



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:34 AM GMT

PDB ID : 2HPY  
Title : Crystallographic model of lumirhodopsin  
Authors : Nakamichi, H.; Okada, T.  
Deposited on : 2006-07-18  
Resolution : 2.80 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.

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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

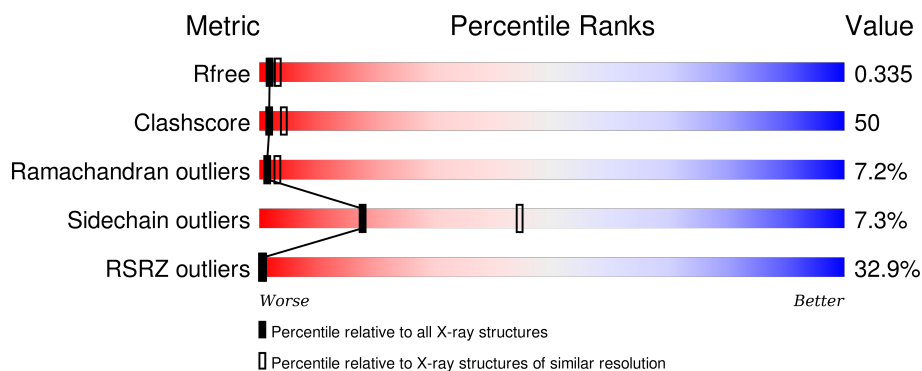
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	349	<div> <div>29%</div> <div>38%</div> <div>53%</div> <div>9%</div> </div>
1	B	349	<div> <div>36%</div> <div>34%</div> <div>55%</div> <div>10%</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
10	HTG	A	1507	-	-	-	X
10	HTG	B	1509	-	-	-	X
6	ZN	B	963	-	-	-	X
7	RET	A	1296	-	-	-	X
7	RET	B	1296	-	-	-	X
8	PLM	A	1322	-	-	-	X
8	PLM	B	1322	-	-	-	X
8	PLM	B	1323	-	-	-	X
8	PLM	B	1407	-	-	-	X

## 2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5948 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 Rhodopsin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			
1	B	349	Total	C	N	O	S	0	0	0
			2749	1818	424	481	26			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	2	Total	C	N	O	0	0
			28	16	2	10		
4	B	2	Total	C	N	O	0	0
			28	16	2	10		

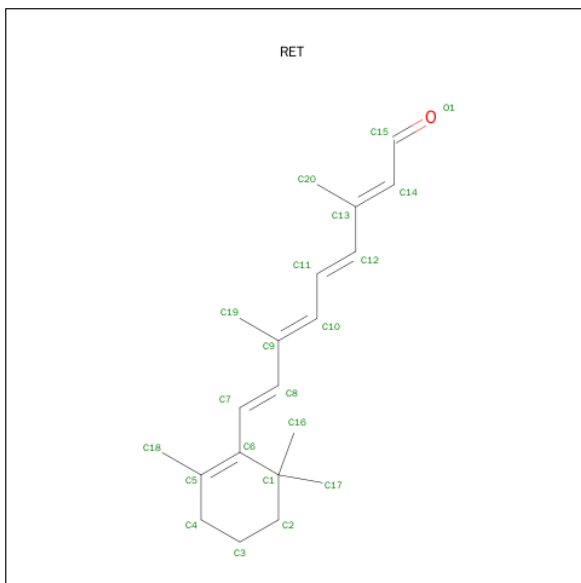
- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	3	Total	Hg	0	0
			3	3		
5	A	3	Total	Hg	0	0
			3	3		

- Molecule 6 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Zn	0	0
			3	3		
6	A	4	Total	Zn	0	0
			4	4		

- Molecule 7 is RETINAL (three-letter code: RET) (formula: C<sub>20</sub>H<sub>28</sub>O).



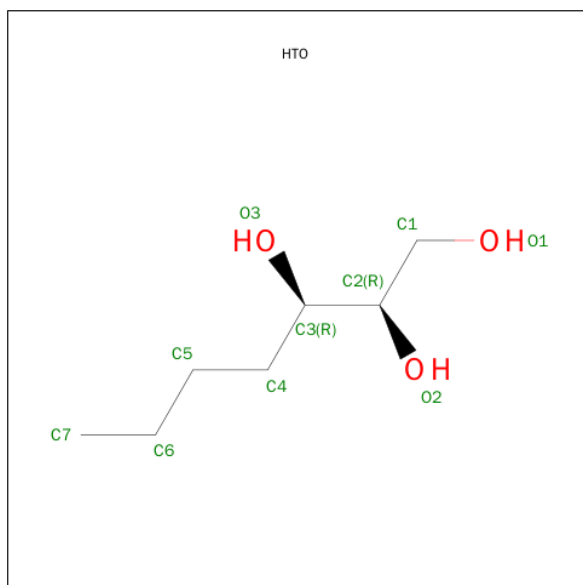
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C	0	0
			20	20		
7	B	1	Total	C	0	0
			20	20		

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: C<sub>16</sub>H<sub>32</sub>O<sub>2</sub>).



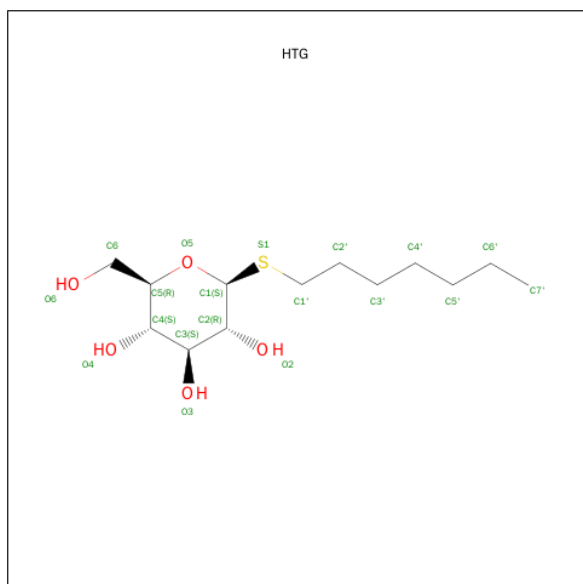
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	16	1		
8	A	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C		0	0
			16	16			
8	A	1	Total	C		0	0
			16	16			

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C<sub>7</sub>H<sub>16</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			10	7	3		

- Molecule 10 is HEPTYL 1-THIOHEXOPYRANOSIDE (three-letter code: HTG) (formula:  $C_{13}H_{26}O_5S$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	O	S	0	0
			19	13	5	1		
10	A	1	Total	C	O	S	0	0
			19	13	5	1		

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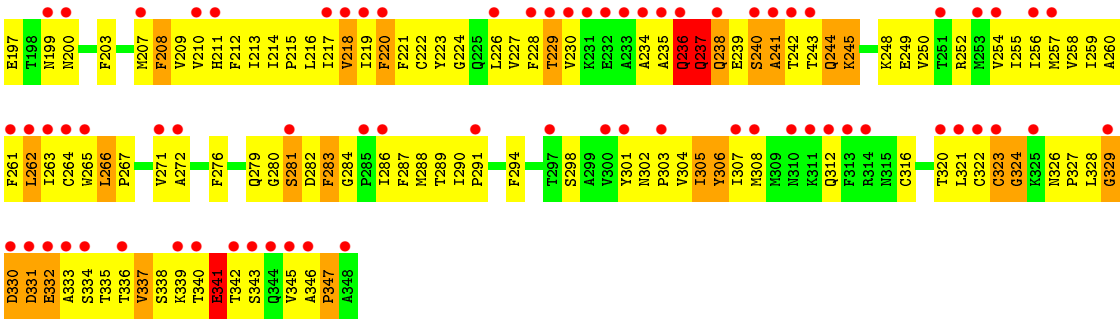
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	A	1	Total	C	O	S	0	0
			19	13	5	1		
10	B	1	Total	C	O	S	0	0
			19	13	5	1		

- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	37	Total	O	0	0
			37	37		
11	B	29	Total	O	0	0
			29	29		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.72Å 96.72Å 150.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 35.05 – 2.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.80) 87.3 (35.05-2.79)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.88 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.218 , 0.238 0.346 , 0.335	Depositor DCC
$R_{free}$ test set	1530 reflections (5.41%)	DCC
Wilson B-factor (Å <sup>2</sup> )	64.8	Xtriage
Anisotropy	0.474	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.15 , 33.5	EDS
Estimated twinning fraction	0.138 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 29870 reflections	Xtriage
$F_o, F_c$ correlation	0.79	EDS
Total number of atoms	5948	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% 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: HTG, ZN, BMA, NAG, ACE, HTO, RET, PLM, HG, MAN

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	0.65	0/2831	0.70	0/3859
1	B	0.65	0/2831	0.68	0/3859
All	All	0.65	0/5662	0.69	0/7718

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	306	TYR	Sidechain

### 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	2749	0	2709	257	1
1	B	2749	0	2709	327	0
2	A	39	0	34	1	0
3	B	50	0	43	0	0
4	A	28	0	25	0	0
4	B	28	0	25	1	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	4	0	0	0	0
6	B	3	0	0	0	0
7	A	20	0	27	2	0
7	B	20	0	27	2	0
8	A	50	0	89	7	0
8	B	50	0	89	4	0
9	B	10	0	16	1	0
10	A	38	0	52	3	0
10	B	38	0	52	4	1
11	A	37	0	0	6	0
11	B	29	0	0	10	0
All	All	5948	0	5897	584	1

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 50.

All (584) 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:B:298:SER:HA	1:B:301:TYR:CE2	1.81	1.15
1:A:298:SER:HA	1:A:301:TYR:CE2	1.82	1.15
1:A:67:LYS:HB2	1:A:337:VAL:HB	1.38	1.02
1:B:64:GLN:HG3	1:B:339:LYS:HE2	1.39	1.02
1:A:345:VAL:HG12	1:A:347:PRO:HD3	1.45	0.98
1:B:337:VAL:HB	1:B:343:SER:HA	1.45	0.97
1:A:94:THR:HB	1:A:113:GLU:OE2	1.63	0.97
1:B:239:GLU:HB2	1:B:245:LYS:HD2	1.44	0.95
1:B:122:GLU:HG3	1:B:167:CYS:SG	2.06	0.94
1:A:65:HIS:ND1	1:A:338:SER:HA	1.81	0.94
1:A:88:PHE:HB3	8:B:1323:PLM:HB1	1.49	0.94
1:A:50:LEU:HD21	1:B:50:LEU:HB2	1.50	0.93
1:B:245:LYS:HA	1:B:245:LYS:HE3	1.51	0.92
1:A:239:GLU:HG2	1:A:248:LYS:NZ	1.85	0.91
1:B:298:SER:HB2	11:B:2036:HOH:O	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:LYS:NZ	1:B:248:LYS:HD2	1.91	0.86
1:A:316:CYS:SG	1:A:337:VAL:HG13	2.15	0.85
1:A:332:GLU:C	1:A:334:SER:H	1.77	0.85
1:B:183:MET:HE3	1:B:289:THR:HG21	1.57	0.84
1:A:65:HIS:HB3	1:A:337:VAL:HG22	1.60	0.84
1:B:157:VAL:O	1:B:161:TRP:HB2	1.78	0.83
1:B:346:ALA:N	1:B:347:PRO:HD3	1.93	0.83
1:B:298:SER:HA	1:B:301:TYR:HE2	1.40	0.83
1:A:298:SER:HA	1:A:301:TYR:CD2	2.14	0.83
1:B:271:VAL:HG21	1:B:291:PRO:HG3	1.61	0.82
1:B:72:LEU:HD22	1:B:250:VAL:HG13	1.59	0.82
1:B:67:LYS:HB3	1:B:337:VAL:CG1	2.10	0.82
1:B:267:PRO:HG2	11:B:2019:HOH:O	1.80	0.81
1:B:210:VAL:HA	1:B:214:ILE:HD12	1.60	0.81
1:A:341:GLU:CG	1:A:342:THR:H	1.94	0.81
1:A:77:LEU:O	1:A:81:VAL:HG23	1.80	0.81
7:A:1296:RET:H181	7:A:1296:RET:H8	1.63	0.80
1:A:307:ILE:O	1:A:307:ILE:HG22	1.80	0.80
1:A:298:SER:HA	1:A:301:TYR:HE2	1.42	0.80
1:A:326:ASN:O	1:A:328:LEU:HD22	1.83	0.79
1:A:239:GLU:HG2	1:A:248:LYS:HZ1	1.46	0.79
1:B:87:VAL:HA	1:B:91:PHE:HB2	1.65	0.79
1:A:90:GLY:O	1:A:94:THR:HG22	1.83	0.78
1:A:253:MET:HE1	1:A:306:TYR:HA	1.65	0.78
1:A:341:GLU:HG3	1:A:342:THR:N	1.98	0.77
1:B:312:GLN:HA	1:B:332:GLU:HG2	1.65	0.77
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.65	0.77
1:A:161:TRP:O	1:A:165:LEU:HB2	1.84	0.77
1:A:267:PRO:HG2	11:A:964:HOH:O	1.84	0.77
1:B:67:LYS:HE3	1:B:312:GLN:HG3	1.67	0.77
1:A:245:LYS:HZ2	1:A:245:LYS:HA	1.49	0.77
1:A:245:LYS:NZ	1:A:245:LYS:HA	2.00	0.77
1:A:87:VAL:O	1:A:91:PHE:HB2	1.85	0.76
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.67	0.76
1:A:112:LEU:HD22	1:A:116:PHE:HE2	1.51	0.76
1:B:332:GLU:HB3	1:B:335:THR:O	1.85	0.76
1:B:248:LYS:O	1:B:252:ARG:HG3	1.83	0.76
1:B:338:SER:HB2	1:B:341:GLU:HG3	1.66	0.76
1:A:345:VAL:HG12	1:A:347:PRO:CD	2.16	0.75
1:B:209:VAL:HA	1:B:213:ILE:HB	1.68	0.75
1:B:67:LYS:H	1:B:337:VAL:CG2	2.00	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:LEU:N	1:A:267:PRO:HD2	2.02	0.74
1:A:67:LYS:HB2	1:A:337:VAL:CB	2.15	0.73
1:B:213:ILE:O	1:B:217:ILE:HG13	1.87	0.73
1:B:230:VAL:HG23	1:B:248:LYS:HD3	1.70	0.73
1:A:308:MET:HE1	1:B:42:ALA:N	2.04	0.73
1:B:337:VAL:HA	1:B:342:THR:O	1.89	0.72
1:B:139:VAL:HG11	1:B:230:VAL:HG12	1.71	0.72
1:A:253:MET:CE	1:A:306:TYR:HA	2.19	0.72
1:B:96:TYR:HE2	1:B:104:VAL:CG2	2.03	0.72
1:B:337:VAL:CB	1:B:343:SER:HA	2.19	0.72
1:B:94:THR:CG2	1:B:113:GLU:HG2	2.19	0.72
1:A:341:GLU:OE1	1:A:342:THR:HG22	1.88	0.72
1:A:150:GLU:O	1:A:154:ILE:HG13	1.90	0.72
1:A:85:PHE:O	1:A:89:GLY:HA3	1.89	0.71
1:A:325:LYS:HE3	1:A:341:GLU:OE1	1.90	0.71
7:B:1296:RET:H181	7:B:1296:RET:H8	1.73	0.71
1:B:126:TRP:CH2	1:B:215:PRO:HG3	2.25	0.71
1:B:234:ALA:HA	1:B:245:LYS:NZ	2.05	0.71
1:A:100:HIS:CE1	10:B:1509:HTG:O6	2.44	0.71
1:A:212:PHE:C	1:A:215:PRO:HD2	2.11	0.71
1:B:237:GLN:NE2	1:B:237:GLN:H	1.89	0.71
1:A:341:GLU:HG3	1:A:342:THR:H	1.55	0.70
1:A:302:ASN:HB2	11:A:2017:HOH:O	1.89	0.70
1:B:303:PRO:O	1:B:307:ILE:HG13	1.91	0.70
1:A:254:VAL:O	1:A:258:VAL:HG23	1.90	0.70
1:A:326:ASN:HD21	1:A:328:LEU:HD11	1.55	0.70
1:B:67:LYS:N	1:B:337:VAL:HG21	2.06	0.70
1:B:74:TYR:HE2	1:B:150:GLU:HG2	1.57	0.70
1:B:195:HIS:HB3	1:B:200:ASN:ND2	2.07	0.70
1:B:64:GLN:HG3	1:B:339:LYS:HB2	1.74	0.69
1:B:301:TYR:HE1	11:B:2008:HOH:O	1.75	0.69
1:B:257:MET:HG2	1:B:305:ILE:HG21	1.74	0.69
1:B:64:GLN:CG	1:B:339:LYS:HB2	2.22	0.69
1:B:77:LEU:O	1:B:81:VAL:HG23	1.92	0.69
1:B:307:ILE:HG22	1:B:307:ILE:O	1.92	0.69
1:A:67:LYS:H	1:A:337:VAL:HG23	1.57	0.69
1:B:338:SER:HB2	1:B:341:GLU:CG	2.23	0.69
1:B:59:LEU:O	1:B:63:VAL:HG23	1.93	0.68
1:B:54:ILE:HD11	1:B:303:PRO:HB2	1.73	0.68
1:B:169:ALA:HB3	1:B:170:PRO:HD3	1.75	0.68
1:B:239:GLU:HB3	1:B:244:GLN:HE22	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LEU:HD12	1:B:77:LEU:HD11	1.75	0.68
1:A:212:PHE:O	1:A:215:PRO:HD2	1.94	0.68
1:B:337:VAL:HA	1:B:342:THR:C	2.13	0.68
1:B:337:VAL:HG23	1:B:338:SER:N	2.09	0.68
1:B:129:VAL:HG13	1:B:218:VAL:HG11	1.74	0.68
1:B:143:MET:HG2	1:B:146:PHE:HB3	1.76	0.68
1:A:65:HIS:ND1	1:A:337:VAL:O	2.27	0.68
1:A:167:CYS:HB2	1:A:207:MET:SD	2.34	0.68
1:B:238:GLN:HG3	1:B:241:ALA:H	1.59	0.68
1:B:143:MET:HG2	1:B:146:PHE:CB	2.24	0.67
1:A:191:TYR:O	1:A:279:GLN:HG2	1.93	0.67
1:A:341:GLU:CG	1:A:342:THR:N	2.57	0.67
1:B:94:THR:HG22	1:B:113:GLU:CG	2.25	0.67
1:B:94:THR:HG22	1:B:113:GLU:HG2	1.75	0.67
1:A:213:ILE:O	1:A:217:ILE:HG12	1.93	0.67
1:A:75:ILE:O	1:A:79:LEU:HB2	1.95	0.67
1:B:332:GLU:OE2	1:B:334:SER:HB2	1.94	0.67
1:A:332:GLU:C	1:A:334:SER:N	2.49	0.66
1:B:129:VAL:CG1	1:B:218:VAL:HG11	2.25	0.66
1:A:70:THR:H	1:A:73:ASN:HD22	1.42	0.66
1:B:129:VAL:HG13	1:B:218:VAL:CG1	2.26	0.66
1:A:181:GLU:OE2	1:A:188:GLY:HA3	1.96	0.66
1:B:65:HIS:HB2	1:B:68:LEU:HD12	1.77	0.66
1:A:239:GLU:HG2	1:A:248:LYS:HZ2	1.61	0.66
1:B:54:ILE:CD1	1:B:303:PRO:HB2	2.25	0.66
1:B:67:LYS:HB3	1:B:337:VAL:HG11	1.78	0.65
1:B:67:LYS:HD3	1:B:337:VAL:HG13	1.78	0.65
1:A:97:THR:HG21	1:A:185:CYS:HA	1.77	0.65
1:A:238:GLN:HA	1:A:242:THR:HA	1.79	0.65
1:A:137:VAL:HA	1:A:142:PRO:CD	2.27	0.65
1:A:239:GLU:HB3	1:A:244:GLN:CD	2.17	0.65
1:B:266:LEU:N	1:B:267:PRO:HD2	2.11	0.65
1:A:325:LYS:HE2	1:A:327:PRO:HD3	1.79	0.65
1:A:99:LEU:HD11	10:B:1509:HTG:H3'1	1.77	0.65
1:B:237:GLN:O	1:B:238:GLN:HB3	1.97	0.65
1:A:103:PHE:CE2	1:A:180:PRO:HB3	2.31	0.65
1:A:300:VAL:O	1:A:302:ASN:N	2.30	0.64
1:A:97:THR:CG2	1:A:185:CYS:HA	2.27	0.64
1:A:338:SER:HB2	1:A:341:GLU:HG2	1.79	0.64
1:B:67:LYS:HZ1	1:B:332:GLU:HG3	1.63	0.64
1:B:195:HIS:CE1	1:B:197:GLU:HB3	2.32	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:85:PHE:O	1:B:89:GLY:N	2.29	0.64
1:B:131:LEU:HD23	1:B:254:VAL:HG13	1.80	0.63
1:B:238:GLN:HA	1:B:242:THR:HA	1.79	0.63
1:A:337:VAL:O	1:A:338:SER:OG	2.17	0.63
1:A:235:ALA:HB3	1:A:239:GLU:OE1	1.98	0.63
1:A:103:PHE:CZ	1:A:187:CYS:SG	2.92	0.63
1:A:326:ASN:OD1	1:A:328:LEU:HD13	1.99	0.63
1:A:110:CYS:HB3	11:A:2045:HOH:O	1.99	0.63
1:A:227:VAL:HG13	1:A:228:PHE:N	2.13	0.63
1:B:199:ASN:ND2	11:B:2005:HOH:O	2.31	0.62
1:A:283:PHE:HB2	1:A:287:PHE:CD2	2.35	0.62
1:A:303:PRO:O	1:A:307:ILE:HG13	2.00	0.62
1:A:271:VAL:HG21	1:A:291:PRO:HG3	1.80	0.62
1:A:304:VAL:O	1:A:308:MET:CG	2.47	0.62
1:A:322:CYS:O	1:A:324:GLY:N	2.32	0.62
1:A:57:LEU:HD23	8:A:1322:PLM:HD2	1.81	0.62
1:A:96:TYR:HE2	1:A:104:VAL:HG21	1.65	0.61
1:B:6:GLY:HA3	1:B:9:PHE:CZ	2.34	0.61
1:B:150:GLU:O	1:B:154:ILE:HD13	2.00	0.61
1:A:35:TRP:HZ3	1:A:39:MET:SD	2.23	0.61
1:A:342:THR:O	1:A:342:THR:HG23	2.01	0.61
1:A:234:ALA:HB2	1:A:248:LYS:HG2	1.82	0.61
1:A:75:ILE:HG21	1:A:131:LEU:HD13	1.82	0.61
1:B:96:TYR:HE2	1:B:104:VAL:HG22	1.66	0.61
1:B:236:GLN:HB2	1:B:237:GLN:NE2	2.15	0.61
1:B:302:ASN:HB2	11:B:2016:HOH:O	2.00	0.61
1:B:337:VAL:HB	1:B:343:SER:CA	2.26	0.60
1:A:67:LYS:H	1:A:337:VAL:CG2	2.13	0.60
1:B:113:GLU:OE1	1:B:187:CYS:HB2	2.01	0.60
1:A:224:GLY:O	1:A:227:VAL:HG12	2.01	0.60
1:B:76:LEU:HD13	1:B:306:TYR:CG	2.36	0.60
1:A:65:HIS:HB3	1:A:337:VAL:CG2	2.31	0.60
1:A:253:MET:HE1	1:A:306:TYR:HD1	1.67	0.60
1:A:180:PRO:HA	1:A:186:SER:O	2.00	0.60
1:A:312:GLN:NE2	1:A:337:VAL:HG12	2.16	0.60
1:A:59:LEU:O	1:A:59:LEU:HD12	2.01	0.60
1:B:327:PRO:HB2	1:B:331:ASP:OD2	2.02	0.60
1:B:75:ILE:HG13	1:B:131:LEU:CD1	2.32	0.60
1:B:143:MET:HA	1:B:143:MET:CE	2.32	0.60
1:A:93:THR:O	1:A:96:TYR:N	2.34	0.59
1:A:59:LEU:HD13	1:A:77:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:96:TYR:HE2	1:B:104:VAL:HG21	1.67	0.59
1:B:54:ILE:HG23	1:B:55:ASN:N	2.17	0.59
1:B:195:HIS:HB3	1:B:200:ASN:HD21	1.67	0.59
1:B:64:GLN:HG3	1:B:339:LYS:CE	2.24	0.59
1:A:137:VAL:HA	1:A:142:PRO:HD2	1.85	0.59
1:A:65:HIS:ND1	1:A:338:SER:CA	2.61	0.59
1:A:66:LYS:HD2	1:A:66:LYS:N	2.18	0.59
1:B:46:LEU:HD12	8:B:1407:PLM:HD2	1.85	0.59
1:B:67:LYS:HB3	1:B:337:VAL:CG2	2.32	0.59
1:B:122:GLU:HA	1:B:122:GLU:OE1	2.02	0.59
1:B:143:MET:HA	1:B:143:MET:HE2	1.84	0.59
1:A:307:ILE:CG2	1:A:307:ILE:O	2.51	0.59
1:B:119:LEU:HD23	1:B:120:GLY:N	2.17	0.59
1:B:245:LYS:HZ1	1:B:248:LYS:HD2	1.68	0.58
1:A:239:GLU:HB3	1:A:244:GLN:NE2	2.18	0.58
1:A:212:PHE:HB2	7:A:1296:RET:H32	1.84	0.58
1:B:220:PHE:O	1:B:223:TYR:HB3	2.04	0.58
1:B:183:MET:CE	1:B:289:THR:HG21	2.32	0.58
1:A:210:VAL:HG12	1:A:210:VAL:O	2.02	0.58
1:B:67:LYS:NZ	1:B:332:GLU:HG3	2.17	0.58
1:A:304:VAL:O	1:A:308:MET:HG2	2.04	0.58
1:B:67:LYS:NZ	1:B:336:THR:HA	2.18	0.58
1:B:234:ALA:HB1	1:B:245:LYS:HE2	1.86	0.58
1:B:241:ALA:HB1	1:B:243:THR:HG22	1.86	0.58
1:A:6:GLY:HA3	1:A:9:PHE:CZ	2.38	0.58
1:B:36:GLN:O	1:B:39:MET:HB2	2.04	0.58
1:A:178:TYR:HA	1:A:188:GLY:O	2.04	0.57
1:B:332:GLU:O	1:B:333:ALA:HB3	2.04	0.57
1:A:218:VAL:O	1:A:218:VAL:HG12	2.04	0.57
1:B:180:PRO:HG2	11:B:2023:HOH:O	2.03	0.57
1:B:302:ASN:HB2	1:B:303:PRO:HD3	1.86	0.57
1:B:48:ILE:HD12	1:B:95:LEU:HD22	1.85	0.57
1:A:192:TYR:O	1:A:279:GLN:HB3	2.03	0.57
1:A:189:ILE:CG2	1:A:190:ASP:N	2.68	0.57
1:A:326:ASN:ND2	1:A:328:LEU:HD21	2.19	0.56
1:B:312:GLN:HA	1:B:332:GLU:CG	2.34	0.56
1:B:239:GLU:HB3	1:B:244:GLN:NE2	2.19	0.56
1:B:326:ASN:O	1:B:328:LEU:HD22	2.04	0.56
1:B:283:PHE:N	1:B:283:PHE:CD1	2.74	0.56
1:B:67:LYS:HZ2	1:B:336:THR:HA	1.70	0.56
1:B:239:GLU:HB2	1:B:245:LYS:CD	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:THR:O	1:B:95:LEU:HB3	2.05	0.56
1:B:170:PRO:HB2	1:B:171:PRO:HD3	1.88	0.56
1:B:259:ILE:HG22	1:B:263:ILE:HD12	1.85	0.56
1:A:250:VAL:O	1:A:254:VAL:HG23	2.04	0.56
1:A:65:HIS:HB2	1:A:68:LEU:HD12	1.86	0.56
1:B:226:LEU:HD12	1:B:226:LEU:N	2.20	0.56
1:B:167:CYS:HB2	1:B:211:HIS:NE2	2.21	0.56
1:A:70:THR:HG23	1:A:73:ASN:ND2	2.21	0.56
1:A:175:TRP:CZ2	1:A:203:PHE:HA	2.41	0.56
1:A:298:SER:CA	1:A:301:TYR:CE2	2.75	0.56
1:A:230:VAL:HG23	1:A:248:LYS:HE2	1.88	0.56
1:B:298:SER:HA	1:B:301:TYR:CD2	2.37	0.55
1:B:129:VAL:HG22	1:B:219:ILE:HG13	1.88	0.55
1:B:244:GLN:O	1:B:248:LYS:HG3	2.05	0.55
1:B:345:VAL:C	1:B:347:PRO:HD3	2.26	0.55
8:A:1322:PLM:H61	1:B:88:PHE:HE1	1.69	0.55
1:A:346:ALA:N	1:A:347:PRO:HD3	2.21	0.55
1:B:234:ALA:HA	1:B:245:LYS:HZ3	1.71	0.55
1:B:245:LYS:CE	1:B:248:LYS:HD2	2.36	0.55
1:A:338:SER:CB	1:A:341:GLU:HG2	2.36	0.55
1:B:57:LEU:HD21	1:B:321:LEU:HD21	1.89	0.55
1:B:326:ASN:HB3	1:B:328:LEU:CD2	2.37	0.55
1:B:33:GLU:HB2	1:B:36:GLN:HG3	1.89	0.55
1:B:212:PHE:O	1:B:216:LEU:HD23	2.07	0.54
1:B:208:PHE:O	1:B:213:ILE:HD12	2.06	0.54
1:A:103:PHE:HE2	1:A:180:PRO:HB3	1.70	0.54
1:B:135:ARG:HA	1:B:135:ARG:NE	2.22	0.54
1:A:311:LYS:HG2	1:A:331:ASP:O	2.06	0.54
1:B:337:VAL:HA	1:B:342:THR:HG23	1.90	0.54
1:B:78:ASN:O	1:B:81:VAL:N	2.40	0.54
1:A:267:PRO:O	1:A:271:VAL:HG23	2.07	0.54
1:B:143:MET:CG	1:B:146:PHE:HB3	2.37	0.54
1:B:136:TYR:HA	1:B:226:LEU:HD11	1.88	0.54
1:B:238:GLN:HG3	1:B:241:ALA:N	2.21	0.54
1:A:79:LEU:HD11	1:A:124:ALA:HA	1.90	0.54
1:A:267:PRO:HA	10:A:1507:HTG:H6'1	1.90	0.54
1:B:67:LYS:CE	1:B:312:GLN:HG3	2.35	0.54
1:B:234:ALA:HA	1:B:245:LYS:HZ2	1.73	0.54
1:A:139:VAL:HG11	1:A:226:LEU:HG	1.90	0.54
1:A:157:VAL:O	1:A:161:TRP:HD1	1.91	0.54
1:B:237:GLN:H	1:B:237:GLN:HE21	1.55	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:332:GLU:O	1:A:334:SER:N	2.42	0.53
1:A:237:GLN:O	1:A:238:GLN:HB3	2.07	0.53
1:A:232:GLU:HA	1:A:252:ARG:HD3	1.91	0.53
1:A:85:PHE:O	1:A:89:GLY:CA	2.57	0.53
1:B:288:MET:HG3	1:B:288:MET:O	2.06	0.53
1:A:227:VAL:CG1	1:A:228:PHE:N	2.71	0.53
1:A:311:LYS:CE	1:A:330:ASP:HB2	2.38	0.53
1:B:245:LYS:HZ3	1:B:248:LYS:HD2	1.71	0.53
1:B:326:ASN:C	1:B:328:LEU:HD22	2.29	0.53
1:B:263:ILE:O	1:B:294:PHE:HE2	1.92	0.53
1:B:54:ILE:O	1:B:57:LEU:HB3	2.09	0.53
1:A:266:LEU:N	1:A:267:PRO:CD	2.71	0.53
1:A:311:LYS:O	1:A:315:ASN:ND2	2.40	0.53
1:B:283:PHE:HB2	1:B:287:PHE:CD2	2.44	0.53
1:B:64:GLN:HG2	1:B:339:LYS:HB2	1.91	0.53
1:B:322:CYS:HA	8:B:1322:PLM:O1	2.08	0.53
1:A:53:PRO:O	1:A:57:LEU:HB2	2.09	0.53
1:B:139:VAL:HG21	1:B:226:LEU:HD23	1.92	0.52
1:B:238:GLN:HG3	1:B:241:ALA:CA	2.39	0.52
1:B:332:GLU:CB	1:B:335:THR:O	2.57	0.52
1:B:235:ALA:HB3	1:B:239:GLU:OE1	2.09	0.52
1:A:300:VAL:O	1:A:303:PRO:HD2	2.08	0.52
1:A:321:LEU:HD13	8:A:1322:PLM:H72	1.91	0.52
1:B:283:PHE:HB2	1:B:287:PHE:HD2	1.73	0.52
1:B:286:ILE:O	1:B:290:ILE:HG12	2.09	0.52
1:B:221:PHE:O	1:B:224:GLY:N	2.37	0.52
1:A:96:TYR:CE2	1:A:104:VAL:HG21	2.43	0.52
1:B:139:VAL:CG1	1:B:230:VAL:HG12	2.39	0.52
1:B:207:MET:SD	1:B:211:HIS:HD2	2.33	0.52
1:B:103:PHE:CZ	1:B:187:CYS:SG	3.03	0.52
1:B:32:ALA:HB1	1:B:36:GLN:OE1	2.10	0.52
1:A:158:ALA:O	1:A:162:VAL:HG23	2.10	0.52
1:B:337:VAL:CA	1:B:342:THR:HG23	2.40	0.52
1:B:129:VAL:HG22	1:B:219:ILE:CG1	2.40	0.52
1:A:237:GLN:CD	1:A:237:GLN:H	2.14	0.51
1:A:156:GLY:O	1:A:159:PHE:HB3	2.10	0.51
1:B:129:VAL:C	1:B:131:LEU:N	2.64	0.51
1:A:133:ILE:O	1:A:136:TYR:N	2.44	0.51
1:B:332:GLU:OE1	1:B:332:GLU:O	2.29	0.51
1:A:139:VAL:HG11	1:A:230:VAL:HG12	1.91	0.51
1:A:169:ALA:N	1:A:170:PRO:CD	2.73	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:146:PHE:HE1	1:B:152:HIS:NE2	2.09	0.51
2:A:504:NAG:C7	2:A:505:NAG:H61	2.40	0.51
1:B:67:LYS:HZ2	1:B:335:THR:C	2.14	0.51
1:B:284:GLY:O	1:B:287:PHE:HB3	2.10	0.51
1:B:239:GLU:CB	1:B:244:GLN:HE22	2.23	0.51
1:A:300:VAL:C	1:A:302:ASN:H	2.14	0.51
1:B:171:PRO:HA	1:B:175:TRP:O	2.11	0.51
1:B:35:TRP:O	1:B:39:MET:HG2	2.11	0.51
1:B:50:LEU:C	1:B:50:LEU:CD2	2.79	0.50
1:B:171:PRO:HG2	1:B:189:ILE:HD11	1.92	0.50
1:B:230:VAL:HG23	1:B:248:LYS:CD	2.39	0.50
1:A:239:GLU:HB3	1:A:244:GLN:OE1	2.10	0.50
1:A:251:THR:C	1:A:253:MET:N	2.64	0.50
8:A:1322:PLM:H91	1:B:49:MET:SD	2.51	0.50
1:B:170:PRO:HB3	1:B:175:TRP:HB3	1.94	0.50
1:A:110:CYS:SG	1:A:180:PRO:HD3	2.51	0.50
1:A:52:PHE:HB3	1:A:53:PRO:CD	2.42	0.50
1:A:67:LYS:HB2	1:A:337:VAL:CG2	2.42	0.50
1:A:36:GLN:O	1:A:39:MET:HB2	2.11	0.50
1:A:44:MET:HB2	1:A:95:LEU:HD13	1.94	0.50
1:A:104:VAL:C	1:A:106:GLY:H	2.16	0.50
1:A:77:LEU:O	1:A:77:LEU:HD12	2.12	0.50
1:A:308:MET:HE1	1:B:41:ALA:C	2.32	0.50
1:B:330:ASP:O	1:B:331:ASP:O	2.29	0.50
1:A:59:LEU:O	1:A:63:VAL:HG23	2.12	0.50
1:A:304:VAL:O	1:A:308:MET:HG3	2.11	0.49
1:B:64:GLN:HA	1:B:339:LYS:HD3	1.93	0.49
1:B:123:ILE:HG13	1:B:164:ALA:HB3	1.94	0.49
1:A:247:GLU:HA	1:A:247:GLU:OE1	2.11	0.49
1:B:301:TYR:O	1:B:305:ILE:HG13	2.12	0.49
1:B:340:THR:HG23	1:B:341:GLU:N	2.27	0.49
1:B:67:LYS:HZ2	1:B:336:THR:CA	2.25	0.49
1:B:346:ALA:N	1:B:347:PRO:CD	2.71	0.49
1:A:88:PHE:HA	1:A:92:THR:HG23	1.94	0.49
1:B:129:VAL:C	1:B:131:LEU:H	2.15	0.49
1:A:286:ILE:O	1:A:290:ILE:HG12	2.13	0.49
1:A:283:PHE:HB2	1:A:287:PHE:HD2	1.76	0.49
1:B:227:VAL:HG13	1:B:228:PHE:N	2.26	0.49
1:A:139:VAL:HG21	1:A:230:VAL:HG11	1.95	0.49
1:A:276:PHE:O	1:A:279:GLN:HG3	2.13	0.49
1:B:227:VAL:CG1	1:B:228:PHE:N	2.75	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLU:HB3	1:B:244:GLN:OE1	2.13	0.49
1:B:133:ILE:N	1:B:133:ILE:HD13	2.28	0.49
1:B:67:LYS:N	1:B:337:VAL:CG2	2.66	0.48
1:A:42:ALA:O	1:A:45:PHE:HB3	2.13	0.48
1:A:91:PHE:HA	1:A:94:THR:CG2	2.43	0.48
1:B:78:ASN:OD1	1:B:157:VAL:HG13	2.12	0.48
9:B:1401:HTO:H72	10:B:1509:HTG:H3'2	1.95	0.48
1:A:240:SER:O	1:A:241:ALA:HB2	2.12	0.48
1:A:12:PRO:HD3	11:A:2064:HOH:O	2.11	0.48
1:B:265:TRP:C	1:B:267:PRO:HD2	2.33	0.48
1:A:321:LEU:C	1:A:323:CYS:H	2.16	0.48
1:B:93:THR:O	1:B:96:TYR:HB3	2.12	0.48
1:B:78:ASN:O	1:B:79:LEU:C	2.51	0.48
1:A:245:LYS:NZ	1:A:245:LYS:CA	2.76	0.48
1:B:282:ASP:HB2	4:B:805:NAG:H62	1.96	0.48
1:A:153:ALA:O	1:A:157:VAL:HG23	2.13	0.48
1:B:104:VAL:C	1:B:106:GLY:H	2.17	0.48
1:B:283:PHE:HD1	1:B:283:PHE:H	1.59	0.48
1:B:259:ILE:C	1:B:261:PHE:H	2.17	0.48
1:B:123:ILE:HG13	1:B:164:ALA:CB	2.44	0.48
1:B:67:LYS:HB3	1:B:337:VAL:HG13	1.91	0.48
1:A:126:TRP:NE1	1:A:163:MET:HB3	2.28	0.48
1:A:302:ASN:CB	1:A:303:PRO:HD3	2.43	0.48
1:B:281:SER:OG	1:B:282:ASP:N	2.47	0.48
1:B:136:TYR:CE2	1:B:142:PRO:HG2	2.49	0.48
1:B:321:LEU:C	1:B:323:CYS:H	2.16	0.48
1:A:135:ARG:HA	1:A:135:ARG:NE	2.29	0.48
1:B:126:TRP:NE1	1:B:163:MET:HB3	2.29	0.47
1:A:232:GLU:HB3	1:A:252:ARG:HD3	1.96	0.47
1:B:151:ASN:HD21	1:B:152:HIS:CE1	2.32	0.47
1:B:261:PHE:C	1:B:263:ILE:H	2.17	0.47
1:B:280:GLY:O	1:B:281:SER:O	2.32	0.47
1:A:311:LYS:HE3	1:A:331:ASP:O	2.15	0.47
1:B:238:GLN:HB2	1:B:242:THR:OG1	2.14	0.47
1:B:67:LYS:HD3	1:B:336:THR:C	2.35	0.47
1:A:59:LEU:C	1:A:59:LEU:HD12	2.34	0.47
1:A:311:LYS:NZ	1:A:330:ASP:HB2	2.29	0.47
1:B:67:LYS:H	1:B:337:VAL:HG22	1.77	0.47
1:A:94:THR:HB	1:A:113:GLU:CD	2.30	0.47
1:B:126:TRP:HA	1:B:126:TRP:CE3	2.48	0.47
1:A:175:TRP:NE1	1:A:203:PHE:HB2	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:SER:CA	1:A:301:TYR:HE2	2.20	0.47
1:B:238:GLN:HG3	1:B:241:ALA:C	2.34	0.47
1:B:240:SER:O	1:B:241:ALA:CB	2.62	0.47
1:A:232:GLU:CA	1:A:252:ARG:HD3	2.45	0.47
1:A:122:GLU:HG3	1:A:167:CYS:SG	2.54	0.47
1:B:200:ASN:HB3	11:B:2044:HOH:O	2.14	0.47
1:B:76:LEU:HD13	1:B:306:TYR:CD1	2.50	0.47
1:B:178:TYR:HA	1:B:188:GLY:O	2.15	0.47
1:B:126:TRP:CZ3	1:B:215:PRO:HG3	2.50	0.47
1:B:8:ASN:HA	1:B:8:ASN:HD22	1.50	0.47
1:A:278:HIS:O	1:A:280:GLY:N	2.48	0.47
1:B:64:GLN:HA	1:B:339:LYS:NZ	2.29	0.47
1:A:200:ASN:O	1:A:204:VAL:HG23	2.15	0.47
1:A:148:PHE:HA	1:A:152:HIS:ND1	2.30	0.47
1:B:154:ILE:HD12	1:B:154:ILE:N	2.30	0.46
1:B:328:LEU:O	1:B:329:GLY:C	2.53	0.46
8:B:1322:PLM:H52	8:B:1323:PLM:H61	1.97	0.46
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.39	0.46
1:B:68:LEU:HB3	1:B:73:ASN:HD22	1.80	0.46
1:A:253:MET:HE1	1:A:306:TYR:CD1	2.50	0.46
1:A:231:LYS:HB2	1:A:231:LYS:NZ	2.30	0.46
1:B:341:GLU:OE1	1:B:342:THR:HG22	2.15	0.46
1:A:300:VAL:C	1:A:302:ASN:N	2.69	0.46
1:B:150:GLU:O	1:B:154:ILE:CD1	2.63	0.46
1:A:130:VAL:HG12	1:A:130:VAL:O	2.14	0.46
1:A:251:THR:O	1:A:253:MET:N	2.49	0.46
1:B:304:VAL:O	1:B:308:MET:HG3	2.16	0.46
1:B:58:THR:O	1:B:59:LEU:C	2.52	0.46
1:A:130:VAL:HG21	1:A:160:THR:CG2	2.45	0.46
1:A:70:THR:HG23	1:A:73:ASN:HD22	1.80	0.46
1:B:132:ALA:O	1:B:222:CYS:SG	2.70	0.46
1:B:336:THR:O	1:B:337:VAL:O	2.33	0.46
1:B:160:THR:O	1:B:162:VAL:N	2.49	0.46
1:B:165:LEU:C	1:B:167:CYS:H	2.19	0.46
1:A:267:PRO:HA	10:A:1507:HTG:C6'	2.45	0.46
1:A:231:LYS:HZ2	1:A:233:ALA:HB3	1.81	0.46
1:B:33:GLU:O	1:B:36:GLN:HB2	2.16	0.46
1:B:160:THR:C	1:B:162:VAL:H	2.20	0.45
1:A:251:THR:O	1:A:252:ARG:C	2.55	0.45
1:A:321:LEU:HD13	8:A:1322:PLM:H51	1.97	0.45
1:B:64:GLN:HA	1:B:339:LYS:HZ2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:237:GLN:N	1:B:237:GLN:HE21	2.14	0.45
1:B:57:LEU:HD13	1:B:57:LEU:C	2.36	0.45
1:B:68:LEU:HA	1:B:73:ASN:ND2	2.32	0.45
1:B:244:GLN:OE1	1:B:248:LYS:HE2	2.16	0.45
1:A:88:PHE:HA	1:A:92:THR:CG2	2.47	0.45
1:B:129:VAL:CG2	1:B:219:ILE:HD11	2.47	0.45
1:A:74:TYR:CE2	1:A:150:GLU:HG2	2.52	0.45
1:A:137:VAL:O	1:A:141:LYS:HA	2.15	0.45
1:A:28:GLN:HB3	1:A:31:LEU:HD12	1.98	0.45
1:B:259:ILE:C	1:B:261:PHE:N	2.69	0.45
1:B:67:LYS:HZ2	1:B:336:THR:N	2.15	0.45
1:B:307:ILE:O	1:B:307:ILE:CG2	2.61	0.45
1:A:134:GLU:HG2	1:A:148:PHE:CD2	2.51	0.45
1:B:160:THR:C	1:B:162:VAL:N	2.70	0.45
1:A:290:ILE:HB	1:A:291:PRO:CD	2.47	0.45
1:B:119:LEU:C	1:B:119:LEU:HD23	2.36	0.45
1:B:65:HIS:NE2	1:B:320:THR:OG1	2.49	0.45
1:B:126:TRP:HB3	1:B:160:THR:HG22	1.97	0.45
1:B:33:GLU:HB3	1:B:35:TRP:CD1	2.52	0.45
1:B:237:GLN:O	1:B:238:GLN:CB	2.65	0.44
1:A:75:ILE:HG13	1:A:131:LEU:HD13	1.98	0.44
1:A:231:LYS:HB2	1:A:231:LYS:HZ2	1.81	0.44
1:A:312:GLN:HB2	1:A:332:GLU:HG3	1.99	0.44
1:A:134:GLU:HG2	1:A:148:PHE:CE2	2.53	0.44
1:A:305:ILE:HG12	10:A:1508:HTG:H6'2	1.99	0.44
1:B:67:LYS:HE2	1:B:316:CYS:SG	2.57	0.44
1:A:307:ILE:HG12	1:A:313:PHE:CE2	2.52	0.44
1:B:35:TRP:CZ3	1:B:39:MET:HG3	2.52	0.44
1:B:240:SER:O	1:B:241:ALA:HB2	2.18	0.44
1:A:256:ILE:HA	1:A:256:ILE:HD13	1.85	0.44
1:A:256:ILE:HG22	1:A:305:ILE:HD13	1.99	0.44
1:A:322:CYS:HA	8:A:1322:PLM:O1	2.17	0.44
1:B:264:CYS:SG	1:B:298:SER:HB3	2.57	0.44
1:A:264:CYS:SG	1:A:295:ALA:O	2.76	0.44
1:B:244:GLN:HE21	1:B:245:LYS:N	2.16	0.44
1:A:35:TRP:CZ3	1:A:39:MET:SD	3.08	0.44
1:A:326:ASN:ND2	1:A:328:LEU:CD2	2.81	0.44
1:A:342:THR:C	1:A:344:GLN:H	2.21	0.44
1:A:93:THR:HG22	1:A:94:THR:N	2.32	0.44
1:B:124:ALA:O	1:B:128:LEU:HG	2.17	0.44
1:B:167:CYS:SG	1:B:207:MET:CE	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:VAL:HG23	1:B:219:ILE:HD11	2.00	0.44
1:B:102:TYR:CE2	1:B:104:VAL:HA	2.53	0.44
1:B:148:PHE:CD1	1:B:152:HIS:HB2	2.52	0.44
1:B:44:MET:O	1:B:48:ILE:HG13	2.17	0.44
1:A:327:PRO:O	1:A:328:LEU:C	2.56	0.44
1:B:238:GLN:CG	1:B:241:ALA:H	2.29	0.44
1:B:143:MET:CB	1:B:146:PHE:HB3	2.48	0.44
1:A:259:ILE:C	1:A:261:PHE:H	2.21	0.44
1:A:338:SER:HB2	1:A:341:GLU:CG	2.47	0.43
1:A:301:TYR:HE1	11:A:2020:HOH:O	2.01	0.43
1:A:50:LEU:HD21	1:B:50:LEU:CB	2.36	0.43
1:B:171:PRO:HA	1:B:176:SER:O	2.18	0.43
1:A:115:PHE:O	1:A:118:THR:N	2.51	0.43
1:B:171:PRO:HG2	1:B:189:ILE:CD1	2.48	0.43
1:B:162:VAL:O	1:B:165:LEU:N	2.50	0.43
1:B:50:LEU:O	1:B:52:PHE:N	2.51	0.43
1:A:112:LEU:HD22	1:A:116:PHE:CE2	2.41	0.43
1:B:110:CYS:HB3	11:B:2060:HOH:O	2.18	0.43
1:B:262:LEU:HB3	1:B:266:LEU:HD22	2.00	0.43
1:B:189:ILE:HG22	1:B:190:ASP:N	2.32	0.43
1:A:137:VAL:O	1:A:137:VAL:HG12	2.17	0.43
1:A:224:GLY:O	1:A:227:VAL:CG1	2.66	0.43
1:B:221:PHE:CD1	1:B:221:PHE:C	2.92	0.43
1:A:314:ARG:O	1:A:317:MET:HB3	2.19	0.43
1:B:156:GLY:HA2	1:B:159:PHE:HB3	2.00	0.43
1:A:336:THR:C	1:A:337:VAL:HG12	2.38	0.43
1:A:268:TYR:HA	1:A:291:PRO:HB2	1.99	0.43
1:B:85:PHE:O	1:B:89:GLY:CA	2.65	0.43
1:A:199:ASN:HB3	1:A:202:SER:OG	2.19	0.43
1:A:338:SER:OG	1:A:341:GLU:OE2	2.34	0.43
1:A:264:CYS:SG	1:A:298:SER:HB3	2.59	0.43
1:A:238:GLN:HA	1:A:242:THR:CA	2.48	0.43
1:B:96:TYR:CE2	1:B:104:VAL:HG21	2.51	0.43
1:A:262:LEU:HB3	1:A:266:LEU:HD22	2.01	0.42
1:B:54:ILE:CG2	1:B:55:ASN:N	2.81	0.42
1:B:106:GLY:HA3	1:B:107:PRO:HD2	1.89	0.42
1:B:152:HIS:O	1:B:155:MET:HB2	2.20	0.42
1:B:47:LEU:HA	1:B:47:LEU:HD23	1.86	0.42
1:B:22:SER:C	1:B:24:PHE:H	2.22	0.42
1:B:193:THR:HA	1:B:194:PRO:HD3	1.92	0.42
1:B:183:MET:CE	1:B:286:ILE:HD13	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:266:LEU:N	1:B:267:PRO:CD	2.79	0.42
1:A:56:PHE:O	1:A:59:LEU:HB3	2.19	0.42
1:A:49:MET:SD	1:B:54:ILE:HB	2.59	0.42
1:B:189:ILE:CG2	1:B:190:ASP:N	2.81	0.42
1:B:288:MET:CG	1:B:288:MET:O	2.68	0.42
1:A:8:ASN:HA	1:A:8:ASN:HD22	1.50	0.42
1:A:330:ASP:OD2	1:B:100:HIS:CE1	2.72	0.42
1:B:65:HIS:N	1:B:65:HIS:CD2	2.87	0.42
1:A:238:GLN:HG2	1:A:239:GLU:N	2.34	0.42
1:A:167:CYS:C	1:A:170:PRO:HD2	2.40	0.42
1:A:227:VAL:CG1	1:A:228:PHE:H	2.32	0.42
1:A:218:VAL:O	1:A:218:VAL:CG1	2.67	0.42
1:B:259:ILE:O	1:B:261:PHE:N	2.52	0.42
1:B:115:PHE:CD1	1:B:172:LEU:HD11	2.54	0.42
1:B:255:ILE:HG22	1:B:256:ILE:N	2.34	0.42
1:B:209:VAL:O	1:B:214:ILE:HG13	2.19	0.42
1:A:253:MET:HE3	1:A:306:TYR:HA	1.99	0.42
1:B:85:PHE:O	1:B:89:GLY:HA3	2.20	0.42
1:B:134:GLU:CD	1:B:135:ARG:HH21	2.22	0.42
1:B:224:GLY:O	1:B:227:VAL:HG12	2.19	0.42
1:A:99:LEU:HD23	1:A:99:LEU:HA	1.79	0.42
1:A:44:MET:O	1:A:48:ILE:HG13	2.20	0.42
1:B:183:MET:HE1	1:B:286:ILE:HD13	2.02	0.42
1:A:115:PHE:O	1:A:116:PHE:C	2.56	0.42
1:B:199:ASN:HB3	11:B:2005:HOH:O	2.19	0.42
1:A:124:ALA:HB2	11:A:2030:HOH:O	2.20	0.42
1:A:225:GLN:C	1:A:227:VAL:H	2.21	0.42
1:A:35:TRP:O	1:A:38:SER:HB2	2.20	0.42
1:B:250:VAL:O	1:B:254:VAL:HG23	2.20	0.42
1:B:171:PRO:HG3	1:B:176:SER:HB3	2.02	0.42
1:B:191:TYR:CE2	1:B:272:ALA:HB1	2.55	0.42
1:B:301:TYR:CD1	1:B:301:TYR:C	2.93	0.41
1:B:167:CYS:HB2	1:B:211:HIS:CD2	2.55	0.41
1:A:239:GLU:CG	1:A:248:LYS:HZ2	2.31	0.41
1:B:146:PHE:CE1	1:B:152:HIS:NE2	2.86	0.41
1:A:40:LEU:O	1:A:44:MET:HG2	2.20	0.41
1:A:345:VAL:CG1	1:A:347:PRO:HD3	2.33	0.41
7:B:1296:RET:H201	11:B:2018:HOH:O	2.20	0.41
1:B:135:ARG:NH2	1:B:138:VAL:HG21	2.35	0.41
1:B:50:LEU:HD23	1:B:50:LEU:C	2.41	0.41
1:B:129:VAL:O	1:B:133:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:CH2	1:A:215:PRO:HG3	2.55	0.41
1:A:22:SER:C	1:A:24:PHE:H	2.22	0.41
1:B:276:PHE:O	1:B:279:GLN:HG3	2.21	0.41
1:A:347:PRO:HB2	1:A:348:ALA:H	1.58	0.41
1:A:62:THR:CG2	1:A:77:LEU:HD22	2.49	0.41
1:A:337:VAL:CG2	1:A:338:SER:N	2.83	0.41
1:B:68:LEU:CA	1:B:73:ASN:HD22	2.34	0.41
1:B:338:SER:CB	1:B:341:GLU:CD	2.88	0.41
1:B:322:CYS:O	1:B:324:GLY:N	2.53	0.41
1:B:50:LEU:C	1:B:52:PHE:N	2.74	0.41
1:B:224:GLY:O	1:B:227:VAL:HB	2.21	0.41
1:A:260:ALA:HB2	8:A:1410:PLM:HE2	2.02	0.41
1:B:64:GLN:CG	1:B:339:LYS:HE2	2.29	0.41
1:B:189:ILE:HA	1:B:189:ILE:HD13	1.94	0.41
1:B:283:PHE:HA	10:B:1506:HTG:H61	2.03	0.41
1:B:239:GLU:OE1	1:B:239:GLU:HA	2.20	0.41
1:A:227:VAL:O	1:A:231:LYS:HG2	2.21	0.41
1:B:140:CYS:O	1:B:141:LYS:C	2.58	0.41
1:B:27:PRO:HB3	1:B:29:TYR:CE2	2.56	0.41
1:A:72:LEU:HG	1:A:76:LEU:HD12	2.02	0.41
1:B:226:LEU:CD1	1:B:226:LEU:N	2.83	0.41
1:A:169:ALA:O	1:A:172:LEU:HB2	2.21	0.41
1:B:175:TRP:NE1	1:B:203:PHE:HB2	2.35	0.41
1:B:244:GLN:NE2	1:B:245:LYS:N	2.68	0.40
1:B:130:VAL:HG21	1:B:160:THR:HG23	2.03	0.40
1:B:158:ALA:O	1:B:162:VAL:HG23	2.21	0.40
1:B:52:PHE:C	1:B:52:PHE:CD1	2.94	0.40
1:B:125:LEU:HB2	1:B:261:PHE:CZ	2.57	0.40
1:A:232:GLU:CB	1:A:252:ARG:HD3	2.51	0.40
1:B:94:THR:HG22	1:B:113:GLU:HG3	2.00	0.40
1:B:258:VAL:O	1:B:261:PHE:HB3	2.20	0.40
1:B:332:GLU:O	1:B:333:ALA:CB	2.68	0.40
1:B:75:ILE:HG13	1:B:131:LEU:HD12	2.03	0.40
1:A:236:GLN:O	1:A:245:LYS:HD2	2.21	0.40
1:B:64:GLN:NE2	1:B:65:HIS:NE2	2.70	0.40
1:B:137:VAL:HG12	1:B:137:VAL:O	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:344:GLN:NE2	10:B:1509:HTG:O6[4_564]	2.19	0.01

## 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	347/349 (99%)	264 (76%)	57 (16%)	26 (8%)	<b>1</b>	<b>3</b>
1	B	347/349 (99%)	254 (73%)	69 (20%)	24 (7%)	<b>1</b>	<b>3</b>
All	All	694/698 (99%)	518 (75%)	126 (18%)	50 (7%)	<b>1</b>	<b>3</b>

All (50) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	SER
1	A	241	ALA
1	A	323	CYS
1	A	328	LEU
1	A	341	GLU
1	B	229	THR
1	B	240	SER
1	B	241	ALA
1	B	281	SER
1	B	331	ASP
1	B	337	VAL
1	B	341	GLU
1	B	347	PRO
1	A	195	HIS
1	A	229	THR
1	A	279	GLN
1	A	281	SER
1	A	301	TYR
1	A	324	GLY
1	A	329	GLY

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Mol	Chain	Res	Type
1	A	335	THR
1	A	347	PRO
1	B	195	HIS
1	B	237	GLN
1	B	323	CYS
1	B	324	GLY
1	A	87	VAL
1	A	93	THR
1	A	94	THR
1	A	115	PHE
1	A	119	LEU
1	A	167	CYS
1	A	338	SER
1	B	236	GLN
1	B	238	GLN
1	A	89	GLY
1	A	201	GLU
1	B	51	GLY
1	B	161	TRP
1	B	260	ALA
1	A	141	LYS
1	A	145	ASN
1	B	262	LEU
1	B	87	VAL
1	B	218	VAL
1	B	329	GLY
1	B	133	ILE
1	A	337	VAL
1	B	141	LYS
1	B	305	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	296/296 (100%)	276 (93%)	20 (7%)	20 49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	296/296 (100%)	273 (92%)	23 (8%)	16	41
All	All	592/592 (100%)	549 (93%)	43 (7%)	17	44

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	76	LEU
1	A	78	ASN
1	A	100	HIS
1	A	119	LEU
1	A	131	LEU
1	A	135	ARG
1	A	143	MET
1	A	165	LEU
1	A	179	ILE
1	A	191	TYR
1	A	237	GLN
1	A	244	GLN
1	A	245	LYS
1	A	266	LEU
1	A	302	ASN
1	A	332	GLU
1	A	336	THR
1	A	337	VAL
1	A	343	SER
1	B	8	ASN
1	B	50	LEU
1	B	70	THR
1	B	104	VAL
1	B	134	GLU
1	B	135	ARG
1	B	143	MET
1	B	148	PHE
1	B	161	TRP
1	B	185	CYS
1	B	208	PHE
1	B	220	PHE
1	B	229	THR
1	B	236	GLN
1	B	237	GLN
1	B	244	GLN

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Mol	Chain	Res	Type
1	B	245	LYS
1	B	249	GLU
1	B	266	LEU
1	B	283	PHE
1	B	330	ASP
1	B	332	GLU
1	B	341	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	73	ASN
1	A	100	HIS
1	A	237	GLN
1	A	302	ASN
1	A	312	GLN
1	A	326	ASN
1	B	8	ASN
1	B	64	GLN
1	B	73	ASN
1	B	151	ASN
1	B	237	GLN
1	B	244	GLN
1	B	302	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

11 carbohydrates 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	$\# Z  > 2$
2	MAN	A	503	2	11,11,12	0.77	0	14,15,17	0.84	0
2	NAG	A	504	2	14,14,15	0.76	0	15,19,21	0.87	0
2	NAG	A	505	1,2	14,14,15	0.62	0	15,19,21	0.86	0
4	NAG	A	704	4	14,14,15	0.61	0	15,19,21	1.05	1 (6%)
4	NAG	A	705	1,4	14,14,15	0.54	0	15,19,21	0.89	1 (6%)
3	BMA	B	602	3	11,11,12	0.81	0	14,15,17	0.90	1 (7%)
3	BMA	B	603	3	11,11,12	0.79	0	14,15,17	0.72	0
3	NAG	B	604	3	14,14,15	0.63	0	15,19,21	1.02	1 (6%)
3	NAG	B	605	1,3	14,14,15	0.59	0	15,19,21	0.62	0
4	NAG	B	804	4	14,14,15	0.63	0	15,19,21	0.72	0
4	NAG	B	805	1,4	14,14,15	0.63	0	15,19,21	0.85	1 (6%)

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
2	MAN	A	503	2	-	0/2/19/22	0/1/1/1
2	NAG	A	504	2	-	0/6/23/26	0/1/1/1
2	NAG	A	505	1,2	-	0/6/23/26	0/1/1/1
4	NAG	A	704	4	-	0/6/23/26	0/1/1/1
4	NAG	A	705	1,4	-	0/6/23/26	0/1/1/1
3	BMA	B	602	3	-	0/2/19/22	0/1/1/1
3	BMA	B	603	3	-	0/2/19/22	0/1/1/1
3	NAG	B	604	3	-	0/6/23/26	0/1/1/1
3	NAG	B	605	1,3	-	0/6/23/26	0/1/1/1
4	NAG	B	804	4	-	0/6/23/26	0/1/1/1
4	NAG	B	805	1,4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	704	NAG	C2-N2-C7	-3.45	118.61	123.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604	NAG	C2-N2-C7	-3.04	119.13	123.04
4	A	705	NAG	C2-N2-C7	-3.00	119.18	123.04
4	B	805	NAG	C2-N2-C7	-2.40	119.95	123.04
3	B	602	BMA	C1-O5-C5	2.41	115.30	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	NAG	1	0
2	A	505	NAG	1	0
4	B	805	NAG	1	0

## 5.6 Ligand geometry

Of 26 ligands modelled in this entry, 13 are monoatomic - leaving 13 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
7	RET	A	1296	1	19,20,21	2.51	3 (15%)	27,27,28	2.02	7 (25%)
8	PLM	A	1322	1	16,16,17	0.94	1 (6%)	15,15,17	0.61	0
8	PLM	A	1323	1	16,16,17	0.94	1 (6%)	15,15,17	0.53	0
8	PLM	A	1410	-	15,15,17	1.77	3 (20%)	14,14,17	3.31	5 (35%)
10	HTG	A	1507	-	19,19,19	3.11	8 (42%)	22,24,24	2.95	2 (9%)
10	HTG	A	1508	-	19,19,19	2.37	8 (42%)	22,24,24	3.52	2 (9%)
7	RET	B	1296	1	19,20,21	2.16	3 (15%)	27,27,28	1.88	7 (25%)
8	PLM	B	1322	1	16,16,17	0.98	1 (6%)	15,15,17	0.44	0
8	PLM	B	1323	1	16,16,17	0.95	1 (6%)	15,15,17	0.45	0
9	HTO	B	1401	-	9,9,9	1.63	1 (11%)	8,10,10	1.15	1 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	PLM	B	1407	-	15,15,17	1.71	3 (20%)	14,14,17	3.29	6 (42%)
10	HTG	B	1506	-	19,19,19	2.93	8 (42%)	22,24,24	2.57	2 (9%)
10	HTG	B	1509	-	19,19,19	2.66	8 (42%)	22,24,24	2.95	1 (4%)

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
7	RET	A	1296	1	-	0/13/30/31	0/1/1/1
8	PLM	A	1322	1	-	0/14/14/15	0/0/0/0
8	PLM	A	1323	1	-	0/14/14/15	0/0/0/0
8	PLM	A	1410	-	-	0/13/13/15	0/0/0/0
10	HTG	A	1507	-	-	0/10/30/30	0/1/1/1
10	HTG	A	1508	-	-	0/10/30/30	0/1/1/1
7	RET	B	1296	1	-	0/13/30/31	0/1/1/1
8	PLM	B	1322	1	-	0/14/14/15	0/0/0/0
8	PLM	B	1323	1	-	0/14/14/15	0/0/0/0
9	HTO	B	1401	-	-	0/10/10/10	0/0/0/0
8	PLM	B	1407	-	-	0/13/13/15	0/0/0/0
10	HTG	B	1506	-	-	0/10/30/30	0/1/1/1
10	HTG	B	1509	-	-	0/10/30/30	0/1/1/1

All (49) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1410	PLM	CC-CB	-4.69	1.24	1.51
8	B	1407	PLM	CC-CB	-4.49	1.25	1.51
8	A	1322	PLM	O1-C1	-3.58	1.22	1.42
8	B	1322	PLM	O1-C1	-3.51	1.23	1.42
8	A	1323	PLM	O1-C1	-3.48	1.23	1.42
8	A	1410	PLM	CB-CA	-3.26	1.32	1.51
8	B	1323	PLM	O1-C1	-3.24	1.24	1.42
8	B	1407	PLM	CB-CA	-3.06	1.33	1.51
8	A	1410	PLM	CD-CC	-2.90	1.34	1.51
8	B	1407	PLM	CD-CC	-2.71	1.35	1.51
7	A	1296	RET	C15-C14	-2.11	1.40	1.49
10	B	1509	HTG	C6-C5	2.10	1.59	1.51
10	A	1508	HTG	C1-S1	2.29	1.84	1.80
7	B	1296	RET	C17-C1	2.32	1.58	1.53
10	A	1508	HTG	C1'-S1	2.35	1.84	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1509	HTG	C1-S1	2.77	1.85	1.80
10	A	1508	HTG	C1-C2	2.98	1.59	1.53
10	A	1508	HTG	C4-C3	3.01	1.60	1.52
10	A	1507	HTG	C1'-S1	3.02	1.85	1.81
10	A	1508	HTG	C3-C2	3.03	1.60	1.52
10	B	1509	HTG	C4-C3	3.06	1.60	1.52
10	B	1506	HTG	C1'-S1	3.08	1.85	1.81
10	A	1508	HTG	O5-C5	3.13	1.52	1.44
10	B	1509	HTG	C3-C2	3.15	1.60	1.52
10	B	1509	HTG	O5-C5	3.24	1.52	1.44
10	B	1506	HTG	C1-C2	3.24	1.59	1.53
10	B	1506	HTG	C4-C3	3.25	1.60	1.52
10	A	1507	HTG	C4-C3	3.25	1.60	1.52
10	B	1506	HTG	O5-C5	3.32	1.52	1.44
10	A	1507	HTG	O5-C5	3.41	1.52	1.44
10	A	1507	HTG	C4-C5	3.61	1.60	1.53
10	A	1507	HTG	C3-C2	3.72	1.62	1.52
10	A	1508	HTG	C4-C5	3.73	1.61	1.53
10	B	1506	HTG	C4-C5	3.79	1.61	1.53
9	B	1401	HTO	C3-C2	3.79	1.63	1.52
10	B	1509	HTG	C1-C2	3.95	1.60	1.53
10	B	1506	HTG	C3-C2	3.97	1.62	1.52
10	A	1507	HTG	C1-C2	4.33	1.61	1.53
10	B	1506	HTG	C1-S1	4.34	1.87	1.80
10	B	1509	HTG	C4-C5	4.61	1.62	1.53
10	A	1507	HTG	C1-S1	5.30	1.89	1.80
7	B	1296	RET	C1-C6	5.56	1.61	1.53
7	B	1296	RET	C5-C6	6.14	1.44	1.34
10	A	1508	HTG	O5-C1	6.45	1.53	1.42
7	A	1296	RET	C1-C6	7.05	1.63	1.53
7	A	1296	RET	C5-C6	7.05	1.45	1.34
10	B	1509	HTG	O5-C1	7.28	1.54	1.42
10	B	1506	HTG	O5-C1	8.20	1.56	1.42
10	A	1507	HTG	O5-C1	8.59	1.57	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1296	RET	C11-C10-C9	-4.73	120.36	127.20
7	B	1296	RET	C11-C10-C9	-3.64	121.94	127.20
7	B	1296	RET	C8-C9-C10	-3.57	113.23	118.98
7	A	1296	RET	C8-C9-C10	-2.87	114.36	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1296	RET	C18-C5-C4	-2.46	108.77	113.43
9	B	1401	HTO	O3-C3-C4	-2.33	104.17	109.35
10	A	1507	HTG	O5-C1-C2	-2.33	107.03	110.19
7	B	1296	RET	C18-C5-C4	-2.02	109.60	113.43
10	A	1508	HTG	O5-C5-C6	2.04	111.52	106.36
10	B	1506	HTG	O5-C5-C6	2.11	111.68	106.36
8	B	1407	PLM	C9-C8-C7	2.12	125.50	114.53
8	A	1410	PLM	CE-CD-CC	2.19	125.86	114.53
7	A	1296	RET	C8-C7-C6	2.25	134.09	127.32
7	A	1296	RET	C2-C1-C6	2.38	114.13	110.36
8	A	1410	PLM	C5-C4-C3	2.41	126.99	114.53
8	B	1407	PLM	C5-C4-C3	2.42	127.00	114.53
8	B	1407	PLM	CE-CD-CC	2.49	127.40	114.53
7	A	1296	RET	C19-C9-C10	2.50	126.59	122.90
7	B	1296	RET	C2-C1-C6	2.53	114.36	110.36
7	B	1296	RET	C8-C7-C6	2.68	135.37	127.32
7	B	1296	RET	C19-C9-C10	2.86	127.12	122.90
8	A	1410	PLM	CC-CB-CA	3.08	130.46	114.53
8	B	1407	PLM	CC-CB-CA	3.11	130.59	114.53
7	B	1296	RET	C18-C5-C6	5.08	129.60	124.61
7	A	1296	RET	C18-C5-C6	5.69	130.19	124.61
8	B	1407	PLM	CA-C9-C8	7.22	151.83	114.53
8	A	1410	PLM	CA-C9-C8	7.38	152.62	114.53
8	B	1407	PLM	CD-CC-CB	8.00	155.85	114.53
8	A	1410	PLM	CD-CC-CB	8.13	156.51	114.53
10	B	1506	HTG	C1'-S1-C1	11.30	115.88	100.30
10	A	1507	HTG	C1'-S1-C1	13.18	118.47	100.30
10	B	1509	HTG	C1'-S1-C1	13.29	118.62	100.30
10	A	1508	HTG	C1'-S1-C1	15.96	122.30	100.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1296	RET	2	0
8	A	1322	PLM	6	0
8	A	1410	PLM	1	0
10	A	1507	HTG	2	0
10	A	1508	HTG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	1296	RET	2	0
8	B	1322	PLM	2	0
8	B	1323	PLM	2	0
9	B	1401	HTO	1	0
8	B	1407	PLM	1	0
10	B	1506	HTG	1	0
10	B	1509	HTG	3	1

## 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	348/349 (99%)	1.50	102 (29%) <b>1</b> <b>0</b>	48, 61, 135, 149	228 (65%)
1	B	348/349 (99%)	1.75	127 (36%) <b>0</b> <b>0</b>	48, 64, 154, 163	228 (65%)
All	All	696/698 (99%)	1.63	229 (32%) <b>0</b> <b>0</b>	48, 63, 147, 163	456 (65%)

All (229) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	ALA	9.9
1	B	232	GLU	9.5
1	B	344	GLN	7.8
1	B	142	PRO	7.5
1	B	342	THR	6.7
1	A	328	LEU	6.5
1	B	233	ALA	6.3
1	B	148	PHE	6.0
1	B	145	ASN	5.8
1	A	142	PRO	5.8
1	B	242	THR	5.7
1	A	240	SER	5.6
1	A	348	ALA	5.5
1	B	234	ALA	5.2
1	B	345	VAL	5.2
1	A	235	ALA	5.0
1	A	333	ALA	5.0
1	B	321	LEU	5.0
1	A	60	TYR	5.0
1	B	140	CYS	4.8
1	A	228	PHE	4.8
1	A	335	THR	4.6
1	A	147	ARG	4.6
1	A	243	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	146	PHE	4.6
1	B	107	PRO	4.5
1	A	97	THR	4.5
1	B	340	THR	4.3
1	B	143	MET	4.3
1	B	68	LEU	4.3
1	B	231	LYS	4.2
1	A	236	GLN	4.2
1	B	235	ALA	4.2
1	B	286	ILE	4.0
1	A	86	MET	4.0
1	B	334	SER	4.0
1	B	229	THR	3.9
1	B	339	LYS	3.9
1	B	240	SER	3.9
1	B	163	MET	3.7
1	A	145	ASN	3.7
1	A	180	PRO	3.7
1	A	224	GLY	3.7
1	B	281	SER	3.7
1	A	33	GLU	3.6
1	B	311	LYS	3.6
1	B	65	HIS	3.6
1	A	314	ARG	3.6
1	A	304	VAL	3.6
1	B	230	VAL	3.6
1	B	264	CYS	3.5
1	A	105	PHE	3.5
1	B	144	SER	3.5
1	A	159	PHE	3.5
1	A	167	CYS	3.5
1	A	16	LYS	3.5
1	B	228	PHE	3.4
1	B	243	THR	3.4
1	A	65	HIS	3.4
1	A	252	ARG	3.4
1	A	334	SER	3.4
1	A	307	ILE	3.4
1	A	118	THR	3.3
1	B	251	THR	3.3
1	B	220	PHE	3.3
1	A	234	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	96	TYR	3.3
1	B	185	CYS	3.2
1	B	219	ILE	3.2
1	B	312	GLN	3.2
1	B	38	SER	3.2
1	B	329	GLY	3.2
1	B	313	PHE	3.2
1	B	322	CYS	3.2
1	B	199	ASN	3.2
1	A	264	CYS	3.2
1	B	146	PHE	3.1
1	B	253	MET	3.1
1	A	233	ALA	3.1
1	B	332	GLU	3.1
1	A	39	MET	3.0
1	B	184	GLN	3.0
1	A	315	ASN	3.0
1	A	64	GLN	3.0
1	A	23	PRO	3.0
1	B	19	VAL	3.0
1	A	265	TRP	3.0
1	B	330	ASP	3.0
1	B	200	ASN	2.9
1	A	132	ALA	2.9
1	A	280	GLY	2.9
1	B	301	TYR	2.9
1	A	302	ASN	2.9
1	A	301	TYR	2.9
1	A	14	SER	2.8
1	B	125	LEU	2.8
1	B	104	VAL	2.8
1	B	336	THR	2.8
1	B	147	ARG	2.8
1	A	250	VAL	2.8
1	A	189	ILE	2.7
1	B	261	PHE	2.7
1	A	84	LEU	2.7
1	A	295	ALA	2.7
1	A	324	GLY	2.7
1	A	155	MET	2.7
1	A	215	PRO	2.7
1	B	62	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	116	PHE	2.7
1	B	254	VAL	2.7
1	B	167	CYS	2.6
1	B	262	LEU	2.6
1	A	104	VAL	2.6
1	B	343	SER	2.6
1	A	120	GLY	2.6
1	A	237	GLN	2.6
1	B	263	ILE	2.6
1	B	61	VAL	2.6
1	A	176	SER	2.5
1	B	186	SER	2.5
1	B	257	MET	2.5
1	A	125	LEU	2.5
1	B	60	TYR	2.5
1	B	168	ALA	2.5
1	B	272	ALA	2.5
1	B	118	THR	2.5
1	A	102	TYR	2.5
1	A	306	TYR	2.5
1	A	251	THR	2.5
1	A	197	GLU	2.5
1	A	281	SER	2.5
1	B	99	LEU	2.5
1	B	291	PRO	2.5
1	A	100	HIS	2.5
1	A	88	PHE	2.5
1	A	76	LEU	2.4
1	B	46	LEU	2.4
1	B	74	TYR	2.4
1	A	32	ALA	2.4
1	B	346	ALA	2.4
1	A	121	GLY	2.4
1	B	103	PHE	2.4
1	B	87	VAL	2.4
1	B	218	VAL	2.4
1	B	180	PRO	2.4
1	A	269	ALA	2.4
1	A	316	CYS	2.4
1	A	126	TRP	2.4
1	B	73	ASN	2.4
1	B	271	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	182	GLY	2.4
1	A	49	MET	2.4
1	B	96	TYR	2.4
1	B	303	PRO	2.3
1	A	185	CYS	2.3
1	B	47	LEU	2.3
1	B	256	ILE	2.3
1	B	236	GLN	2.3
1	B	310	ASN	2.3
1	B	101	GLY	2.3
1	B	333	ALA	2.3
1	B	307	ILE	2.3
1	A	303	PRO	2.3
1	B	265	TRP	2.3
1	B	308	MET	2.3
1	B	37	PHE	2.3
1	A	41	ALA	2.3
1	A	42	ALA	2.3
1	B	207	MET	2.3
1	A	190	ASP	2.3
1	A	110	CYS	2.3
1	A	310	ASN	2.3
1	A	156	GLY	2.3
1	A	143	MET	2.3
1	B	97	THR	2.3
1	A	196	GLU	2.2
1	A	242	THR	2.2
1	B	226	LEU	2.2
1	A	71	PRO	2.2
1	B	21	ARG	2.2
1	B	241	ALA	2.2
1	A	74	TYR	2.2
1	B	50	LEU	2.2
1	B	314	ARG	2.2
1	B	187	CYS	2.2
1	A	294	PHE	2.2
1	A	73	ASN	2.2
1	B	98	SER	2.2
1	A	34	PRO	2.2
1	B	285	PRO	2.2
1	A	17	THR	2.2
1	A	75	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	79	LEU	2.2
1	A	297	THR	2.2
1	B	238	GLN	2.2
1	B	131	LEU	2.1
1	A	98	SER	2.1
1	A	93	THR	2.1
1	B	320	THR	2.1
1	A	148	PHE	2.1
1	A	128	LEU	2.1
1	B	43	TYR	2.1
1	A	317	MET	2.1
1	B	124	ALA	2.1
1	A	182	GLY	2.1
1	B	56	PHE	2.1
1	B	211	HIS	2.1
1	B	297	THR	2.1
1	B	192	TYR	2.1
1	B	176	SER	2.1
1	B	100	HIS	2.1
1	B	83	ASP	2.1
1	B	331	ASP	2.1
1	A	127	SER	2.1
1	A	77	LEU	2.1
1	B	81	VAL	2.1
1	B	210	VAL	2.1
1	B	153	ALA	2.1
1	A	45	PHE	2.0
1	B	127	SER	2.0
1	A	211	HIS	2.0
1	B	217	ILE	2.0
1	B	325	LYS	2.0
1	A	109	GLY	2.0
1	A	241	ALA	2.0
1	B	323	CYS	2.0
1	A	219	ILE	2.0
1	B	141	LYS	2.0
1	B	300	VAL	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

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
4	NAG	B	805	14/15	0.90	0.30	0.45	65,69,71,77	0
3	BMA	B	602	11/12	0.49	0.38	-0.24	120,122,122,124	0
3	NAG	B	605	14/15	0.91	0.23	-0.25	63,64,69,75	0
2	NAG	A	505	14/15	0.90	0.16	-0.67	66,68,74,75	0
4	NAG	A	705	14/15	0.86	0.17	-1.48	70,75,80,84	0
3	NAG	B	604	14/15	0.82	0.32	-	77,83,90,97	0
4	NAG	A	704	14/15	0.80	0.34	-	91,94,99,101	0
2	MAN	A	503	11/12	0.83	0.29	-	94,97,97,99	0
4	NAG	B	804	14/15	0.79	0.34	-	84,89,91,92	0
3	BMA	B	603	11/12	0.64	0.30	-	104,108,112,116	0
2	NAG	A	504	14/15	0.88	0.27	-	79,82,87,92	0

### 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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
8	PLM	A	1322	17/18	0.65	0.52	4.18	94,104,110,110	0
7	RET	A	1296	20/21	0.70	0.51	3.11	50,52,54,55	20
10	HTG	A	1507	19/19	0.76	0.40	2.27	99,113,115,116	0
8	PLM	B	1407	16/18	0.65	0.46	2.16	75,82,87,88	0
7	RET	B	1296	20/21	0.72	0.42	1.87	51,52,54,54	20
6	ZN	B	963	1/1	0.39	0.45	1.84	93,93,93,93	1
8	PLM	B	1322	17/18	0.68	0.46	1.04	105,108,109,110	0
8	PLM	B	1323	17/18	0.70	0.46	0.92	117,122,124,124	0
10	HTG	B	1506	19/19	0.73	0.37	0.76	88,93,97,99	0
8	PLM	A	1323	17/18	0.70	0.33	0.53	98,105,113,114	0
10	HTG	B	1509	19/19	0.70	0.43	0.49	93,95,100,100	0
6	ZN	A	962	1/1	0.81	0.33	0.19	80,80,80,80	1

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	PLM	A	1410	16/18	0.82	0.33	-0.05	74,77,79,79	0
5	HG	A	903	1/1	0.98	0.22	-0.44	96,96,96,96	1
5	HG	B	904	1/1	0.93	0.24	-0.45	109,109,109,109	1
10	HTG	A	1508	19/19	0.79	0.27	-0.47	72,78,82,85	0
5	HG	B	906	1/1	0.78	0.23	-0.67	121,121,121,121	1
9	HTO	B	1401	10/10	0.75	0.24	-2.07	56,60,62,63	0
5	HG	A	901	1/1	0.94	0.20	-2.80	82,82,82,82	1
5	HG	B	902	1/1	0.96	0.17	-2.85	80,80,80,80	1
6	ZN	A	959	1/1	0.94	0.04	-	92,92,92,92	1
6	ZN	A	2011	1/1	0.96	0.15	-	53,53,53,53	1
6	ZN	A	957	1/1	0.97	0.09	-	53,53,53,53	1
6	ZN	B	958	1/1	0.96	0.11	-	43,43,43,43	1
5	HG	A	905	1/1	0.86	0.39	-	99,99,99,99	1
6	ZN	B	956	1/1	0.96	0.09	-	60,60,60,60	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.