



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:27 PM GMT

PDB ID : 1TQ2
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 : 2004-06-16
Resolution : 2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

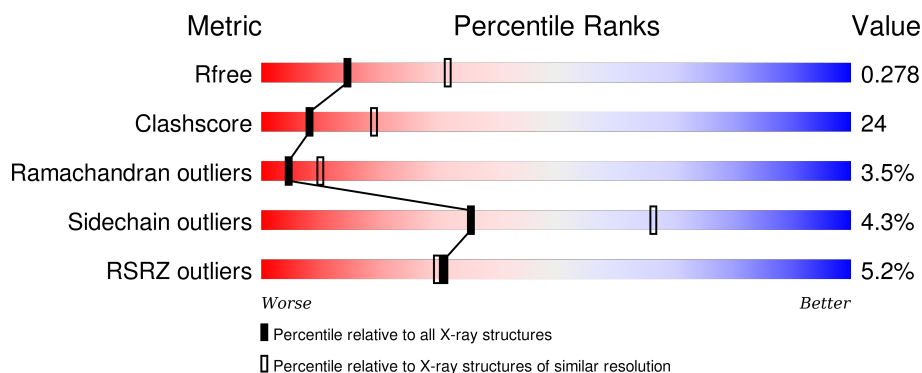
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	422	
1	B	422	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MPD	B	1000	-	-	X	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6573 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	395	Total	C	N	O	S	0	0	0
			3200	2065	524	597	14			
1	B	392	Total	C	N	O	S	0	0	0
			3181	2053	520	594	14			

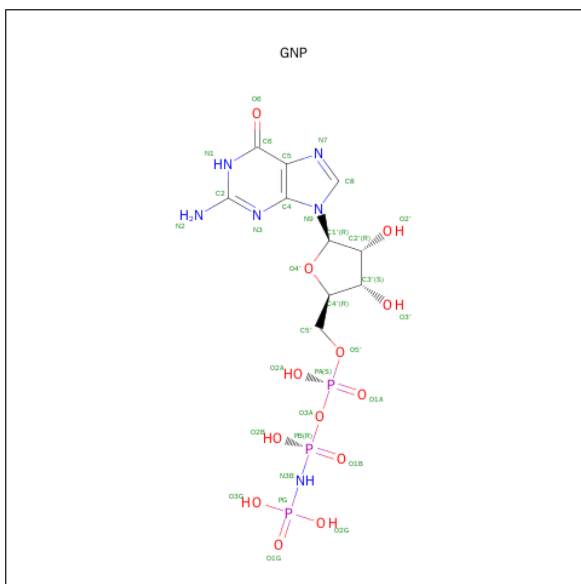
There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	412	LYS	-	CLONING ARTIFACT	UNP Q9QZ85
A	413	LEU	-	CLONING ARTIFACT	UNP Q9QZ85
A	414	GLY	-	CLONING ARTIFACT	UNP Q9QZ85
A	415	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
A	416	LEU	-	CLONING ARTIFACT	UNP Q9QZ85
A	417	GLU	-	CLONING ARTIFACT	UNP Q9QZ85
A	418	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
A	419	PRO	-	CLONING ARTIFACT	UNP Q9QZ85
A	420	HIS	-	CLONING ARTIFACT	UNP Q9QZ85
A	421	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
A	422	ASP	-	CLONING ARTIFACT	UNP Q9QZ85
B	412	LYS	-	CLONING ARTIFACT	UNP Q9QZ85
B	413	LEU	-	CLONING ARTIFACT	UNP Q9QZ85
B	414	GLY	-	CLONING ARTIFACT	UNP Q9QZ85
B	415	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
B	416	LEU	-	CLONING ARTIFACT	UNP Q9QZ85
B	417	GLU	-	CLONING ARTIFACT	UNP Q9QZ85
B	418	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
B	419	PRO	-	CLONING ARTIFACT	UNP Q9QZ85
B	420	HIS	-	CLONING ARTIFACT	UNP Q9QZ85
B	421	ARG	-	CLONING ARTIFACT	UNP Q9QZ85
B	422	ASP	-	CLONING ARTIFACT	UNP Q9QZ85

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Mg 1 1	0	0

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{13}\text{P}_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 32	C 10	N 6	O 13	P 3	0	0
3	B	1	Total 32	C 10	N 6	O 13	P 3	0	0

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $\text{C}_6\text{H}_{14}\text{O}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			8	6	2		

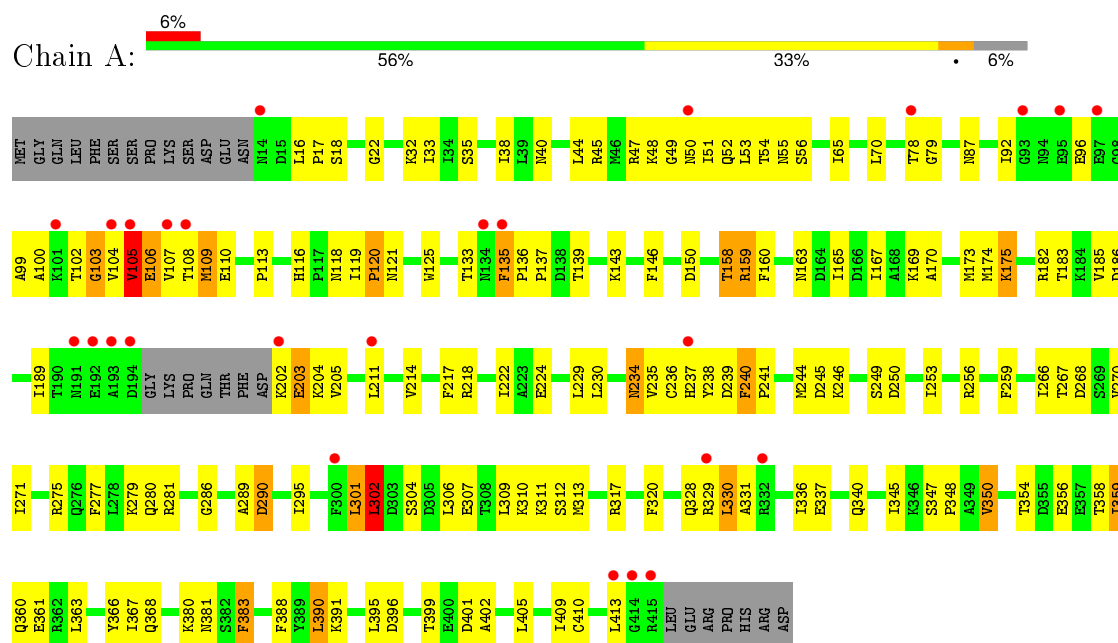
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	50	Total	O	0	0
			50	50		
5	B	69	Total	O	0	0
			69	69		

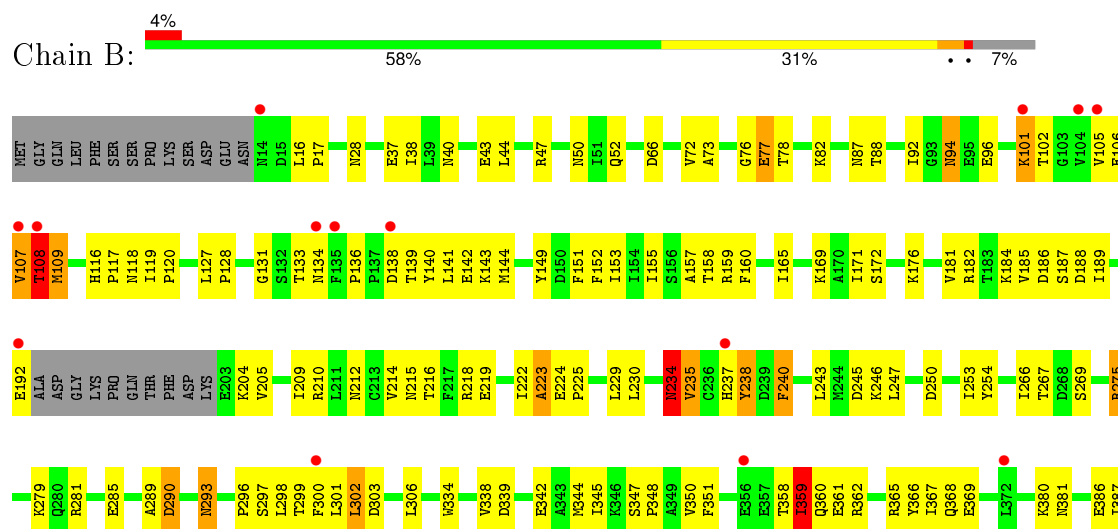
3 Residue-property plots

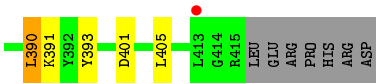
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: interferon-inducible GTPase



• Molecule 1: interferon-inducible GTPase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.86Å 92.67Å 142.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.70 19.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	93.1 (20.00-2.70) 93.4 (19.96-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.13	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.20 (at 2.71Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.222 , 0.280 0.222 , 0.278	Depositor DCC
R_{free} test set	1419 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	54.5	Xtriage
Anisotropy	0.386	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 28362 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6573	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.14% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, MPD, GNP

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	0.39	0/3264	0.61	0/4404
1	B	0.41	0/3245	0.60	0/4379
All	All	0.40	0/6509	0.60	0/8783

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	3200	0	3236	172	0
1	B	3181	0	3216	152	0
2	B	1	0	0	0	0
3	A	32	0	13	2	0
3	B	32	0	13	2	0
4	B	8	0	14	7	0
5	A	50	0	0	10	0
5	B	69	0	0	11	0
All	All	6573	0	6492	317	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 24.

All (317) 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:B:105:VAL:HG12	1:B:106:GLU:H	1.24	1.01
1:A:340:GLN:HG3	5:A:506:HOH:O	1.68	0.90
1:A:45:ARG:HD3	1:A:53:LEU:HB3	1.56	0.88
1:B:159:ARG:HB3	1:B:216:THR:HG21	1.57	0.86
1:A:87:ASN:HD21	1:A:100:ALA:H	1.27	0.82
1:A:306:LEU:HD11	1:A:310:LYS:HE3	1.61	0.82
1:B:94:ASN:HD22	1:B:102:THR:HG21	1.45	0.80
1:A:44:LEU:HD13	1:B:44:LEU:HD13	1.63	0.80
1:A:202:LYS:HG2	1:A:203:GLU:H	1.47	0.80
1:B:365:ARG:O	1:B:369:GLU:HG3	1.82	0.79
1:A:354:THR:HG22	1:A:356:GLU:H	1.47	0.78
1:B:92:ILE:HD11	1:B:117:PRO:HG3	1.63	0.78
1:A:230:LEU:HD22	1:A:240:PHE:CD1	2.18	0.78
1:B:281:ARG:HH11	1:B:281:ARG:HG2	1.50	0.77
1:A:202:LYS:HG2	1:A:203:GLU:HG2	1.67	0.77
1:B:359:ILE:O	1:B:359:ILE:HG12	1.83	0.77
5:A:511:HOH:O	1:B:138:ASP:HB3	1.86	0.76
1:A:301:LEU:O	1:A:302:LEU:HB2	1.85	0.75
1:B:298:LEU:HD11	1:B:301:LEU:HD22	1.69	0.74
1:A:359:ILE:HD13	1:A:363:LEU:HG	1.70	0.74
1:B:253:ILE:HB	4:B:1000:MPD:HM2	1.69	0.74
1:A:367:ILE:HG13	1:A:390:LEU:HD13	1.68	0.73
1:B:289:ALA:O	1:B:290:ASP:HB2	1.88	0.73
1:B:215:ASN:HD22	1:B:218:ARG:HH12	1.34	0.73
1:A:78:THR:HA	3:A:500:GNP:O1G	1.89	0.72
1:B:105:VAL:HG12	1:B:106:GLU:N	2.03	0.72
1:A:302:LEU:HD12	1:A:304:SER:H	1.53	0.72
1:A:92:ILE:HD11	1:A:99:ALA:HA	1.73	0.71
1:A:266:ILE:HG13	1:A:267:THR:N	2.07	0.70
1:A:189:ILE:HD11	1:A:202:LYS:HD3	1.74	0.69
1:B:209:ILE:HA	1:B:212:ASN:HD22	1.56	0.69
1:A:267:THR:HG22	1:A:268:ASP:N	2.08	0.69
1:A:102:THR:HB	1:A:105:VAL:HG22	1.75	0.69
1:A:358:THR:OG1	1:A:361:GLU:HG3	1.92	0.68
1:B:94:ASN:HD22	1:B:102:THR:CG2	2.07	0.68
1:B:47:ARG:HH11	1:B:47:ARG:HG3	1.57	0.68
1:A:211:LEU:HA	1:A:214:VAL:HG12	1.77	0.66
1:B:266:ILE:HG13	1:B:267:THR:HG23	1.78	0.66
1:A:202:LYS:CG	1:A:203:GLU:H	2.09	0.65
1:B:246:LYS:HE2	1:B:250:ASP:OD1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:296:PRO:HA	1:B:386:GLU:HG2	1.76	0.65
1:A:51:ILE:HA	1:A:54:THR:HG22	1.77	0.65
1:A:214:VAL:HG23	1:A:224:GLU:HG3	1.79	0.65
1:B:358:THR:OG1	1:B:361:GLU:HG3	1.97	0.65
1:B:73:ALA:HB2	1:B:149:TYR:CG	2.32	0.64
1:A:158:THR:OG1	1:A:159:ARG:N	2.31	0.64
1:B:158:THR:HA	1:B:182:ARG:HH21	1.63	0.63
1:B:105:VAL:CG1	1:B:106:GLU:H	2.07	0.63
1:A:238:TYR:O	1:A:241:PRO:HD2	1.99	0.63
1:A:106:GLU:C	1:A:108:THR:H	2.02	0.63
1:A:33:ILE:H	1:A:280:GLN:NE2	1.97	0.62
1:B:108:THR:HG23	1:B:128:PRO:HB3	1.82	0.62
1:A:202:LYS:HG2	1:A:203:GLU:N	2.14	0.62
1:A:51:ILE:HA	1:A:54:THR:CG2	2.30	0.62
1:B:350:VAL:HG23	1:B:351:PHE:CD2	2.35	0.62
1:B:92:ILE:HD11	1:B:117:PRO:CG	2.30	0.61
1:A:236:CYS:HB2	1:A:266:ILE:HD12	1.82	0.61
1:A:211:LEU:O	1:A:214:VAL:HG12	2.01	0.61
1:B:235:VAL:HB	1:B:266:ILE:HG21	1.83	0.61
1:A:51:ILE:N	1:A:51:ILE:HD12	2.16	0.61
1:B:275:ARG:O	1:B:279:LYS:HG3	2.01	0.60
1:A:169:LYS:HD3	1:B:169:LYS:HD3	1.83	0.60
1:B:386:GLU:HG3	5:B:1558:HOH:O	2.01	0.60
1:A:120:PRO:O	1:A:121:ASN:HB2	2.01	0.60
1:A:33:ILE:H	1:A:280:GLN:HE22	1.49	0.60
1:A:301:LEU:O	1:A:302:LEU:CB	2.49	0.59
1:A:313:MET:O	1:A:317:ARG:HG3	2.02	0.59
1:A:135:PHE:HD2	1:A:135:PHE:N	1.99	0.59
1:A:347:SER:HB2	1:A:401:ASP:OD2	2.02	0.59
1:A:405:LEU:O	1:A:409:ILE:HG13	2.03	0.59
1:A:70:LEU:HD12	1:A:150:ASP:OD2	2.02	0.59
1:A:186:ASP:O	1:A:189:ILE:HG22	2.01	0.59
1:B:345:ILE:HB	1:B:401:ASP:CG	2.23	0.59
1:B:16:LEU:HB2	1:B:17:PRO:HD3	1.83	0.59
1:A:189:ILE:HD11	1:A:202:LYS:CD	2.33	0.58
1:A:135:PHE:N	1:A:135:PHE:CD2	2.68	0.58
1:B:159:ARG:HB3	1:B:216:THR:CG2	2.29	0.58
1:B:254:TYR:H	4:B:1000:MPD:HM1	1.68	0.58
1:A:79:GLY:H	3:A:500:GNP:HNB3	1.49	0.58
1:A:337:GLU:O	1:A:340:GLN:HB2	2.03	0.58
1:A:70:LEU:HD22	1:A:259:PHE:HB2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LYS:HE3	1:B:127:LEU:O	2.03	0.58
1:B:223:ALA:O	1:B:225:PRO:HD3	2.04	0.58
1:B:297:SER:HB3	1:B:299:THR:HG23	1.85	0.57
1:A:306:LEU:CD1	1:A:310:LYS:HE3	2.32	0.57
1:B:159:ARG:CZ	1:B:212:ASN:HB3	2.35	0.56
1:A:53:LEU:HA	1:A:56:SER:HB3	1.86	0.56
1:B:50:ASN:HD21	1:B:52:GLN:HG2	1.69	0.56
1:B:157:ALA:HB1	1:B:184:LYS:HD2	1.88	0.56
1:A:170:ALA:O	1:A:174:MET:HG2	2.06	0.56
1:B:101:LYS:HD2	1:B:105:VAL:HG13	1.88	0.56
1:A:336:ILE:HG13	5:A:506:HOH:O	2.05	0.56
1:A:256:ARG:HB3	1:A:277:PHE:HE2	1.70	0.56
1:B:136:PRO:HB2	1:B:138:ASP:OD1	2.06	0.55
1:B:159:ARG:NH1	1:B:212:ASN:HB3	2.21	0.55
1:A:320:PHE:CZ	1:A:399:THR:HG22	2.42	0.55
1:B:101:LYS:HD2	1:B:105:VAL:CG1	2.36	0.55
1:B:281:ARG:NH1	1:B:281:ARG:HG2	2.22	0.55
1:A:116:HIS:HB3	1:A:119:ILE:O	2.07	0.55
1:A:51:ILE:H	1:A:51:ILE:HD12	1.72	0.55
1:A:281:ARG:HH11	1:A:281:ARG:HG2	1.72	0.55
1:B:165:ILE:HG23	1:B:222:ILE:HD12	1.89	0.55
1:B:188:ASP:O	1:B:205:VAL:HG11	2.06	0.54
1:B:359:ILE:O	1:B:359:ILE:CG1	2.54	0.54
1:B:298:LEU:C	1:B:300:PHE:H	2.11	0.54
1:A:104:VAL:HG22	5:A:512:HOH:O	2.06	0.54
1:A:312:SER:OG	1:A:391:LYS:HD3	2.08	0.54
1:A:350:VAL:HG13	1:A:366:TYR:HE2	1.73	0.54
1:B:38:ILE:HG13	4:B:1000:MPD:H51	1.89	0.54
1:B:359:ILE:N	5:B:1564:HOH:O	2.37	0.53
1:B:50:ASN:HB3	5:B:1508:HOH:O	2.08	0.53
1:B:78:THR:HA	3:B:1500:GNP:O1G	2.08	0.53
1:A:165:ILE:N	1:A:165:ILE:HD12	2.22	0.53
1:B:367:ILE:HG13	1:B:390:LEU:HD13	1.90	0.53
1:A:32:LYS:HA	1:A:280:GLN:HE22	1.74	0.53
1:B:185:VAL:O	1:B:189:ILE:HG12	2.07	0.53
1:A:320:PHE:CE2	1:A:399:THR:HG22	2.44	0.53
1:A:329:ARG:HH11	1:A:329:ARG:HG2	1.73	0.53
1:A:51:ILE:CA	1:A:54:THR:HG22	2.37	0.53
1:A:395:LEU:O	1:A:399:THR:HG23	2.09	0.53
1:A:267:THR:HG22	1:A:268:ASP:H	1.74	0.53
1:B:108:THR:HG22	5:B:1503:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:136:PRO:HD2	1:B:139:THR:OG1	2.09	0.52
1:A:246:LYS:HE3	1:A:250:ASP:OD1	2.10	0.52
1:A:309:LEU:HD11	1:A:390:LEU:HD23	1.92	0.52
1:A:44:LEU:CD1	1:B:44:LEU:HD13	2.36	0.52
1:A:236:CYS:CB	1:A:266:ILE:HD12	2.40	0.52
1:B:254:TYR:H	4:B:1000:MPD:CM	2.22	0.52
1:A:240:PHE:HB3	1:A:241:PRO:HD3	1.91	0.52
1:A:133:THR:HB	1:A:135:PHE:CD2	2.45	0.52
1:A:217:PHE:HB3	1:A:222:ILE:HD11	1.92	0.52
1:A:165:ILE:H	1:A:165:ILE:HD12	1.75	0.52
1:A:249:SER:HA	1:A:256:ARG:HH21	1.73	0.52
1:A:380:LYS:HG2	1:A:381:ASN:ND2	2.25	0.52
1:A:52:GLN:H	1:A:52:GLN:CD	2.12	0.52
1:B:138:ASP:CG	1:B:139:THR:N	2.64	0.51
1:A:40:ASN:O	1:A:44:LEU:HB2	2.10	0.51
1:A:183:THR:HG22	1:A:230:LEU:HD11	1.93	0.51
1:A:345:ILE:HB	1:A:401:ASP:CG	2.31	0.51
1:A:229:LEU:O	1:A:239:ASP:HB2	2.10	0.51
1:B:107:VAL:O	1:B:109:MET:HG3	2.11	0.51
1:B:298:LEU:CD1	1:B:301:LEU:HD13	2.41	0.51
1:A:48:LYS:HE2	1:B:47:ARG:CZ	2.40	0.50
1:A:240:PHE:HD2	1:A:244:MET:CE	2.23	0.50
1:A:175:LYS:O	1:A:175:LYS:HG2	2.12	0.50
1:A:359:ILE:O	1:A:359:ILE:HD13	2.11	0.50
1:A:33:ILE:HG21	1:A:280:GLN:HB3	1.94	0.50
1:A:266:ILE:HG12	1:A:270:VAL:HG21	1.94	0.50
1:B:358:THR:C	1:B:360:GLN:H	2.15	0.50
1:B:94:ASN:ND2	1:B:102:THR:CG2	2.74	0.50
1:B:88:THR:HG21	1:B:235:VAL:HG13	1.94	0.50
1:A:107:VAL:O	1:A:108:THR:HG23	2.11	0.50
1:A:281:ARG:NH1	1:A:281:ARG:HG2	2.27	0.50
1:A:202:LYS:HE2	1:A:203:GLU:OE2	2.12	0.50
1:A:183:THR:HG22	1:A:230:LEU:CD1	2.42	0.50
1:A:146:PHE:CE1	1:A:174:MET:HG3	2.47	0.50
1:A:410:CYS:O	1:A:413:LEU:HG	2.11	0.50
1:B:298:LEU:HD11	1:B:301:LEU:HD13	1.93	0.50
1:A:267:THR:CG2	1:A:268:ASP:N	2.74	0.50
1:B:134:ASN:HA	5:B:1560:HOH:O	2.11	0.50
1:A:133:THR:HA	5:A:513:HOH:O	2.10	0.49
1:B:367:ILE:CG1	1:B:390:LEU:HD13	2.42	0.49
1:A:214:VAL:O	1:A:218:ARG:HD3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:PRO:HB3	1:A:125:TRP:CZ3	2.47	0.49
1:A:45:ARG:CD	1:A:53:LEU:HB3	2.36	0.49
1:A:271:ILE:HG23	1:A:320:PHE:CD2	2.48	0.49
1:B:345:ILE:HB	1:B:401:ASP:OD1	2.13	0.49
1:A:102:THR:HB	1:A:105:VAL:CG2	2.41	0.49
1:B:238:TYR:N	1:B:238:TYR:CD2	2.80	0.49
1:A:33:ILE:HG22	1:A:280:GLN:NE2	2.28	0.49
1:B:77:GLU:HG2	1:B:78:THR:N	2.28	0.49
1:A:289:ALA:O	1:A:290:ASP:HB2	2.13	0.49
1:A:103:GLY:HA2	5:A:501:HOH:O	2.12	0.49
1:B:37:GLU:HB2	5:B:1527:HOH:O	2.13	0.49
1:A:48:LYS:HE2	1:B:47:ARG:NH2	2.28	0.48
1:A:173:MET:CE	1:B:169:LYS:HA	2.43	0.48
1:B:380:LYS:O	1:B:381:ASN:HB2	2.13	0.48
1:A:217:PHE:CD2	1:A:222:ILE:HD11	2.49	0.48
1:A:202:LYS:CG	1:A:203:GLU:N	2.73	0.48
1:B:77:GLU:HG2	1:B:78:THR:H	1.79	0.48
1:A:106:GLU:C	1:A:108:THR:N	2.63	0.48
1:B:116:HIS:HB3	1:B:119:ILE:O	2.13	0.48
1:A:136:PRO:HD2	1:A:139:THR:HB	1.95	0.48
1:B:108:THR:CG2	1:B:128:PRO:HB3	2.43	0.48
1:B:302:LEU:H	1:B:302:LEU:HD12	1.79	0.48
1:A:354:THR:HG22	1:A:356:GLU:N	2.23	0.47
1:B:301:LEU:HD21	1:B:306:LEU:HD13	1.96	0.47
1:B:222:ILE:O	1:B:223:ALA:O	2.32	0.47
1:B:138:ASP:OD2	1:B:139:THR:HG23	2.15	0.47
1:A:54:THR:HG23	1:A:55:ASN:N	2.30	0.47
1:A:165:ILE:HG22	1:A:169:LYS:HE3	1.96	0.47
1:B:141:LEU:HD12	1:B:141:LEU:C	2.35	0.47
1:B:28:ASN:HB2	5:B:1561:HOH:O	2.13	0.47
1:A:120:PRO:O	1:A:121:ASN:CB	2.63	0.47
1:A:182:ARG:HB3	1:A:229:LEU:HD23	1.96	0.47
1:B:118:ASN:O	1:B:120:PRO:HD3	2.15	0.47
1:A:106:GLU:OE1	1:A:109:MET:HA	2.15	0.46
1:A:203:GLU:C	1:A:205:VAL:H	2.18	0.46
1:B:215:ASN:HA	1:B:218:ARG:NH1	2.30	0.46
1:A:159:ARG:O	1:A:160:PHE:HB2	2.15	0.46
1:B:334:TRP:HZ3	1:B:344:MET:SD	2.38	0.46
1:B:159:ARG:O	1:B:160:PHE:C	2.53	0.46
1:B:347:SER:N	1:B:348:PRO:CD	2.79	0.46
1:A:301:LEU:HD21	1:A:306:LEU:HD23	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:TYR:HB3	4:B:1000:MPD:H32	1.97	0.46
1:A:113:PRO:HB3	1:A:125:TRP:CH2	2.51	0.46
1:B:254:TYR:HD2	4:B:1000:MPD:HM1	1.80	0.46
1:B:338:VAL:O	1:B:342:GLU:HG3	2.16	0.46
1:A:306:LEU:O	1:A:310:LYS:HG3	2.16	0.46
1:B:362:ARG:HB3	1:B:362:ARG:NH1	2.31	0.46
1:B:212:ASN:O	1:B:216:THR:HG23	2.16	0.45
1:B:215:ASN:HA	1:B:218:ARG:HH12	1.80	0.45
1:B:362:ARG:HG3	1:B:365:ARG:HH21	1.81	0.45
1:A:108:THR:C	1:A:110:GLU:H	2.20	0.45
1:B:302:LEU:HD12	1:B:302:LEU:N	2.31	0.45
1:B:210:ARG:O	1:B:214:VAL:HG23	2.16	0.45
1:B:185:VAL:HG21	1:B:229:LEU:HB3	1.98	0.45
1:B:347:SER:N	1:B:348:PRO:HD3	2.31	0.45
1:A:47:ARG:HG2	1:A:47:ARG:HH11	1.81	0.45
1:B:229:LEU:O	1:B:238:TYR:HB3	2.16	0.45
1:A:48:LYS:HE2	1:B:47:ARG:NH1	2.32	0.45
1:B:153:ILE:HG23	1:B:181:VAL:HG21	1.98	0.45
1:B:348:PRO:HB3	5:B:1544:HOH:O	2.17	0.45
1:B:234:ASN:OD1	1:B:237:HIS:CE1	2.69	0.45
1:A:367:ILE:HG13	1:A:390:LEU:CD1	2.44	0.45
1:A:214:VAL:HG22	1:A:218:ARG:HD3	1.99	0.45
1:A:301:LEU:HD21	1:A:306:LEU:HB2	1.98	0.45
1:A:133:THR:C	1:A:135:PHE:H	2.21	0.45
1:A:182:ARG:HD3	1:A:182:ARG:C	2.38	0.45
1:A:163:ASN:O	1:A:167:ILE:HG13	2.17	0.45
1:B:298:LEU:C	1:B:300:PHE:N	2.70	0.44
1:B:47:ARG:HH11	1:B:47:ARG:CG	2.22	0.44
1:B:43:GLU:CD	1:B:47:ARG:HH12	2.20	0.44
1:B:246:LYS:HE2	1:B:250:ASP:CG	2.38	0.44
1:A:240:PHE:CB	1:A:241:PRO:HD3	2.48	0.44
1:A:136:PRO:HD2	1:A:139:THR:CB	2.47	0.44
1:B:133:THR:O	1:B:134:ASN:HB2	2.17	0.44
1:B:293:ASN:HD22	1:B:293:ASN:C	2.20	0.44
1:A:87:ASN:ND2	1:A:100:ALA:H	2.04	0.44
1:A:320:PHE:HB3	1:A:402:ALA:HB2	1.99	0.44
1:B:47:ARG:NH1	1:B:47:ARG:CG	2.79	0.44
1:B:66:ASP:OD2	1:B:281:ARG:NH2	2.50	0.44
1:B:187:SER:C	1:B:189:ILE:H	2.21	0.44
1:A:234:ASN:ND2	1:A:237:HIS:CE1	2.86	0.44
1:A:92:ILE:CD1	1:A:99:ALA:HA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:50:ASN:O	1:A:54:THR:HG22	2.18	0.44
1:B:281:ARG:NH1	1:B:285:GLU:OE1	2.51	0.43
1:A:328:GLN:C	1:A:330:LEU:H	2.22	0.43
1:A:241:PRO:O	1:A:245:ASP:HB2	2.17	0.43
1:A:119:ILE:C	1:A:120:PRO:O	2.56	0.43
1:A:173:MET:HE1	1:B:172:SER:HB2	2.00	0.43
1:A:18:SER:O	1:A:22:GLY:N	2.46	0.43
1:B:176:LYS:HG2	5:B:1553:HOH:O	2.18	0.43
1:A:359:ILE:CD1	1:A:363:LEU:HG	2.44	0.43
1:B:223:ALA:C	1:B:225:PRO:HD3	2.39	0.43
1:A:345:ILE:HG13	1:A:348:PRO:CD	2.48	0.43
1:B:230:LEU:HD22	1:B:240:PHE:CD2	2.53	0.43
1:A:45:ARG:HD3	1:A:53:LEU:CB	2.39	0.43
1:A:266:ILE:CG1	1:A:267:THR:N	2.79	0.43
1:B:192:GLU:OE2	1:B:192:GLU:HA	2.18	0.43
1:A:16:LEU:HB2	1:A:17:PRO:HD3	2.00	0.43
1:B:76:GLY:N	1:B:82:LYS:HD3	2.34	0.43
1:B:72:VAL:HG13	1:B:151:PHE:CE1	2.53	0.43
1:B:152:PHE:CD1	1:B:152:PHE:N	2.85	0.43
1:B:87:ASN:HB3	1:B:92:ILE:O	2.19	0.42
1:A:396:ASP:HB3	5:A:531:HOH:O	2.19	0.42
1:A:35:SER:OG	1:A:38:ILE:HG12	2.19	0.42
1:B:40:ASN:O	1:B:44:LEU:HB2	2.19	0.42
1:B:138:ASP:CG	1:B:139:THR:H	2.22	0.42
1:A:391:LYS:HE3	5:A:527:HOH:O	2.19	0.42
1:B:101:LYS:H	1:B:101:LYS:HG2	1.59	0.42
1:B:108:THR:O	1:B:108:THR:HG22	2.18	0.42
1:A:119:ILE:CG2	5:A:502:HOH:O	2.68	0.42
1:A:70:LEU:HD23	1:A:259:PHE:CD1	2.54	0.42
1:A:234:ASN:ND2	1:A:237:HIS:ND1	2.66	0.42
1:B:405:LEU:HA	1:B:405:LEU:HD23	1.90	0.42
1:A:275:ARG:HB2	1:A:399:THR:HG21	2.00	0.42
1:B:139:THR:O	1:B:143:LYS:HG2	2.20	0.42
1:B:298:LEU:O	1:B:298:LEU:HG	2.19	0.42
1:B:215:ASN:O	1:B:219:GLU:HG2	2.19	0.42
1:A:135:PHE:CD1	1:A:143:LYS:HG3	2.54	0.42
1:A:47:ARG:HG2	1:A:47:ARG:NH1	2.34	0.42
1:A:307:GLU:O	1:A:311:LYS:HG3	2.20	0.42
1:A:234:ASN:HD22	1:A:234:ASN:HA	1.57	0.42
1:A:51:ILE:C	1:A:54:THR:HG22	2.40	0.42
1:A:175:LYS:HD3	1:A:175:LYS:C	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:293:ASN:ND2	1:B:293:ASN:C	2.73	0.42
1:A:119:ILE:HG23	5:A:502:HOH:O	2.18	0.42
1:A:33:ILE:HG12	1:A:33:ILE:O	2.20	0.42
1:A:183:THR:HA	1:A:230:LEU:O	2.19	0.41
1:B:186:ASP:OD1	3:B:1500:GNP:N1	2.41	0.41
1:B:131:GLY:HA2	5:B:1560:HOH:O	2.19	0.41
1:B:140:TYR:O	1:B:144:MET:HG2	2.20	0.41
1:B:47:ARG:NH1	1:B:47:ARG:HG3	2.31	0.41
1:A:267:THR:CG2	1:A:268:ASP:H	2.33	0.41
1:B:152:PHE:CG	1:B:171:ILE:HD13	2.55	0.41
1:A:331:ALA:HA	1:A:336:ILE:HG22	2.02	0.41
1:B:73:ALA:HB2	1:B:149:TYR:CD1	2.56	0.41
1:A:275:ARG:HD3	1:A:279:LYS:HD2	2.02	0.41
1:B:298:LEU:CD1	1:B:301:LEU:HB2	2.50	0.41
1:A:49:GLY:O	1:A:51:ILE:HD12	2.21	0.41
1:A:185:VAL:HG11	1:A:229:LEU:HB3	2.02	0.41
1:B:230:LEU:C	1:B:230:LEU:HD12	2.41	0.41
1:A:33:ILE:HG12	1:A:65:ILE:HD13	2.02	0.41
4:B:1000:MPD:H12	5:B:1562:HOH:O	2.21	0.41
1:B:222:ILE:HG22	1:B:225:PRO:HG3	2.03	0.41
1:B:158:THR:OG1	1:B:159:ARG:N	2.50	0.40
1:A:286:GLY:HA2	1:A:388:PHE:CE1	2.56	0.40
1:B:298:LEU:HD11	1:B:301:LEU:CD2	2.46	0.40
1:B:387:ILE:O	1:B:391:LYS:HG3	2.22	0.40
1:B:243:LEU:O	1:B:247:LEU:HG	2.21	0.40
1:B:82:LYS:HA	1:B:155:ILE:HD12	2.04	0.40
1:B:366:TYR:CD1	1:B:393:TYR:CE2	3.10	0.40
1:A:295:ILE:HG12	1:A:383:PHE:CZ	2.56	0.40
1:B:139:THR:HA	1:B:142:GLU:HB2	2.03	0.40
1:A:211:LEU:CA	1:A:214:VAL:HG12	2.49	0.40
1:B:108:THR:HG23	1:B:128:PRO:CB	2.47	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	391/422 (93%)	345 (88%)	31 (8%)	15 (4%)	4	9
1	B	388/422 (92%)	343 (88%)	33 (8%)	12 (3%)	5	12
All	All	779/844 (92%)	688 (88%)	64 (8%)	27 (4%)	4	10

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	GLU
1	A	203	GLU
1	A	235	VAL
1	A	302	LEU
1	B	107	VAL
1	B	223	ALA
1	A	96	GLU
1	A	105	VAL
1	A	158	THR
1	B	234	ASN
1	A	103	GLY
1	A	204	LYS
1	B	96	GLU
1	A	301	LEU
1	A	350	VAL
1	B	77	GLU
1	B	108	THR
1	B	238	TYR
1	B	302	LEU
1	A	290	ASP
1	A	120	PRO
1	B	94	ASN
1	B	204	LYS
1	B	290	ASP
1	A	253	ILE
1	B	359	ILE
1	A	137	PRO

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	359/386 (93%)	344 (96%)	15 (4%)	36	68
1	B	358/386 (93%)	342 (96%)	16 (4%)	34	65
All	All	717/772 (93%)	686 (96%)	31 (4%)	35	66

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	VAL
1	A	109	MET
1	A	118	ASN
1	A	135	PHE
1	A	159	ARG
1	A	175	LYS
1	A	234	ASN
1	A	240	PHE
1	A	302	LEU
1	A	330	LEU
1	A	359	ILE
1	A	360	GLN
1	A	368	GLN
1	A	383	PHE
1	A	390	LEU
1	B	101	LYS
1	B	108	THR
1	B	109	MET
1	B	224	GLU
1	B	234	ASN
1	B	235	VAL
1	B	240	PHE
1	B	245	ASP
1	B	269	SER
1	B	275	ARG
1	B	293	ASN
1	B	303	ASP
1	B	339	ASP
1	B	359	ILE
1	B	368	GLN
1	B	390	LEU

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

Mol	Chain	Res	Type
1	A	87	ASN
1	A	215	ASN
1	A	220	ASN
1	A	234	ASN
1	A	258	ASN
1	A	276	GLN
1	A	280	GLN
1	A	293	ASN
1	A	328	GLN
1	A	381	ASN
1	B	50	ASN
1	B	94	ASN
1	B	118	ASN
1	B	134	ASN
1	B	163	ASN
1	B	191	ASN
1	B	207	GLN
1	B	212	ASN
1	B	215	ASN
1	B	258	ASN
1	B	293	ASN
1	B	368	GLN
1	B	374	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 1 is monoatomic - leaving 3 for Mogul analysis.

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	GNP	A	500	-	28,34,34	4.16	16 (57%)	33,54,54	3.59	17 (51%)
4	MPD	B	1000	-	6,7,7	0.60	0	7,10,10	0.38	0
3	GNP	B	1500	2	28,34,34	4.13	16 (57%)	33,54,54	3.59	17 (51%)

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	GNP	A	500	-	-	0/12/38/38	0/3/3/3
4	MPD	B	1000	-	-	0/5/5/5	0/0/0/0
3	GNP	B	1500	2	-	0/12/38/38	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1500	GNP	PB-O2B	-8.40	1.33	1.56
3	A	500	GNP	PB-O2B	-8.32	1.33	1.56
3	B	1500	GNP	PG-O2G	-4.56	1.44	1.56
3	A	500	GNP	PG-O2G	-4.54	1.44	1.56
3	B	1500	GNP	C2-N2	-3.05	1.27	1.34
3	A	500	GNP	C2-N2	-2.91	1.28	1.34
3	B	1500	GNP	PB-O3A	-2.84	1.55	1.59
3	A	500	GNP	PB-O3A	-2.60	1.55	1.59
3	B	1500	GNP	C5'-C4'	-2.08	1.44	1.51
3	A	500	GNP	C2'-C3'	2.07	1.59	1.53
3	B	1500	GNP	O4'-C4'	2.26	1.50	1.45
3	A	500	GNP	C8-N7	2.34	1.39	1.34
3	B	1500	GNP	C8-N7	2.51	1.39	1.34
3	A	500	GNP	O2'-C2'	2.52	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1500	GNP	O2'-C2'	2.55	1.49	1.43
3	A	500	GNP	O4'-C4'	2.55	1.50	1.45
3	B	1500	GNP	C5-C4	2.58	1.46	1.40
3	B	1500	GNP	PB-O1B	2.66	1.49	1.46
3	A	500	GNP	C5-C4	2.69	1.46	1.40
3	A	500	GNP	PB-O1B	2.83	1.49	1.46
3	A	500	GNP	O6-C6	4.63	1.35	1.24
3	B	1500	GNP	O3'-C3'	4.68	1.54	1.43
3	A	500	GNP	O3'-C3'	4.78	1.54	1.43
3	B	1500	GNP	O6-C6	4.81	1.36	1.24
3	A	500	GNP	PB-N3B	5.31	1.77	1.63
3	B	1500	GNP	O4'-C1'	5.42	1.48	1.41
3	B	1500	GNP	PB-N3B	5.50	1.77	1.63
3	A	500	GNP	O4'-C1'	5.71	1.48	1.41
3	B	1500	GNP	C2-N1	8.91	1.51	1.35
3	A	500	GNP	C2-N1	9.08	1.51	1.35
3	B	1500	GNP	PG-O1G	11.58	1.59	1.46
3	A	500	GNP	PG-O1G	11.79	1.59	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1500	GNP	C6-C5-C4	-10.04	108.90	120.90
3	A	500	GNP	C6-C5-C4	-9.97	108.98	120.90
3	B	1500	GNP	C4-C5-N7	-8.54	101.62	109.48
3	A	500	GNP	C4-C5-N7	-8.27	101.87	109.48
3	A	500	GNP	N3-C2-N1	-6.20	117.99	127.44
3	B	1500	GNP	N3-C2-N1	-6.08	118.19	127.44
3	B	1500	GNP	O3'-C3'-C4'	-4.67	97.05	111.05
3	A	500	GNP	O3'-C3'-C4'	-4.66	97.07	111.05
3	A	500	GNP	O1G-PG-N3B	-4.55	104.92	111.90
3	B	1500	GNP	O1G-PG-N3B	-4.24	105.39	111.90
3	B	1500	GNP	O3G-PG-O1G	-3.23	104.91	113.49
3	A	500	GNP	O3G-PG-O1G	-3.22	104.92	113.49
3	B	1500	GNP	C1'-N9-C4	-2.80	122.72	126.94
3	B	1500	GNP	O3'-C3'-C2'	-2.76	102.84	111.83
3	A	500	GNP	O3'-C3'-C2'	-2.75	102.89	111.83
3	B	1500	GNP	N2-C2-N1	-2.71	112.72	117.20
3	A	500	GNP	O2G-PG-O1G	-2.71	106.30	113.49
3	A	500	GNP	N2-C2-N1	-2.69	112.75	117.20
3	A	500	GNP	C1'-N9-C4	-2.65	122.94	126.94
3	B	1500	GNP	O2G-PG-O1G	-2.52	106.80	113.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	GNP	O4'-C4'-C3'	-2.48	100.16	105.15
3	B	1500	GNP	O4'-C4'-C3'	-2.37	100.38	105.15
3	B	1500	GNP	O3G-PG-O2G	2.03	113.60	107.58
3	A	500	GNP	O3G-PG-O2G	2.17	114.02	107.58
3	A	500	GNP	O3A-PB-N3B	2.50	113.31	106.44
3	B	1500	GNP	C5-C6-N1	2.56	127.09	123.59
3	A	500	GNP	C5-C6-N1	2.62	127.16	123.59
3	B	1500	GNP	O3A-PB-N3B	2.68	113.81	106.44
3	A	500	GNP	C2'-C3'-C4'	3.85	110.52	102.61
3	B	1500	GNP	C2'-C3'-C4'	3.99	110.81	102.61
3	B	1500	GNP	N2-C2-N3	5.89	129.09	117.80
3	A	500	GNP	N2-C2-N3	5.97	129.25	117.80
3	B	1500	GNP	C4'-O4'-C1'	6.75	117.14	109.72
3	A	500	GNP	C4'-O4'-C1'	6.87	117.26	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	500	GNP	2	0
4	B	1000	MPD	7	0
3	B	1500	GNP	2	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	395/422 (93%)	0.13	26 (6%) 22 20	25, 55, 98, 109	0
1	B	392/422 (92%)	0.05	15 (3%) 44 44	27, 52, 93, 103	0
All	All	787/844 (93%)	0.09	41 (5%) 31 30	25, 53, 96, 109	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	VAL	7.0
1	A	414	GLY	5.7
1	B	108	THR	5.5
1	B	105	VAL	4.9
1	A	107	VAL	4.4
1	A	194	ASP	4.3
1	B	104	VAL	4.3
1	B	192	GLU	4.2
1	A	193	ALA	4.1
1	A	101	LYS	3.9
1	A	237	HIS	3.5
1	B	134	ASN	3.5
1	A	300	PHE	3.5
1	A	105	VAL	3.5
1	B	135	PHE	3.3
1	A	192	GLU	3.2
1	A	134	ASN	3.1
1	B	300	PHE	3.0
1	A	413	LEU	3.0
1	A	191	ASN	2.9
1	A	108	THR	2.9
1	A	50	ASN	2.7
1	B	413	LEU	2.7
1	A	415	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	14	ASN	2.6
1	A	202	LYS	2.5
1	B	101	LYS	2.5
1	A	332	ARG	2.4
1	A	97	GLU	2.3
1	B	372	LEU	2.3
1	A	329	ARG	2.3
1	A	78	THR	2.2
1	B	356	GLU	2.2
1	A	95	GLU	2.2
1	B	138	ASP	2.2
1	B	107	VAL	2.2
1	A	93	GLY	2.2
1	A	211	LEU	2.1
1	A	14	ASN	2.1
1	B	237	HIS	2.1
1	A	135	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(\AA^2)	Q<0.9
4	MPD	B	1000	8/8	0.83	0.30	8.58	66,68,72,73	0
3	GNP	A	500	32/32	0.80	0.32	0.71	109,109,114,115	32
2	MG	B	1501	1/1	0.93	0.35	-0.02	55,55,55,55	1
3	GNP	B	1500	32/32	0.90	0.21	-0.17	68,71,72,74	32

6.5 Other polymers

There are no such residues in this entry.