



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:56 AM GMT

PDB ID : 3QBT
Title : Crystal structure of OCRL1 540-678 in complex with Rab8a:GppNHp
Authors : Hou, X.; Hagemann, N.; Schoebel, S.; Blankenfeldt, W.; Goody, R.S.; Erdmann, K.S.; Itzen, A.
Deposited on : 2011-01-14
Resolution : 2.00 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

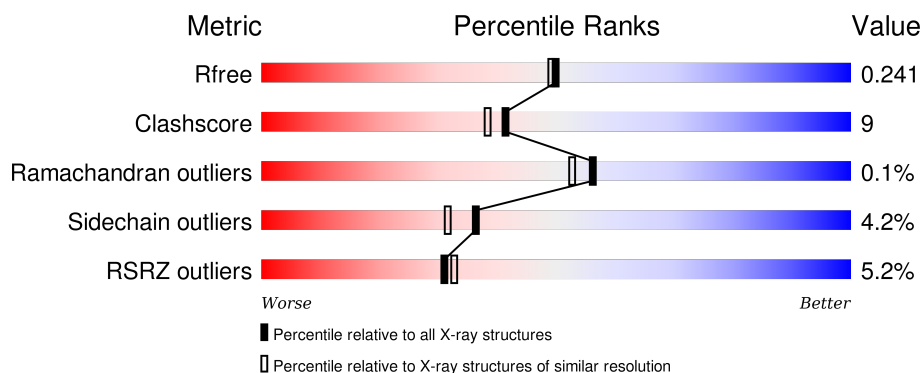
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	6249 (2.00-2.00)
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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	174	<div> <div>5%</div> <div>80% 15% ...</div> </div>
1	C	174	<div> <div>4%</div> <div>86% 11% ...</div> </div>
1	E	174	<div> <div>3%</div> <div>85% 11% ...</div> </div>
1	G	174	<div> <div>2%</div> <div>78% 17% ...</div> </div>
2	B	140	<div> <div>9%</div> <div>79% 11% 7%</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	140	<div> <div>%</div> <div> </div> <div>79% 11% • 7%</div> </div>
2	F	140	<div> <div>14%</div> <div> </div> <div>74% 21% • •</div> </div>
2	H	140	<div> <div>4%</div> <div> </div> <div>78% 19% • •</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	SO4	D	2	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10400 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 Ras-related protein Rab-8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	170	Total	C	N	O	S	0	0	0
			1373	874	237	255	7			
1	C	171	Total	C	N	O	S	0	0	0
			1381	878	238	258	7			
1	E	169	Total	C	N	O	S	0	0	0
			1364	868	235	254	7			
1	G	169	Total	C	N	O	S	0	0	0
			1364	868	235	254	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	GLY	-	EXPRESSION TAG	UNP P61006
A	4	HIS	-	EXPRESSION TAG	UNP P61006
A	5	MET	-	EXPRESSION TAG	UNP P61006
C	3	GLY	-	EXPRESSION TAG	UNP P61006
C	4	HIS	-	EXPRESSION TAG	UNP P61006
C	5	MET	-	EXPRESSION TAG	UNP P61006
E	3	GLY	-	EXPRESSION TAG	UNP P61006
E	4	HIS	-	EXPRESSION TAG	UNP P61006
E	5	MET	-	EXPRESSION TAG	UNP P61006
G	3	GLY	-	EXPRESSION TAG	UNP P61006
G	4	HIS	-	EXPRESSION TAG	UNP P61006
G	5	MET	-	EXPRESSION TAG	UNP P61006

- Molecule 2 is a protein called Inositol polyphosphate 5-phosphatase OCRL-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	130	Total	C	N	O	S	0	0	0
			1072	684	177	207	4			
2	D	130	Total	C	N	O	S	0	0	0
			1072	684	177	207	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	139	Total	C	N	O	S	0	0	0
			1162	741	196	221	4			
2	H	139	Total	C	N	O	S	0	0	0
			1162	741	196	221	4			

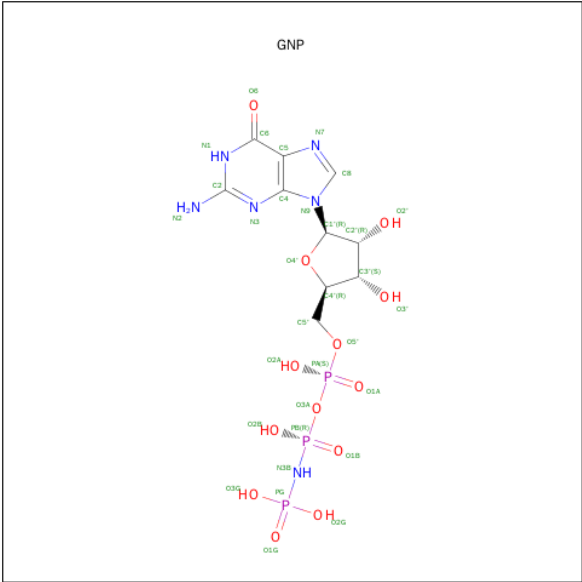
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	539	GLY	-	EXPRESSION TAG	UNP Q01968
D	539	GLY	-	EXPRESSION TAG	UNP Q01968
F	539	GLY	-	EXPRESSION TAG	UNP Q01968
H	539	GLY	-	EXPRESSION TAG	UNP Q01968

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

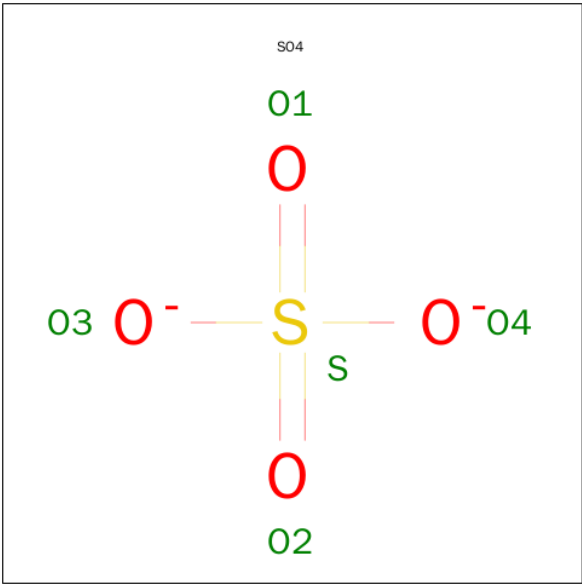
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-GUANYLATE ESTER (three-letter code: GNP) (formula: C₁₀H₁₇N₆O₁₃P₃).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

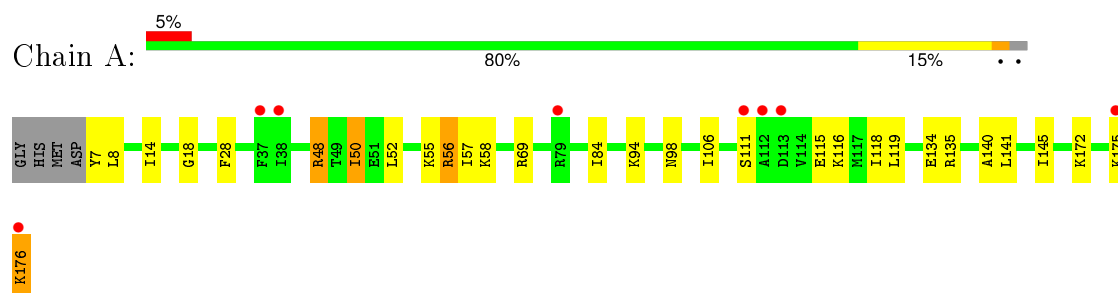
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total	O	0	0
			39	39		
6	C	65	Total	O	0	0
			65	65		
6	E	31	Total	O	0	0
			31	31		
6	G	32	Total	O	0	0
			32	32		
6	B	40	Total	O	0	0
			40	40		
6	D	47	Total	O	0	0
			47	47		
6	F	20	Total	O	0	0
			20	20		
6	H	34	Total	O	0	0
			34	34		

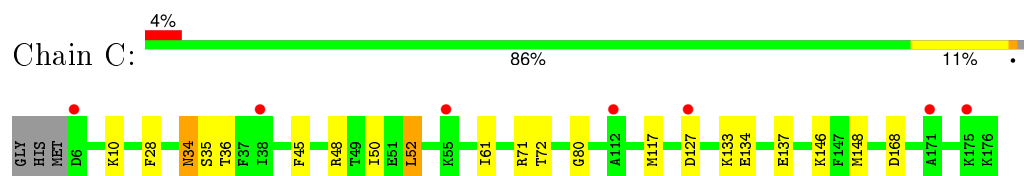
3 Residue-property plots [i](#)

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.

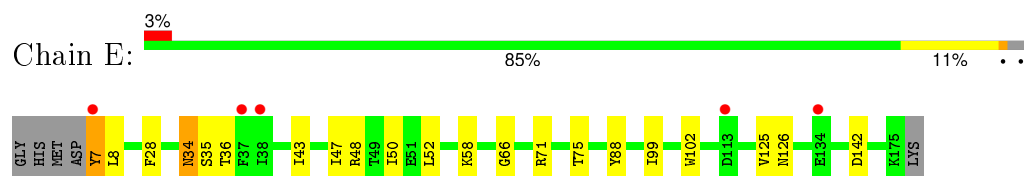
- Molecule 1: Ras-related protein Rab-8A



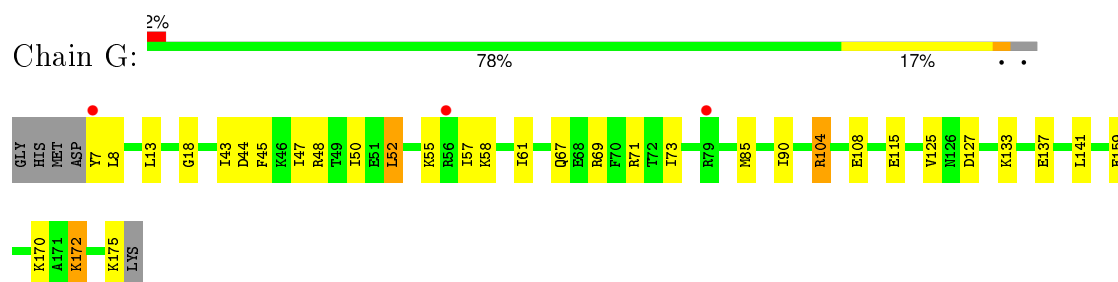
- Molecule 1: Ras-related protein Rab-8A



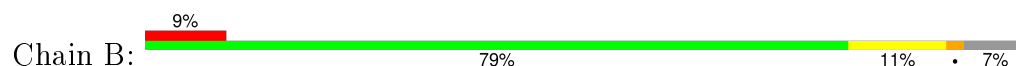
- Molecule 1: Ras-related protein Rab-8A



- Molecule 1: Ras-related protein Rab-8A

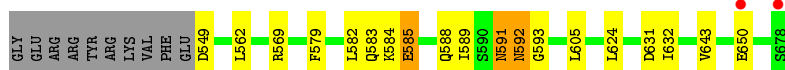
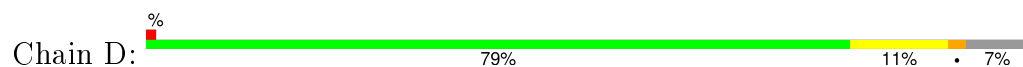


- Molecule 2: Inositol polyphosphate 5-phosphatase OCRL-1

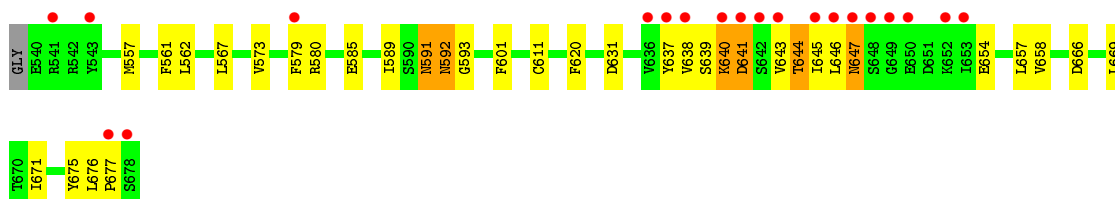
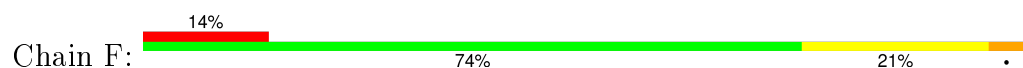




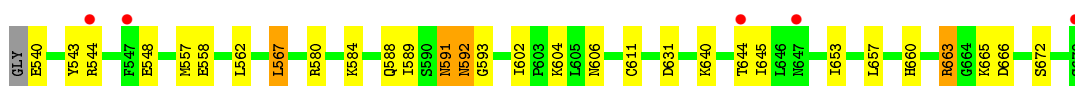
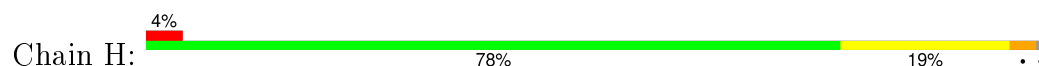
- Molecule 2: Inositol polyphosphate 5-phosphatase OCRL-1



- Molecule 2: Inositol polyphosphate 5-phosphatase OCRL-1



- Molecule 2: Inositol polyphosphate 5-phosphatase OCRL-1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.15Å 55.34Å 173.84Å 90.00° 91.93° 90.00°	Depositor
Resolution (Å)	47.38 – 2.00 47.38 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.3 (47.38-2.00) 98.3 (47.38-2.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.208 , 0.241 0.209 , 0.241	Depositor DCC
R_{free} test set	4996 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	29.3	Xtriage
Anisotropy	0.019	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 56.2	EDS
Estimated twinning fraction	0.025 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	0 of 99857 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	10400	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 50.07 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 6.8166e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, GNP, 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	0.68	0/1393	0.69	0/1865
1	C	0.72	0/1401	0.72	0/1876
1	E	0.65	0/1384	0.65	0/1854
1	G	0.68	0/1384	0.69	1/1854 (0.1%)
2	B	0.63	0/1096	0.69	0/1481
2	D	0.70	0/1096	0.71	0/1481
2	F	0.63	0/1188	0.68	0/1602
2	H	0.74	0/1188	0.69	0/1602
All	All	0.68	0/10130	0.69	1/13615 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	104	ARG	NE-CZ-NH1	5.70	123.15	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1373	0	1392	30	0
1	C	1381	0	1396	18	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	1364	0	1379	21	0
1	G	1364	0	1379	29	1
2	B	1072	0	1043	20	0
2	D	1072	0	1043	14	0
2	F	1162	0	1134	30	0
2	H	1162	0	1134	26	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
3	E	1	0	0	0	0
3	G	1	0	0	0	0
4	A	32	0	13	1	0
4	C	32	0	13	0	0
4	E	32	0	13	0	0
4	G	32	0	13	1	0
5	B	5	0	0	0	0
5	D	5	0	0	0	0
6	A	39	0	0	1	0
6	B	40	0	0	1	0
6	C	65	0	0	3	0
6	D	47	0	0	1	0
6	E	31	0	0	0	0
6	F	20	0	0	0	0
6	G	32	0	0	3	0
6	H	34	0	0	0	0
All	All	10400	0	9952	171	1

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 9.

All (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:580:ARG:HH21	2:H:640:LYS:HE2	1.35	0.88
2:H:567:LEU:HD13	2:H:589:ILE:HG22	1.57	0.85
1:E:88:TYR:CD1	1:E:99:ILE:HD11	2.13	0.84
1:C:34:ASN:ND2	1:C:36:THR:H	1.77	0.81
1:E:34:ASN:ND2	1:E:36:THR:H	1.81	0.79
2:H:580:ARG:NH2	2:H:640:LYS:HE2	1.97	0.78
1:G:67:GLN:NE2	1:G:69:ARG:HH12	1.81	0.77
2:F:580:ARG:NH2	2:F:640:LYS:HE3	1.99	0.77
1:G:115:GLU:OE1	1:G:172:LYS:HE3	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:590:SER:OG	2:B:629:THR:HG22	1.85	0.76
1:A:50:ILE:CD1	1:A:57:ILE:HB	2.16	0.75
2:B:552:ARG:NH2	6:B:293:HOH:O	2.20	0.74
1:C:34:ASN:HD22	1:C:36:THR:H	1.35	0.74
1:A:14:ILE:CD1	1:A:106:ILE:HD11	2.18	0.74
1:A:50:ILE:HD11	1:A:57:ILE:HB	1.70	0.74
2:B:554:MET:HA	2:H:557:MET:HE1	1.68	0.73
2:B:652:LYS:HG2	2:B:653:ILE:H	1.54	0.73
2:H:663:ARG:HH11	2:H:663:ARG:HG3	1.54	0.72
1:E:34:ASN:HD22	1:E:36:THR:H	1.36	0.72
1:E:125:VAL:HG12	1:E:125:VAL:O	1.89	0.71
1:E:7:TYR:HD1	1:E:8:LEU:H	1.37	0.71
1:G:104:ARG:HD3	1:G:108:GLU:OE2	1.91	0.70
1:G:67:GLN:HE22	1:G:69:ARG:HH12	1.37	0.69
1:E:66:GLY:O	1:E:71:ARG:NH1	2.25	0.69
2:F:580:ARG:HH11	2:F:639:SER:HB2	1.58	0.68
1:G:8:LEU:HD13	1:G:58:LYS:HE2	1.76	0.65
2:F:567:LEU:HD22	2:F:589:ILE:HG22	1.79	0.65
1:G:125:VAL:O	1:G:125:VAL:HG12	1.96	0.65
2:D:579:PHE:CD1	2:D:643:VAL:HG11	2.32	0.65
2:F:580:ARG:NH1	2:F:639:SER:HB2	2.13	0.64
2:F:580:ARG:HH22	2:F:640:LYS:HE3	1.60	0.64
1:E:7:TYR:HD1	1:E:8:LEU:N	1.94	0.63
2:B:588:GLN:HG2	2:B:631:ASP:OD1	1.96	0.63
2:F:591:ASN:C	2:F:591:ASN:HD22	2.02	0.63
1:E:71:ARG:HD2	1:E:102:TRP:CH2	2.34	0.62
2:D:588:GLN:HG2	2:D:631:ASP:OD1	2.00	0.62
2:D:549:ASP:HB3	6:D:447:HOH:O	1.99	0.62
1:E:34:ASN:HD22	1:E:34:ASN:C	2.02	0.62
1:G:69:ARG:HH11	1:G:69:ARG:HG2	1.65	0.61
2:H:591:ASN:HD22	2:H:593:GLY:H	1.48	0.61
1:C:34:ASN:C	1:C:34:ASN:HD22	2.04	0.60
2:F:580:ARG:HA	2:F:637:TYR:CZ	2.37	0.60
2:F:638:VAL:HG11	2:F:675:TYR:CE1	2.35	0.60
2:H:591:ASN:ND2	2:H:593:GLY:H	1.99	0.60
1:A:14:ILE:HD11	1:A:106:ILE:HD11	1.83	0.60
1:G:13:LEU:HD23	1:G:85:MET:HB2	1.83	0.60
2:H:592:ASN:HD22	2:H:592:ASN:H	1.48	0.60
1:E:7:TYR:CD1	1:E:8:LEU:N	2.66	0.59
1:C:28:PHE:CE2	1:C:48:ARG:HG2	2.38	0.58
2:B:591:ASN:HD22	2:B:593:GLY:H	1.50	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ARG:NH2	6:C:185:HOH:O	2.36	0.58
1:A:69:ARG:HG2	1:A:69:ARG:HH11	1.67	0.57
1:A:14:ILE:HD13	1:A:106:ILE:HD11	1.83	0.57
1:G:7:TYR:HE2	1:G:55:LYS:CD	2.17	0.57
2:H:591:ASN:C	2:H:591:ASN:HD22	2.08	0.57
1:G:71:ARG:NH2	6:G:191:HOH:O	2.38	0.56
1:A:135:ARG:HG2	1:A:135:ARG:HH11	1.70	0.56
2:F:591:ASN:HD22	2:F:593:GLY:H	1.53	0.56
2:F:591:ASN:ND2	2:F:593:GLY:H	2.04	0.56
1:C:80:GLY:HA2	2:H:645:ILE:HG22	1.88	0.56
2:B:652:LYS:HG2	2:B:653:ILE:N	2.19	0.56
2:B:591:ASN:C	2:B:591:ASN:HD22	2.09	0.56
1:A:56:ARG:HH22	2:B:554:MET:CE	2.18	0.55
2:B:579:PHE:CD1	2:B:643:VAL:HG11	2.41	0.55
1:G:67:GLN:NE2	1:G:69:ARG:NH1	2.50	0.55
1:E:50:ILE:HD12	1:E:52:LEU:HD13	1.89	0.54
1:C:72:THR:HG22	2:D:605:LEU:HD11	1.88	0.54
1:C:34:ASN:HD22	1:C:35:SER:N	2.06	0.54
1:C:133:LYS:O	1:C:137:GLU:HG3	2.07	0.54
2:D:589:ILE:HG12	2:D:632:ILE:CD1	2.37	0.54
1:A:134:GLU:HG3	6:A:187:HOH:O	2.08	0.53
1:G:7:TYR:HE2	1:G:55:LYS:HD2	1.73	0.53
1:A:50:ILE:HD13	1:A:57:ILE:HB	1.89	0.53
1:A:176:LYS:CG	2:F:640:LYS:HE2	2.39	0.52
2:H:540:GLU:HG2	2:H:543:TYR:CD1	2.45	0.52
1:A:28:PHE:CE2	1:A:48:ARG:HG2	2.45	0.52
2:H:663:ARG:NH1	2:H:663:ARG:HG3	2.20	0.52
1:A:48:ARG:HD2	2:B:552:ARG:CZ	2.40	0.52
2:H:558:GLU:O	2:H:562:LEU:HD13	2.10	0.52
1:A:8:LEU:HD13	1:A:58:LYS:HD2	1.92	0.52
2:D:592:ASN:H	2:D:592:ASN:HD22	1.57	0.52
1:E:142:ASP:OD2	2:B:580:ARG:NH2	2.44	0.51
2:D:579:PHE:CD1	2:D:643:VAL:CG1	2.94	0.51
1:A:18:GLY:H	4:A:200:GNP:HNB3	1.59	0.50
1:A:176:LYS:HG3	2:F:579:PHE:CZ	2.46	0.50
2:F:592:ASN:HD22	2:F:592:ASN:H	1.58	0.50
2:D:582:LEU:HD21	2:D:584:LYS:HE2	1.92	0.50
1:G:52:LEU:HD22	1:G:57:ILE:HD12	1.93	0.50
2:B:591:ASN:ND2	2:B:593:GLY:H	2.09	0.50
2:F:643:VAL:HG13	2:F:644:THR:H	1.75	0.50
2:D:591:ASN:C	2:D:591:ASN:HD22	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:LYS:O	1:A:176:LYS:C	2.50	0.49
1:A:84:ILE:HD13	1:A:106:ILE:HD12	1.94	0.49
2:D:589:ILE:HG12	2:D:632:ILE:HD11	1.94	0.49
2:H:567:LEU:HD13	2:H:589:ILE:CG2	2.34	0.49
2:F:567:LEU:HD22	2:F:589:ILE:CG2	2.43	0.49
2:H:588:GLN:HG3	2:H:631:ASP:OD1	2.12	0.49
1:C:10:LYS:NZ	6:C:546:HOH:O	2.46	0.49
1:G:57:ILE:HD11	1:G:170:LYS:HD2	1.94	0.48
2:F:643:VAL:HG13	2:F:644:THR:N	2.28	0.48
1:A:50:ILE:HD13	1:A:57:ILE:O	2.13	0.48
2:H:592:ASN:HD22	2:H:592:ASN:N	2.09	0.48
2:D:591:ASN:HD22	2:D:593:GLY:H	1.62	0.48
1:G:18:GLY:H	4:G:200:GNP:HNB3	1.62	0.48
2:F:611:CYS:HB3	2:F:657:LEU:CD2	2.44	0.48
2:B:640:LYS:HA	2:B:643:VAL:HG22	1.97	0.47
2:F:579:PHE:CD2	2:F:580:ARG:HG2	2.50	0.46
1:G:52:LEU:HB2	1:G:57:ILE:HD12	1.98	0.46
2:D:569:ARG:HH12	2:D:585:GLU:HG2	1.80	0.46
1:C:80:GLY:CA	2:H:645:ILE:HG22	2.45	0.46
1:G:172:LYS:HA	1:G:175:LYS:HE2	1.96	0.46
1:C:117:MET:CE	1:C:148:MET:CE	2.94	0.46
1:E:34:ASN:HD22	1:E:35:SER:N	2.14	0.46
1:G:48:ARG:NH2	1:G:159:GLU:OE1	2.49	0.45
1:C:45:PHE:HA	1:C:61:ILE:O	2.16	0.45
1:A:111:SER:OG	2:F:647:ASN:ND2	2.49	0.45
2:F:641:ASP:OD2	2:F:641:ASP:N	2.50	0.45
1:G:133:LYS:HE3	1:G:137:GLU:OE2	2.16	0.45
1:A:118:ILE:HD11	1:A:145:ILE:HD11	1.98	0.44
2:H:611:CYS:HB3	2:H:657:LEU:CD2	2.47	0.44
2:D:582:LEU:HD21	2:D:584:LYS:CE	2.47	0.44
2:H:602:ILE:HD13	2:H:660:HIS:HB2	1.97	0.44
1:C:117:MET:HE2	1:C:148:MET:CE	2.47	0.44
1:E:71:ARG:O	1:E:75:THR:HG23	2.17	0.44
2:F:654:GLU:HA	2:F:671:ILE:O	2.17	0.44
2:B:592:ASN:HD22	2:B:592:ASN:N	2.16	0.44
1:G:7:TYR:HE2	1:G:55:LYS:HD3	1.82	0.44
1:E:88:TYR:CG	1:E:99:ILE:HD11	2.51	0.43
2:B:554:MET:HA	2:H:557:MET:CE	2.42	0.43
1:C:146:LYS:HZ2	1:C:168:ASP:CG	2.21	0.43
2:H:544:ARG:O	2:H:548:GLU:HG3	2.18	0.43
2:B:592:ASN:HD22	2:B:592:ASN:H	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:567:LEU:HD23	2:B:567:LEU:N	2.33	0.43
1:A:115:GLU:OE1	1:A:172:LYS:HD2	2.19	0.43
1:A:176:LYS:HG3	2:F:579:PHE:CE2	2.54	0.43
2:F:676:LEU:HA	2:F:677:PRO:HD2	1.86	0.43
2:F:601:PHE:HA	2:F:658:VAL:O	2.19	0.43
2:D:591:ASN:ND2	2:D:593:GLY:H	2.16	0.43
1:E:47:ILE:C	1:E:47:ILE:HD12	2.39	0.42
1:G:133:LYS:NZ	6:G:212:HOH:O	2.52	0.42
1:E:28:PHE:CE2	1:E:48:ARG:HG2	2.54	0.42
1:E:8:LEU:HD13	1:E:58:LYS:CG	2.49	0.42
1:A:56:ARG:HH22	2:B:554:MET:HE2	1.84	0.42
1:A:69:ARG:HG2	1:A:69:ARG:NH1	2.33	0.42
1:C:117:MET:CE	1:C:148:MET:HE3	2.49	0.42
1:G:43:ILE:HG22	2:H:666:ASP:HB2	2.01	0.42
2:F:567:LEU:CD1	2:F:669:LEU:HD21	2.50	0.42
1:G:73:ILE:HD12	2:H:604:LYS:HB3	2.01	0.42
1:G:44:ASP:OD2	2:H:665:LYS:HE2	2.20	0.42
1:G:67:GLN:HG3	6:G:193:HOH:O	2.20	0.42
1:E:43:ILE:HG22	2:F:666:ASP:HB2	2.02	0.41
1:A:106:ILE:HG21	1:A:116:LYS:HD3	2.01	0.41
1:C:50:ILE:HD12	1:C:52:LEU:HD13	2.02	0.41
2:F:557:MET:O	2:F:561:PHE:HD1	2.03	0.41
1:A:50:ILE:H	1:A:50:ILE:HD13	1.85	0.41
1:G:125:VAL:O	1:G:125:VAL:CG1	2.66	0.41
2:F:591:ASN:ND2	2:F:591:ASN:C	2.72	0.41
2:B:567:LEU:HD22	2:B:589:ILE:HG22	2.01	0.41
1:G:50:ILE:HD12	1:G:52:LEU:HD13	2.01	0.41
1:G:45:PHE:HA	1:G:61:ILE:O	2.20	0.41
1:E:34:ASN:ND2	1:E:34:ASN:C	2.73	0.41
2:H:653:ILE:O	2:H:672:SER:HA	2.21	0.41
2:H:611:CYS:HB3	2:H:657:LEU:HD21	2.03	0.41
2:F:573:VAL:O	2:F:585:GLU:OE1	2.38	0.41
2:F:592:ASN:HD22	2:F:592:ASN:N	2.16	0.40
1:A:140:ALA:HB1	1:A:145:ILE:O	2.21	0.40
1:C:134:GLU:HB2	6:C:214:HOH:O	2.20	0.40
1:E:125:VAL:CG1	1:E:125:VAL:O	2.60	0.40
1:A:7:TYR:HE2	1:A:55:LYS:HG3	1.86	0.40
1:G:69:ARG:NH1	1:G:69:ARG:HG2	2.36	0.40
1:A:94:LYS:HE3	1:A:98:ASN:HD21	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:ASP:OD1	1:G:127:ASP:OD1[3_545]	2.09	0.11

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	168/174 (97%)	164 (98%)	4 (2%)	0	100	100
1	C	169/174 (97%)	166 (98%)	3 (2%)	0	100	100
1	E	167/174 (96%)	162 (97%)	5 (3%)	0	100	100
1	G	167/174 (96%)	163 (98%)	4 (2%)	0	100	100
2	B	128/140 (91%)	124 (97%)	4 (3%)	0	100	100
2	D	128/140 (91%)	126 (98%)	2 (2%)	0	100	100
2	F	137/140 (98%)	134 (98%)	2 (2%)	1 (1%)	26	19
2	H	137/140 (98%)	136 (99%)	1 (1%)	0	100	100
All	All	1201/1256 (96%)	1175 (98%)	25 (2%)	1 (0%)	56	53

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	640	LYS

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	147/150 (98%)	140 (95%)	7 (5%)	31	26
1	C	148/150 (99%)	146 (99%)	2 (1%)	74	77
1	E	146/150 (97%)	143 (98%)	3 (2%)	61	63
1	G	146/150 (97%)	141 (97%)	5 (3%)	44	41
2	B	124/133 (93%)	119 (96%)	5 (4%)	38	33
2	D	124/133 (93%)	117 (94%)	7 (6%)	26	20
2	F	133/133 (100%)	123 (92%)	10 (8%)	17	11
2	H	133/133 (100%)	126 (95%)	7 (5%)	28	22
All	All	1101/1132 (97%)	1055 (96%)	46 (4%)	36	31

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	50	ILE
1	A	52	LEU
1	A	56	ARG
1	A	119	LEU
1	A	141	LEU
1	A	176	LYS
1	C	34	ASN
1	C	52	LEU
1	E	7	TYR
1	E	34	ASN
1	E	126	ASN
1	G	47	ILE
1	G	52	LEU
1	G	90	ILE
1	G	141	LEU
1	G	172	LYS
2	B	556	ARG
2	B	562	LEU
2	B	567	LEU
2	B	591	ASN
2	B	592	ASN
2	D	562	LEU
2	D	583	GLN
2	D	585	GLU
2	D	591	ASN
2	D	592	ASN

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Mol	Chain	Res	Type
2	D	624	LEU
2	D	650	GLU
2	F	562	LEU
2	F	591	ASN
2	F	592	ASN
2	F	620	PHE
2	F	631	ASP
2	F	641	ASP
2	F	644	THR
2	F	645	ILE
2	F	646	LEU
2	F	647	ASN
2	H	567	LEU
2	H	584	LYS
2	H	591	ASN
2	H	592	ASN
2	H	606	ASN
2	H	644	THR
2	H	663	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	34	ASN
1	E	34	ASN
1	E	126	ASN
1	E	155	ASN
1	E	157	ASN
1	E	160	ASN
1	G	67	GLN
1	G	157	ASN
2	B	588	GLN
2	B	591	ASN
2	B	592	ASN
2	B	609	GLN
2	D	591	ASN
2	D	592	ASN
2	D	609	GLN
2	F	583	GLN
2	F	591	ASN
2	F	592	ASN
2	F	609	GLN

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Mol	Chain	Res	Type
2	H	591	ASN
2	H	592	ASN
2	H	594	GLN
2	H	598	HIS
2	H	609	GLN
2	H	647	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 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	$\# Z > 2$
4	GNP	A	200	3	28,34,34	1.66	7 (25%)	33,54,54	1.83	10 (30%)
5	SO4	B	1	-	4,4,4	0.22	0	6,6,6	0.23	0
4	GNP	C	200	3	28,34,34	2.00	7 (25%)	33,54,54	2.00	10 (30%)
5	SO4	D	2	-	4,4,4	0.28	0	6,6,6	0.31	0
4	GNP	E	200	3	28,34,34	1.82	7 (25%)	33,54,54	1.86	7 (21%)
4	GNP	G	200	3	28,34,34	1.61	6 (21%)	33,54,54	1.94	8 (24%)

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	GNP	A	200	3	-	1/12/38/38	0/3/3/3
5	SO4	B	1	-	-	0/0/0/0	0/0/0/0
4	GNP	C	200	3	-	1/12/38/38	0/3/3/3
5	SO4	D	2	-	-	0/0/0/0	0/0/0/0
4	GNP	E	200	3	-	1/12/38/38	0/3/3/3
4	GNP	G	200	3	-	1/12/38/38	0/3/3/3

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	200	GNP	PB-O2B	-4.06	1.45	1.56
4	G	200	GNP	PB-O2B	-3.47	1.47	1.56
4	A	200	GNP	PB-O2B	-3.22	1.47	1.56
4	E	200	GNP	PB-O2B	-3.11	1.48	1.56
4	E	200	GNP	PA-O1A	-2.16	1.43	1.51
4	E	200	GNP	PA-O2A	-2.07	1.46	1.54
4	A	200	GNP	PA-O2A	-2.05	1.46	1.54
4	C	200	GNP	PA-O2A	-2.01	1.46	1.54
4	G	200	GNP	PB-O3A	2.06	1.61	1.59
4	G	200	GNP	C2-N1	2.09	1.39	1.35
4	A	200	GNP	C6-N1	2.17	1.37	1.33
4	A	200	GNP	C2-N1	2.20	1.39	1.35
4	C	200	GNP	C2-N1	2.29	1.39	1.35
4	G	200	GNP	PG-O1G	2.54	1.49	1.46
4	G	200	GNP	PB-O1B	2.95	1.49	1.46
4	E	200	GNP	C2-N1	2.96	1.40	1.35
4	A	200	GNP	PB-O3A	3.05	1.62	1.59
4	C	200	GNP	PB-O1B	3.42	1.50	1.46
4	C	200	GNP	PB-O3A	3.43	1.63	1.59
4	C	200	GNP	C6-N1	3.51	1.39	1.33
4	E	200	GNP	PG-O1G	3.78	1.50	1.46
4	E	200	GNP	C6-N1	3.78	1.40	1.33
4	G	200	GNP	C6-N1	3.97	1.40	1.33
4	A	200	GNP	O4'-C1'	3.97	1.46	1.41
4	A	200	GNP	PG-O1G	4.16	1.50	1.46
4	E	200	GNP	O4'-C1'	4.44	1.46	1.41
4	C	200	GNP	PG-O1G	5.84	1.52	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	200	GNP	N3-C2-N1	-4.79	120.15	127.44
4	G	200	GNP	N3-C2-N1	-4.40	120.74	127.44
4	C	200	GNP	N3-C2-N1	-4.20	121.05	127.44
4	G	200	GNP	C5-C6-N1	-4.03	118.07	123.59
4	A	200	GNP	N3-C2-N1	-3.77	121.71	127.44
4	E	200	GNP	C5-C6-N1	-3.65	118.60	123.59
4	A	200	GNP	O1B-PB-N3B	-3.64	106.31	111.90
4	A	200	GNP	O1G-PG-N3B	-3.63	106.33	111.90
4	C	200	GNP	O3G-PG-O1G	-3.59	103.96	113.49
4	C	200	GNP	O1B-PB-N3B	-3.50	106.53	111.90
4	C	200	GNP	C5-C6-N1	-3.23	119.17	123.59
4	G	200	GNP	PA-O3A-PB	-2.90	122.94	132.67
4	G	200	GNP	O1B-PB-N3B	-2.80	107.60	111.90
4	C	200	GNP	C4-C5-N7	-2.72	106.98	109.48
4	E	200	GNP	C4-C5-N7	-2.67	107.02	109.48
4	C	200	GNP	O1G-PG-N3B	-2.67	107.81	111.90
4	G	200	GNP	O1G-PG-N3B	-2.62	107.88	111.90
4	E	200	GNP	PA-O3A-PB	-2.59	123.98	132.67
4	G	200	GNP	O3A-PA-O5'	-2.41	96.55	102.94
4	A	200	GNP	O2G-PG-O1G	-2.39	107.13	113.49
4	E	200	GNP	O2G-PG-O1G	-2.34	107.27	113.49
4	A	200	GNP	PA-O3A-PB	-2.13	125.52	132.67
4	C	200	GNP	O3A-PB-N3B	-2.10	100.66	106.44
4	A	200	GNP	C4-C5-N7	-2.09	107.55	109.48
4	A	200	GNP	O3G-PG-O1G	-2.07	107.99	113.49
4	A	200	GNP	O3G-PG-O2G	2.15	113.95	107.58
4	C	200	GNP	C6-N1-C2	2.27	119.08	115.94
4	C	200	GNP	N2-C2-N3	2.66	122.91	117.80
4	E	200	GNP	C6-N1-C2	2.81	119.84	115.94
4	A	200	GNP	N2-C2-N3	2.99	123.54	117.80
4	G	200	GNP	C6-N1-C2	3.35	120.59	115.94
4	A	200	GNP	O2B-PB-O1B	3.74	117.80	110.00
4	E	200	GNP	O2B-PB-O1B	3.88	118.09	110.00
4	G	200	GNP	O2B-PB-O1B	4.26	118.90	110.00
4	C	200	GNP	O2B-PB-O1B	4.74	119.90	110.00

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	200	GNP	O1B-PB-N3B-PG
4	G	200	GNP	O1B-PB-N3B-PG
4	A	200	GNP	O1B-PB-N3B-PG

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Mol	Chain	Res	Type	Atoms
4	C	200	GNP	O1B-PB-N3B-PG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	200	GNP	1	0
4	G	200	GNP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	170/174 (97%)	0.34	8 (4%) 35 37	20, 33, 56, 79	1 (0%)
1	C	171/174 (98%)	0.24	7 (4%) 41 42	16, 29, 56, 69	1 (0%)
1	E	169/174 (97%)	0.25	5 (2%) 54 55	25, 41, 63, 76	0
1	G	169/174 (97%)	0.14	3 (1%) 71 72	21, 35, 53, 71	1 (0%)
2	B	130/140 (92%)	0.52	13 (10%) 9 10	25, 40, 75, 81	0
2	D	130/140 (92%)	0.26	2 (1%) 76 77	20, 33, 63, 69	0
2	F	139/140 (99%)	0.77	20 (14%) 3 4	30, 50, 80, 87	0
2	H	139/140 (99%)	0.26	5 (3%) 46 48	24, 38, 54, 66	0
All	All	1217/1256 (96%)	0.33	63 (5%) 31 33	16, 37, 65, 87	3 (0%)

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	647	ASN	5.8
1	G	7	TYR	5.7
2	F	646	LEU	5.1
1	A	176	LYS	4.5
2	H	678	SER	4.3
2	B	644	THR	4.3
2	F	648	SER	4.2
1	G	56	ARG	4.0
2	F	638	VAL	3.7
2	F	649	GLY	3.6
1	E	7	TYR	3.6
2	F	677	PRO	3.5
1	C	112	ALA	3.5
2	F	543	TYR	3.4
2	F	579	PHE	3.3
2	F	641	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
2	F	643	VAL	3.2
2	D	678	SER	3.2
2	F	642	SER	3.1
1	C	175	LYS	3.1
2	F	678	SER	3.0
2	F	645	ILE	3.0
2	F	637	TYR	2.9
2	B	646	LEU	2.9
1	E	134	GLU	2.8
1	C	6	ASP	2.8
1	A	175	LYS	2.8
2	F	653	ILE	2.7
2	H	547	PHE	2.7
1	E	37	PHE	2.7
1	E	113	ASP	2.6
2	B	678	SER	2.6
1	A	38	ILE	2.6
1	A	112	ALA	2.6
2	B	579	PHE	2.5
2	F	650	GLU	2.5
2	F	640	LYS	2.5
2	H	544	ARG	2.5
2	B	643	VAL	2.5
2	F	541	ARG	2.5
2	B	554	MET	2.4
2	H	644	THR	2.4
2	B	645	ILE	2.3
2	H	647	ASN	2.3
1	A	113	ASP	2.3
1	C	38	ILE	2.3
2	B	651	ASP	2.2
1	C	127	ASP	2.2
2	B	676	LEU	2.2
1	A	79	ARG	2.2
2	B	623	TYR	2.2
2	B	640	LYS	2.1
2	B	648	SER	2.1
1	C	171	ALA	2.1
2	F	636	VAL	2.1
1	A	111	SER	2.1
2	F	652	LYS	2.1
1	E	38	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	79	ARG	2.1
2	B	550	SER	2.1
1	A	37	PHE	2.1
2	D	650	GLU	2.0
1	C	55	LYS	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(Å ²)	Q<0.9
5	SO4	D	2	5/5	0.86	0.17	3.31	65,65,68,70	0
3	MG	C	201	1/1	1.00	0.16	0.30	18,18,18,18	0
4	GNP	G	200	32/32	0.98	0.13	0.27	21,24,29,32	0
4	GNP	C	200	32/32	0.99	0.14	0.22	15,21,26,30	0
4	GNP	E	200	32/32	0.99	0.12	-0.11	23,28,32,38	0
4	GNP	A	200	32/32	0.98	0.13	-0.20	18,24,30,36	0
5	SO4	B	1	5/5	0.89	0.13	-0.22	63,64,66,68	0
3	MG	A	201	1/1	0.99	0.12	-0.41	24,24,24,24	0
3	MG	E	201	1/1	0.97	0.09	-0.96	30,30,30,30	0
3	MG	G	201	1/1	0.99	0.07	-2.25	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.