WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Dec 16, 2023 – 08:05 am GMT

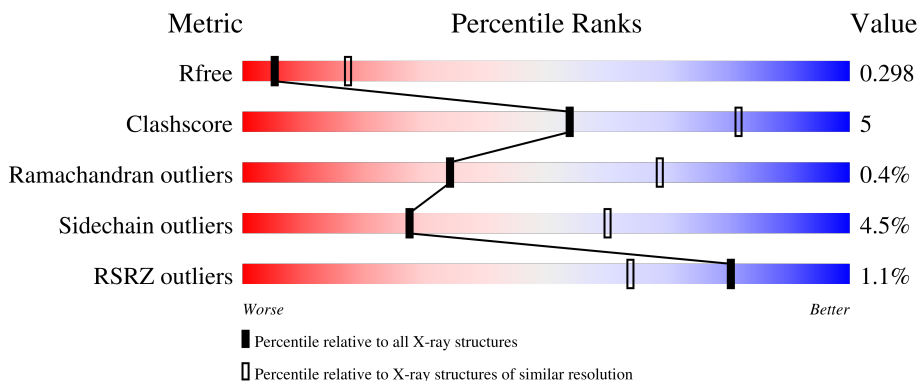|		
PDB ID	:	4A09
Title	:	Structure of hsDDB1-drDDB2 bound to a 15 bp CPD-duplex (purine at D-1 position) at 3.1 A resolution (CPD 2)
Authors	:	Scrima, A.; Fischer, E.S.; Iwai, S.; Gut, H.; Thoma, N.H.
Deposited on	:	2011-09-08
Resolution	:	3.10 Å(reported)

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	Percentile Ranks	Value
Rfree		0.298
Clashscore		5
Ramachandran outliers		0.4%
Sidechain outliers		4.5%
RSRZ outliers		1.1%

Worse *Better*

█ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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 <=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	%: 81% 14% · 5%
2	B	382	75% 16% · 7%
3	G	14	50% 36% 14%
4	H	16	6%: 62% 25% 6% 6%

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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 8646	C 5484	N 1453	O 1662	S 47	0	0	0

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 2839	C 1804	N 498	O 526	S 11	0	0	0

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 (three-letter code: 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 ann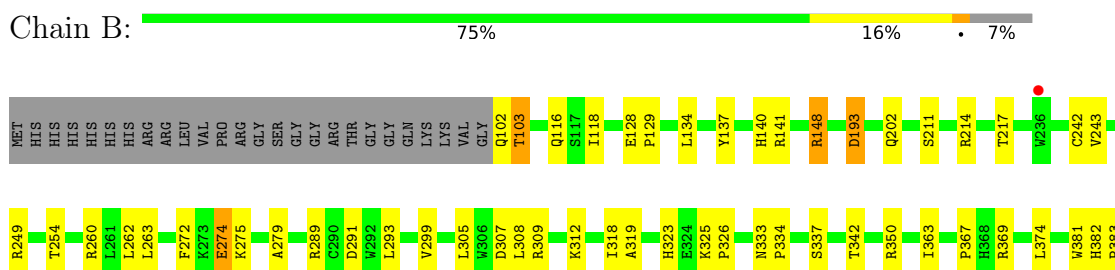otated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (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
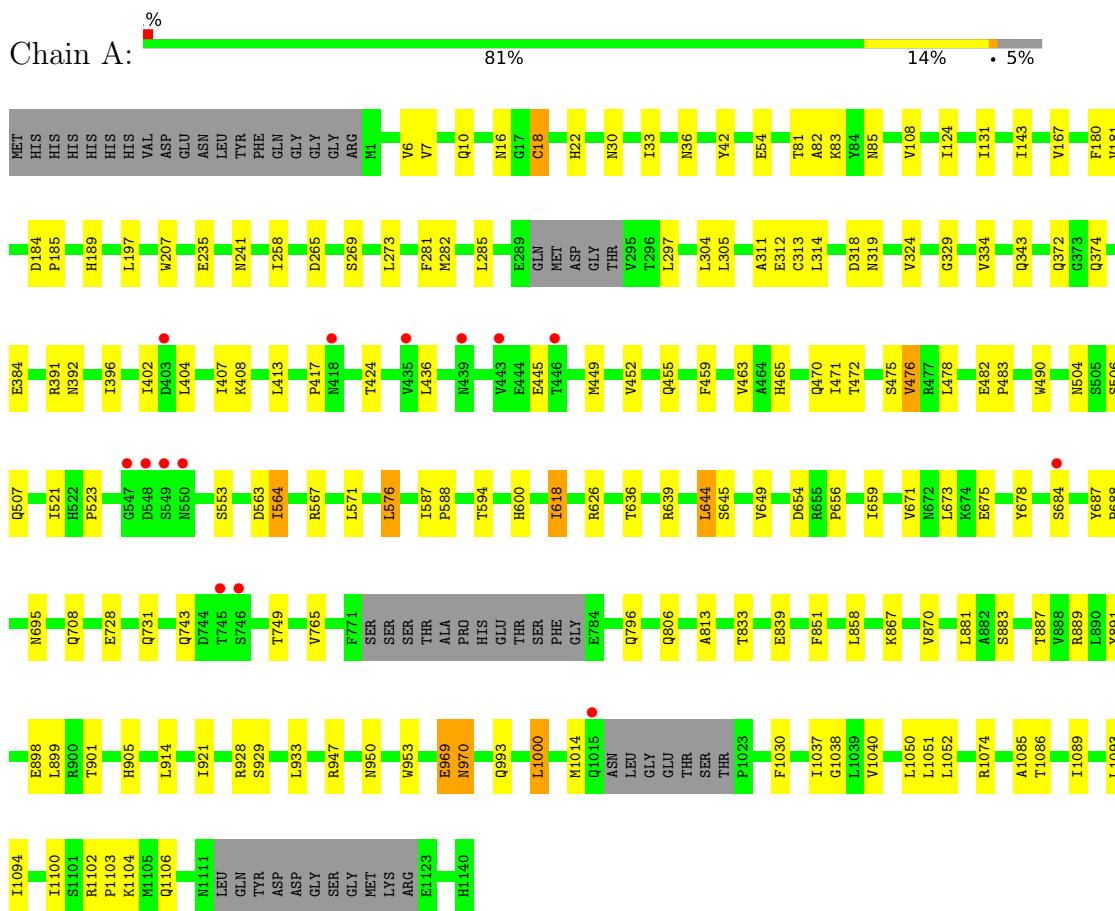
• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

I388 V389 R392 Y393 P394 D395 D402 T405 I408 R421 L441 A442 S443 F447 L450 I451 W452 N453 R454 E455 ASP THR

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

Chain G:

| 50% | 36% | 14% |

G1 G2 T3 G4 A5 A6 A7 T8 G15

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

6%

Chain H:

| 62% | 25% | 6% | 6% |

C1 C2 T3 C8 T9 C15 DC
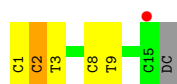
4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 , 45.3	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CA, 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	0.32	0/8803	0.51	0/11924
2	B	0.32	0/2913	0.52	0/3957
3	G	0.61	0/308	1.03	1/473 (0.2%)
4	H	0.77	0/323	1.24	1/494 (0.2%)
All	All	0.35	0/12347	0.56	2/16848 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	5	DA	P-O3'-C3'	5.15	125.88	119.70
4	H	2	DC	P-O3'-C3'	5.01	125.71	119.70

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	8646	0	8626	80	0
2	B	2839	0	2785	38	0
3	G	313	0	170	5	0
4	H	292	0	172	4	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	126	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 (126) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:969:GLU:HG2	1:A:970:ASN:N	2.22	0.53
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
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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 ⓘ

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	1095/1159 (94%)	1011 (92%)	80 (7%)	4 (0%)	34	69
2	B	352/382 (92%)	327 (93%)	23 (6%)	2 (1%)	25	59
All	All	1447/1541 (94%)	1338 (92%)	103 (7%)	6 (0%)	34	69

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

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Mol	Chain	Res	Type
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%)	923 (95%)	44 (5%)	27	59
2	B	313/335 (93%)	300 (96%)	13 (4%)	30	62
All	All	1280/1349 (95%)	1223 (96%)	57 (4%)	27	60

All (57) 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	207	TRP
1	A	235	GLU
1	A	241	ASN
1	A	304	LEU
1	A	312	GLU
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	449	MET
1	A	476	VAL
1	A	478	LEU
1	A	563	ASP
1	A	576	LEU
1	A	587	ILE
1	A	594	THR

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Mol	Chain	Res	Type
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	708	GLN
1	A	728	GLU
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	969	GLU
1	A	970	ASN
1	A	993	GLN
1	A	1000	LEU
1	A	1050	LEU
1	A	1052	LEU
1	A	1086	THR
1	A	1093	LEU
1	A	1106	GLN
2	B	103	THR
2	B	116	GLN
2	B	148	ARG
2	B	202	GLN
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	393	TYR
2	B	453	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	30	ASN

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Mol	Chain	Res	Type
1	A	85	ASN
1	A	156	ASN
1	A	234	GLN
1	A	240	HIS
1	A	241	ASN
1	A	267	ASN
1	A	374	GLN
1	A	392	ASN
1	A	456	GLN
1	A	481	GLN
1	A	504	ASN
1	A	522	HIS
1	A	683	ASN
1	A	727	GLN
1	A	796	GLN
1	A	806	GLN
1	A	809	GLN
1	A	885	ASN
1	A	950	ASN
1	A	970	ASN
1	A	990	GLN
1	A	1034	ASN
1	A	1049	ASN
1	A	1055	GLN
1	A	1106	GLN
2	B	102	GLN
2	B	107	HIS
2	B	119	HIS
2	B	159	HIS
2	B	181	ASN
2	B	269	HIS
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	1.54	8 (19%)	62,74,77	2.70	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	-	15/22/109/110	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	4.20	1.51	1.45
3	G	8	TTD	C1'-N1	3.51	1.50	1.45
3	G	8	TTD	PB-O5P	3.50	1.63	1.50
3	G	8	TTD	C2-N1	3.32	1.43	1.36
3	G	8	TTD	C6-N1	3.00	1.51	1.46
3	G	8	TTD	C2T-N1T	2.43	1.41	1.36
3	G	8	TTD	C6T-N1T	2.22	1.50	1.46
3	G	8	TTD	O4'-C1'	2.07	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	6.71	121.91	116.06
3	G	8	TTD	C5T-C4T-N3T	6.71	121.90	116.06
3	G	8	TTD	N3-C2-N1	5.72	122.62	116.69
3	G	8	TTD	N3T-C2T-N1T	5.09	121.97	116.69
3	G	8	TTD	O4-C4-C5	-4.50	119.28	122.88
3	G	8	TTD	C4-N3-C2	-3.55	121.21	126.67
3	G	8	TTD	C4'-O4R-C1R	-3.51	100.96	109.45
3	G	8	TTD	O4T-C4T-C5T	-3.44	120.13	122.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	8	TTD	C4T-N3T-C2T	-3.35	121.52	126.67
3	G	8	TTD	O2-C2-N3	-3.03	115.85	121.50
3	G	8	TTD	C2R-C1R-N1T	-2.91	111.66	115.59
3	G	8	TTD	C2'-C1'-N1	-2.63	112.03	115.59
3	G	8	TTD	C5-C5T-C6T	2.36	91.31	88.38
3	G	8	TTD	O4R-C1R-C2R	-2.34	101.82	106.25
3	G	8	TTD	O2T-C2T-N1T	-2.07	120.27	123.49
3	G	8	TTD	O2T-C2T-N3T	-2.04	117.71	121.50

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	8	TTD	C2'-C3R-O3R-PB
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'-C4R-C5'-O5'
3	G	8	TTD	O4'-C1'-N1-C6
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	C3R-O3R-PB-O5R
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	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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	1105/1159 (95%)	0.03	14 (1%)	77	59	39, 56, 80, 96	0
2	B	354/382 (92%)	-0.13	1 (0%)	94	88	33, 49, 66, 75	0
3	G	13/14 (92%)	0.51	0	100	100	56, 73, 100, 102	0
4	H	15/16 (93%)	0.48	1 (6%)	17	7	47, 74, 107, 108	0
All	All	1487/1571 (94%)	0.00	16 (1%)	80	64	33, 54, 79, 108	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	547	GLY	3.5
1	A	446	THR	3.3
1	A	418	ASN	3.2
1	A	746	SER	3.2
1	A	439	ASN	2.9
1	A	548	ASP	2.7
1	A	435	VAL	2.7
1	A	745	THR	2.6
1	A	549	SER	2.5
1	A	403	ASP	2.4
1	A	684	SER	2.3
1	A	550	ASN	2.3
4	H	15	DC	2.2
1	A	443	VAL	2.2
2	B	236	TRP	2.2
1	A	1015	GLN	2.0

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

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	0.91	0.24	63,66,66,66	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	0.96	0.31	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.