



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:56 PM GMT

PDB ID : 1HZX
Title : CRYSTAL STRUCTURE OF BOVINE RHODOPSIN
Authors : Teller, D.C.; Okada, T.; Behnke, C.A.; Palczewski, K.; Stenkamp, R.E.
Deposited on : 2001-01-26
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
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) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

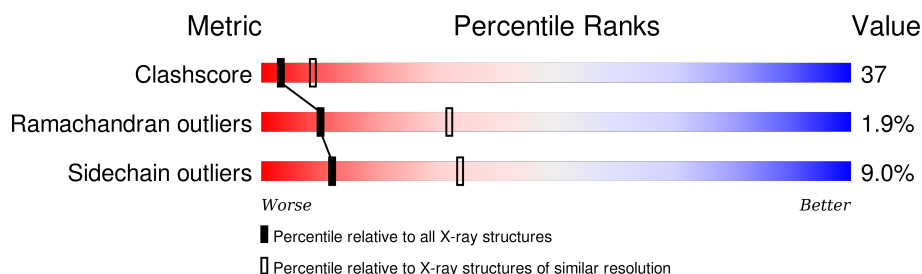
1 Overall quality at a glance ⓘ

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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (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 ≥ 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	349	
1	B	349	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	BNG	B	1506	-	-	X	-

2 Entry composition [i](#)

There are 11 unique types of molecules in this entry. The entry contains 5551 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	341	Total	C	N	O	S	0	0	0
			2685	1783	413	463	26			
1	B	302	Total	C	N	O	S	0	0	0
			2398	1603	366	404	25			

- 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		

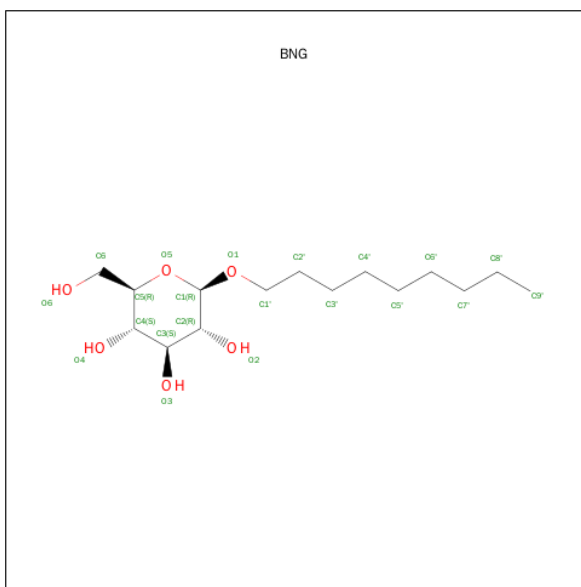
- Molecule 3 is a polymer of unknown type called SUGAR (4-MER).

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 SUGAR (B-NONYLGLUCOSIDE) (three-letter code: BNG) (formula: C₁₅H₃₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	B	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	A	1	Total	C	O	0	0
			21	15	6		
5	B	1	Total	C	O	0	0
			21	15	6		

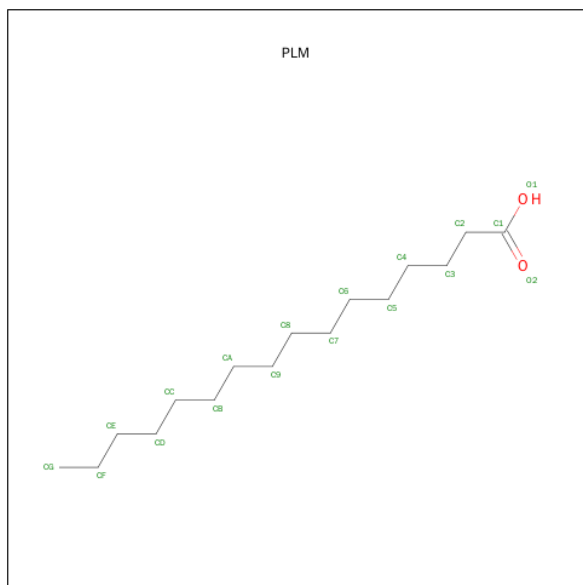
- Molecule 6 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

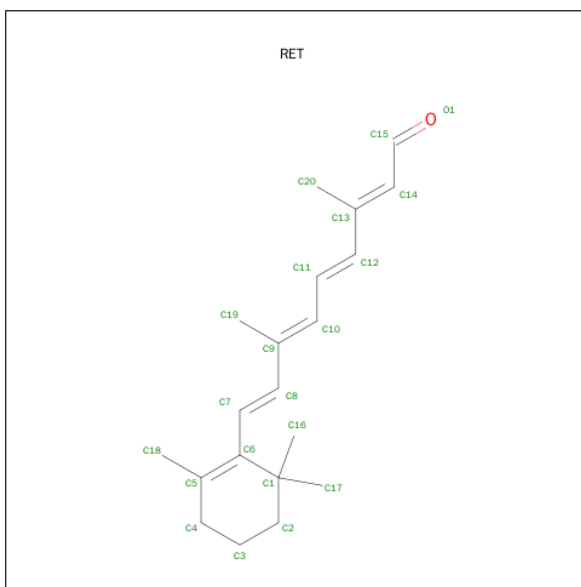
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	3	Total	Zn	0	0
			3	3		
7	A	4	Total	Zn	0	0
			4	4		

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: $C_{16}H_{32}O_2$).



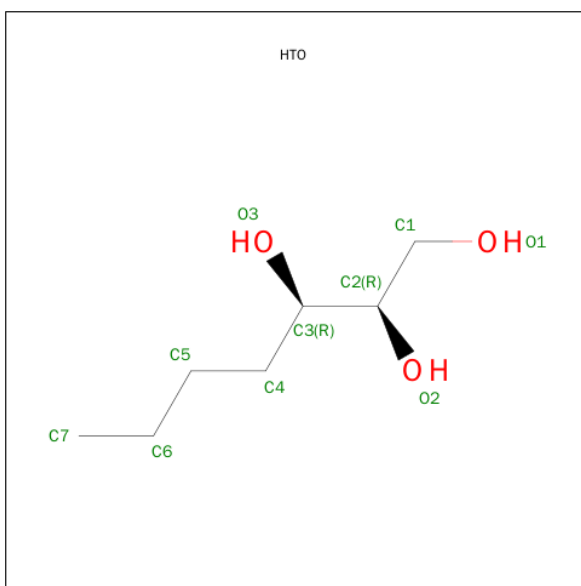
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	16	1		
8	A	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		

- Molecule 9 is RETINAL (three-letter code: RET) (formula: $C_{20}H_{28}O$).



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

- Molecule 10 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: $C_7H_{16}O_3$).



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

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

- Molecule 11 is water.

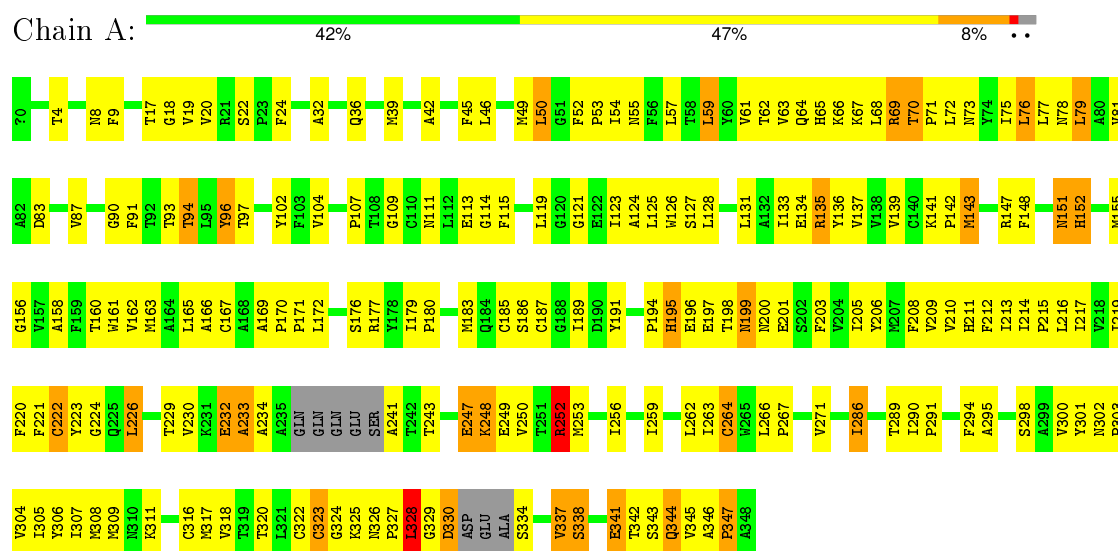
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	7	Total	O	0	0
			7	7		
11	B	5	Total	O	0	0
			5	5		

3 Residue-property plots

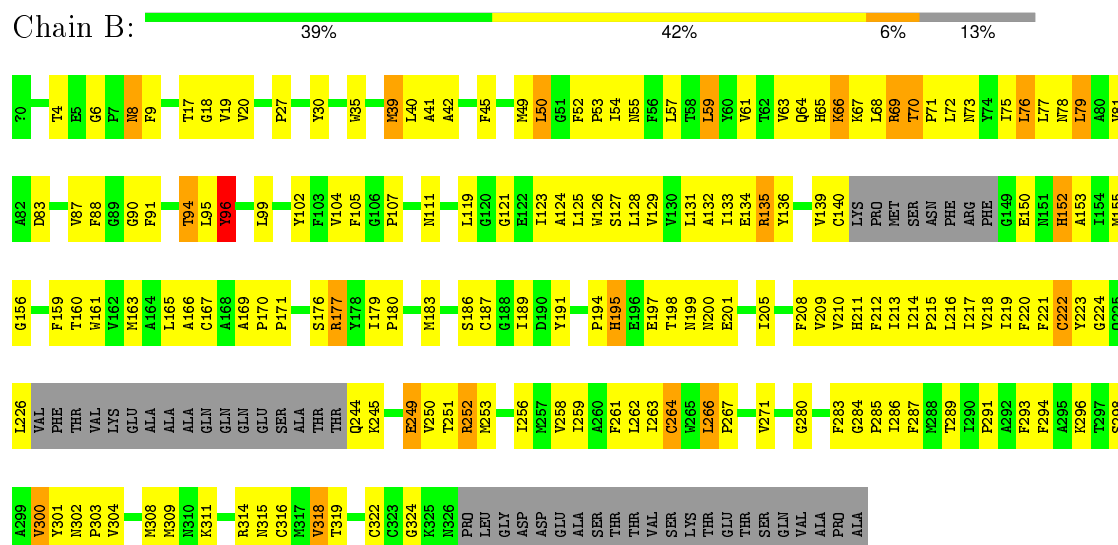
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

Note EDS was not executed.

• Molecule 1: RHODOPSIN



• Molecule 1: RHODOPSIN



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 41	Depositor
Cell constants a, b, c, α , β , γ	97.25Å 97.25Å 149.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	69.8 (30.00-2.80)	Depositor
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	?	Depositor
R, R_{free}	0.175 , 0.212	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5551	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, BMA, NAG, ACE, HTO, RET, PLM, BNG, 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	0.53	2/2765 (0.1%)	0.74	2/3767 (0.1%)
1	B	0.53	2/2472 (0.1%)	0.72	1/3368 (0.0%)
All	All	0.53	4/5237 (0.1%)	0.73	3/7135 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	96	TYR	CB-CG	-5.68	1.43	1.51
1	A	96	TYR	CB-CG	-5.49	1.43	1.51
1	B	249	GLU	CD-OE1	-5.28	1.19	1.25
1	A	249	GLU	CD-OE1	-5.18	1.20	1.25

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	B	177	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	252	ARG	NE-CZ-NH2	5.24	122.92	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2685	0	2655	232	1
1	B	2398	0	2368	198	0
2	A	39	0	34	5	0
3	B	50	0	43	2	0
4	A	28	0	25	2	0
4	B	28	0	25	1	0
5	A	105	0	150	10	0
5	B	42	0	60	10	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
7	A	4	0	0	0	0
7	B	3	0	0	0	1
8	A	34	0	62	1	0
8	B	17	0	31	1	0
9	A	20	0	27	1	0
9	B	20	0	27	1	0
10	A	40	0	64	5	0
10	B	20	0	32	2	0
11	A	7	0	0	0	0
11	B	5	0	0	1	0
All	All	5551	0	5603	415	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 37.

All (415) 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:328:LEU:HB2	1:B:96:TYR:CE2	1.67	1.29
1:A:50:LEU:HD12	1:B:50:LEU:HD12	1.11	1.09
1:A:50:LEU:HD12	1:B:50:LEU:CD1	1.83	1.09
1:A:65:HIS:HB3	1:A:337:VAL:HG22	1.38	1.06
1:A:328:LEU:HB2	1:B:96:TYR:HE2	1.04	1.02
1:B:136:TYR:HA	1:B:226:LEU:HD11	1.42	1.01
1:B:72:LEU:HD22	1:B:250:VAL:HG13	1.39	1.01
1:A:142:PRO:HB2	1:A:143:MET:HE2	1.46	0.97
1:A:230:VAL:HG23	1:A:248:LYS:HG3	1.48	0.94
1:A:75:ILE:HG21	1:A:131:LEU:HD21	1.49	0.93
1:A:67:LYS:H	1:A:337:VAL:HG23	1.34	0.92
1:A:50:LEU:CD1	1:B:50:LEU:HD12	1.99	0.91
1:A:241:ALA:HB3	1:A:243:THR:HG22	1.54	0.90
1:A:65:HIS:ND1	1:A:338:SER:HA	1.85	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ILE:HG21	1:B:131:LEU:HD21	1.55	0.88
1:A:9:PHE:HA	1:A:179:ILE:HD11	1.55	0.86
1:B:136:TYR:CA	1:B:226:LEU:HD11	2.07	0.84
1:A:67:LYS:HB2	1:A:337:VAL:HB	1.58	0.84
1:B:212:PHE:O	1:B:216:LEU:HD23	1.77	0.83
1:A:328:LEU:HD22	1:A:328:LEU:N	1.93	0.83
1:A:91:PHE:HA	1:A:94:THR:CG2	2.08	0.82
1:A:212:PHE:O	1:A:216:LEU:HD23	1.79	0.82
1:A:346:ALA:N	1:A:347:PRO:HD3	1.95	0.81
1:A:325:LYS:HG2	1:A:326:ASN:H	1.43	0.81
1:B:311:LYS:HG2	1:B:314:ARG:HH21	1.45	0.81
1:A:54:ILE:HG12	1:B:49:MET:HE2	1.65	0.78
1:A:328:LEU:HB3	1:B:105:PHE:HZ	1.48	0.77
1:B:91:PHE:HA	1:B:94:THR:CG2	2.14	0.77
1:B:50:LEU:HD23	1:B:54:ILE:HD12	1.66	0.77
1:B:68:LEU:O	1:B:69:ARG:HD2	1.86	0.76
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.67	0.76
1:A:136:TYR:HA	1:A:226:LEU:HD11	1.67	0.76
1:B:314:ARG:O	1:B:318:VAL:HG12	1.85	0.76
1:B:161:TRP:O	1:B:165:LEU:HD23	1.87	0.75
1:B:139:VAL:HB	1:B:226:LEU:CD2	2.17	0.75
1:B:9:PHE:HA	1:B:179:ILE:HD11	1.68	0.74
1:A:230:VAL:HG23	1:A:248:LYS:CG	2.17	0.74
1:A:65:HIS:ND1	1:A:337:VAL:O	2.20	0.74
1:A:214:ILE:HB	1:A:215:PRO:HD3	1.69	0.73
1:A:90:GLY:O	1:A:94:THR:HG22	1.89	0.73
1:B:209:VAL:HA	1:B:213:ILE:HD12	1.71	0.73
1:A:316:CYS:SG	1:A:337:VAL:HG13	2.29	0.73
1:B:304:VAL:O	1:B:308:MET:HG2	1.90	0.72
2:A:504:NAG:H83	2:A:505:NAG:H62	1.70	0.72
1:A:304:VAL:O	1:A:308:MET:HG2	1.90	0.72
1:B:126:TRP:CH2	1:B:215:PRO:HG3	2.25	0.72
1:B:139:VAL:HB	1:B:226:LEU:HD23	1.72	0.72
1:B:90:GLY:O	1:B:94:THR:HG22	1.89	0.72
1:A:68:LEU:C	1:A:69:ARG:HD2	2.09	0.71
1:B:244:GLN:HB2	1:B:245:LYS:HD2	1.72	0.71
1:B:311:LYS:HG2	1:B:314:ARG:NH2	2.06	0.70
1:A:161:TRP:O	1:A:165:LEU:HD23	1.90	0.70
1:B:314:ARG:NH1	10:B:1401:HTO:H51	2.06	0.70
1:B:322:CYS:C	1:B:324:GLY:H	1.93	0.70
1:A:65:HIS:HD1	1:A:338:SER:HA	1.53	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:O	1:A:69:ARG:HD2	1.93	0.69
1:A:9:PHE:HA	1:A:179:ILE:CD1	2.22	0.69
1:B:135:ARG:HD2	1:B:251:THR:OG1	1.93	0.69
1:B:68:LEU:HB3	1:B:73:ASN:HD22	1.57	0.69
1:A:230:VAL:CG2	1:A:248:LYS:HG3	2.20	0.69
1:B:127:SER:O	1:B:131:LEU:HD23	1.92	0.69
1:A:346:ALA:H	1:A:347:PRO:HD3	1.58	0.68
1:B:128:LEU:HD22	1:B:258:VAL:HG22	1.76	0.68
1:A:50:LEU:CD2	1:A:54:ILE:HD11	2.23	0.68
1:A:209:VAL:HA	1:A:213:ILE:HD12	1.73	0.68
1:A:127:SER:O	1:A:131:LEU:HD23	1.93	0.68
1:B:91:PHE:CZ	1:B:296:LYS:HB3	2.30	0.67
1:A:126:TRP:CE2	1:A:163:MET:HB3	2.30	0.67
1:B:285:PRO:HD2	5:B:1506:BNG:H8'1	1.76	0.67
1:A:199:ASN:HD22	1:A:199:ASN:N	1.92	0.67
1:A:267:PRO:HA	5:A:1503:BNG:H7'1	1.76	0.67
1:B:66:LYS:HD2	1:B:67:LYS:H	1.60	0.66
1:A:134:GLU:HA	1:A:148:PHE:CE2	2.30	0.66
1:A:151:ASN:OD1	1:A:152:HIS:CE1	2.49	0.66
1:A:50:LEU:CD2	1:A:54:ILE:CD1	2.73	0.66
1:A:213:ILE:O	1:A:217:ILE:HD13	1.95	0.65
1:B:75:ILE:HG13	1:B:131:LEU:HD21	1.77	0.65
1:B:68:LEU:C	1:B:69:ARG:HD2	2.16	0.65
1:A:266:LEU:N	1:A:267:PRO:HD2	2.10	0.65
1:A:151:ASN:OD1	1:A:152:HIS:ND1	2.30	0.65
1:B:266:LEU:N	1:B:267:PRO:HD2	2.12	0.65
1:B:55:ASN:ND2	1:B:83:ASP:HB3	2.12	0.65
1:A:308:MET:HE3	1:B:99:LEU:HD21	1.78	0.64
1:A:65:HIS:HB3	1:A:337:VAL:CG2	2.22	0.64
1:A:75:ILE:CG2	1:A:131:LEU:HD21	2.25	0.64
1:A:50:LEU:HD21	1:A:54:ILE:HD11	1.78	0.64
1:B:208:PHE:O	1:B:213:ILE:HG13	1.98	0.63
1:A:208:PHE:O	1:A:213:ILE:HG13	1.97	0.63
1:A:75:ILE:O	1:A:79:LEU:HD22	1.99	0.63
1:A:142:PRO:HB2	1:A:143:MET:CE	2.25	0.63
1:B:213:ILE:O	1:B:217:ILE:HD13	1.97	0.63
1:A:300:VAL:O	1:A:303:PRO:HD2	1.99	0.63
1:A:68:LEU:HB3	1:A:73:ASN:HD22	1.63	0.63
1:B:139:VAL:CB	1:B:226:LEU:HD23	2.28	0.63
1:B:284:GLY:H	5:B:1506:BNG:H5'2	1.63	0.63
1:B:75:ILE:O	1:B:78:ASN:HB3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:H	1:A:337:VAL:HG21	1.63	0.62
1:B:300:VAL:O	1:B:303:PRO:HD2	2.00	0.62
1:B:39:MET:HE3	1:B:39:MET:HA	1.82	0.61
1:A:328:LEU:N	1:A:328:LEU:CD2	2.63	0.61
1:A:308:MET:HE1	1:B:41:ALA:HB1	1.82	0.61
1:A:201:GLU:O	1:A:205:ILE:HG13	2.01	0.61
1:A:197:GLU:O	1:A:197:GLU:HG2	2.01	0.61
1:B:284:GLY:H	5:B:1506:BNG:H3'1	1.64	0.61
1:A:65:HIS:HD1	1:A:337:VAL:C	2.05	0.61
1:A:75:ILE:O	1:A:78:ASN:HB3	2.00	0.61
1:B:75:ILE:CG2	1:B:131:LEU:HD21	2.30	0.60
1:A:102:TYR:CE2	1:A:104:VAL:HA	2.35	0.60
1:A:49:MET:CE	1:B:53:PRO:HB2	2.32	0.60
1:A:68:LEU:N	1:A:337:VAL:HG21	2.15	0.60
1:B:199:ASN:N	1:B:199:ASN:HD22	1.97	0.60
1:B:201:GLU:O	1:B:205:ILE:HG13	2.01	0.60
1:B:102:TYR:CE2	1:B:104:VAL:HA	2.36	0.60
1:B:152:HIS:N	1:B:152:HIS:ND1	2.47	0.60
1:B:132:ALA:O	1:B:222:CYS:SG	2.60	0.60
1:A:267:PRO:O	1:A:271:VAL:HG23	2.01	0.60
1:A:50:LEU:HD23	1:A:54:ILE:CD1	2.32	0.60
1:A:65:HIS:HD1	1:A:338:SER:CA	2.15	0.60
1:B:210:VAL:HA	1:B:214:ILE:HD12	1.83	0.59
1:B:322:CYS:C	1:B:324:GLY:N	2.56	0.59
1:A:252:ARG:HH21	5:A:1501:BNG:C6	2.14	0.59
1:B:298:SER:HA	1:B:301:TYR:CE2	2.37	0.59
1:A:328:LEU:HB3	1:B:105:PHE:CZ	2.34	0.59
1:B:9:PHE:HA	1:B:179:ILE:CD1	2.33	0.59
1:A:328:LEU:CB	1:B:96:TYR:CE2	2.62	0.59
1:A:75:ILE:HG22	1:A:79:LEU:CD2	2.32	0.59
1:A:54:ILE:HG12	1:B:49:MET:CE	2.31	0.59
1:B:126:TRP:CZ3	1:B:215:PRO:HG3	2.37	0.59
1:B:59:LEU:HD12	1:B:77:LEU:HD11	1.84	0.59
1:A:308:MET:CE	1:B:41:ALA:HB1	2.33	0.59
1:A:134:GLU:HG2	1:A:148:PHE:CD2	2.37	0.59
1:B:170:PRO:HB2	1:B:171:PRO:HD3	1.85	0.59
1:B:222:CYS:O	1:B:226:LEU:HD12	2.02	0.58
1:A:135:ARG:NE	1:A:135:ARG:HA	2.18	0.58
1:A:230:VAL:HA	1:A:248:LYS:HE3	1.84	0.58
1:A:9:PHE:CA	1:A:179:ILE:HD11	2.29	0.58
1:B:267:PRO:O	1:B:271:VAL:HG23	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:THR:O	1:A:342:THR:HG23	2.04	0.58
1:A:75:ILE:HG13	1:A:131:LEU:HD21	1.85	0.58
1:A:294:PHE:HB2	10:A:1403:HTO:H41	1.86	0.58
1:B:125:LEU:O	1:B:128:LEU:HB2	2.04	0.58
1:A:49:MET:HE3	1:B:53:PRO:HB2	1.86	0.58
1:A:67:LYS:N	1:A:337:VAL:HG23	2.13	0.57
1:B:271:VAL:HG21	1:B:291:PRO:HG3	1.85	0.57
1:A:67:LYS:HB2	1:A:337:VAL:CB	2.33	0.57
1:A:125:LEU:O	1:A:128:LEU:HB2	2.05	0.57
1:A:262:LEU:HB3	1:A:266:LEU:HD22	1.87	0.57
1:B:284:GLY:N	5:B:1506:BNG:H5'2	2.20	0.57
1:A:342:THR:HA	1:A:344:GLN:CD	2.24	0.57
4:A:704:NAG:H82	4:A:705:NAG:O6	2.04	0.57
1:A:65:HIS:HB2	1:A:68:LEU:HD12	1.87	0.56
1:B:136:TYR:HA	1:B:226:LEU:CD1	2.28	0.56
1:A:325:LYS:HG2	1:A:326:ASN:N	2.17	0.56
1:B:256:ILE:HA	1:B:259:ILE:HD12	1.87	0.56
1:A:290:ILE:HG23	10:A:1403:HTO:H42	1.86	0.56
1:B:50:LEU:CD2	1:B:54:ILE:HD12	2.34	0.56
1:A:298:SER:HA	1:A:301:TYR:CE2	2.41	0.56
1:A:76:LEU:HD22	1:A:306:TYR:CD2	2.40	0.56
1:A:135:ARG:NH1	1:A:247:GLU:HG3	2.20	0.56
1:A:67:LYS:HD3	1:A:343:SER:O	2.06	0.56
1:B:75:ILE:HG13	1:B:131:LEU:CD2	2.36	0.56
1:B:50:LEU:CD2	1:B:54:ILE:CD1	2.84	0.55
1:B:75:ILE:HG22	1:B:79:LEU:CD2	2.35	0.55
1:B:189:ILE:HB	1:B:191:TYR:CE1	2.41	0.55
1:A:139:VAL:HB	1:A:226:LEU:HD21	1.87	0.55
1:B:245:LYS:HD2	1:B:245:LYS:N	2.20	0.55
1:A:91:PHE:HA	1:A:94:THR:HG23	1.89	0.55
1:A:195:HIS:HB3	1:A:200:ASN:HD21	1.71	0.55
1:A:136:TYR:CA	1:A:226:LEU:HD11	2.34	0.55
1:B:50:LEU:HD21	1:B:54:ILE:HD11	1.89	0.55
5:A:1500:BNG:H3'1	1:B:35:TRP:HB2	1.89	0.55
1:A:119:LEU:O	1:A:123:ILE:HG13	2.07	0.55
1:B:139:VAL:HB	1:B:226:LEU:HD21	1.87	0.55
1:A:4:THR:HG21	1:A:20:VAL:HG11	1.88	0.55
1:A:199:ASN:ND2	1:A:199:ASN:N	2.55	0.55
1:B:68:LEU:CB	1:B:73:ASN:HD22	2.20	0.55
1:B:128:LEU:HB3	1:B:219:ILE:HD13	1.89	0.54
1:A:187:CYS:O	9:A:1296:RET:H12	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:HA	1:A:214:ILE:HD12	1.88	0.54
1:A:195:HIS:HB3	1:A:200:ASN:ND2	2.23	0.54
1:A:346:ALA:N	1:A:347:PRO:CD	2.70	0.54
1:B:72:LEU:HD22	1:B:250:VAL:CG1	2.26	0.54
1:B:197:GLU:O	1:B:197:GLU:CG	2.55	0.54
1:B:283:PHE:HA	5:B:1506:BNG:H3'1	1.89	0.54
1:B:66:LYS:HD2	1:B:67:LYS:N	2.23	0.53
1:A:345:VAL:HB	1:A:347:PRO:HD3	1.89	0.53
1:B:75:ILE:O	1:B:79:LEU:HD22	2.09	0.53
1:A:308:MET:CE	1:B:41:ALA:CB	2.87	0.53
1:B:179:ILE:HG13	1:B:180:PRO:HD2	1.90	0.53
1:B:284:GLY:H	5:B:1506:BNG:C3'	2.22	0.53
1:B:18:GLY:HA2	3:B:605:NAG:C1	2.38	0.53
1:A:139:VAL:HB	1:A:226:LEU:CD2	2.38	0.53
1:B:135:ARG:NE	1:B:135:ARG:HA	2.22	0.52
1:B:4:THR:HG21	1:B:20:VAL:HG11	1.90	0.52
1:A:137:VAL:O	1:A:141:LYS:HA	2.08	0.52
1:A:256:ILE:HA	1:A:259:ILE:HD12	1.91	0.52
1:A:342:THR:OG1	1:A:344:GLN:HG2	2.09	0.52
1:B:17:THR:OG1	1:B:19:VAL:HG12	2.09	0.52
1:B:19:VAL:HG22	1:B:19:VAL:O	2.09	0.52
1:B:252:ARG:O	1:B:256:ILE:HG12	2.10	0.52
1:B:199:ASN:N	1:B:199:ASN:ND2	2.58	0.52
1:B:280:GLY:O	4:B:805:NAG:H82	2.09	0.52
1:A:318:VAL:HG11	1:A:328:LEU:CD2	2.40	0.52
1:A:57:LEU:HD23	1:A:61:VAL:HG23	1.91	0.52
1:B:152:HIS:O	1:B:155:MET:HB2	2.09	0.51
1:A:59:LEU:O	1:A:63:VAL:HG12	2.11	0.51
1:B:221:PHE:O	1:B:224:GLY:N	2.43	0.51
1:A:328:LEU:HD22	1:A:328:LEU:H	1.73	0.51
1:A:222:CYS:O	1:A:226:LEU:HD12	2.10	0.51
1:A:126:TRP:CH2	1:A:215:PRO:HG3	2.44	0.51
1:B:220:PHE:O	1:B:223:TYR:HB3	2.11	0.51
1:A:322:CYS:O	1:A:323:CYS:SG	2.69	0.51
1:A:75:ILE:HG22	1:A:79:LEU:HD21	1.92	0.51
1:A:62:THR:HG21	1:A:77:LEU:HB2	1.92	0.51
1:A:327:PRO:O	1:A:329:GLY:N	2.43	0.50
1:A:54:ILE:CG1	1:B:49:MET:HE2	2.39	0.50
1:A:65:HIS:CE1	1:A:338:SER:OG	2.63	0.50
1:A:183:MET:HG3	1:A:289:THR:OG1	2.11	0.50
1:A:57:LEU:O	1:A:57:LEU:HD23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:HIS:O	1:A:155:MET:HB2	2.10	0.50
1:B:315:ASN:O	1:B:318:VAL:HG13	2.11	0.50
1:B:119:LEU:O	1:B:123:ILE:HG13	2.11	0.50
1:B:156:GLY:O	1:B:159:PHE:HB3	2.12	0.50
1:A:334:SER:N	10:A:1404:HTO:HO3	2.10	0.49
1:A:197:GLU:O	1:A:197:GLU:CG	2.60	0.49
1:A:305:ILE:HA	5:A:1500:BNG:H8'2	1.94	0.49
1:A:220:PHE:O	1:A:223:TYR:HB3	2.13	0.49
1:B:262:LEU:HB3	1:B:266:LEU:HD22	1.95	0.49
1:A:126:TRP:NE1	1:A:163:MET:HB3	2.28	0.49
1:B:59:LEU:HD12	1:B:77:LEU:CD1	2.42	0.49
1:A:64:GLN:NE2	1:A:320:THR:OG1	2.45	0.49
1:A:189:ILE:HB	1:A:191:TYR:CE1	2.48	0.49
1:A:68:LEU:HG	1:A:337:VAL:HG21	1.93	0.49
1:B:42:ALA:O	1:B:45:PHE:HB3	2.13	0.49
1:B:107:PRO:O	1:B:111:ASN:ND2	2.46	0.49
1:B:87:VAL:HA	1:B:91:PHE:HB2	1.94	0.49
1:B:136:TYR:HB2	1:B:222:CYS:SG	2.52	0.48
1:B:75:ILE:CG1	1:B:131:LEU:HD21	2.42	0.48
1:B:87:VAL:O	1:B:91:PHE:HB2	2.11	0.48
1:B:195:HIS:HB3	1:B:200:ASN:ND2	2.28	0.48
1:B:180:PRO:HA	1:B:186:SER:O	2.13	0.48
1:B:244:GLN:HB2	1:B:245:LYS:CD	2.42	0.48
1:A:139:VAL:O	1:A:229:THR:HG21	2.13	0.48
1:B:59:LEU:O	1:B:63:VAL:HG12	2.13	0.48
1:A:46:LEU:HD13	10:A:1400:HTO:H71	1.96	0.48
1:A:252:ARG:O	1:A:256:ILE:HG12	2.13	0.48
1:B:39:MET:HA	1:B:39:MET:CE	2.44	0.48
1:A:17:THR:OG1	1:A:19:VAL:HG12	2.14	0.48
1:A:76:LEU:HD22	1:A:306:TYR:CG	2.48	0.48
1:A:230:VAL:CA	1:A:248:LYS:HE3	2.44	0.48
1:A:75:ILE:HG13	1:A:131:LEU:CD2	2.43	0.48
1:B:287:PHE:HB2	5:B:1506:BNG:H4'1	1.96	0.48
1:A:55:ASN:ND2	1:A:83:ASP:HB3	2.29	0.48
1:A:32:ALA:HB1	1:A:36:GLN:OE1	2.14	0.48
1:B:195:HIS:HB3	1:B:200:ASN:HD21	1.78	0.47
1:B:50:LEU:HD23	1:B:54:ILE:CD1	2.40	0.47
1:A:139:VAL:HG12	1:A:229:THR:HB	1.96	0.47
1:B:77:LEU:O	1:B:81:VAL:HG23	2.14	0.47
1:A:311:LYS:NZ	1:A:330:ASP:H	2.12	0.47
1:A:107:PRO:O	1:A:111:ASN:ND2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:LEU:HB2	1:B:96:TYR:CD2	2.39	0.47
1:B:68:LEU:CA	1:B:73:ASN:HD22	2.27	0.47
1:A:271:VAL:HG21	1:A:291:PRO:HG3	1.96	0.47
1:B:91:PHE:O	1:B:94:THR:HG23	2.15	0.47
1:A:134:GLU:HA	1:A:148:PHE:HE2	1.75	0.47
1:B:57:LEU:C	1:B:57:LEU:HD23	2.34	0.47
1:A:167:CYS:HB2	1:A:211:HIS:CG	2.50	0.47
1:B:183:MET:HG3	1:B:289:THR:OG1	2.14	0.47
1:A:66:LYS:O	1:A:69:ARG:HD3	2.15	0.47
4:A:704:NAG:H3	4:A:704:NAG:H83	1.97	0.47
1:B:72:LEU:HD11	1:B:253:MET:CE	2.45	0.47
1:B:187:CYS:O	9:B:1296:RET:H12	2.15	0.47
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.96	0.47
1:A:308:MET:HE2	1:B:42:ALA:N	2.29	0.47
1:B:287:PHE:HB2	5:B:1506:BNG:H3'2	1.97	0.47
1:A:52:PHE:HB3	1:A:53:PRO:CD	2.46	0.46
1:A:57:LEU:C	1:A:57:LEU:HD23	2.35	0.46
1:A:230:VAL:HB	1:A:248:LYS:HE3	1.97	0.46
1:A:230:VAL:HG13	1:A:230:VAL:O	2.16	0.46
1:B:65:HIS:HB2	1:B:68:LEU:HD12	1.97	0.46
1:A:308:MET:CE	1:B:99:LEU:HD21	2.44	0.46
1:B:125:LEU:HB2	1:B:261:PHE:CZ	2.50	0.46
1:A:45:PHE:O	1:A:49:MET:HB2	2.15	0.46
1:A:252:ARG:HH21	5:A:1501:BNG:H62	1.78	0.46
1:A:148:PHE:HD1	1:A:152:HIS:CD2	2.34	0.46
1:A:322:CYS:C	1:A:323:CYS:SG	2.94	0.46
1:A:327:PRO:HA	1:A:328:LEU:HD22	1.96	0.46
1:A:53:PRO:HB2	1:B:49:MET:HE1	1.97	0.46
1:A:42:ALA:O	1:A:45:PHE:HB3	2.15	0.46
1:B:301:TYR:HE1	11:B:2008:HOH:O	1.98	0.46
1:B:167:CYS:HB2	1:B:211:HIS:CG	2.50	0.46
1:A:156:GLY:O	1:A:160:THR:HG23	2.15	0.46
1:A:75:ILE:HG21	1:A:131:LEU:CD2	2.36	0.46
1:A:114:GLY:HA2	1:A:187:CYS:O	2.16	0.46
1:A:180:PRO:HA	1:A:186:SER:O	2.15	0.46
1:A:18:GLY:HA2	2:A:505:NAG:C1	2.46	0.46
5:A:1500:BNG:C3'	1:B:35:TRP:HB2	2.46	0.46
1:B:298:SER:HA	1:B:301:TYR:CD2	2.49	0.46
1:A:19:VAL:HG22	1:A:19:VAL:O	2.16	0.46
1:A:72:LEU:HD22	1:A:250:VAL:HG13	1.98	0.46
1:A:327:PRO:C	1:A:328:LEU:HD22	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ILE:CG1	1:A:131:LEU:HD21	2.46	0.45
1:B:133:ILE:O	1:B:134:GLU:C	2.55	0.45
1:B:9:PHE:CA	1:B:179:ILE:HD11	2.40	0.45
1:A:152:HIS:N	1:A:152:HIS:HD1	2.14	0.45
1:A:263:ILE:O	1:A:294:PHE:HE2	1.99	0.45
1:A:167:CYS:HB2	1:A:211:HIS:CE1	2.51	0.45
1:B:64:GLN:O	1:B:64:GLN:HG2	2.17	0.45
1:A:139:VAL:HG11	1:A:230:VAL:HG12	1.97	0.45
1:B:128:LEU:HD22	1:B:258:VAL:CG2	2.44	0.45
1:A:155:MET:CE	1:A:155:MET:HA	2.47	0.45
1:B:6:GLY:C	1:B:8:ASN:H	2.19	0.45
1:A:68:LEU:CB	1:A:73:ASN:HD22	2.28	0.45
1:A:230:VAL:HG22	1:A:230:VAL:O	2.17	0.45
1:A:179:ILE:HG13	1:A:180:PRO:HD2	1.99	0.45
1:B:163:MET:O	1:B:166:ALA:HB3	2.16	0.45
1:B:41:ALA:O	1:B:95:LEU:HD13	2.17	0.45
5:A:1500:BNG:H1'1	1:B:35:TRP:HA	1.97	0.45
1:B:75:ILE:HG22	1:B:79:LEU:HD21	1.99	0.45
1:A:87:VAL:O	1:A:91:PHE:HB2	2.17	0.45
1:B:322:CYS:HA	8:B:1322:PLM:O2	2.15	0.45
1:A:133:ILE:O	1:A:134:GLU:C	2.55	0.45
1:B:266:LEU:N	1:B:267:PRO:CD	2.79	0.44
1:B:57:LEU:HD23	1:B:57:LEU:O	2.17	0.44
2:A:504:NAG:N2	2:A:505:NAG:H61	2.33	0.44
1:B:167:CYS:HB2	1:B:211:HIS:CE1	2.53	0.44
1:A:128:LEU:HB3	1:A:219:ILE:HD13	1.98	0.44
1:A:298:SER:HA	1:A:301:TYR:CD2	2.53	0.44
1:B:91:PHE:HA	1:B:94:THR:HG23	1.96	0.44
1:B:214:ILE:HB	1:B:215:PRO:CD	2.44	0.44
1:A:87:VAL:HA	1:A:91:PHE:HB2	2.00	0.44
1:A:266:LEU:N	1:A:267:PRO:CD	2.79	0.44
3:B:604:NAG:H82	3:B:605:NAG:H62	2.00	0.44
1:B:253:MET:HA	1:B:309:MET:CE	2.48	0.44
1:A:291:PRO:O	1:A:295:ALA:HB2	2.17	0.44
1:B:195:HIS:HB3	1:B:198:THR:HG22	2.00	0.44
1:B:52:PHE:HB3	1:B:53:PRO:CD	2.48	0.44
1:B:50:LEU:HD21	1:B:54:ILE:CD1	2.47	0.44
1:A:67:LYS:O	1:A:69:ARG:N	2.51	0.44
1:A:126:TRP:CZ3	1:A:215:PRO:HG3	2.53	0.44
1:B:209:VAL:O	1:B:214:ILE:HG13	2.18	0.43
1:A:50:LEU:CD2	1:A:54:ILE:HD12	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:LEU:CA	1:A:73:ASN:HD22	2.31	0.43
1:A:163:MET:O	1:A:166:ALA:HB3	2.18	0.43
1:B:244:GLN:HB2	1:B:245:LYS:CE	2.49	0.43
1:A:203:PHE:O	1:A:206:TYR:HB3	2.19	0.43
1:A:334:SER:N	10:A:1404:HTO:H2	2.34	0.43
1:A:9:PHE:C	1:A:179:ILE:HD11	2.40	0.43
1:A:347:PRO:HG3	5:A:1504:BNG:O3	2.19	0.43
8:A:1322:PLM:H72	1:B:88:PHE:HE1	1.84	0.43
1:B:136:TYR:CB	1:B:226:LEU:HD11	2.48	0.42
1:B:284:GLY:HA3	5:B:1506:BNG:H6'1	2.00	0.42
1:A:195:HIS:HB3	1:A:198:THR:HG22	2.01	0.42
1:A:169:ALA:N	1:A:170:PRO:CD	2.81	0.42
1:A:121:GLY:O	1:A:124:ALA:HB3	2.18	0.42
1:B:70:THR:O	1:B:71:PRO:C	2.56	0.42
1:B:66:LYS:HZ3	1:B:67:LYS:HG2	1.85	0.42
1:A:302:ASN:CB	1:A:303:PRO:HD3	2.50	0.42
1:B:20:VAL:HA	1:B:30:TYR:CZ	2.55	0.42
1:A:253:MET:HA	1:A:309:MET:CE	2.49	0.42
1:B:244:GLN:C	1:B:245:LYS:HD2	2.40	0.42
1:A:176:SER:OG	1:A:189:ILE:HG23	2.19	0.42
1:A:167:CYS:HB2	1:A:211:HIS:CD2	2.55	0.42
1:B:79:LEU:HG	1:B:302:ASN:ND2	2.33	0.42
1:A:194:PRO:O	1:A:195:HIS:C	2.58	0.42
1:B:57:LEU:HD23	1:B:61:VAL:HG23	2.02	0.42
1:A:97:THR:HG21	1:A:185:CYS:HA	2.02	0.42
1:B:121:GLY:O	1:B:124:ALA:HB3	2.20	0.42
1:B:285:PRO:CD	5:B:1506:BNG:H8'1	2.47	0.42
1:A:77:LEU:O	1:A:81:VAL:HG23	2.20	0.42
1:B:156:GLY:O	1:B:160:THR:HG23	2.20	0.42
1:A:64:GLN:O	1:A:64:GLN:HG2	2.19	0.42
1:B:126:TRP:CE2	1:B:163:MET:HB3	2.55	0.41
1:B:155:MET:CE	1:B:155:MET:HA	2.50	0.41
2:A:504:NAG:C8	2:A:505:NAG:H62	2.44	0.41
5:A:1500:BNG:H7'2	1:B:39:MET:HE3	2.02	0.41
1:A:66:LYS:HA	1:A:69:ARG:NH1	2.35	0.41
1:B:136:TYR:O	1:B:140:CYS:HB2	2.20	0.41
1:B:76:LEU:HA	1:B:79:LEU:HD23	2.02	0.41
1:A:4:THR:HG23	2:A:505:NAG:H83	2.01	0.41
1:A:152:HIS:N	1:A:152:HIS:ND1	2.67	0.41
1:A:318:VAL:HG11	1:A:327:PRO:HA	2.02	0.41
1:A:230:VAL:CB	1:A:248:LYS:HE3	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ALA:N	1:B:170:PRO:CD	2.83	0.41
1:A:97:THR:CG2	1:A:185:CYS:HA	2.51	0.41
1:B:40:LEU:HD22	1:B:293:PHE:CE2	2.55	0.41
1:A:22:SER:C	1:A:24:PHE:H	2.23	0.41
1:B:176:SER:OG	1:B:189:ILE:HG23	2.20	0.41
1:A:115:PHE:CD1	1:A:172:LEU:HD11	2.55	0.41
1:B:316:CYS:O	1:B:319:THR:HB	2.21	0.41
1:A:221:PHE:O	1:A:224:GLY:N	2.53	0.41
1:B:135:ARG:HG3	1:B:226:LEU:HD22	2.03	0.41
1:B:301:TYR:HA	10:B:1406:HTO:H11	2.03	0.41
1:B:264:CYS:HA	1:B:294:PHE:CE2	2.56	0.41
1:A:91:PHE:O	1:A:94:THR:HG23	2.21	0.41
1:A:135:ARG:HH12	1:A:247:GLU:HG3	1.85	0.41
1:A:264:CYS:HA	1:A:294:PHE:CE2	2.55	0.41
1:B:263:ILE:O	1:B:294:PHE:HE2	2.03	0.41
1:A:307:ILE:HD13	1:A:317:MET:SD	2.60	0.41
1:A:93:THR:HG21	1:A:109:GLY:CA	2.51	0.41
1:B:315:ASN:HA	1:B:315:ASN:HD22	1.63	0.41
1:B:68:LEU:HA	1:B:73:ASN:ND2	2.36	0.40
1:B:197:GLU:HG3	1:B:197:GLU:O	2.21	0.40
1:B:194:PRO:O	1:B:195:HIS:C	2.60	0.40
1:A:286:ILE:HB	5:A:1505:BNG:H3'1	2.03	0.40
1:A:158:ALA:O	1:A:162:VAL:HG23	2.21	0.40
1:A:76:LEU:HD13	1:A:306:TYR:CE1	2.56	0.40
1:B:129:VAL:HG13	1:B:218:VAL:HG11	2.03	0.40
1:B:150:GLU:HA	1:B:153:ALA:HB3	2.03	0.40
1:A:65:HIS:HB2	1:A:68:LEU:CD1	2.52	0.40
1:B:167:CYS:HB2	1:B:211:HIS:CD2	2.56	0.40
1:A:109:GLY:O	1:A:113:GLU:HB2	2.21	0.40
1:A:233:ALA:O	1:A:234:ALA:HB2	2.22	0.40
1:A:39:MET:CE	1:A:39:MET:HA	2.50	0.40
1:A:70:THR:O	1:A:71:PRO:C	2.59	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:196:GLU:OE2	7:B:958:ZN:ZN[2_654]	1.56	0.64

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	335/349 (96%)	275 (82%)	50 (15%)	10 (3%)	5	18
1	B	296/349 (85%)	256 (86%)	38 (13%)	2 (1%)	26	62
All	All	631/698 (90%)	531 (84%)	88 (14%)	12 (2%)	10	32

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	ALA
1	A	328	LEU
1	A	341	GLU
1	A	195	HIS
1	A	232	GLU
1	A	324	GLY
1	A	337	VAL
1	A	323	CYS
1	A	347	PRO
1	B	195	HIS
1	A	338	SER
1	B	300	VAL

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	289/296 (98%)	262 (91%)	27 (9%)	11	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	257/296 (87%)	235 (91%)	22 (9%)	13	36
All	All	546/592 (92%)	497 (91%)	49 (9%)	12	34

All (49) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	50	LEU
1	A	59	LEU
1	A	69	ARG
1	A	70	THR
1	A	76	LEU
1	A	79	LEU
1	A	94	THR
1	A	96	TYR
1	A	135	ARG
1	A	143	MET
1	A	147	ARG
1	A	151	ASN
1	A	152	HIS
1	A	199	ASN
1	A	222	CYS
1	A	226	LEU
1	A	232	GLU
1	A	247	GLU
1	A	248	LYS
1	A	252	ARG
1	A	264	CYS
1	A	286	ILE
1	A	328	LEU
1	A	330	ASP
1	A	341	GLU
1	A	344	GLN
1	B	8	ASN
1	B	27	PRO
1	B	39	MET
1	B	50	LEU
1	B	59	LEU
1	B	66	LYS
1	B	69	ARG
1	B	70	THR
1	B	76	LEU

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Mol	Chain	Res	Type
1	B	79	LEU
1	B	94	THR
1	B	96	TYR
1	B	135	ARG
1	B	152	HIS
1	B	177	ARG
1	B	222	CYS
1	B	249	GLU
1	B	252	ARG
1	B	264	CYS
1	B	266	LEU
1	B	286	ILE
1	B	318	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	64	GLN
1	A	199	ASN
1	A	302	ASN
1	A	315	ASN
1	B	8	ASN
1	B	64	GLN
1	B	111	ASN
1	B	199	ASN
1	B	302	ASN
1	B	312	GLN
1	B	315	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	0.67	0	14,15,17	0.75	0
2	NAG	A	504	2	14,14,15	0.64	0	15,19,21	0.89	0
2	NAG	A	505	1,2	14,14,15	0.66	0	15,19,21	0.71	0
4	NAG	A	704	4	14,14,15	0.81	0	15,19,21	0.79	0
4	NAG	A	705	1,4	14,14,15	0.54	0	15,19,21	0.84	1 (6%)
3	BMA	B	602	3	11,11,12	0.67	0	14,15,17	0.72	0
3	BMA	B	603	3	11,11,12	0.72	0	14,15,17	0.64	0
3	NAG	B	604	3	14,14,15	0.50	0	15,19,21	0.91	1 (6%)
3	NAG	B	605	1,3	14,14,15	0.47	0	15,19,21	0.79	1 (6%)
4	NAG	B	804	4	14,14,15	0.78	0	15,19,21	0.65	0
4	NAG	B	805	1,4	14,14,15	0.65	0	15,19,21	0.70	0

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	-	1/6/23/26	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	-	1/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604	NAG	C2-N2-C7	-2.79	119.45	123.04
4	A	705	NAG	C2-N2-C7	-2.31	120.07	123.04
3	B	605	NAG	C2-N2-C7	-2.13	120.31	123.04

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	805	NAG	O7-C7-N2-C2
4	A	705	NAG	O7-C7-N2-C2

There are no ring outliers.

7 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	NAG	3	0
2	A	505	NAG	5	0
4	A	704	NAG	2	0
4	A	705	NAG	1	0
3	B	604	NAG	1	0
3	B	605	NAG	2	0
4	B	805	NAG	1	0

5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 13 are monoatomic - leaving 18 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	$\# Z > 2$
9	RET	A	1296	1	19,20,21	1.69	5 (26%)	27,27,28	1.88	9 (33%)
8	PLM	A	1322	1	16,16,17	0.33	0	14,15,17	0.56	0
8	PLM	A	1323	1	16,16,17	0.50	0	14,15,17	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	HTO	A	1400	-	9,9,9	1.53	2 (22%)	8,10,10	0.74	0
10	HTO	A	1403	-	9,9,9	1.42	1 (11%)	8,10,10	0.54	0
10	HTO	A	1404	-	9,9,9	1.54	1 (11%)	8,10,10	0.75	0
10	HTO	A	1405	-	9,9,9	1.24	1 (11%)	8,10,10	0.51	0
5	BNG	A	1500	-	21,21,21	1.26	3 (14%)	26,26,26	0.60	0
5	BNG	A	1501	-	21,21,21	1.23	2 (9%)	26,26,26	0.64	0
5	BNG	A	1503	-	21,21,21	1.21	3 (14%)	26,26,26	0.61	0
5	BNG	A	1504	-	21,21,21	1.28	3 (14%)	26,26,26	0.62	0
5	BNG	A	1505	-	21,21,21	1.36	3 (14%)	26,26,26	0.67	0
9	RET	B	1296	1	19,20,21	1.47	3 (15%)	27,27,28	1.91	9 (33%)
8	PLM	B	1322	1	16,16,17	0.42	0	14,15,17	0.49	0
10	HTO	B	1401	-	9,9,9	1.44	1 (11%)	8,10,10	0.90	0
10	HTO	B	1406	-	9,9,9	1.53	2 (22%)	8,10,10	0.81	0
5	BNG	B	1502	-	21,21,21	1.39	2 (9%)	26,26,26	0.65	0
5	BNG	B	1506	-	21,21,21	1.34	3 (14%)	26,26,26	0.64	0

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
9	RET	A	1296	1	-	0/13/30/31	0/1/1/1
8	PLM	A	1322	1	-	0/13/14/15	0/0/0/0
8	PLM	A	1323	1	-	0/13/14/15	0/0/0/0
10	HTO	A	1400	-	-	0/10/10/10	0/0/0/0
10	HTO	A	1403	-	-	0/10/10/10	0/0/0/0
10	HTO	A	1404	-	-	0/10/10/10	0/0/0/0
10	HTO	A	1405	-	-	0/10/10/10	0/0/0/0
5	BNG	A	1500	-	-	0/12/32/32	0/1/1/1
5	BNG	A	1501	-	-	0/12/32/32	0/1/1/1
5	BNG	A	1503	-	-	0/12/32/32	0/1/1/1
5	BNG	A	1504	-	-	0/12/32/32	0/1/1/1
5	BNG	A	1505	-	-	0/12/32/32	0/1/1/1
9	RET	B	1296	1	-	0/13/30/31	0/1/1/1
8	PLM	B	1322	1	-	0/13/14/15	0/0/0/0
10	HTO	B	1401	-	-	0/10/10/10	0/0/0/0
10	HTO	B	1406	-	-	0/10/10/10	0/0/0/0
5	BNG	B	1502	-	-	0/12/32/32	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	BNG	B	1506	-	-	0/12/32/32	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	1296	RET	C1-C6	-2.49	1.50	1.53
5	A	1505	BNG	C4-C5	2.03	1.57	1.53
10	A	1400	HTO	C4-C3	2.11	1.56	1.52
5	A	1503	BNG	C4-C5	2.13	1.57	1.53
9	B	1296	RET	C12-C13	2.17	1.50	1.45
9	B	1296	RET	C18-C5	2.18	1.54	1.51
9	A	1296	RET	C17-C1	2.22	1.58	1.53
5	A	1500	BNG	C4-C5	2.24	1.57	1.53
5	B	1506	BNG	C4-C5	2.36	1.58	1.53
9	B	1296	RET	C17-C1	2.38	1.58	1.53
10	B	1406	HTO	C4-C3	2.38	1.57	1.52
5	A	1504	BNG	C4-C5	2.39	1.58	1.53
9	A	1296	RET	C5-C6	2.61	1.38	1.34
5	A	1503	BNG	O1-C1	2.62	1.44	1.40
5	A	1504	BNG	O1-C1	2.71	1.45	1.40
5	A	1500	BNG	O1-C1	2.75	1.45	1.40
5	A	1501	BNG	O1-C1	2.88	1.45	1.40
5	A	1501	BNG	O5-C1	3.03	1.49	1.41
10	A	1405	HTO	C3-C2	3.04	1.61	1.52
5	B	1506	BNG	O1-C1	3.09	1.45	1.40
5	A	1504	BNG	O5-C1	3.10	1.49	1.41
9	A	1296	RET	C18-C5	3.13	1.56	1.51
9	A	1296	RET	C2-C1	3.14	1.61	1.54
5	A	1505	BNG	O5-C1	3.15	1.49	1.41
5	A	1500	BNG	O5-C1	3.16	1.49	1.41
5	A	1503	BNG	O5-C1	3.21	1.50	1.41
5	B	1506	BNG	O5-C1	3.27	1.50	1.41
5	B	1502	BNG	O5-C1	3.30	1.50	1.41
10	B	1406	HTO	C3-C2	3.36	1.62	1.52
10	A	1403	HTO	C3-C2	3.42	1.62	1.52
5	A	1505	BNG	O1-C1	3.46	1.46	1.40
10	A	1400	HTO	C3-C2	3.54	1.62	1.52
10	A	1404	HTO	C3-C2	3.55	1.62	1.52
10	B	1401	HTO	C3-C2	3.59	1.62	1.52
5	B	1502	BNG	O1-C1	3.69	1.46	1.40

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	1296	RET	C19-C9-C8	-3.17	112.82	118.10
9	B	1296	RET	C8-C7-C6	-2.87	118.71	127.32
9	A	1296	RET	C19-C9-C8	-2.64	113.69	118.10
9	A	1296	RET	C17-C1-C2	-2.32	100.46	108.79
9	A	1296	RET	C3-C4-C5	-2.30	110.22	113.87
9	B	1296	RET	C18-C5-C6	2.10	126.67	124.61
9	A	1296	RET	C10-C11-C12	2.26	130.01	123.13
9	A	1296	RET	C8-C9-C10	2.49	122.99	118.98
9	B	1296	RET	C17-C1-C6	2.68	114.51	110.30
9	B	1296	RET	C10-C11-C12	2.74	131.47	123.13
9	B	1296	RET	C8-C9-C10	2.84	123.56	118.98
9	A	1296	RET	C7-C8-C9	2.89	130.62	126.22
9	B	1296	RET	C7-C8-C9	3.01	130.81	126.22
9	A	1296	RET	C2-C1-C6	3.17	115.38	110.36
9	B	1296	RET	C2-C1-C6	3.58	116.02	110.36
9	A	1296	RET	C17-C1-C6	3.91	116.44	110.30
9	B	1296	RET	C11-C12-C13	4.45	139.42	126.32
9	A	1296	RET	C11-C12-C13	4.50	139.56	126.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	1296	RET	1	0
8	A	1322	PLM	1	0
10	A	1400	HTO	1	0
10	A	1403	HTO	2	0
10	A	1404	HTO	2	0
5	A	1500	BNG	5	0
5	A	1501	BNG	2	0
5	A	1503	BNG	1	0
5	A	1504	BNG	1	0
5	A	1505	BNG	1	0
9	B	1296	RET	1	0
8	B	1322	PLM	1	0
10	B	1401	HTO	1	0
10	B	1406	HTO	1	0
5	B	1506	BNG	10	0

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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.