



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:41 PM GMT

PDB ID : 4A0B  
Title : STRUCTURE OF HSDDDB1-DRDDDB2 BOUND TO A 16 BP CPD-DUPLEX  
(PYRIMIDINE AT D-1 POSITION) AT 3.8 Å RESOLUTION (CPD 4)  
Authors : Scrima, A.; Fischer, E.S.; Iwai, S.; Gut, H.; Thoma, N.H.  
Deposited on : 2011-09-08  
Resolution : 3.80 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.

---

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

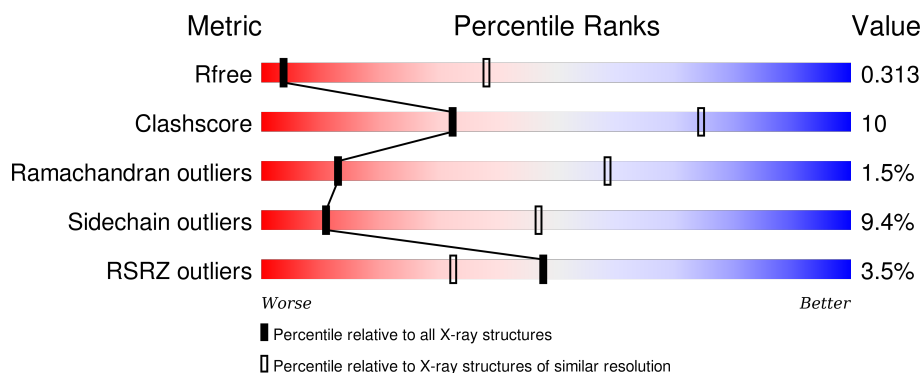
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 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>6%</div> <div> <div></div> <div>65%</div> <div>25%</div> <div>6%</div> </div> </div>
1	C	1159	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>27%</div> <div>6%</div> </div> </div>
2	B	382	<div> <div></div> <div> <div></div> <div>63%</div> <div>26%</div> <div>7%</div> </div> </div>
2	D	382	<div> <div></div> <div> <div></div> <div>65%</div> <div>24%</div> <div>7%</div> </div> </div>
3	G	15	<div> <div></div> <div> <div></div> <div>47%</div> <div>47%</div> <div>7%</div> </div> </div>

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
3	I	15	 60% 27% 13%
4	H	16	 44% 38% 6% 13%
4	J	16	 75% 6% 19%

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23938 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	1090	Total	C	N	O	S	0	0	0
			8543	5423	1443	1631	46			
1	C	1095	Total	C	N	O	S	0	0	0
			8582	5447	1449	1639	47			

There are 40 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	SER	GLU	ENGINEERED MUTATION	UNP Q16531
C	-18	MET	-	EXPRESSION TAG	UNP Q16531
C	-17	HIS	-	EXPRESSION TAG	UNP Q16531
C	-16	HIS	-	EXPRESSION TAG	UNP Q16531
C	-15	HIS	-	EXPRESSION TAG	UNP Q16531
C	-14	HIS	-	EXPRESSION TAG	UNP Q16531

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	HIS	-	EXPRESSION TAG	UNP Q16531
C	-12	HIS	-	EXPRESSION TAG	UNP Q16531
C	-11	VAL	-	EXPRESSION TAG	UNP Q16531
C	-10	ASP	-	EXPRESSION TAG	UNP Q16531
C	-9	GLU	-	EXPRESSION TAG	UNP Q16531
C	-8	ASN	-	EXPRESSION TAG	UNP Q16531
C	-7	LEU	-	EXPRESSION TAG	UNP Q16531
C	-6	TYR	-	EXPRESSION TAG	UNP Q16531
C	-5	PHE	-	EXPRESSION TAG	UNP Q16531
C	-4	GLN	-	EXPRESSION TAG	UNP Q16531
C	-3	GLY	-	EXPRESSION TAG	UNP Q16531
C	-2	GLY	-	EXPRESSION TAG	UNP Q16531
C	-1	GLY	-	EXPRESSION TAG	UNP Q16531
C	0	ARG	-	EXPRESSION TAG	UNP Q16531
C	224	SER	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			
2	D	355	Total	C	N	O	S	0	0	0
			2843	1806	499	527	11			

There are 40 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

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
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
D	76	MET	-	EXPRESSION TAG	UNP Q2YDS1
D	77	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	78	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	79	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	80	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	81	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	82	HIS	-	EXPRESSION TAG	UNP Q2YDS1
D	83	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	84	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	85	LEU	-	EXPRESSION TAG	UNP Q2YDS1
D	86	VAL	-	EXPRESSION TAG	UNP Q2YDS1
D	87	PRO	-	EXPRESSION TAG	UNP Q2YDS1
D	88	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	89	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	90	SER	-	EXPRESSION TAG	UNP Q2YDS1
D	91	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	92	GLY	-	EXPRESSION TAG	UNP Q2YDS1
D	93	ARG	-	EXPRESSION TAG	UNP Q2YDS1
D	180	GLN	LEU	VARIANT	UNP Q2YDS1
D	214	ARG	TRP	VARIANT	UNP Q2YDS1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	14	Total	C	N	O	P	0	0	0
			312	149	61	88	14			
3	I	13	Total	C	N	O	P	0	0	0
			290	139	56	82	13			

- 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	14	Total	C	N	O	P	0	0	0
			274	133	44	84	13			

*Continued on next page...*

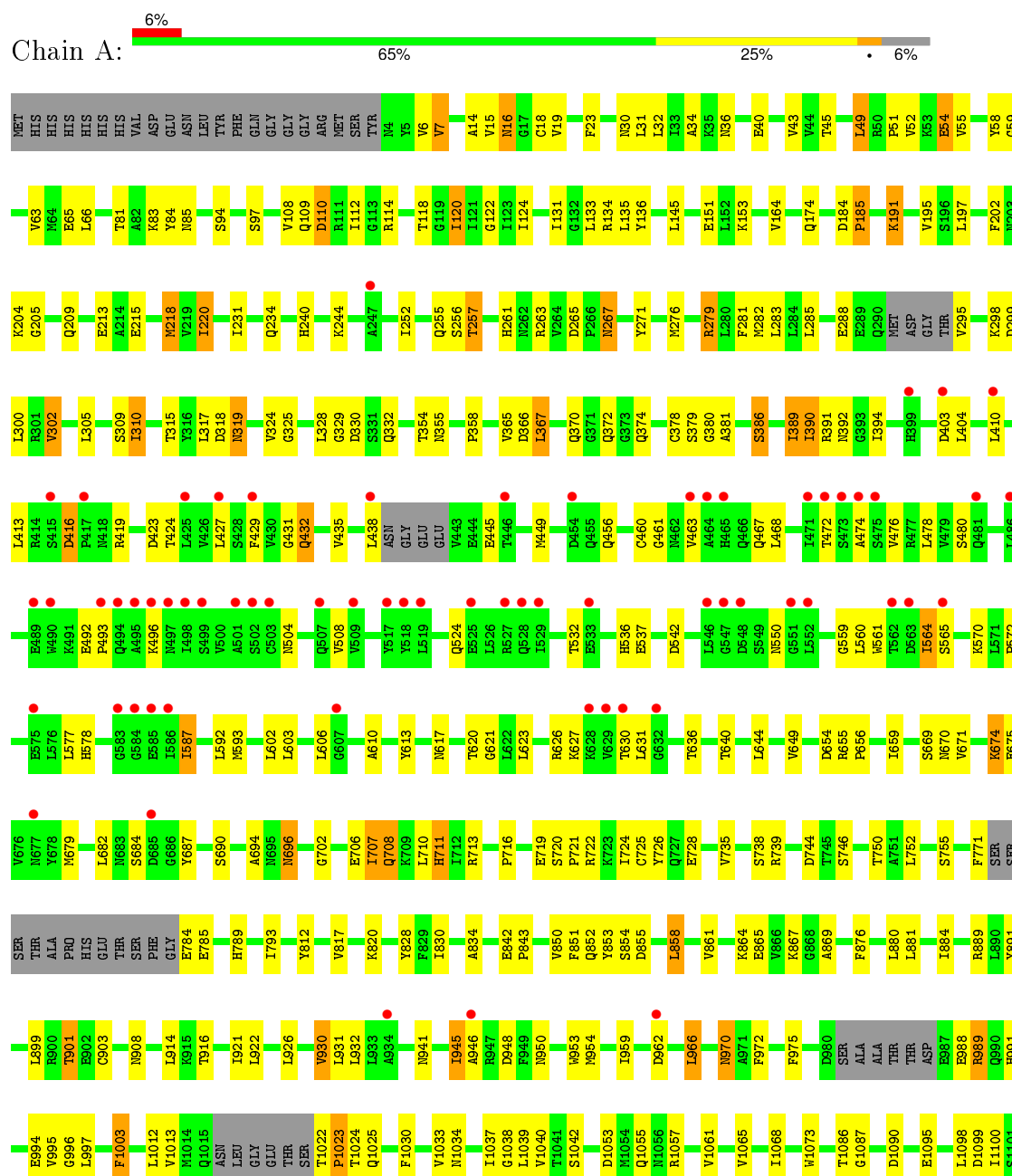
*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	13	Total	C	N	O	P	0	0	0
			255	124	41	78	12			

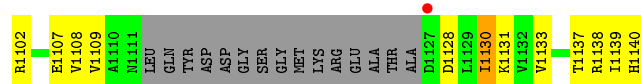
### 3 Residue-property plots

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.

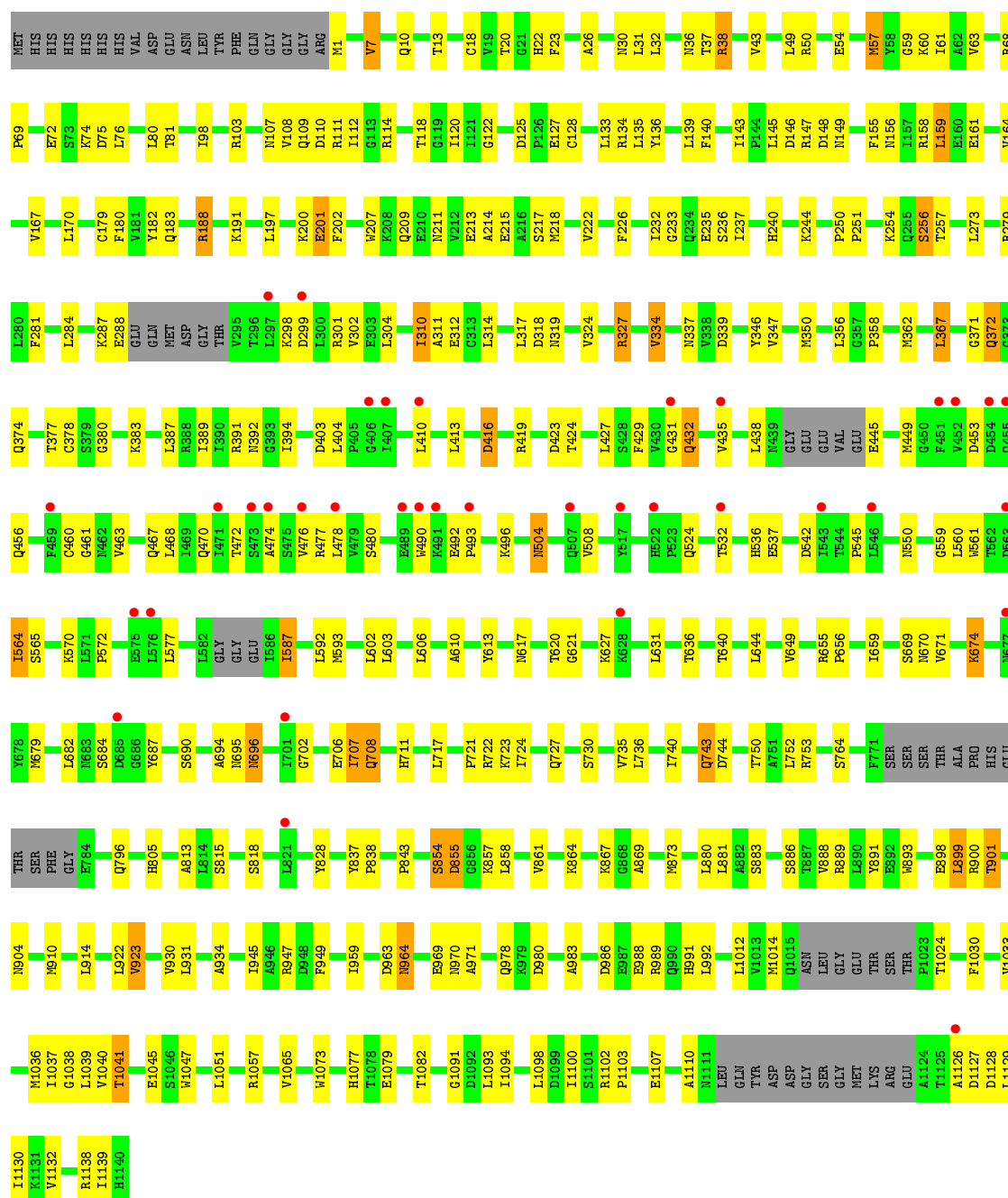
#### • Molecule 1: DNA DAMAGE-BINDING PROTEIN 1





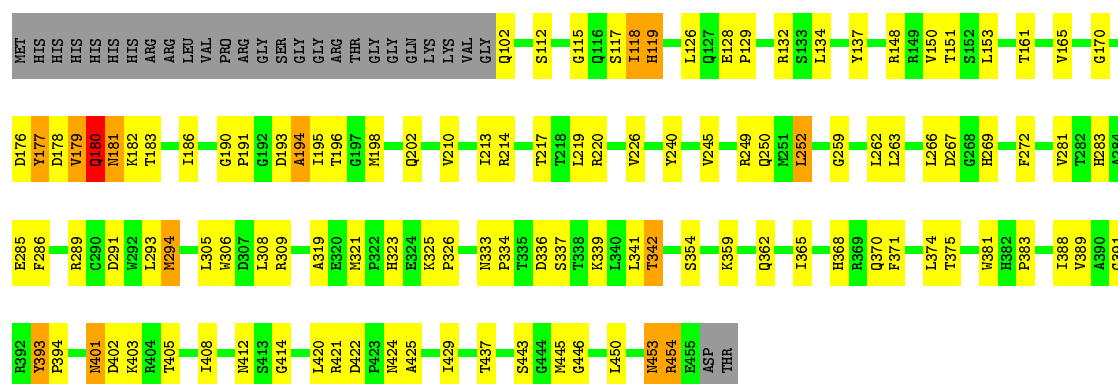


• Molecule 1: DNA DAMAGE-BINDING PROTEIN 1



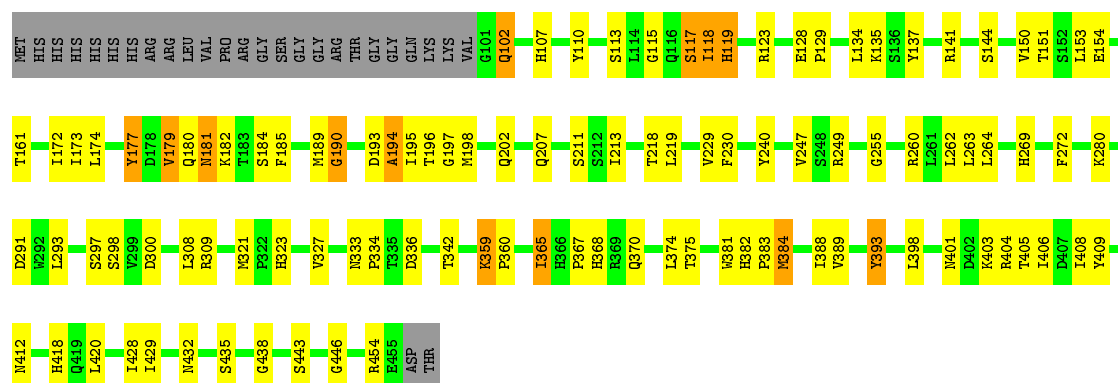
• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2





• Molecule 2: DNA DAMAGE-BINDING PROTEIN 2

Chain D: 65% 24% 7%



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

Chain G: 47% 47% 7%



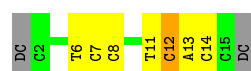
• Molecule 3: 5'-D(\*DGP\*GP\*TP\*GP\*AP\*AP\*AP\*(TTD)P\*AP\*GP\*CP\*AP\*GP\*DGP)-3',

Chain I: 60% 27% 13%



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

Chain H: 44% 38% 6% 13%



• 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 2 <sub>1</sub> 2 <sub>1</sub> 2 <sub>1</sub>	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	113.10Å 145.90Å 224.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.72 – 3.80 47.72 – 3.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.72-3.80) 99.8 (47.72-3.80)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.34 (at 3.77Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.243 , 0.319 0.240 , 0.313	Depositor DCC
$R_{free}$ test set	1862 reflections (5.26%)	DCC
Wilson B-factor (Å <sup>2</sup> )	102.6	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 61.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	1 of 37280 reflections (0.003%)	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	23938	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 19.23% 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: 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	0.37	0/8697	0.56	0/11777
1	C	0.37	0/8737	0.56	0/11831
2	B	0.37	0/2913	0.57	0/3957
2	D	0.37	0/2917	0.57	0/3962
3	G	0.63	0/306	1.13	2/470 (0.4%)
3	I	0.61	0/281	1.09	0/431
4	H	0.66	0/304	1.35	3/465 (0.6%)
4	J	0.65	0/283	1.17	1/433 (0.2%)
All	All	0.39	0/24438	0.61	6/33326 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	15	DG	P-O3'-C3'	5.89	126.77	119.70
4	J	12	DC	P-O3'-C3'	5.46	126.25	119.70
4	H	11	DT	C4-C5-C7	5.34	122.20	119.00
4	H	11	DT	C6-C5-C7	-5.21	119.77	122.90
4	H	12	DC	P-O3'-C3'	5.16	125.89	119.70
3	G	12	DG	P-O3'-C3'	5.10	125.82	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	8543	0	8538	184	0
1	C	8582	0	8588	177	0
2	B	2839	0	2785	63	0
2	D	2843	0	2788	66	0
3	G	312	0	171	8	0
3	I	290	0	160	4	0
4	H	274	0	160	6	0
4	J	255	0	149	0	0
All	All	23938	0	23339	494	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 10.

All (494) 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:40:GLU:HG2	1:A:54:GLU:HG3	1.44	0.97
1:A:864:LYS:HG3	1:A:899:LEU:HB2	1.51	0.93
1:A:204:LYS:HG2	1:A:205:GLY:H	1.33	0.91
1:C:391:ARG:HH21	1:C:711:HIS:HD2	1.18	0.90
2:D:102:GLN:HG3	2:D:107:HIS:HB3	1.54	0.89
1:A:972:PHE:HD1	1:A:1003:PHE:HB3	1.39	0.87
1:C:843:PRO:HG2	1:C:869:ALA:HB2	1.57	0.85
1:A:655:ARG:HD3	1:A:1138:ARG:NH1	1.92	0.84
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.61	0.82
1:A:151:GLU:HB2	1:A:153:LYS:HD2	1.59	0.82
1:C:889:ARG:HE	1:C:904:ASN:HD21	1.25	0.82
2:B:128:GLU:HG3	2:B:129:PRO:HD3	1.62	0.81
2:D:128:GLU:HG3	2:D:129:PRO:HD3	1.63	0.80
1:A:392:ASN:HB2	1:A:1012:LEU:HB3	1.63	0.80
2:B:161:THR:O	2:B:176:ASP:HB2	1.80	0.80
1:C:964:ASN:HB3	1:C:978:GLN:HG2	1.62	0.80
1:C:837:TYR:HB3	1:C:838:PRO:HD2	1.65	0.77
1:C:59:GLY:HA2	1:C:1073:TRP:CZ3	2.19	0.77
1:A:282:MET:HB2	1:A:305:LEU:HD11	1.65	0.76
2:D:263:LEU:HB3	2:D:272:PHE:HB3	1.67	0.75
2:B:339:LYS:HE3	2:B:412:ASN:HD21	1.53	0.74
2:B:214:ARG:HD3	3:G:9:TTD:H5A3	1.69	0.74
1:C:391:ARG:HH21	1:C:711:HIS:CD2	2.04	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1022:THR:N	1:A:1023:PRO:HD3	2.01	0.73
2:D:177:TYR:HD1	2:D:177:TYR:H	1.37	0.73
1:A:63:VAL:HG11	1:A:122:GLY:HA3	1.70	0.73
1:C:146:ASP:HB2	1:C:149:ASN:HB2	1.71	0.73
1:C:394:ILE:HD12	1:C:670:ASN:O	1.91	0.71
2:B:323:HIS:NE2	2:B:342:THR:HG21	2.06	0.71
2:D:150:VAL:HG12	2:D:446:GLY:O	1.92	0.70
1:C:170:LEU:HD11	1:C:179:CYS:HB2	1.73	0.70
2:B:134:LEU:HA	2:B:137:TYR:CD1	2.27	0.70
1:A:996:GLY:HA2	1:A:1087:GLY:HA3	1.74	0.70
1:A:972:PHE:CD1	1:A:1003:PHE:HB3	2.25	0.69
1:A:655:ARG:HD3	1:A:1138:ARG:HH11	1.53	0.69
1:C:1102:ARG:HG3	1:C:1103:PRO:HD3	1.73	0.69
1:A:1033:VAL:HG11	2:B:115:GLY:HA3	1.74	0.69
1:A:394:ILE:HD12	1:A:670:ASN:O	1.93	0.68
1:A:631:LEU:HD23	1:A:1138:ARG:HH22	1.58	0.68
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.76	0.68
1:A:903:CYS:SG	1:A:941:ASN:HA	2.34	0.68
2:D:323:HIS:NE2	2:D:342:THR:HG21	2.08	0.67
2:D:207:GLN:HB3	2:D:219:LEU:HD21	1.77	0.67
2:B:443:SER:HB2	2:B:450:LEU:HB2	1.77	0.66
1:A:81:THR:HG22	1:A:83:LYS:H	1.58	0.66
1:C:857:LYS:HG3	1:C:858:LEU:H	1.61	0.66
1:A:1003:PHE:HZ	2:B:112:SER:O	1.79	0.65
1:C:31:LEU:HD23	1:C:49:LEU:HD21	1.79	0.65
1:A:110:ASP:HB2	1:A:136:TYR:CE1	2.31	0.65
1:A:656:PRO:HB2	1:A:671:VAL:HB	1.79	0.65
2:D:174:LEU:HB3	2:D:184:SER:HB3	1.78	0.65
1:C:1047:TRP:HZ3	1:C:1132:VAL:HG13	1.63	0.64
1:C:22:HIS:HB3	1:C:26:ALA:HA	1.77	0.64
1:A:191:LYS:HG2	1:A:209:GLN:HG3	1.79	0.64
1:A:570:LYS:HG2	1:A:572:PRO:HD2	1.80	0.63
2:D:128:GLU:HG3	2:D:129:PRO:CD	2.28	0.63
1:C:358:PRO:HD2	1:C:380:GLY:HA2	1.81	0.63
1:C:922:LEU:HD22	1:C:959:ILE:HG13	1.81	0.63
1:C:63:VAL:HG11	1:C:122:GLY:HA3	1.81	0.63
1:C:656:PRO:HB2	1:C:671:VAL:HB	1.79	0.62
1:A:726:TYR:HE2	1:A:728:GLU:HG2	1.63	0.62
1:C:423:ASP:HA	1:C:438:LEU:HD12	1.81	0.62
2:B:305:LEU:HD12	2:B:319:ALA:HB3	1.81	0.62
1:A:234:GLN:HG3	1:A:257:THR:HG22	1.80	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:LYS:HG2	1:A:205:GLY:N	2.12	0.62
1:A:423:ASP:HA	1:A:438:LEU:HD12	1.81	0.62
2:D:123:ARG:HD3	2:D:384:MET:O	2.00	0.62
1:A:577:LEU:HD23	1:A:621:GLY:HA3	1.82	0.61
1:C:577:LEU:HD23	1:C:621:GLY:HA3	1.83	0.61
2:D:151:THR:HA	2:D:375:THR:HG21	1.83	0.61
1:A:59:GLY:HA2	1:A:1073:TRP:NE1	2.15	0.61
2:D:181:ASN:HD22	2:D:182:LYS:N	1.99	0.61
2:B:119:HIS:ND1	2:B:119:HIS:C	2.54	0.61
1:C:112:ILE:HD12	2:D:293:LEU:HD13	1.83	0.61
1:A:271:TYR:HB2	1:A:283:LEU:HB3	1.83	0.60
2:D:134:LEU:HA	2:D:137:TYR:CD1	2.36	0.60
2:B:194:ALA:HB3	2:B:213:ILE:HD12	1.83	0.60
1:A:771:PHE:HZ	1:A:865:GLU:HG3	1.65	0.60
1:A:492:GLU:HG2	1:A:493:PRO:HD2	1.83	0.60
1:C:492:GLU:HG2	1:C:493:PRO:HD2	1.83	0.60
1:A:133:LEU:HD23	1:A:135:LEU:HD21	1.83	0.60
3:G:6:DA:H1'	3:G:7:DA:H5'	1.84	0.60
2:D:119:HIS:ND1	2:D:119:HIS:C	2.55	0.60
1:C:7:VAL:HG13	1:C:1091:GLY:HA3	1.84	0.60
2:B:150:VAL:HG12	2:B:446:GLY:O	2.02	0.60
1:A:726:TYR:CE2	1:A:728:GLU:HG2	2.37	0.59
1:C:690:SER:HA	1:C:702:GLY:O	2.02	0.59
1:A:14:ALA:HB3	1:A:1034:ASN:HD22	1.67	0.59
1:A:706:GLU:OE1	1:A:711:HIS:HB2	2.02	0.59
1:A:298:LYS:HD3	1:A:299:ASP:HB2	1.84	0.59
2:D:102:GLN:HG3	2:D:107:HIS:CB	2.30	0.59
1:C:883:SER:HB2	1:C:914:LEU:HD11	1.85	0.59
1:A:1003:PHE:CZ	2:B:112:SER:O	2.55	0.59
1:C:334:VAL:HG21	1:C:347:VAL:HG12	1.85	0.59
1:A:358:PRO:O	1:A:379:SER:HA	2.03	0.58
1:C:723:LYS:HB2	1:C:736:LEU:HD12	1.83	0.58
1:C:273:LEU:HB2	1:C:281:PHE:HB2	1.85	0.58
1:A:682:LEU:HB2	1:A:690:SER:O	2.03	0.58
1:A:690:SER:HA	1:A:702:GLY:O	2.03	0.58
1:A:649:VAL:HG13	1:A:659:ILE:HB	1.84	0.58
1:A:1095:GLU:HG2	1:A:1137:THR:HG22	1.85	0.58
1:C:374:GLN:HE22	1:C:391:ARG:HA	1.69	0.58
1:C:1079:GLU:OE2	2:D:123:ARG:NH2	2.36	0.57
1:A:84:TYR:HB3	1:A:108:VAL:HG23	1.87	0.57
2:D:194:ALA:HB3	2:D:213:ILE:HD12	1.86	0.57

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:570:LYS:HG2	1:C:572:PRO:HD2	1.86	0.57
2:D:179:VAL:HB	2:D:181:ASN:ND2	2.19	0.57
2:B:129:PRO:HA	2:B:132:ARG:HH11	1.69	0.57
1:C:649:VAL:HG13	1:C:659:ILE:HB	1.86	0.57
1:C:682:LEU:HB2	1:C:690:SER:O	2.05	0.57
2:B:325:LYS:HB3	2:B:326:PRO:HD2	1.86	0.57
1:C:161:GLU:OE2	1:C:191:LYS:HE3	2.05	0.56
1:A:358:PRO:HD2	1:A:380:GLY:HA2	1.86	0.56
1:A:828:TYR:HE1	1:A:861:VAL:HG21	1.69	0.56
1:C:1051:LEU:HD22	1:C:1094:ILE:HD13	1.87	0.56
2:B:193:ASP:HA	2:B:214:ARG:HB3	1.88	0.56
1:C:201:GLU:HG3	1:C:202:PHE:N	2.21	0.56
1:C:334:VAL:HG21	1:C:347:VAL:CG1	2.35	0.56
1:A:630:THR:HG21	1:A:1130:ILE:CG1	2.36	0.56
1:C:949:PHE:CZ	1:C:991:HIS:HA	2.41	0.55
1:A:1061:VAL:HG11	1:A:1108:VAL:CG1	2.36	0.55
1:C:23:PHE:H	1:C:30:ASN:ND2	2.04	0.55
2:B:240:TYR:HE1	2:B:262:LEU:HD13	1.70	0.55
2:D:406:ILE:HD11	2:D:429:ILE:HG21	1.88	0.55
2:D:141:ARG:HD2	2:D:177:TYR:HB2	1.88	0.55
1:C:394:ILE:HA	1:C:706:GLU:HG3	1.87	0.55
1:A:467:GLN:HG2	1:A:480:SER:HA	1.89	0.55
1:A:876:PHE:HD1	1:A:916:THR:HG1	1.53	0.55
2:B:453:ASN:HD22	2:B:454:ARG:N	2.05	0.55
2:D:119:HIS:HD1	2:D:119:HIS:C	2.10	0.55
1:A:328:LEU:HD23	1:A:381:ALA:HB3	1.89	0.55
1:C:391:ARG:NH2	1:C:711:HIS:HD2	1.96	0.55
1:A:1030:PHE:CZ	1:A:1038:GLY:HA3	2.42	0.55
1:A:394:ILE:HA	1:A:706:GLU:HG3	1.89	0.54
1:C:857:LYS:HG3	1:C:858:LEU:N	2.21	0.54
2:B:286:PHE:HE2	2:B:308:LEU:HD21	1.72	0.54
3:G:6:DA:H2"	3:G:7:DA:OP2	2.08	0.54
1:A:881:LEU:HD13	1:A:914:LEU:HD23	1.88	0.54
1:C:110:ASP:HB2	1:C:136:TYR:CE1	2.43	0.54
1:C:182:TYR:OH	1:C:209:GLN:OE1	2.23	0.53
1:A:670:ASN:HD21	1:A:1138:ARG:HD3	1.74	0.53
1:A:329:GLY:HA2	1:A:355:ASN:HB3	1.90	0.53
1:A:834:ALA:HB2	1:A:869:ALA:HA	1.90	0.53
1:C:120:ILE:HG23	1:C:135:LEU:HD23	1.90	0.53
1:A:309:SER:HB3	1:A:332:GLN:HG2	1.89	0.53
2:B:151:THR:HA	2:B:375:THR:HG21	1.89	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:297:SER:HB2	2:D:327:VAL:HG12	1.90	0.53
1:C:10:GLN:HB3	1:C:1037:ILE:H	1.73	0.53
1:C:232:ILE:HG12	1:C:237:ILE:CD1	2.39	0.53
3:G:3:DG:N2	4:H:14:DC:O2	2.42	0.53
2:D:173:ILE:HG13	2:D:184:SER:O	2.08	0.53
1:C:854:SER:O	1:C:855:ASP:HB3	2.08	0.53
1:C:889:ARG:HE	1:C:904:ASN:ND2	2.01	0.53
2:D:161:THR:HA	2:D:177:TYR:CE1	2.44	0.53
1:A:204:LYS:CG	1:A:205:GLY:H	2.10	0.52
1:A:830:ILE:HG12	1:A:850:VAL:HG13	1.91	0.52
1:A:267:ASN:N	1:A:267:ASN:OD1	2.41	0.52
1:C:888:VAL:HG21	1:C:923:VAL:HG11	1.92	0.52
1:C:1047:TRP:CZ3	1:C:1132:VAL:HG13	2.45	0.52
1:C:492:GLU:OE1	1:C:496:LYS:HB2	2.10	0.52
1:C:1041:THR:HG21	1:C:1139:ILE:HD12	1.90	0.52
1:A:921:ILE:O	1:A:932:LEU:HD12	2.08	0.52
1:C:837:TYR:HB3	1:C:838:PRO:CD	2.39	0.52
3:G:9:TTD:H5R1	3:G:11:DA:C8	2.44	0.52
2:D:403:LYS:HB3	2:D:405:THR:HG23	1.92	0.52
1:C:387:LEU:HG	1:C:717:LEU:HD11	1.90	0.52
1:C:188:ARG:HD2	1:C:215:GLU:H	1.74	0.52
1:A:7:VAL:HG23	1:A:1039:LEU:HB3	1.92	0.52
1:C:68:ARG:HB2	1:C:75:ASP:OD1	2.10	0.52
2:B:339:LYS:HE3	2:B:412:ASN:ND2	2.22	0.52
4:H:7:DC:C2'	4:H:8:DC:H5'	2.39	0.52
2:D:181:ASN:HD22	2:D:182:LYS:H	1.58	0.52
1:C:467:GLN:HG2	1:C:480:SER:HA	1.92	0.52
1:A:1061:VAL:HG11	1:A:1108:VAL:HG12	1.91	0.51
1:C:38:ARG:HG3	1:C:54:GLU:OE2	2.10	0.51
2:D:197:GLY:N	2:D:211:SER:OG	2.40	0.51
1:A:404:LEU:HD21	1:A:427:LEU:HD13	1.93	0.51
1:C:934:ALA:HB2	1:C:945:ILE:HD11	1.92	0.51
1:C:404:LEU:HD21	1:C:427:LEU:HD13	1.92	0.51
2:B:250:GLN:HA	2:B:266:LEU:HD12	1.92	0.51
1:C:476:VAL:HG21	1:C:508:VAL:HG11	1.93	0.51
2:B:263:LEU:HB2	2:B:272:PHE:HB3	1.92	0.51
1:A:472:THR:HG23	1:A:474:ALA:H	1.76	0.51
1:A:1025:GLN:HB3	1:A:1042:SER:HB2	1.92	0.51
1:A:492:GLU:OE1	1:A:496:LYS:HB2	2.10	0.50
1:A:950:ASN:HB2	1:A:994:GLU:OE2	2.11	0.50
1:A:476:VAL:HG21	1:A:508:VAL:HG11	1.93	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:LYS:HD3	1:C:299:ASP:HB2	1.93	0.50
1:C:394:ILE:HD11	1:C:669:SER:HB3	1.92	0.50
1:A:134:ARG:HH11	1:A:164:VAL:HB	1.75	0.50
1:C:460:CYS:SG	1:C:461:GLY:N	2.84	0.50
1:C:429:PHE:HB2	1:C:432:GLN:HB2	1.94	0.50
1:A:744:ASP:HB2	1:A:750:THR:OG1	2.12	0.50
1:C:31:LEU:HD13	1:C:317:LEU:HD21	1.92	0.50
1:A:988:GLU:HA	1:A:991:HIS:CD2	2.47	0.50
1:C:413:LEU:HD11	1:C:468:LEU:HG	1.94	0.50
2:D:388:ILE:O	2:D:408:ILE:HA	2.12	0.50
1:C:232:ILE:HG12	1:C:237:ILE:HD12	1.93	0.50
1:C:288:GLU:OE1	1:C:298:LYS:HG3	2.12	0.50
2:D:161:THR:HA	2:D:177:TYR:OH	2.12	0.50
1:C:828:TYR:CE1	1:C:861:VAL:HG21	2.47	0.50
1:A:724:ILE:HG13	1:A:735:VAL:HG22	1.92	0.50
1:C:617:ASN:HB2	1:C:620:THR:OG1	2.12	0.50
2:D:240:TYR:HE1	2:D:262:LEU:HD13	1.77	0.50
1:A:631:LEU:HD23	1:A:1138:ARG:NH2	2.25	0.49
1:A:58:TYR:HB2	1:A:1068:ILE:HB	1.93	0.49
1:A:365:VAL:HG12	1:A:367:LEU:HG	1.94	0.49
1:A:81:THR:HB	1:A:85:ASN:H	1.77	0.49
1:A:460:CYS:SG	1:A:461:GLY:N	2.85	0.49
2:D:230:PHE:HB3	2:D:264:LEU:HD22	1.95	0.49
1:A:394:ILE:HD11	1:A:669:SER:HB3	1.93	0.49
1:A:630:THR:HG21	1:A:1130:ILE:HG13	1.93	0.49
2:B:170:GLY:HA2	2:B:195:ILE:HD12	1.94	0.49
1:A:220:ILE:HG23	1:A:261:HIS:CE1	2.46	0.49
1:C:914:LEU:HG	1:C:923:VAL:HG12	1.93	0.49
1:A:830:ILE:HG23	1:A:850:VAL:HG22	1.95	0.49
2:B:263:LEU:CB	2:B:272:PHE:HB3	2.43	0.49
1:A:15:VAL:HG11	1:A:325:GLY:HA3	1.92	0.49
1:C:843:PRO:CG	1:C:869:ALA:HB2	2.36	0.49
1:C:537:GLU:HB2	1:C:561:TRP:HB2	1.95	0.49
1:A:285:LEU:HG	1:A:300:LEU:HD21	1.94	0.49
2:B:259:GLY:HA2	2:B:281:VAL:HG23	1.95	0.49
1:C:374:GLN:NE2	1:C:391:ARG:HA	2.27	0.48
1:A:429:PHE:HB2	1:A:432:GLN:HB2	1.95	0.48
2:B:286:PHE:CE2	2:B:308:LEU:HD21	2.48	0.48
1:C:923:VAL:HG23	1:C:931:LEU:HB3	1.95	0.48
1:C:226:PHE:HZ	1:C:287:LYS:HE2	1.78	0.48
1:A:413:LEU:HD11	1:A:468:LEU:HG	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:GLU:HB2	1:A:561:TRP:HB2	1.95	0.48
1:C:140:PHE:HB2	1:C:159:LEU:HD12	1.95	0.48
1:A:997:LEU:N	1:A:1086:THR:O	2.45	0.48
1:C:10:GLN:HG2	1:C:356:LEU:HD12	1.95	0.48
2:B:333:ASN:HB3	2:B:381:TRP:CE2	2.48	0.48
1:C:764:SER:HG	1:C:805:HIS:HD1	1.61	0.48
1:C:18:CYS:HA	1:C:32:LEU:O	2.13	0.48
1:C:214:ALA:O	1:C:215:GLU:HB2	2.14	0.48
1:C:107:ASN:OD1	1:C:109:GLN:HG2	2.13	0.48
1:A:416:ASP:HB2	1:A:419:ARG:HB3	1.96	0.48
1:C:969:GLU:OE1	1:C:971:ALA:HB3	2.13	0.48
1:C:410:LEU:HD11	1:C:694:ALA:HB3	1.95	0.48
2:B:388:ILE:O	2:B:408:ILE:HA	2.14	0.48
1:A:410:LEU:HD11	1:A:694:ALA:HB3	1.95	0.48
2:B:128:GLU:HG3	2:B:129:PRO:CD	2.39	0.48
1:A:1095:GLU:HG2	1:A:1137:THR:CG2	2.43	0.48
1:A:1024:THR:HG21	1:A:1139:ILE:HD13	1.95	0.48
1:C:7:VAL:HG23	1:C:1039:LEU:HB3	1.96	0.47
1:A:134:ARG:NH1	1:A:164:VAL:HB	2.29	0.47
1:A:195:VAL:HG22	1:A:202:PHE:HE1	1.79	0.47
2:D:172:ILE:HD11	2:D:195:ILE:HD11	1.96	0.47
1:C:135:LEU:HB2	1:C:136:TYR:CD1	2.48	0.47
1:A:1055:GLN:HE22	1:A:1090:ASP:H	1.60	0.47
2:D:297:SER:HB2	2:D:327:VAL:CG1	2.45	0.47
2:D:333:ASN:HB3	2:D:381:TRP:CE2	2.49	0.47
1:C:472:THR:HG23	1:C:474:ALA:H	1.78	0.47
1:C:706:GLU:C	1:C:708:GLN:H	2.18	0.47
1:C:922:LEU:CD2	1:C:959:ILE:HG13	2.45	0.47
1:A:252:ILE:HG22	1:A:281:PHE:HE1	1.79	0.47
1:C:235:GLU:HG2	1:C:254:LYS:HG3	1.96	0.47
1:C:378:CYS:HB3	1:C:721:PRO:HB2	1.97	0.47
1:A:389:ILE:HD12	1:A:713:ARG:HB3	1.97	0.47
1:A:378:CYS:HB3	1:A:721:PRO:HG2	1.97	0.47
1:C:587:ILE:H	1:C:587:ILE:HD13	1.80	0.47
1:C:256:SER:HB3	1:C:257:THR:H	1.61	0.47
1:A:1053:ASP:O	1:A:1057:ARG:HG3	2.15	0.47
2:B:119:HIS:C	2:B:119:HIS:HD1	2.16	0.47
2:D:367:PRO:HB2	2:D:393:TYR:O	2.15	0.47
1:C:312:GLU:HG3	1:C:327:ARG:HD3	1.97	0.47
1:C:167:VAL:HG13	1:C:180:PHE:HB3	1.97	0.47
1:C:764:SER:OG	1:C:805:HIS:ND1	2.47	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:LEU:HD12	1:A:610:ALA:HB3	1.97	0.47
1:C:139:LEU:HB3	1:C:156:ASN:HD22	1.80	0.47
1:A:722:ARG:NH1	1:A:738:SER:OG	2.48	0.47
1:C:57:MET:HG3	1:C:61:ILE:HD11	1.96	0.47
1:A:1133:VAL:O	1:A:1137:THR:HG23	2.16	0.46
2:B:341:LEU:HD21	2:B:388:ILE:HG23	1.97	0.46
1:A:391:ARG:HB3	1:A:711:HIS:HB3	1.97	0.46
1:A:631:LEU:HD12	1:A:636:THR:HG21	1.97	0.46
1:A:889:ARG:HD3	1:A:901:THR:HB	1.97	0.46
2:B:178:ASP:C	2:B:180:GLN:H	2.19	0.46
3:I:2:DG:H2''	3:I:3:DG:C8	2.50	0.46
1:C:964:ASN:HB3	1:C:978:GLN:CG	2.40	0.46
2:D:117:SER:O	2:D:119:HIS:N	2.48	0.46
2:D:135:LYS:HG2	2:D:418:HIS:CE1	2.51	0.46
1:A:536:HIS:HB2	1:A:560:LEU:HB3	1.98	0.46
2:D:404:ARG:NH1	2:D:428:ILE:HG13	2.30	0.46
1:C:310:ILE:HG23	1:C:383:LYS:HE3	1.98	0.46
1:C:207:TRP:CH2	1:C:240:HIS:HB2	2.50	0.46
1:C:374:GLN:HE21	1:C:374:GLN:HA	1.79	0.46
3:G:9:TTD:O2	3:G:9:TTD:O4'	2.33	0.46
2:D:388:ILE:HB	2:D:409:TYR:HB2	1.98	0.46
1:C:431:GLY:HA2	1:C:456:GLN:HB2	1.97	0.46
2:B:391:GLY:HA3	2:B:429:ILE:O	2.14	0.46
1:A:282:MET:O	1:A:302:VAL:HA	2.16	0.46
4:H:6:DT:H1'	4:H:7:DC:H5'	1.98	0.46
1:A:431:GLY:HA2	1:A:456:GLN:HB2	1.98	0.46
1:C:631:LEU:HD12	1:C:636:THR:HG21	1.98	0.46
1:A:966:LEU:HD11	1:A:1040:VAL:HG21	1.98	0.46
3:I:9:TTD:H2''	3:I:9:TTD:H6	1.76	0.46
1:C:986:ASP:HA	1:C:989:ARG:HG2	1.98	0.45
2:D:255:GLY:HA2	2:D:260:ARG:O	2.16	0.45
2:B:240:TYR:CE1	2:B:262:LEU:HD13	2.51	0.45
1:C:1033:VAL:HG11	2:D:115:GLY:HA3	1.98	0.45
2:B:245:VAL:HG12	2:B:252:LEU:HB2	1.97	0.45
1:C:114:ARG:HH12	2:D:412:ASN:HD21	1.63	0.45
1:C:603:LEU:HD23	1:C:613:TYR:HB3	1.99	0.45
1:C:592:LEU:HD21	1:C:640:THR:HG23	1.98	0.45
1:C:372:GLN:CG	1:C:374:GLN:HG2	2.46	0.45
1:C:60:LYS:O	1:C:81:THR:HA	2.16	0.45
1:A:114:ARG:NE	2:B:336:ASP:OD2	2.47	0.45
1:C:606:LEU:HD12	1:C:610:ALA:HB3	1.98	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:CB	1:A:185:PRO:HD2	2.37	0.45
1:C:467:GLN:HE22	1:C:524:GLN:H	1.64	0.45
1:C:383:LYS:HG2	1:C:753:ARG:NH1	2.31	0.45
1:A:43:VAL:HG22	1:A:52:VAL:HG22	1.98	0.45
1:C:536:HIS:HB2	1:C:560:LEU:HB3	1.97	0.45
2:B:334:PRO:HG2	2:B:383:PRO:HA	1.99	0.45
1:A:16:ASN:HB3	1:A:34:ALA:O	2.16	0.45
2:B:153:LEU:HD12	2:B:165:VAL:HG22	1.99	0.45
4:H:12:DC:H2"	4:H:13:DA:OP2	2.15	0.45
1:A:617:ASN:HB2	1:A:620:THR:OG1	2.17	0.45
3:I:3:DG:H2"	3:I:4:DT:H71	1.99	0.45
1:A:626:ARG:H	1:A:1102:ARG:HB2	1.81	0.45
1:A:131:ILE:HG13	1:A:145:LEU:HD11	1.98	0.44
1:A:603:LEU:HD23	1:A:613:TYR:HB3	1.99	0.44
2:D:218:THR:HG22	2:D:229:VAL:HA	1.99	0.44
2:D:435:SER:O	2:D:438:GLY:N	2.50	0.44
1:A:989:ARG:HA	1:A:989:ARG:NE	2.32	0.44
1:A:869:ALA:O	1:A:884:ILE:HA	2.17	0.44
1:C:127:GLU:O	1:C:128:CYS:HB2	2.18	0.44
1:A:922:LEU:HB2	1:A:959:ILE:HD11	1.99	0.44
1:A:120:ILE:H	1:A:120:ILE:HG13	1.55	0.44
1:C:424:THR:HG23	1:C:435:VAL:HG13	2.00	0.44
1:A:94:SER:HB3	1:A:97:SER:HB2	2.00	0.44
1:A:631:LEU:CD2	1:A:1138:ARG:HH22	2.27	0.44
1:A:84:TYR:HB2	1:A:109:GLN:HB3	2.00	0.44
1:A:684:SER:HB3	1:A:687:TYR:HB2	1.98	0.44
1:C:470:GLN:OE1	1:C:477:ARG:HD3	2.17	0.44
1:C:69:PRO:HG2	1:C:76:LEU:HD12	1.99	0.44
1:A:213:GLU:HG2	1:A:215:GLU:H	1.82	0.44
1:A:19:VAL:HG11	1:A:66:LEU:H	1.81	0.44
1:C:889:ARG:NE	1:C:904:ASN:HD21	2.04	0.44
1:C:1079:GLU:HG2	1:C:1079:GLU:O	2.18	0.44
1:C:80:LEU:HD22	1:C:133:LEU:HD11	1.99	0.44
1:C:1102:ARG:HG3	1:C:1103:PRO:CD	2.45	0.44
1:A:424:THR:HG23	1:A:435:VAL:HG13	1.98	0.44
1:A:390:ILE:HD12	1:A:1037:ILE:HD11	2.00	0.44
1:C:1057:ARG:HH12	1:C:1110:ALA:HB3	1.82	0.44
2:D:179:VAL:HB	2:D:181:ASN:HD21	1.83	0.44
1:A:309:SER:CB	1:A:332:GLN:HG2	2.48	0.44
1:C:416:ASP:HB2	1:C:419:ARG:HB3	1.99	0.44
1:A:926:LEU:HD21	2:B:126:LEU:HD11	1.99	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:403:LYS:HB3	2:B:405:THR:HG23	1.99	0.44
2:B:161:THR:O	2:B:176:ASP:CB	2.60	0.44
1:A:1128:ASP:HA	1:A:1130:ILE:HG22	1.99	0.44
1:C:893:TRP:HE3	1:C:899:LEU:HD13	1.83	0.44
1:C:992:LEU:HD23	1:C:992:LEU:HA	1.91	0.44
1:A:255:GLN:H	1:A:255:GLN:HG2	1.58	0.43
1:A:324:VAL:HB	1:A:332:GLN:HB2	1.99	0.43
1:C:72:GLU:OE1	1:C:103:ARG:NH2	2.51	0.43
1:C:684:SER:HB3	1:C:687:TYR:HB2	1.99	0.43
2:D:298:SER:HB3	2:D:300:ASP:OD1	2.18	0.43
1:A:828:TYR:CE1	1:A:861:VAL:HG21	2.52	0.43
1:A:23:PHE:H	1:A:30:ASN:ND2	2.16	0.43
2:D:365:ILE:HG23	2:D:398:LEU:HD21	2.00	0.43
1:C:392:ASN:CB	1:C:1012:LEU:HB3	2.48	0.43
2:D:382:HIS:CG	2:D:383:PRO:HD2	2.54	0.43
2:D:161:THR:CA	2:D:177:TYR:CE1	3.01	0.43
1:A:231:ILE:HD13	1:A:240:HIS:HD2	1.83	0.43
2:B:393:TYR:HD1	2:B:393:TYR:C	2.22	0.43
1:C:724:ILE:HG13	1:C:735:VAL:HG22	2.01	0.43
1:C:374:GLN:HE22	1:C:391:ARG:CA	2.30	0.43
3:G:9:TTD:H2"	3:G:9:TTD:H6	1.95	0.43
2:D:177:TYR:CD1	2:D:177:TYR:N	2.73	0.43
1:C:108:VAL:HG11	1:C:143:ILE:HD11	1.99	0.43
1:A:31:LEU:HD13	1:A:317:LEU:HD21	2.00	0.43
2:D:432:ASN:OD1	2:D:443:SER:OG	2.32	0.43
1:A:1022:THR:N	1:A:1023:PRO:CD	2.78	0.43
1:C:736:LEU:HD22	1:C:813:ALA:HB1	2.01	0.43
2:B:333:ASN:HA	2:B:334:PRO:HD3	1.89	0.43
2:D:110:TYR:O	2:D:113:SER:HB3	2.19	0.43
2:B:362:GLN:HG2	2:B:414:GLY:HA3	2.00	0.43
2:D:359:LYS:HA	2:D:360:PRO:HD3	1.91	0.43
1:C:371:GLY:O	1:C:1014:MET:HG2	2.18	0.43
1:C:843:PRO:HG2	1:C:869:ALA:CB	2.37	0.43
1:A:889:ARG:HD2	1:A:891:TYR:CE2	2.53	0.43
1:A:592:LEU:HD21	1:A:640:THR:HG23	2.00	0.43
1:C:644:LEU:HB3	1:C:707:ILE:HD13	2.01	0.43
1:C:197:LEU:HD23	1:C:197:LEU:H	1.83	0.43
1:C:889:ARG:HD3	1:C:901:THR:HB	1.99	0.42
1:C:334:VAL:CG2	1:C:347:VAL:HG12	2.48	0.42
2:B:393:TYR:CD1	2:B:393:TYR:C	2.92	0.42
1:C:183:GLN:NE2	1:C:188:ARG:HH21	2.16	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1030:PHE:HE2	1:C:1040:VAL:HG23	1.85	0.42
1:C:59:GLY:HA2	1:C:1073:TRP:CE3	2.53	0.42
1:A:310:ILE:HG21	1:A:328:LEU:HD13	2.01	0.42
2:D:393:TYR:CD1	2:D:393:TYR:C	2.93	0.42
1:A:644:LEU:HB3	1:A:707:ILE:HD13	2.00	0.42
1:A:112:ILE:HG23	2:B:354:SER:HB2	2.02	0.42
1:A:719:GLU:HG2	1:A:755:SER:HB2	2.01	0.42
2:B:294:MET:HB3	2:B:306:TRP:HB2	2.01	0.42
1:A:467:GLN:HE22	1:A:524:GLN:H	1.65	0.42
1:C:392:ASN:HB3	1:C:1012:LEU:HB3	2.00	0.42
1:A:593:MET:HB3	1:A:602:LEU:HD23	2.01	0.42
1:C:337:ASN:O	1:C:346:TYR:HB3	2.19	0.42
2:D:154:GLU:HG3	2:D:198:MET:O	2.19	0.42
1:A:49:LEU:N	1:A:49:LEU:HD12	2.35	0.42
1:C:743:GLN:HG2	1:C:744:ASP:O	2.19	0.42
2:B:193:ASP:O	2:B:213:ILE:HB	2.20	0.42
1:A:390:ILE:CD1	1:A:1037:ILE:HD11	2.50	0.42
1:A:234:GLN:HG3	1:A:257:THR:CG2	2.46	0.42
1:A:876:PHE:HD1	1:A:916:THR:OG1	2.02	0.42
1:C:232:ILE:CG2	1:C:233:GLY:N	2.82	0.42
1:C:727:GLN:HE21	1:C:730:SER:HB2	1.83	0.42
1:A:587:ILE:H	1:A:587:ILE:HD13	1.84	0.42
2:B:210:VAL:O	2:B:217:THR:HA	2.19	0.42
1:A:954:MET:HE2	1:A:975:PHE:HZ	1.85	0.42
1:C:374:GLN:NE2	1:C:391:ARG:HG3	2.35	0.42
1:A:793:ILE:HG21	1:A:853:TYR:CD1	2.54	0.42
2:B:161:THR:HA	2:B:177:TYR:OH	2.19	0.42
1:C:38:ARG:HA	1:C:38:ARG:HD2	1.85	0.42
1:A:255:GLN:HG3	1:A:279:ARG:HH12	1.85	0.42
2:B:422:ASP:OD2	2:B:424:ASN:HB2	2.19	0.42
1:C:284:LEU:HD22	1:C:301:ARG:HH21	1.84	0.42
2:D:128:GLU:N	2:D:129:PRO:HD2	2.35	0.42
2:B:161:THR:HA	2:B:177:TYR:CZ	2.54	0.42
2:B:148:ARG:HD3	3:G:9:TTD:OP1	2.20	0.42
1:C:593:MET:HB3	1:C:602:LEU:HD23	2.02	0.42
1:C:250:PRO:HA	1:C:251:PRO:HD3	1.88	0.42
1:A:842:GLU:HG2	1:A:843:PRO:HD2	2.00	0.42
2:D:393:TYR:C	2:D:393:TYR:HD1	2.24	0.42
1:C:542:ASP:OD2	1:C:593:MET:HG2	2.20	0.42
1:C:695:ASN:N	1:C:695:ASN:OD1	2.48	0.42
1:A:706:GLU:C	1:A:708:GLN:H	2.23	0.41

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:708:GLN:HA	1:C:708:GLN:OE1	2.20	0.41
2:D:406:ILE:HG13	2:D:429:ILE:HD13	2.02	0.41
2:D:280:LYS:O	2:D:298:SER:HA	2.19	0.41
1:C:559:GLY:HA2	1:C:565:SER:O	2.21	0.41
2:D:161:THR:HA	2:D:177:TYR:CZ	2.55	0.41
1:A:234:GLN:HE21	1:A:257:THR:HG23	1.85	0.41
1:A:880:LEU:HB3	1:A:891:TYR:HB2	2.02	0.41
1:C:880:LEU:O	1:C:891:TYR:N	2.52	0.41
1:A:578:HIS:CE1	1:A:623:LEU:H	2.38	0.41
2:D:153:LEU:O	2:D:154:GLU:HG2	2.20	0.41
1:A:654:ASP:HA	1:A:675:GLU:HA	2.03	0.41
1:A:953:TRP:O	1:A:970:ASN:HB2	2.21	0.41
1:A:288:GLU:HB2	1:A:298:LYS:HB2	2.02	0.41
1:C:188:ARG:HD2	1:C:215:GLU:N	2.33	0.41
1:C:1030:PHE:CZ	1:C:1038:GLY:HA3	2.55	0.41
1:A:908:ASN:HD21	1:A:931:LEU:HD13	1.84	0.41
2:D:189:MET:HG3	2:D:190:GLY:N	2.36	0.41
1:A:708:GLN:HA	1:A:708:GLN:OE1	2.21	0.41
1:A:65:GLU:HB2	1:A:124:ILE:HD12	2.02	0.41
4:H:7:DC:H2'	4:H:8:DC:H5'	2.03	0.41
2:B:283:HIS:NE2	2:B:285:GLU:HB2	2.36	0.41
2:B:394:PRO:HB3	2:B:402:ASP:HB3	2.02	0.41
1:A:970:ASN:HA	1:A:970:ASN:HD22	1.68	0.41
1:C:311:ALA:HB2	1:C:324:VAL:HG12	2.02	0.41
1:A:789:HIS:CD2	1:A:812:TYR:HA	2.56	0.41
1:A:218:MET:HG2	1:A:261:HIS:CD2	2.56	0.41
2:D:189:MET:O	2:D:193:ASP:HB2	2.21	0.41
1:C:362:MET:HB3	1:C:377:THR:HG22	2.03	0.41
1:A:930:VAL:HG23	1:A:948:ASP:HB3	2.02	0.41
1:C:881:LEU:HD13	1:C:914:LEU:CD2	2.51	0.41
2:B:371:PHE:HE1	4:H:8:DC:O2	2.03	0.41
3:I:3:DG:H2''	3:I:4:DT:C7	2.51	0.41
1:C:983:ALA:HB3	1:C:989:ARG:HE	1.86	0.41
1:A:23:PHE:H	1:A:30:ASN:HD22	1.68	0.41
1:C:134:ARG:NH1	1:C:164:VAL:HB	2.35	0.41
1:C:43:VAL:HG23	1:C:50:ARG:HB2	2.03	0.41
1:C:1077:HIS:CE1	1:C:1082:THR:HG1	2.39	0.41
1:A:851:PHE:HB3	1:A:858:LEU:HD21	2.02	0.41
2:B:289:ARG:HD3	2:B:337:SER:HB2	2.03	0.41
1:C:504:ASN:HD22	1:C:545:PRO:HD3	1.86	0.41
1:A:945:ILE:HG22	1:A:946:ALA:N	2.36	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:PRO:HD2	1:C:380:GLY:CA	2.50	0.41
1:C:881:LEU:CD1	1:C:914:LEU:HD23	2.51	0.41
1:A:988:GLU:O	1:A:991:HIS:HB2	2.21	0.41
2:B:425:ALA:HB1	2:B:445:MET:SD	2.61	0.41
1:A:386:SER:HB3	1:A:716:PRO:HA	2.03	0.40
1:A:719:GLU:OE1	1:A:739:ARG:HB3	2.21	0.40
1:A:542:ASP:OD2	1:A:593:MET:HG2	2.20	0.40
1:C:727:GLN:HG3	1:C:818:SER:OG	2.21	0.40
1:A:559:GLY:HA2	1:A:565:SER:O	2.22	0.40
2:D:207:GLN:HB3	2:D:219:LEU:CD2	2.50	0.40
2:B:180:GLN:HB3	2:B:181:ASN:H	1.68	0.40
2:B:220:ARG:HD2	2:B:226:VAL:HG22	2.02	0.40
1:C:155:PHE:CD2	1:C:200:LYS:HG2	2.56	0.40
1:C:476:VAL:HG13	1:C:490:TRP:HB3	2.03	0.40
1:A:988:GLU:HA	1:A:991:HIS:HD2	1.85	0.40
2:D:333:ASN:HA	2:D:334:PRO:HD3	1.85	0.40
2:B:401:ASN:HA	2:B:401:ASN:HD22	1.57	0.40
1:C:10:GLN:O	1:C:1036:MET:HG2	2.21	0.40
1:A:390:ILE:HG22	1:A:710:LEU:HD12	2.02	0.40
1:A:231:ILE:HD13	1:A:240:HIS:CD2	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	1076/1159 (93%)	960 (89%)	100 (9%)	16 (2%)	13	59
1	C	1081/1159 (93%)	953 (88%)	114 (10%)	14 (1%)	15	61
2	B	352/382 (92%)	307 (87%)	36 (10%)	9 (3%)	7	48
2	D	353/382 (92%)	318 (90%)	30 (8%)	5 (1%)	14	59
All	All	2862/3082 (93%)	2538 (89%)	280 (10%)	44 (2%)	13	59

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	118	ILE
2	B	183	THR
2	B	194	ALA
1	C	707	ILE
1	C	855	ASP
1	A	674	LYS
1	A	707	ILE
1	A	854	SER
1	A	945	ILE
2	B	179	VAL
2	B	190	GLY
1	C	674	LYS
2	D	118	ILE
2	D	190	GLY
2	D	194	ALA
2	D	368	HIS
1	A	367	LEU
2	B	180	GLN
1	C	36	ASN
1	C	367	LEU
2	D	117	SER
1	A	185	PRO
1	A	319	ASN
1	A	696	ASN
2	B	117	SER
1	C	696	ASN
1	C	1128	ASP
1	A	36	ASN
1	A	51	PRO
1	A	330	ASP
1	A	504	ASN
2	B	191	PRO
1	C	111	ARG
1	C	463	VAL
1	C	504	ASN
1	C	963	ASP
1	C	1100	ILE
1	C	1126	ALA
1	A	463	VAL
1	A	1109	VAL
2	B	368	HIS
1	A	1023	PRO

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	564	ILE
1	C	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	957/1015 (94%)	873 (91%)	84 (9%)	12	50
1	C	962/1015 (95%)	870 (90%)	92 (10%)	10	46
2	B	313/335 (93%)	278 (89%)	35 (11%)	7	38
2	D	313/335 (93%)	284 (91%)	29 (9%)	11	47
All	All	2545/2700 (94%)	2305 (91%)	240 (9%)	11	47

All (240) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	VAL
1	A	16	ASN
1	A	18	CYS
1	A	32	LEU
1	A	45	THR
1	A	49	LEU
1	A	54	GLU
1	A	55	VAL
1	A	110	ASP
1	A	118	THR
1	A	120	ILE
1	A	174	GLN
1	A	191	LYS
1	A	197	LEU
1	A	218	MET
1	A	220	ILE
1	A	244	LYS
1	A	256	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	257	THR
1	A	263	ARG
1	A	265	ASP
1	A	267	ASN
1	A	276	MET
1	A	279	ARG
1	A	295	VAL
1	A	302	VAL
1	A	310	ILE
1	A	315	THR
1	A	318	ASP
1	A	319	ASN
1	A	354	THR
1	A	366	ASP
1	A	370	GLN
1	A	372	GLN
1	A	374	GLN
1	A	386	SER
1	A	389	ILE
1	A	390	ILE
1	A	403	ASP
1	A	416	ASP
1	A	432	GLN
1	A	445	GLU
1	A	449	MET
1	A	478	LEU
1	A	532	THR
1	A	550	ASN
1	A	564	ILE
1	A	587	ILE
1	A	627	LYS
1	A	674	LYS
1	A	679	MET
1	A	696	ASN
1	A	708	GLN
1	A	711	HIS
1	A	720	SER
1	A	725	CYS
1	A	746	SER
1	A	752	LEU
1	A	784	GLU
1	A	785	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	817	VAL
1	A	820	LYS
1	A	852	GLN
1	A	855	ASP
1	A	858	LEU
1	A	867	LYS
1	A	901	THR
1	A	930	VAL
1	A	962	ASP
1	A	966	LEU
1	A	970	ASN
1	A	989	ARG
1	A	995	VAL
1	A	1003	PHE
1	A	1013	VAL
1	A	1065	VAL
1	A	1098	LEU
1	A	1099	ASP
1	A	1100	ILE
1	A	1107	GLU
1	A	1130	ILE
1	A	1131	LYS
1	A	1140	HIS
2	B	102	GLN
2	B	118	ILE
2	B	119	HIS
2	B	177	TYR
2	B	179	VAL
2	B	180	GLN
2	B	181	ASN
2	B	182	LYS
2	B	186	ILE
2	B	196	THR
2	B	198	MET
2	B	202	GLN
2	B	219	LEU
2	B	249	ARG
2	B	252	LEU
2	B	267	ASP
2	B	269	HIS
2	B	291	ASP
2	B	293	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	294	MET
2	B	309	ARG
2	B	321	MET
2	B	342	THR
2	B	359	LYS
2	B	365	ILE
2	B	370	GLN
2	B	374	LEU
2	B	389	VAL
2	B	393	TYR
2	B	401	ASN
2	B	420	LEU
2	B	421	ARG
2	B	437	THR
2	B	453	ASN
2	B	454	ARG
1	C	1	MET
1	C	7	VAL
1	C	13	THR
1	C	20	THR
1	C	37	THR
1	C	38	ARG
1	C	57	MET
1	C	74	LYS
1	C	98	ILE
1	C	118	THR
1	C	125	ASP
1	C	145	LEU
1	C	147	ARG
1	C	148	ASP
1	C	158	ARG
1	C	159	LEU
1	C	188	ARG
1	C	201	GLU
1	C	211	ASN
1	C	213	GLU
1	C	217	SER
1	C	218	MET
1	C	222	VAL
1	C	236	SER
1	C	244	LYS
1	C	256	SER

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	279	ARG
1	C	302	VAL
1	C	304	LEU
1	C	310	ILE
1	C	314	LEU
1	C	318	ASP
1	C	319	ASN
1	C	327	ARG
1	C	334	VAL
1	C	339	ASP
1	C	350	MET
1	C	367	LEU
1	C	372	GLN
1	C	389	ILE
1	C	403	ASP
1	C	416	ASP
1	C	432	GLN
1	C	445	GLU
1	C	449	MET
1	C	453	ASP
1	C	478	LEU
1	C	532	THR
1	C	550	ASN
1	C	564	ILE
1	C	587	ILE
1	C	627	LYS
1	C	655	ARG
1	C	674	LYS
1	C	679	MET
1	C	696	ASN
1	C	708	GLN
1	C	722	ARG
1	C	740	ILE
1	C	743	GLN
1	C	750	THR
1	C	752	LEU
1	C	796	GLN
1	C	815	SER
1	C	854	SER
1	C	864	LYS
1	C	867	LYS
1	C	873	MET

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type
1	C	886	SER
1	C	898	GLU
1	C	899	LEU
1	C	900	ARG
1	C	901	THR
1	C	910	MET
1	C	923	VAL
1	C	930	VAL
1	C	947	ARG
1	C	964	ASN
1	C	970	ASN
1	C	980	ASP
1	C	988	GLU
1	C	1024	THR
1	C	1041	THR
1	C	1045	GLU
1	C	1065	VAL
1	C	1093	LEU
1	C	1098	LEU
1	C	1107	GLU
1	C	1127	ASP
1	C	1129	LEU
1	C	1130	ILE
1	C	1138	ARG
2	D	102	GLN
2	D	118	ILE
2	D	119	HIS
2	D	144	SER
2	D	177	TYR
2	D	179	VAL
2	D	180	GLN
2	D	181	ASN
2	D	185	PHE
2	D	196	THR
2	D	202	GLN
2	D	247	VAL
2	D	249	ARG
2	D	269	HIS
2	D	291	ASP
2	D	308	LEU
2	D	309	ARG
2	D	321	MET

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	D	336	ASP
2	D	359	LYS
2	D	365	ILE
2	D	370	GLN
2	D	374	LEU
2	D	384	MET
2	D	389	VAL
2	D	393	TYR
2	D	401	ASN
2	D	420	LEU
2	D	454	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	30	ASN
1	A	149	ASN
1	A	209	GLN
1	A	234	GLN
1	A	261	HIS
1	A	343	GLN
1	A	467	GLN
1	A	507	GLN
1	A	528	GLN
1	A	550	ASN
1	A	648	ASN
1	A	670	ASN
1	A	672	ASN
1	A	677	ASN
1	A	727	GLN
1	A	796	GLN
1	A	806	GLN
1	A	845	GLN
1	A	904	ASN
1	A	908	ASN
1	A	970	ASN
1	A	991	HIS
1	A	1034	ASN
1	A	1055	GLN
2	B	202	GLN
2	B	370	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
2	B	401	ASN
2	B	412	ASN
2	B	419	GLN
2	B	453	ASN
1	C	30	ASN
1	C	105	HIS
1	C	183	GLN
1	C	240	HIS
1	C	261	HIS
1	C	319	ASN
1	C	374	GLN
1	C	467	GLN
1	C	507	GLN
1	C	528	GLN
1	C	550	ASN
1	C	648	ASN
1	C	670	ASN
1	C	677	ASN
1	C	711	HIS
1	C	727	GLN
1	C	731	GLN
1	C	796	GLN
1	C	845	GLN
1	C	904	ASN
1	C	1034	ASN
2	D	102	GLN
2	D	181	ASN
2	D	202	GLN
2	D	370	GLN
2	D	373	HIS
2	D	401	ASN
2	D	412	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are 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	9	3	40,45,46	1.63	7 (17%)	58,74,77	2.26	16 (27%)
3	TTD	I	9	3	40,45,46	1.55	7 (17%)	58,74,77	2.16	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	9	3	-	0/22/109/110	0/3/6/6
3	TTD	I	9	3	-	0/22/109/110	0/3/6/6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	9	TTD	C2T-N1T	2.26	1.41	1.36
3	G	9	TTD	C6T-N1T	2.29	1.50	1.46
3	I	9	TTD	O4'-C1'	2.37	1.47	1.42
3	I	9	TTD	C2T-N1T	2.64	1.42	1.36
3	I	9	TTD	C6T-N1T	2.80	1.51	1.46
3	I	9	TTD	C6-N1	2.82	1.51	1.46
3	G	9	TTD	O4'-C1'	2.82	1.48	1.42
3	I	9	TTD	C2-N1	3.15	1.43	1.36
3	G	9	TTD	C6-N1	3.33	1.51	1.46
3	G	9	TTD	C2-N1	3.47	1.43	1.36
3	I	9	TTD	C1'-N1	3.99	1.51	1.45
3	I	9	TTD	C1R-N1T	4.01	1.51	1.45
3	G	9	TTD	C1R-N1T	4.42	1.51	1.45
3	G	9	TTD	C1'-N1	4.48	1.51	1.45

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	9	TTD	O4-C4-C5	-3.87	119.76	122.92
3	I	9	TTD	O4-C4-C5	-3.53	120.04	122.92

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	9	TTD	O4T-C4T-C5T	-3.42	120.13	122.92
3	I	9	TTD	C4'-O4R-C1R	-3.33	101.04	109.46
3	G	9	TTD	C4-N3-C2	-3.26	120.97	126.84
3	G	9	TTD	O4R-C1R-C2R	-3.25	99.80	106.28
3	I	9	TTD	C4T-N3T-C2T	-3.06	121.34	126.84
3	I	9	TTD	C2R-C1R-N1T	-3.04	111.48	115.64
3	I	9	TTD	C4-N3-C2	-2.97	121.50	126.84
3	G	9	TTD	O4T-C4T-C5T	-2.96	120.50	122.92
3	G	9	TTD	O2-C2-N3	-2.95	115.71	121.48
3	G	9	TTD	C4'-O4R-C1R	-2.89	102.16	109.46
3	G	9	TTD	C4T-N3T-C2T	-2.84	121.73	126.84
3	G	9	TTD	O2T-C2T-N1T	-2.80	119.14	123.36
3	I	9	TTD	O2-C2-N3	-2.52	116.55	121.48
3	G	9	TTD	C5-C6-N1	-2.20	112.59	115.70
3	I	9	TTD	O4R-C1R-C2R	-2.13	102.03	106.28
3	I	9	TTD	O2T-C2T-N1T	-2.13	120.15	123.36
3	G	9	TTD	O4R-C4'-C5R	2.03	116.58	109.32
3	G	9	TTD	C5-C5T-C6T	2.24	91.20	88.37
3	I	9	TTD	C5-C5T-C6T	2.44	91.45	88.37
3	G	9	TTD	C2R-C1R-N1T	4.75	122.15	115.64
3	I	9	TTD	N3T-C2T-N1T	5.26	122.08	116.82
3	G	9	TTD	N3T-C2T-N1T	5.55	122.37	116.82
3	I	9	TTD	N3-C2-N1	5.74	122.57	116.82
3	G	9	TTD	C5T-C4T-N3T	5.82	121.07	116.01
3	G	9	TTD	C5-C4-N3	5.88	121.12	116.01
3	I	9	TTD	C5-C4-N3	6.54	121.69	116.01
3	G	9	TTD	N3-C2-N1	6.73	123.56	116.82
3	I	9	TTD	C5T-C4T-N3T	6.76	121.88	116.01

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	9	TTD	5	0
3	I	9	TTD	1	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

There are no ligands in this entry.

## 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, 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	1090/1159 (94%)	0.15	68 (6%)	24	14	68, 109, 228, 265	0
1	C	1095/1159 (94%)	0.05	36 (3%)	50	34	70, 106, 215, 247	0
2	B	354/382 (92%)	-0.26	0	100	100	77, 98, 133, 144	0
2	D	355/382 (92%)	-0.19	0	100	100	74, 103, 147, 175	0
3	G	13/15 (86%)	-0.53	0	100	100	128, 164, 217, 229	0
3	I	12/15 (80%)	-0.31	0	100	100	167, 206, 232, 286	0
4	H	14/16 (87%)	-0.19	0	100	100	131, 154, 223, 232	0
4	J	13/16 (81%)	0.35	0	100	100	196, 230, 337, 374	0
All	All	2946/3144 (93%)	0.02	104 (3%)	48	32	68, 106, 219, 374	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	583	GLY	6.3
1	A	584	GLY	6.3
1	A	497	ASN	4.9
1	A	548	ASP	4.8
1	A	547	GLY	4.5
1	A	498	ILE	4.4
1	A	496	LYS	4.3
1	C	490	TRP	4.3
1	A	415	SER	4.1
1	A	429	PHE	4.0
1	C	575	GLU	3.9
1	A	628	LYS	3.7
1	A	518	TYR	3.6
1	A	463	VAL	3.6
1	A	494	GLN	3.6
1	A	495	ALA	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	410	LEU	3.5
1	C	406	GLY	3.4
1	A	499	SER	3.4
1	A	519	LEU	3.4
1	A	685	ASP	3.3
1	A	481	GLN	3.3
1	A	509	VAL	3.3
1	A	546	LEU	3.3
1	A	490	TRP	3.2
1	A	632	GLY	3.2
1	C	576	LEU	3.0
1	A	399	HIS	3.0
1	A	552	LEU	3.0
1	C	454	ASP	3.0
1	A	464	ALA	3.0
1	A	507	GLN	2.9
1	A	1127	ASP	2.9
1	A	247	ALA	2.9
1	A	525	GLU	2.8
1	A	493	PRO	2.8
1	A	630	THR	2.8
1	C	410	LEU	2.8
1	A	446	THR	2.8
1	A	486	LEU	2.7
1	A	563	ASP	2.7
1	C	563	ASP	2.7
1	C	1126	ALA	2.7
1	C	471	ILE	2.7
1	A	417	PRO	2.7
1	C	532	THR	2.7
1	C	628	LYS	2.6
1	C	459	PHE	2.6
1	A	677	ASN	2.6
1	A	527	ARG	2.5
1	A	475	SER	2.5
1	A	425	LEU	2.5
1	A	934	ALA	2.5
1	C	491	LYS	2.5
1	C	517	TYR	2.5
1	A	575	GLU	2.5
1	A	471	ILE	2.4
1	C	431	GLY	2.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	503	CYS	2.4
1	C	451	PHE	2.4
1	A	473	SER	2.4
1	A	629	VAL	2.4
1	A	427	LEU	2.4
1	A	528	GLN	2.4
1	C	522	HIS	2.4
1	A	501	ALA	2.4
1	C	489	GLU	2.3
1	A	465	HIS	2.3
1	C	478	LEU	2.3
1	C	685	ASP	2.3
1	C	407	ILE	2.3
1	A	517	TYR	2.3
1	A	489	GLU	2.2
1	A	562	THR	2.2
1	A	454	ASP	2.2
1	C	455	GLN	2.2
1	A	585	GLU	2.2
1	C	299	ASP	2.2
1	C	435	VAL	2.2
1	A	607	GLY	2.2
1	C	474	ALA	2.2
1	C	493	PRO	2.2
1	C	507	GLN	2.2
1	A	472	THR	2.2
1	A	586	ILE	2.1
1	C	543	ILE	2.1
1	C	476	VAL	2.1
1	A	946	ALA	2.1
1	A	962	ASP	2.1
1	A	474	ALA	2.1
1	A	529	ILE	2.1
1	C	701	ILE	2.1
1	A	533	GLU	2.1
1	A	551	GLY	2.1
1	C	821	LEU	2.1
1	C	546	LEU	2.1
1	A	403	ASP	2.1
1	A	438	LEU	2.1
1	A	565	SER	2.1
1	C	297	LEU	2.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	473	SER	2.0
1	A	502	SER	2.0
1	C	452	VAL	2.0
1	C	677	ASN	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( $\text{\AA}^2$ )	Q<0.9
3	TTD	G	9	40/41	0.89	0.23	-	128,141,161,167	0
3	TTD	I	9	40/41	0.83	0.28	-	164,193,226,236	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.