



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:05 AM UTC

PDB ID : 4A09 / pdb_00004a09
Title : Structure of hsDDB1-drDDB2 bound to a 15 bp CPD-duplex (purine at D-1 position) at 3.1 Å resolution (CPD 2)
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Deposited on : 2011-09-08
Resolution : 3.10 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

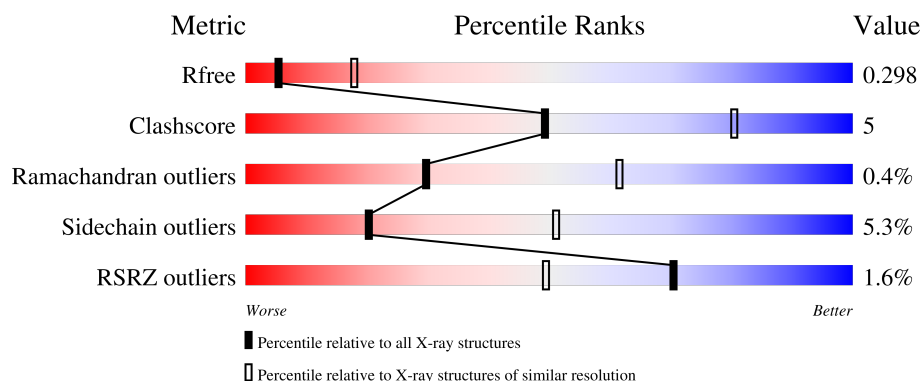
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	 2% 80% 14% • 5%
2	B	382	 % 74% 17% • 7%
3	G	14	 50% 43% 7%
4	H	16	 6% 62% 31% 6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 12113 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	0	0	0
			8646	5484	1453	1662	47			

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	354	Total	C	N	O	S	0	0	0
			2839	1804	498	526	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(*GP*GP*TP*GP*AP*AP*AP*(TTD)P*AP*GP*C P*AP*GP*GP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	14	Total	C	N	O	P	0	0	0
			313	149	64	86	14			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	15	Total	C	N	O	P	0	0	0
			292	142	44	92	14			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

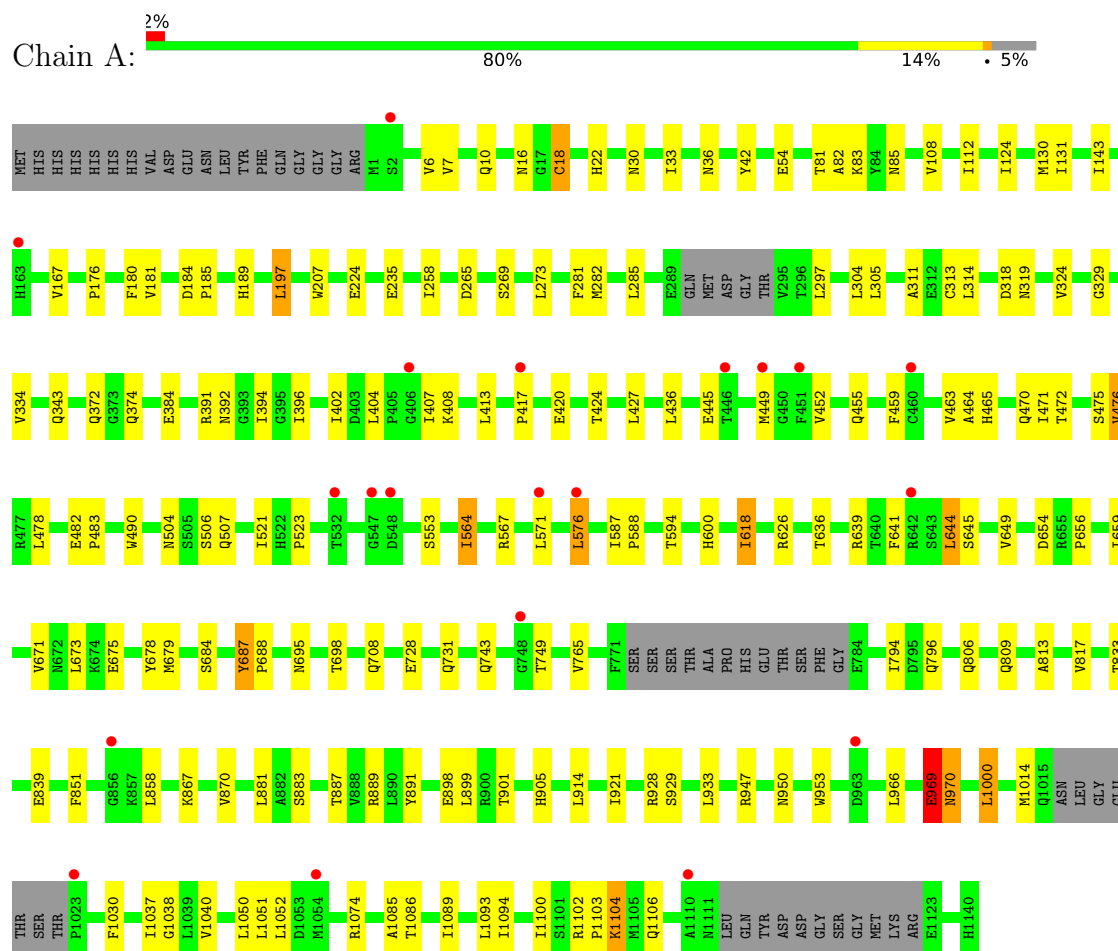
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total 16	O 16	0	0
6	B	4	Total 4	O 4	0	0
6	G	2	Total 2	O 2	0	0

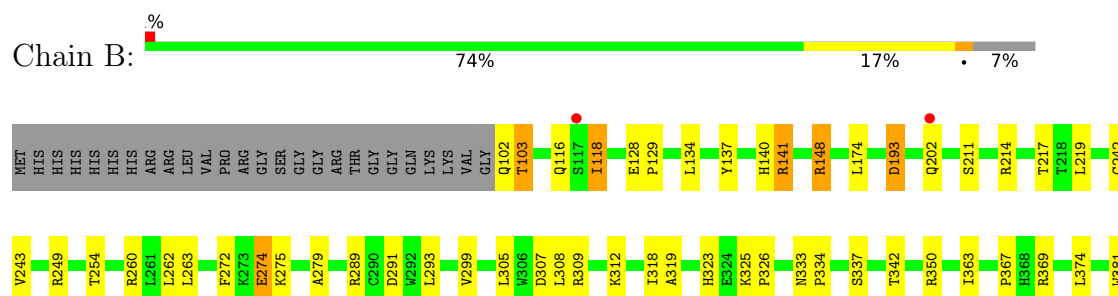
3 Residue-property plots

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

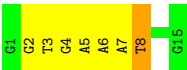


• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2





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



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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	111.65Å 122.94Å 154.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.27 – 3.10 48.27 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.27-3.10) 99.8 (48.27-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.55 (at 3.12Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.245 , 0.308 0.239 , 0.298	Depositor DCC
R_{free} test set	1955 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	62.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12113	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.45% 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: TTD, CA

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	0.41	0/8803	0.72	4/11924 (0.0%)
2	B	0.41	0/2913	0.72	0/3957
3	G	0.19	0/308	0.73	0/473
4	H	0.27	0/323	0.87	0/494
All	All	0.40	0/12347	0.73	4/16848 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	687	TYR	CA-C-N	5.65	126.90	119.84
1	A	687	TYR	C-N-CA	5.65	126.90	119.84
1	A	464	ALA	N-CA-C	5.44	116.89	111.07
1	A	969	GLU	N-CA-C	5.04	116.65	109.14

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	8646	0	8626	82	0
2	B	2839	0	2785	39	0
3	G	313	0	170	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	292	0	172	4	0
5	B	1	0	0	0	0
6	A	16	0	0	0	0
6	B	4	0	0	0	0
6	G	2	0	0	0	0
All	All	12113	0	11753	129	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 5.

All (129) 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:81:THR:HG22	1:A:83:LYS:H	1.41	0.86
1:A:167:VAL:HG12	1:A:180:PHE:HB3	1.65	0.78
1:A:482:GLU:HB3	1:A:483:PRO:HD3	1.67	0.75
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.70	0.71
1:A:329:GLY:HA3	1:A:384:GLU:HG2	1.73	0.70
2:B:141:ARG:HH11	2:B:141:ARG:HG2	1.55	0.70
2:B:249:ARG:HE	2:B:291:ASP:HB3	1.58	0.68
4:H:1:DC:H2''	4:H:2:DC:C5	2.29	0.67
2:B:323:HIS:NE2	2:B:342:THR:HG21	2.10	0.66
2:B:350:ARG:HG2	2:B:363:ILE:HG12	1.77	0.65
4:H:1:DC:H2''	4:H:2:DC:H5	1.62	0.65
1:A:654:ASP:HA	1:A:675:GLU:HG3	1.78	0.64
1:A:18:CYS:HB2	1:A:313:CYS:SG	2.37	0.64
1:A:507:GLN:NE2	1:A:553:SER:H	1.93	0.64
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.80	0.64
1:A:197:LEU:H	1:A:197:LEU:HD23	1.63	0.62
1:A:413:LEU:HB3	1:A:424:THR:HB	1.82	0.62
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.82	0.61
2:B:211:SER:HB3	2:B:243:VAL:HG13	1.82	0.60
1:A:839:GLU:H	2:B:103:THR:HG21	1.66	0.60
2:B:193:ASP:HB2	2:B:214:ARG:HD3	1.84	0.59
1:A:402:ILE:HG22	1:A:404:LEU:HD13	1.83	0.59
2:B:443:SER:HB2	2:B:450:LEU:HB2	1.84	0.58
2:B:263:LEU:HB2	2:B:272:PHE:HB3	1.84	0.57
1:A:953:TRP:HB2	1:A:970:ASN:HB2	1.85	0.57
1:A:16:ASN:HD22	1:A:36:ASN:H	1.53	0.56
2:B:307:ASP:OD1	2:B:309:ARG:HG2	2.05	0.55
1:A:476:VAL:HG13	1:A:490:TRP:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:305:LEU:HD12	2:B:319:ALA:HB3	1.89	0.54
1:A:273:LEU:HB2	1:A:281:PHE:HB2	1.89	0.54
2:B:369:ARG:HH21	2:B:395:ASP:HA	1.73	0.53
2:B:140:HIS:HB2	2:B:453:ASN:HB2	1.91	0.53
1:A:969:GLU:HG2	1:A:970:ASN:N	2.22	0.53
2:B:134:LEU:HA	2:B:137:TYR:CD1	2.45	0.52
1:A:1089:ILE:HG21	1:A:1094:ILE:HD11	1.91	0.51
2:B:279:ALA:HB1	2:B:299:VAL:HG23	1.90	0.51
2:B:388:ILE:O	2:B:408:ILE:HA	2.10	0.51
2:B:367:PRO:HG2	2:B:392:ARG:HG3	1.92	0.51
1:A:567:ARG:HH11	1:A:576:LEU:HD21	1.76	0.51
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.26	0.51
1:A:504:ASN:HD22	1:A:506:SER:H	1.59	0.50
1:A:905:HIS:CD2	1:A:933:LEU:HD21	2.47	0.50
1:A:870:VAL:HA	1:A:883:SER:O	2.12	0.49
1:A:81:THR:HB	1:A:85:ASN:HB2	1.93	0.49
1:A:507:GLN:HE22	1:A:553:SER:H	1.58	0.49
2:B:102:GLN:O	2:B:103:THR:HG22	2.13	0.49
2:B:141:ARG:HH11	2:B:141:ARG:CG	2.21	0.49
2:B:260:ARG:HA	2:B:275:LYS:HA	1.95	0.49
2:B:289:ARG:HD2	2:B:337:SER:HB2	1.95	0.49
1:A:684:SER:HB3	1:A:687:TYR:HB2	1.95	0.48
1:A:184:ASP:HB2	1:A:185:PRO:CD	2.40	0.48
1:A:452:VAL:HB	1:A:470:GLN:HE22	1.78	0.48
1:A:504:ASN:ND2	1:A:506:SER:H	2.10	0.48
1:A:851:PHE:HB3	1:A:858:LEU:HD22	1.96	0.48
1:A:130:MET:HE3	1:A:176:PRO:HG2	1.94	0.48
1:A:813:ALA:HA	1:A:833:THR:HG22	1.96	0.47
1:A:285:LEU:HB3	1:A:297:LEU:HD11	1.96	0.47
2:B:307:ASP:HB2	2:B:318:ILE:HD11	1.97	0.47
1:A:929:SER:HB2	1:A:950:ASN:O	2.14	0.47
2:B:441:LEU:HB3	2:B:452:TRP:HB2	1.97	0.47
1:A:329:GLY:HA3	1:A:384:GLU:CG	2.41	0.46
2:B:242:CYS:O	2:B:254:THR:HG23	2.14	0.46
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.98	0.46
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.51	0.46
3:G:4:DG:H2''	3:G:5:DA:C8	2.51	0.46
1:A:459:PHE:HB3	1:A:471:ILE:HD12	1.98	0.46
4:H:2:DC:C2'	4:H:3:DT:H71	2.46	0.46
2:B:279:ALA:CB	2:B:299:VAL:HG23	2.46	0.45
2:B:382:HIS:CG	2:B:383:PRO:HD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1089:ILE:CG2	1:A:1094:ILE:HD11	2.46	0.45
1:A:731:GLN:HA	1:A:796:GLN:NE2	2.32	0.45
1:A:1100:ILE:HD12	1:A:1104:LYS:HB3	1.99	0.45
1:A:507:GLN:HE22	1:A:553:SER:N	2.15	0.45
1:A:891:TYR:HB3	1:A:899:LEU:HG	1.98	0.45
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.81	0.44
1:A:928:ARG:HG2	1:A:947:ARG:HH12	1.82	0.44
1:A:374:GLN:HE21	1:A:391:ARG:HB2	1.82	0.44
3:G:8:TTD:O4'	3:G:8:TTD:O2	2.36	0.44
1:A:282:MET:HB2	1:A:305:LEU:HD11	1.99	0.44
2:B:333:ASN:HB3	2:B:381:TRP:CE2	2.52	0.44
1:A:181:VAL:HA	1:A:189:HIS:O	2.18	0.44
1:A:436:LEU:HA	1:A:445:GLU:HA	2.00	0.44
2:B:148:ARG:HA	2:B:447:PHE:CE2	2.52	0.44
1:A:649:VAL:HG22	1:A:659:ILE:HB	2.00	0.44
1:A:463:VAL:HB	1:A:521:ILE:HG21	2.00	0.43
2:B:334:PRO:HG2	2:B:383:PRO:HA	1.99	0.43
2:B:405:THR:HG22	2:B:421:ARG:HB2	1.99	0.43
2:B:141:ARG:CG	2:B:141:ARG:NH1	2.80	0.43
1:A:10:GLN:HB3	1:A:1037:ILE:HB	2.01	0.43
1:A:564:ILE:HG23	1:A:588:PRO:HD3	2.00	0.43
1:A:1000:LEU:HD11	1:A:1030:PHE:CE1	2.53	0.43
1:A:258:ILE:HD13	1:A:273:LEU:HD13	2.01	0.43
1:A:472:THR:HG23	1:A:475:SER:H	1.84	0.43
2:B:394:PRO:HB3	2:B:402:ASP:HB3	2.00	0.43
1:A:372:GLN:HA	1:A:1014:MET:HG2	2.00	0.43
3:G:2:DG:H2''	3:G:3:DT:OP2	2.18	0.43
1:A:600:HIS:CD2	1:A:618:ILE:HG12	2.54	0.43
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.54	0.43
1:A:22:HIS:HA	1:A:30:ASN:HD22	1.84	0.43
1:A:504:ASN:HD21	1:A:507:GLN:HG2	1.83	0.43
2:B:272:PHE:CZ	2:B:274:GLU:HB2	2.54	0.42
1:A:33:ILE:HD12	1:A:42:TYR:HE2	1.83	0.42
2:B:217:THR:OG1	2:B:254:THR:HG21	2.19	0.42
4:H:8:DC:H1'	4:H:9:DT:H71	2.02	0.42
1:A:265:ASP:OD2	1:A:269:SER:HB2	2.19	0.42
2:B:325:LYS:HB3	2:B:326:PRO:HD2	2.00	0.42
2:B:367:PRO:HB2	2:B:393:TYR:O	2.20	0.42
1:A:396:ILE:HG12	1:A:673:LEU:HD11	2.01	0.42
1:A:921:ILE:HB	1:A:933:LEU:HB2	2.02	0.42
1:A:928:ARG:HG2	1:A:947:ARG:NH1	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:TYR:C	2:B:393:TYR:CD1	2.98	0.42
1:A:455:GLN:HB3	1:A:472:THR:OG1	2.19	0.41
2:B:128:GLU:N	2:B:129:PRO:HD2	2.35	0.41
3:G:6:DA:H2''	3:G:7:DA:OP2	2.20	0.41
1:A:1074:ARG:O	1:A:1085:ALA:HB2	2.20	0.41
3:G:8:TTD:H2''	3:G:8:TTD:H6	1.68	0.41
1:A:743:GLN:HA	1:A:749:THR:HG22	2.02	0.41
1:A:108:VAL:HG11	1:A:143:ILE:HD11	2.02	0.41
1:A:765:VAL:HG12	1:A:806:GLN:HB3	2.03	0.41
1:A:81:THR:CG2	1:A:82:ALA:N	2.83	0.41
1:A:571:LEU:HD23	1:A:571:LEU:HA	1.90	0.41
1:A:641:PHE:HB3	1:A:679:MET:HE1	2.01	0.41
1:A:644:LEU:HG	1:A:645:SER:H	1.86	0.41
1:A:6:VAL:HG22	1:A:1040:VAL:HG22	2.02	0.41
1:A:81:THR:HG22	1:A:82:ALA:N	2.35	0.40
1:A:408:LYS:HA	1:A:678:TYR:CE2	2.55	0.40
2:B:382:HIS:CD2	2:B:383:PRO:HD2	2.56	0.40
1:A:311:ALA:HB2	1:A:324:VAL:HG13	2.02	0.40
1:A:465:HIS:CD2	1:A:523:PRO:HD3	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	1095/1159 (94%)	1011 (92%)	80 (7%)	4 (0%)	30 61
2	B	352/382 (92%)	327 (93%)	23 (6%)	2 (1%)	21 52
All	All	1447/1541 (94%)	1338 (92%)	103 (7%)	6 (0%)	30 61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	407	ILE
1	A	417	PRO
1	A	688	PRO
2	B	193	ASP
2	B	118	ILE
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	967/1014 (95%)	915 (95%)	52 (5%)	20	50
2	B	313/335 (93%)	297 (95%)	16 (5%)	21	52
All	All	1280/1349 (95%)	1212 (95%)	68 (5%)	20	51

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	18	CYS
1	A	54	GLU
1	A	112	ILE
1	A	197	LEU
1	A	207	TRP
1	A	224	GLU
1	A	235	GLU
1	A	304	LEU
1	A	314	LEU
1	A	318	ASP
1	A	319	ASN
1	A	334	VAL
1	A	343	GLN
1	A	392	ASN
1	A	394	ILE
1	A	420	GLU
1	A	427	LEU

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Mol	Chain	Res	Type
1	A	449	MET
1	A	476	VAL
1	A	478	LEU
1	A	576	LEU
1	A	587	ILE
1	A	594	THR
1	A	618	ILE
1	A	626	ARG
1	A	636	THR
1	A	639	ARG
1	A	644	LEU
1	A	695	ASN
1	A	698	THR
1	A	708	GLN
1	A	728	GLU
1	A	794	ILE
1	A	809	GLN
1	A	817	VAL
1	A	867	LYS
1	A	881	LEU
1	A	887	THR
1	A	898	GLU
1	A	901	THR
1	A	914	LEU
1	A	966	LEU
1	A	969	GLU
1	A	970	ASN
1	A	1000	LEU
1	A	1050	LEU
1	A	1052	LEU
1	A	1086	THR
1	A	1093	LEU
1	A	1104	LYS
1	A	1106	GLN
2	B	103	THR
2	B	116	GLN
2	B	118	ILE
2	B	141	ARG
2	B	148	ARG
2	B	174	LEU
2	B	202	GLN
2	B	219	LEU

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Mol	Chain	Res	Type
2	B	262	LEU
2	B	274	GLU
2	B	293	LEU
2	B	308	LEU
2	B	312	LYS
2	B	374	LEU
2	B	389	VAL
2	B	453	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	16	ASN
1	A	30	ASN
1	A	85	ASN
1	A	109	GLN
1	A	156	ASN
1	A	209	GLN
1	A	234	GLN
1	A	241	ASN
1	A	267	ASN
1	A	374	GLN
1	A	439	ASN
1	A	456	GLN
1	A	465	HIS
1	A	504	ASN
1	A	522	HIS
1	A	531	HIS
1	A	683	ASN
1	A	789	HIS
1	A	790	ASN
1	A	796	GLN
1	A	809	GLN
1	A	877	ASN
1	A	885	ASN
1	A	907	ASN
1	A	950	ASN
1	A	970	ASN
1	A	990	GLN
1	A	993	GLN
1	A	1034	ASN

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Mol	Chain	Res	Type
1	A	1049	ASN
1	A	1055	GLN
1	A	1056	ASN
1	A	1070	HIS
1	A	1106	GLN
1	A	1140	HIS
2	B	102	GLN
2	B	107	HIS
2	B	116	GLN
2	B	119	HIS
2	B	121	GLN
2	B	159	HIS
2	B	181	ASN
2	B	269	HIS
2	B	362	GLN
2	B	370	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 ⓘ

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	8	3	42,45,46	1.57	8 (19%)	61,74,77	2.71	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	8	3	-	16/22/109/110	0/5/6/6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	8	TTD	C1R-N1T	4.15	1.51	1.45
3	G	8	TTD	PB-O5P	3.61	1.63	1.50
3	G	8	TTD	C2-N1	3.55	1.43	1.36
3	G	8	TTD	C1'-N1	3.48	1.50	1.45
3	G	8	TTD	C6-N1	3.06	1.51	1.46
3	G	8	TTD	C2T-N1T	2.61	1.41	1.36
3	G	8	TTD	C6T-N1T	2.26	1.50	1.46
3	G	8	TTD	O4'-C1'	2.06	1.47	1.42

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	8	TTD	O4R-C1R-N1T	12.26	123.18	108.65
3	G	8	TTD	C5-C4-N3	6.93	121.91	116.09
3	G	8	TTD	C5T-C4T-N3T	6.92	121.90	116.09
3	G	8	TTD	N3-C2-N1	5.58	122.62	116.78
3	G	8	TTD	N3T-C2T-N1T	4.95	121.97	116.78
3	G	8	TTD	O4-C4-C5	-3.68	119.28	122.71
3	G	8	TTD	C4-N3-C2	-3.62	121.21	126.67
3	G	8	TTD	C4'-O4R-C1R	-3.60	100.96	109.51
3	G	8	TTD	C4T-N3T-C2T	-3.41	121.52	126.67
3	G	8	TTD	O2-C2-N3	-3.06	115.85	121.49
3	G	8	TTD	C2R-C1R-N1T	-2.91	111.66	115.59
3	G	8	TTD	O4T-C4T-C5T	-2.77	120.13	122.71
3	G	8	TTD	C2'-C1'-N1	-2.63	112.03	115.59
3	G	8	TTD	C5-C5T-C6T	2.52	91.31	88.36
3	G	8	TTD	O4R-C1R-C2R	-2.37	101.82	106.25
3	G	8	TTD	O2T-C2T-N1T	-2.11	120.27	123.44
3	G	8	TTD	O2T-C2T-N3T	-2.05	117.71	121.49

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	8	TTD	C2'-C3R-O3R-PB

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Mol	Chain	Res	Type	Atoms
3	G	8	TTD	O4'-C1'-N1-C2
3	G	8	TTD	C5R-O5R-PB-O3R
3	G	8	TTD	O4R-C4'-C5R-O5R
3	G	8	TTD	C3'-C4'-C5R-O5R
3	G	8	TTD	O4'-C1'-N1-C6
3	G	8	TTD	O4'-C4R-C5'-O5'
3	G	8	TTD	C2R-C1R-N1T-C6T
3	G	8	TTD	O4R-C1R-N1T-C6T
3	G	8	TTD	C4R-C5'-O5'-P
3	G	8	TTD	C2'-C1'-N1-C6
3	G	8	TTD	O4R-C1R-N1T-C2T
3	G	8	TTD	C2R-C1R-N1T-C2T
3	G	8	TTD	C3R-O3R-PB-O5P
3	G	8	TTD	C3R-O3R-PB-O4P
3	G	8	TTD	C4'-C5R-O5R-PB

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	8	TTD	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

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	1105/1159 (95%)	0.30	20 (1%) 67 47	39, 56, 80, 96	0
2	B	354/382 (92%)	0.12	3 (0%) 82 65	33, 49, 66, 75	0
3	G	13/14 (92%)	0.73	0 100 100	56, 73, 100, 102	0
4	H	15/16 (93%)	0.79	1 (6%) 24 13	47, 74, 107, 108	0
All	All	1487/1571 (94%)	0.27	24 (1%) 70 49	33, 54, 79, 108	0

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	117	SER	4.4
1	A	547	GLY	3.7
1	A	2	SER	3.1
1	A	451	PHE	2.8
1	A	460	CYS	2.8
1	A	449	MET	2.7
1	A	571	LEU	2.7
1	A	856	GLY	2.5
1	A	548	ASP	2.4
1	A	406	GLY	2.3
1	A	1110	ALA	2.3
2	B	453	ASN	2.3
1	A	417	PRO	2.2
1	A	446	THR	2.2
4	H	1	DC	2.1
1	A	642	ARG	2.1
1	A	748	GLY	2.1
1	A	163	HIS	2.1
1	A	963	ASP	2.1
2	B	202	GLN	2.1
1	A	576	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	532	THR	2.0
1	A	1023	PRO	2.0
1	A	1054	MET	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	8	40/41	0.85	0.15	63,66,66,66	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
5	CA	B	1456	1/1	0.99	0.17	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.