



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:16 AM UTC

PDB ID : 3EI1 / pdb_00003ei1
Title : Structure of hsDDB1-drDDB2 bound to a 14 bp 6-4 photoproduct containing DNA-duplex
Authors : Scrima, A.; Thoma, N.H.
Deposited on : 2008-09-15
Resolution : 2.80 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

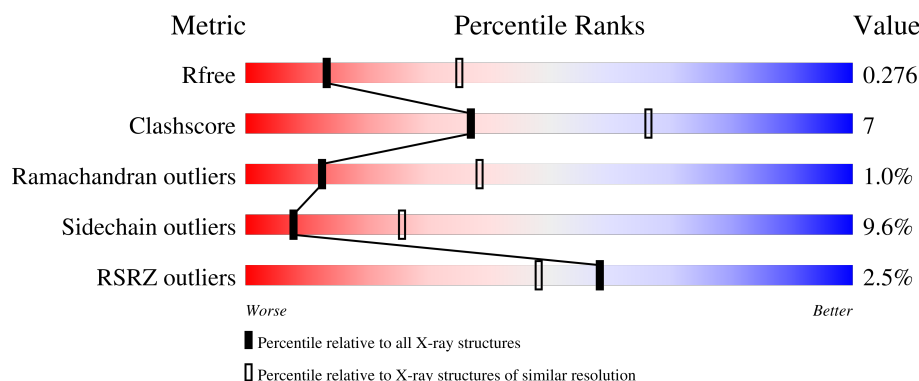
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 of 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	
2	B	383	
3	G	14	
4	H	14	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12326 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
1	A	1105	Total	C	N	O	S	23	4	0
			8698	5516	1468	1666	48			

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
2	B	355	Total	C	N	O	S	0	1	0
			2854	1812	503	528	11			

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

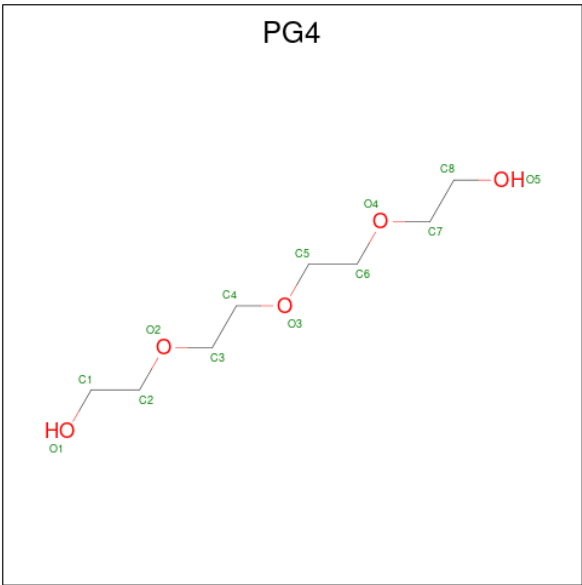
- Molecule 3 is a DNA chain called 5'-D(*DAP*DCP*DGP*DCP*DGP*DAP*(64T)P*(5PY)P*DGP*DCP*DGP*DCP*DCP*DC)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	14	Total	C	N	O	P	0	0	0
			281	134	52	82	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	14	Total	C	N	O	P	0	0	0
			287	136	56	82	13			

- Molecule 5 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



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

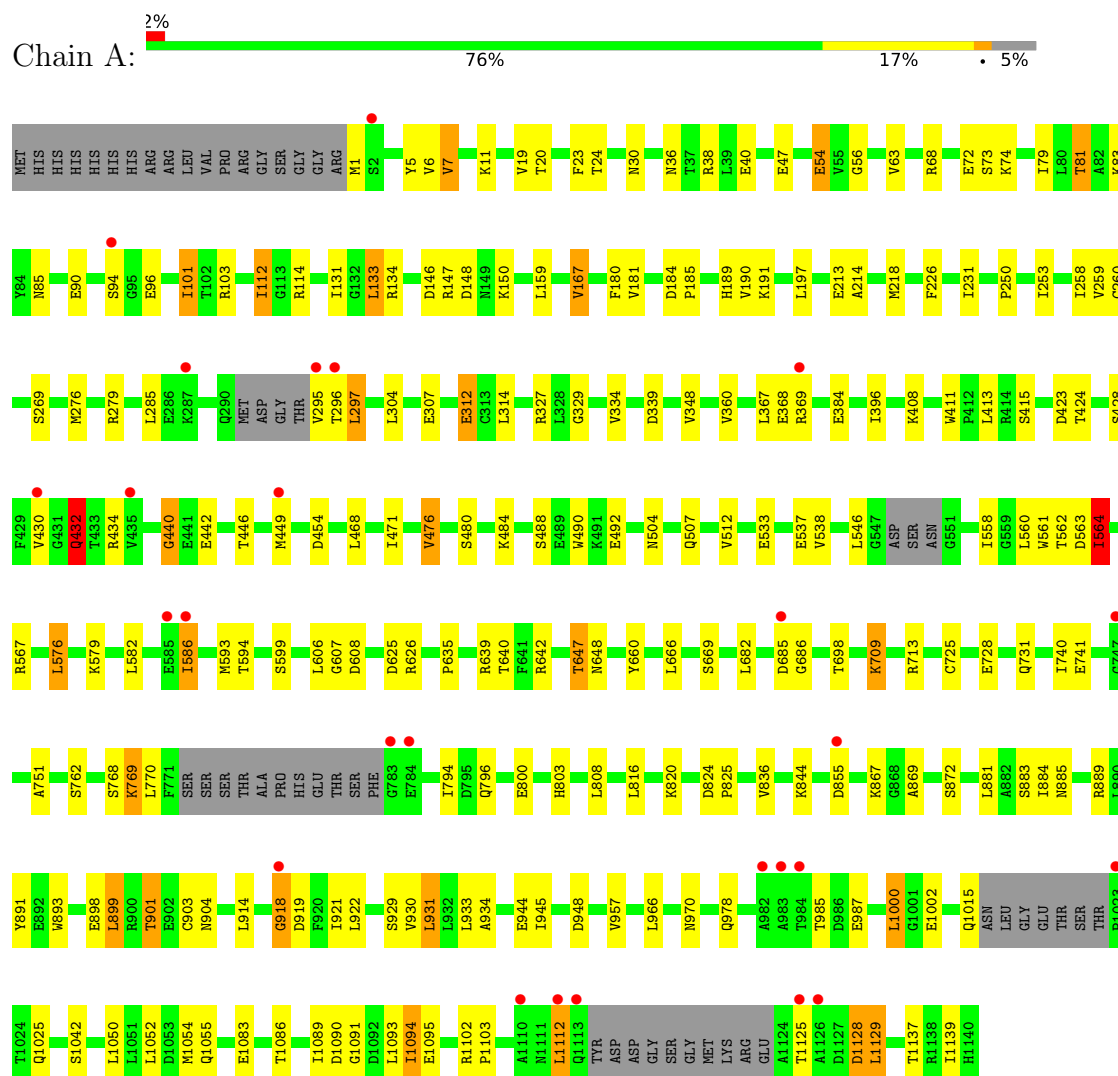
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	136	Total	O	0	0
			136	136		
6	B	49	Total	O	0	0
			49	49		
6	G	4	Total	O	0	0
			4	4		
6	H	4	Total	O	0	0
			4	4		

3 Residue-property plots [i](#)

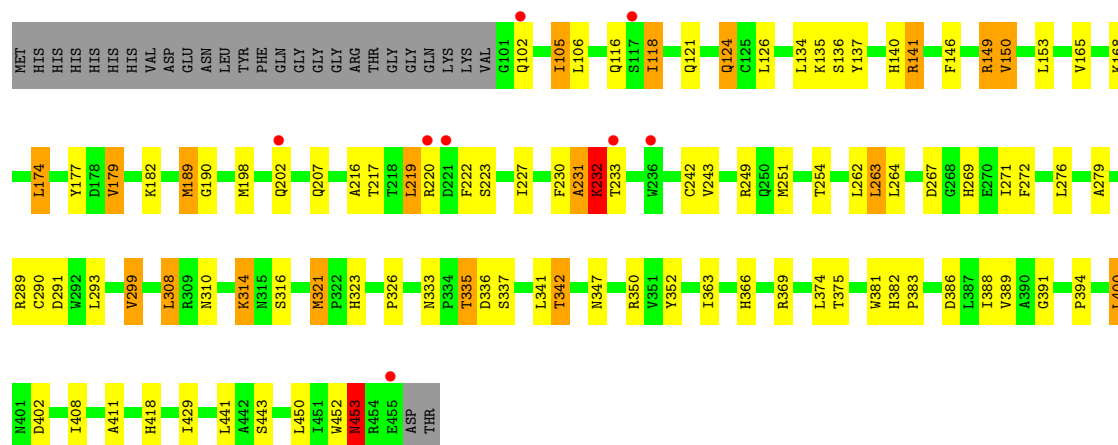
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA damage-binding protein 1

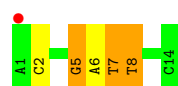


• Molecule 2: DNA damage-binding protein 2

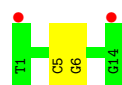
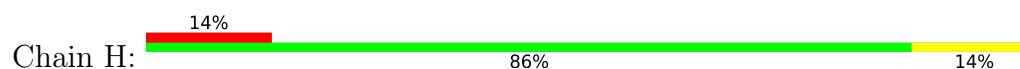




• Molecule 3: 5'-D(*DAP*DCP*DGP*DCP*DGP*DAP*(64T)P*(5PY)P*DGP*DCP*DGP*DCP*DCP*DC)-3'



• Molecule 4: 5'-D(*DTP*DGP*DGP*DGP*DCP*DGP*DCP*DAP*DAP*DTP*DCP*DGP*DCP*DG)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	112.74Å 123.60Å 158.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 50.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-2.80) 97.5 (50.00-2.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.220 , 0.278 0.219 , 0.276	Depositor DCC
R_{free} test set	2724 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.4	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	0.92	EDS
Total number of atoms	12326	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PG4, 64T, 5PY

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	0.48	0/8855	0.77	2/11989 (0.0%)
2	B	0.51	1/2928 (0.0%)	0.81	2/3976 (0.1%)
3	G	0.28	0/269	0.87	1/410 (0.2%)
4	H	0.27	0/322	0.79	0/496
All	All	0.48	1/12374 (0.0%)	0.78	5/16871 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	453	ASN	C-N	8.52	1.45	1.33

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	432	GLN	N-CA-C	6.54	116.91	108.34
2	B	230	PHE	N-CA-C	-5.70	106.31	113.72
2	B	146	PHE	N-CA-C	5.44	117.76	108.90
3	G	5	DG	P-O3'-C3'	5.26	128.10	120.20
1	A	929	SER	CB-CA-C	-5.06	110.72	116.54

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	8698	0	8686	111	0
2	B	2854	0	2800	57	0
3	G	281	0	158	4	0
4	H	287	0	158	1	0
5	A	13	0	18	0	0
6	A	136	0	0	1	0
6	B	49	0	0	1	0
6	G	4	0	0	0	0
6	H	4	0	0	0	0
All	All	12326	0	11820	170	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 7.

All (170) 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:23:PHE:H	1:A:30:ASN:HD22	1.12	0.98
1:A:504:ASN:HD21	1:A:507:GLN:HE21	0.94	0.93
1:A:889:ARG:HH11	1:A:904:ASN:HD21	1.17	0.92
1:A:504:ASN:HD21	1:A:507:GLN:NE2	1.67	0.91
1:A:23:PHE:H	1:A:30:ASN:ND2	1.72	0.88
1:A:1055:GLN:HE22	1:A:1090:ASP:H	1.20	0.86
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.58	0.84
1:A:81:THR:HG21	1:A:85:ASN:HD22	1.43	0.83
1:A:889:ARG:NH1	1:A:904:ASN:HD21	1.77	0.81
1:A:1:MET:HA	1:A:978:GLN:HE22	1.43	0.81
2:B:323:HIS:NE2	2:B:342:THR:HG21	1.98	0.79
1:A:440:GLY:O	1:A:686:GLY:HA3	1.82	0.78
1:A:312:GLU:HG3	1:A:327:ARG:CD	2.14	0.77
2:B:263:LEU:HB2	2:B:272:PHE:HB3	1.69	0.75
1:A:869:ALA:H	1:A:885:ASN:HD21	1.36	0.73
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.73	0.71
1:A:1055:GLN:NE2	1:A:1090:ASP:H	1.88	0.70
2:B:231:ALA:O	2:B:232:LYS:HB2	1.91	0.70
1:A:582:LEU:HA	1:A:626:ARG:HH22	1.57	0.69
1:A:889:ARG:HD3	1:A:901:THR:HB	1.74	0.68
1:A:504:ASN:ND2	1:A:507:GLN:HE21	1.79	0.68
1:A:934:ALA:HB2	1:A:945:ILE:HD11	1.76	0.67
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.77	0.67
2:B:441:LEU:HB3	2:B:452:TRP:HB2	1.77	0.67
1:A:642:ARG:HH11	1:A:647:THR:HG22	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLY:HA3	1:A:384:GLU:HG3	1.78	0.66
2:B:216:ALA:HB3	2:B:231:ALA:HB1	1.78	0.65
1:A:81:THR:HG21	1:A:85:ASN:ND2	2.11	0.64
1:A:889:ARG:HG3	1:A:904:ASN:ND2	2.12	0.64
2:B:121:GLN:HA	2:B:124:GLN:HB3	1.80	0.64
1:A:564:ILE:O	1:A:564:ILE:HG22	1.97	0.64
1:A:329:GLY:HA3	1:A:384:GLU:CG	2.27	0.64
1:A:970[B]:ASN:OD1	1:A:970[B]:ASN:C	2.42	0.62
2:B:400:LEU:HD23	2:B:400:LEU:H	1.64	0.62
2:B:141:ARG:NE	2:B:177:TYR:O	2.31	0.61
1:A:259:VAL:HG21	1:A:276:MET:HE2	1.82	0.61
3:G:7:64T:H2"	3:G:8:5PY:N3	2.15	0.61
2:B:140:HIS:HB2	2:B:453:ASN:HB2	1.83	0.60
1:A:112:ILE:HD13	2:B:290:CYS:HB2	1.82	0.60
1:A:218:MET:HE1	1:A:260:CYS:HA	1.84	0.59
1:A:90:GLU:HB3	1:A:101:ILE:HG22	1.83	0.59
1:A:413:LEU:HB3	1:A:424:THR:HB	1.84	0.59
1:A:415:SER:HB3	1:A:423:ASP:OD2	2.02	0.59
2:B:141:ARG:HG3	2:B:141:ARG:NH1	2.17	0.58
1:A:312:GLU:HG3	1:A:327:ARG:HD2	1.85	0.58
2:B:242:CYS:O	2:B:254:THR:HG23	2.03	0.58
2:B:350:ARG:HG2	2:B:363:ILE:HG12	1.84	0.58
1:A:312:GLU:HG3	1:A:327:ARG:HD3	1.86	0.58
2:B:141:ARG:HH11	2:B:141:ARG:CG	2.17	0.57
2:B:321:MET:HG2	2:B:352:TYR:CE2	2.40	0.56
1:A:253:ILE:HD12	1:A:258:ILE:HD11	1.87	0.56
1:A:24:THR:H	1:A:30:ASN:HD21	1.53	0.56
2:B:394:PRO:HB3	2:B:402:ASP:HB3	1.87	0.56
1:A:38:ARG:HH21	1:A:56:GLY:HA3	1.71	0.55
1:A:606:LEU:C	1:A:608:ASP:H	2.13	0.55
1:A:869:ALA:H	1:A:885:ASN:ND2	2.03	0.55
1:A:931:LEU:HD21	1:A:944:GLU:HG3	1.88	0.55
2:B:388:ILE:O	2:B:408:ILE:HA	2.07	0.54
1:A:546:LEU:HD11	1:A:593:MET:HB3	1.89	0.54
1:A:889:ARG:HD2	1:A:891:TYR:CE1	2.42	0.54
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.90	0.54
1:A:564:ILE:O	1:A:564:ILE:CG2	2.56	0.53
1:A:1025:GLN:HB3	1:A:1042:SER:HB2	1.90	0.53
1:A:190:VAL:HG21	1:A:231:ILE:HD11	1.90	0.53
1:A:889:ARG:HG3	1:A:904:ASN:HD21	1.72	0.53
2:B:216:ALA:CB	2:B:231:ALA:HB1	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:893:TRP:HE3	1:A:899:LEU:HD13	1.73	0.53
2:B:299:VAL:HA	2:B:326:PRO:HB3	1.89	0.53
1:A:872:SER:H	1:A:883:SER:HB2	1.75	0.52
2:B:137:TYR:HA	2:B:453:ASN:O	2.09	0.52
1:A:1054:MET:SD	1:A:1129:LEU:HD11	2.49	0.52
2:B:153:LEU:HD12	2:B:165:VAL:HG22	1.91	0.52
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.75	0.52
1:A:24:THR:H	1:A:30:ASN:ND2	2.07	0.52
1:A:640:THR:HG22	6:A:1221:HOH:O	2.10	0.52
1:A:922:LEU:HD11	1:A:930:VAL:CG1	2.40	0.51
2:B:141:ARG:NH1	2:B:141:ARG:CG	2.74	0.50
4:H:5:DC:H2'	4:H:6:DG:C8	2.47	0.50
1:A:72:GLU:CD	1:A:103:ARG:HH22	2.20	0.50
1:A:669:SER:HA	1:A:709:LYS:HE3	1.94	0.50
1:A:768:SER:HB3	1:A:808:LEU:HD11	1.94	0.50
1:A:1125:THR:H	1:A:1128:ASP:HB2	1.76	0.50
2:B:141:ARG:HG3	2:B:141:ARG:HH11	1.75	0.49
1:A:480:SER:O	1:A:484:LYS:HA	2.11	0.49
2:B:207:GLN:HB3	2:B:219:LEU:HD21	1.95	0.48
1:A:114:ARG:NE	2:B:336:ASP:OD2	2.35	0.48
1:A:449:MET:HA	1:A:449:MET:HE2	1.96	0.48
1:A:11:LYS:HD2	1:A:38:ARG:HD2	1.95	0.48
2:B:279:ALA:HB1	2:B:299:VAL:HG22	1.95	0.48
1:A:40:GLU:HG2	1:A:54:GLU:HG3	1.95	0.47
1:A:648:ASN:HD22	1:A:660:TYR:HB3	1.79	0.47
3:G:8:5PY:H6	3:G:8:5PY:H2'	1.44	0.47
1:A:893:TRP:CE3	1:A:899:LEU:HD13	2.49	0.47
2:B:135:LYS:HA	2:B:418:HIS:CE1	2.49	0.47
2:B:116:GLN:O	2:B:118:ILE:HG13	2.15	0.47
1:A:1054:MET:HE2	1:A:1094:ILE:HG12	1.95	0.47
2:B:443:SER:HB2	2:B:450:LEU:HB2	1.96	0.47
1:A:329:GLY:HA3	1:A:384:GLU:HG2	1.97	0.47
1:A:250:PRO:HG2	1:A:253:ILE:HG12	1.95	0.47
1:A:411:TRP:HZ3	1:A:428:SER:HB2	1.80	0.47
2:B:323:HIS:CD2	2:B:342:THR:HG21	2.49	0.47
1:A:81:THR:HG22	1:A:85:ASN:H	1.79	0.46
1:A:607:GLY:HA2	1:A:635:PRO:HA	1.97	0.46
1:A:23:PHE:N	1:A:30:ASN:ND2	2.52	0.46
1:A:769:LYS:HD2	1:A:769:LYS:H	1.80	0.46
2:B:310:ASN:O	2:B:310:ASN:CG	2.59	0.46
1:A:181:VAL:HA	1:A:189:HIS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:921:ILE:HB	1:A:933:LEU:HB2	1.97	0.46
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.45	0.46
3:G:5:DG:H2'	3:G:6:DA:OP2	2.15	0.46
1:A:226:PHE:HE1	1:A:296:THR:HA	1.81	0.46
2:B:269:HIS:CE1	2:B:271:ILE:HG12	2.50	0.46
1:A:561:TRP:O	1:A:563:ASP:N	2.48	0.45
2:B:251:MET:HB2	2:B:264:LEU:O	2.16	0.45
1:A:1055:GLN:NE2	1:A:1090:ASP:N	2.62	0.45
1:A:131:ILE:HG22	1:A:133:LEU:HD13	1.99	0.45
1:A:918:GLY:O	1:A:919:ASP:HB2	2.17	0.45
1:A:63:VAL:O	1:A:79:ILE:HA	2.17	0.45
2:B:174:LEU:HB2	2:B:222:PHE:CE2	2.52	0.44
1:A:81:THR:HG23	1:A:83:LYS:H	1.82	0.44
2:B:341:LEU:HB2	2:B:381:TRP:CZ2	2.51	0.44
1:A:213:GLU:HG2	1:A:214:ALA:N	2.31	0.44
1:A:538:VAL:HG22	1:A:558:ILE:HD11	1.99	0.44
1:A:883:SER:C	1:A:884:ILE:HG13	2.42	0.44
2:B:289:ARG:NH2	2:B:335:THR:O	2.51	0.44
1:A:725:CYS:SG	1:A:816:LEU:HG	2.58	0.44
2:B:249:ARG:HE	2:B:291:ASP:HB3	1.83	0.44
2:B:134:LEU:HD13	2:B:408:ILE:HD13	1.99	0.43
3:G:2:DC:H2'	3:G:2:DC:OP2	2.17	0.43
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.33	0.43
2:B:333:ASN:HD21	2:B:336:ASP:HB2	1.83	0.43
1:A:68:ARG:HH21	1:A:74:LYS:HA	1.82	0.43
1:A:576:LEU:HD21	1:A:579:LYS:HB2	2.00	0.43
1:A:538:VAL:HA	1:A:560:LEU:HD23	2.01	0.43
1:A:889:ARG:HH11	1:A:889:ARG:HG3	1.83	0.43
2:B:391:GLY:HA3	2:B:429:ILE:O	2.19	0.43
1:A:5:TYR:CE2	1:A:7:VAL:HG13	2.54	0.43
1:A:762:SER:O	1:A:803:HIS:HA	2.18	0.43
1:A:824:ASP:HA	1:A:825:PRO:HD2	1.93	0.43
1:A:586:ILE:HG21	1:A:608:ASP:HB2	2.00	0.43
1:A:432:GLN:NE2	1:A:434:ARG:HH22	2.17	0.43
1:A:471:ILE:HG12	1:A:476:VAL:HB	2.01	0.43
2:B:105:ILE:O	2:B:105:ILE:HG12	2.19	0.43
2:B:308:LEU:HD12	2:B:308:LEU:HA	1.90	0.42
2:B:267:ASP:OD2	2:B:267:ASP:N	2.51	0.42
2:B:336:ASP:O	2:B:337:SER:HB2	2.20	0.42
2:B:207:GLN:NE2	2:B:227:ILE:HD13	2.34	0.42
2:B:386:ASP:HB3	2:B:411:ALA:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LYS:NZ	6:B:505:HOH:O	2.52	0.42
2:B:149:ARG:HD3	2:B:375:THR:OG1	2.19	0.42
2:B:276:LEU:HA	2:B:314:LYS:HB2	2.00	0.42
1:A:741:GLU:HG2	1:A:751:ALA:HA	2.02	0.42
2:B:149:ARG:HG2	2:B:150:VAL:N	2.35	0.42
2:B:382:HIS:CG	2:B:383:PRO:HD2	2.55	0.42
2:B:347:ASN:HA	2:B:366:HIS:O	2.20	0.41
1:A:492:GLU:HG3	1:A:512:VAL:HG11	2.02	0.41
2:B:179:VAL:HG13	2:B:182:LYS:HB3	2.01	0.41
1:A:148:ASP:O	1:A:150:LYS:N	2.49	0.41
1:A:836:VAL:CG2	2:B:106:LEU:HD12	2.50	0.41
1:A:7:VAL:HG13	1:A:1091:GLY:HA3	2.02	0.41
1:A:869:ALA:O	1:A:884:ILE:HA	2.20	0.41
1:A:285:LEU:HB3	1:A:297:LEU:HD11	2.03	0.41
1:A:408:LYS:HE3	1:A:430:VAL:HG22	2.02	0.41
2:B:105:ILE:HD12	2:B:126:LEU:HD21	2.02	0.41
1:A:948:ASP:OD1	1:A:948:ASP:C	2.64	0.40
1:A:134:ARG:HD2	1:A:134:ARG:C	2.46	0.40
1:A:259:VAL:HG21	1:A:276:MET:CE	2.50	0.40
1:A:1095:GLU:HG2	1:A:1137:THR:HG22	2.04	0.40
2:B:217:THR:OG1	2:B:254:THR:HG21	2.22	0.40
2:B:333:ASN:HB3	2:B:381:TRP:CE2	2.57	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	1097/1158 (95%)	1023 (93%)	64 (6%)	10 (1%)	14	41
2	B	354/383 (92%)	327 (92%)	23 (6%)	4 (1%)	11	36
All	All	1451/1541 (94%)	1350 (93%)	87 (6%)	14 (1%)	12	38

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLU
1	A	367	LEU
1	A	369	ARG
1	A	918	GLY
2	B	231	ALA
2	B	232	LYS
1	A	1112	LEU
1	A	562	THR
1	A	36	ASN
1	A	855	ASP
2	B	190	GLY
2	B	189	MET
1	A	440	GLY
1	A	564	ILE

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	973/1014 (96%)	883 (91%)	90 (9%)	8	27
2	B	314/336 (94%)	279 (89%)	35 (11%)	6	20
All	All	1287/1350 (95%)	1162 (90%)	125 (10%)	8	25

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	VAL
1	A	19	VAL
1	A	20	THR
1	A	47	GLU
1	A	54	GLU
1	A	73	SER
1	A	81	THR
1	A	94	SER

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Mol	Chain	Res	Type
1	A	96	GLU
1	A	101	ILE
1	A	112	ILE
1	A	133	LEU
1	A	146	ASP
1	A	147	ARG
1	A	159	LEU
1	A	167	VAL
1	A	191	LYS
1	A	197	LEU
1	A	269	SER
1	A	279	ARG
1	A	295	VAL
1	A	297	LEU
1	A	304	LEU
1	A	307	GLU
1	A	312	GLU
1	A	314	LEU
1	A	334	VAL
1	A	339	ASP
1	A	348	VAL
1	A	360	VAL
1	A	396	ILE
1	A	432	GLN
1	A	442	GLU
1	A	446	THR
1	A	454	ASP
1	A	468	LEU
1	A	476	VAL
1	A	488	SER
1	A	533	GLU
1	A	537	GLU
1	A	564	ILE
1	A	567	ARG
1	A	576	LEU
1	A	586	ILE
1	A	594	THR
1	A	599	SER
1	A	625	ASP
1	A	639	ARG
1	A	647	THR
1	A	666	LEU

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Mol	Chain	Res	Type
1	A	682	LEU
1	A	685	ASP
1	A	698	THR
1	A	709	LYS
1	A	713[A]	ARG
1	A	713[B]	ARG
1	A	728	GLU
1	A	740	ILE
1	A	769	LYS
1	A	770	LEU
1	A	794	ILE
1	A	800	GLU
1	A	820	LYS
1	A	844	LYS
1	A	867	LYS
1	A	881	LEU
1	A	898	GLU
1	A	899	LEU
1	A	901	THR
1	A	903	CYS
1	A	914	LEU
1	A	931	LEU
1	A	957	VAL
1	A	966	LEU
1	A	985	THR
1	A	987	GLU
1	A	1000	LEU
1	A	1015	GLN
1	A	1050	LEU
1	A	1052	LEU
1	A	1083	GLU
1	A	1086	THR
1	A	1089	ILE
1	A	1093	LEU
1	A	1094	ILE
1	A	1112	LEU
1	A	1128	ASP
1	A	1129	LEU
1	A	1139	ILE
2	B	102	GLN
2	B	105	ILE
2	B	118	ILE

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Mol	Chain	Res	Type
2	B	124	GLN
2	B	136	SER
2	B	141	ARG
2	B	149	ARG
2	B	150	VAL
2	B	174	LEU
2	B	179	VAL
2	B	189	MET
2	B	198	MET
2	B	202	GLN
2	B	219	LEU
2	B	220[A]	ARG
2	B	220[B]	ARG
2	B	223	SER
2	B	232	LYS
2	B	233	THR
2	B	243	VAL
2	B	262	LEU
2	B	263	LEU
2	B	293	LEU
2	B	299	VAL
2	B	308	LEU
2	B	314	LYS
2	B	316	SER
2	B	321	MET
2	B	335	THR
2	B	342	THR
2	B	369	ARG
2	B	374	LEU
2	B	389	VAL
2	B	400	LEU
2	B	453	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	85	ASN
1	A	186	GLN
1	A	234	GLN
1	A	432	GLN
1	A	455	GLN

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Mol	Chain	Res	Type
1	A	465	HIS
1	A	497	ASN
1	A	507	GLN
1	A	520	GLN
1	A	617	ASN
1	A	648	ASN
1	A	670	ASN
1	A	727	GLN
1	A	731	GLN
1	A	790	ASN
1	A	796	GLN
1	A	806	GLN
1	A	809	GLN
1	A	845	GLN
1	A	852	GLN
1	A	859	GLN
1	A	885	ASN
1	A	904	ASN
1	A	907	ASN
1	A	964	ASN
1	A	978	GLN
1	A	990	GLN
1	A	1034	ASN
1	A	1055	GLN
1	A	1056	ASN
2	B	102	GLN
2	B	107	HIS
2	B	119	HIS
2	B	121	GLN
2	B	124	GLN
2	B	206	ASN
2	B	250	GLN
2	B	269	HIS
2	B	315	ASN
2	B	401	ASN
2	B	424	ASN
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 ⓘ

2 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$
3	5PY	G	8	3	16,20,21	1.10	2 (12%)	19,28,31	1.38	1 (5%)
3	64T	G	7	3	17,22,23	1.68	2 (11%)	23,33,36	1.73	5 (21%)

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	5PY	G	8	3	-	4/7/21/22	0/2/2/2
3	64T	G	7	3	-	0/7/40/41	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7	64T	C2-N1	-5.49	1.28	1.35
3	G	7	64T	C6-N1	2.61	1.49	1.46
3	G	8	5PY	C6-C5	2.52	1.39	1.35
3	G	8	5PY	C2-N1	-2.16	1.35	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	7	64T	O4'-C1'-N1	4.43	113.88	108.39
3	G	8	5PY	C5-C4-N3	-3.92	118.53	125.19
3	G	7	64T	N3-C2-N1	3.83	120.50	116.65
3	G	7	64T	C2'-C1'-N1	-3.20	111.79	115.59
3	G	7	64T	C4-N3-C2	-2.35	123.12	126.67
3	G	7	64T	C6-C5-C4	-2.10	107.26	114.37

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	8	5PY	O4'-C1'-N1-C6
3	G	8	5PY	O4'-C1'-N1-C2
3	G	8	5PY	C2'-C1'-N1-C6
3	G	8	5PY	C2'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	8	5PY	2	0
3	G	7	64T	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	0.61	0	11,11,11	0.47	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	-	-	3/10/10/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1141	PG4	C3-C4-O3-C5
5	A	1141	PG4	C8-C7-O4-C6
5	A	1141	PG4	O3-C5-C6-O4

There are no ring outliers.

No monomer is involved in short contacts.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	1105/1158 (95%)	0.09	26 (2%) 59 49	12, 42, 63, 87	9 (0%)
2	B	355/383 (92%)	0.10	8 (2%) 61 51	23, 39, 55, 65	1 (0%)
3	G	12/14 (85%)	1.05	1 (8%) 17 12	52, 81, 113, 116	0
4	H	14/14 (100%)	0.98	2 (14%) 6 5	52, 79, 105, 112	0
All	All	1486/1569 (94%)	0.10	37 (2%) 58 48	12, 42, 63, 116	10 (0%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	455	GLU	5.2
1	A	585	GLU	4.1
2	B	202	GLN	3.5
1	A	855	ASP	3.3
4	H	1	DT	3.1
1	A	984	THR	3.1
1	A	1112	LEU	3.1
1	A	983	ALA	2.9
2	B	117	SER	2.9
1	A	1023	PRO	2.8
1	A	1113	GLN	2.7
3	G	1	DA	2.7
1	A	982	ALA	2.6
1	A	1125	THR	2.6
1	A	1126	ALA	2.6
4	H	14	DG	2.5
1	A	295	VAL	2.5
2	B	221	ASP	2.5
1	A	918	GLY	2.5
2	B	236	TRP	2.4
1	A	2	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	586	ILE	2.4
2	B	102	GLN	2.3
1	A	94	SER	2.3
1	A	1110	ALA	2.2
1	A	449	MET	2.2
1	A	296	THR	2.2
1	A	287	LYS	2.2
1	A	747	GLY	2.1
1	A	369	ARG	2.1
2	B	220[A]	ARG	2.1
1	A	783	GLY	2.1
2	B	233	THR	2.1
1	A	784	GLU	2.1
1	A	685	ASP	2.0
1	A	430	VAL	2.0
1	A	435	VAL	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	64T	G	7	21/22	0.76	0.15	80,81,81,81	0
3	5PY	G	8	19/20	0.84	0.14	71,77,79,80	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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($\text{\AA}^2$)	Q<0.9
5	PG4	A	1141	13/13	0.90	0.14	57,59,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.