



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:00 AM UTC

PDB ID : 1TQD / pdb_00001tqd
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 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

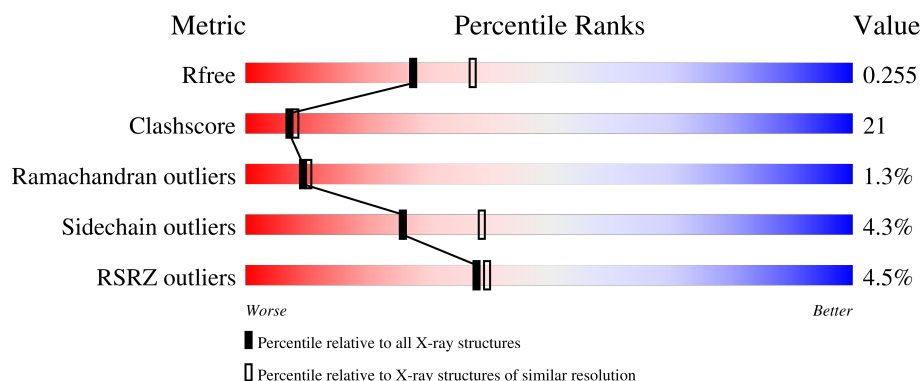
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	413	
1	B	413	

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
1	A	385	Total	C	N	O	S	0	0	0
			3136	2024	516	582	14			
1	B	379	Total	C	N	O	S	0	0	0
			3100	1998	510	578	14			

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

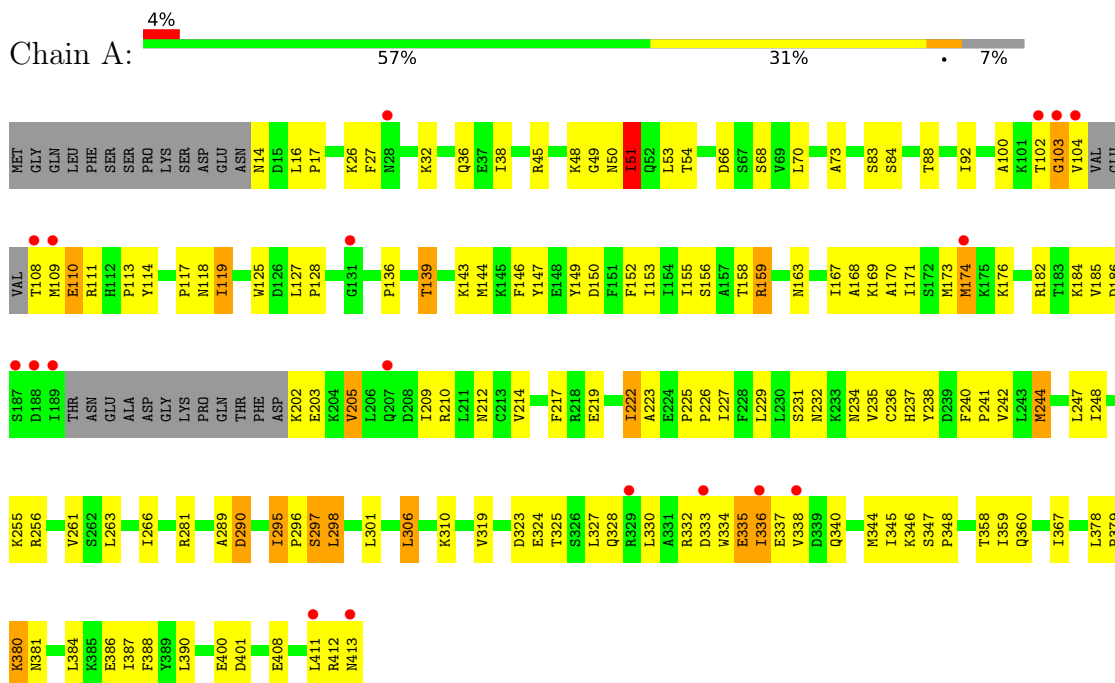
- Molecule 4 is water.

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

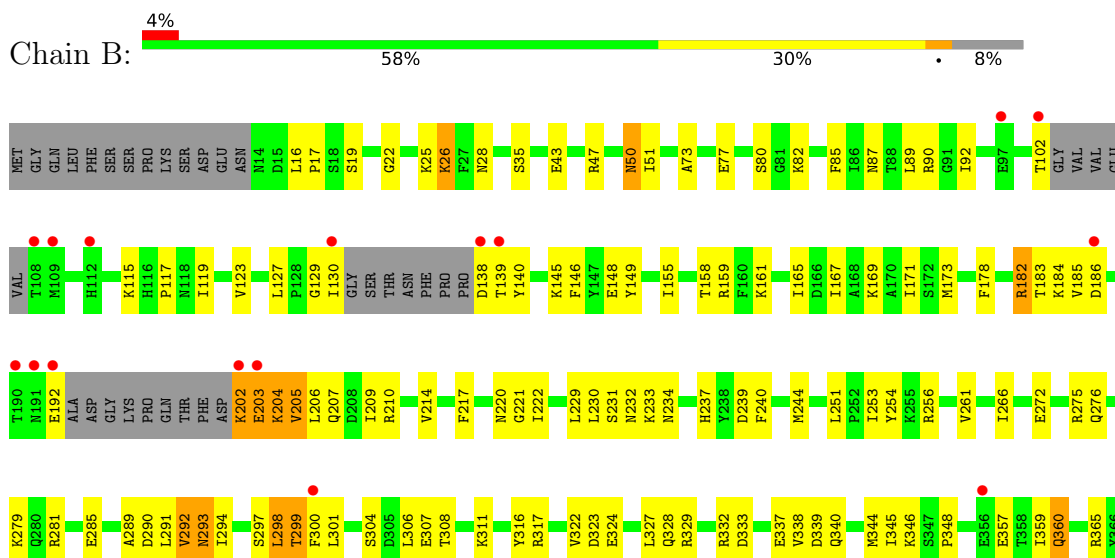
3 Residue-property plots

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: interferon-inducible GTPase



• Molecule 1: interferon-inducible GTPase



I367	Q368	E369	L372	L384	K385	E386	I387	F388	Y389	L390	D396	M397	V398	D401	E408	L411	R412	M413
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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 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.30) 95.9 (20.00-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.56 (at 2.31Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.214 , 0.258 0.211 , 0.255	Depositor DCC
R_{free} test set	8448 reflections (9.10%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.173	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 49.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
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

Xtriage'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

5.1 Standard geometry

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

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	0.41	0/3199	0.91	6/4313 (0.1%)
1	B	0.42	0/3159	0.93	10/4254 (0.2%)
All	All	0.42	0/6358	0.92	16/8567 (0.2%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	VAL	N-CA-C	-8.41	101.63	113.07
1	A	205	VAL	N-CA-C	-7.52	103.58	112.98
1	B	256	ARG	N-CA-C	7.02	118.58	111.07
1	A	384	LEU	N-CA-C	-6.97	101.13	110.55
1	B	299	THR	N-CA-C	-6.91	104.84	113.20
1	B	384	LEU	N-CA-C	-6.19	101.36	110.52
1	A	235	VAL	N-CA-C	5.91	117.36	110.62
1	A	346	LYS	N-CA-C	5.83	121.05	113.88
1	B	146	PHE	N-CA-C	5.74	118.31	111.71
1	A	110	GLU	N-CA-C	5.62	115.53	108.45
1	B	119	ILE	CA-C-N	5.53	125.89	119.47
1	B	119	ILE	C-N-CA	5.53	125.89	119.47
1	B	19	SER	N-CA-C	-5.51	105.35	111.36
1	B	389	TYR	N-CA-C	-5.43	105.52	111.82
1	A	256	ARG	N-CA-C	5.28	116.72	111.07
1	B	239	ASP	N-CA-C	5.04	119.07	113.02

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	3136	0	3175	142	0
1	B	3100	0	3137	123	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	260	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 21.

All (260) 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:174:MET:HE3	1:A:176:LYS:HG3	1.47	0.97
1:B:344:MET:HE1	1:B:408:GLU:HG3	1.56	0.88
1:A:51:ILE:HD13	1:A:51:ILE:O	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:A:146:PHE:HB2	1:A:174:MET:HE1	1.64	0.80
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	0.76
1:A:168:ALA:HB1	1:B:173:MET:HE1	1.67	0.76
1:B:50:ASN:HB3	4:B:2299:HOH:O	1.86	0.75
1:A:244:MET:HE3	1:A:244:MET:HA	1.68	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:A:168:ALA:CB	1:B:173:MET:HE1	2.18	0.73
1:B:292:VAL:HG13	1:B:294:ILE:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD12	1:A:119:ILE:N	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:84:SER:O	1:A:88:THR:HG23	1.91	0.69
1:A:240:PHE:HB3	1:A:241:PRO:HD3	1.75	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:344:MET:HE1	1:A:408:GLU:HG2	1.75	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:HB2	1:B:202:LYS:NZ	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
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:B:129:GLY:C	1:B:130:ILE:HD12	2.23	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:43:GLU:OE2	1:B:47:ARG:NH1	2.31	0.63
1:B:254:TYR:CD2	3:B:2000:MES:H52	2.33	0.63
1:B:184:LYS:HG2	1:B:232:ASN:ND2	2.13	0.62
1:B:186:ASP:HB3	1:B:231:SER:HB2	1.79	0.62
1:A:159:ARG:HH11	1:A:212:ASN:HB3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:ARG:HD2	1:B:333:ASP:OD1	1.99	0.62
1:A:103:GLY:O	1:A:104:VAL:HB	1.98	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:B:306:LEU:HD11	1:B:359:ILE:HD13	1.82	0.61
1:B:412:ARG:HG2	1:B:412:ARG:HH11	1.65	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:A:100:ALA:HA	1:A:114:TYR:CE2	2.36	0.59
1:B:87:ASN:HB3	1:B:92:ILE:O	2.02	0.59
1:B:289:ALA:O	1:B:290:ASP:HB2	2.01	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:B:244:MET:HE2	1:B:266:ILE:HD11	1.84	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: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:B:82:LYS:NZ	1:B:127:LEU:O	2.37	0.57
1:A:83:SER:OG	1:A:102:THR:HA	2.04	0.56
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:344:MET:CE	1:B:408:GLU:HG3	2.32	0.55
1:B:138:ASP:C	1:B:140:TYR:H	2.13	0.55
1:B:16:LEU:HD21	1:B:291:LEU:HD12	1.88	0.55
1:A:45:ARG:HD3	1:A:53:LEU:HB3	1.89	0.54
1:A:295:ILE:HD12	1:A:295:ILE:O	2.07	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:336:ILE:HG23	1:A:340:GLN:CD	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:367:ILE:HG13	1:B:390:LEU:HD13	1.90	0.53
1:A:296:PRO:O	1:A:297:SER:C	2.51	0.53
1:B:26:LYS:O	1:B:26:LYS:HG2	2.08	0.53
1:B:138:ASP:C	1:B:140:TYR:N	2.64	0.53
1:A:360:GLN:HB2	4:A:665:HOH:O	2.09	0.53
1:B:206:LEU:HD12	1:B:206:LEU:N	2.24	0.53
1:A:167:ILE:O	1:A:171:ILE:HG13	2.09	0.52
1:B:202:LYS:HB2	1:B:202:LYS:HZ2	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:B:293:ASN:C	1:B:293:ASN:ND2	2.68	0.51
1:A:146:PHE:CD1	1:A:174:MET:SD	3.03	0.51
1:B:244:MET:HE2	1:B:266:ILE:CD1	2.41	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:A:345:ILE:HB	1:A:401:ASP:CG	2.36	0.50
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:B:298:LEU:HD23	1:B:300:PHE:O	2.12	0.50
1:A:49:GLY:O	1:A:51:ILE:N	2.40	0.50
1:B:35:SER:HB3	3:B:2000:MES:H22	1.93	0.50
1:B:130:ILE:O	4:B:2280:HOH:O	2.20	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:SER:O	1:A:182:ARG:HD2	2.12	0.49
1:A:68:SER:OG	1:A:255:LYS:HG2	2.13	0.49
1:A:222:ILE:HG23	1:A:223:ALA:O	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:168:ALA:HB3	1:B:173:MET:HE1	1.95	0.48
1:A:222:ILE:HG13	1:B:173:MET:HG2	1.94	0.48
1:B:387:ILE:HG22	4:B:2219:HOH:O	2.12	0.48
1:B:372:LEU:C	1:B:372:LEU:HD13	2.38	0.48
1:B:158:THR:OG1	1:B:159:ARG:N	2.43	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:411:LEU:C	1:B:411:LEU:HD13	2.40	0.47
1:A:70:LEU:HD12	1:A:150:ASP:CG	2.39	0.47
1:A:337:GLU:O	1:A:338:VAL:C	2.58	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:A:173:MET:HA	1:A:173:MET:HE3	1.97	0.46
1:A:48:LYS:HE3	1:B:47:ARG:NH2	2.30	0.46
1:A:234:ASN:O	1:A:237:HIS:HB2	2.15	0.46
1:B:293:ASN:C	1:B:293:ASN:HD22	2.23	0.46
1:A:226:PRO:HD3	4:A:564:HOH:O	2.15	0.46
1:B:204:LYS:HZ2	1:B:204:LYS:CB	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: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:B:345:ILE:HB	1:B:401:ASP:CG	2.42	0.45
1:A:298:LEU:HB2	1:A:367:ILE:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:GLU:OE2	1:B:161:LYS:HE2	2.17	0.45
1:B:165:ILE:HD12	1:B:220:ASN:HB2	1.98	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:178:PHE:C	1:B:178:PHE:CD1	2.95	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:CB	1:B:329:ARG:HH11	2.30	0.44
1:B:357:GLU:CD	1:B:365:ARG:HH21	2.25	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:174:MET:HE3	1:A:176:LYS:CG	2.31	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:N	1:A:119:ILE:CD1	2.78	0.43
1:A:146:PHE:CD1	1:A:146:PHE:C	2.96	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:A:205:VAL:HG12	1:A:205:VAL:O	2.17	0.43
1:B:372:LEU:HD13	1:B:372:LEU:O	2.18	0.43
1:A:104:VAL:CG2	4:A:640:HOH:O	2.66	0.43
1:A:380:LYS:O	1:A:381:ASN:HB2	2.17	0.43
1:B:307:GLU:O	1:B:311:LYS:HG3	2.18	0.43
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:336:ILE:CG2	1:A:340:GLN:CD	2.92	0.42
1:A:408:GLU:O	1:A:412:ARG:HG3	2.19	0.42
1:A:174:MET:CE	1:A:176:LYS:HG3	2.34	0.42
1:A:51:ILE:O	1:A:51:ILE:CD1	2.58	0.42
1:A:236:CYS:HB3	1:A:266:ILE:HD12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ASP:O	1:B:327:LEU:HG	2.19	0.42
1:A:66:ASP:CG	1:A:281:ARG:HH21	2.28	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: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:A:411:LEU:HD13	1:A:411:LEU:C	2.45	0.41
1:B:203:GLU:CD	1:B:204:LYS:HG2	2.45	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:380:LYS:HB2	1:A:380:LYS:NZ	2.36	0.41
1:B:316:TYR:HB3	1:B:398:VAL:HG21	2.03	0.41
1:B:317:ARG:HD2	1:B:322:VAL:O	2.21	0.41
1:A:244:MET:HE3	1:A:247:LEU:HD12	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:A:167:ILE:HD13	1:A:167:ILE:HA	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:A:332:ARG:O	1:A:333:ASP:C	2.64	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: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:B:275:ARG:O	1:B:279:LYS:HG3	2.21	0.40
1:A:16:LEU:HB2	1:A:17:PRO:HD3	2.02	0.40
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%)	6	6
1	B	371/413 (90%)	347 (94%)	21 (6%)	3 (1%)	16	20
All	All	750/826 (91%)	694 (92%)	46 (6%)	10 (1%)	9	10

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%)	336 (95%)	17 (5%)	23	35
1	B	349/378 (92%)	336 (96%)	13 (4%)	30	45
All	All	702/756 (93%)	672 (96%)	30 (4%)	26	39

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	51	ILE
1	A	119	ILE
1	A	139	THR
1	A	159	ARG
1	A	174	MET
1	A	203	GLU
1	A	219	GLU
1	A	222	ILE
1	A	244	MET
1	A	295	ILE
1	A	298	LEU
1	A	306	LEU
1	A	359	ILE
1	A	380	LYS
1	A	390	LEU
1	A	400	GLU
1	B	26	LYS
1	B	28	ASN
1	B	182	ARG
1	B	202	LYS
1	B	204	LYS
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	387	ILE
1	B	390	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	118	ASN
1	A	232	ASN
1	A	258	ASN
1	A	381	ASN
1	A	413	ASN
1	B	191	ASN

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Mol	Chain	Res	Type
1	B	207	GLN
1	B	212	ASN
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 oligosaccharides 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	1.41	3 (25%)	15,16,16	6.06	7 (46%)
2	SO4	B	1000	-	4,4,4	0.39	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	2.78	1.53	1.47
3	B	2000	MES	C3-N4	2.47	1.53	1.46
3	B	2000	MES	C5-N4	2.12	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	-13.44	79.72	106.00
3	B	2000	MES	O3S-S-O1S	-10.94	84.04	111.40
3	B	2000	MES	O1S-S-C8	10.76	122.99	106.73
3	B	2000	MES	O3S-S-O2S	-9.39	87.90	111.40
3	B	2000	MES	O2S-S-C8	5.31	114.75	106.73
3	B	2000	MES	C2-C3-N4	-2.34	106.57	110.12
3	B	2000	MES	O1-C2-C3	-2.22	106.98	111.77

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 ⓘ

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, 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%)	0.34	18 (4%) 36 38	22, 37, 62, 71	0
1	B	379/413 (91%)	0.17	16 (4%) 40 42	18, 34, 57, 66	0
All	All	764/826 (92%)	0.26	34 (4%) 38 40	18, 36, 60, 71	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	103	GLY	6.4
1	B	130	ILE	4.1
1	A	102	THR	4.0
1	B	203	GLU	3.8
1	A	108	THR	3.8
1	A	338	VAL	3.6
1	A	413	ASN	3.6
1	A	188	ASP	3.4
1	A	336	ILE	3.3
1	A	411	LEU	3.3
1	B	108	THR	3.2
1	B	97	GLU	3.1
1	A	189	ILE	3.0
1	B	190	THR	3.0
1	B	102	THR	2.9
1	B	191	ASN	2.9
1	A	187	SER	2.8
1	A	174	MET	2.8
1	B	356	GLU	2.6
1	A	131	GLY	2.6
1	A	109	MET	2.5
1	B	109	MET	2.4
1	A	207	GLN	2.3
1	B	138	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	300	PHE	2.3
1	B	112	HIS	2.2
1	B	202	LYS	2.2
1	A	329	ARG	2.1
1	A	28	ASN	2.1
1	A	333	ASP	2.1
1	B	186	ASP	2.1
1	B	139	THR	2.0
1	B	192	GLU	2.0
1	A	104	VAL	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($\text{\AA}^2$)	Q<0.9
3	MES	B	2000	12/12	0.70	0.16	39,45,62,66	0
2	SO4	B	1000	5/5	0.90	0.20	55,56,58,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.