



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:38 PM GMT

PDB ID : 4A08  
Title : STRUCTURE OF HSDDDB1-DRDDB2 BOUND TO A 13 BP CPD-DUPLEX  
(PURINE AT D-1 POSITION) AT 3.0 Å RESOLUTION (CPD 1)  
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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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

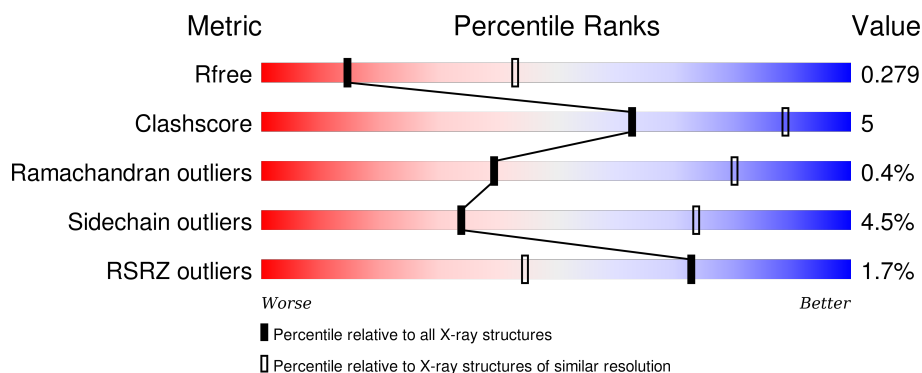
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1159	<div> <div>2%</div> <div>80%</div> <div>13%</div> <div>6%</div> </div>
2	B	382	<div> <div>%</div> <div>73%</div> <div>20%</div> <div>8%</div> </div>
3	G	13	<div> <div>8%</div> <div>54%</div> <div>15%</div> <div>8%</div> <div>23%</div> </div>
4	H	14	<div> <div>50%</div> <div>43%</div> <div>7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	MES	A	2141	-	-	-	X
5	MES	A	2142	-	-	-	X

## 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\*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 (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



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 (three-letter code: CA) (formula: Ca).

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

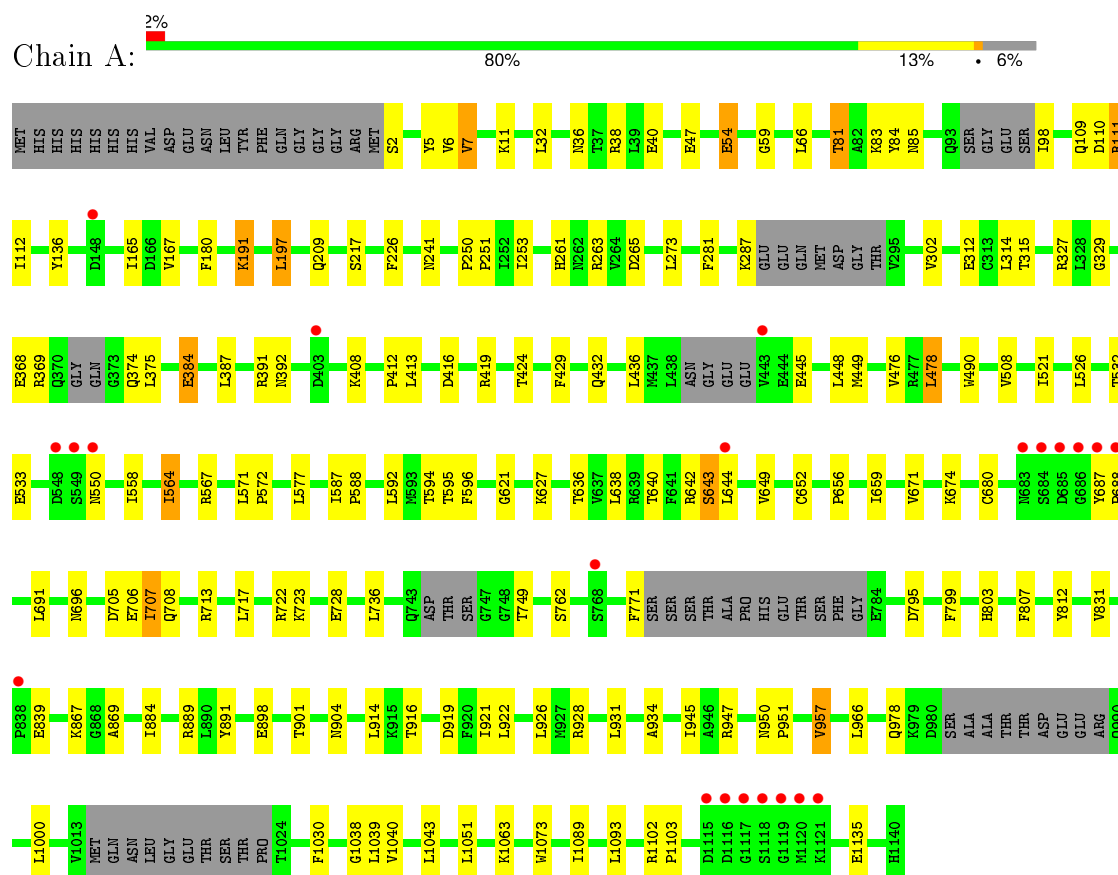
- Molecule 7 is water.

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

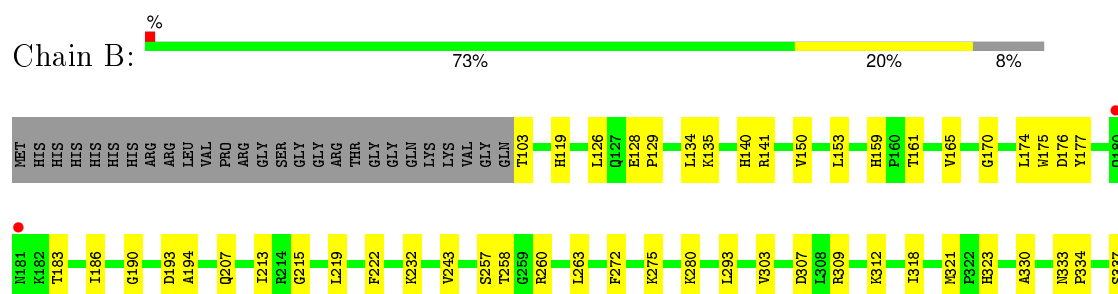
### 3 Residue-property plots

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

#### • Molecule 1: DNA DAMAGE-BINDING PROTEIN 1



#### • Molecule 2: DNA DAMAGE-BINDING PROTEIN 2





- Molecule 3: 5'-D(\*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\*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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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 (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.5	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 40.3	EDS
Estimated twinning fraction	0.021 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 37310 reflections	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	11866	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.32	0/8662	0.50	0/11729
2	B	0.31	0/2898	0.49	0/3938
3	G	0.61	0/206	1.01	1/313 (0.3%)
4	H	0.69	0/297	1.05	0/456
All	All	0.34	0/12063	0.54	1/16436 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	2	DC	P-O3'-C3'	5.67	126.50	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	8509	0	8508	85	0
2	B	2824	0	2766	34	0
3	G	225	0	124	2	0
4	H	266	0	145	6	0
5	A	24	0	24	2	0
6	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	124	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 (124) 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: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:HH11	1:A:263:ARG:HG2	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:HD3	1:A:111:ARG:H	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:B:330:ALA:HA	2:B:341:LEU:O	2.11	0.51
1:A:7:VAL:HG23	1:A:1039:LEU:HB3	1.93	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:931:LEU:HG	1:A:947:ARG:HB3	1.96	0.47
1:A:926:LEU:HD21	2:B:126:LEU:HD11	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
3:G:7:TTD:H2''	3:G:7:TTD:H6	1.64	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
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
2:B:141:ARG:NE	2:B:177:TYR:O	2.47	0.46
1:A:197:LEU:H	1:A:197:LEU:HD23	1.78	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:170:GLY:HA2	2:B:193:ASP:O	2.17	0.45
1:A:594:THR:HG22	1:A:595:THR:H	1.82	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:1051:LEU:HB2	1:A:1089:ILE:HD13	2.00	0.44
1:A:577:LEU:HD23	1:A:621:GLY:HA3	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:762:SER:O	1:A:803:HIS:HA	2.18	0.43
1:A:191:LYS:HG2	1:A:209:GLN:HG3	2.01	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:CD	1:A:111:ARG:N	2.81	0.43
1:A:263:ARG:HH11	1:A:263:ARG:CG	2.30	0.42
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.53	0.42
1:A:508:VAL:HG23	1:A:521:ILE:HD11	2.00	0.42
1:A:795:ASP:O	1:A:799:PHE:HA	2.19	0.42
1:A:368:GLU:O	1:A:369:ARG:HB2	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: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
1:A:596:PHE:HZ	1:A:649:VAL:HG12	1.85	0.41
2:B:159:HIS:CD2	2:B:161:THR:H	2.37	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:346:ARG:HA	2:B:369:ARG:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:LEU:HD13	1:A:66:LEU:HD11	2.03	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
1:A:571:LEU:N	1:A:572:PRO:HD2	2.35	0.41
2:B:406:ILE:HB	2:B:420:LEU:HB2	2.02	0.41
2:B:367:PRO:HB2	2:B:393:TYR:O	2.20	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%)	46	84
2	B	351/382 (92%)	330 (94%)	19 (5%)	2 (1%)	30	72
All	All	1421/1541 (92%)	1323 (93%)	93 (6%)	5 (0%)	39	80

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	215	GLY
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%)	905 (96%)	43 (4%)	34	74
2	B	311/335 (93%)	297 (96%)	14 (4%)	34	74
All	All	1259/1349 (93%)	1202 (96%)	57 (4%)	34	74

All (57) 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	191	LYS
1	A	197	LEU
1	A	241	ASN
1	A	265	ASP
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
1	A	478	LEU
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

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Mol	Chain	Res	Type
1	A	705	ASP
1	A	707	ILE
1	A	728	GLU
1	A	749	THR
1	A	771	PHE
1	A	867	LYS
1	A	898	GLU
1	A	901	THR
1	A	914	LEU
1	A	919	ASP
1	A	957	VAL
1	A	966	LEU
1	A	1000	LEU
1	A	1063	LYS
1	A	1093	LEU
1	A	1135	GLU
2	B	119	HIS
2	B	134	LEU
2	B	150	VAL
2	B	174	LEU
2	B	232	LYS
2	B	243	VAL
2	B	293	LEU
2	B	309	ARG
2	B	312	LYS
2	B	359	LYS
2	B	374	LEU
2	B	384	MET
2	B	389	VAL
2	B	454	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	93	GLN
1	A	209	GLN
1	A	241	ASN
1	A	261	HIS
1	A	374	GLN
1	A	456	GLN
1	A	467	GLN

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Mol	Chain	Res	Type
1	A	528	GLN
1	A	648	ASN
1	A	677	ASN
1	A	696	ASN
1	A	796	GLN
1	A	797	HIS
1	A	859	GLN
1	A	877	ASN
1	A	907	ASN
1	A	950	ASN
1	A	990	GLN
2	B	159	HIS
2	B	269	HIS
2	B	401	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	7	3	40,45,46	1.68	9 (22%)	58,74,77	2.12	14 (24%)

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	-	0/22/109/110	0/3/6/6

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	7	TTD	O4'-C1'	2.06	1.47	1.42
3	G	7	TTD	C5T-C4T	2.09	1.55	1.51
3	G	7	TTD	C6T-N1T	2.61	1.50	1.46
3	G	7	TTD	C2T-N1T	2.70	1.42	1.36
3	G	7	TTD	C6-N1	3.00	1.51	1.46
3	G	7	TTD	C2-N1	3.24	1.43	1.36
3	G	7	TTD	PB-O5P	3.26	1.63	1.51
3	G	7	TTD	C1'-N1	3.58	1.50	1.45
3	G	7	TTD	C1R-N1T	4.97	1.52	1.45

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	7	TTD	O4-C4-C5	-3.77	119.85	122.92
3	G	7	TTD	C2'-C1'-N1	-3.32	111.10	115.64
3	G	7	TTD	O4T-C4T-C5T	-3.02	120.46	122.92
3	G	7	TTD	C4-N3-C2	-2.98	121.48	126.84
3	G	7	TTD	C4'-O4R-C1R	-2.90	102.12	109.46
3	G	7	TTD	O2-C2-N3	-2.74	116.12	121.48
3	G	7	TTD	C4T-N3T-C2T	-2.72	121.94	126.84
3	G	7	TTD	O4R-C1R-C2R	-2.26	101.78	106.28
3	G	7	TTD	O2T-C2T-N1T	-2.16	120.10	123.36
3	G	7	TTD	C5-C5T-C6T	2.67	91.75	88.37
3	G	7	TTD	N3T-C2T-N1T	5.14	121.96	116.82
3	G	7	TTD	N3-C2-N1	5.76	122.58	116.82
3	G	7	TTD	C5-C4-N3	6.20	121.39	116.01
3	G	7	TTD	C5T-C4T-N3T	6.22	121.41	116.01

There are no chirality outliers.

There are no torsion outliers.

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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

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	2141	-	11,12,12	0.71	0	14,16,16	8.97	8 (57%)
5	MES	A	2142	-	11,12,12	0.87	1 (9%)	14,16,16	8.98	8 (57%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2142	MES	O1S-S	2.14	1.52	1.45

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2142	MES	O1S-S-C8	-24.72	85.81	106.91
5	A	2141	MES	O2S-S-C8	-24.30	86.17	106.91
5	A	2141	MES	O1S-S-C8	-21.08	88.92	106.91
5	A	2142	MES	O2S-S-C8	-20.61	89.32	106.91
5	A	2142	MES	C6-C5-N4	-2.28	106.67	110.12
5	A	2141	MES	C6-C5-N4	-2.28	106.67	110.12
5	A	2142	MES	C7-N4-C5	2.52	117.73	111.27
5	A	2141	MES	C7-N4-C3	3.13	119.30	111.27
5	A	2141	MES	C7-N4-C5	3.14	119.32	111.27
5	A	2141	MES	O3S-S-O1S	3.28	119.23	111.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2141	MES	O3S-S-O2S	3.49	119.73	111.61
5	A	2142	MES	O3S-S-O2S	3.77	120.37	111.61
5	A	2142	MES	O3S-S-O1S	3.86	120.60	111.61
5	A	2142	MES	C7-N4-C3	4.25	122.17	111.27
5	A	2142	MES	C5-N4-C3	5.17	120.10	108.90
5	A	2141	MES	C5-N4-C3	5.76	121.38	108.90

There are no chirality outliers.

There are no torsion outliers.

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1088/1159 (93%)	-0.04	22 (2%) 68 39	30, 47, 68, 82	0
2	B	353/382 (92%)	-0.13	2 (0%) 90 73	32, 46, 60, 65	0
3	G	9/13 (69%)	0.72	1 (11%) 7 3	59, 69, 93, 98	0
4	H	13/14 (92%)	0.27	0 100 100	57, 72, 79, 79	0
All	All	1463/1568 (93%)	-0.06	25 (1%) 73 45	30, 47, 67, 98	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	181	ASN	4.6
1	A	1117	GLY	3.6
1	A	687	TYR	3.3
1	A	686	GLY	3.3
1	A	1116	ASP	3.3
1	A	683	ASN	3.2
1	A	685	ASP	3.2
1	A	1115	ASP	3.0
1	A	1120	MET	2.9
2	B	180	GLN	2.9
1	A	548	ASP	2.9
1	A	403	ASP	2.8
3	G	2	DC	2.8
1	A	1121	LYS	2.7
1	A	549	SER	2.5
1	A	443	VAL	2.4
1	A	838	PRO	2.4
1	A	550	ASN	2.3
1	A	684	SER	2.3
1	A	644	LEU	2.2
1	A	148	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1118	SER	2.2
1	A	1119	GLY	2.1
1	A	768	SER	2.0
1	A	688	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	TTD	G	7	40/41	0.90	0.20	-	64,66,67,67	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MES	A	2141	12/12	0.77	0.41	3.99	116,116,117,117	0
5	MES	A	2142	12/12	0.86	0.29	3.55	83,84,84,84	0
6	CA	B	1456	1/1	0.92	0.09	-2.25	56,56,56,56	0
6	CA	H	1015	1/1	0.79	0.31	-	78,78,78,78	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.