Full wwPDB X-ray Structure Validation Report (i)

Dec 13, 2023 – 10:41 am GMT

PDB ID	:	4A0A
Title	:	Structure of hsDDB1-drDDB2 bound to a 16 bp CPD-duplex (pyrimidine at D-1 position) at 3.6 A resolution (CPD 3)
Authors	:	Scrima, A.; Fischer, E.S.; Iwai, S.; Gut, H.; Thoma, N.H.
Deposited on	:	2011-09-08
Resolution	:	3.60 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 (i) 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 (i)) were used in the production of this report:

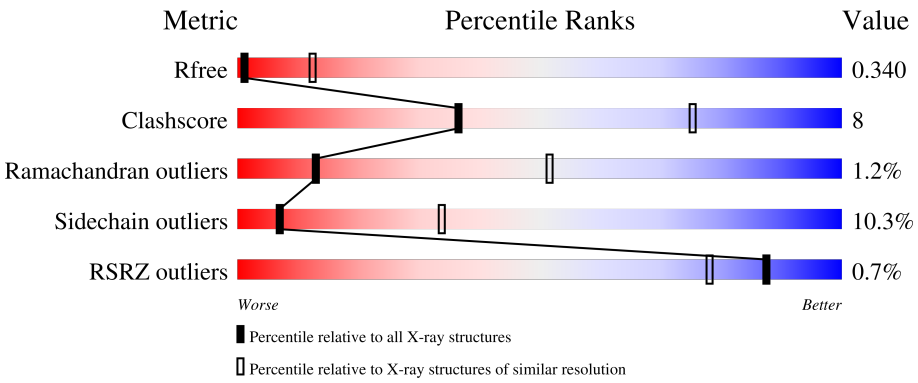
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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	52% 13% • 33%
2	B	382	2% 65% 25% • 7%
3	C	15	33% 47% 20%
4	D	16	56% 38% 6%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 9619 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	780	6129	3901	1025	1169	34	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	224	LYS	GLU	engineered mutation	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	2843	1806	499	527	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*CP*AP*GP*DGP)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
3	C	15	334	159	66	94	15	0	0	0

- 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
			Total	C	N	O	P			
4	D	16	312	151	50	96	15	0	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

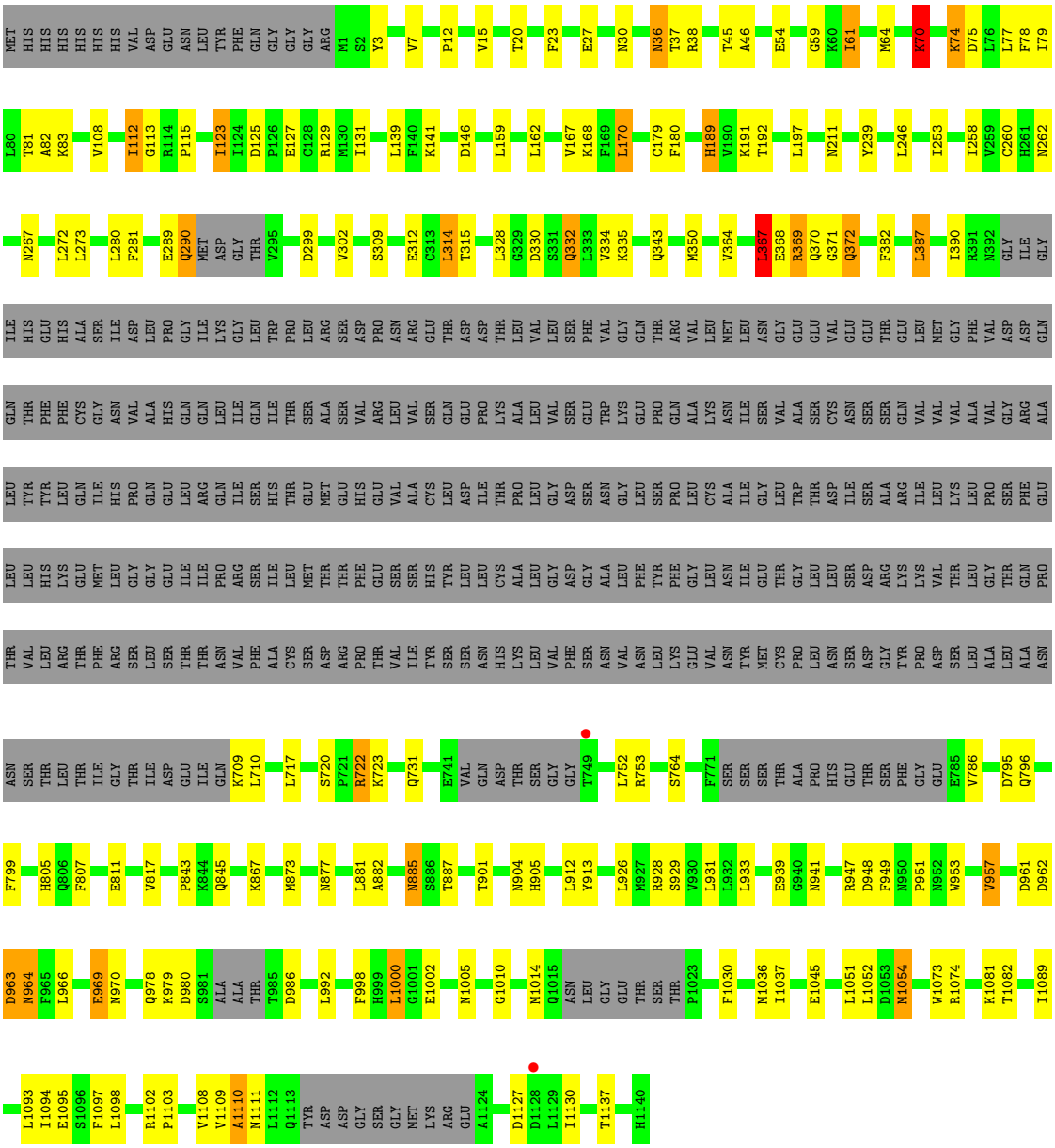
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
5	C	1	1	1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

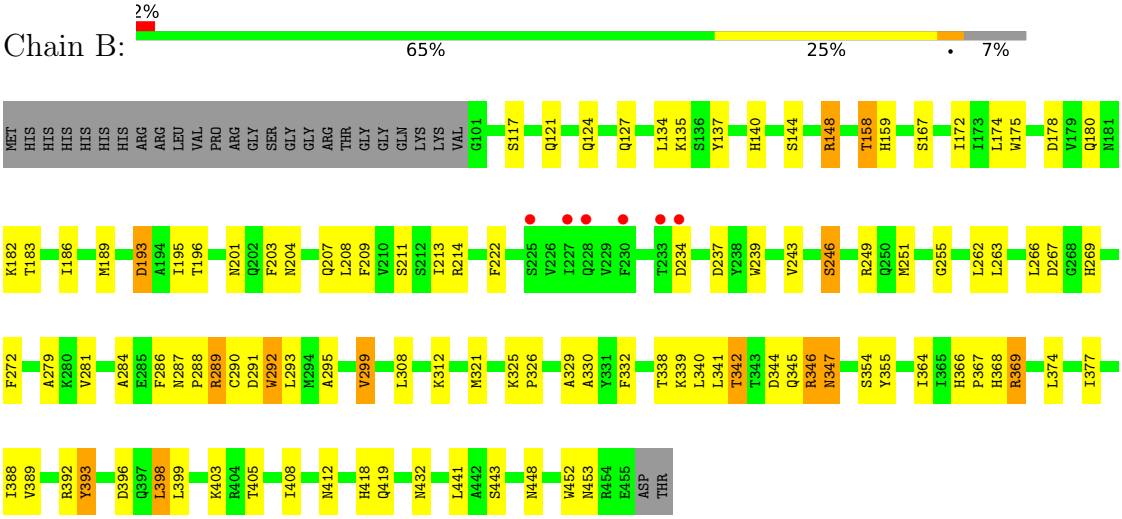
- Molecule 1: DNA DAMAGE-BINDING PROTEIN 1

Chain A: 52% 13% • 33%



• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

Chain B:



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

Chain C:

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

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	155.64Å 227.14Å 114.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.25 – 3.60 46.25 – 3.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (46.25-3.60) 99.5 (46.25-3.60)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.23 (at 3.57Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.263 , 0.347 0.259 , 0.340	Depositor DCC
R_{free} test set	1188 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	71.3	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.24 , 2.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.85	EDS
Total number of atoms	9619	wwPDB-VP
Average B, all atoms (Å^2)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% of the height of the origin peak. No significant pseudotranslation is detected.*

[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 (i)

5.1 Standard geometry (i)

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	0.36	0/6236	0.55	1/8429 (0.0%)
2	B	0.36	0/2917	0.55	0/3962
3	C	0.61	0/331	1.00	2/509 (0.4%)
4	D	0.66	0/346	1.14	1/529 (0.2%)
All	All	0.39	0/9830	0.60	4/13429 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	9	DA	P-O3'-C3'	5.89	126.77	119.70
1	A	367	LEU	CA-CB-CG	5.49	127.93	115.30
3	C	15	DG	P-O3'-C3'	5.29	126.04	119.70
3	C	12	DG	P-O3'-C3'	5.14	125.87	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	6129	0	6105	90	0
2	B	2843	0	2788	55	0
3	C	334	0	182	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	312	0	182	4	0
5	C	1	0	0	0	0
All	All	9619	0	9257	149	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 8.

All (149) 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:928:ARG:HG2	1:A:928:ARG:HH11	1.40	0.84
1:A:969:GLU:HG2	1:A:970:ASN:N	1.99	0.78
1:A:369:ARG:HG2	1:A:370:GLN:N	1.98	0.78
1:A:38:ARG:HH12	1:A:54:GLU:HB3	1.48	0.77
1:A:127:GLU:HB2	1:A:129:ARG:HD2	1.66	0.77
2:B:325:LYS:HB3	2:B:326:PRO:HD2	1.67	0.76
1:A:112:ILE:HG23	2:B:354:SER:HB2	1.70	0.71
2:B:292:TRP:H	2:B:292:TRP:HD1	1.39	0.71
1:A:369:ARG:HG2	1:A:370:GLN:H	1.55	0.70
1:A:390:ILE:HD13	1:A:1037:ILE:HD11	1.75	0.68
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.58	0.68
4:D:5:DC:H1'	4:D:6:DT:H5'	1.74	0.68
1:A:253:ILE:HD11	1:A:302:VAL:HG11	1.76	0.67
1:A:969:GLU:HG2	1:A:970:ASN:H	1.58	0.67
2:B:211:SER:HB3	2:B:243:VAL:HG23	1.78	0.66
1:A:1051:LEU:HD22	1:A:1094:ILE:HD13	1.79	0.64
1:A:948:ASP:O	1:A:949:PHE:HB2	1.97	0.64
1:A:112:ILE:HG23	2:B:354:SER:CB	2.27	0.64
1:A:998:PHE:CZ	1:A:1074:ARG:HD2	2.33	0.64
1:A:36:ASN:O	1:A:61:ILE:HD12	1.98	0.64
1:A:112:ILE:CG2	2:B:354:SER:HB2	2.28	0.63
2:B:330:ALA:HA	2:B:341:LEU:O	1.99	0.62
1:A:258:ILE:HD12	1:A:258:ILE:H	1.65	0.61
1:A:81:THR:HG22	1:A:83:LYS:H	1.66	0.61
1:A:926:LEU:O	1:A:953:TRP:HA	2.00	0.60
1:A:108:VAL:HB	1:A:141:LYS:HD3	1.85	0.59
1:A:1051:LEU:HA	1:A:1054:MET:HB2	1.86	0.57
1:A:369:ARG:CG	1:A:370:GLN:H	2.18	0.56
1:A:1095:GLU:HG2	1:A:1137:THR:HG22	1.85	0.56
1:A:964:ASN:HB3	1:A:978:GLN:HE21	1.69	0.56
2:B:201:ASN:HB3	2:B:204:ASN:O	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:441:LEU:HB3	2:B:452:TRP:HB2	1.88	0.55
1:A:887:THR:CG2	1:A:904:ASN:HD22	2.20	0.55
4:D:9:DA:H1'	4:D:10:DT:H5'	1.87	0.55
3:C:12:DG:H1'	3:C:13:DC:H5'	1.88	0.55
3:C:15:DG:H1'	3:C:16:DG:H5'	1.90	0.54
1:A:70:LYS:H	1:A:70:LYS:HD2	1.72	0.54
2:B:263:LEU:HB3	2:B:272:PHE:HB3	1.90	0.54
2:B:158:THR:OG1	2:B:159:HIS:N	2.41	0.53
3:C:4:DT:H2"	3:C:5:DG:C8	2.43	0.53
1:A:887:THR:HG21	1:A:904:ASN:ND2	2.24	0.53
1:A:709:LYS:HD3	1:A:710:LEU:HG	1.91	0.53
1:A:928:ARG:HG2	1:A:928:ARG:NH1	2.16	0.53
1:A:961:ASP:O	1:A:963:ASP:N	2.42	0.52
1:A:887:THR:HG21	1:A:904:ASN:HD22	1.74	0.52
3:C:15:DG:H2"	3:C:16:DG:OP2	2.09	0.52
1:A:197:LEU:H	1:A:197:LEU:HD23	1.75	0.52
1:A:371:GLY:HA3	1:A:1014:MET:HG3	1.91	0.52
2:B:332:PHE:HA	2:B:339:LYS:O	2.11	0.51
2:B:341:LEU:HD21	2:B:388:ILE:HG23	1.92	0.51
1:A:189:HIS:HB3	1:A:211:ASN:HA	1.93	0.51
2:B:193:ASP:HB2	2:B:214:ARG:H	1.77	0.50
2:B:389:VAL:HG12	2:B:408:ILE:HG12	1.91	0.50
1:A:23:PHE:H	1:A:30:ASN:HD22	1.60	0.50
1:A:167:VAL:HG13	1:A:180:PHE:HB3	1.93	0.50
2:B:405:THR:HG21	2:B:419:GLN:HE21	1.76	0.50
3:C:9:TTD:O4'	3:C:9:TTD:O2	2.29	0.50
1:A:260:CYS:SG	1:A:314:LEU:HD22	2.51	0.49
1:A:764:SER:O	1:A:805:HIS:HA	2.12	0.49
2:B:279:ALA:HB1	2:B:299:VAL:HG13	1.93	0.49
2:B:172:ILE:HB	2:B:186:ILE:HB	1.93	0.49
1:A:364:VAL:HG11	1:A:1010:GLY:HA3	1.95	0.49
2:B:267:ASP:OD1	2:B:269:HIS:HD2	1.95	0.49
1:A:262:ASN:HB2	1:A:314:LEU:O	2.13	0.48
2:B:148:ARG:HH11	2:B:148:ARG:HB3	1.78	0.48
1:A:64:MET:HA	1:A:78:PHE:O	2.14	0.48
1:A:123:ILE:HG21	1:A:168:LYS:HA	1.96	0.48
2:B:249:ARG:HB2	2:B:291:ASP:HB2	1.96	0.48
2:B:284:ALA:HA	2:B:295:ALA:O	2.14	0.48
1:A:64:MET:HG2	1:A:77:LEU:HD11	1.95	0.47
1:A:61:ILE:HG23	1:A:79:ILE:HG23	1.97	0.47
2:B:211:SER:HB3	2:B:243:VAL:CG2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:MET:HB3	1:A:882:ALA:HA	1.96	0.47
2:B:140:HIS:HB2	2:B:453:ASN:HB3	1.96	0.47
2:B:209:PHE:HB3	2:B:243:VAL:HG11	1.96	0.47
1:A:112:ILE:HD13	2:B:290:CYS:HB2	1.96	0.47
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.30	0.47
4:D:6:DT:H2"	4:D:7:DC:OP2	2.15	0.46
1:A:722:ARG:O	1:A:723:LYS:HG3	2.16	0.46
2:B:174:LEU:HB2	2:B:222:PHE:CE1	2.50	0.46
1:A:1000:LEU:HD13	1:A:1002:GLU:HB2	1.97	0.46
1:A:964:ASN:ND2	1:A:964:ASN:H	2.14	0.46
2:B:135:LYS:HA	2:B:418:HIS:CE1	2.51	0.46
1:A:387:LEU:HD12	1:A:717:LEU:HD21	1.99	0.46
1:A:807:PHE:HB3	1:A:811:GLU:OE1	2.15	0.46
2:B:366:HIS:O	2:B:368:HIS:ND1	2.48	0.46
1:A:843:PRO:HG2	1:A:885:ASN:HD21	1.81	0.45
1:A:272:LEU:HD22	1:A:280:LEU:HD11	1.98	0.45
1:A:139:LEU:HG	2:B:355:TYR:HB2	1.98	0.45
1:A:913:TYR:HB2	1:A:957:VAL:HG23	1.97	0.45
2:B:392:ARG:HD2	2:B:405:THR:OG1	2.17	0.45
1:A:170:LEU:HD12	1:A:179:CYS:HB2	1.97	0.45
1:A:947:ARG:HA	1:A:992:LEU:HD12	1.96	0.45
2:B:368:HIS:HB2	2:B:377:ILE:HD12	1.99	0.45
2:B:167:SER:H	2:B:195:ILE:HD12	1.82	0.45
1:A:1097:PHE:HE1	1:A:1108:VAL:HG11	1.82	0.45
1:A:939:GLU:HB3	1:A:941:ASN:HD22	1.82	0.45
2:B:292:TRP:CD1	2:B:292:TRP:N	2.77	0.45
1:A:309:SER:N	1:A:332:GLN:OE1	2.47	0.44
2:B:134:LEU:HA	2:B:137:TYR:CD1	2.52	0.44
2:B:144:SER:HB3	2:B:448:ASN:HA	1.98	0.44
1:A:38:ARG:NH1	1:A:54:GLU:HB3	2.24	0.44
1:A:162:LEU:HD21	2:B:355:TYR:CZ	2.52	0.44
1:A:1000:LEU:HD11	1:A:1030:PHE:CZ	2.53	0.44
2:B:246:SER:HB2	2:B:286:PHE:CG	2.53	0.44
2:B:325:LYS:HE2	2:B:346:ARG:HG3	1.99	0.44
1:A:45:THR:O	1:A:46:ALA:C	2.55	0.44
1:A:731:GLN:HA	1:A:796:GLN:NE2	2.28	0.44
2:B:326:PRO:HG2	2:B:345:GLN:HB2	2.00	0.44
3:C:8:DT:H3'	3:C:9:TTD:H5"	1.99	0.44
2:B:332:PHE:CE1	2:B:340:LEU:HD13	2.53	0.44
1:A:335:LYS:HB2	1:A:350:MET:HG3	1.99	0.43
2:B:213:ILE:HG12	2:B:239:TRP:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:TRP:HA	2:B:183:THR:HG22	2.01	0.43
1:A:81:THR:HG22	1:A:82:ALA:N	2.33	0.43
1:A:1110:ALA:HB1	1:A:1111:ASN:HD22	1.84	0.43
2:B:127:GLN:HE21	2:B:127:GLN:HB3	1.71	0.43
2:B:325:LYS:HB3	2:B:326:PRO:CD	2.44	0.43
3:C:1:DG:H2"	3:C:2:DG:C8	2.54	0.43
2:B:369:ARG:HE	2:B:369:ARG:HB3	1.73	0.43
1:A:239:TYR:HB3	1:A:246:LEU:HB3	2.01	0.43
1:A:372:GLN:HB2	1:A:1014:MET:HA	2.01	0.43
1:A:953:TRP:HB2	1:A:970:ASN:HB2	2.00	0.43
2:B:388:ILE:O	2:B:408:ILE:HA	2.19	0.42
2:B:366:HIS:CE1	2:B:368:HIS:HB3	2.54	0.42
1:A:113:GLY:H	2:B:338:THR:HG22	1.84	0.42
1:A:928:ARG:NH1	1:A:928:ARG:CG	2.79	0.42
1:A:290:GLN:HE21	1:A:290:GLN:HA	1.84	0.42
1:A:905:HIS:CE1	1:A:933:LEU:HD21	2.54	0.42
1:A:1098:LEU:HD22	1:A:1130:ILE:HG13	2.00	0.42
2:B:255:GLY:HA3	2:B:281:VAL:HB	2.02	0.42
2:B:347:ASN:HB3	2:B:367:PRO:HA	2.00	0.42
1:A:246:LEU:HD11	1:A:299:ASP:HA	2.00	0.42
2:B:289:ARG:HH11	2:B:289:ARG:HB2	1.85	0.42
1:A:113:GLY:O	1:A:115:PRO:HD3	2.20	0.42
1:A:382:PHE:H	1:A:720:SER:HB3	1.85	0.41
1:A:74:LYS:HE2	1:A:74:LYS:HB3	1.95	0.41
4:D:12:DC:H1'	4:D:13:DA:C8	2.55	0.41
1:A:332:GLN:HG3	1:A:334:VAL:HG23	2.02	0.41
1:A:969:GLU:CG	1:A:970:ASN:N	2.74	0.41
2:B:367:PRO:HB2	2:B:393:TYR:O	2.21	0.41
1:A:273:LEU:HB2	1:A:281:PHE:HB2	2.01	0.41
1:A:368:GLU:O	1:A:370:GLN:HG2	2.20	0.41
2:B:287:ASN:HA	2:B:288:PRO:HD3	1.90	0.41
1:A:795:ASP:O	1:A:799:PHE:HA	2.20	0.41
1:A:3:TYR:CE1	1:A:1045:GLU:HG3	2.56	0.40
2:B:329:ALA:O	2:B:342:THR:HA	2.22	0.40
1:A:59:GLY:HA2	1:A:1073:TRP:CZ3	2.57	0.40
1:A:78:PHE:CE1	1:A:131:ILE:HD13	2.56	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	764/1159 (66%)	681 (89%)	73 (10%)	10 (1%)	12	50
2	B	353/382 (92%)	314 (89%)	36 (10%)	3 (1%)	19	59
All	All	1117/1541 (72%)	995 (89%)	109 (10%)	13 (1%)	13	51

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	962	ASP
1	A	112	ILE
1	A	1110	ALA
2	B	189	MET
1	A	70	LYS
1	A	330	ASP
1	A	885	ASN
2	B	117	SER
1	A	929	SER
2	B	398	LEU
1	A	36	ASN
1	A	367	LEU
1	A	951	PRO

5.3.2 Protein sidechains (i)

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	679/1015 (67%)	617 (91%)	62 (9%)	9	39

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	313/335 (93%)	273 (87%)	40 (13%)	4 24
All	All	992/1350 (74%)	890 (90%)	102 (10%)	7 34

All (102) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	VAL
1	A	12	PRO
1	A	15	VAL
1	A	20	THR
1	A	27	GLU
1	A	37	THR
1	A	61	ILE
1	A	70	LYS
1	A	74	LYS
1	A	75	ASP
1	A	123	ILE
1	A	125	ASP
1	A	146	ASP
1	A	159	LEU
1	A	170	LEU
1	A	189	HIS
1	A	191	LYS
1	A	192	THR
1	A	267	ASN
1	A	289	GLU
1	A	290	GLN
1	A	312	GLU
1	A	314	LEU
1	A	315	THR
1	A	328	LEU
1	A	332	GLN
1	A	343	GLN
1	A	367	LEU
1	A	369	ARG
1	A	372	GLN
1	A	387	LEU
1	A	722	ARG
1	A	752	LEU
1	A	753	ARG
1	A	786	VAL
1	A	817	VAL

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Mol	Chain	Res	Type
1	A	845	GLN
1	A	867	LYS
1	A	877	ASN
1	A	881	LEU
1	A	901	THR
1	A	912	LEU
1	A	931	LEU
1	A	957	VAL
1	A	963	ASP
1	A	964	ASN
1	A	966	LEU
1	A	969	GLU
1	A	979	LYS
1	A	980	ASP
1	A	986	ASP
1	A	1000	LEU
1	A	1005	ASN
1	A	1036	MET
1	A	1052	LEU
1	A	1054	MET
1	A	1081	LYS
1	A	1082	THR
1	A	1089	ILE
1	A	1093	LEU
1	A	1109	VAL
1	A	1127	ASP
2	B	121	GLN
2	B	124	GLN
2	B	148	ARG
2	B	158	THR
2	B	178	ASP
2	B	180	GLN
2	B	182	LYS
2	B	193	ASP
2	B	196	THR
2	B	203	PHE
2	B	207	GLN
2	B	208	LEU
2	B	234	ASP
2	B	237	ASP
2	B	246	SER
2	B	251	MET

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Mol	Chain	Res	Type
2	B	262	LEU
2	B	266	LEU
2	B	289	ARG
2	B	292	TRP
2	B	293	LEU
2	B	299	VAL
2	B	308	LEU
2	B	312	LYS
2	B	321	MET
2	B	342	THR
2	B	344	ASP
2	B	346	ARG
2	B	347	ASN
2	B	364	ILE
2	B	369	ARG
2	B	374	LEU
2	B	393	TYR
2	B	396	ASP
2	B	398	LEU
2	B	399	LEU
2	B	403	LYS
2	B	412	ASN
2	B	432	ASN
2	B	443	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	30	ASN
1	A	109	GLN
1	A	156	ASN
1	A	189	HIS
1	A	290	GLN
1	A	370	GLN
1	A	392	ASN
1	A	727	GLN
1	A	790	ASN
1	A	796	GLN
1	A	806	GLN
1	A	885	ASN
1	A	904	ASN

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Mol	Chain	Res	Type
1	A	941	ASN
1	A	964	ASN
1	A	978	GLN
1	A	990	GLN
1	A	1015	GLN
1	A	1055	GLN
1	A	1111	ASN
2	B	121	GLN
2	B	124	GLN
2	B	127	GLN
2	B	269	HIS
2	B	347	ASN
2	B	370	GLN
2	B	373	HIS
2	B	418	HIS
2	B	432	ASN
2	B	453	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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	C	9	3	42,45,46	1.82	10 (23%)	62,74,77	2.39	16 (25%)

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	C	9	3	-	12/22/109/110	0/5/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	9	TTD	C1R-N1T	4.74	1.51	1.45
3	C	9	TTD	C1'-N1	4.59	1.51	1.45
3	C	9	TTD	C5'-C4R	3.64	1.62	1.51
3	C	9	TTD	C2-N1	3.49	1.43	1.36
3	C	9	TTD	C6-N1	3.48	1.52	1.46
3	C	9	TTD	PB-O5P	3.10	1.61	1.50
3	C	9	TTD	C2T-N1T	2.71	1.41	1.36
3	C	9	TTD	O4'-C1'	2.46	1.47	1.42
3	C	9	TTD	C5T-C4T	2.18	1.55	1.51
3	C	9	TTD	C6T-N1T	2.10	1.49	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	9	TTD	O4R-C1R-N1T	8.41	118.62	108.65
3	C	9	TTD	C5T-C4T-N3T	6.58	121.79	116.06
3	C	9	TTD	N3-C2-N1	6.07	122.99	116.69
3	C	9	TTD	C5-C4-N3	6.07	121.35	116.06
3	C	9	TTD	N3T-C2T-N1T	4.41	121.27	116.69
3	C	9	TTD	O4-C4-C5	-3.85	119.80	122.88
3	C	9	TTD	C4-N3-C2	-3.50	121.28	126.67
3	C	9	TTD	O4T-C4T-C5T	-3.45	120.12	122.88
3	C	9	TTD	O4'-C4R-C5'	3.32	120.31	109.37
3	C	9	TTD	O2-C2-N3	-3.26	115.42	121.50
3	C	9	TTD	C4T-N3T-C2T	-3.11	121.88	126.67
3	C	9	TTD	C4'-O4R-C1R	-2.88	102.49	109.45
3	C	9	TTD	O4R-C1R-C2R	-2.29	101.92	106.25
3	C	9	TTD	O4'-C1'-N1	2.06	111.09	108.65
3	C	9	TTD	O2T-C2T-N1T	-2.04	120.32	123.49
3	C	9	TTD	C3R-C2'-C1'	2.03	106.80	102.91

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	9	TTD	C2'-C3R-O3R-PB
3	C	9	TTD	O4'-C1'-N1-C2

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Mol	Chain	Res	Type	Atoms
3	C	9	TTD	O4R-C4'-C5R-O5R
3	C	9	TTD	O4'-C1'-N1-C6
3	C	9	TTD	O4'-C4R-C5'-O5'
3	C	9	TTD	C3'-C4'-C5R-O5R
3	C	9	TTD	C3R-C4R-C5'-O5'
3	C	9	TTD	C2R-C1R-N1T-C6T
3	C	9	TTD	C2R-C1R-N1T-C2T
3	C	9	TTD	O4R-C1R-N1T-C6T
3	C	9	TTD	O4R-C1R-N1T-C2T
3	C	9	TTD	C5R-O5R-PB-O3R

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	9	TTD	2	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	780/1159 (67%)	-0.31	2 (0%)	94	88	54, 68, 96, 117	0
2	B	355/382 (92%)	-0.25	6 (1%)	70	55	54, 73, 97, 102	0
3	C	14/15 (93%)	-0.68	0	100	100	82, 105, 114, 119	0
4	D	16/16 (100%)	-0.46	0	100	100	67, 91, 124, 127	0
All	All	1165/1572 (74%)	-0.29	8 (0%)	87	78	54, 69, 100, 127	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1128	ASP	2.5
2	B	225	SER	2.4
2	B	227	ILE	2.2
2	B	233	THR	2.2
2	B	234	ASP	2.1
2	B	228	GLN	2.1
1	A	749	THR	2.0
2	B	230	PHE	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	C	9	40/41	0.92	0.16	85,92,96,96	0

6.3 Carbohydrates (i)

There are no monosaccharides 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	C	1017	1/1	0.85	0.16	77,77,77,77	0

6.5 Other polymers (i)

There are no such residues in this entry.