



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:11 AM UTC

PDB ID : 4A08 / pdb_00004a08
Title : Structure of hsDDB1-drDDB2 bound to a 13 bp CPD-duplex (purine at D-1 position) at 3.0 Å resolution (CPD 1)
Authors : Scrima, A.; Fischer, E.S.; Iwai, S.; Gut, H.; Thoma, N.H.
Deposited on : 2011-09-08
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

<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

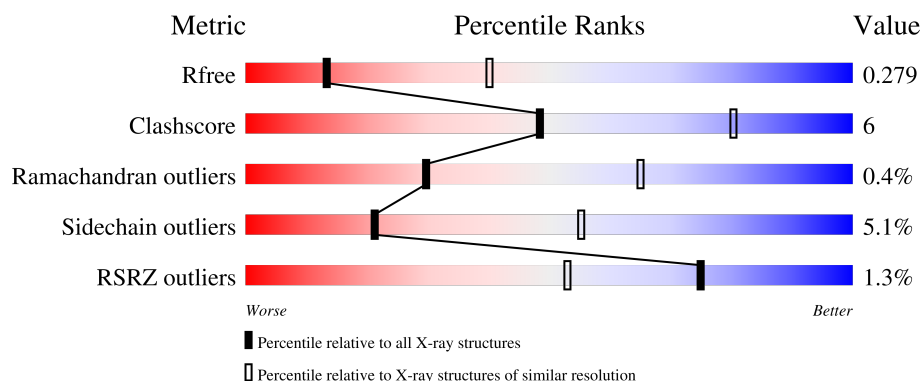
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	1159	79% 13% 6%
2	B	382	72% 20% 8%
3	G	13	54% 15% 8% 23%
4	H	14	50% 43% 7%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 11866 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	1088	Total	C	N	O	S	0	0	0
			8509	5412	1436	1615	46			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP Q16531
A	-17	HIS	-	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	VAL	-	expression tag	UNP Q16531
A	-10	ASP	-	expression tag	UNP Q16531
A	-9	GLU	-	expression tag	UNP Q16531
A	-8	ASN	-	expression tag	UNP Q16531
A	-7	LEU	-	expression tag	UNP Q16531
A	-6	TYR	-	expression tag	UNP Q16531
A	-5	PHE	-	expression tag	UNP Q16531
A	-4	GLN	-	expression tag	UNP Q16531
A	-3	GLY	-	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
A	194	ALA	GLU	engineered mutation	UNP Q16531

- Molecule 2 is a protein called DNA DAMAGE-BINDING PROTEIN 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	353	Total	C	N	O	S	0	0	0
			2824	1796	493	524	11			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	MET	-	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	HIS	-	expression tag	UNP Q2YDS1
B	83	ARG	-	expression tag	UNP Q2YDS1
B	84	ARG	-	expression tag	UNP Q2YDS1
B	85	LEU	-	expression tag	UNP Q2YDS1
B	86	VAL	-	expression tag	UNP Q2YDS1
B	87	PRO	-	expression tag	UNP Q2YDS1
B	88	ARG	-	expression tag	UNP Q2YDS1
B	89	GLY	-	expression tag	UNP Q2YDS1
B	90	SER	-	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
B	180	GLN	LEU	variant	UNP Q2YDS1
B	214	ARG	TRP	variant	UNP Q2YDS1

- Molecule 3 is a DNA chain called 5'-D(*AP*CP*GP*CP*GP*AP*(TTD)P*GP*CP*GP*C P*CP*C)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	10	Total	C	N	O	P	0	0	0
			225	106	41	67	11			

- Molecule 4 is a DNA chain called 5'-D(*TP*GP*GP*GP*CP*GP*CP*CP*CP*TP*CP*G P*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	13	Total	C	N	O	P	0	0	0
			266	124	50	79	13			

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Ca	0	0
			1	1		
6	H	1	Total	Ca	0	0
			1	1		

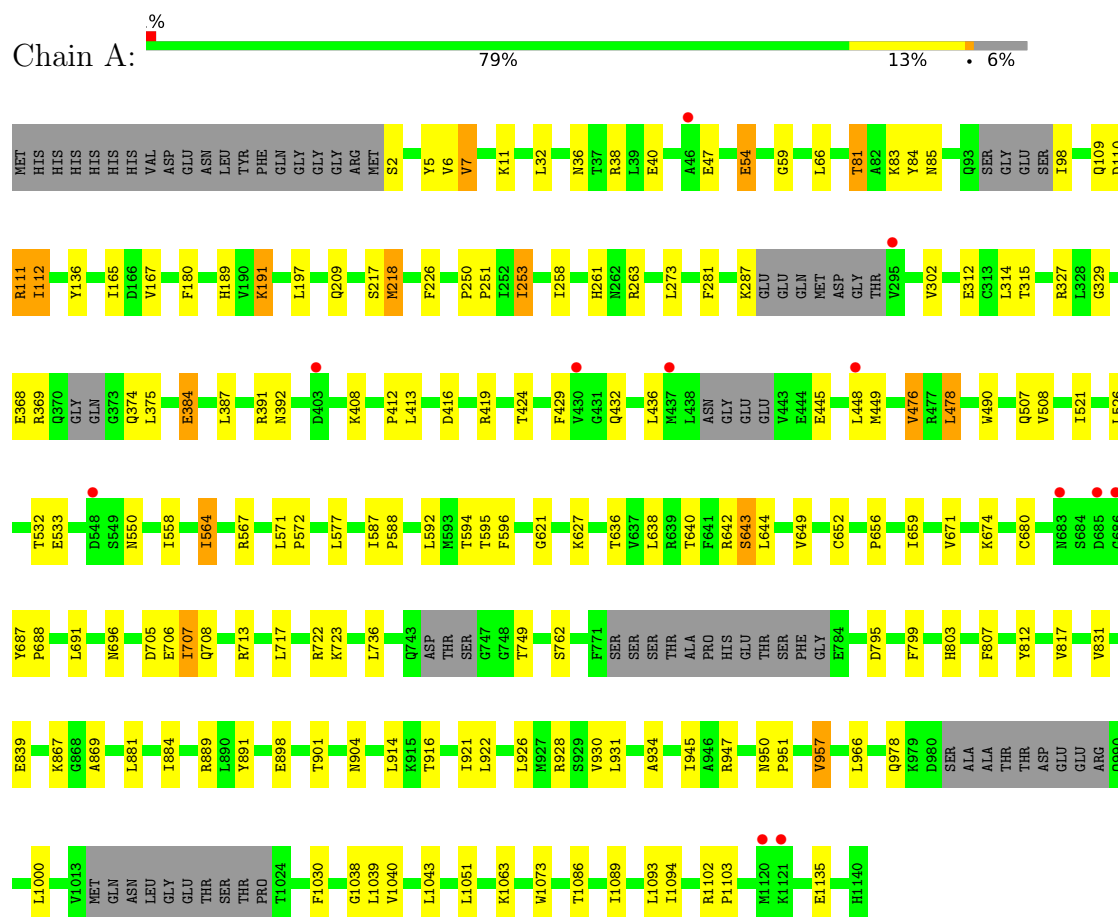
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	11	Total	O	0	0
			11	11		
7	B	5	Total	O	0	0
			5	5		

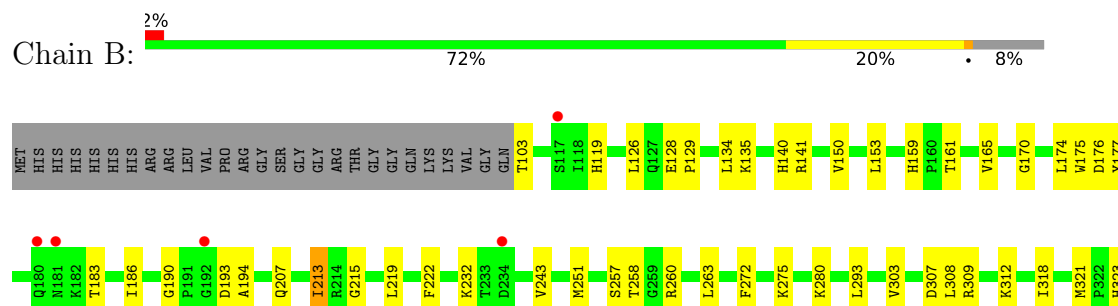
3 Residue-property plots

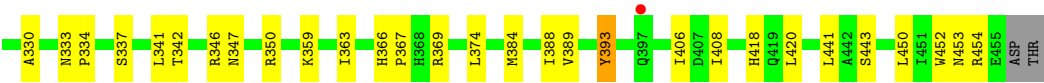
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

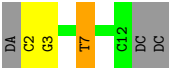


• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

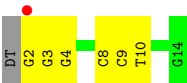




● Molecule 3: 5'-D(*AP*CP*GP*CP*GP*AP*(TTD)P*GP*CP*GP*CP*CP*C)-3'



● Molecule 4: 5'-D(*TP*GP*GP*GP*CP*GP*CP*CP*TP*CP*GP*CP*G)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	114.37Å 116.70Å 137.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.62 – 3.00 48.62 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.62-3.00) 99.4 (48.62-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.04 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.234 , 0.294 0.229 , 0.279	Depositor DCC
R_{free} test set	1866 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	55.5	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	11866	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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: CA, MES, TTD

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	0.42	0/8662	0.70	0/11729
2	B	0.40	0/2898	0.72	2/3938 (0.1%)
3	G	0.21	0/206	0.75	0/313
4	H	0.33	0/297	0.77	0/456
All	All	0.41	0/12063	0.71	2/16436 (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	393	TYR	CA-C-N	5.00	125.00	119.90
2	B	393	TYR	C-N-CA	5.00	125.00	119.90

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	8509	0	8508	88	0
2	B	2824	0	2766	35	0
3	G	225	0	124	2	0
4	H	266	0	145	6	0
5	A	24	0	24	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	0	0
6	H	1	0	0	0	0
7	A	11	0	0	0	0
7	B	5	0	0	0	0
All	All	11866	0	11567	128	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 6.

All (128) 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:329:GLY:HA3	1:A:384:GLU:HG2	1.59	0.82
2:B:140:HIS:HB2	2:B:453:ASN:HB2	1.66	0.77
1:A:218:MET:HE3	1:A:261:HIS:HD2	1.49	0.77
1:A:707:ILE:O	1:A:708:GLN:HB2	1.89	0.70
1:A:81:THR:HG22	1:A:85:ASN:H	1.55	0.70
1:A:263:ARG:HG2	1:A:263:ARG:HH11	1.56	0.69
2:B:307:ASP:HB2	2:B:318:ILE:HD11	1.77	0.67
2:B:443:SER:HB2	2:B:450:LEU:HB2	1.77	0.66
1:A:649:VAL:HG13	1:A:659:ILE:HB	1.76	0.65
1:A:11:LYS:HD2	1:A:38:ARG:HD2	1.76	0.65
4:H:8:DC:H2''	4:H:9:DC:H5'	1.77	0.65
2:B:176:ASP:H	2:B:183:THR:HG22	1.63	0.64
1:A:643:SER:O	1:A:688:PRO:HB2	1.98	0.63
1:A:110:ASP:HB2	1:A:136:TYR:HE2	1.64	0.63
4:H:9:DC:H1'	4:H:10:DT:H71	1.81	0.62
1:A:167:VAL:HG12	1:A:180:PHE:HB3	1.80	0.62
1:A:110:ASP:HB2	1:A:136:TYR:CE2	2.35	0.61
1:A:707:ILE:HD11	1:A:713:ARG:HD2	1.82	0.61
2:B:128:GLU:HG3	2:B:129:PRO:HD3	1.82	0.60
1:A:429:PHE:HB2	1:A:432:GLN:HB2	1.85	0.59
2:B:207:GLN:HB3	2:B:219:LEU:HD21	1.86	0.58
2:B:350:ARG:HG2	2:B:363:ILE:HG12	1.86	0.58
1:A:111:ARG:H	1:A:111:ARG:HD3	1.68	0.58
1:A:111:ARG:HD3	1:A:111:ARG:N	2.19	0.57
3:G:2:DC:H2''	3:G:3:DG:OP2	2.04	0.57
1:A:922:LEU:HD23	1:A:957:VAL:HG13	1.87	0.56
1:A:165:ILE:HG21	1:A:217:SER:HA	1.88	0.56
2:B:323:HIS:NE2	2:B:342:THR:HG21	2.21	0.56
1:A:413:LEU:HB3	1:A:424:THR:HB	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:592:LEU:HD21	1:A:640:THR:HG23	1.87	0.55
1:A:889:ARG:HG3	1:A:904:ASN:OD1	2.07	0.55
1:A:564:ILE:HG23	1:A:588:PRO:HD3	1.89	0.54
1:A:312:GLU:HG3	1:A:327:ARG:HB2	1.89	0.54
2:B:251:MET:HE1	2:B:263:LEU:HD23	1.89	0.53
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.91	0.53
2:B:194:ALA:HB3	2:B:213:ILE:HD12	1.91	0.53
1:A:218:MET:HE3	1:A:261:HIS:CD2	2.38	0.53
2:B:186:ILE:HD11	2:B:222:PHE:HA	1.92	0.52
1:A:928:ARG:HG2	1:A:947:ARG:HH22	1.75	0.52
1:A:7:VAL:HG23	1:A:1039:LEU:HB3	1.93	0.51
2:B:330:ALA:HA	2:B:341:LEU:O	2.11	0.51
1:A:226:PHE:HZ	1:A:287:LYS:HG2	1.75	0.51
2:B:159:HIS:HD2	2:B:161:THR:H	1.59	0.51
4:H:8:DC:H2''	4:H:9:DC:C5'	2.41	0.50
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.92	0.50
1:A:532:THR:HG22	1:A:533:GLU:N	2.25	0.50
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	1.92	0.50
2:B:303:VAL:HB	2:B:321:MET:HB2	1.94	0.49
1:A:81:THR:HG23	1:A:83:LYS:H	1.78	0.49
1:A:391:ARG:NH2	1:A:708:GLN:HA	2.28	0.48
1:A:416:ASP:HB2	1:A:419:ARG:HD2	1.95	0.48
1:A:112:ILE:HD11	2:B:337:SER:O	2.13	0.48
2:B:347:ASN:HA	2:B:366:HIS:O	2.13	0.48
1:A:926:LEU:HD21	2:B:126:LEU:HD11	1.96	0.47
1:A:931:LEU:HG	1:A:947:ARG:HB3	1.96	0.47
1:A:84:TYR:HB2	1:A:109:GLN:HB3	1.96	0.47
1:A:5:TYR:HB2	1:A:1043:LEU:HD11	1.96	0.47
1:A:636:THR:HA	1:A:652:CYS:O	2.14	0.47
2:B:128:GLU:HG3	2:B:129:PRO:CD	2.44	0.47
1:A:412:PRO:HD3	1:A:680:CYS:HB2	1.97	0.47
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.96	0.47
3:G:7:TTD:H6	3:G:7:TTD:H2''	1.64	0.47
1:A:253:ILE:HD11	1:A:302:VAL:HG11	1.97	0.47
1:A:644:LEU:HD23	1:A:706:GLU:HG2	1.96	0.47
1:A:197:LEU:H	1:A:197:LEU:HD23	1.78	0.46
2:B:141:ARG:NE	2:B:177:TYR:O	2.47	0.46
1:A:81:THR:HG22	1:A:85:ASN:N	2.26	0.46
1:A:2:SER:N	1:A:978:GLN:OE1	2.49	0.46
5:A:2142:MES:H32	5:A:2142:MES:H81	1.61	0.46
1:A:478:LEU:HD12	1:A:526:LEU:HG	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:722:ARG:NH2	1:A:812:TYR:OH	2.49	0.46
2:B:135:LYS:HA	2:B:418:HIS:CE1	2.51	0.45
1:A:707:ILE:CD1	1:A:713:ARG:HD2	2.45	0.45
2:B:153:LEU:HD12	2:B:165:VAL:HG22	1.99	0.45
2:B:175:TRP:HD1	2:B:183:THR:HG21	1.82	0.45
2:B:388:ILE:O	2:B:408:ILE:HA	2.17	0.45
1:A:594:THR:HG22	1:A:595:THR:H	1.82	0.45
2:B:170:GLY:HA2	2:B:193:ASP:O	2.17	0.45
1:A:40:GLU:HG2	1:A:54:GLU:HG2	1.98	0.45
1:A:261:HIS:CE1	5:A:2142:MES:O2S	2.70	0.45
2:B:263:LEU:HD13	2:B:272:PHE:HB3	1.98	0.44
1:A:112:ILE:O	1:A:112:ILE:HG12	2.18	0.44
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.53	0.44
1:A:577:LEU:HD23	1:A:621:GLY:HA3	2.00	0.44
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	2.00	0.44
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.53	0.44
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.85	0.44
1:A:916:THR:HG22	1:A:921:ILE:HG12	2.00	0.44
1:A:391:ARG:HH22	1:A:708:GLN:HA	1.83	0.44
2:B:441:LEU:HB3	2:B:452:TRP:HB2	2.00	0.44
4:H:9:DC:H1'	4:H:10:DT:C7	2.47	0.43
1:A:374:GLN:HG2	1:A:391:ARG:HG2	2.00	0.43
1:A:191:LYS:HG2	1:A:209:GLN:HG3	2.01	0.43
1:A:762:SER:O	1:A:803:HIS:HA	2.18	0.43
1:A:889:ARG:HD2	1:A:891:TYR:CE2	2.54	0.43
2:B:257:SER:HA	2:B:280:LYS:HG3	2.01	0.43
1:A:111:ARG:N	1:A:111:ARG:CD	2.81	0.43
1:A:263:ARG:HH11	1:A:263:ARG:CG	2.30	0.42
1:A:508:VAL:HG23	1:A:521:ILE:HD11	2.00	0.42
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.53	0.42
1:A:368:GLU:O	1:A:369:ARG:HB2	2.19	0.42
1:A:795:ASP:O	1:A:799:PHE:HA	2.19	0.42
1:A:253:ILE:CD1	1:A:302:VAL:HG11	2.50	0.42
1:A:934:ALA:HB2	1:A:945:ILE:HD11	2.02	0.42
4:H:3:DG:H2'	4:H:4:DG:C8	2.55	0.42
1:A:436:LEU:HD23	1:A:445:GLU:HB3	2.01	0.42
1:A:218:MET:HE1	1:A:258:ILE:HG22	2.01	0.41
1:A:839:GLU:H	2:B:103:THR:HG21	1.85	0.41
1:A:312:GLU:HG3	1:A:327:ARG:HD3	2.01	0.41
1:A:558:ILE:HG23	1:A:567:ARG:HB2	2.03	0.41
1:A:674:LYS:H	1:A:674:LYS:HG3	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:596:PHE:HZ	1:A:649:VAL:HG12	1.85	0.41
1:A:869:ALA:O	1:A:884:ILE:HA	2.21	0.41
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.35	0.41
2:B:159:HIS:CD2	2:B:161:THR:H	2.37	0.41
1:A:32:LEU:HD13	1:A:66:LEU:HD11	2.03	0.41
2:B:346:ARG:HA	2:B:369:ARG:HA	2.03	0.41
1:A:571:LEU:N	1:A:572:PRO:HD2	2.35	0.41
1:A:723:LYS:HB2	1:A:736:LEU:HB2	2.03	0.41
2:B:260:ARG:HA	2:B:275:LYS:HA	2.02	0.41
2:B:367:PRO:HB2	2:B:393:TYR:O	2.20	0.41
2:B:406:ILE:HB	2:B:420:LEU:HB2	2.02	0.41
1:A:387:LEU:HG	1:A:717:LEU:HD11	2.03	0.41
2:B:258:THR:HG22	4:H:2:DG:C8	2.56	0.41
1:A:312:GLU:CG	1:A:327:ARG:HB2	2.51	0.40
1:A:950:ASN:HA	1:A:951:PRO:HD3	1.97	0.40
2:B:333:ASN:HA	2:B:334:PRO:HD3	1.87	0.40
1:A:807:PHE:CZ	1:A:831:VAL:HG11	2.56	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	
1	A	1070/1159 (92%)	993 (93%)	74 (7%)	3 (0%)	36	70
2	B	351/382 (92%)	330 (94%)	19 (5%)	2 (1%)	21	56
All	All	1421/1541 (92%)	1323 (93%)	93 (6%)	5 (0%)	30	65

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	215	GLY

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Mol	Chain	Res	Type
2	B	190	GLY
1	A	36	ASN
1	A	643	SER
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	948/1014 (94%)	900 (95%)	48 (5%)	21	55
2	B	311/335 (93%)	295 (95%)	16 (5%)	21	55
All	All	1259/1349 (93%)	1195 (95%)	64 (5%)	21	55

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	47	GLU
1	A	54	GLU
1	A	81	THR
1	A	98	ILE
1	A	111	ARG
1	A	112	ILE
1	A	189	HIS
1	A	191	LYS
1	A	218	MET
1	A	253	ILE
1	A	314	LEU
1	A	315	THR
1	A	375	LEU
1	A	384	GLU
1	A	392	ASN
1	A	408	LYS
1	A	448	LEU
1	A	449	MET

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Mol	Chain	Res	Type
1	A	476	VAL
1	A	478	LEU
1	A	507	GLN
1	A	550	ASN
1	A	587	ILE
1	A	627	LYS
1	A	638	LEU
1	A	642	ARG
1	A	687	TYR
1	A	691	LEU
1	A	696	ASN
1	A	705	ASP
1	A	707	ILE
1	A	749	THR
1	A	817	VAL
1	A	867	LYS
1	A	881	LEU
1	A	898	GLU
1	A	901	THR
1	A	914	LEU
1	A	930	VAL
1	A	957	VAL
1	A	966	LEU
1	A	1000	LEU
1	A	1063	LYS
1	A	1086	THR
1	A	1093	LEU
1	A	1094	ILE
1	A	1135	GLU
2	B	119	HIS
2	B	134	LEU
2	B	150	VAL
2	B	174	LEU
2	B	213	ILE
2	B	232	LYS
2	B	243	VAL
2	B	293	LEU
2	B	308	LEU
2	B	309	ARG
2	B	312	LYS
2	B	359	LYS
2	B	374	LEU

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Mol	Chain	Res	Type
2	B	384	MET
2	B	389	VAL
2	B	454	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	93	GLN
1	A	163	HIS
1	A	183	GLN
1	A	209	GLN
1	A	241	ASN
1	A	261	HIS
1	A	262	ASN
1	A	374	GLN
1	A	397	HIS
1	A	399	HIS
1	A	456	GLN
1	A	465	HIS
1	A	467	GLN
1	A	528	GLN
1	A	550	ASN
1	A	648	ASN
1	A	711	HIS
1	A	727	GLN
1	A	731	GLN
1	A	859	GLN
1	A	877	ASN
1	A	907	ASN
1	A	950	ASN
1	A	990	GLN
1	A	991	HIS
1	A	993	GLN
1	A	1056	ASN
1	A	1106	GLN
1	A	1113	GLN
1	A	1140	HIS
2	B	121	GLN
2	B	140	HIS
2	B	187	GLN
2	B	202	GLN

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Mol	Chain	Res	Type
2	B	269	HIS
2	B	362	GLN
2	B	401	ASN
2	B	418	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	TTD	G	7	3	42,45,46	1.74	9 (21%)	61,74,77	2.57	17 (27%)

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	TTD	G	7	3	-	14/22/109/110	0/5/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7	TTD	C1R-N1T	5.13	1.52	1.45
3	G	7	TTD	C1'-N1	3.71	1.50	1.45
3	G	7	TTD	C2-N1	3.57	1.43	1.36
3	G	7	TTD	PB-O5P	3.54	1.63	1.50
3	G	7	TTD	C6-N1	3.08	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7	TTD	C2T-N1T	2.97	1.42	1.36
3	G	7	TTD	C6T-N1T	2.66	1.50	1.46
3	G	7	TTD	C5T-C4T	2.18	1.55	1.51
3	G	7	TTD	O4'-C1'	2.14	1.47	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	7	TTD	O4R-C1R-N1T	11.43	122.20	108.65
3	G	7	TTD	C5T-C4T-N3T	6.33	121.41	116.09
3	G	7	TTD	C5-C4-N3	6.32	121.39	116.09
3	G	7	TTD	N3-C2-N1	5.54	122.58	116.78
3	G	7	TTD	N3T-C2T-N1T	4.95	121.96	116.78
3	G	7	TTD	C4-N3-C2	-3.44	121.48	126.67
3	G	7	TTD	C2'-C1'-N1	-3.32	111.10	115.59
3	G	7	TTD	C4T-N3T-C2T	-3.14	121.94	126.67
3	G	7	TTD	C4'-O4R-C1R	-3.11	102.12	109.51
3	G	7	TTD	O4-C4-C5	-3.08	119.85	122.71
3	G	7	TTD	O2-C2-N3	-2.91	116.12	121.49
3	G	7	TTD	C5-C5T-C6T	2.90	91.75	88.36
3	G	7	TTD	O4'-C1'-N1	2.61	111.74	108.65
3	G	7	TTD	O4T-C4T-C5T	-2.42	120.46	122.71
3	G	7	TTD	O4R-C1R-C2R	-2.39	101.78	106.25
3	G	7	TTD	O2T-C2T-N1T	-2.23	120.10	123.44
3	G	7	TTD	O4'-C4R-C5'	2.11	116.09	109.33

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	7	TTD	C2'-C3R-O3R-PB
3	G	7	TTD	O4'-C1'-N1-C2
3	G	7	TTD	C5R-O5R-PB-O3R
3	G	7	TTD	O4R-C4'-C5R-O5R
3	G	7	TTD	C3'-C4'-C5R-O5R
3	G	7	TTD	O4'-C1'-N1-C6
3	G	7	TTD	C2R-C1R-N1T-C6T
3	G	7	TTD	O4'-C4R-C5'-O5'
3	G	7	TTD	C4R-C5'-O5'-P
3	G	7	TTD	O4R-C1R-N1T-C6T
3	G	7	TTD	C2'-C1'-N1-C6
3	G	7	TTD	O4R-C1R-N1T-C2T

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Mol	Chain	Res	Type	Atoms
3	G	7	TTD	C3R-O3R-PB-O4P
3	G	7	TTD	C2R-C1R-N1T-C2T

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	7	TTD	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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$
5	MES	A	2142	-	12,12,12	2.16	2 (16%)	15,16,16	5.86	9 (60%)
5	MES	A	2141	-	12,12,12	2.17	1 (8%)	15,16,16	5.91	9 (60%)

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	MES	A	2142	-	-	2/6/14/14	0/1/1/1
5	MES	A	2141	-	-	5/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2141	MES	C8-S	-7.11	1.67	1.77
5	A	2142	MES	C8-S	-6.83	1.68	1.77
5	A	2142	MES	O1S-S	2.43	1.52	1.45

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2142	MES	O1S-S-C8	-13.84	85.81	106.73
5	A	2141	MES	O2S-S-C8	-13.60	86.17	106.73
5	A	2141	MES	O1S-S-C8	-11.79	88.92	106.73
5	A	2142	MES	O2S-S-C8	-11.52	89.32	106.73
5	A	2141	MES	O3S-S-C8	-10.47	85.51	106.00
5	A	2142	MES	O3S-S-C8	-10.11	86.23	106.00
5	A	2141	MES	C5-N4-C3	5.82	121.38	108.84
5	A	2142	MES	C5-N4-C3	5.23	120.10	108.84
5	A	2142	MES	C7-N4-C3	4.10	122.17	111.24
5	A	2142	MES	O3S-S-O1S	3.68	120.60	111.40
5	A	2142	MES	O3S-S-O2S	3.59	120.37	111.40
5	A	2141	MES	O3S-S-O2S	3.33	119.73	111.40
5	A	2141	MES	O3S-S-O1S	3.13	119.23	111.40
5	A	2141	MES	C7-N4-C5	3.03	119.32	111.24
5	A	2141	MES	C7-N4-C3	3.02	119.30	111.24
5	A	2142	MES	C7-N4-C5	2.43	117.73	111.24
5	A	2142	MES	C6-C5-N4	-2.27	106.67	110.12
5	A	2141	MES	C6-C5-N4	-2.27	106.67	110.12

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2141	MES	N4-C7-C8-S
5	A	2141	MES	C7-C8-S-O1S
5	A	2141	MES	C7-C8-S-O2S
5	A	2141	MES	C7-C8-S-O3S
5	A	2142	MES	C8-C7-N4-C3
5	A	2142	MES	N4-C7-C8-S
5	A	2141	MES	C8-C7-N4-C5

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2142	MES	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1088/1159 (93%)	0.19	12 (1%) 78 57	30, 47, 68, 82	0
2	B	353/382 (92%)	0.13	6 (1%) 69 45	32, 46, 60, 65	0
3	G	9/13 (69%)	0.91	0 100 100	59, 69, 93, 98	0
4	H	13/14 (92%)	1.05	1 (7%) 19 10	57, 72, 79, 79	0
All	All	1463/1568 (93%)	0.19	19 (1%) 75 53	30, 47, 67, 98	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	403	ASP	3.3
2	B	181	ASN	2.8
1	A	683	ASN	2.7
4	H	2	DG	2.6
1	A	430	VAL	2.5
1	A	437	MET	2.4
2	B	117	SER	2.4
1	A	1120	MET	2.3
1	A	46	ALA	2.3
1	A	548	ASP	2.2
1	A	686	GLY	2.2
1	A	685	ASP	2.2
2	B	180	GLN	2.2
2	B	192	GLY	2.2
2	B	234	ASP	2.1
1	A	448	LEU	2.1
2	B	397	GLN	2.1
1	A	1121	LYS	2.0
1	A	295	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	TTD	G	7	40/41	0.85	0.14	64,66,67,67	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(Å ²)	Q<0.9
6	CA	H	1015	1/1	0.72	0.20	78,78,78,78	0
5	MES	A	2142	12/12	0.73	0.25	83,84,84,84	0
5	MES	A	2141	12/12	0.82	0.24	116,116,117,117	0
6	CA	B	1456	1/1	0.96	0.04	56,56,56,56	0

6.5 Other polymers [i](#)

There are no such residues in this entry.