



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 05:28 am BST

PDB ID : 1TQD
Title : Crystal structure of IIGP1: a paradigm for interferon inducible p47 resistance GTPases
Authors : Ghosh, A.; Uthaiiah, R.; Howard, J.; Herrmann, C.; Wolf, E.
Deposited on : 2004-06-17
Resolution : 2.30 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

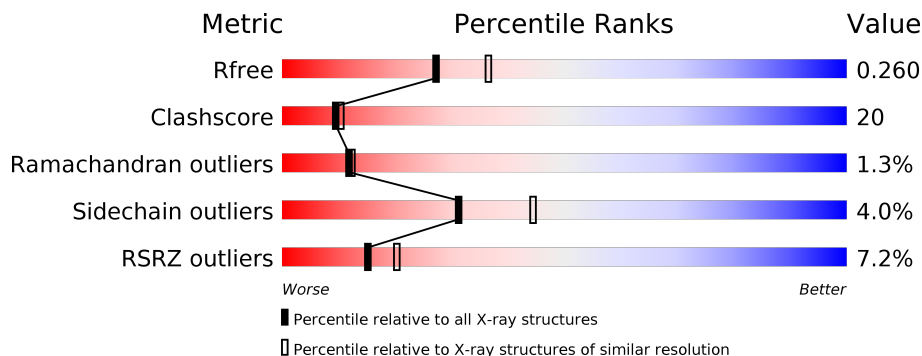
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	413	<div style="display: flex; align-items: center;"> <div style="width: 8%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 59%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 31%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">8% 59% 31% • 7%</p>
1	B	413	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 61%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 28%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: orange; margin-right: 5px;"></div> <div style="width: 8%; height: 10px; background-color: grey;"></div> </div> <p style="font-size: small; margin-top: 5px;">5% 61% 28% • 8%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6867 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 interferon-inducible GTPase.

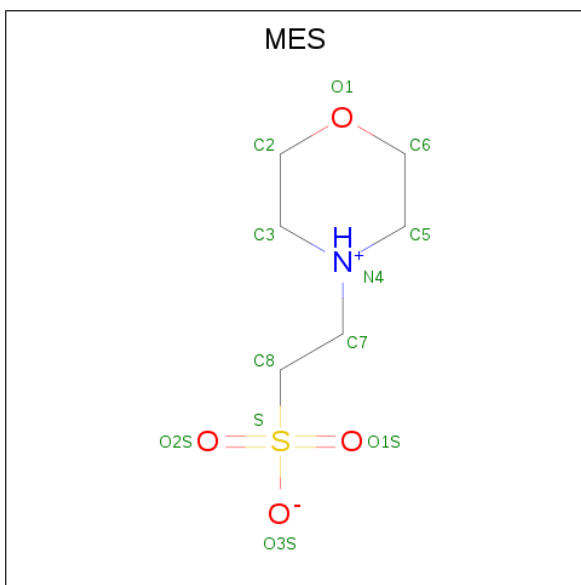
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	385	Total 3136	C 2024	N 516	O 582	S 14	0	0	0
1	B	379	Total 3100	C 1998	N 510	O 578	S 14	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	Total 5	O 4	S 1	0	0

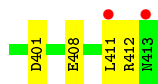
- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	B	1	12	6	1	4	1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	279	Total	O	0	0
			279	279		
4	B	335	Total	O	0	0
			335	335		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	83.07Å 93.67Å 139.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.30 24.76 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 96.0 (24.76-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.56 (at 2.31Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.258 0.215 , 0.260	Depositor DCC
R_{free} test set	8448 reflections (9.10%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtrriage
Anisotropy	0.173	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6867	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, MES

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	0.37	0/3199	0.58	0/4313
1	B	0.37	0/3159	0.59	0/4254
All	All	0.37	0/6358	0.59	0/8567

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 [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	3136	0	3175	133	0
1	B	3100	0	3137	117	0
2	B	5	0	0	1	0
3	B	12	0	13	5	0
4	A	279	0	0	16	0
4	B	335	0	0	10	0
All	All	6867	0	6325	247	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 20.

All (247) 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:51:ILE:O	1:A:51:ILE:HD13	1.75	0.87
1:A:136:PRO:HD2	1:A:139:THR:HG21	1.57	0.86
1:A:298:LEU:HD11	1:A:301:LEU:HD13	1.58	0.84
1:A:110:GLU:HB2	4:A:667:HOH:O	1.77	0.82
1:A:336:ILE:HG21	1:A:340:GLN:HB2	1.59	0.82
1:A:358:THR:HB	4:A:664:HOH:O	1.79	0.82
1:A:50:ASN:O	1:A:54:THR:HG23	1.79	0.81
1:B:92:ILE:HD11	1:B:117:PRO:HG2	1.66	0.78
1:A:306:LEU:HD22	1:A:310:LYS:HE3	1.67	0.77
1:A:127:LEU:HD22	1:A:144:MET:HE3	1.68	0.75
1:B:50:ASN:HB3	4:B:2299:HOH:O	1.86	0.75
1:B:22:GLY:HA2	1:B:25:LYS:HD3	1.67	0.74
1:A:336:ILE:CG2	1:A:340:GLN:HB2	2.17	0.74
1:A:184:LYS:HG2	1:A:232:ASN:ND2	2.03	0.73
1:B:292:VAL:HG13	1:B:294:ILE:H	1.53	0.73
1:B:298:LEU:HD21	1:B:301:LEU:HB2	1.71	0.73
1:A:92:ILE:HD11	1:A:117:PRO:HG3	1.71	0.72
1:A:108:THR:HG23	1:A:128:PRO:HB3	1.70	0.72
1:A:26:LYS:HG3	4:A:417:HOH:O	1.89	0.71
1:A:336:ILE:HB	4:A:668:HOH:O	1.91	0.70
1:A:244:MET:HG3	1:A:263:LEU:HD13	1.72	0.70
1:A:335:GLU:HG3	1:A:336:ILE:HG13	1.74	0.70
1:A:119:ILE:N	1:A:119:ILE:HD12	2.07	0.69
1:B:185:VAL:HG21	1:B:229:LEU:HB3	1.74	0.69
1:A:298:LEU:HD21	1:A:301:LEU:HB2	1.74	0.69
1:A:240:PHE:HB3	1:A:241:PRO:HD3	1.75	0.69
1:A:84:SER:O	1:A:88:THR:HG23	1.91	0.69
1:A:234:ASN:HB2	1:A:237:HIS:ND1	2.07	0.69
1:A:45:ARG:HB3	1:A:54:THR:HG22	1.74	0.68
1:B:204:LYS:HG3	1:B:207:GLN:HE21	1.58	0.68
1:B:204:LYS:HZ2	1:B:204:LYS:HB3	1.58	0.68
1:A:185:VAL:HG21	1:A:229:LEU:HB3	1.76	0.67
1:A:289:ALA:O	1:A:290:ASP:HB2	1.94	0.67
1:A:139:THR:O	1:A:143:LYS:HG2	1.95	0.67
1:B:204:LYS:HG3	1:B:207:GLN:NE2	2.09	0.67
1:A:38:ILE:HD13	4:A:535:HOH:O	1.93	0.67
1:B:202:LYS:NZ	1:B:202:LYS:HB2	2.10	0.66
1:B:139:THR:HA	4:B:2030:HOH:O	1.96	0.66
1:B:50:ASN:HA	4:B:2285:HOH:O	1.95	0.66
1:A:182:ARG:NH1	1:A:209:ILE:HG23	2.11	0.65
1:A:324:GLU:O	1:A:328:GLN:HG3	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:LEU:HD22	1:A:144:MET:CE	2.27	0.65
1:A:234:ASN:HB2	1:A:237:HIS:CE1	2.32	0.65
1:A:306:LEU:CD2	1:A:310:LYS:HE3	2.26	0.64
1:A:184:LYS:HG2	1:A:232:ASN:HD21	1.62	0.64
1:A:186:ASP:HB3	1:A:231:SER:OG	1.97	0.64
1:A:111:ARG:HD2	4:A:473:HOH:O	1.97	0.64
1:A:217:PHE:HB3	1:A:222:ILE:HG22	1.80	0.63
1:A:169:LYS:HD3	1:B:169:LYS:HD3	1.79	0.63
1:B:254:TYR:CD2	3:B:2000:MES:H52	2.33	0.63
1:B:43:GLU:OE2	1:B:47:ARG:NH1	2.31	0.63
1:B:186:ASP:HB3	1:B:231:SER:HB2	1.79	0.62
1:B:184:LYS:HG2	1:B:232:ASN:ND2	2.13	0.62
1:A:103:GLY:O	1:A:104:VAL:HB	1.98	0.62
1:A:159:ARG:HH11	1:A:212:ASN:HB3	1.64	0.62
1:B:332:ARG:HD2	1:B:333:ASP:OD1	1.99	0.62
1:B:307:GLU:HG3	1:B:311:LYS:HE2	1.80	0.62
1:B:329:ARG:NH1	1:B:329:ARG:HB2	2.15	0.62
1:A:330:LEU:HD21	1:A:334:TRP:CZ2	2.34	0.61
1:A:244:MET:HE3	1:A:247:LEU:HD12	1.82	0.61
1:B:306:LEU:HD11	1:B:359:ILE:HD13	1.82	0.61
1:B:412:ARG:HH11	1:B:412:ARG:HG2	1.65	0.61
1:B:289:ALA:O	1:B:290:ASP:HB2	2.01	0.61
1:B:158:THR:O	1:B:182:ARG:HD3	2.02	0.60
1:B:254:TYR:HD2	3:B:2000:MES:H52	1.67	0.60
1:B:344:MET:CE	1:B:408:GLU:HG3	2.32	0.60
1:A:100:ALA:HA	1:A:114:TYR:CE2	2.36	0.59
1:B:129:GLY:C	1:B:130:ILE:HD12	2.23	0.59
1:B:87:ASN:HB3	1:B:92:ILE:O	2.02	0.59
1:B:306:LEU:HD11	1:B:359:ILE:CD1	2.32	0.59
1:A:136:PRO:HD2	1:A:139:THR:CG2	2.32	0.59
1:A:334:TRP:O	1:A:335:GLU:HB3	2.03	0.59
1:A:412:ARG:NH2	4:A:625:HOH:O	2.36	0.58
1:B:85:PHE:O	1:B:89:LEU:HD23	2.02	0.58
1:A:174:MET:HE3	1:A:176:LYS:HG3	1.84	0.58
1:A:261:VAL:HG13	1:A:319:VAL:HG22	1.84	0.58
1:B:205:VAL:O	1:B:209:ILE:HG13	2.04	0.58
1:B:367:ILE:CG1	1:B:390:LEU:HD13	2.34	0.58
1:A:118:ASN:HB2	1:A:119:ILE:HD12	1.85	0.58
1:A:210:ARG:O	1:A:214:VAL:HG23	2.04	0.57
1:A:174:MET:CE	1:A:176:LYS:HG3	2.34	0.57
1:A:83:SER:OG	1:A:102:THR:HA	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ARG:O	1:B:285:GLU:HG3	2.04	0.56
1:B:324:GLU:HG2	4:B:2200:HOH:O	2.05	0.56
1:B:230:LEU:HD13	1:B:240:PHE:CE2	2.40	0.56
1:A:45:ARG:CB	1:A:54:THR:HG22	2.35	0.56
1:A:335:GLU:O	1:A:336:ILE:HB	2.06	0.55
1:B:82:LYS:NZ	1:B:127:LEU:O	2.37	0.55
1:B:16:LEU:HD21	1:B:291:LEU:HD12	1.88	0.55
1:A:295:ILE:O	1:A:295:ILE:HD12	2.07	0.54
1:A:45:ARG:HD3	1:A:53:LEU:HB3	1.89	0.54
1:A:242:VAL:HG13	4:A:608:HOH:O	2.07	0.54
1:B:338:VAL:HG23	1:B:339:ASP:N	2.21	0.54
1:B:230:LEU:HD22	1:B:240:PHE:CD2	2.42	0.54
1:A:159:ARG:NH1	1:A:212:ASN:HB3	2.23	0.53
1:B:317:ARG:NH1	1:B:348:PRO:HG3	2.24	0.53
1:B:367:ILE:HG13	1:B:390:LEU:HD13	1.90	0.53
1:B:26:LYS:O	1:B:26:LYS:HG2	2.08	0.53
1:A:360:GLN:HB2	4:A:665:HOH:O	2.09	0.53
1:B:206:LEU:N	1:B:206:LEU:HD12	2.24	0.53
1:A:167:ILE:O	1:A:171:ILE:HG13	2.09	0.52
1:B:202:LYS:HZ2	1:B:202:LYS:HB2	1.72	0.52
1:A:169:LYS:O	1:A:173:MET:HG2	2.09	0.52
1:B:337:GLU:O	1:B:340:GLN:HB2	2.08	0.52
1:B:43:GLU:HG2	1:B:47:ARG:NH1	2.23	0.52
1:A:323:ASP:O	1:A:327:LEU:HG	2.09	0.52
1:A:92:ILE:HD11	1:A:117:PRO:CG	2.40	0.52
1:A:378:LEU:HB3	1:A:379:PRO:HD2	1.93	0.51
1:B:328:GLN:HG2	1:B:338:VAL:HG11	1.93	0.51
1:A:159:ARG:HD2	4:A:685:HOH:O	2.09	0.51
1:A:330:LEU:HD21	1:A:334:TRP:CH2	2.45	0.51
1:A:128:PRO:HD2	1:A:144:MET:CE	2.40	0.51
1:A:298:LEU:HA	1:A:386:GLU:OE2	2.10	0.51
1:B:234:ASN:O	1:B:237:HIS:HB2	2.11	0.51
1:B:92:ILE:HD11	1:B:117:PRO:CG	2.37	0.51
1:A:146:PHE:CD1	1:A:174:MET:SD	3.03	0.51
1:B:138:ASP:C	1:B:140:TYR:H	2.13	0.51
1:B:138:ASP:C	1:B:140:TYR:N	2.64	0.51
1:B:43:GLU:HG2	1:B:47:ARG:HH11	1.76	0.51
1:A:298:LEU:CD2	1:A:301:LEU:HB2	2.41	0.51
1:B:115:LYS:HG2	1:B:123:VAL:HG22	1.93	0.51
3:B:2000:MES:H22	4:B:2073:HOH:O	2.10	0.50
1:B:344:MET:HE2	1:B:408:GLU:HG3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:PRO:O	1:A:139:THR:HG23	2.11	0.50
1:B:304:SER:O	1:B:308:THR:HG23	2.12	0.50
1:A:336:ILE:HG23	1:A:340:GLN:CD	2.32	0.50
1:B:298:LEU:HD23	1:B:300:PHE:O	2.12	0.50
1:A:168:ALA:HB1	1:B:173:MET:HE3	1.93	0.50
1:A:49:GLY:O	1:A:51:ILE:N	2.40	0.50
1:B:130:ILE:O	4:B:2280:HOH:O	2.20	0.50
1:B:35:SER:HB3	3:B:2000:MES:H22	1.93	0.50
1:A:163:ASN:ND2	4:A:479:HOH:O	2.45	0.50
1:A:217:PHE:HE1	1:A:227:ILE:HD11	1.77	0.50
1:B:158:THR:OG1	1:B:159:ARG:N	2.43	0.50
1:A:146:PHE:CD1	1:A:147:TYR:N	2.80	0.50
1:A:289:ALA:O	1:A:290:ASP:CB	2.60	0.49
1:A:386:GLU:HG3	4:A:555:HOH:O	2.11	0.49
1:B:192:GLU:HB2	4:B:2020:HOH:O	2.12	0.49
1:A:156:SER:O	1:A:182:ARG:HD2	2.12	0.49
1:A:222:ILE:HG23	1:A:223:ALA:O	2.13	0.49
1:A:68:SER:OG	1:A:255:LYS:HG2	2.13	0.49
1:B:253:ILE:HB	3:B:2000:MES:O1	2.12	0.49
1:B:169:LYS:O	1:B:173:MET:HB2	2.13	0.49
1:B:412:ARG:HG2	1:B:412:ARG:NH1	2.28	0.49
1:B:332:ARG:NH2	1:B:333:ASP:OD1	2.46	0.48
1:A:70:LEU:HD12	1:A:150:ASP:OD2	2.12	0.48
1:A:231:SER:HB2	1:A:238:TYR:CE1	2.47	0.48
1:B:272:GLU:O	1:B:276:GLN:HG3	2.13	0.48
1:A:296:PRO:O	1:A:297:SER:C	2.51	0.48
1:A:222:ILE:HG13	1:B:173:MET:HG2	1.94	0.48
1:B:344:MET:HE1	1:B:408:GLU:HG3	1.96	0.48
1:B:387:ILE:HG22	4:B:2219:HOH:O	2.12	0.48
1:A:146:PHE:HB2	1:A:174:MET:HE1	1.96	0.48
1:B:17:PRO:HB2	1:B:47:ARG:NH1	2.29	0.48
1:B:184:LYS:HG2	1:B:232:ASN:HD22	1.79	0.47
1:A:110:GLU:HA	1:A:128:PRO:HG2	1.96	0.47
1:A:347:SER:N	1:A:348:PRO:CD	2.77	0.47
1:A:32:LYS:HE2	1:A:36:GLN:HG2	1.96	0.47
1:B:210:ARG:O	1:B:214:VAL:HG23	2.14	0.47
1:B:165:ILE:HD12	1:B:220:ASN:CB	2.45	0.47
1:B:367:ILE:HG12	1:B:390:LEU:HD13	1.96	0.47
1:A:152:PHE:CG	1:A:171:ILE:HD13	2.49	0.46
1:B:293:ASN:ND2	1:B:293:ASN:C	2.68	0.46
1:A:234:ASN:O	1:A:237:HIS:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:LYS:HE3	1:B:47:ARG:NH2	2.30	0.46
1:A:244:MET:CE	1:A:244:MET:HA	2.45	0.46
1:A:226:PRO:HD3	4:A:564:HOH:O	2.15	0.46
1:B:204:LYS:CB	1:B:204:LYS:HZ2	2.28	0.46
1:A:111:ARG:HD3	4:A:460:HOH:O	2.15	0.46
1:A:169:LYS:CE	1:A:222:ILE:HD13	2.45	0.46
1:A:345:ILE:HB	1:A:401:ASP:CG	2.36	0.46
1:B:73:ALA:HB2	1:B:149:TYR:CG	2.51	0.46
1:B:386:GLU:HG2	1:B:387:ILE:N	2.30	0.46
1:B:145:LYS:HD3	1:B:148:GLU:OE2	2.16	0.46
1:B:192:GLU:HG2	4:B:2063:HOH:O	2.15	0.45
1:A:298:LEU:HB2	1:A:367:ILE:HD12	1.98	0.45
1:B:165:ILE:HD12	1:B:220:ASN:HB2	1.98	0.45
1:B:77:GLU:OE2	1:B:161:LYS:HE2	2.17	0.45
1:A:73:ALA:HB2	1:A:149:TYR:CG	2.52	0.45
1:B:80:SER:OG	1:B:82:LYS:HG3	2.16	0.45
1:A:248:ILE:HD11	1:A:263:LEU:HD11	1.98	0.45
1:A:325:THR:HA	1:A:328:GLN:OE1	2.17	0.45
1:A:102:THR:O	1:A:104:VAL:N	2.50	0.44
1:B:234:ASN:HB3	1:B:237:HIS:CG	2.52	0.44
1:A:210:ARG:HH21	1:A:229:LEU:HG	1.82	0.44
1:A:336:ILE:HG21	1:A:340:GLN:CB	2.39	0.44
1:B:329:ARG:HH11	1:B:329:ARG:CB	2.30	0.44
1:A:413:ASN:N	1:A:413:ASN:HD22	2.14	0.44
1:A:202:LYS:HB3	4:A:676:HOH:O	2.16	0.44
1:A:334:TRP:CG	1:A:412:ARG:NH1	2.86	0.44
1:A:158:THR:OG1	1:A:159:ARG:N	2.48	0.44
1:A:223:ALA:O	1:A:225:PRO:HD3	2.17	0.44
1:B:298:LEU:CD2	1:B:301:LEU:HB2	2.44	0.44
1:A:119:ILE:CD1	1:A:119:ILE:N	2.78	0.43
1:B:186:ASP:OD2	1:B:233:LYS:HG2	2.18	0.43
1:B:338:VAL:HG23	1:B:339:ASP:H	1.84	0.43
1:A:335:GLU:HG3	1:A:336:ILE:N	2.33	0.43
1:B:90:ARG:HB3	1:B:117:PRO:HD3	1.99	0.43
1:B:167:ILE:O	1:B:171:ILE:HG13	2.18	0.43
1:B:372:LEU:C	1:B:372:LEU:HD13	2.38	0.43
1:A:205:VAL:O	1:A:205:VAL:HG12	2.17	0.43
1:A:380:LYS:O	1:A:381:ASN:HB2	2.17	0.43
1:B:372:LEU:O	1:B:372:LEU:HD13	2.18	0.43
1:A:104:VAL:CG2	4:A:640:HOH:O	2.66	0.43
1:B:307:GLU:O	1:B:311:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:27:PHE:O	1:A:32:LYS:NZ	2.52	0.43
1:A:153:ILE:HG22	1:A:155:ILE:HG13	2.01	0.43
1:B:346:LYS:HD2	4:B:2187:HOH:O	2.19	0.43
1:B:365:ARG:O	1:B:369:GLU:HG3	2.18	0.43
1:A:70:LEU:HD12	1:A:150:ASP:CG	2.39	0.42
1:A:408:GLU:O	1:A:412:ARG:HG3	2.19	0.42
1:B:411:LEU:HD13	1:B:411:LEU:C	2.40	0.42
1:A:236:CYS:HB3	1:A:266:ILE:HD12	2.02	0.42
1:A:51:ILE:O	1:A:51:ILE:CD1	2.58	0.42
1:B:323:ASP:O	1:B:327:LEU:HG	2.19	0.42
1:B:43:GLU:CG	1:B:47:ARG:NH1	2.82	0.42
1:A:182:ARG:HH11	1:A:209:ILE:HG23	1.79	0.42
1:A:337:GLU:O	1:A:338:VAL:C	2.58	0.42
1:B:203:GLU:HG2	1:B:204:LYS:HG2	2.02	0.42
1:B:203:GLU:OE1	1:B:204:LYS:HG2	2.18	0.42
1:B:230:LEU:HD22	1:B:240:PHE:CG	2.54	0.42
1:B:297:SER:OG	1:B:299:THR:HG23	2.20	0.42
1:B:359:ILE:HG23	1:B:360:GLN:N	2.34	0.42
1:B:293:ASN:HD22	1:B:293:ASN:C	2.23	0.41
1:B:155:ILE:HG23	1:B:183:THR:HG23	2.02	0.41
1:A:113:PRO:HB3	1:A:125:TRP:CZ3	2.55	0.41
1:A:240:PHE:N	1:A:241:PRO:CD	2.83	0.41
1:B:102:THR:HB	2:B:1000:SO4:O2	2.21	0.41
1:B:217:PHE:O	1:B:222:ILE:HG22	2.21	0.41
1:A:173:MET:HE3	1:A:173:MET:HA	2.02	0.41
1:A:380:LYS:NZ	1:A:380:LYS:HB2	2.36	0.41
1:B:317:ARG:HD2	1:B:322:VAL:O	2.21	0.41
1:B:316:TYR:HB3	1:B:398:VAL:HG21	2.03	0.41
1:A:298:LEU:HD21	1:A:301:LEU:CB	2.48	0.41
1:B:130:ILE:HD12	1:B:130:ILE:N	2.36	0.41
1:B:275:ARG:HH21	1:B:396:ASP:HA	1.86	0.41
1:B:345:ILE:HB	1:B:401:ASP:CG	2.42	0.41
1:A:167:ILE:HA	1:A:167:ILE:HD13	1.87	0.40
1:A:169:LYS:HE2	1:A:222:ILE:HD13	2.03	0.40
1:A:170:ALA:O	1:A:174:MET:HG2	2.21	0.40
1:B:329:ARG:NH1	1:B:329:ARG:CB	2.84	0.40
1:A:184:LYS:CG	1:A:232:ASN:HD21	2.29	0.40
1:B:275:ARG:O	1:B:279:LYS:HG3	2.21	0.40
1:B:51:ILE:CD1	1:B:51:ILE:N	2.85	0.40
1:B:51:ILE:N	1:B:51:ILE:HD12	2.36	0.40
1:A:16:LEU:HB2	1:A:17:PRO:HD3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:ILE:HG13	1:A:388:PHE:N	2.37	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	379/413 (92%)	347 (92%)	25 (7%)	7 (2%)	8	7
1	B	371/413 (90%)	347 (94%)	21 (6%)	3 (1%)	19	23
All	All	750/826 (91%)	694 (92%)	46 (6%)	10 (1%)	12	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	103	GLY
1	A	297	SER
1	A	335	GLU
1	A	336	ILE
1	A	51	ILE
1	A	290	ASP
1	B	203	GLU
1	A	109	MET
1	B	50	ASN
1	B	221	GLY

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	353/378 (93%)	340 (96%)	13 (4%)	34	48
1	B	349/378 (92%)	334 (96%)	15 (4%)	29	40
All	All	702/756 (93%)	674 (96%)	28 (4%)	31	44

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	51	ILE
1	A	101	LYS
1	A	139	THR
1	A	159	ARG
1	A	188	ASP
1	A	203	GLU
1	A	208	ASP
1	A	222	ILE
1	A	244	MET
1	A	303	ASP
1	A	390	LEU
1	A	400	GLU
1	B	26	LYS
1	B	28	ASN
1	B	50	ASN
1	B	159	ARG
1	B	182	ARG
1	B	202	LYS
1	B	237	HIS
1	B	240	PHE
1	B	251	LEU
1	B	261	VAL
1	B	292	VAL
1	B	293	ASN
1	B	298	LEU
1	B	360	GLN
1	B	390	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	220	ASN
1	A	232	ASN
1	A	258	ASN
1	A	293	ASN
1	A	413	ASN
1	B	207	GLN
1	B	232	ASN
1	B	258	ASN
1	B	293	ASN
1	B	368	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 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	MES	B	2000	-	12,12,12	1.38	3 (25%)	14,16,16	7.14	7 (50%)
2	SO4	B	1000	-	4,4,4	0.29	0	6,6,6	0.11	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
3	MES	B	2000	-	-	4/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2000	MES	C7-N4	2.75	1.53	1.47
3	B	2000	MES	C3-N4	2.41	1.53	1.46
3	B	2000	MES	C5-N4	2.07	1.52	1.46

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2000	MES	O3S-S-C8	-16.11	79.72	105.77
3	B	2000	MES	O1S-S-C8	13.35	122.99	106.92
3	B	2000	MES	O3S-S-O1S	-11.15	84.04	111.27
3	B	2000	MES	O3S-S-O2S	-9.57	87.90	111.27
3	B	2000	MES	O2S-S-C8	6.50	114.75	106.92
3	B	2000	MES	C2-C3-N4	-2.33	106.57	110.10
3	B	2000	MES	O1-C2-C3	-2.19	106.98	111.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2000	MES	C8-C7-N4-C3
3	B	2000	MES	C8-C7-N4-C5
3	B	2000	MES	C7-C8-S-O3S
3	B	2000	MES	C7-C8-S-O1S

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2000	MES	5	0
2	B	1000	SO4	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	385/413 (93%)	0.47	34 (8%) 10 13	22, 37, 62, 71	0
1	B	379/413 (91%)	0.26	21 (5%) 25 31	18, 34, 57, 66	0
All	All	764/826 (92%)	0.36	55 (7%) 15 20	18, 36, 60, 71	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	GLY	7.6
1	A	109	MET	5.7
1	B	192	GLU	4.9
1	A	336	ILE	4.7
1	B	190	THR	4.6
1	B	202	LYS	4.6
1	B	203	GLU	4.5
1	B	108	THR	4.5
1	A	411	LEU	4.4
1	A	134	ASN	4.4
1	A	108	THR	4.0
1	B	191	ASN	4.0
1	A	413	ASN	4.0
1	B	97	GLU	3.9
1	B	109	MET	3.7
1	A	202	LYS	3.6
1	B	102	THR	3.5
1	A	102	THR	3.5
1	A	233	LYS	3.4
1	A	79	GLY	3.4
1	A	207	GLN	3.4
1	A	203	GLU	3.3
1	A	187	SER	3.2
1	B	233	LYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	207	GLN	3.1
1	A	234	ASN	3.0
1	A	51	ILE	3.0
1	A	333	ASP	3.0
1	A	131	GLY	2.9
1	B	413	ASN	2.8
1	A	74	VAL	2.8
1	A	153	ILE	2.8
1	A	97	GLU	2.8
1	B	74	VAL	2.7
1	A	188	ASP	2.7
1	B	73	ALA	2.6
1	B	14	ASN	2.6
1	A	337	GLU	2.6
1	A	95	GLU	2.5
1	B	139	THR	2.4
1	A	332	ARG	2.4
1	B	300	PHE	2.4
1	A	154	ILE	2.3
1	B	411	LEU	2.3
1	A	329	ARG	2.3
1	B	189	ILE	2.3
1	A	75	THR	2.3
1	B	356	GLU	2.2
1	A	73	ALA	2.1
1	A	218	ARG	2.1
1	A	181	VAL	2.1
1	A	50	ASN	2.1
1	A	186	ASP	2.1
1	A	104	VAL	2.0
1	B	219	GLU	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. 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(\AA^2)	Q<0.9
3	MES	B	2000	12/12	0.75	0.32	39,45,62,66	0
2	SO4	B	1000	5/5	0.94	0.33	55,56,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.