



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:42 pm BST

PDB ID : 3EI2
Title : Structure of hsDDB1-drDDB2 bound to a 16 bp abasic site containing DNA-duplex
Authors : Scrima, A.; Thoma, N.H.
Deposited on : 2008-09-15
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

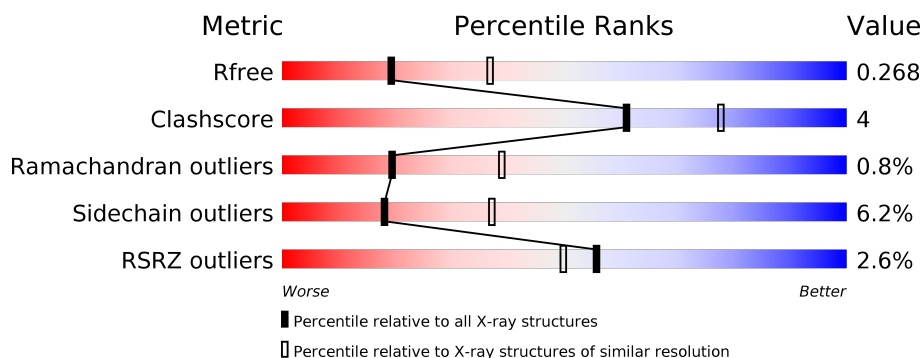
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1158	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>12%</div> <div>• 5%</div> </div> </div>
2	B	383	<div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div>
3	G	16	<div> <div>25%</div> <div>94%</div> <div>6%</div> </div>
4	H	16	<div> <div>13%</div> <div>75%</div> <div>19%</div> <div>6%</div> </div>

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12465 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1103	8714	5523	1471	1671	49	41	8	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	EXPRESSION TAG	UNP Q16531
A	-16	HIS	-	EXPRESSION TAG	UNP Q16531
A	-15	HIS	-	EXPRESSION TAG	UNP Q16531
A	-14	HIS	-	EXPRESSION TAG	UNP Q16531
A	-13	HIS	-	EXPRESSION TAG	UNP Q16531
A	-12	HIS	-	EXPRESSION TAG	UNP Q16531
A	-11	HIS	-	EXPRESSION TAG	UNP Q16531
A	-10	ARG	-	EXPRESSION TAG	UNP Q16531
A	-9	ARG	-	EXPRESSION TAG	UNP Q16531
A	-8	LEU	-	EXPRESSION TAG	UNP Q16531
A	-7	VAL	-	EXPRESSION TAG	UNP Q16531
A	-6	PRO	-	EXPRESSION TAG	UNP Q16531
A	-5	ARG	-	EXPRESSION TAG	UNP Q16531
A	-4	GLY	-	EXPRESSION TAG	UNP Q16531
A	-3	SER	-	EXPRESSION TAG	UNP Q16531
A	-2	GLY	-	EXPRESSION TAG	UNP Q16531
A	-1	GLY	-	EXPRESSION TAG	UNP Q16531
A	0	ARG	-	EXPRESSION TAG	UNP Q16531

- Molecule 2 is a protein called DNA damage-binding protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	355	2854	1812	503	528	11	0	1	0

There are 19 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	75	MET	-	EXPRESSION TAG	UNP Q2YDS1
B	76	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	77	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	78	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	79	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	80	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	81	HIS	-	EXPRESSION TAG	UNP Q2YDS1
B	82	VAL	-	EXPRESSION TAG	UNP Q2YDS1
B	83	ASP	-	EXPRESSION TAG	UNP Q2YDS1
B	84	GLU	-	EXPRESSION TAG	UNP Q2YDS1
B	85	ASN	-	EXPRESSION TAG	UNP Q2YDS1
B	86	LEU	-	EXPRESSION TAG	UNP Q2YDS1
B	87	TYR	-	EXPRESSION TAG	UNP Q2YDS1
B	88	PHE	-	EXPRESSION TAG	UNP Q2YDS1
B	89	GLN	-	EXPRESSION TAG	UNP Q2YDS1
B	90	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	91	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	92	GLY	-	EXPRESSION TAG	UNP Q2YDS1
B	93	ARG	-	EXPRESSION TAG	UNP Q2YDS1

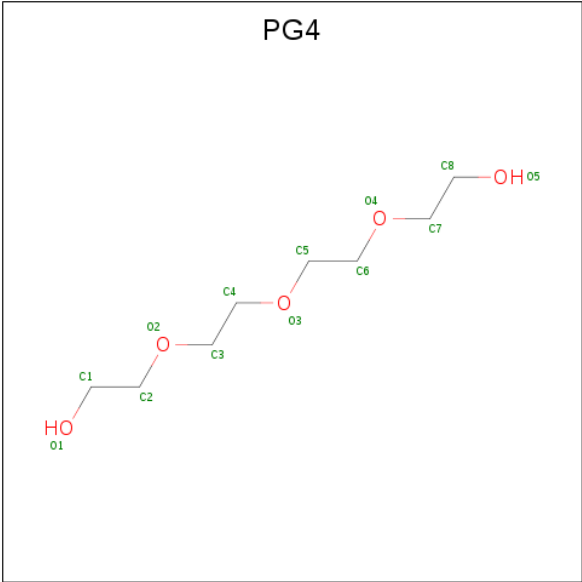
- Molecule 3 is a DNA chain called 5'-D(*DAP*DAP*DAP*DTP*DGP*DAP*DAP*DTP*(3 DR)P*DAP*DAP*DGP*DCP*DAP*DGP*DG)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	15	Total	C	N	O	P	0	0	0
			305	144	62	84	15			

- Molecule 4 is a DNA chain called 5'-D(*DCP*DCP*DTP*DGP*DCP*DTP*DTP*DTP*DA P*DTP*DTP*DCP*DAP*DTP*DTP*DT)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	15	Total	C	N	O	P	0	0	0
			297	146	43	94	14			

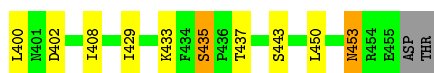
- Molecule 5 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 6 is water.

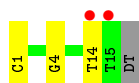
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	209	Total	O	0	0
			209	209		
6	B	65	Total	O	0	0
			65	65		
6	G	4	Total	O	0	0
			4	4		
6	H	4	Total	O	0	0
			4	4		



- Molecule 3: 5'-D(*DAP*DAP*DAP*DTP*DGP*DAP*DAP*DTP*(3DR)P*DAP*DAP*DGP*DCP*DAP*DGP*DG)-3'



- Molecule 4: 5'-D(*DCP*DCP*DTP*DGP*DCP*DTP*DTP*DTP*DAP*DTP*DTP*DCP*DA P*DTP*DTP*DT)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	113.21Å 123.48Å 159.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60 48.91 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.60) 99.9 (48.91-2.60)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.47 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.220 , 0.268 0.219 , 0.268	Depositor DCC
R_{free} test set	3506 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	49.9	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	12465	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, 3DR

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	0.38	2/8875 (0.0%)	0.56	0/12017
2	B	0.37	0/2928	0.59	0/3976
3	G	0.64	0/331	1.11	0/507
4	H	0.84	1/329 (0.3%)	1.44	3/505 (0.6%)
All	All	0.40	3/12463 (0.0%)	0.63	3/17005 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	18	CYS	CB-SG	-5.11	1.73	1.81
1	A	903	CYS	CB-SG	-5.10	1.73	1.81
4	H	14	DT	C5-C7	5.08	1.53	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	DC	P-O3'-C3'	6.73	127.78	119.70
4	H	4	DG	O4'-C1'-N9	6.17	112.32	108.00
4	H	14	DT	O4'-C1'-N1	5.26	111.68	108.00

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	8714	0	8687	83	0
2	B	2854	0	2800	24	0
3	G	305	0	165	0	0
4	H	297	0	175	0	0
5	A	13	0	18	0	0
6	A	209	0	0	2	0
6	B	65	0	0	1	0
6	G	4	0	0	0	0
6	H	4	0	0	0	0
All	All	12465	0	11845	107	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 4.

All (107) 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:482:GLU:HG2	1:A:483:PRO:HD3	1.42	1.02
1:A:18:CYS:HB2	1:A:313:CYS:SG	2.12	0.89
2:B:323:HIS:NE2	2:B:342:THR:HG21	1.89	0.87
1:A:23:PHE:H	1:A:30:ASN:HD22	1.21	0.86
1:A:329:GLY:HA3	1:A:384:GLU:HG2	1.54	0.86
1:A:81:THR:HG21	1:A:85:ASN:HD22	1.41	0.85
1:A:329:GLY:HA3	1:A:384:GLU:CG	2.15	0.76
1:A:23:PHE:H	1:A:30:ASN:ND2	1.83	0.76
1:A:507:GLN:HE22	1:A:553:SER:H	1.34	0.73
1:A:1055:GLN:HE22	1:A:1090:ASP:H	1.37	0.73
1:A:507:GLN:NE2	1:A:553:SER:H	1.89	0.70
2:B:263:LEU:HB2	2:B:272:PHE:HB3	1.73	0.70
1:A:889:ARG:HD3	1:A:901:THR:HB	1.73	0.69
1:A:722:ARG:NH2	1:A:812[B]:TYR:OH	2.26	0.69
1:A:482:GLU:HG2	1:A:483:PRO:CD	2.21	0.68
1:A:648:ASN:HD22	1:A:660:TYR:HB3	1.59	0.67
2:B:443:SER:HB2	2:B:450:LEU:HB2	1.76	0.67
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.76	0.65
2:B:249:ARG:HE	2:B:291:ASP:HB3	1.64	0.62
1:A:413:LEU:HB3	1:A:424:THR:HB	1.82	0.62
1:A:504:ASN:HD21	1:A:507:GLN:HE21	1.48	0.62
1:A:889:ARG:HG3	1:A:904:ASN:ND2	2.16	0.61
1:A:7:VAL:HG13	1:A:1091:GLY:HA3	1.81	0.61
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.84	0.59
1:A:922:LEU:HD23	1:A:957:VAL:HG13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:THR:HG23	6:A:1142:HOH:O	2.02	0.59
1:A:889:ARG:HG3	1:A:904:ASN:HD21	1.67	0.59
1:A:851:PHE:HB3	1:A:858:LEU:HD22	1.85	0.58
1:A:890:LEU:HB3	1:A:903:CYS:HB2	1.84	0.58
1:A:903:CYS:HB3	1:A:942:PHE:CE1	2.39	0.58
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.86	0.57
2:B:242:CYS:O	2:B:254:THR:HG23	2.05	0.57
2:B:140:HIS:HB2	2:B:453:ASN:HB2	1.88	0.55
1:A:289:GLU:HA	1:A:295:VAL:HA	1.89	0.55
1:A:285:LEU:HB3	1:A:297:LEU:HD11	1.89	0.54
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.88	0.54
1:A:596:PHE:HB3	1:A:661:SER:HB2	1.88	0.54
1:A:218:MET:CE	1:A:261:HIS:HD2	2.21	0.53
2:B:299:VAL:HA	2:B:326:PRO:HB3	1.89	0.53
1:A:931:LEU:HD21	1:A:944:GLU:HG3	1.90	0.53
2:B:217:THR:OG1	2:B:254:THR:HG21	2.10	0.52
1:A:578:HIS:CD2	1:A:623:LEU:H	2.28	0.51
1:A:417:PRO:HB3	1:A:481:GLN:HG2	1.94	0.50
1:A:504:ASN:HD21	1:A:507:GLN:NE2	2.10	0.49
1:A:893:TRP:HE3	1:A:899:LEU:HD13	1.77	0.49
2:B:211:SER:HB3	2:B:243:VAL:HG13	1.94	0.49
1:A:1054:MET:SD	1:A:1129:LEU:HD11	2.52	0.49
2:B:256:ASP:OD1	2:B:260:ARG:HB2	2.13	0.49
2:B:433:LYS:HG2	6:B:482:HOH:O	2.12	0.48
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.78	0.48
1:A:389:ILE:HD13	1:A:713:ARG:HG2	1.96	0.48
1:A:1136:LEU:O	1:A:1139:ILE:HG12	2.13	0.48
2:B:394:PRO:HB3	2:B:402:ASP:HB3	1.96	0.47
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.44	0.47
1:A:578:HIS:HE1	1:A:580:GLU:OE1	1.96	0.47
2:B:272:PHE:HE1	2:B:312:LYS:HA	1.78	0.47
1:A:482:GLU:H	1:A:482:GLU:CD	2.18	0.47
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.50	0.47
1:A:23:PHE:N	1:A:30:ASN:ND2	2.59	0.47
1:A:385:GLY:HA3	1:A:719:GLU:O	2.14	0.47
1:A:770:LEU:HD13	1:A:865:GLU:HB2	1.96	0.47
1:A:356:LEU:HD21	1:A:712:ILE:HD13	1.97	0.47
1:A:218:MET:HE2	1:A:261:HIS:HD2	1.80	0.47
1:A:507:GLN:HE22	1:A:553:SER:N	2.09	0.47
1:A:548:ASP:C	1:A:548:ASP:OD2	2.54	0.46
1:A:1048:TYR:O	1:A:1052:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.97	0.46
1:A:480:SER:O	1:A:484:LYS:HA	2.16	0.46
1:A:43:VAL:HG21	1:A:50:ARG:CZ	2.45	0.46
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.97	0.45
1:A:312:GLU:HG3	1:A:327:ARG:HD2	1.98	0.45
1:A:1109:VAL:O	1:A:1111:ASN:N	2.42	0.45
1:A:869:ALA:H	1:A:885:ASN:ND2	2.14	0.45
2:B:388:ILE:O	2:B:408:ILE:HA	2.17	0.45
1:A:538:VAL:HG22	1:A:558:ILE:HD11	1.99	0.44
1:A:1055:GLN:NE2	1:A:1090:ASP:H	2.09	0.44
1:A:740:ILE:HG23	1:A:785:GLU:HG3	1.99	0.44
1:A:921:ILE:HB	1:A:933:LEU:HB2	1.99	0.44
1:A:312:GLU:HG3	1:A:327:ARG:CD	2.47	0.44
1:A:492:GLU:HG2	1:A:493:PRO:HD2	1.99	0.44
1:A:1057:ARG:HH12	1:A:1110:ALA:HB3	1.82	0.44
1:A:329:GLY:CA	1:A:384:GLU:HG2	2.37	0.44
1:A:658:VAL:HG11	1:A:707:ILE:HG12	1.98	0.44
1:A:889:ARG:CD	1:A:901:THR:HB	2.45	0.43
1:A:1097:PHE:O	1:A:1100:ILE:HG12	2.18	0.43
2:B:367:PRO:HG2	2:B:392:ARG:HG3	2.01	0.43
2:B:105:ILE:HD12	2:B:126:LEU:HD21	2.01	0.43
1:A:893:TRP:CE3	1:A:899:LEU:HD13	2.54	0.43
1:A:1055:GLN:HE22	1:A:1090:ASP:N	2.11	0.43
2:B:382:HIS:CG	2:B:383:PRO:HD2	2.54	0.43
1:A:640:THR:HG22	6:A:1349:HOH:O	2.18	0.42
1:A:372:GLN:NE2	1:A:391:ARG:HD3	2.33	0.42
2:B:383:PRO:HG3	2:B:435:SER:O	2.18	0.42
2:B:279:ALA:HB1	2:B:299:VAL:HG22	2.02	0.42
2:B:391:GLY:HA3	2:B:429:ILE:O	2.20	0.42
1:A:329:GLY:HA3	1:A:384:GLU:HG3	2.00	0.42
1:A:230:ILE:HD11	1:A:285:LEU:HD21	2.02	0.42
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.35	0.42
1:A:564:ILE:HG22	1:A:582:LEU:HB2	2.02	0.42
2:B:289[B]:ARG:NH2	2:B:335:THR:O	2.53	0.42
2:B:323:HIS:CD2	2:B:342:THR:HG21	2.53	0.42
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.54	0.41
1:A:870:VAL:HA	1:A:883:SER:O	2.21	0.41
1:A:24:THR:H	1:A:30:ASN:ND2	2.19	0.41
2:B:347:ASN:HA	2:B:366:HIS:O	2.20	0.40
2:B:354:SER:HA	2:B:357:TRP:CE2	2.56	0.40
1:A:596:PHE:HB3	1:A:661:SER:CB	2.52	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	1099/1158 (95%)	1041 (95%)	50 (4%)	8 (1%)	22	43
2	B	354/383 (92%)	333 (94%)	17 (5%)	4 (1%)	14	30
All	All	1453/1541 (94%)	1374 (95%)	67 (5%)	12 (1%)	19	39

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	367	LEU
1	A	855	ASP
1	A	1110	ALA
2	B	117	SER
1	A	372	GLN
1	A	1109	VAL
1	A	36	ASN
2	B	190	GLY
1	A	242	GLY
2	B	291	ASP
2	B	118	ILE
1	A	564	ILE

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	976/1014 (96%)	919 (94%)	57 (6%)	20	40
2	B	314/336 (94%)	291 (93%)	23 (7%)	14	28
All	All	1290/1350 (96%)	1210 (94%)	80 (6%)	18	37

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	81	THR
1	A	99	ASP
1	A	133	LEU
1	A	147	ARG
1	A	159	LEU
1	A	167	VAL
1	A	191	LYS
1	A	241	ASN
1	A	267[A]	ASN
1	A	267[B]	ASN
1	A	304	LEU
1	A	314	LEU
1	A	334	VAL
1	A	339	ASP
1	A	360	VAL
1	A	370	GLN
1	A	392	ASN
1	A	396	ILE
1	A	449	MET
1	A	468	LEU
1	A	476	VAL
1	A	482	GLU
1	A	533	GLU
1	A	567	ARG
1	A	576	LEU
1	A	599	SER
1	A	625	ASP
1	A	647	THR
1	A	674	LYS
1	A	682	LEU
1	A	696	ASN
1	A	698	THR
1	A	713	ARG
1	A	728	GLU

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Mol	Chain	Res	Type
1	A	809	GLN
1	A	820	LYS
1	A	844	LYS
1	A	864	LYS
1	A	867	LYS
1	A	881	LEU
1	A	898	GLU
1	A	899	LEU
1	A	901	THR
1	A	914	LEU
1	A	931	LEU
1	A	957	VAL
1	A	966	LEU
1	A	970	ASN
1	A	984	THR
1	A	1000	LEU
1	A	1014	MET
1	A	1052	LEU
1	A	1086	THR
1	A	1093	LEU
1	A	1106	GLN
1	A	1129	LEU
2	B	111	LYS
2	B	116	GLN
2	B	134	LEU
2	B	148	ARG
2	B	174	LEU
2	B	179	VAL
2	B	219	LEU
2	B	243	VAL
2	B	254	THR
2	B	262	LEU
2	B	274	GLU
2	B	293	LEU
2	B	299	VAL
2	B	308	LEU
2	B	312	LYS
2	B	321	MET
2	B	374	LEU
2	B	389	VAL
2	B	393	TYR
2	B	400	LEU

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Mol	Chain	Res	Type
2	B	435	SER
2	B	437	THR
2	B	453	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	30	ASN
1	A	85	ASN
1	A	156	ASN
1	A	241	ASN
1	A	261	HIS
1	A	372	GLN
1	A	374	GLN
1	A	392	ASN
1	A	455	GLN
1	A	507	GLN
1	A	578	HIS
1	A	648	ASN
1	A	670	ASN
1	A	727	GLN
1	A	796	GLN
1	A	885	ASN
1	A	904	ASN
1	A	907	ASN
1	A	908	ASN
1	A	991	HIS
1	A	1034	ASN
1	A	1055	GLN
2	B	107	HIS
2	B	269	HIS
2	B	370	GLN
2	B	453	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	3DR	G	9	3	8,11,12	0.41	0	9,14,17	1.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	3DR	G	9	3	-	1/3/15/16	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	9	3DR	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	$\# Z > 2$
5	PG4	A	1141	-	12,12,12	0.58	0	11,11,11	0.49	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PG4	A	1141	-	-	6/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1141	PG4	O2-C3-C4-O3
5	A	1141	PG4	O1-C1-C2-O2
5	A	1141	PG4	O4-C7-C8-O5
5	A	1141	PG4	C5-C6-O4-C7
5	A	1141	PG4	O3-C5-C6-O4
5	A	1141	PG4	C1-C2-O2-C3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1103/1158 (95%)	-0.00	32 (2%) 51 45	24, 44, 63, 81	8 (0%)
2	B	355/383 (92%)	-0.06	0 100 100	26, 40, 58, 67	0
3	G	14/16 (87%)	0.86	4 (28%) 0 0	45, 71, 110, 114	0
4	H	15/16 (93%)	0.52	2 (13%) 3 2	45, 72, 103, 107	0
All	All	1487/1573 (94%)	-0.00	38 (2%) 56 50	24, 43, 64, 114	8 (0%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	47	GLU	3.7
1	A	295	VAL	3.5
1	A	296	THR	3.4
1	A	548	ASP	3.4
1	A	437	MET	3.4
1	A	1024	THR	3.3
1	A	856	GLY	3.3
3	G	2	DA	3.2
1	A	439	ASN	3.2
1	A	438	LEU	3.1
1	A	855	ASP	3.0
3	G	3	DA	2.9
1	A	243	ASP	2.8
1	A	685	ASP	2.6
1	A	290	GLN	2.6
1	A	94	SER	2.6
1	A	441	GLU	2.6
3	G	4	DT	2.6
1	A	983	ALA	2.6
1	A	745	THR	2.5
1	A	288	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	H	15	DT	2.4
1	A	368	GLU	2.4
1	A	748	GLY	2.3
1	A	1047	TRP	2.3
1	A	443	VAL	2.3
1	A	1023	PRO	2.2
1	A	1	MET	2.2
1	A	746	SER	2.2
1	A	419	ARG	2.2
1	A	1015	GLN	2.1
4	H	14	DT	2.1
1	A	1109	VAL	2.1
1	A	984	THR	2.1
1	A	301	ARG	2.1
1	A	420	GLU	2.1
3	G	5	DG	2.0
1	A	442	GLU	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	3DR	G	9	11/12	0.95	0.20	62,64,66,66	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. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PG4	A	1141	13/13	0.91	0.18	57,58,63,63	0

6.5 Other polymers ⓘ

There are no such residues in this entry.