



Full wwPDB X-ray Structure Validation Report ⓘ

May 21, 2020 – 09:34 pm BST

PDB ID : 5YK7
Title : Crystal Structure of Mdm12-Mmm1 complex
Authors : Jeong, H.; Park, J.; Lee, C.
Deposited on : 2017-10-12
Resolution : 3.80 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

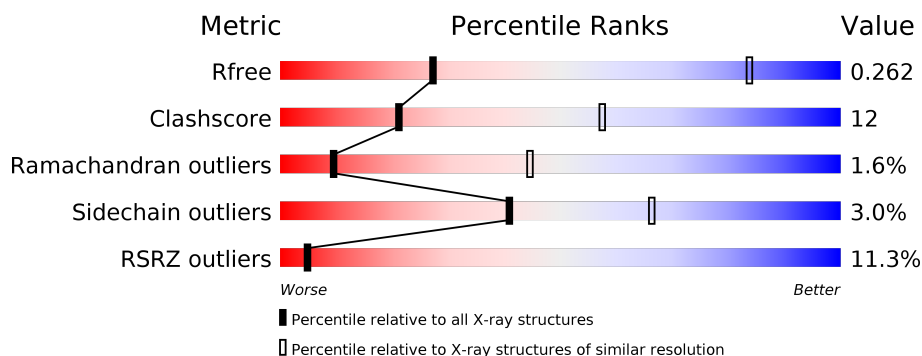
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.80 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	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

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 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	255	<div> <div>6%</div> <div>58%</div> <div>27%</div> <div>•</div> <div>13%</div> </div>
1	C	255	<div> <div>5%</div> <div>60%</div> <div>25%</div> <div>•</div> <div>14%</div> </div>
2	B	208	<div> <div>17%</div> <div>68%</div> <div>25%</div> <div>•</div> <div>5%</div> </div>
2	D	208	<div> <div>15%</div> <div>65%</div> <div>29%</div> <div>6%</div> </div>

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
3	PO4	B	301	-	-	-	X

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 6817 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 Maintenance of mitochondrial morphology protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	221	Total	C	N	O	S	0	0	0
			1817	1168	307	337	5			
1	C	220	Total	C	N	O	S	0	0	0
			1810	1164	306	335	5			

- Molecule 2 is a protein called Mitochondrial distribution and morphology protein 12.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	197	Total	C	N	O	S	0	0	0
			1583	1021	252	304	6			
2	D	196	Total	C	N	O	S	0	0	0
			1577	1018	251	302	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	110	GLY	-	linker	UNP Q92328
B	111	GLY	-	linker	UNP Q92328
B	112	SER	-	linker	UNP Q92328
B	113	GLY	-	linker	UNP Q92328
B	114	GLY	-	linker	UNP Q92328
B	183	GLY	-	linker	UNP Q92328
B	184	GLY	-	linker	UNP Q92328
D	110	GLY	-	linker	UNP Q92328
D	111	GLY	-	linker	UNP Q92328
D	112	SER	-	linker	UNP Q92328
D	113	GLY	-	linker	UNP Q92328
D	114	GLY	-	linker	UNP Q92328
D	183	GLY	-	linker	UNP Q92328
D	184	GLY	-	linker	UNP Q92328

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

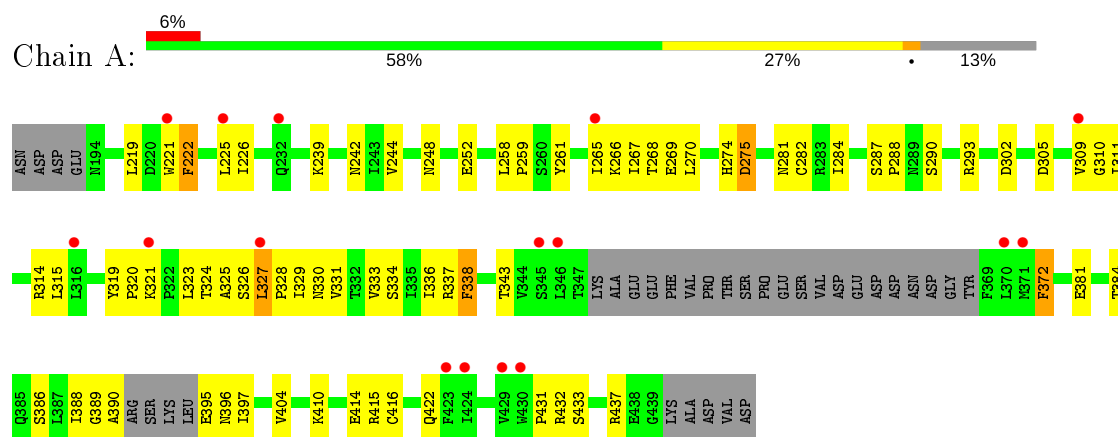


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	C	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		

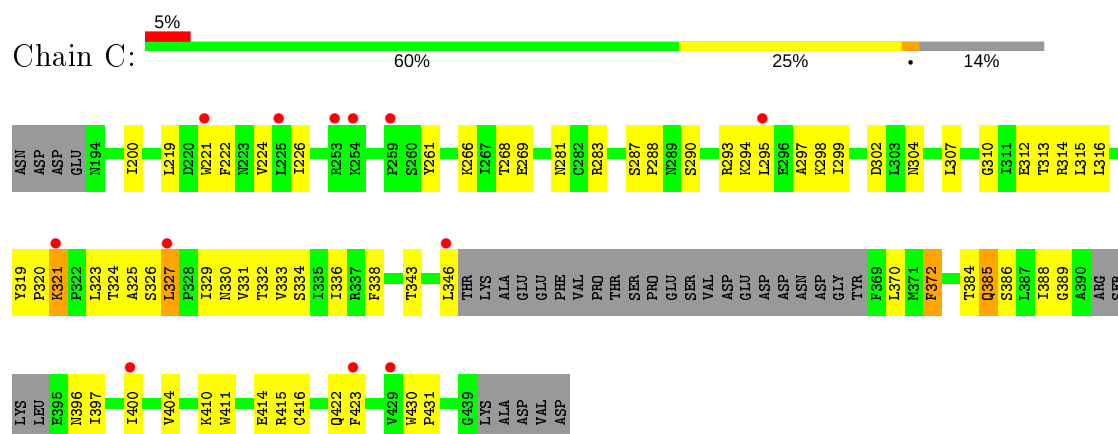
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

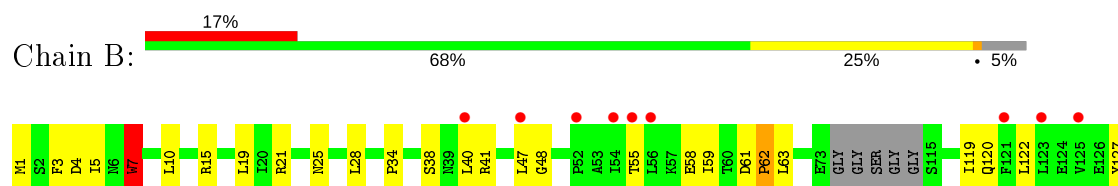
- Molecule 1: Maintenance of mitochondrial morphology protein 1

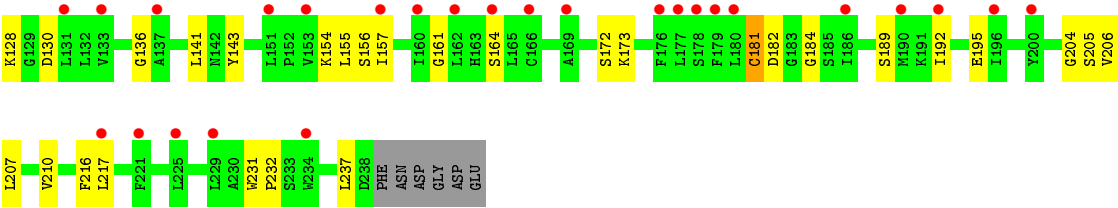


- Molecule 1: Maintenance of mitochondrial morphology protein 1

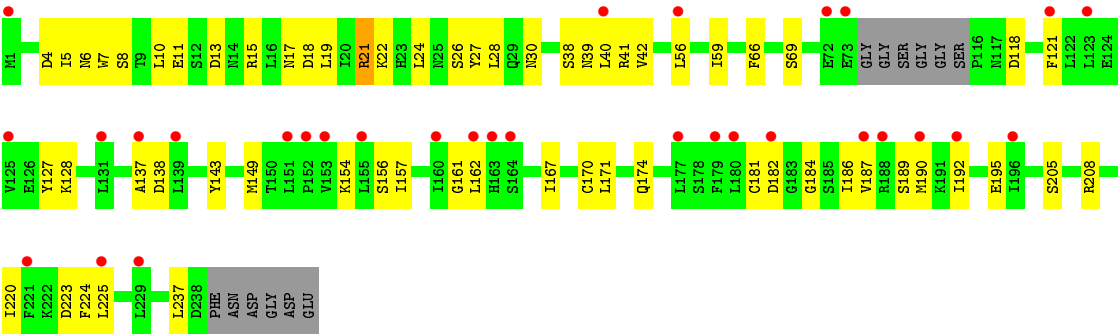


- Molecule 2: Mitochondrial distribution and morphology protein 12





● Molecule 2: Mitochondrial distribution and morphology protein 12



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	87.56 Å 87.56 Å 436.88 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.14 – 3.80 39.14 – 3.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (39.14-3.80) 99.6 (39.14-3.80)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.56 (at 3.76 Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.238 , 0.262 0.238 , 0.262	Depositor DCC
R_{free} test set	916 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	170.4	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 172.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.448 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6817	wwPDB-VP
Average B, all atoms (Å ²)	240.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.26	0/1856	0.49	0/2513
1	C	0.27	0/1849	0.49	0/2503
2	B	0.27	0/1613	0.48	0/2184
2	D	0.26	0/1607	0.47	0/2175
All	All	0.26	0/6925	0.48	0/9375

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	1817	0	1820	57	0
1	C	1810	0	1813	55	0
2	B	1583	0	1585	35	0
2	D	1577	0	1581	41	0
3	A	10	0	0	1	0
3	B	5	0	0	0	0
3	C	10	0	0	1	0
3	D	5	0	0	0	0
All	All	6817	0	6799	165	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 12.

All (165) 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)
2:B:21:ARG:O	2:B:25:ASN:HB2	1.69	0.93
2:D:18:ASP:O	2:D:22:LYS:HB2	1.77	0.84
1:A:431:PRO:HB3	1:C:422:GLN:HE22	1.48	0.78
1:A:343:THR:O	1:A:372:PHE:HA	1.87	0.74
2:D:24:LEU:HB3	2:D:42:VAL:HG21	1.69	0.73
1:C:307:LEU:O	1:C:334:SER:HA	1.88	0.72
1:A:422:GLN:HE22	1:C:431:PRO:HB3	1.55	0.72
1:C:321:LYS:HG3	2:D:10:LEU:HD11	1.72	0.71
1:A:410:LYS:O	1:A:414:GLU:HB2	1.91	0.71
1:A:239:LYS:HA	1:A:242:ASN:HB2	1.71	0.70
1:C:343:THR:O	1:C:372:PHE:HA	1.91	0.70
2:D:17:ASN:O	2:D:21:ARG:HB2	1.91	0.69
1:C:315:LEU:H	1:C:326:SER:HB2	1.58	0.68
2:B:204:GLY:HA2	2:B:207:LEU:HD12	1.75	0.68
1:A:333:VAL:HG22	1:A:384:THR:HG23	1.76	0.67
2:B:58:GLU:HB2	2:B:122:LEU:HB3	1.75	0.67
2:D:26:SER:O	2:D:30:ASN:ND2	2.27	0.67
2:B:164:SER:HB2	2:B:181:CYS:HB2	1.74	0.67
2:D:143:TYR:HD1	2:D:208:ARG:HH22	1.41	0.67
1:A:325:ALA:HB2	2:B:5:ILE:HG13	1.75	0.67
2:B:154:LYS:HG3	2:B:195:GLU:HB3	1.75	0.66
2:B:61:ASP:HB3	2:B:62:PRO:HD3	1.78	0.66
2:D:156:SER:O	2:D:192:ILE:HA	1.95	0.66
1:C:269:GLU:HB3	1:C:310:GLY:HA3	1.78	0.64
1:A:416:CYS:SG	1:A:422:GLN:NE2	2.71	0.64
1:C:283:ARG:O	1:C:297:ALA:HA	1.99	0.62
1:C:397:ILE:HG21	2:D:59:ILE:HG23	1.82	0.61
1:C:321:LYS:HD2	2:D:10:LEU:HD21	1.83	0.61
1:C:333:VAL:HG22	1:C:384:THR:HG23	1.82	0.61
1:A:315:LEU:H	1:A:326:SER:HB2	1.66	0.61
2:D:154:LYS:HG3	2:D:195:GLU:HB3	1.83	0.60
1:A:324:THR:HA	2:B:5:ILE:HD11	1.84	0.60
2:D:162:LEU:HD11	2:D:186:ILE:HD12	1.83	0.60
1:C:416:CYS:SG	1:C:422:GLN:NE2	2.75	0.60
1:A:259:PRO:HB3	1:A:261:TYR:CZ	2.38	0.59
2:D:13:ASP:OD1	2:D:15:ARG:NH2	2.36	0.59
1:C:325:ALA:HB2	2:D:5:ILE:HG12	1.86	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:287:SER:OG	1:C:290:SER:OG	2.18	0.57
2:B:156:SER:O	2:B:192:ILE:HA	2.05	0.57
2:B:143:TYR:CG	2:B:205:SER:HB2	2.40	0.56
1:A:270:LEU:HD13	1:A:309:VAL:HG22	1.87	0.56
1:A:222:PHE:O	1:A:226:ILE:HB	2.06	0.55
1:C:290:SER:HB2	1:C:293:ARG:HD2	1.89	0.55
1:A:315:LEU:HD12	1:A:327:LEU:HD11	1.89	0.55
1:C:315:LEU:N	1:C:326:SER:HB2	2.20	0.55
1:A:314:ARG:HB3	1:A:326:SER:HB2	1.90	0.54
1:C:302:ASP:HA	1:C:338:PHE:O	2.07	0.54
1:A:248:ASN:O	1:A:252:GLU:HG3	2.08	0.54
2:D:157:ILE:HG12	2:D:192:ILE:HG12	1.90	0.53
1:A:433:SER:HB3	1:C:415:ARG:HH21	1.73	0.53
2:D:187:VAL:HG21	2:D:225:LEU:HD12	1.91	0.52
2:B:58:GLU:HB2	2:B:122:LEU:HD23	1.91	0.52
1:C:290:SER:HB2	1:C:293:ARG:HB2	1.92	0.52
1:A:422:GLN:NE2	1:C:431:PRO:HB3	2.22	0.52
1:A:266:LYS:HE2	1:A:268:THR:HG22	1.92	0.51
1:A:320:PRO:HD3	2:B:237:LEU:HD12	1.92	0.51
1:A:275:ASP:N	1:A:305:ASP:OD2	2.38	0.51
1:A:325:ALA:HB1	2:B:4:ASP:H	1.76	0.51
1:C:314:ARG:HB3	1:C:326:SER:HB2	1.91	0.51
2:D:161:GLY:HA3	2:D:189:SER:HB2	1.93	0.51
1:A:225:LEU:HB3	1:C:346:LEU:HD12	1.93	0.51
2:D:181:CYS:HB3	2:D:186:ILE:HG22	1.91	0.51
1:C:283:ARG:HD2	1:C:298:LYS:HD3	1.93	0.51
2:D:28:LEU:HD13	2:D:40:LEU:HB3	1.93	0.50
1:A:311:ILE:HB	1:A:331:VAL:HB	1.94	0.50
1:A:269:GLU:O	1:A:310:GLY:N	2.37	0.50
1:A:415:ARG:HB3	1:A:422:GLN:HE21	1.77	0.50
1:C:313:THR:HG22	1:C:314:ARG:H	1.77	0.50
1:C:329:ILE:HG22	1:C:331:VAL:HG22	1.94	0.49
1:A:327:LEU:HD13	1:A:329:ILE:HD11	1.94	0.49
1:A:330:ASN:O	1:A:386:SER:HA	2.11	0.49
2:B:63:LEU:HG	2:B:120:GLN:HE22	1.77	0.49
1:C:324:THR:HA	2:D:5:ILE:HD11	1.95	0.49
1:A:284:ILE:HG21	1:C:224:VAL:HG11	1.95	0.49
1:A:221:TRP:CZ2	1:C:219:LEU:HD21	2.48	0.48
1:A:327:LEU:HD23	2:B:3:PHE:CE1	2.48	0.48
2:D:38:SER:HB3	2:D:138:ASP:HB2	1.95	0.48
1:A:333:VAL:HG21	1:A:404:VAL:HG11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:118:ASP:HB3	2:D:171:LEU:HA	1.94	0.48
2:B:5:ILE:HG22	2:B:7:TRP:HA	1.96	0.48
2:D:15:ARG:O	2:D:19:LEU:HB2	2.13	0.48
1:A:290:SER:HB2	1:A:293:ARG:HB2	1.95	0.48
1:A:431:PRO:HB3	1:C:422:GLN:NE2	2.22	0.48
1:C:330:ASN:O	1:C:386:SER:HA	2.12	0.48
1:A:274:HIS:N	1:A:305:ASP:OD2	2.46	0.48
1:A:395:GLU:O	1:A:397:ILE:N	2.47	0.47
1:A:415:ARG:NH2	3:A:502:PO4:O4	2.38	0.47
2:B:141:LEU:HD13	2:B:206:VAL:HA	1.95	0.47
1:C:411:TRP:HD1	1:C:415:ARG:HH11	1.62	0.47
1:A:219:LEU:HD21	1:C:221:TRP:CZ2	2.49	0.47
1:A:432:ARG:HA	3:C:501:PO4:O3	2.15	0.47
1:C:315:LEU:HD12	1:C:327:LEU:HD11	1.96	0.47
2:B:10:LEU:HD13	2:B:47:LEU:HD23	1.97	0.47
2:B:157:ILE:HG12	2:B:192:ILE:HG12	1.95	0.47
1:C:410:LYS:O	1:C:414:GLU:HB2	2.14	0.47
2:D:121:PHE:O	2:D:167:ILE:HA	2.15	0.47
2:B:155:LEU:HD22	2:B:217:LEU:HD22	1.97	0.47
2:B:41:ARG:O	2:B:136:GLY:N	2.48	0.46
1:C:312:GLU:HA	1:C:329:ILE:O	2.15	0.46
2:D:8:SER:O	2:D:11:GLU:HG2	2.15	0.46
2:B:1:MET:HB2	2:B:55:THR:HG23	1.98	0.46
2:D:27:TYR:HA	2:D:30:ASN:HD21	1.81	0.46
1:A:337:ARG:HB3	1:A:381:GLU:HG3	1.96	0.46
1:A:325:ALA:HB3	2:B:3:PHE:HD2	1.81	0.46
1:C:320:PRO:HA	1:C:321:LYS:HA	1.48	0.45
1:C:200:ILE:HG23	1:C:295:LEU:HD11	1.97	0.45
2:D:4:ASP:OD1	2:D:4:ASP:N	2.44	0.45
2:B:59:ILE:HD12	2:B:120:GLN:O	2.15	0.45
1:A:388:ILE:O	1:A:390:ALA:N	2.50	0.45
2:B:182:ASP:O	2:B:184:GLY:N	2.43	0.45
2:B:34:PRO:HD3	2:B:216:PHE:CZ	2.51	0.45
1:C:304:ASN:HA	1:C:336:ILE:O	2.16	0.45
2:B:172:SER:N	2:B:173:LYS:HA	2.32	0.44
1:C:430:TRP:CD2	1:C:431:PRO:HD2	2.52	0.44
1:C:400:ILE:O	1:C:404:VAL:HG23	2.17	0.44
2:D:39:ASN:OD1	2:D:41:ARG:HG2	2.18	0.44
1:C:329:ILE:HD13	1:C:388:ILE:HG23	2.00	0.44
1:A:437:ARG:HD2	1:C:423:PHE:HD2	1.83	0.44
2:B:63:LEU:HD23	2:B:63:LEU:HA	1.66	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ASN:O	1:C:299:ILE:HA	2.18	0.44
1:C:261:TYR:O	1:C:315:LEU:HA	2.18	0.43
1:A:265:ILE:HG23	1:A:311:ILE:HG23	2.00	0.43
2:D:220:ILE:HA	2:D:223:ASP:HB2	2.00	0.43
2:D:128:LYS:HD2	2:D:128:LYS:HA	1.82	0.43
1:A:329:ILE:HG22	1:A:331:VAL:HG22	1.99	0.43
2:D:39:ASN:O	2:D:137:ALA:HA	2.18	0.43
1:A:219:LEU:HD12	1:A:282:CYS:HB2	2.00	0.43
2:D:170:CYS:HA	2:D:174:GLN:O	2.19	0.43
1:A:261:TYR:CE1	2:B:119:ILE:HG13	2.53	0.42
1:C:370:LEU:O	1:C:423:PHE:HA	2.19	0.42
2:D:186:ILE:HG13	2:D:187:VAL:N	2.34	0.42
1:A:328:PRO:O	1:A:388:ILE:HA	2.19	0.42
1:A:415:ARG:HB3	1:A:422:GLN:NE2	2.34	0.42
1:C:321:LYS:HD3	1:C:321:LYS:HA	1.58	0.42
2:D:143:TYR:CG	2:D:205:SER:HB2	2.53	0.42
1:A:261:TYR:O	1:A:315:LEU:HA	2.19	0.42
2:D:190:MET:HE3	2:D:190:MET:HB2	1.93	0.42
2:D:27:TYR:CE2	2:D:224:PHE:HB2	2.54	0.42
1:C:314:ARG:HB3	1:C:326:SER:CB	2.48	0.42
2:D:190:MET:HG2	2:D:192:ILE:HG13	2.02	0.42
1:C:332:THR:OG1	1:C:385:GLN:HG2	2.19	0.42
2:D:181:CYS:HB3	2:D:186:ILE:CG2	2.50	0.42
2:B:48:GLY:HA3	2:B:130:ASP:O	2.20	0.42
1:C:327:LEU:HD21	2:D:56:LEU:HD22	2.02	0.42
1:A:244:VAL:HG23	1:A:270:LEU:HD23	2.01	0.41
1:C:327:LEU:HD13	1:C:329:ILE:HD11	2.01	0.41
2:B:231:TRP:CD2	2:B:232:PRO:HA	2.55	0.41
1:C:333:VAL:HG11	1:C:404:VAL:HG11	2.01	0.41
1:A:267:ILE:HA	1:A:310:GLY:O	2.20	0.41
2:D:225:LEU:HD23	2:D:225:LEU:HA	1.87	0.41
2:D:6:ASN:C	2:D:8:SER:H	2.23	0.41
1:A:305:ASP:O	1:A:336:ILE:HA	2.20	0.41
2:B:161:GLY:HA3	2:B:189:SER:HB3	2.02	0.41
1:C:266:LYS:HE2	1:C:268:THR:HG22	2.01	0.41
1:A:302:ASP:HA	1:A:338:PHE:O	2.20	0.41
2:D:66:PHE:O	2:D:69:SER:OG	2.25	0.41
1:A:320:PRO:HA	1:A:321:LYS:HA	1.77	0.41
1:C:226:ILE:HA	1:C:226:ILE:HD13	1.92	0.41
2:B:207:LEU:HA	2:B:210:VAL:HB	2.02	0.41
2:B:28:LEU:HD22	2:B:40:LEU:HD13	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:LEU:HD23	1:C:326:SER:HB3	2.03	0.41
2:B:128:LYS:HD2	2:B:128:LYS:HA	1.93	0.40
1:A:258:LEU:HG	1:A:259:PRO:HD2	2.02	0.40
1:A:287:SER:HA	1:A:288:PRO:HD3	1.98	0.40
1:C:288:PRO:C	1:C:290:SER:H	2.24	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	215/255 (84%)	195 (91%)	15 (7%)	5 (2%)	6	38
1	C	214/255 (84%)	198 (92%)	12 (6%)	4 (2%)	8	42
2	B	193/208 (93%)	174 (90%)	17 (9%)	2 (1%)	15	52
2	D	192/208 (92%)	173 (90%)	17 (9%)	2 (1%)	15	52
All	All	814/926 (88%)	740 (91%)	61 (8%)	13 (2%)	9	44

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	396	ASN
1	A	389	GLY
2	B	62	PRO
2	D	184	GLY
2	D	237	LEU
1	A	281	ASN
1	A	323	LEU
1	A	319	TYR
1	C	319	TYR
1	C	323	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	7	TRP
1	C	321	LYS
1	C	389	GLY

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	204/235 (87%)	198 (97%)	6 (3%)	42	67
1	C	203/235 (86%)	197 (97%)	6 (3%)	41	66
2	B	182/188 (97%)	176 (97%)	6 (3%)	38	65
2	D	181/188 (96%)	176 (97%)	5 (3%)	43	68
All	All	770/846 (91%)	747 (97%)	23 (3%)	41	66

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	222	PHE
1	A	275	ASP
1	A	327	LEU
1	A	334	SER
1	A	338	PHE
1	A	372	PHE
2	B	7	TRP
2	B	15	ARG
2	B	19	LEU
2	B	38	SER
2	B	127	TYR
2	B	181	CYS
1	C	222	PHE
1	C	294	LYS
1	C	327	LEU
1	C	372	PHE
1	C	385	GLN
1	C	396	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	7	TRP
2	D	21	ARG
2	D	127	TYR
2	D	149	MET
2	D	182	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	422	GLN
1	C	422	GLN
2	D	30	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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	$\# Z > 2$
3	PO4	A	502	-	4,4,4	0.93	0	6,6,6	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PO4	C	502	-	4,4,4	0.92	0	6,6,6	0.42	0
3	PO4	D	301	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	A	501	-	4,4,4	0.92	0	6,6,6	0.43	0
3	PO4	B	301	-	4,4,4	0.92	0	6,6,6	0.44	0
3	PO4	C	501	-	4,4,4	0.96	0	6,6,6	0.41	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	PO4	1	0
3	C	501	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	221/255 (86%)	0.19	16 (7%) 15 12	157, 234, 326, 394	0
1	C	220/255 (86%)	0.18	12 (5%) 25 21	158, 237, 335, 461	0
2	B	197/208 (94%)	0.59	35 (17%) 1 1	166, 227, 345, 448	0
2	D	196/208 (94%)	0.54	31 (15%) 2 2	154, 219, 332, 432	0
All	All	834/926 (90%)	0.36	94 (11%) 5 5	154, 230, 333, 461	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	345	SER	7.5
2	B	192	ILE	4.6
1	A	346	LEU	4.2
2	D	180	LEU	4.0
1	C	346	LEU	4.0
1	A	423	PHE	4.0
2	B	160	ILE	4.0
2	D	73	GLU	4.0
2	D	153	VAL	3.9
1	C	321	LYS	3.8
1	C	254	LYS	3.8
2	B	196	ILE	3.6
2	B	180	LEU	3.5
2	D	151	LEU	3.5
2	D	190	MET	3.5
2	D	196	ILE	3.5
2	B	54	ILE	3.5
2	B	234	TRP	3.4
2	B	131	LEU	3.4
2	B	177	LEU	3.4
2	B	157	ILE	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	163	HIS	3.2
2	B	229	LEU	3.2
2	D	192	ILE	3.2
1	A	225	LEU	3.2
2	B	123	LEU	3.1
2	D	179	PHE	3.1
2	B	221	PHE	3.1
2	B	178	SER	3.1
1	A	430	TRP	3.1
2	B	162	LEU	3.1
2	B	169	ALA	3.0
2	D	40	LEU	3.0
2	D	152	PRO	3.0
2	B	137	ALA	2.9
2	B	179	PHE	2.9
2	D	56	LEU	2.9
1	A	370	LEU	2.8
1	A	316	LEU	2.8
1	C	295	LEU	2.8
1	C	225	LEU	2.8
2	D	162	LEU	2.8
2	D	1	MET	2.8
2	D	160	ILE	2.8
2	B	133	VAL	2.7
2	B	121	PHE	2.7
1	C	259	PRO	2.7
2	B	166	CYS	2.7
2	D	182	ASP	2.7
2	D	125	VAL	2.6
2	D	137	ALA	2.6
2	D	221	PHE	2.6
2	B	55	THR	2.6
1	A	265	ILE	2.5
1	A	327	LEU	2.5
2	B	52	PRO	2.5
2	B	56	LEU	2.5
2	B	164	SER	2.5
2	D	155	LEU	2.5
2	D	164	SER	2.5
2	D	121	PHE	2.5
2	B	225	LEU	2.5
1	A	321	LYS	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	232	GLN	2.4
2	D	187	VAL	2.4
2	B	153	VAL	2.4
1	C	327	LEU	2.4
2	B	47	LEU	2.4
2	B	190	MET	2.3
2	B	186	ILE	2.3
2	D	139	LEU	2.3
1	C	400	ILE	2.3
2	D	177	LEU	2.3
1	A	371	MET	2.3
2	D	225	LEU	2.3
1	A	424	ILE	2.3
2	D	72	GLU	2.3
2	D	131	LEU	2.3
1	C	221	TRP	2.2
2	B	176	PHE	2.2
2	D	229	LEU	2.2
1	A	429	VAL	2.2
2	B	125	VAL	2.2
1	A	309	VAL	2.2
1	C	429	VAL	2.2
1	C	253	ARG	2.2
1	C	423	PHE	2.1
2	B	151	LEU	2.1
2	B	217	LEU	2.1
1	A	221	TRP	2.1
2	D	123	LEU	2.1
2	B	40	LEU	2.1
2	D	188	ARG	2.1
2	B	200	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

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. 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	PO4	C	501	5/5	0.55	0.15	225,230,249,284	0
3	PO4	B	301	5/5	0.60	0.40	260,267,269,275	0
3	PO4	C	502	5/5	0.64	0.20	267,288,291,293	0
3	PO4	A	501	5/5	0.71	0.27	270,275,281,281	0
3	PO4	D	301	5/5	0.72	0.35	247,262,277,293	0
3	PO4	A	502	5/5	0.78	0.18	228,232,256,267	0

6.5 Other polymers [i](#)

There are no such residues in this entry.