



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:24 AM GMT

PDB ID : 3EI1
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
<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

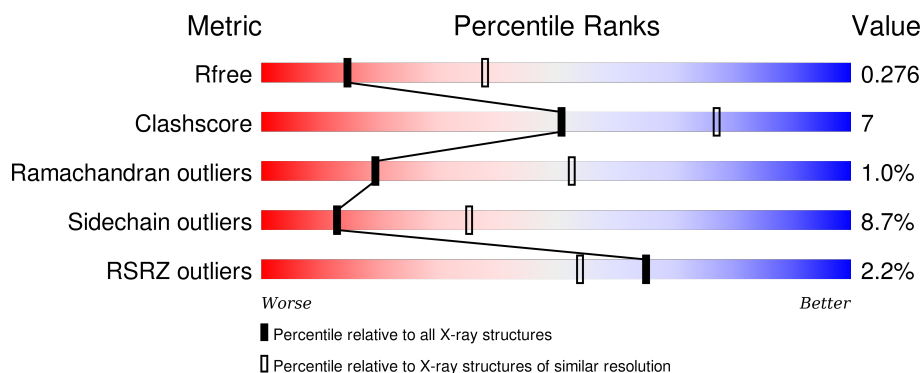
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (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 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	1158	<div> <div>2%</div> <div>77%</div> <div>17%</div> <div>• 5%</div> </div>
2	B	383	<div> <div>%</div> <div>68%</div> <div>21%</div> <div>• • 7%</div> </div>
3	G	14	<div> <div>21%</div> <div>64%</div> <div>29%</div> <div>7%</div> </div>
4	H	14	<div> <div>14%</div> <div>79%</div> <div>21%</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	PG4	A	1141	-	-	-	X

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
			Total	C	N	O	S			
1	A	1105	8698	5516	1468	1666	48	23	4	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

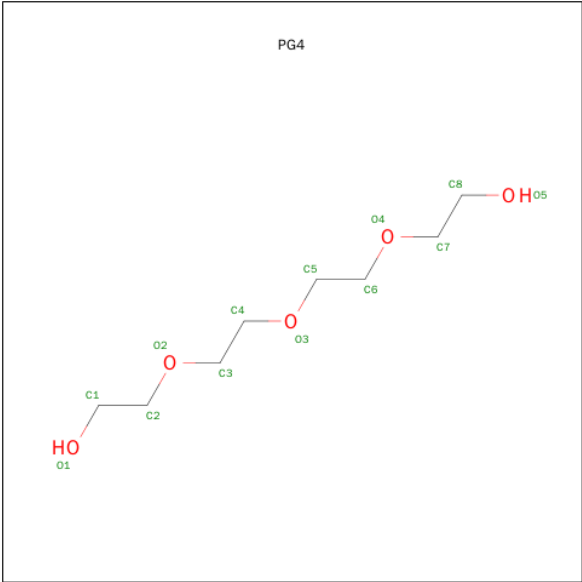
- Molecule 3 is a DNA chain called 5'-D(*DAP*DCP*DGP*DCP*DGP*DAP*(64T)P*(5PY)P*DGP*DCP*DGP*DCP*DCP*DC)-3'.

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 (three-letter code: PG4) (formula: C₈H₁₈O₅).



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

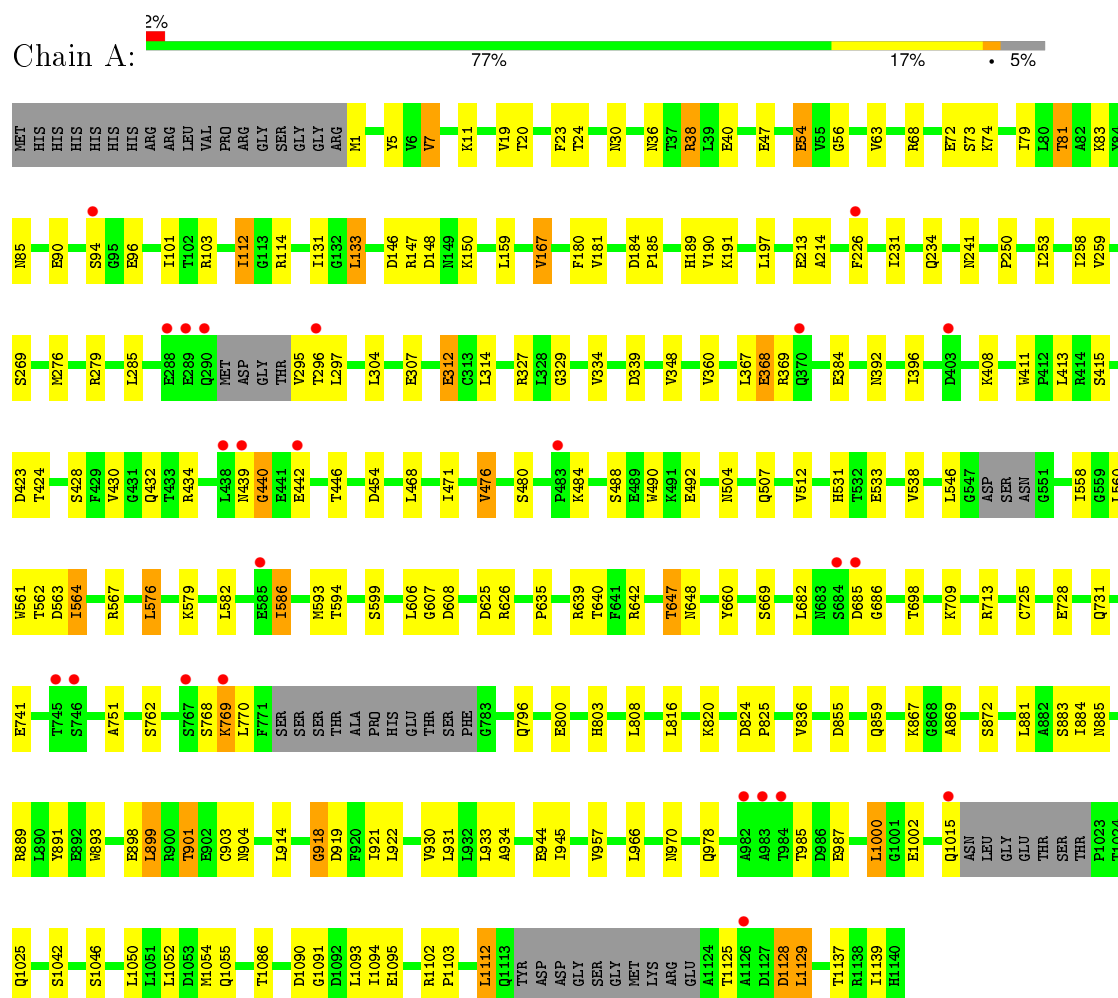
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	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		

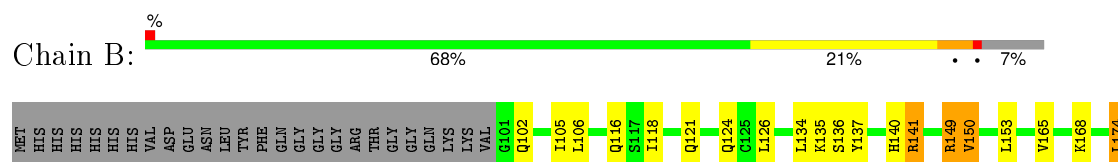
3 Residue-property plots

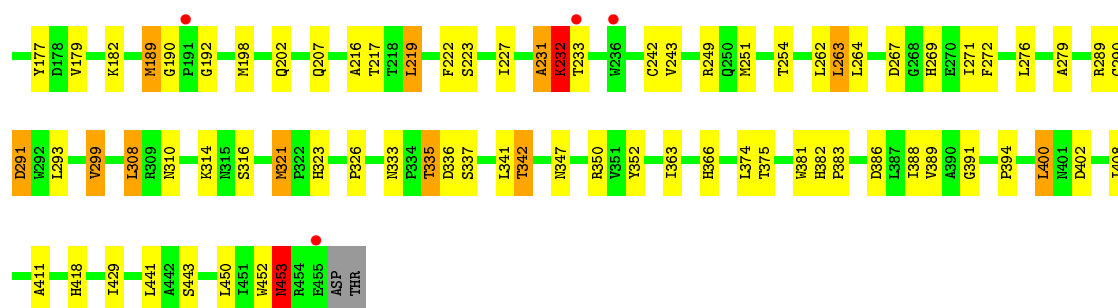
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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



• Molecule 2: DNA damage-binding protein 2

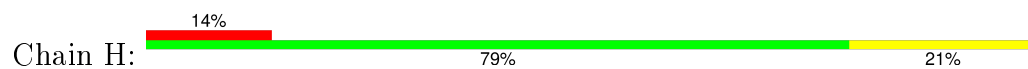




● Molecule 3: 5'-D(*DAP*DCP*DGP*DCP*DGP*DAP*(64T)P*(5PY)P*DGP*DCP*DGP*DCP*DCP*DC)-3'



● 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 48.72 – 2.80	Depositor EDS
% Data completeness (in resolution range)	97.4 (50.00-2.80) 97.5 (48.72-2.80)	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 (5.34%)	DCC
Wilson B-factor (Å ²)	48.4	Xtriage
Anisotropy	0.085	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 53748 reflections	Xtriage
F_o, F_c correlation	0.91	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, 0.375 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: 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	0.39	0/8855	0.58	0/11989
2	B	0.39	1/2928 (0.0%)	0.60	0/3976
3	G	0.74	0/269	1.18	1/410 (0.2%)
4	H	0.77	0/322	1.24	1/496 (0.2%)
All	All	0.41	1/12374 (0.0%)	0.63	2/16871 (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	5.11	1.45	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5	DG	P-O3'-C3'	7.00	128.10	119.70
4	H	2	DG	P-O3'-C3'	6.14	127.07	119.70

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	8698	0	8686	104	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	2854	0	2800	58	0
3	G	281	0	158	5	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	164	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 (164) 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
2:B:400:LEU:H	2:B:400:LEU:HD23	1.64	0.62
2:B:141:ARG:NE	2:B:177:TYR:O	2.31	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:90:GLU:HB3	1:A:101:ILE:HG22	1.83	0.59
1:A:415:SER:HB3	1:A:423:ASP:OD2	2.02	0.59
1:A:413:LEU:HB3	1:A:424:THR:HB	1.84	0.59
2:B:141:ARG:NH1	2:B:141:ARG:HG3	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
1:A:970[B]:ASN:OD1	1:A:970[B]:ASN:C	2.42	0.57
2:B:141:ARG:CG	2:B:141:ARG:HH11	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:606:LEU:C	1:A:608:ASP:H	2.13	0.50
4:H:5:DC:H2'	4:H:6:DG:C8	2.47	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: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
3:G:8:5PY:H6	3:G:8:5PY:H2'	1.44	0.47
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
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
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
2:B:323:HIS:CD2	2:B:342:THR:HG21	2.49	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
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:H	1:A:769:LYS:HD2	1.80	0.46
1:A:181:VAL:HA	1:A:189:HIS:O	2.15	0.46
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:GLU:CD	1:A:103:ARG:HH22	2.20	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
2:B:289:ARG:NH2	2:B:335:THR:O	2.51	0.44
2:B:249:ARG:HE	2:B:291:ASP:HB3	1.83	0.44
1:A:725:CYS:SG	1:A:816:LEU:HG	2.58	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
2:B:333:ASN:HD21	2:B:336:ASP:HB2	1.83	0.43
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.33	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:889:ARG:HH11	1:A:889:ARG:HG3	1.83	0.43
1:A:538:VAL:HA	1:A:560:LEU:HD23	2.01	0.43
2:B:391:GLY:HA3	2:B:429:ILE:O	2.19	0.43
2:B:105:ILE:HG12	2:B:105:ILE:O	2.19	0.43
1:A:762:SER:O	1:A:803:HIS:HA	2.18	0.43
1:A:5:TYR:CE2	1:A:7:VAL:HG13	2.54	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:471:ILE:HG12	1:A:476:VAL:HB	2.01	0.43
1:A:432:GLN:NE2	1:A:434:ARG:HH22	2.17	0.43
2:B:308:LEU:HD12	2:B:308:LEU:HA	1.90	0.42
2:B:336:ASP:O	2:B:337:SER:HB2	2.20	0.42
2:B:267:ASP:OD2	2:B:267:ASP:N	2.51	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
2:B:168:LYS:NZ	6:B:505:HOH:O	2.52	0.42
2:B:276:LEU:HA	2:B:314:LYS:HB2	2.00	0.42
2:B:149:ARG:HD3	2:B:375:THR:OG1	2.19	0.42
1:A:741:GLU:HG2	1:A:751:ALA:HA	2.02	0.42
2:B:192:GLY:HA3	3:G:8:5PY:H72	2.01	0.42
2:B:149:ARG:HG2	2:B:150:VAL:N	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:382:HIS:CG	2:B:383:PRO:HD2	2.55	0.42
2:B:310:ASN:CG	2:B:310:ASN:O	2.59	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:869:ALA:O	1:A:884:ILE:HA	2.20	0.41
1:A:7:VAL:HG13	1:A:1091:GLY:HA3	2.02	0.41
1:A:259:VAL:HG21	1:A:276:MET:CE	2.50	0.41
1:A:285:LEU:HB3	1:A:297:LEU:HD11	2.03	0.41
2:B:105:ILE:HD12	2:B:126:LEU:HD21	2.02	0.41
1:A:408:LYS:HE3	1:A:430:VAL:HG22	2.02	0.41
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%)	21	55
2	B	354/383 (92%)	327 (92%)	23 (6%)	4 (1%)	17	50
All	All	1451/1541 (94%)	1350 (93%)	87 (6%)	14 (1%)	19	52

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLU
1	A	367	LEU

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Mol	Chain	Res	Type
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%)	888 (91%)	85 (9%)	13	35
2	B	314/336 (94%)	286 (91%)	28 (9%)	12	34
All	All	1287/1350 (95%)	1174 (91%)	113 (9%)	13	35

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	19	VAL
1	A	20	THR
1	A	38	ARG
1	A	47	GLU
1	A	54	GLU
1	A	73	SER
1	A	81	THR
1	A	94	SER
1	A	96	GLU
1	A	112	ILE

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Mol	Chain	Res	Type
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	234	GLN
1	A	241	ASN
1	A	269	SER
1	A	279	ARG
1	A	295	VAL
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	368	GLU
1	A	392	ASN
1	A	396	ILE
1	A	439	ASN
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	531	HIS
1	A	533	GLU
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	682	LEU
1	A	685	ASP

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Mol	Chain	Res	Type
1	A	698	THR
1	A	713[A]	ARG
1	A	713[B]	ARG
1	A	728	GLU
1	A	769	LYS
1	A	770	LEU
1	A	800	GLU
1	A	820	LYS
1	A	859	GLN
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	957	VAL
1	A	966	LEU
1	A	985	THR
1	A	987	GLU
1	A	1000	LEU
1	A	1015	GLN
1	A	1046	SER
1	A	1050	LEU
1	A	1052	LEU
1	A	1086	THR
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	136	SER
2	B	141	ARG
2	B	149	ARG
2	B	150	VAL
2	B	174	LEU
2	B	189	MET
2	B	198	MET
2	B	202	GLN
2	B	219	LEU

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Mol	Chain	Res	Type
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	291	ASP
2	B	293	LEU
2	B	299	VAL
2	B	308	LEU
2	B	316	SER
2	B	321	MET
2	B	335	THR
2	B	342	THR
2	B	374	LEU
2	B	389	VAL
2	B	400	LEU
2	B	453	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	85	ASN
1	A	93	GLN
1	A	241	ASN
1	A	374	GLN
1	A	392	ASN
1	A	432	GLN
1	A	455	GLN
1	A	465	HIS
1	A	497	ASN
1	A	507	GLN
1	A	648	ASN
1	A	670	ASN
1	A	727	GLN
1	A	796	GLN
1	A	806	GLN
1	A	809	GLN
1	A	885	ASN
1	A	904	ASN
1	A	978	GLN

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Mol	Chain	Res	Type
1	A	991	HIS
1	A	1034	ASN
1	A	1055	GLN
1	A	1111	ASN
2	B	102	GLN
2	B	107	HIS
2	B	269	HIS
2	B	370	GLN
2	B	401	ASN
2	B	419	GLN
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	64T	G	7	3	16,22,23	1.71	3 (18%)	22,33,36	1.68	5 (22%)
3	5PY	G	8	3	12,20,21	0.39	0	18,28,31	1.86	3 (16%)

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7	64T	C2-N1	-4.85	1.28	1.35
3	G	7	64T	C6-N1	2.41	1.49	1.46
3	G	7	64T	C1'-N1	2.80	1.49	1.45

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	8	5PY	C5-C4-N3	-5.37	118.53	124.82
3	G	7	64T	C2'-C1'-N1	-3.19	111.79	115.66
3	G	7	64T	C6-C5-C4	-2.15	107.26	112.82
3	G	7	64T	C4-N3-C2	-2.07	123.12	126.84
3	G	8	5PY	C6-C5-C4	2.05	118.42	115.54
3	G	7	64T	N3-C2-N1	3.91	120.50	116.60
3	G	7	64T	O4'-C1'-N1	4.06	113.88	108.40
3	G	8	5PY	C4-N3-C2	4.08	122.03	115.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

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

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	0.62	0	11,11,11	0.48	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	-	-	0/10/10/10	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

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	1105/1158 (95%)	-0.07	24 (2%) 65 54	23, 42, 63, 87	5 (0%)
2	B	355/383 (92%)	-0.09	4 (1%) 82 74	23, 39, 55, 65	0
3	G	12/14 (85%)	1.00	3 (25%) 1 0	52, 81, 113, 116	0
4	H	14/14 (100%)	0.80	2 (14%) 4 2	52, 79, 105, 112	0
All	All	1486/1569 (94%)	-0.06	33 (2%) 65 54	23, 42, 64, 116	5 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	GLN	4.7
1	A	984	THR	4.4
4	H	14	DG	3.8
3	G	1	DA	3.6
1	A	403	ASP	3.3
2	B	455	GLU	3.1
1	A	983	ALA	3.1
1	A	746	SER	3.0
4	H	1	DT	2.9
1	A	296	THR	2.8
2	B	233	THR	2.8
1	A	1126	ALA	2.7
1	A	685	ASP	2.7
1	A	684	SER	2.6
1	A	289	GLU	2.5
1	A	1015	GLN	2.5
1	A	226	PHE	2.4
2	B	191	PRO	2.4
1	A	585	GLU	2.3
1	A	745	THR	2.3
1	A	94	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	982	ALA	2.3
1	A	442	GLU	2.3
1	A	370	GLN	2.2
3	G	3	DG	2.2
3	G	4	DC	2.1
1	A	288	GLU	2.1
1	A	439	ASN	2.1
1	A	438	LEU	2.1
1	A	769	LYS	2.1
1	A	767	SER	2.0
2	B	236	TRP	2.0
1	A	483	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
3	5PY	G	8	19/20	0.88	0.26	-	71,77,79,80	0
3	64T	G	7	21/22	0.90	0.25	-	80,81,81,81	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	PG4	A	1141	13/13	0.88	0.27	3.69	57,59,64,64	0

6.5 Other polymers [i](#)

There are no such residues in this entry.