



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 05:44 AM GMT

PDB ID : 2IS6
Title : Crystal structure of UvrD-DNA-ADPMgF3 ternary complex
Authors : Yang, W.; Lee, J.Y.
Deposited on : 2006-10-16
Resolution : 2.20 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

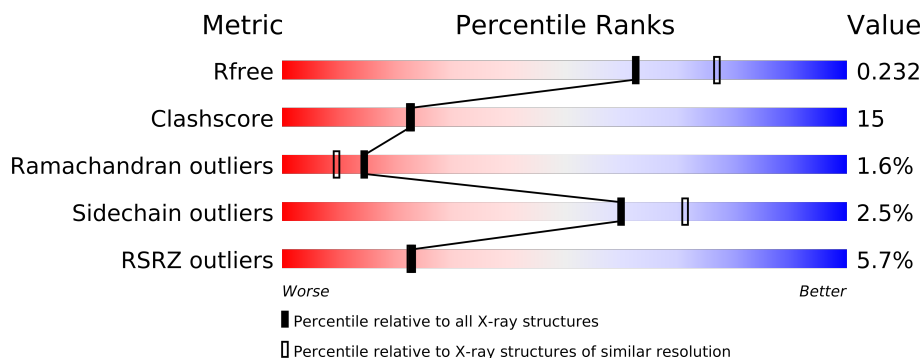
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	C	25	
1	D	25	
2	A	680	
2	B	680	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	MG	A	681	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11795 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DNA chain called 5'-D(*CP*GP*AP*GP*CP*AP*CP*TP*GP*CP*AP*GP*TP*GP*CP*TP*CP*GP*TP*TP*GP*TP*TP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	23	Total	C	N	O	P	0	0	0
			468	224	82	140	22			
1	D	23	Total	C	N	O	P	0	0	0
			468	224	82	140	22			

- Molecule 2 is a protein called DNA helicase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	654	Total	C	N	O	S	0	0	0
			5155	3224	939	966	26			
2	B	652	Total	C	N	O	S	0	0	0
			5127	3208	930	962	27			

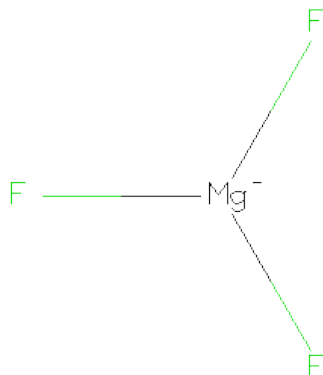
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	399	VAL	ALA	ENGINEERED	UNP P03018
B	399	VAL	ALA	ENGINEERED	UNP P03018

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

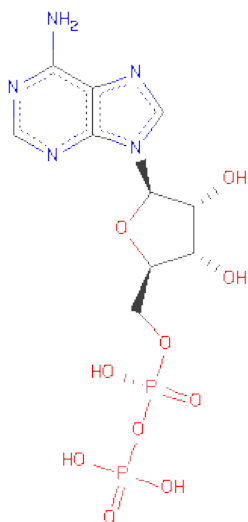
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		

- Molecule 4 is TRIFLUOROMAGNESATE (three-letter code: MGF) (formula: F₃Mg).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	F	Mg	0	0
			4	3	1		
4	B	1	Total	F	Mg	0	0
			4	3	1		

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	
			27	10	5	10	2	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



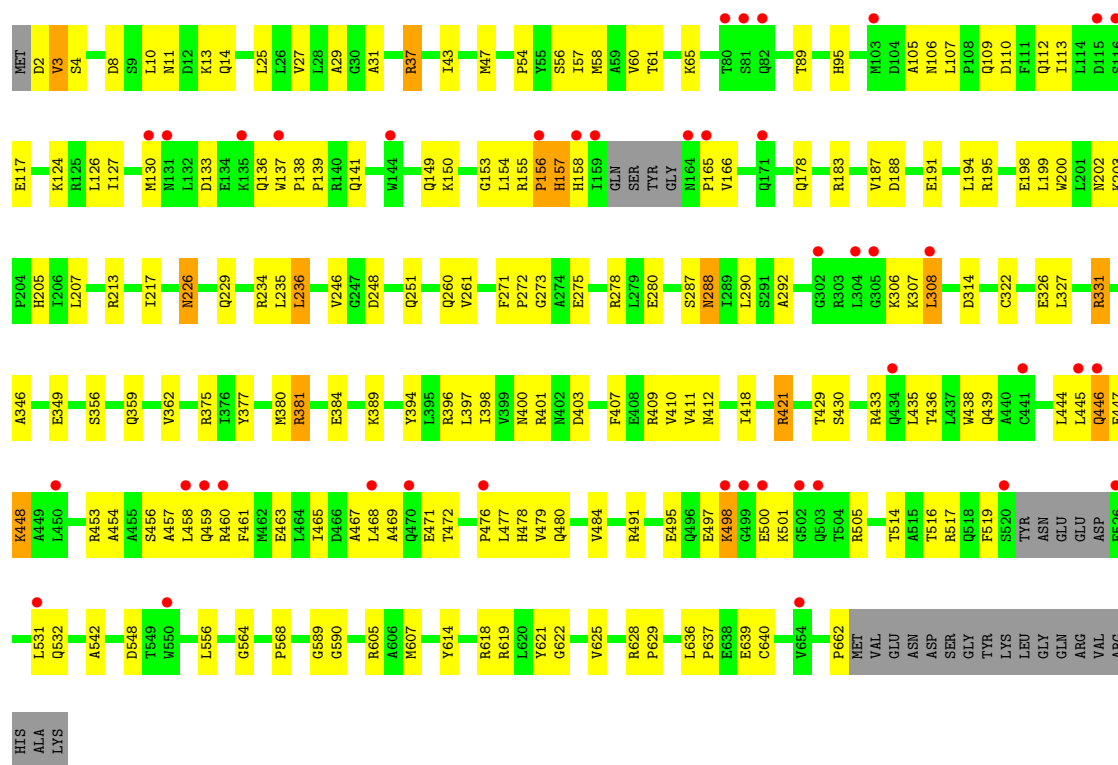
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	243	Total	O	0	0
			243	243		
7	B	239	Total	O	0	0
			239	239		
7	C	15	Total	O	0	0
			15	15		
7	D	10	Total	O	0	0
			10	10		

● Molecule 2: DNA helicase II

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.34Å 96.61Å 110.93Å 90.00° 94.05° 90.00°	Depositor
Resolution (Å)	29.94 – 2.20 48.01 – 2.20	Depositor EDS
% Data completeness (in resolution range)	89.1 (29.94-2.20) 89.2 (48.01-2.20)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 2.20Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.210 , 0.240 0.204 , 0.232	Depositor DCC
R_{free} test set	9797 reflections (11.17%)	DCC
Wilson B-factor (Å ²)	37.7	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 49.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 102183 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11795	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, MGF, ADP

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	C	0.30	0/523	0.73	0/806
1	D	0.29	0/523	0.71	0/806
2	A	0.33	0/5251	0.57	1/7107 (0.0%)
2	B	0.34	0/5220	0.54	1/7062 (0.0%)
All	All	0.33	0/11517	0.57	2/15781 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	662	PRO	N-CA-CB	5.71	110.15	103.30
2	A	653	PRO	N-CA-CB	5.35	109.72	103.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	468	0	262	14	0
1	D	468	0	262	24	0
2	A	5155	0	4971	135	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	5127	0	4969	152	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	6	0	8	2	0
7	A	243	0	0	5	0
7	B	239	0	0	11	0
7	C	15	0	0	1	0
7	D	10	0	0	0	0
All	All	11795	0	10496	320	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (320) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:4:DG:H2''	1:D:5:DC:H5''	1.38	0.99
1:D:5:DC:H2''	1:D:6:DA:C8	2.07	0.90
1:C:18:DG:H2''	1:C:19:DT:H5'	1.52	0.89
2:A:155:ARG:H	2:A:158:HIS:HD2	1.17	0.88
2:A:401:ARG:NH1	2:A:465:ILE:HG22	1.93	0.83
2:B:375:ARG:CZ	2:B:548:ASP:HB2	2.11	0.81
2:A:23:SER:HA	2:A:242:LYS:HD2	1.62	0.80
1:C:13:DT:H2''	1:C:14:DG:C8	2.20	0.77
2:B:468:LEU:O	2:B:472:THR:HG22	1.87	0.74
2:A:475:MET:HB3	2:A:479:VAL:HG13	1.69	0.74
1:D:4:DG:C2'	1:D:5:DC:H5''	2.17	0.73
2:A:491:ARG:O	2:A:495:GLU:HG3	1.87	0.73
1:D:11:DA:H2''	1:D:12:DG:C8	2.25	0.72
1:C:18:DG:C2'	1:C:19:DT:H5'	2.19	0.72
2:A:25:LEU:HD11	2:A:277:ILE:HG13	1.72	0.72
2:A:475:MET:HB3	2:A:479:VAL:CG1	2.19	0.72
2:A:401:ARG:HH11	2:A:465:ILE:HG22	1.53	0.71
2:B:396:ARG:HD2	2:B:403:ASP:OD2	1.91	0.71
2:B:438:TRP:HZ3	2:B:465:ILE:HD12	1.56	0.70
2:A:150:LYS:NZ	2:A:178:GLN:HE22	1.89	0.70
2:B:183:ARG:HD2	2:B:435:LEU:HA	1.73	0.70
2:A:443:GLU:HA	2:A:446:GLN:HG2	1.73	0.70
1:D:6:DA:H1'	1:D:7:DC:H5''	1.72	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:112:GLN:CD	2:B:396:ARG:HD3	2.11	0.70
2:B:112:GLN:HG2	2:B:396:ARG:HH11	1.58	0.69
2:A:155:ARG:H	2:A:158:HIS:CD2	2.05	0.68
2:B:226:ASN:HD21	2:B:229:GLN:HG3	1.58	0.67
2:B:150:LYS:NZ	2:B:178:GLN:HE22	1.92	0.67
2:B:459:GLN:O	2:B:463:GLU:HG3	1.94	0.67
2:A:503:GLN:O	2:A:506:ILE:HG22	1.95	0.67
2:A:25:LEU:HD21	2:A:277:ILE:HD12	1.77	0.66
2:A:1:MET:H3	2:A:5:TYR:HE2	1.44	0.66
2:A:564:GLY:H	2:A:605:ARG:NH2	1.92	0.66
2:A:47:MET:CE	2:A:54:PRO:HG3	2.26	0.66
2:A:477:LEU:HG	2:A:516:THR:HB	1.77	0.65
2:B:436:THR:OG1	2:B:439:GLN:HG3	1.97	0.65
2:B:155:ARG:HB3	2:B:156:PRO:HD2	1.78	0.65
2:B:136:GLN:HE21	2:B:137:TRP:HE1	1.45	0.64
2:A:260:GLN:HG2	7:A:801:HOH:O	1.97	0.64
2:B:187:VAL:HG13	2:B:191:GLU:CG	2.28	0.64
2:B:290:LEU:HD11	2:B:308:LEU:HD13	1.79	0.64
2:A:511:GLU:OE2	2:A:546:GLN:HG3	1.98	0.64
2:B:477:LEU:HG	2:B:516:THR:HB	1.80	0.63
2:B:628:ARG:HB2	2:B:628:ARG:NH2	2.13	0.63
2:A:208:GLN:O	2:A:212:GLU:HG3	1.98	0.63
2:B:628:ARG:HH21	2:B:628:ARG:CB	2.12	0.62
2:A:1:MET:N	2:A:5:TYR:HE2	1.98	0.61
1:C:6:DA:H1'	1:C:7:DC:H5''	1.83	0.61
2:B:191:GLU:OE2	2:B:195:ARG:HD3	2.00	0.60
2:B:398:ILE:HG23	2:B:469:ALA:HA	1.82	0.60
2:A:472:THR:HB	2:A:480:GLN:HG3	1.83	0.60
1:D:11:DA:H2''	1:D:12:DG:H8	1.63	0.60
2:A:356:SER:H	2:A:359:GLN:NE2	2.00	0.60
1:D:6:DA:H2''	1:D:7:DC:H5'	1.83	0.60
2:A:443:GLU:O	2:A:447:GLU:HG3	2.02	0.60
2:B:187:VAL:HG13	2:B:191:GLU:HG3	1.83	0.59
2:A:156:PRO:HB2	2:A:175:GLN:HE21	1.66	0.59
2:A:643:GLU:HG2	2:A:645:ARG:CZ	2.33	0.59
2:B:445:LEU:HD13	2:B:459:GLN:HB2	1.83	0.59
2:A:565:LEU:HD22	6:A:701:GOL:H11	1.85	0.59
2:A:287:SER:HB3	2:A:314:ASP:HA	1.85	0.59
1:D:19:DT:H2''	1:D:20:DT:OP1	2.02	0.58
2:B:202:ASN:O	2:B:203:LYS:HD2	2.03	0.58
2:B:226:ASN:C	2:B:226:ASN:HD22	2.06	0.58
2:A:140:ARG:HH11	2:A:140:ARG:HG3	1.69	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:461:PHE:CZ	2:B:465:ILE:HD11	2.39	0.58
2:A:150:LYS:HZ1	2:A:178:GLN:HE22	1.52	0.57
2:B:472:THR:HG23	2:B:480:GLN:HE21	1.69	0.57
2:A:601:VAL:O	2:A:605:ARG:CD	2.53	0.57
2:A:387:GLU:CD	2:A:505:ARG:HG3	2.24	0.57
2:B:29:ALA:O	2:B:248:ASP:HB2	2.04	0.57
1:D:6:DA:H2''	1:D:7:DC:C5'	2.35	0.57
2:B:326:GLU:CG	2:B:618:ARG:HB2	2.35	0.57
2:B:226:ASN:ND2	2:B:229:GLN:H	2.03	0.57
2:A:170:TRP:CE3	2:A:170:TRP:HA	2.40	0.57
2:A:472:THR:CB	2:A:480:GLN:HG3	2.35	0.56
2:A:601:VAL:O	2:A:605:ARG:HD3	2.05	0.56
2:B:637:PRO:HG2	2:B:640:CYS:SG	2.45	0.56
2:B:207:LEU:HD22	2:B:235:LEU:HD21	1.88	0.56
2:A:567:PHE:CE2	6:A:701:GOL:H2	2.40	0.56
2:A:590:GLY:C	2:A:592:LEU:H	2.06	0.56
2:A:140:ARG:HG3	2:A:140:ARG:NH1	2.21	0.56
2:B:47:MET:CE	2:B:54:PRO:HG3	2.36	0.56
2:B:381:ARG:HA	2:B:381:ARG:NE	2.21	0.55
2:B:56:SER:HA	2:B:213:ARG:O	2.06	0.55
2:A:303:ARG:C	2:A:305:GLY:H	2.08	0.55
2:A:47:MET:HE1	2:A:54:PRO:HG3	1.87	0.55
2:A:346:ALA:HB3	2:A:349:GLU:HG3	1.88	0.55
2:B:331:ARG:HB3	2:B:331:ARG:HH11	1.72	0.55
2:B:107:LEU:HD21	2:B:195:ARG:NH1	2.22	0.54
2:B:618:ARG:HD3	7:B:829:HOH:O	2.07	0.54
2:A:288:ASN:HB2	2:A:314:ASP:O	2.07	0.54
2:B:381:ARG:H	2:B:384:GLU:HG3	1.73	0.54
2:A:476:PRO:HD2	2:A:479:VAL:HG11	1.90	0.54
2:A:538:ALA:O	2:A:542:ALA:HB2	2.07	0.54
2:B:124:LYS:HG2	2:B:139:PRO:HG2	1.90	0.54
2:A:503:GLN:O	2:A:507:GLU:HG3	2.08	0.54
2:B:429:THR:OG1	2:B:444:LEU:HD11	2.07	0.54
2:A:156:PRO:HA	2:A:171:GLN:NE2	2.24	0.53
2:A:442:ARG:HD3	2:A:462:MET:HE1	1.91	0.53
2:B:430:SER:HA	2:B:435:LEU:HD12	1.90	0.53
2:B:105:ALA:O	2:B:106:ASN:HB3	2.08	0.53
2:B:346:ALA:HB3	2:B:349:GLU:HG3	1.90	0.53
2:B:43:ILE:HG23	2:B:57:ILE:HD13	1.91	0.53
2:A:61:THR:O	2:A:89:THR:HA	2.09	0.53
2:B:261:VAL:HG23	7:B:905:HOH:O	2.08	0.53
2:B:47:MET:HE1	2:B:54:PRO:HG3	1.90	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:506:ILE:HD12	2:A:509:LEU:HD12	1.91	0.53
2:A:605:ARG:N	2:A:605:ARG:HD2	2.24	0.53
2:B:497:GLU:OE1	2:B:505:ARG:HD2	2.09	0.52
2:A:163:GLY:O	2:A:164:ASN:C	2.48	0.52
2:A:170:TRP:HE3	2:A:170:TRP:HA	1.75	0.52
2:A:222:PHE:O	2:A:225:THR:HG23	2.10	0.52
2:B:421:ARG:HD2	2:B:421:ARG:N	2.24	0.52
2:A:137:TRP:CZ3	2:A:166:VAL:HA	2.45	0.52
2:A:470:GLN:HG3	7:A:919:HOH:O	2.09	0.52
2:B:153:GLY:HA2	2:B:194:LEU:HD13	1.90	0.52
2:B:11:ASN:OD1	2:B:14:GLN:HG3	2.10	0.52
2:B:326:GLU:HG3	2:B:618:ARG:HB2	1.92	0.51
1:D:10:DC:H2''	1:D:11:DA:C5'	2.39	0.51
1:D:10:DC:H2''	1:D:11:DA:H5'	1.92	0.51
2:B:356:SER:H	2:B:359:GLN:NE2	2.08	0.51
2:A:194:LEU:O	2:A:198:GLU:HG3	2.11	0.51
2:A:361:ARG:O	2:A:365:GLU:HG3	2.09	0.51
2:A:472:THR:HG22	2:A:475:MET:SD	2.51	0.51
2:B:430:SER:HB3	2:B:435:LEU:O	2.09	0.51
1:D:18:DG:H21	1:D:19:DT:H71	1.75	0.51
2:B:389:LYS:HB3	2:B:409:ARG:NE	2.25	0.51
2:B:25:LEU:HD12	2:B:275:GLU:O	2.10	0.51
2:B:226:ASN:ND2	2:B:229:GLN:HG3	2.24	0.51
2:A:592:LEU:HD21	7:A:934:HOH:O	2.10	0.51
2:A:592:LEU:HD21	2:A:631:ARG:NH1	2.26	0.50
2:B:61:THR:O	2:B:89:THR:HA	2.11	0.50
2:A:375:ARG:CZ	2:A:548:ASP:HB3	2.41	0.50
2:A:156:PRO:HA	2:A:171:GLN:HE22	1.76	0.50
2:A:102:HIS:NE2	2:A:109:GLN:HB2	2.27	0.50
2:A:389:LYS:HB3	2:A:409:ARG:NE	2.26	0.50
2:A:514:THR:O	2:A:517:ARG:HB3	2.12	0.50
2:A:164:ASN:OD1	2:A:166:VAL:HG23	2.12	0.50
2:A:102:HIS:CE1	2:A:109:GLN:HB2	2.46	0.50
2:B:375:ARG:NE	2:B:548:ASP:HB2	2.27	0.50
2:B:133:ASP:HB3	2:B:136:GLN:HB3	1.93	0.50
2:A:576:GLU:HG3	2:A:579:MET:CG	2.42	0.50
2:A:480:GLN:O	2:A:484:VAL:HG23	2.11	0.50
2:A:114:LEU:CD1	2:A:118:ASP:HB3	2.41	0.50
2:A:500:GLU:O	2:A:504:THR:HG22	2.12	0.50
2:A:442:ARG:NH1	2:A:462:MET:HE2	2.27	0.49
2:B:37:ARG:HD2	7:B:790:HOH:O	2.11	0.49
2:B:456:SER:O	2:B:460:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:263:ASN:HB2	7:A:721:HOH:O	2.11	0.49
2:A:376:ILE:HG12	2:A:556:LEU:HB2	1.94	0.49
2:B:394:TYR:O	2:B:398:ILE:HG13	2.13	0.49
2:B:194:LEU:O	2:B:198:GLU:HG3	2.12	0.49
2:B:133:ASP:HB3	2:B:136:GLN:CB	2.42	0.49
2:B:381:ARG:HB3	7:B:835:HOH:O	2.12	0.49
2:A:494:TYR:CE2	2:A:505:ARG:HD3	2.47	0.49
2:A:126:LEU:O	2:A:130:MET:HG3	2.13	0.49
2:A:130:MET:O	2:A:131:ASN:HB2	2.13	0.48
2:B:531:LEU:HD23	2:B:531:LEU:O	2.14	0.48
2:A:79:GLY:C	2:A:81:SER:H	2.16	0.48
2:A:401:ARG:HB3	2:A:438:TRP:CD2	2.48	0.48
2:B:31:ALA:HB2	2:B:251:GLN:NE2	2.29	0.48
2:B:435:LEU:HB2	2:B:439:GLN:OE1	2.14	0.48
2:B:498:LYS:C	2:B:500:GLU:H	2.16	0.48
1:D:9:DG:H3'	2:B:421:ARG:HB2	1.95	0.48
1:D:5:DC:P	2:A:124:LYS:HE2	2.54	0.48
1:C:2:DG:H2''	1:C:3:DA:OP2	2.14	0.48
2:B:149:GLN:HG3	2:B:154:LEU:HB2	1.95	0.48
2:B:394:TYR:CE1	2:B:410:VAL:HB	2.49	0.47
2:B:331:ARG:HH11	2:B:331:ARG:CB	2.27	0.47
2:B:568:PRO:HA	2:B:607:MET:HB2	1.96	0.47
2:A:408:GLU:HG2	2:A:437:LEU:CD1	2.44	0.47
2:A:364:GLU:HG3	2:A:374:TYR:CZ	2.49	0.47
2:B:447:GLU:O	2:B:448:LYS:C	2.52	0.47
2:B:628:ARG:NH2	2:B:628:ARG:CB	2.73	0.47
2:B:199:LEU:O	2:B:203:LYS:HB2	2.14	0.47
2:A:588:GLU:CB	2:A:591:ARG:HD2	2.44	0.47
2:B:476:PRO:HB2	2:B:479:VAL:HG23	1.96	0.47
1:D:18:DG:H21	1:D:19:DT:C7	2.27	0.47
1:D:23:DT:H2'	7:B:766:HOH:O	2.12	0.47
2:A:601:VAL:O	2:A:605:ARG:HD2	2.15	0.47
1:C:6:DA:H2''	1:C:7:DC:H5'	1.95	0.47
2:A:442:ARG:HH11	2:A:462:MET:HE2	1.78	0.47
2:B:380:MET:SD	2:B:384:GLU:HB2	2.54	0.47
2:B:165:PRO:HG2	2:B:166:VAL:H	1.79	0.47
2:A:476:PRO:O	2:A:479:VAL:HG12	2.15	0.47
2:B:618:ARG:O	2:B:625:VAL:HG22	2.15	0.47
2:B:453:ARG:CG	2:B:454:ALA:N	2.78	0.47
2:A:56:SER:HA	2:A:213:ARG:O	2.15	0.47
2:A:481:THR:O	2:A:485:ILE:HG13	2.14	0.47
2:A:1:MET:N	2:A:5:TYR:CE2	2.79	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:A:564:GLY:H	2:A:605:ARG:HH21	1.59	0.47
2:B:27:VAL:HB	2:B:246:VAL:HG12	1.97	0.47
2:A:150:LYS:NZ	2:A:178:GLN:NE2	2.60	0.47
2:A:60:VAL:HG22	2:A:61:THR:N	2.30	0.47
2:A:290:LEU:HD11	2:A:308:LEU:HD13	1.96	0.47
2:A:27:VAL:HB	2:A:246:VAL:HG12	1.97	0.46
2:B:13:LYS:HG2	2:B:278:ARG:O	2.14	0.46
2:B:397:LEU:O	2:B:401:ARG:HD2	2.16	0.46
7:C:596:HOH:O	2:B:619:ARG:HD3	2.14	0.46
2:B:619:ARG:NH1	2:B:622:GLY:O	2.48	0.46
2:B:155:ARG:O	2:B:157:HIS:N	2.48	0.46
2:B:480:GLN:O	2:B:484:VAL:HG23	2.15	0.46
2:B:429:THR:O	2:B:433:ARG:HG2	2.15	0.46
2:A:97:LEU:HD13	7:A:789:HOH:O	2.15	0.46
2:B:497:GLU:O	2:B:498:LYS:C	2.54	0.46
2:B:290:LEU:HD11	2:B:308:LEU:CD1	2.45	0.46
2:B:110:ASP:OD1	2:B:532:GLN:HG2	2.16	0.46
2:A:282:ASN:HB2	2:A:308:LEU:HD22	1.97	0.46
2:A:308:LEU:HA	2:A:308:LEU:HD23	1.82	0.46
2:B:126:LEU:HG	2:B:130:MET:CE	2.46	0.46
2:A:126:LEU:CD1	2:A:177:TYR:HA	2.46	0.45
2:B:411:VAL:HG13	2:B:412:ASN:N	2.31	0.45
2:B:331:ARG:NH1	2:B:331:ARG:HB3	2.31	0.45
2:B:2:ASP:O	2:B:3:VAL:C	2.54	0.45
2:B:150:LYS:HZ1	2:B:178:GLN:HE22	1.63	0.45
2:B:292:ALA:HB1	2:B:636:LEU:HD22	1.99	0.45
2:B:564:GLY:H	2:B:605:ARG:NH2	2.15	0.45
2:A:494:TYR:O	2:A:497:GLU:HB2	2.17	0.45
1:C:11:DA:H2''	1:C:12:DG:C8	2.51	0.45
2:B:112:GLN:OE1	2:B:396:ARG:HD3	2.17	0.45
2:B:384:GLU:OE2	2:B:542:ALA:HB1	2.16	0.45
1:D:5:DC:H2''	1:D:6:DA:N7	2.29	0.45
2:B:234:ARG:HD3	7:B:903:HOH:O	2.17	0.45
2:A:475:MET:CE	2:A:479:VAL:HG22	2.47	0.44
2:A:16:GLU:O	2:A:20:ALA:HB2	2.17	0.44
2:A:459:GLN:HG3	2:A:463:GLU:OE2	2.17	0.44
2:A:114:LEU:HD12	2:A:118:ASP:HB3	1.99	0.44
2:B:138:PRO:O	2:B:141:GLN:HB2	2.17	0.44
1:D:21:DG:H2'	1:D:21:DG:H8	1.71	0.44
2:A:226:ASN:ND2	2:A:229:GLN:H	2.15	0.44
2:A:542:ALA:C	2:A:544:GLU:H	2.21	0.44
2:A:411:VAL:HA	2:A:461:PHE:CZ	2.52	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:18:DG:H1'	1:C:19:DT:H5'	1.99	0.44
2:A:226:ASN:C	2:A:226:ASN:HD22	2.21	0.44
2:B:327:LEU:HD23	2:B:362:VAL:HG13	1.98	0.44
2:B:271:PHE:HA	2:B:272:PRO:HD3	1.83	0.44
1:D:15:DC:H2''	1:D:16:DT:H72	1.99	0.44
2:A:401:ARG:HH22	2:A:469:ALA:CB	2.29	0.44
2:A:41:HIS:CD2	2:A:77:LEU:HD22	2.53	0.44
1:C:6:DA:H2''	1:C:7:DC:C5'	2.48	0.43
2:A:374:TYR:HA	2:A:553:ALA:HB1	2.00	0.43
2:A:133:ASP:HB3	2:A:136:GLN:CB	2.48	0.43
1:C:12:DG:H2''	1:C:13:DT:OP2	2.19	0.43
1:D:18:DG:C4	2:B:621:TYR:HD2	2.36	0.43
2:B:60:VAL:HG22	2:B:61:THR:N	2.33	0.43
2:B:418:ILE:HD11	2:B:458:LEU:HA	2.00	0.43
2:B:457:ALA:O	2:B:460:ARG:HB3	2.17	0.43
2:B:446:GLN:HE21	2:B:447:GLU:N	2.17	0.43
2:B:110:ASP:CG	2:B:532:GLN:HE21	2.21	0.43
2:B:260:GLN:HG2	7:B:808:HOH:O	2.17	0.43
2:A:398:ILE:HD11	2:A:468:LEU:HB3	2.00	0.43
2:A:156:PRO:CB	2:A:175:GLN:HE21	2.28	0.43
2:B:322:CYS:HB2	2:B:614:TYR:CZ	2.53	0.43
2:A:155:ARG:N	2:A:158:HIS:HD2	1.99	0.43
2:B:155:ARG:CB	2:B:156:PRO:HD2	2.48	0.43
2:B:10:LEU:HB3	2:B:14:GLN:HB2	2.01	0.43
2:B:280:GLU:HG3	7:B:837:HOH:O	2.18	0.43
2:B:95:HIS:CD2	2:B:113:ILE:HD11	2.54	0.43
2:B:401:ARG:HH22	2:B:469:ALA:CB	2.32	0.42
2:B:202:ASN:C	2:B:203:LYS:HD2	2.38	0.42
2:A:542:ALA:C	2:A:544:GLU:N	2.73	0.42
2:A:79:GLY:C	2:A:81:SER:N	2.72	0.42
2:B:614:TYR:CE2	2:B:629:PRO:HG3	2.53	0.42
2:B:467:ALA:O	2:B:471:GLU:HG3	2.19	0.42
2:A:127:ILE:HG23	2:A:132:LEU:HB2	2.02	0.42
2:B:65:LYS:HE2	2:B:377:TYR:CG	2.54	0.42
1:C:20:DT:OP1	2:A:584:MET:HG2	2.20	0.42
2:B:628:ARG:HH21	2:B:628:ARG:HB3	1.81	0.42
2:B:127:ILE:HD12	2:B:139:PRO:HG3	2.02	0.42
2:B:2:ASP:O	2:B:4:SER:N	2.53	0.42
1:D:6:DA:C1'	1:D:7:DC:H5''	2.46	0.42
2:A:159:ILE:HG13	2:A:171:GLN:NE2	2.34	0.42
2:A:590:GLY:C	2:A:592:LEU:N	2.72	0.42
1:C:4:DG:H2''	1:C:5:DC:H5'	2.02	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:590:GLY:HA2	7:B:857:HOH:O	2.20	0.42
2:B:226:ASN:HB2	7:B:739:HOH:O	2.20	0.42
1:D:19:DT:OP1	1:D:19:DT:O4'	2.37	0.42
2:A:115:ASP:CG	2:A:389:LYS:HZ1	2.22	0.42
2:B:639:GLU:CD	2:B:639:GLU:H	2.23	0.42
2:B:155:ARG:C	2:B:157:HIS:H	2.23	0.42
2:A:485:ILE:HG22	2:A:491:ARG:HB2	2.02	0.42
2:B:478:HIS:HB3	2:B:517:ARG:HA	2.02	0.42
2:B:556:LEU:N	2:B:556:LEU:HD12	2.35	0.42
2:B:288:ASN:HA	2:B:288:ASN:HD22	1.70	0.42
2:B:188:ASP:OD1	2:B:191:GLU:N	2.47	0.41
2:A:442:ARG:HH11	2:A:462:MET:CE	2.32	0.41
2:A:303:ARG:O	2:A:305:GLY:N	2.52	0.41
2:A:137:TRP:CH2	2:A:166:VAL:HA	2.55	0.41
2:B:273:GLY:O	2:B:275:GLU:HG2	2.20	0.41
2:A:325:ASN:HA	2:A:617:THR:O	2.20	0.41
2:B:126:LEU:HG	2:B:130:MET:HE1	2.03	0.41
2:B:491:ARG:O	2:B:495:GLU:HG3	2.20	0.41
2:B:4:SER:O	2:B:8:ASP:OD1	2.39	0.41
2:B:200:TRP:CH2	2:B:236:LEU:HG	2.55	0.41
2:A:164:ASN:HB3	2:A:167:GLU:HB3	2.02	0.41
2:A:303:ARG:C	2:A:305:GLY:N	2.73	0.41
2:B:418:ILE:CD1	2:B:458:LEU:HA	2.50	0.41
2:A:441:CYS:O	2:A:445:LEU:HG	2.21	0.41
2:A:643:GLU:OE1	2:A:645:ARG:NH2	2.54	0.41
2:A:60:VAL:O	2:A:219:VAL:HA	2.21	0.41
2:A:364:GLU:HG3	2:A:374:TYR:OH	2.20	0.41
1:D:15:DC:C2'	1:D:16:DT:H72	2.51	0.41
1:C:15:DC:H2''	1:C:16:DT:OP2	2.21	0.41
2:B:287:SER:HB3	2:B:314:ASP:HA	2.03	0.41
2:A:203:LYS:CB	2:A:206:ILE:HD12	2.51	0.41
2:B:117:GLU:OE1	2:B:389:LYS:HE3	2.20	0.41
2:B:109:GLN:HG3	2:B:110:ASP:N	2.36	0.41
1:C:18:DG:C1'	1:C:19:DT:H5'	2.51	0.40
2:B:514:THR:O	2:B:517:ARG:HB3	2.21	0.40
2:A:160:GLN:HB2	2:A:160:GLN:HE21	1.68	0.40
2:B:191:GLU:O	2:B:195:ARG:HB2	2.22	0.40
2:B:203:LYS:HG3	2:B:205:HIS:CE1	2.56	0.40
1:D:10:DC:OP2	2:B:421:ARG:HB2	2.21	0.40
2:A:576:GLU:HG3	2:A:579:MET:HG3	2.03	0.40
2:B:478:HIS:CE1	2:B:479:VAL:HG23	2.56	0.40
2:B:37:ARG:CD	7:B:790:HOH:O	2.69	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:453:ARG:CG	2:B:454:ALA:H	2.34	0.40
2:B:397:LEU:HD11	2:B:407:PHE:HA	2.04	0.40
2:B:58:MET:HE2	2:B:217:ILE:HG23	2.04	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	
2	A	650/680 (96%)	610 (94%)	31 (5%)	9 (1%)	16	12
2	B	646/680 (95%)	608 (94%)	26 (4%)	12 (2%)	12	7
All	All	1296/1360 (95%)	1218 (94%)	57 (4%)	21 (2%)	14	9

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	3	VAL
2	B	158	HIS
2	B	448	LYS
2	B	501	LYS
2	B	589	GLY
2	A	304	LEU
2	A	307	LYS
2	B	307	LYS
2	B	519	PHE
2	A	305	GLY
2	B	156	PRO
2	B	306	LYS
2	B	498	LYS
2	A	454	ALA
2	A	498	LYS
2	B	400	ASN
2	A	2	ASP

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Mol	Chain	Res	Type
2	A	134	GLU
2	A	164	ASN
2	B	157	HIS
2	A	308	LEU

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	
2	A	522/574 (91%)	505 (97%)	17 (3%)	50	60
2	B	523/574 (91%)	514 (98%)	9 (2%)	73	84
All	All	1045/1148 (91%)	1019 (98%)	26 (2%)	60	71

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	37	ARG
2	A	103	MET
2	A	160	GLN
2	A	170	TRP
2	A	175	GLN
2	A	195	ARG
2	A	208	GLN
2	A	226	ASN
2	A	235	LEU
2	A	288	ASN
2	A	298	GLU
2	A	308	LEU
2	A	424	ASP
2	A	442	ARG
2	A	483	ARG
2	A	497	GLU
2	A	605	ARG
2	B	37	ARG
2	B	226	ASN
2	B	236	LEU
2	B	288	ASN

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Mol	Chain	Res	Type
2	B	308	LEU
2	B	331	ARG
2	B	381	ARG
2	B	421	ARG
2	B	446	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	119	GLN
2	A	136	GLN
2	A	147	ASN
2	A	158	HIS
2	A	160	GLN
2	A	175	GLN
2	A	178	GLN
2	A	226	ASN
2	A	227	ASN
2	A	265	GLN
2	A	269	ASN
2	A	288	ASN
2	A	359	GLN
2	A	400	ASN
2	A	459	GLN
2	A	496	GLN
2	B	119	GLN
2	B	136	GLN
2	B	147	ASN
2	B	149	GLN
2	B	175	GLN
2	B	178	GLN
2	B	226	ASN
2	B	227	ASN
2	B	288	ASN
2	B	359	GLN
2	B	369	GLN
2	B	446	GLN
2	B	470	GLN
2	B	480	GLN
2	B	503	GLN
2	B	508	ASN
2	B	551	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 7 ligands modelled in this entry, 2 are monoatomic - leaving 5 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	MGF	A	699	3,5,7	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	A	700	3,4	29,29,29	2.70	12 (41%)	45,45,45	2.57	13 (28%)
6	GOL	A	701	-	5,5,5	0.26	0	5,5,5	0.21	0
4	MGF	B	701	3,5,7	0,3,3	0.00	-	0,3,3	0.00	-
5	ADP	B	702	3,4	29,29,29	2.63	10 (34%)	45,45,45	2.55	13 (28%)

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	MGF	A	699	3,5,7	-	0/0/0/0	0/0/0/0
5	ADP	A	700	3,4	-	0/16/32/32	0/1/3/3
6	GOL	A	701	-	-	0/4/4/4	0/0/0/0
4	MGF	B	701	3,5,7	-	0/0/0/0	0/0/0/0
5	ADP	B	702	3,4	-	0/16/32/32	0/1/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	700	ADP	C5-C4	5.94	1.53	1.40
5	A	700	ADP	C2-N1	5.72	1.45	1.33
5	B	702	ADP	C2-N1	5.54	1.44	1.33
5	B	702	ADP	C5-C4	5.46	1.52	1.40
5	A	700	ADP	C2'-C1'	-5.41	1.45	1.53
5	B	702	ADP	C2'-C1'	-5.01	1.46	1.53
5	B	702	ADP	C4-N3	4.87	1.43	1.35
5	B	702	ADP	C2-N3	4.86	1.41	1.32
5	A	700	ADP	C4-N3	4.78	1.42	1.35
5	A	700	ADP	C2-N3	4.67	1.41	1.32
5	A	700	ADP	C4-N9	-4.21	1.31	1.37
5	B	702	ADP	C4-N9	-4.13	1.31	1.37
5	B	702	ADP	PB-O3B	3.06	1.65	1.54
5	A	700	ADP	PB-O3B	3.02	1.65	1.54
5	A	700	ADP	PB-O2B	-2.94	1.44	1.54
5	B	702	ADP	PB-O2B	-2.83	1.44	1.54
5	A	700	ADP	C3'-C4'	-2.67	1.45	1.53
5	A	700	ADP	C8-N9	2.32	1.40	1.36
5	B	702	ADP	C6-C5	2.21	1.55	1.42
5	B	702	ADP	C3'-C4'	-2.18	1.47	1.53
5	A	700	ADP	C6-C5	2.13	1.54	1.42
5	A	700	ADP	C5-N7	-2.12	1.32	1.40

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	702	ADP	N3-C2-N1	-9.88	120.45	128.71
5	A	700	ADP	N3-C2-N1	-9.62	120.66	128.71
5	A	700	ADP	N6-C6-N1	4.96	129.09	119.36
5	A	700	ADP	O4'-C1'-N9	-4.79	103.98	108.44
5	B	702	ADP	O4'-C1'-N9	-4.77	104.00	108.44
5	B	702	ADP	N6-C6-N1	4.76	128.72	119.36
5	A	700	ADP	C2-N1-C6	4.62	127.12	118.77
5	B	702	ADP	C2-N1-C6	4.44	126.78	118.77
5	B	702	ADP	N3-C4-N9	4.11	132.86	125.43
5	A	700	ADP	N3-C4-N9	4.10	132.83	125.43
5	B	702	ADP	C4-C5-N7	-3.85	106.23	109.52
5	A	700	ADP	C4-C5-N7	-3.81	106.26	109.52
5	B	702	ADP	C1'-N9-C4	-3.34	120.86	126.64
5	A	700	ADP	C1'-N9-C4	-3.24	121.03	126.64
5	A	700	ADP	C4'-O4'-C1'	3.10	113.12	109.75
5	A	700	ADP	O5'-PA-O1A	3.06	121.37	109.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	702	ADP	O5'-PA-O1A	2.72	120.04	109.37
5	B	702	ADP	C8-N9-C4	2.69	108.95	106.90
5	A	700	ADP	O2A-PA-O1A	-2.69	97.21	112.21
5	B	702	ADP	C4'-O4'-C1'	2.67	112.65	109.75
5	A	700	ADP	O2B-PB-O1B	2.51	118.64	110.44
5	B	702	ADP	O2A-PA-O1A	-2.46	98.45	112.21
5	B	702	ADP	O4'-C1'-C2'	-2.41	103.07	106.77
5	A	700	ADP	O4'-C1'-C2'	-2.41	103.08	106.77
5	B	702	ADP	O2B-PB-O1B	2.37	118.18	110.44
5	A	700	ADP	C8-N9-C4	2.36	108.70	106.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	23/25 (92%)	0.35	1 (4%) 34 34	35, 83, 122, 136	0
1	D	23/25 (92%)	0.40	1 (4%) 34 34	38, 82, 108, 113	0
2	A	654/680 (96%)	0.25	33 (5%) 28 27	25, 49, 85, 104	1 (0%)
2	B	652/680 (95%)	0.27	42 (6%) 19 18	26, 54, 94, 106	0
All	All	1352/1410 (95%)	0.27	77 (5%) 23 23	25, 52, 92, 136	1 (0%)

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	159	ILE	7.8
2	B	499	GLY	6.9
2	B	304	LEU	6.1
2	A	499	GLY	5.9
2	A	590	GLY	5.8
2	A	526	GLU	5.6
2	A	166	VAL	5.1
2	A	648	ALA	5.0
2	A	81	SER	4.7
2	A	547	ALA	4.6
2	B	158	HIS	4.6
2	A	500	GLU	4.5
2	B	450	LEU	4.5
2	A	651	SER	4.4
2	A	656	HIS	4.4
2	A	649	THR	4.4
2	B	445	LEU	4.3
2	B	302	GLY	4.3
2	B	144	TRP	4.2
2	B	137	TRP	4.2
2	B	305	GLY	4.1

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Mol	Chain	Res	Type	RSRZ
2	B	654	VAL	4.1
2	A	304	LEU	4.0
2	B	500	GLU	3.9
2	B	156	PRO	3.9
2	B	81	SER	3.8
2	B	446	GLN	3.7
2	A	650	VAL	3.7
2	A	496	GLN	3.6
2	A	82	GLN	3.4
2	B	503	GLN	3.4
2	B	82	GLN	3.4
2	A	305	GLY	3.3
2	A	523	GLU	3.3
2	B	80	THR	3.2
2	A	543	GLY	3.2
2	B	165	PRO	3.2
2	A	1	MET	3.2
2	A	527	ASP	3.1
2	B	550	TRP	3.0
2	A	5	TYR	2.9
2	A	80	THR	2.8
2	B	130	MET	2.8
2	A	165	PRO	2.8
2	B	458	LEU	2.7
2	B	470	GLN	2.7
2	A	502	GLY	2.7
2	A	497	GLU	2.6
2	B	441	CYS	2.6
2	B	520	SER	2.5
2	B	131	ASN	2.5
2	B	460	ARG	2.5
2	B	476	PRO	2.5
2	B	459	GLN	2.5
2	A	137	TRP	2.4
2	A	376	ILE	2.4
2	B	468	LEU	2.3
2	A	558	THR	2.3
1	D	19	DT	2.3
2	B	135	LYS	2.3
2	A	301	ASN	2.2
2	B	103	MET	2.2
2	A	302	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	502	GLY	2.2
2	B	308	LEU	2.2
2	A	498	LYS	2.1
2	B	531	LEU	2.1
2	A	63	THR	2.1
2	B	526	GLU	2.1
2	B	115	ASP	2.1
2	A	546	GLN	2.0
2	B	164	ASN	2.0
2	B	498	LYS	2.0
2	B	116	SER	2.0
2	B	434	GLN	2.0
1	C	1	DC	2.0
2	B	171	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	MG	A	681	1/1	0.22	2.70	36,36,36,36	0
6	GOL	A	701	6/6	0.25	1.80	65,68,69,69	0
4	MGF	B	701	4/4	0.12	0.85	29,31,34,36	0
5	ADP	B	702	27/27	0.12	0.70	29,34,43,44	0
3	MG	B	681	1/1	0.12	0.12	33,33,33,33	0
4	MGF	A	699	4/4	0.15	0.07	33,33,35,35	0
5	ADP	A	700	27/27	0.14	-0.03	29,36,43,45	0

6.5 Other polymers ⓘ

There are no such residues in this entry.