Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:27 PM GMT

PDB ID	:	1P16
Title	:	Structure of an mRNA capping enzyme bound to the phosphorylated carboxyl-terminal domain of RNA polymerase II
Authors	:	Fabrega, C.; Shen, V.; Shuman, S.; Lima, C.D.
Deposited on	:	2003-04-11
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

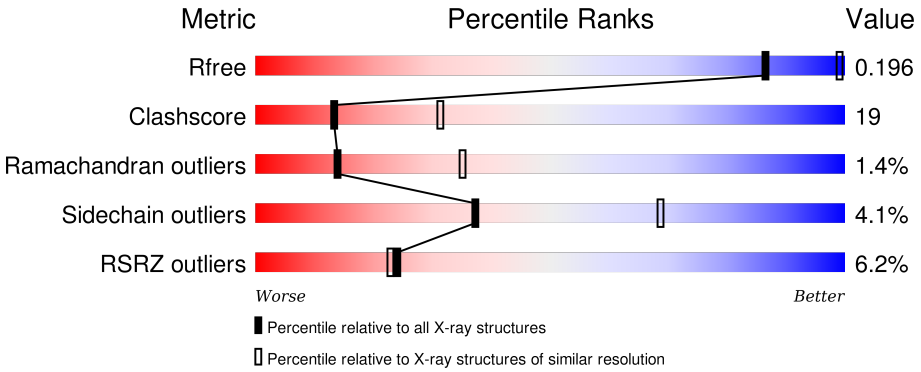
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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 <=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	395	4% 61% 35%
1	B	395	5% 58% 35% 5%
2	C	21	10% 19% 19% 5% 57%
2	D	21	48% 57% 14% 5% 5% 19%

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	G	A	1167	-	-	-	X
5	GTP	B	5001	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7016 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 mRNA capping enzyme alpha subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	Se	0	0	0
			3208	2041	550	604	6	7			
1	B	377	Total	C	N	O	S	Se	0	0	0
			3099	1979	530	577	6	7			

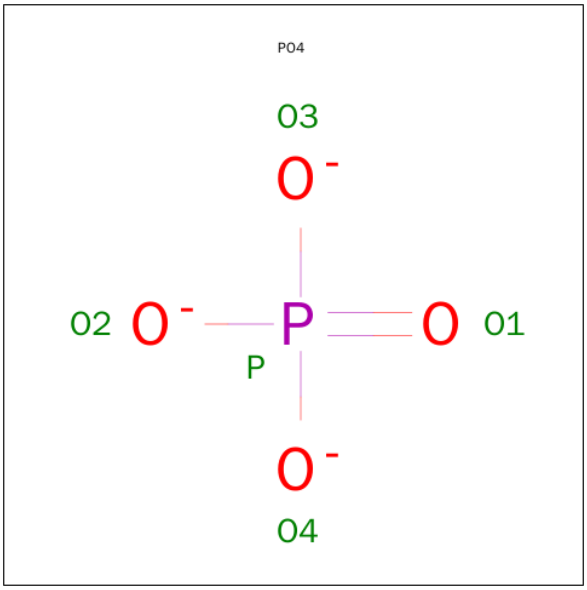
There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	CLONING ARTIFACT	UNP P78587
A	2	VAL	ILE	ENGINEERED	UNP P78587
A	28	MSE	MET	CLONING ARTIFACT	UNP P78587
A	58	MSE	MET	CLONING ARTIFACT	UNP P78587
A	171	MSE	MET	CLONING ARTIFACT	UNP P78587
A	199	MSE	MET	CLONING ARTIFACT	UNP P78587
A	212	MSE	MET	CLONING ARTIFACT	UNP P78587
A	338	MSE	MET	CLONING ARTIFACT	UNP P78587
B	1	MSE	MET	CLONING ARTIFACT	UNP P78587
B	2	VAL	ILE	ENGINEERED	UNP P78587
B	28	MSE	MET	CLONING ARTIFACT	UNP P78587
B	58	MSE	MET	CLONING ARTIFACT	UNP P78587
B	171	MSE	MET	CLONING ARTIFACT	UNP P78587
B	199	MSE	MET	CLONING ARTIFACT	UNP P78587
B	212	MSE	MET	CLONING ARTIFACT	UNP P78587
B	338	MSE	MET	CLONING ARTIFACT	UNP P78587

- Molecule 2 is a protein called phosphorylated peptide from C-terminal of RNA polymerase II.

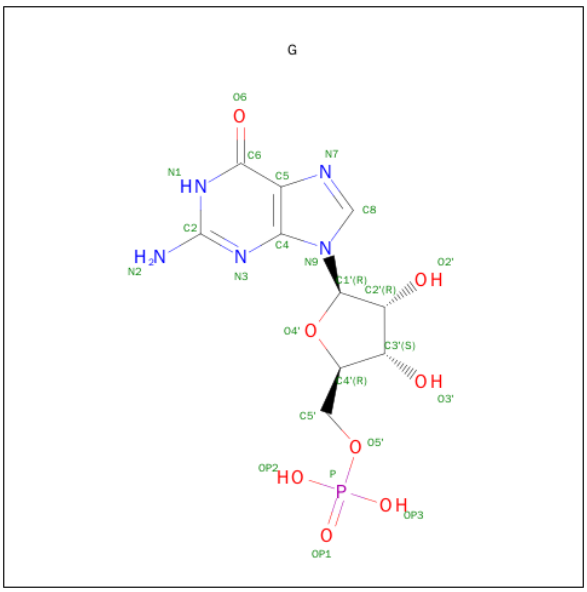
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	9	Total	C	N	O	P	0	0	0
			72	39	9	22	2			
2	D	17	Total	C	N	O	P	0	0	0
			134	76	17	38	3			

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



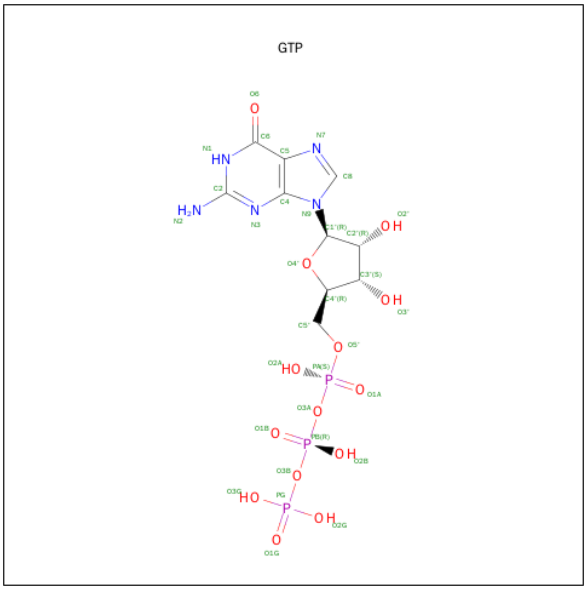
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0

- Molecule 4 is GUANOSINE-5'-MONOPHOSPHATE (three-letter code: G) (formula: $C_{10}H_{14}N_5O_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is water.

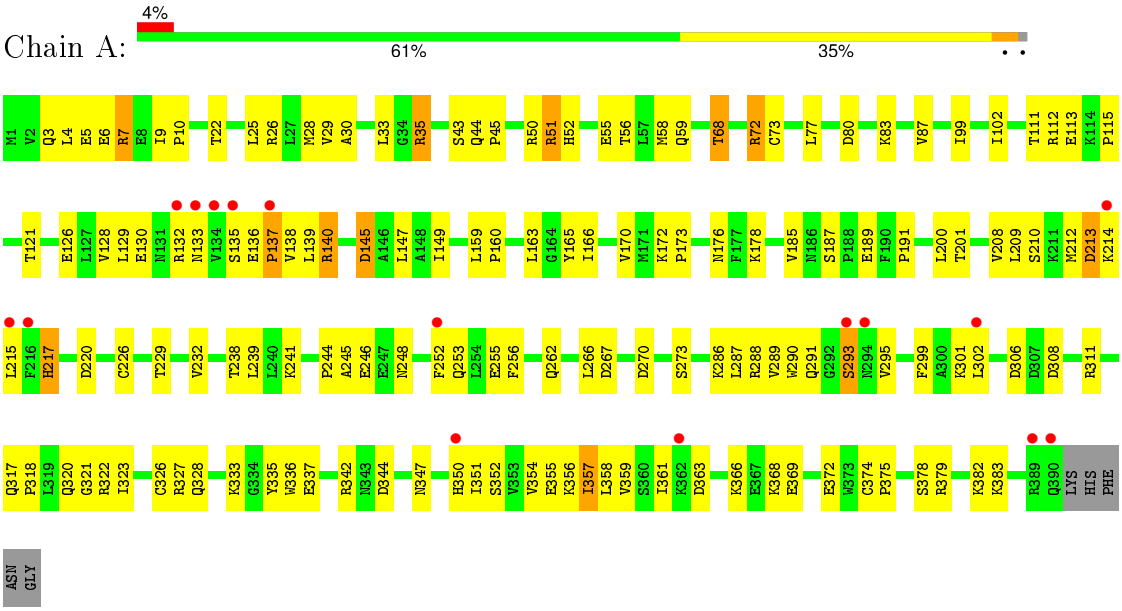
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	208	Total	O	0	0
			208	208		
6	B	197	Total	O	0	0
			197	197		
6	C	10	Total	O	0	0
			10	10		
6	D	18	Total	O	0	0
			18	18		

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 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.

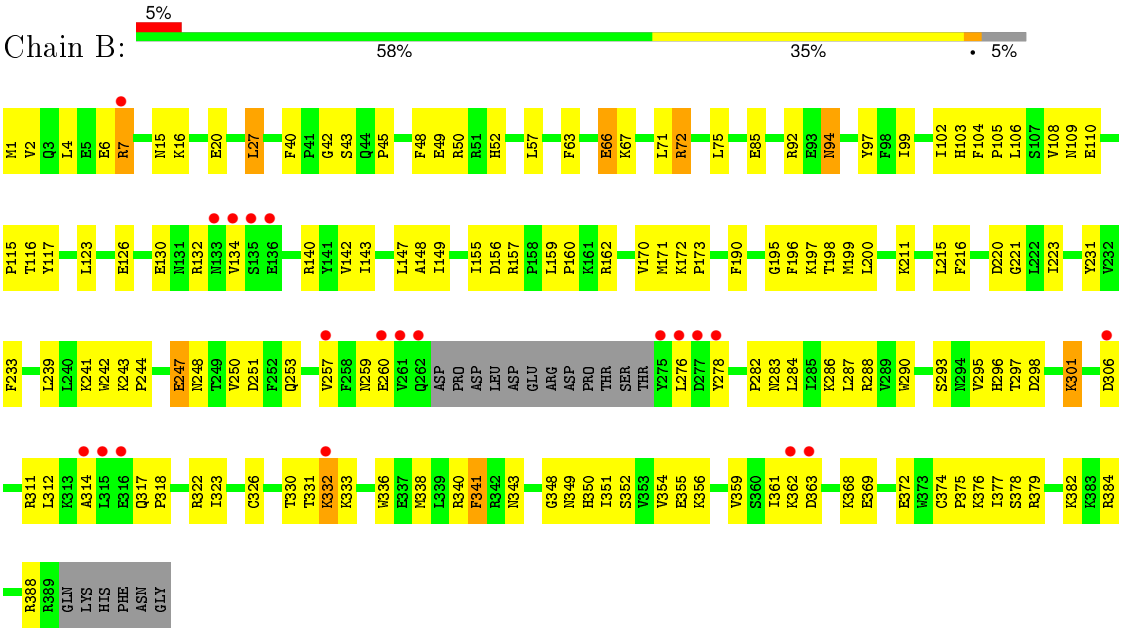
- Molecule 1: mRNA capping enzyme alpha subunit

Chain A:



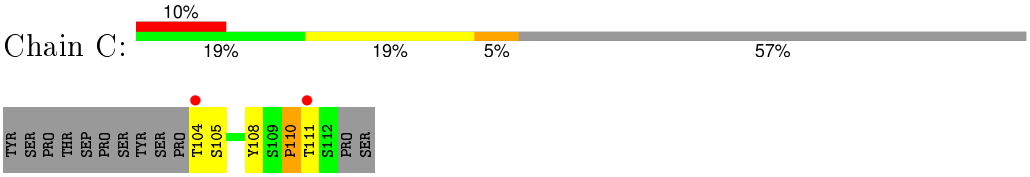
- Molecule 1: mRNA capping enzyme alpha subunit

Chain B:



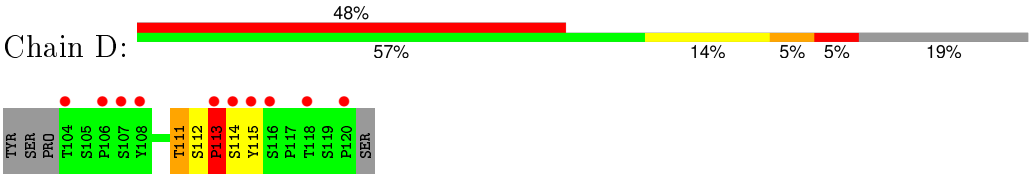
• Molecule 2: phosphorylated peptide from C-terminal of RNA polymerase II

Chain C:



• Molecule 2: phosphorylated peptide from C-terminal of RNA polymerase II

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	47.11Å 124.97Å 92.70Å 90.00° 100.54° 90.00°	Depositor
Resolution (Å)	19.70 – 2.70 19.70 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.7 (19.70-2.70) 95.7 (19.70-2.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.96 (at 2.59Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.200 , 0.266 0.204 , 0.196	Depositor DCC
R_{free} test set	1409 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	40.6	Xtriage
Anisotropy	0.254	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 60.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 30991 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	7016	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GTP, PO4, SEP

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	0.43	0/3277	0.54	0/4423
1	B	0.43	0/3165	0.54	0/4268
2	C	0.36	0/53	0.52	0/71
2	D	0.33	0/107	0.54	0/143
All	All	0.43	0/6602	0.54	0/8905

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	3208	0	3164	117	0
1	B	3099	0	3067	121	0
2	C	72	0	53	6	0
2	D	134	0	103	5	0
3	A	15	0	0	0	0
4	A	23	0	12	0	0
5	B	32	0	12	2	0
6	A	208	0	0	11	0
6	B	197	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	10	0	0	1	0
6	D	18	0	0	2	0
All	All	7016	0	6411	244	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 19.

All (244) 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:366:LYS:HD2	1:A:368:LYS:HE2	1.52	0.90
1:B:288:ARG:HB3	1:B:296:HIS:HB3	1.56	0.88
1:B:253:GLN:HB3	1:B:288:ARG:HB2	1.54	0.87
1:A:111:THR:HG22	1:A:113:GLU:H	1.42	0.83
1:A:132:ARG:HD3	1:A:135:SER:H	1.43	0.83
1:A:256:PHE:H	1:A:320:GLN:HE22	1.28	0.81
1:A:25:LEU:HA	1:A:28:MSE:HE3	1.61	0.80
1:A:4:LEU:HD11	1:A:311:ARG:HB3	1.63	0.79
1:A:212:MSE:HA	1:A:215:LEU:HD13	1.65	0.78
1:B:43:SER:H	1:B:72:ARG:HH22	1.32	0.78
1:A:45:PRO:HB3	1:A:239:LEU:HG	1.65	0.78
1:B:49:GLU:H	1:B:52:HIS:HD2	1.29	0.77
1:A:209:LEU:HA	1:A:212:MSE:HE3	1.67	0.75
1:B:66:GLU:HG2	1:B:215:LEU:HD11	1.67	0.75
1:B:67:LYS:HD3	1:B:223:ILE:HD11	1.69	0.74
1:B:356:LYS:O	1:B:359:VAL:HG22	1.86	0.74
1:B:244:PRO:HB2	1:B:247:GLU:HB2	1.69	0.73
1:A:355:GLU:HA	1:A:358:LEU:HD12	1.71	0.73
1:B:251:ASP:H	1:B:349:ASN:ND2	1.86	0.73
1:A:7:ARG:H	1:A:7:ARG:HD3	1.55	0.71
1:A:10:PRO:HG3	1:A:129:LEU:HG	1.73	0.70
1:A:208:VAL:HG12	1:A:212:MSE:HE2	1.76	0.68
1:A:220:ASP:HB2	6:A:7044:HOH:O	1.94	0.67
1:A:356:LYS:O	1:A:359:VAL:HG22	1.95	0.66
1:A:102:ILE:HB	1:A:191:PRO:HG3	1.77	0.66
1:B:372:GLU:O	1:B:375:PRO:HD2	1.95	0.66
1:B:49:GLU:H	1:B:52:HIS:CD2	2.13	0.65
1:B:251:ASP:H	1:B:349:ASN:HD22	1.44	0.65
1:A:210:SER:HB2	6:A:7037:HOH:O	1.96	0.65
1:B:317:GLN:HE21	1:B:322:ARG:NH1	1.95	0.64
1:B:259:ASN:HD21	1:B:283:ASN:H	1.44	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:VAL:HG23	1:A:299:PHE:HB2	1.79	0.64
1:B:343:ASN:HA	6:B:5020:HOH:O	1.97	0.64
1:A:363:ASP:HB2	6:A:7090:HOH:O	1.97	0.64
1:A:287:LEU:HD21	1:A:302:LEU:HB2	1.80	0.64
1:B:66:GLU:CD	1:B:66:GLU:H	2.00	0.64
1:B:171:MSE:HE3	2:D:115:TYR:OH	1.98	0.64
1:A:50:ARG:HH22	1:A:369:GLU:CD	2.01	0.63
1:A:140:ARG:HH11	1:A:140:ARG:HB2	1.63	0.63
1:A:43:SER:HB3	1:A:232:VAL:O	1.99	0.63
1:B:247:GLU:HG3	6:B:5056:HOH:O	1.99	0.62
1:A:6:GLU:HG2	6:A:7071:HOH:O	1.98	0.62
1:B:50:ARG:HH12	1:B:369:GLU:CD	2.03	0.62
1:B:301:LYS:HG2	6:B:5097:HOH:O	1.99	0.62
1:B:312:LEU:HD21	1:B:338:MSE:HE2	1.80	0.62
1:A:374:CYS:N	1:A:375:PRO:HD2	2.14	0.62
1:A:256:PHE:N	1:A:320:GLN:HE22	1.99	0.61
1:A:255:GLU:HB3	1:A:286:LYS:HG3	1.81	0.61
5:B:5001:GTP:H2'	5:B:5001:GTP:N3	2.15	0.61
1:A:187:SER:OG	1:A:189:GLU:HG2	2.01	0.60
1:B:159:LEU:HD23	1:B:162:ARG:NH2	2.17	0.60
1:A:245:ALA:HA	1:A:248:ASN:ND2	2.17	0.60
1:B:132:ARG:HB2	1:B:216:PHE:HA	1.84	0.59
1:B:220:ASP:HB3	1:B:243:LYS:HE2	1.83	0.59
1:B:171:MSE:HE2	1:B:196:PHE:HB2	1.85	0.59
1:A:214:LYS:HB2	6:A:7164:HOH:O	2.03	0.59
1:A:55:GLU:O	1:A:59:GLN:HG2	2.02	0.59
1:B:351:ILE:O	1:B:355:GLU:HG3	2.04	0.58
1:A:7:ARG:H	1:A:7:ARG:CD	2.11	0.58
1:A:87:VAL:HG21	1:A:102:ILE:HG23	1.84	0.58
1:A:80:ASP:HB3	1:A:83:LYS:HB2	1.86	0.57
1:A:159:LEU:HB3	1:A:160:PRO:HD3	1.87	0.57
1:B:331:THR:HB	1:B:333:LYS:HD2	1.85	0.57
1:B:259:ASN:O	1:B:276:LEU:HA	2.05	0.57
1:A:333:LYS:HG2	6:A:7080:HOH:O	2.05	0.56
1:B:155:ILE:HB	1:B:231:TYR:HB3	1.87	0.55
1:B:159:LEU:HD11	1:B:199:MSE:HE3	1.88	0.55
1:B:171:MSE:HE2	1:B:196:PHE:N	2.22	0.55
1:B:2:VAL:HG12	1:B:338:MSE:HB3	1.88	0.55
1:A:293:SER:O	1:A:295:VAL:HG23	2.07	0.55
1:A:226:CYS:HB3	1:A:229:THR:HG22	1.89	0.54
1:B:75:LEU:HD23	1:B:123:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:ILE:O	1:A:355:GLU:HG3	2.08	0.54
1:B:16:LYS:HB2	1:B:97:TYR:CE2	2.43	0.54
1:A:5:GLU:HG3	6:A:7071:HOH:O	2.07	0.54
1:A:378:SER:O	1:A:382:LYS:HG2	2.08	0.54
1:A:132:ARG:HD3	1:A:135:SER:N	2.18	0.53
1:B:156:ASP:O	1:B:157:ARG:HD3	2.07	0.53
1:A:172:LYS:HB2	1:A:173:PRO:HD3	1.90	0.53
1:B:40:PHE:CE2	1:B:42:GLY:HA3	2.44	0.53
1:A:72:ARG:HD3	1:A:73:CYS:N	2.24	0.53
1:A:253:GLN:HB3	1:A:288:ARG:HG3	1.90	0.52
1:B:374:CYS:HB2	1:B:375:PRO:HD3	1.91	0.52
1:A:130:GLU:O	1:A:137:PRO:HA	2.09	0.52
1:B:312:LEU:HD21	1:B:338:MSE:CE	2.40	0.52
1:B:172:LYS:HB2	1:B:173:PRO:HD3	1.92	0.52
1:A:311:ARG:HH11	1:A:311:ARG:HG3	1.75	0.52
1:B:142:VAL:HA	1:B:195:GLY:O	2.10	0.52
2:C:111:THR:HG23	2:D:111:THR:OG1	2.10	0.52
1:B:45:PRO:HB3	1:B:239:LEU:HG	1.91	0.52
1:A:200:LEU:HA	2:C:110:PRO:HB3	1.91	0.51
1:B:106:LEU:HB3	1:B:116:THR:HB	1.93	0.51
1:A:44:GLN:HA	1:A:44:GLN:HE21	1.76	0.51
1:B:288:ARG:HH11	1:B:298:ASP:N	2.09	0.51
1:A:111:THR:HG22	1:A:113:GLU:N	2.20	0.51
1:A:51:ARG:O	1:A:55:GLU:HB2	2.10	0.51
1:B:248:ASN:HB2	1:B:361:ILE:HG22	1.93	0.51
1:A:215:LEU:HD23	1:A:217:HIS:NE2	2.26	0.51
1:A:213:ASP:HB2	6:A:7036:HOH:O	2.10	0.51
1:B:71:LEU:O	1:B:126:GLU:HA	2.11	0.50
1:B:110:GLU:HG3	1:B:115:PRO:HA	1.93	0.50
1:B:369:GLU:HA	1:B:372:GLU:HG2	1.92	0.50
1:A:246:GLU:HB3	1:A:366:LYS:HE2	1.94	0.50
1:A:350:HIS:O	1:A:354:VAL:HG23	2.12	0.50
1:A:262:GLN:HE22	1:A:273:SER:HB3	1.77	0.49
1:B:340:ARG:HG2	1:B:341:PHE:H	1.78	0.49
1:B:132:ARG:HG3	1:B:215:LEU:O	2.12	0.49
1:B:108:VAL:HG23	1:B:109:ASN:OD1	2.12	0.49
1:B:67:LYS:HB3	1:B:221:GLY:H	1.76	0.49
1:B:155:ILE:HD13	1:B:233:PHE:CZ	2.47	0.49
1:B:148:ALA:C	1:B:149:ILE:HD12	2.33	0.49
1:B:376:LYS:HA	1:B:379:ARG:NH1	2.28	0.49
1:B:170:VAL:C	1:B:173:PRO:HD2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:299:PHE:HZ	1:A:358:LEU:HD11	1.78	0.49
1:B:355:GLU:O	1:B:359:VAL:HG13	2.13	0.48
1:A:50:ARG:NH2	1:A:369:GLU:OE2	2.46	0.48
1:B:159:LEU:N	1:B:160:PRO:HD2	2.29	0.48
1:B:123:LEU:HD13	1:B:143:ILE:HD13	1.95	0.48
1:A:245:ALA:HA	1:A:248:ASN:HD21	1.78	0.48
1:B:350:HIS:O	1:B:354:VAL:HG23	2.12	0.48
1:B:2:VAL:CG1	1:B:338:MSE:HB3	2.43	0.48
1:B:105:PRO:HB3	1:B:110:GLU:OE1	2.14	0.48
1:A:379:ARG:O	1:A:383:LYS:HB2	2.13	0.48
1:B:288:ARG:HA	1:B:297:THR:O	2.14	0.48
1:B:43:SER:H	1:B:72:ARG:NH2	2.07	0.48
1:B:20:GLU:H	1:B:20:GLU:CD	2.18	0.48
1:A:256:PHE:H	1:A:320:GLN:NE2	2.03	0.47
1:A:113:GLU:C	1:A:115:PRO:HD3	2.35	0.47
1:B:110:GLU:CG	1:B:115:PRO:HA	2.45	0.47
1:A:342:ARG:C	1:A:344:ASP:H	2.17	0.47
1:A:311:ARG:NH1	1:A:311:ARG:HG3	2.30	0.47
1:B:43:SER:N	1:B:72:ARG:HH22	2.08	0.47
1:B:63:PHE:CD1	1:B:159:LEU:HD12	2.49	0.47
1:A:201:THR:HG23	2:C:110:PRO:HG3	1.97	0.47
1:B:103:HIS:HE1	1:B:116:THR:O	1.98	0.47
1:A:270:ASP:HB3	1:A:273:SER:OG	2.15	0.47
1:B:198:THR:HA	6:B:5066:HOH:O	2.14	0.46
1:B:99:ILE:N	1:B:99:ILE:HD12	2.29	0.46
1:B:4:LEU:HD21	1:B:312:LEU:HD23	1.97	0.46
1:A:326:CYS:HB3	1:A:337:GLU:O	2.15	0.46
1:A:44:GLN:HA	1:A:44:GLN:NE2	2.31	0.46
1:A:246:GLU:OE1	1:A:366:LYS:HB2	2.16	0.46
1:B:359:VAL:O	1:B:363:ASP:HB2	2.15	0.46
1:A:252:PHE:HB3	1:A:287:LEU:HB3	1.97	0.46
1:B:171:MSE:HE2	1:B:196:PHE:H	1.81	0.46
1:A:111:THR:HG23	6:A:7157:HOH:O	2.15	0.46
1:B:361:ILE:HD12	1:B:362:LYS:HB3	1.98	0.46
1:B:171:MSE:HB3	2:D:115:TYR:CE2	2.51	0.46
1:A:55:GLU:O	1:A:58:MSE:HB2	2.16	0.46
1:B:99:ILE:HG22	1:B:102:ILE:HG21	1.98	0.46
1:A:163:LEU:HB2	2:C:108:TYR:HB3	1.98	0.46
1:A:352:SER:O	1:A:356:LYS:HG3	2.16	0.46
1:B:253:GLN:HA	1:B:323:ILE:HD13	1.97	0.46
1:A:52:HIS:HA	1:A:56:THR:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:317:GLN:HE21	1:B:322:ARG:HH12	1.62	0.45
1:A:286:LYS:HA	1:A:301:LYS:HA	1.97	0.45
1:A:328:GLN:HG2	1:A:336:TRP:CH2	2.52	0.45
1:A:33:LEU:HD12	1:A:35:ARG:HD3	1.98	0.45
1:A:226:CYS:HB3	1:A:229:THR:CG2	2.47	0.45
1:B:384:ARG:HD3	1:B:388:ARG:HH21	1.81	0.45
1:B:293:SER:O	1:B:295:VAL:HG23	2.16	0.45
1:B:147:LEU:HD12	1:B:147:LEU:N	2.32	0.45
1:B:130:GLU:OE2	1:B:140:ARG:HD2	2.17	0.45
1:B:287:LEU:HD11	1:B:336:TRP:HB2	1.97	0.45
1:A:267:ASP:O	1:A:270:ASP:HB3	2.17	0.45
1:B:290:TRP:O	1:B:350:HIS:HA	2.17	0.45
1:A:357:ILE:O	1:A:361:ILE:HG13	2.17	0.45
1:A:147:LEU:N	1:A:147:LEU:HD12	2.32	0.45
1:B:330:THR:C	1:B:332:LYS:H	2.19	0.45
1:B:239:LEU:HD21	5:B:5001:GTP:N2	2.32	0.44
1:A:30:ALA:HB1	1:A:35:ARG:O	2.17	0.44
1:A:308:ASP:HA	1:A:311:ARG:HG3	2.00	0.44
2:C:104:THR:HG22	2:C:105:SEP:N	2.33	0.44
1:B:368:LYS:HG3	1:B:369:GLU:N	2.33	0.44
1:A:317:GLN:HE21	1:A:322:ARG:NH1	2.16	0.44
1:B:250:VAL:HG11	1:B:354:VAL:HG13	1.99	0.44
1:A:145:ASP:C	1:A:166:ILE:HD11	2.38	0.44
1:A:374:CYS:N	1:A:375:PRO:CD	2.81	0.44
1:A:368:LYS:O	1:A:372:GLU:HG2	2.18	0.44
1:A:132:ARG:HG2	1:A:133:ASN:N	2.33	0.44
1:A:255:GLU:OE1	1:A:286:LYS:HE3	2.18	0.44
1:A:68:THR:HG21	1:A:128:VAL:HG11	1.98	0.44
1:A:170:VAL:C	1:A:173:PRO:HD2	2.38	0.43
1:A:317:GLN:HB2	1:A:318:PRO:HD2	2.00	0.43
1:B:286:LYS:HD3	6:B:5100:HOH:O	2.18	0.43
1:B:92:ARG:C	1:B:94:ASN:H	2.21	0.43
1:A:357:ILE:HD13	1:A:357:ILE:O	2.19	0.43
1:A:357:ILE:HD13	1:A:361:ILE:HD11	1.99	0.43
1:A:29:VAL:O	1:A:33:LEU:HG	2.19	0.43
1:B:67:LYS:HB3	1:B:221:GLY:C	2.38	0.43
1:A:354:VAL:HA	1:A:357:ILE:HG22	2.00	0.43
1:B:318:PRO:HB2	6:B:5063:HOH:O	2.19	0.43
1:B:241:LYS:O	1:B:241:LYS:HG3	2.18	0.43
1:A:3:GLN:HB3	6:A:7137:HOH:O	2.19	0.43
1:B:257:VAL:HG11	1:B:284:LEU:HD23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:350:HIS:HD2	1:B:352:SER:OG	2.02	0.43
1:B:27:LEU:HA	1:B:27:LEU:HD12	1.85	0.43
1:B:340:ARG:HG2	1:B:341:PHE:N	2.33	0.43
1:B:6:GLU:HG3	1:B:7:ARG:NH1	2.33	0.43
1:A:241:LYS:O	1:A:241:LYS:HG3	2.19	0.42
1:B:85:GLU:HB2	1:B:117:TYR:CD2	2.54	0.42
1:A:178:LYS:HG3	1:A:185:VAL:HG21	2.01	0.42
1:A:77:LEU:HB2	1:A:121:THR:HB	2.01	0.42
1:A:136:GLU:O	1:A:138:VAL:HG13	2.19	0.42
1:B:296:HIS:HE1	1:B:348:GLY:H	1.68	0.42
1:A:149:ILE:HG13	1:A:165:TYR:HB3	2.02	0.42
1:B:301:LYS:HD2	1:B:301:LYS:H	1.85	0.42
1:A:361:ILE:H	1:A:361:ILE:HG13	1.66	0.42
1:A:270:ASP:OD1	1:A:270:ASP:C	2.58	0.42
1:B:57:LEU:O	1:B:377:ILE:HG23	2.20	0.42
1:B:170:VAL:O	1:B:173:PRO:HD2	2.19	0.42
1:A:226:CYS:HB2	1:A:238:THR:HB	2.01	0.42
1:B:361:ILE:C	1:B:361:ILE:HD12	2.40	0.42
1:B:142:VAL:HG12	1:B:197:LYS:HB2	2.00	0.41
1:B:311:ARG:HG3	1:B:311:ARG:HH11	1.85	0.41
1:A:176:ASN:HA	6:A:7083:HOH:O	2.19	0.41
1:B:351:ILE:HG23	1:B:352:SER:N	2.35	0.41
1:A:252:PHE:CB	1:A:287:LEU:HB3	2.51	0.41
1:B:1:MSE:HE3	6:B:5106:HOH:O	2.19	0.41
2:D:114:SER:HA	6:D:139:HOH:O	2.20	0.41
1:A:102:ILE:HG23	1:A:102:ILE:O	2.20	0.41
1:A:323:ILE:N	1:A:323:ILE:HD12	2.34	0.41
1:A:320:GLN:HE21	1:A:321:GLY:H	1.69	0.41
1:A:10:PRO:HB3	1:A:139:LEU:HD11	2.02	0.41
1:A:99:ILE:O	1:A:102:ILE:HG22	2.20	0.41
1:B:374:CYS:N	1:B:375:PRO:CD	2.84	0.41
1:B:378:SER:O	1:B:382:LYS:HG2	2.21	0.41
1:B:67:LYS:O	1:B:67:LYS:HG3	2.21	0.41
1:B:48:PHE:CB	1:B:242:TRP:HB2	2.51	0.41
1:B:259:ASN:ND2	1:B:283:ASN:H	2.14	0.41
1:B:2:VAL:HG11	1:B:338:MSE:HE3	2.03	0.41
1:B:148:ALA:O	1:B:149:ILE:HD12	2.21	0.41
1:B:384:ARG:O	1:B:388:ARG:HG3	2.21	0.41
1:B:326:CYS:HB3	1:B:336:TRP:HB3	2.02	0.41
2:C:104:THR:HG21	6:C:303:HOH:O	2.20	0.41
1:B:311:ARG:O	1:B:314:ALA:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:ASP:CB	1:B:243:LYS:HE2	2.50	0.41
1:A:333:LYS:C	1:A:335:TYR:H	2.25	0.41
1:B:200:LEU:HA	6:D:129:HOH:O	2.20	0.40
1:A:22:THR:O	1:A:26:ARG:HG3	2.21	0.40
1:A:289:VAL:HG12	1:A:290:TRP:N	2.36	0.40
2:D:112:SEP:O	2:D:113:PRO:C	2.59	0.40
1:B:75:LEU:HD21	1:B:104:PHE:CZ	2.56	0.40
1:A:266:LEU:HD12	1:A:273:SER:HA	2.03	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	388/395 (98%)	343 (88%)	41 (11%)	4 (1%)	19	45
1	B	373/395 (94%)	334 (90%)	35 (9%)	4 (1%)	17	42
2	C	6/21 (29%)	4 (67%)	1 (17%)	1 (17%)	0	0
2	D	12/21 (57%)	8 (67%)	2 (17%)	2 (17%)	0	0
All	All	779/832 (94%)	689 (88%)	79 (10%)	11 (1%)	14	35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	134	VAL
2	D	111	THR
1	A	293	SER
1	A	291	GLN
1	B	211	LYS
2	D	113	PRO
1	B	332	LYS

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Mol	Chain	Res	Type
2	C	110	PRO
1	A	137	PRO
1	B	282	PRO
1	A	244	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	359/356 (101%)	343 (96%)	16 (4%)	34 65
1	B	345/356 (97%)	332 (96%)	13 (4%)	40 71
2	C	7/18 (39%)	7 (100%)	0	100 100
2	D	14/18 (78%)	13 (93%)	1 (7%)	18 41
All	All	725/748 (97%)	695 (96%)	30 (4%)	37 69

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

Mol	Chain	Res	Type
1	A	7	ARG
1	A	9	ILE
1	A	35	ARG
1	A	51	ARG
1	A	68	THR
1	A	72	ARG
1	A	112	ARG
1	A	126	GLU
1	A	140	ARG
1	A	145	ASP
1	A	213	ASP
1	A	217	HIS
1	A	306	ASP
1	A	327	ARG
1	A	347	ASN
1	A	357	ILE
1	B	7	ARG

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Mol	Chain	Res	Type
1	B	15	ASN
1	B	27	LEU
1	B	66	GLU
1	B	72	ARG
1	B	94	ASN
1	B	190	PHE
1	B	247	GLU
1	B	260	GLU
1	B	278	TYR
1	B	301	LYS
1	B	306	ASP
1	B	341	PHE
2	D	113	PRO

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	GLN
1	A	133	ASN
1	A	237	GLN
1	A	248	ASN
1	A	262	GLN
1	A	283	ASN
1	A	317	GLN
1	A	320	GLN
1	B	52	HIS
1	B	59	GLN
1	B	94	ASN
1	B	133	ASN
1	B	259	ASN
1	B	283	ASN
1	B	291	GLN
1	B	296	HIS
1	B	317	GLN
1	B	328	GLN
1	B	349	ASN
1	B	350	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

5 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SEP	C	105	2	8,9,10	2.17	1 (12%)	8,12,14	5.84	3 (37%)
2	SEP	C	112	2	8,9,10	2.15	1 (12%)	8,12,14	5.58	3 (37%)
2	SEP	D	105	2	8,9,10	2.14	1 (12%)	8,12,14	5.59	3 (37%)
2	SEP	D	112	2	8,9,10	2.12	1 (12%)	8,12,14	5.62	4 (50%)
2	SEP	D	119	2	8,9,10	2.13	1 (12%)	8,12,14	5.55	3 (37%)

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
2	SEP	C	105	2	-	0/6/8/10	0/0/0/0
2	SEP	C	112	2	-	0/6/8/10	0/0/0/0
2	SEP	D	105	2	-	0/6/8/10	0/0/0/0
2	SEP	D	112	2	-	0/6/8/10	0/0/0/0
2	SEP	D	119	2	-	0/6/8/10	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	112	SEP	OG-CB	-5.37	1.22	1.44
2	C	105	SEP	OG-CB	-5.35	1.22	1.44
2	D	105	SEP	OG-CB	-5.34	1.22	1.44
2	D	119	SEP	OG-CB	-5.28	1.23	1.44
2	D	112	SEP	OG-CB	-5.09	1.24	1.44

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	112	SEP	O2P-P-O1P	-2.45	102.68	110.58
2	D	105	SEP	O2P-P-O1P	-2.27	103.28	110.58
2	C	105	SEP	O2P-P-O1P	-2.07	103.91	110.58
2	D	119	SEP	O2P-P-O1P	-2.07	103.92	110.58
2	C	112	SEP	O2P-P-O1P	-2.07	103.93	110.58
2	D	112	SEP	O2P-P-OG	2.20	112.89	106.56
2	C	112	SEP	O3P-P-O1P	3.23	120.97	110.58
2	D	119	SEP	O3P-P-O1P	3.24	121.01	110.58
2	D	105	SEP	O3P-P-O1P	3.27	121.10	110.58
2	D	112	SEP	O3P-P-O1P	3.30	121.19	110.58
2	C	105	SEP	O3P-P-O1P	3.32	121.27	110.58
2	D	119	SEP	OG-CB-CA	15.01	121.08	108.27
2	D	112	SEP	OG-CB-CA	15.07	121.13	108.27
2	C	112	SEP	OG-CB-CA	15.08	121.14	108.27
2	D	105	SEP	OG-CB-CA	15.08	121.14	108.27
2	C	105	SEP	OG-CB-CA	15.84	121.79	108.27

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
2	C	105	SEP	1	0
2	D	112	SEP	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

5 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	$\#\|Z\|>2$
4	G	A	1167	1	16,25,26	1.86	3 (18%)	19,37,40	1.87	4 (21%)
3	PO4	A	7001	-	4,4,4	1.04	0	6,6,6	0.27	0
3	PO4	A	7002	-	4,4,4	1.07	0	6,6,6	0.27	0
3	PO4	A	7005	-	4,4,4	1.09	0	6,6,6	0.27	0
5	GTP	B	5001	-	25,34,34	1.92	8 (32%)	34,54,54	2.20	8 (23%)

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
4	G	A	1167	1	-	0/3/25/26	0/3/3/3
3	PO4	A	7001	-	-	0/0/0/0	0/0/0/0
3	PO4	A	7002	-	-	0/0/0/0	0/0/0/0
3	PO4	A	7005	-	-	0/0/0/0	0/0/0/0
5	GTP	B	5001	-	-	0/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	5001	GTP	C2'-C3'	-3.21	1.44	1.53
5	B	5001	GTP	C3'-C4'	-2.36	1.46	1.53
5	B	5001	GTP	C8-N7	-2.33	1.30	1.34
5	B	5001	GTP	PG-O2G	-2.04	1.47	1.54
5	B	5001	GTP	O4'-C1'	2.54	1.44	1.41
4	A	1167	G	C6-N1	2.80	1.38	1.33
5	B	5001	GTP	C6-C5	2.91	1.47	1.41
4	A	1167	G	C4-N3	3.00	1.40	1.35
5	B	5001	GTP	C4-N3	3.01	1.40	1.35
5	B	5001	GTP	C6-N1	4.74	1.41	1.33
4	A	1167	G	O6-C6	4.82	1.36	1.24

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	5001	GTP	C5-C6-N1	-7.91	112.77	123.59
4	A	1167	G	C5-C6-N1	-4.66	117.22	123.59
4	A	1167	G	N2-C2-N3	-3.55	110.99	117.80
5	B	5001	GTP	N3-C2-N1	-3.50	122.12	127.44
4	A	1167	G	C6-C5-C4	-2.78	117.58	120.90
5	B	5001	GTP	C4'-O4'-C1'	-2.45	107.03	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	5001	GTP	O5'-C5'-C4'	2.07	116.76	109.12
5	B	5001	GTP	N2-C2-N1	2.33	121.07	117.20
5	B	5001	GTP	O4'-C4'-C5'	2.54	118.39	109.32
5	B	5001	GTP	C1'-N9-C4	2.61	130.88	126.94
4	A	1167	G	C6-N1-C2	3.24	120.43	115.94
5	B	5001	GTP	C6-N1-C2	6.55	125.03	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	5001	GTP	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, 95^{th} 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	383/395 (96%)	-0.12	16 (4%) 40 39	18, 46, 91, 107	0
1	B	370/395 (93%)	0.01	20 (5%) 29 28	15, 45, 123, 149	0
2	C	7/21 (33%)	2.35	2 (28%) 1 0	104, 105, 113, 116	0
2	D	14/21 (66%)	2.65	10 (71%) 0 0	123, 127, 130, 131	0
All	All	774/832 (93%)	0.02	48 (6%) 24 23	15, 46, 116, 149	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	111	THR	6.0
1	B	261	VAL	5.9
1	A	294	ASN	5.6
2	C	104	THR	5.2
2	D	104	THR	4.9
1	B	135	SER	4.8
1	B	275	TYR	4.7
1	A	293	SER	4.4
1	B	134	VAL	4.1
1	B	262	GLN	3.9
1	B	7	ARG	3.9
2	D	114	SER	3.9
2	D	118	THR	3.8
1	B	276	LEU	3.8
1	A	135	SER	3.8
1	B	316	GLU	3.7
2	D	116	SER	3.7
1	A	389	ARG	3.5
1	A	132	ARG	3.4
1	A	134	VAL	3.2
1	B	278	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	257	VAL	3.2
1	B	306	ASP	3.0
1	A	302	LEU	2.9
1	B	260	GLU	2.8
1	A	362	LYS	2.8
1	A	137	PRO	2.7
2	D	113	PRO	2.7
1	A	390	GLN	2.7
1	A	133	ASN	2.7
1	B	332	LYS	2.7
2	D	108	TYR	2.6
1	B	133	ASN	2.6
2	D	107	SER	2.6
1	B	136	GLU	2.6
1	A	216	PHE	2.6
1	A	215	LEU	2.5
1	B	277	ASP	2.5
1	B	363	ASP	2.4
2	D	115	TYR	2.4
2	D	106	PRO	2.3
1	B	362	LYS	2.3
1	B	315	LEU	2.2
1	A	252	PHE	2.2
1	B	314	ALA	2.2
2	D	120	PRO	2.1
1	A	214	LYS	2.1
1	A	350	HIS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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(Å^2)	Q<0.9
2	SEP	D	105	10/11	0.88	0.26	-	121,123,127,128	0
2	SEP	D	119	10/11	0.85	0.17	-	110,113,121,123	0
2	SEP	D	112	10/11	0.73	0.27	-	110,116,124,125	0
2	SEP	C	112	10/11	0.91	0.21	-	106,108,115,115	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SEP	C	105	10/11	0.87	0.23	-	99,101,106,107	0

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, 95^{th} 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(Å^2)	Q<0.9
5	GTP	B	5001	32/32	0.67	0.39	7.27	71,79,87,87	32
4	G	A	1167	23/24	0.65	0.37	3.44	105,106,108,110	0
3	PO4	A	7001	5/5	0.67	0.47	-	115,115,116,116	0
3	PO4	A	7005	5/5	0.90	0.15	-	96,97,98,98	0
3	PO4	A	7002	5/5	0.76	0.34	-	112,112,112,113	0

6.5 Other polymers (i)

There are no such residues in this entry.