A	332	ALA	2.6
1	C	121	GLY	2.5
1	B	144	HIS	2.5
1	A	122	ALA	2.5
1	A	117	CYS	2.5
1	C	393	PRO	2.5
1	C	159	LYS	2.5
1	B	332	ALA	2.4
1	B	160	ILE	2.4
1	D	583	HIS	2.4
1	C	398	ALA	2.3
1	C	138	ASN	2.3
1	D	581	GLU	2.3
1	C	115	TYR	2.3
1	C	172	ILE	2.2
1	D	272	LYS	2.2
1	D	117	CYS	2.2
1	C	392	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	333	GLN	2.2
1	C	146	ILE	2.2
1	B	333	GLN	2.2
1	B	117	CYS	2.2
1	D	178	ASP	2.2
1	D	365	PRO	2.1
1	D	115	TYR	2.1
1	A	605	ASN	2.0
1	B	98	ALA	2.0
1	B	199	ASN	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 oligosaccharides 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
2	PO4	A	702	5/5	0.85	0.17	71,75,81,82	0
2	PO4	B	702	5/5	0.86	0.15	61,63,65,69	0
2	PO4	D	701	5/5	0.97	0.05	25,33,35,38	0
2	PO4	A	701	5/5	0.98	0.06	21,21,26,29	0
2	PO4	C	701	5/5	0.98	0.06	24,33,37,45	0
2	PO4	B	701	5/5	0.98	0.09	25,28,31,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.