



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:13 AM GMT

PDB ID : 2G87
Title : Crystallographic model of bathorhodopsin
Authors : Nakamichi, H.; Okada, T.
Deposited on : 2006-03-02
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<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

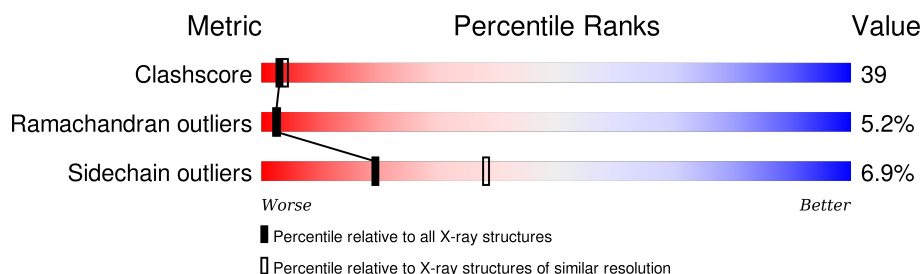
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)

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	

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		

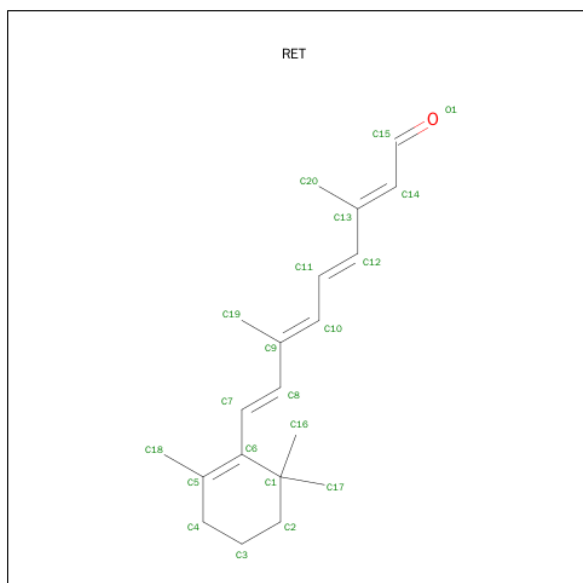
- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

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: C₂₀H₂₈O).



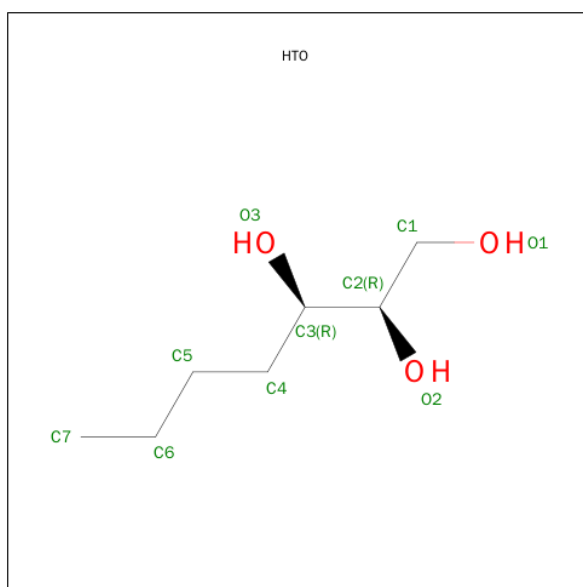
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	C	0	0
			20	20		
7	B	1	Total	C	0	0
			20	20		

- Molecule 8 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



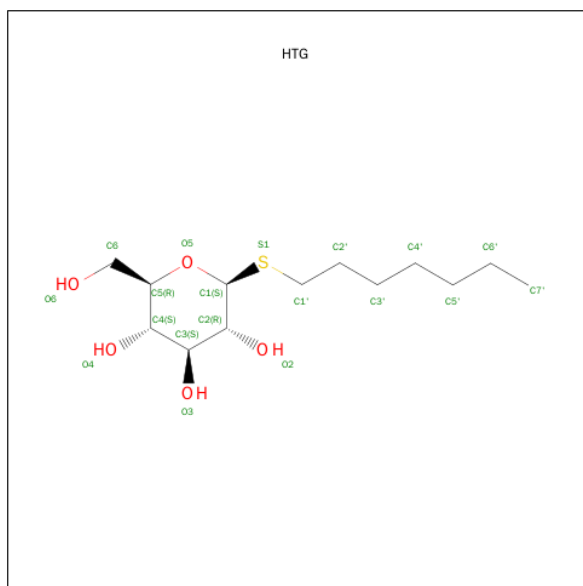
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			17	16	1		
8	A	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C	O	0	0
			17	16	1		
8	B	1	Total	C		0	0
			16	16			
8	A	1	Total	C		0	0
			16	16			

- Molecule 9 is HEPTANE-1,2,3-TRIOL (three-letter code: HTO) (formula: C₇H₁₆O₃).



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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	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.

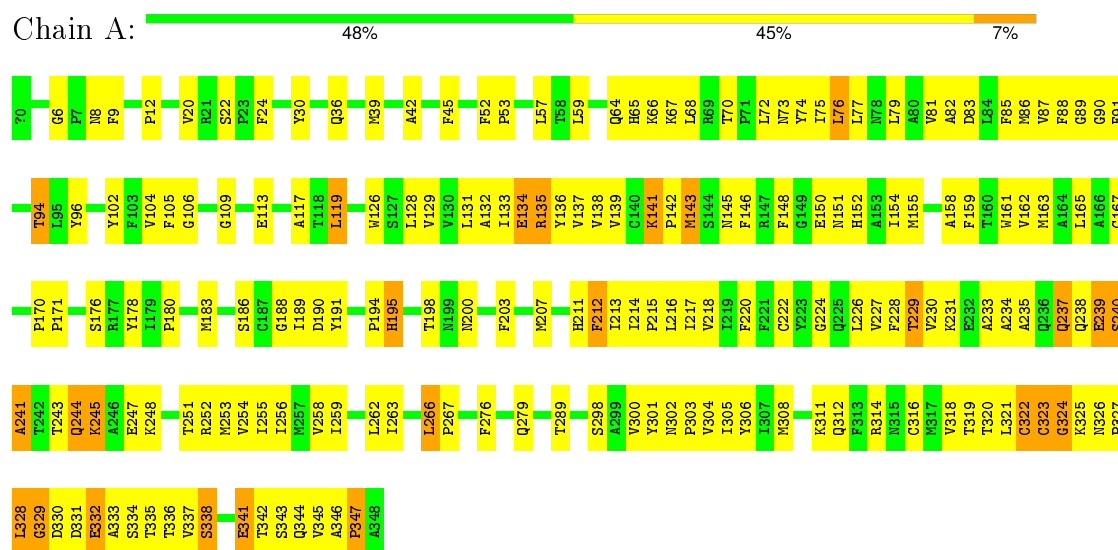
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	37	Total	O	0	0
			37	37		
11	B	29	Total	O	0	0
			29	29		

3 Residue-property plots

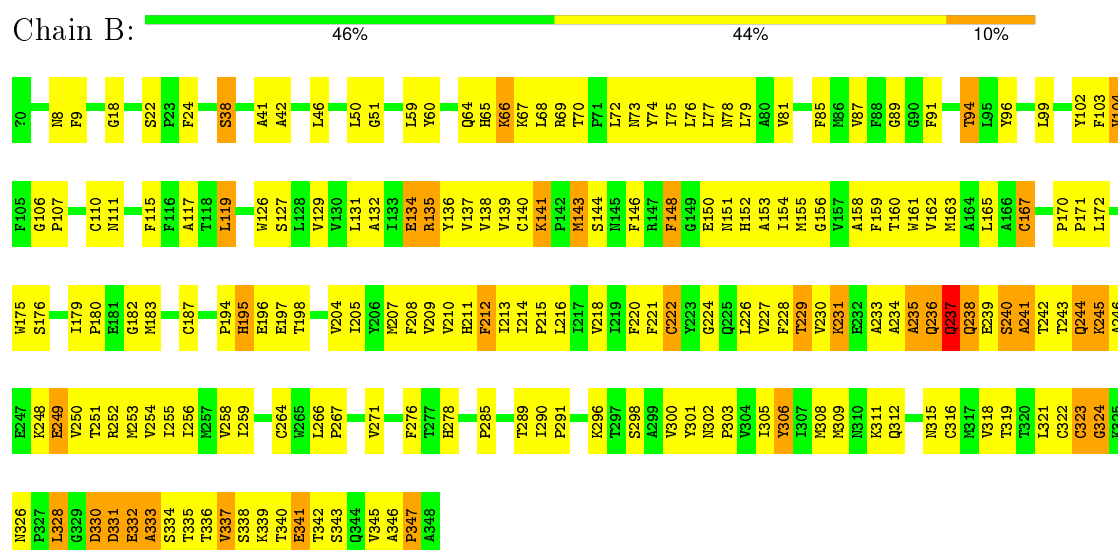
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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	96.49Å 96.49Å 150.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.60	Depositor
% Data completeness (in resolution range)	(Not available) (50.00-2.60)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.178 , 0.181	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5948	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

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	0.61	0/2831	0.67	0/3859
1	B	0.60	0/2831	0.68	0/3859
All	All	0.60	0/5662	0.67	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	2706	217	0
1	B	2749	0	2707	239	0
2	A	39	0	34	1	0
3	B	50	0	43	2	0
4	A	28	0	25	1	0
4	B	28	0	25	0	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	3	0
7	B	20	0	27	4	0
8	A	50	0	89	4	0
8	B	50	0	89	5	0
9	B	10	0	16	1	0
10	A	19	0	26	0	0
10	B	57	0	78	5	0
11	A	37	0	0	3	0
11	B	29	0	0	4	0
All	All	5948	0	5892	454	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (454) 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:312:GLN:HA	1:B:332:GLU:HG2	1.32	1.08
1:A:65:HIS:HB3	1:A:337:VAL:HG22	1.37	1.03
1:A:345:VAL:HG12	1:A:347:PRO:HD3	1.37	1.03
1:B:239:GLU:HB2	1:B:245:LYS:HD2	1.40	1.03
1:B:245:LYS:HA	1:B:245:LYS:HE3	1.39	1.02
1:B:245:LYS:NZ	1:B:248:LYS:HD2	1.76	1.01
1:A:316:CYS:SG	1:A:337:VAL:HG13	2.05	0.96
1:A:311:LYS:HD2	1:A:314:ARG:NH2	1.79	0.96
1:A:326:ASN:O	1:A:328:LEU:HD22	1.71	0.91
1:A:88:PHE:HB3	8:B:1323:PLM:HB1	1.54	0.90
1:B:346:ALA:N	1:B:347:PRO:HD3	1.86	0.90
1:A:94:THR:HB	1:A:113:GLU:OE2	1.73	0.89
1:B:322:CYS:HA	8:B:1322:PLM:O1	1.73	0.88
1:B:72:LEU:HD22	1:B:250:VAL:HG13	1.55	0.87
1:B:239:GLU:HB3	1:B:244:GLN:HE22	1.40	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:337:VAL:HB	1:B:343:SER:HA	1.59	0.85
1:A:91:PHE:HA	1:A:94:THR:CG2	2.06	0.85
1:A:326:ASN:HD21	1:A:328:LEU:HD11	1.41	0.85
1:B:238:GLN:HG3	1:B:241:ALA:H	1.41	0.84
1:B:245:LYS:HZ1	1:B:248:LYS:HD2	1.37	0.84
1:A:70:THR:H	1:A:73:ASN:HD22	1.26	0.83
1:B:170:PRO:HB2	1:B:171:PRO:HD3	1.60	0.82
1:A:341:GLU:OE1	1:A:342:THR:HG22	1.78	0.82
1:B:230:VAL:HG23	1:B:248:LYS:HD3	1.62	0.82
7:A:1296:RET:H8	7:A:1296:RET:H181	1.60	0.82
1:B:75:ILE:HG13	1:B:131:LEU:CD1	2.10	0.82
1:B:91:PHE:HA	1:B:94:THR:CG2	2.09	0.81
1:A:329:GLY:HA2	1:B:96:TYR:CE1	2.18	0.79
1:B:67:LYS:HD3	1:B:337:VAL:HG13	1.65	0.79
1:A:308:MET:HE3	1:B:99:LEU:HD21	1.62	0.79
1:A:96:TYR:HE2	1:A:104:VAL:HG21	1.49	0.78
1:A:345:VAL:HG12	1:A:347:PRO:CD	2.13	0.78
1:B:183:MET:HE3	1:B:289:THR:HG21	1.64	0.77
7:B:1296:RET:H181	7:B:1296:RET:H8	1.66	0.77
1:B:332:GLU:HB3	1:B:335:THR:O	1.85	0.77
1:A:67:LYS:HB2	1:A:337:VAL:HB	1.65	0.77
1:A:341:GLU:CG	1:A:342:THR:H	1.97	0.76
1:A:341:GLU:HG3	1:A:342:THR:N	2.01	0.76
1:B:139:VAL:HG11	1:B:230:VAL:HG12	1.66	0.75
1:A:308:MET:CE	1:B:99:LEU:HD21	2.16	0.75
1:A:59:LEU:HD12	1:A:77:LEU:HD11	1.68	0.75
1:B:337:VAL:HG23	1:B:338:SER:N	2.02	0.75
1:A:304:VAL:O	1:A:308:MET:HG2	1.86	0.75
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.67	0.74
1:A:329:GLY:HA2	1:B:96:TYR:HE1	1.52	0.74
1:A:341:GLU:HG3	1:A:342:THR:H	1.53	0.73
1:B:67:LYS:NZ	1:B:312:GLN:HG3	2.03	0.73
1:B:75:ILE:HG13	1:B:131:LEU:HD11	1.72	0.72
1:A:239:GLU:HB3	1:A:244:GLN:CD	2.09	0.71
1:B:139:VAL:CG1	1:B:230:VAL:HG12	2.20	0.71
1:B:208:PHE:O	1:B:213:ILE:HG13	1.90	0.71
1:A:170:PRO:HB2	1:A:171:PRO:HD3	1.72	0.71
1:A:245:LYS:HA	1:A:245:LYS:NZ	2.06	0.71
1:B:70:THR:H	1:B:73:ASN:HD22	1.39	0.70
1:A:230:VAL:HG23	1:A:248:LYS:HE2	1.73	0.70
1:B:59:LEU:HD13	1:B:77:LEU:HD11	1.73	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:HIS:HB2	1:B:68:LEU:HD12	1.74	0.70
1:A:262:LEU:HB3	1:A:266:LEU:HD22	1.73	0.70
1:A:150:GLU:O	1:A:154:ILE:HG13	1.91	0.70
1:A:245:LYS:HA	1:A:245:LYS:HZ2	1.55	0.70
1:B:9:PHE:HA	1:B:179:ILE:HD11	1.72	0.69
1:B:337:VAL:HA	1:B:342:THR:HG23	1.73	0.69
1:B:234:ALA:HB1	1:B:245:LYS:HE2	1.74	0.69
1:B:67:LYS:HB3	1:B:337:VAL:CG2	2.23	0.69
1:A:332:GLU:C	1:A:334:SER:H	1.95	0.69
1:B:64:GLN:HG3	1:B:339:LYS:HE2	1.74	0.69
1:A:135:ARG:HD3	1:A:251:THR:HA	1.75	0.68
1:A:65:HIS:ND1	1:A:338:SER:HA	2.07	0.68
1:A:325:LYS:HE3	1:A:341:GLU:OE1	1.93	0.68
1:B:239:GLU:HB3	1:B:244:GLN:NE2	2.07	0.68
1:A:239:GLU:HG2	1:A:248:LYS:NZ	2.08	0.68
1:A:183:MET:HE3	1:A:289:THR:HG21	1.76	0.68
1:B:231:LYS:NZ	1:B:233:ALA:HB3	2.09	0.68
1:A:65:HIS:CG	1:A:338:SER:HA	2.27	0.68
1:B:96:TYR:HE2	1:B:104:VAL:HG21	1.59	0.68
1:B:69:ARG:N	1:B:73:ASN:HD22	1.92	0.68
1:B:237:GLN:O	1:B:238:GLN:HB3	1.94	0.67
1:B:132:ALA:O	1:B:222:CYS:SG	2.52	0.67
1:A:239:GLU:HB3	1:A:244:GLN:NE2	2.10	0.67
1:A:75:ILE:HG13	1:A:131:LEU:CD1	2.23	0.67
1:B:70:THR:H	1:B:73:ASN:ND2	1.93	0.67
1:A:314:ARG:O	1:A:318:VAL:HG23	1.93	0.67
1:A:311:LYS:HD2	1:A:314:ARG:HH21	1.57	0.67
1:A:76:LEU:HD22	1:A:306:TYR:CG	2.29	0.67
1:B:255:ILE:O	1:B:259:ILE:HG12	1.94	0.67
1:A:137:VAL:O	1:A:141:LYS:HA	1.94	0.67
1:B:267:PRO:HG2	11:B:2019:HOH:O	1.95	0.67
1:A:161:TRP:O	1:A:165:LEU:HD23	1.95	0.66
1:B:238:GLN:HG3	1:B:241:ALA:N	2.09	0.66
1:A:96:TYR:HE2	1:A:104:VAL:CG2	2.09	0.66
1:B:38:SER:HB3	10:B:1508:HTG:H4'1	1.78	0.65
1:A:126:TRP:CH2	1:A:215:PRO:HG3	2.31	0.65
1:B:183:MET:CE	1:B:289:THR:HG21	2.27	0.65
1:A:198:THR:HG23	1:A:200:ASN:OD1	1.96	0.65
1:A:235:ALA:HB3	1:A:239:GLU:OE1	1.97	0.65
1:B:136:TYR:HA	1:B:226:LEU:HD11	1.78	0.64
1:A:59:LEU:CD1	1:A:77:LEU:HD11	2.26	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLN:HG2	1:B:65:HIS:CD2	2.32	0.64
1:B:312:GLN:HA	1:B:332:GLU:CG	2.17	0.64
1:A:302:ASN:HB2	1:A:303:PRO:HD3	1.80	0.64
1:B:338:SER:HB2	1:B:341:GLU:CG	2.27	0.64
1:B:67:LYS:HZ2	1:B:312:GLN:HG3	1.60	0.64
1:B:341:GLU:HG3	1:B:342:THR:H	1.62	0.64
1:B:245:LYS:HE3	1:B:245:LYS:CA	2.21	0.64
1:A:247:GLU:OE1	1:A:247:GLU:HA	1.96	0.64
1:A:325:LYS:HE2	1:A:327:PRO:HD3	1.80	0.64
1:B:59:LEU:CD1	1:B:77:LEU:HD11	2.27	0.64
1:B:216:LEU:O	1:B:220:PHE:HD2	1.79	0.64
1:A:337:VAL:O	1:A:338:SER:OG	2.16	0.63
1:A:239:GLU:HG2	1:A:248:LYS:HZ2	1.62	0.63
1:B:271:VAL:HG21	1:B:291:PRO:HG3	1.81	0.63
1:A:64:GLN:HE22	1:A:320:THR:HG23	1.64	0.62
1:B:337:VAL:CA	1:B:342:THR:HG23	2.30	0.62
1:A:341:GLU:CG	1:A:342:THR:N	2.61	0.62
1:B:230:VAL:HG23	1:B:248:LYS:CD	2.28	0.62
1:B:239:GLU:CB	1:B:244:GLN:HE22	2.10	0.62
1:B:298:SER:HA	1:B:301:TYR:CD2	2.34	0.62
1:B:337:VAL:HA	1:B:342:THR:O	1.98	0.62
1:A:129:VAL:HG13	1:A:218:VAL:HG11	1.82	0.62
1:A:148:PHE:HA	1:A:152:HIS:ND1	2.15	0.62
1:A:239:GLU:HB3	1:A:244:GLN:OE1	2.00	0.61
1:B:253:MET:HA	1:B:309:MET:SD	2.40	0.61
1:A:251:THR:O	1:A:255:ILE:HG13	2.00	0.61
1:A:189:ILE:HG22	1:A:190:ASP:N	2.15	0.61
1:B:67:LYS:HB3	1:B:337:VAL:HG21	1.82	0.61
1:B:234:ALA:HA	1:B:245:LYS:NZ	2.16	0.61
1:A:298:SER:HA	1:A:301:TYR:CE2	2.36	0.61
1:B:248:LYS:O	1:B:252:ARG:HG3	2.00	0.61
1:B:91:PHE:HA	1:B:94:THR:HG22	1.82	0.61
1:A:312:GLN:HB2	1:A:332:GLU:HG3	1.83	0.60
1:B:298:SER:HA	1:B:301:TYR:CE2	2.34	0.60
1:A:195:HIS:HD1	1:A:198:THR:CG2	2.15	0.60
1:A:237:GLN:O	1:A:238:GLN:HB3	2.01	0.60
1:A:67:LYS:H	1:A:337:VAL:CG2	2.15	0.60
1:A:311:LYS:HZ1	1:A:330:ASP:HB2	1.67	0.60
1:B:67:LYS:HB3	1:B:337:VAL:CG1	2.31	0.60
1:A:65:HIS:HB3	1:A:337:VAL:CG2	2.22	0.59
1:A:212:PHE:O	1:A:216:LEU:HD23	2.02	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:LYS:HZ3	1:B:335:THR:C	2.06	0.59
1:A:326:ASN:OD1	1:A:328:LEU:HD13	2.03	0.59
1:B:65:HIS:CG	1:B:338:SER:HA	2.38	0.59
1:B:338:SER:HB2	1:B:341:GLU:HG3	1.84	0.59
1:A:237:GLN:CD	1:A:237:GLN:H	2.06	0.58
1:A:311:LYS:HD2	1:A:314:ARG:HH22	1.68	0.58
1:A:211:HIS:O	1:A:212:PHE:HB2	2.02	0.58
1:B:239:GLU:HB2	1:B:245:LYS:CD	2.23	0.58
1:A:227:VAL:HG13	1:A:228:PHE:N	2.18	0.58
1:B:238:GLN:HA	1:B:242:THR:HA	1.85	0.58
1:B:143:MET:HA	1:B:143:MET:HE2	1.86	0.57
1:B:64:GLN:HG2	1:B:65:HIS:HD2	1.68	0.57
1:B:245:LYS:HZ2	1:B:248:LYS:HD2	1.64	0.57
1:B:194:PRO:O	1:B:195:HIS:C	2.43	0.57
1:B:209:VAL:O	1:B:214:ILE:HG13	2.05	0.57
1:A:198:THR:CG2	1:A:200:ASN:OD1	2.53	0.57
1:A:267:PRO:HG2	11:A:964:HOH:O	2.03	0.57
1:B:9:PHE:CA	1:B:179:ILE:HD11	2.33	0.57
1:B:235:ALA:HB3	1:B:239:GLU:OE1	2.05	0.57
1:A:90:GLY:O	1:A:94:THR:HG22	2.03	0.57
1:A:311:LYS:NZ	1:A:330:ASP:HB2	2.20	0.57
2:A:504:NAG:C7	2:A:505:NAG:H61	2.35	0.57
1:A:342:THR:O	1:A:342:THR:HG23	2.03	0.56
1:A:75:ILE:HG13	1:A:131:LEU:HD11	1.85	0.56
1:B:119:LEU:HD21	1:B:165:LEU:HD22	1.85	0.56
1:B:96:TYR:HE2	1:B:104:VAL:CG2	2.18	0.56
1:B:69:ARG:HH11	1:B:69:ARG:HG2	1.70	0.56
1:A:139:VAL:HG11	1:A:226:LEU:HG	1.86	0.56
8:B:1322:PLM:H52	8:B:1323:PLM:H61	1.86	0.56
1:A:12:PRO:HD3	11:A:2064:HOH:O	2.04	0.56
1:A:254:VAL:O	1:A:258:VAL:HG23	2.06	0.56
1:B:22:SER:C	1:B:24:PHE:H	2.09	0.56
1:A:321:LEU:HD13	8:A:1322:PLM:H72	1.88	0.56
1:B:246:ALA:O	1:B:249:GLU:HG2	2.06	0.56
1:B:126:TRP:CE2	1:B:163:MET:HB3	2.40	0.56
1:A:183:MET:CE	1:A:289:THR:HG21	2.35	0.56
1:B:224:GLY:O	1:B:227:VAL:HG12	2.06	0.56
1:B:131:LEU:O	1:B:135:ARG:HB2	2.06	0.55
1:B:337:VAL:HA	1:B:342:THR:C	2.27	0.55
1:A:91:PHE:HA	1:A:94:THR:HG22	1.88	0.55
1:B:256:ILE:HG22	1:B:305:ILE:HD13	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:CYS:SG	1:A:207:MET:HG3	2.46	0.55
1:A:65:HIS:HB2	1:A:68:LEU:HD12	1.89	0.55
1:B:345:VAL:C	1:B:347:PRO:HD3	2.26	0.55
1:B:156:GLY:O	1:B:160:THR:HG23	2.07	0.55
1:A:322:CYS:O	1:A:324:GLY:N	2.39	0.55
1:A:244:GLN:OE1	1:A:244:GLN:C	2.45	0.55
1:B:135:ARG:HD3	1:B:251:THR:HA	1.89	0.54
1:B:332:GLU:O	1:B:333:ALA:HB3	2.07	0.54
1:A:135:ARG:NE	1:A:135:ARG:HA	2.22	0.54
1:B:278:HIS:NE2	11:B:2038:HOH:O	2.34	0.54
8:A:1410:PLM:H81	1:B:46:LEU:HD11	1.88	0.54
1:A:91:PHE:HA	1:A:94:THR:HG23	1.87	0.54
1:B:167:CYS:SG	1:B:211:HIS:CD2	3.01	0.54
1:B:330:ASP:O	1:B:331:ASP:O	2.26	0.54
1:A:321:LEU:C	1:A:323:CYS:H	2.10	0.54
1:B:143:MET:HG2	1:B:146:PHE:CB	2.38	0.53
1:B:226:LEU:HD12	1:B:226:LEU:N	2.23	0.53
1:B:311:LYS:HE3	10:B:1509:HTG:O3	2.09	0.53
1:B:216:LEU:O	1:B:220:PHE:CD2	2.60	0.53
1:B:161:TRP:O	1:B:165:LEU:HD23	2.09	0.53
1:A:65:HIS:ND1	1:A:337:VAL:O	2.36	0.53
1:B:167:CYS:O	1:B:170:PRO:HD2	2.09	0.53
1:B:46:LEU:HD12	8:B:1407:PLM:HD2	1.89	0.53
1:A:82:ALA:O	1:A:86:MET:HG3	2.08	0.53
1:B:68:LEU:HA	1:B:73:ASN:ND2	2.24	0.53
1:B:212:PHE:O	1:B:216:LEU:HD23	2.09	0.53
1:B:51:GLY:HA2	1:B:300:VAL:HG12	1.90	0.53
1:B:332:GLU:CB	1:B:335:THR:O	2.54	0.53
1:A:239:GLU:CG	1:A:244:GLN:HE22	2.21	0.53
1:A:67:LYS:HB2	1:A:337:VAL:CB	2.37	0.52
1:B:266:LEU:N	1:B:267:PRO:HD2	2.24	0.52
1:B:332:GLU:OE1	1:B:332:GLU:O	2.26	0.52
1:A:74:TYR:CE2	1:A:150:GLU:HG2	2.44	0.52
1:A:327:PRO:O	1:A:328:LEU:C	2.47	0.52
1:A:231:LYS:HZ1	1:A:233:ALA:HB3	1.75	0.52
1:B:150:GLU:O	1:B:154:ILE:CD1	2.58	0.52
1:A:326:ASN:HD21	1:A:328:LEU:CD1	2.17	0.52
1:B:159:PHE:O	1:B:163:MET:HG2	2.09	0.51
1:B:143:MET:HA	1:B:143:MET:CE	2.40	0.51
1:B:139:VAL:HG21	1:B:226:LEU:HD23	1.92	0.51
1:A:214:ILE:HB	1:A:215:PRO:HD3	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ARG:HD2	1:B:99:LEU:HD13	1.91	0.51
1:A:109:GLY:O	1:A:113:GLU:HB2	2.10	0.51
1:B:67:LYS:HB3	1:B:337:VAL:HG11	1.91	0.51
1:B:254:VAL:O	1:B:258:VAL:HG23	2.09	0.51
1:A:135:ARG:HD3	1:A:251:THR:CA	2.41	0.51
1:B:9:PHE:C	1:B:179:ILE:HD11	2.30	0.51
1:A:224:GLY:O	1:A:227:VAL:HG12	2.11	0.51
1:A:87:VAL:O	1:A:91:PHE:HB2	2.10	0.51
1:A:136:TYR:HA	1:A:226:LEU:HD11	1.91	0.51
1:A:262:LEU:HB3	1:A:266:LEU:CD2	2.40	0.51
1:B:85:PHE:O	1:B:89:GLY:N	2.40	0.51
1:B:127:SER:O	1:B:131:LEU:HD13	2.11	0.51
1:B:67:LYS:N	1:B:337:VAL:HG21	2.26	0.51
1:B:139:VAL:CG1	1:B:226:LEU:HG	2.41	0.51
1:B:167:CYS:SG	1:B:207:MET:HG3	2.51	0.51
1:A:346:ALA:N	1:A:347:PRO:HD3	2.26	0.50
1:A:88:PHE:HB2	8:B:1323:PLM:HF2	1.93	0.50
1:B:67:LYS:NZ	1:B:332:GLU:HG3	2.26	0.50
1:B:129:VAL:HG13	1:B:218:VAL:HG11	1.94	0.50
1:B:67:LYS:HG2	1:B:337:VAL:HG22	1.92	0.50
1:A:94:THR:CB	1:A:113:GLU:OE2	2.54	0.50
1:A:176:SER:HA	1:A:200:ASN:OD1	2.12	0.50
1:B:298:SER:HB2	11:B:2036:HOH:O	2.12	0.50
1:A:325:LYS:HG2	1:A:327:PRO:HD3	1.93	0.50
1:B:321:LEU:C	1:B:323:CYS:H	2.15	0.50
1:A:24:PHE:CD1	1:A:106:GLY:HA2	2.46	0.50
1:B:302:ASN:HB2	11:B:2016:HOH:O	2.11	0.50
1:B:42:ALA:HB2	10:B:1508:HTG:H7'3	1.93	0.50
1:A:259:ILE:O	1:A:263:ILE:HG13	2.12	0.50
1:A:308:MET:CE	1:B:41:ALA:HB1	2.42	0.50
1:B:51:GLY:CA	1:B:300:VAL:HG12	2.42	0.50
1:A:326:ASN:ND2	1:A:328:LEU:HD11	2.18	0.49
1:A:83:ASP:O	1:A:87:VAL:HG23	2.12	0.49
1:A:240:SER:O	1:A:241:ALA:HB2	2.12	0.49
1:B:158:ALA:O	1:B:162:VAL:HG23	2.12	0.49
1:A:67:LYS:H	1:A:337:VAL:HG23	1.75	0.49
1:B:75:ILE:HG21	1:B:131:LEU:HD11	1.95	0.49
1:A:234:ALA:HB2	1:A:248:LYS:HG2	1.93	0.49
1:B:143:MET:HG2	1:B:146:PHE:HB2	1.94	0.49
1:A:139:VAL:HG21	1:A:230:VAL:HG11	1.94	0.49
1:B:195:HIS:HD1	1:B:198:THR:CG2	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:PHE:HA	1:B:179:ILE:CD1	2.41	0.49
1:A:231:LYS:NZ	1:A:233:ALA:HB3	2.28	0.49
1:B:346:ALA:N	1:B:347:PRO:CD	2.66	0.49
1:A:134:GLU:HG2	1:A:148:PHE:CD2	2.48	0.49
1:A:42:ALA:O	1:A:45:PHE:HB3	2.13	0.49
1:A:338:SER:HB2	1:A:341:GLU:HG2	1.94	0.49
1:A:96:TYR:CE2	1:A:104:VAL:HG21	2.40	0.49
1:A:6:GLY:HA3	1:A:9:PHE:CZ	2.48	0.48
1:A:189:ILE:CG2	1:A:190:ASP:N	2.76	0.48
1:B:107:PRO:O	1:B:111:ASN:ND2	2.46	0.48
1:A:70:THR:O	1:A:74:TYR:HD2	1.96	0.48
1:A:239:GLU:OE2	1:A:248:LYS:HD2	2.14	0.48
1:A:318:VAL:O	1:A:322:CYS:SG	2.71	0.48
1:A:311:LYS:HB3	1:A:332:GLU:HG2	1.94	0.48
1:A:161:TRP:O	1:A:165:LEU:HB2	2.13	0.48
1:A:195:HIS:HD1	1:A:198:THR:HG22	1.79	0.48
1:B:240:SER:O	1:B:241:ALA:HB2	2.14	0.48
1:A:72:LEU:HD21	1:A:253:MET:CE	2.44	0.48
1:B:337:VAL:CG2	1:B:338:SER:N	2.70	0.48
1:B:322:CYS:O	1:B:324:GLY:N	2.46	0.48
1:B:134:GLU:O	1:B:138:VAL:HG13	2.14	0.48
1:A:227:VAL:CG1	1:A:228:PHE:N	2.76	0.48
1:A:326:ASN:ND2	1:A:328:LEU:CD1	2.77	0.47
1:B:319:THR:HG21	1:B:341:GLU:OE1	2.14	0.47
1:B:302:ASN:HB2	1:B:303:PRO:HD3	1.96	0.47
1:A:152:HIS:O	1:A:155:MET:HB2	2.14	0.47
1:B:221:PHE:O	1:B:224:GLY:N	2.42	0.47
1:A:337:VAL:CG2	1:A:338:SER:N	2.76	0.47
1:B:238:GLN:HG3	1:B:241:ALA:CA	2.44	0.47
1:A:85:PHE:O	1:A:89:GLY:N	2.47	0.47
1:A:342:THR:OG1	1:A:344:GLN:CD	2.53	0.47
1:A:329:GLY:HA2	1:B:96:TYR:CZ	2.49	0.47
1:B:196:GLU:C	1:B:198:THR:H	2.18	0.47
1:A:151:ASN:ND2	1:A:152:HIS:CD2	2.82	0.47
1:A:66:LYS:HD2	1:A:66:LYS:N	2.29	0.47
1:A:132:ALA:O	1:A:222:CYS:SG	2.73	0.47
1:B:236:GLN:O	1:B:238:GLN:N	2.48	0.47
1:A:70:THR:H	1:A:73:ASN:ND2	2.04	0.47
1:B:170:PRO:CB	1:B:171:PRO:HD3	2.38	0.47
1:B:290:ILE:HB	1:B:291:PRO:CD	2.44	0.47
1:A:298:SER:HA	1:A:301:TYR:CD2	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:66:LYS:HD3	1:B:343:SER:OG	2.15	0.47
1:B:227:VAL:HG13	1:B:228:PHE:N	2.29	0.47
1:A:326:ASN:ND2	1:A:328:LEU:HD21	2.30	0.47
1:B:237:GLN:O	1:B:238:GLN:CB	2.62	0.47
1:A:322:CYS:HA	8:A:1322:PLM:O1	2.14	0.47
1:A:194:PRO:O	1:A:195:HIS:C	2.54	0.47
1:A:302:ASN:HB2	11:A:2017:HOH:O	2.15	0.47
1:B:204:VAL:HG11	1:B:276:PHE:CD1	2.50	0.47
1:B:115:PHE:CD1	1:B:172:LEU:HD11	2.50	0.47
1:A:178:TYR:HA	1:A:188:GLY:O	2.15	0.46
1:B:240:SER:O	1:B:241:ALA:CB	2.63	0.46
1:B:143:MET:CB	1:B:146:PHE:HB3	2.46	0.46
1:B:140:CYS:O	1:B:141:LYS:C	2.53	0.46
1:B:238:GLN:CG	1:B:241:ALA:H	2.21	0.46
1:A:302:ASN:CB	1:A:303:PRO:HD3	2.45	0.46
1:B:256:ILE:HD13	1:B:256:ILE:HA	1.72	0.46
1:B:137:VAL:HG12	1:B:137:VAL:O	2.15	0.46
1:B:76:LEU:HD22	1:B:306:TYR:CG	2.51	0.46
1:A:131:LEU:O	1:A:135:ARG:HB2	2.15	0.46
1:A:137:VAL:HA	1:A:142:PRO:CD	2.46	0.46
1:A:180:PRO:HA	1:A:186:SER:O	2.16	0.46
1:B:239:GLU:OE1	1:B:239:GLU:HA	2.16	0.46
1:B:170:PRO:HB2	1:B:171:PRO:CD	2.39	0.46
1:A:143:MET:HB2	1:A:146:PHE:HB3	1.98	0.46
1:A:300:VAL:O	1:A:303:PRO:HD2	2.16	0.45
1:A:75:ILE:HG21	1:A:131:LEU:HD11	1.97	0.45
1:A:137:VAL:HA	1:A:142:PRO:HD3	1.98	0.45
1:B:227:VAL:CG1	1:B:228:PHE:N	2.79	0.45
1:B:150:GLU:O	1:B:154:ILE:HD12	2.16	0.45
1:B:340:THR:HG23	1:B:341:GLU:N	2.31	0.45
1:B:70:THR:O	1:B:74:TYR:HD2	2.00	0.45
1:B:75:ILE:O	1:B:79:LEU:HD13	2.17	0.45
1:A:230:VAL:HG13	1:A:230:VAL:O	2.16	0.45
1:B:315:ASN:OD1	1:B:331:ASP:O	2.34	0.45
1:B:64:GLN:HE21	1:B:65:HIS:CD2	2.33	0.45
1:A:342:THR:HA	1:A:344:GLN:OE1	2.16	0.45
1:B:134:GLU:OE1	1:B:135:ARG:NH2	2.50	0.45
1:B:150:GLU:O	1:B:153:ALA:HB3	2.17	0.45
1:A:77:LEU:O	1:A:81:VAL:HG23	2.17	0.45
1:B:208:PHE:O	1:B:213:ILE:CG1	2.62	0.45
1:A:266:LEU:N	1:A:267:PRO:HD2	2.31	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:148:PHE:CE1	1:B:152:HIS:HB3	2.51	0.45
1:A:67:LYS:H	1:A:337:VAL:HG21	1.82	0.45
1:B:234:ALA:HA	1:B:245:LYS:HZ3	1.82	0.45
1:A:325:LYS:HE2	1:A:327:PRO:CD	2.45	0.45
1:B:75:ILE:O	1:B:78:ASN:HB3	2.17	0.45
1:A:266:LEU:HD12	1:A:266:LEU:HA	1.78	0.45
1:B:216:LEU:HD12	1:B:220:PHE:HE2	1.82	0.45
1:A:158:ALA:O	1:A:162:VAL:HG23	2.17	0.44
1:B:78:ASN:O	1:B:81:VAL:N	2.49	0.44
1:B:221:PHE:CD1	1:B:221:PHE:C	2.90	0.44
1:B:300:VAL:O	1:B:303:PRO:HD2	2.17	0.44
1:B:205:ILE:O	1:B:209:VAL:HG23	2.17	0.44
1:A:245:LYS:CA	1:A:245:LYS:NZ	2.77	0.44
1:B:148:PHE:CD1	1:B:152:HIS:HB2	2.53	0.44
1:B:332:GLU:OE2	1:B:334:SER:HB2	2.17	0.44
1:A:143:MET:HG2	1:A:146:PHE:HB2	1.98	0.44
1:A:67:LYS:HB2	1:A:337:VAL:CG2	2.48	0.44
1:B:60:TYR:C	1:B:60:TYR:CD1	2.91	0.44
1:A:213:ILE:O	1:A:217:ILE:HG13	2.17	0.44
1:A:191:TYR:OH	7:A:1296:RET:H192	2.18	0.44
1:B:126:TRP:CH2	1:B:215:PRO:HG3	2.53	0.44
1:B:231:LYS:HE3	1:B:231:LYS:HB2	1.81	0.44
1:B:22:SER:C	1:B:24:PHE:N	2.70	0.44
1:A:337:VAL:C	1:A:338:SER:OG	2.56	0.44
1:A:329:GLY:HA2	1:B:96:TYR:OH	2.18	0.43
1:A:39:MET:CE	1:A:39:MET:HA	2.48	0.43
1:A:319:THR:OG1	1:A:327:PRO:HB3	2.18	0.43
1:A:74:TYR:OH	1:A:150:GLU:HG2	2.18	0.43
1:B:102:TYR:CE2	1:B:104:VAL:HA	2.54	0.43
1:B:305:ILE:O	1:B:309:MET:N	2.48	0.43
1:B:139:VAL:HG11	1:B:226:LEU:HG	2.00	0.43
1:A:138:VAL:HG23	1:A:139:VAL:N	2.32	0.43
1:A:231:LYS:HB2	1:A:231:LYS:NZ	2.32	0.43
1:B:244:GLN:O	1:B:248:LYS:HG3	2.18	0.43
1:A:102:TYR:CE2	1:A:104:VAL:HA	2.53	0.43
1:B:301:TYR:CD1	1:B:301:TYR:C	2.91	0.43
1:B:315:ASN:O	1:B:318:VAL:HG12	2.18	0.43
1:B:117:ALA:CB	7:B:1296:RET:H14	2.49	0.43
1:B:18:GLY:HA2	3:B:605:NAG:O5	2.19	0.43
1:B:234:ALA:HA	1:B:245:LYS:HZ1	1.84	0.43
1:B:231:LYS:CE	1:B:233:ALA:HB3	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:LEU:HD12	1:B:220:PHE:CE2	2.54	0.43
1:B:311:LYS:HD2	10:B:1509:HTG:O2	2.19	0.43
1:A:117:ALA:CB	7:A:1296:RET:H14	2.49	0.42
1:B:332:GLU:O	1:B:333:ALA:CB	2.67	0.42
1:A:52:PHE:HB3	1:A:53:PRO:CD	2.50	0.42
1:B:312:GLN:O	1:B:316:CYS:SG	2.78	0.42
1:B:226:LEU:CD1	1:B:226:LEU:N	2.83	0.42
1:A:332:GLU:C	1:A:334:SER:N	2.65	0.42
1:A:133:ILE:O	1:A:136:TYR:N	2.52	0.42
1:B:103:PHE:CZ	1:B:187:CYS:SG	3.12	0.42
1:B:69:ARG:NH1	1:B:69:ARG:HG2	2.32	0.42
1:B:67:LYS:H	1:B:337:VAL:CG2	2.31	0.42
1:B:210:VAL:O	1:B:215:PRO:HD3	2.19	0.42
1:A:129:VAL:O	1:A:133:ILE:HG12	2.18	0.42
9:B:1401:HTO:H72	10:B:1509:HTG:H3'2	2.01	0.42
1:B:238:GLN:HG2	1:B:239:GLU:N	2.34	0.42
1:A:135:ARG:O	1:A:138:VAL:HG22	2.19	0.42
1:A:159:PHE:O	1:A:163:MET:HG2	2.20	0.42
1:B:196:GLU:C	1:B:198:THR:N	2.73	0.42
1:A:6:GLY:HA3	1:A:9:PHE:CE1	2.54	0.42
4:A:704:NAG:H82	4:A:705:NAG:H61	2.01	0.42
1:A:155:MET:HA	1:A:155:MET:CE	2.50	0.42
1:A:104:VAL:CG2	1:A:105:PHE:N	2.83	0.42
1:B:141:LYS:NZ	1:B:144:SER:O	2.38	0.42
1:B:326:ASN:C	1:B:328:LEU:HD22	2.39	0.42
1:A:239:GLU:CB	1:A:244:GLN:OE1	2.68	0.42
1:A:22:SER:C	1:A:24:PHE:H	2.23	0.42
1:A:321:LEU:HD13	8:A:1322:PLM:H51	2.02	0.41
1:B:224:GLY:O	1:B:227:VAL:CG1	2.67	0.41
1:B:18:GLY:HA2	3:B:605:NAG:C1	2.50	0.41
1:B:151:ASN:O	1:B:155:MET:HG2	2.20	0.41
1:B:243:THR:HG23	1:B:244:GLN:N	2.34	0.41
1:B:150:GLU:O	1:B:154:ILE:HD13	2.20	0.41
1:B:99:LEU:HD23	1:B:99:LEU:HA	1.92	0.41
1:B:330:ASP:C	1:B:331:ASP:O	2.58	0.41
1:B:67:LYS:HE2	1:B:336:THR:O	2.21	0.41
1:B:9:PHE:HA	1:B:179:ILE:CG1	2.50	0.41
1:A:216:LEU:HD12	1:A:220:PHE:CE2	2.56	0.41
1:B:326:ASN:HB3	1:B:328:LEU:CD2	2.51	0.41
1:A:119:LEU:HA	1:A:119:LEU:HD23	1.89	0.41
1:A:256:ILE:HG22	1:A:305:ILE:HD13	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:VAL:HA	1:A:30:TYR:CZ	2.56	0.41
1:A:326:ASN:C	1:A:328:LEU:H	2.23	0.41
1:B:243:THR:CG2	1:B:244:GLN:N	2.83	0.41
1:A:332:GLU:O	1:A:333:ALA:HB3	2.20	0.41
1:A:241:ALA:C	1:A:243:THR:N	2.74	0.41
1:A:36:GLN:O	1:A:39:MET:HB2	2.20	0.41
1:B:182:GLY:HA2	1:B:285:PRO:O	2.21	0.41
1:B:87:VAL:O	1:B:91:PHE:HB2	2.20	0.41
1:A:170:PRO:CB	1:A:171:PRO:HD3	2.45	0.41
1:A:67:LYS:HG2	1:A:343:SER:OG	2.21	0.41
1:B:117:ALA:HB1	7:B:1296:RET:H14	2.03	0.41
1:A:170:PRO:HB2	1:A:203:PHE:CE1	2.56	0.41
1:A:134:GLU:HG2	1:A:148:PHE:CE2	2.55	0.41
1:A:64:GLN:NE2	1:A:320:THR:HG23	2.34	0.41
1:A:72:LEU:HD21	1:A:253:MET:HE1	2.03	0.41
1:B:59:LEU:HA	1:B:77:LEU:CD1	2.51	0.40
1:B:110:CYS:SG	1:B:180:PRO:HD3	2.61	0.40
1:A:231:LYS:NZ	1:A:231:LYS:CB	2.85	0.40
1:B:67:LYS:CE	1:B:312:GLN:HG3	2.51	0.40
1:A:338:SER:CB	1:A:341:GLU:HG2	2.51	0.40
1:B:207:MET:CE	7:B:1296:RET:H161	2.51	0.40
1:A:276:PHE:O	1:A:279:GLN:HG3	2.21	0.40
1:B:238:GLN:HG3	1:B:241:ALA:C	2.42	0.40
1:B:91:PHE:CZ	1:B:296:LYS:HB3	2.56	0.40
1:A:229:THR:HG22	1:A:230:VAL:H	1.87	0.40
1:A:126:TRP:CE2	1:A:163:MET:HB3	2.56	0.40
1:A:85:PHE:O	1:A:89:GLY:HA3	2.21	0.40
1:A:128:LEU:HA	1:A:128:LEU:HD23	1.77	0.40
1:B:175:TRP:O	1:B:176:SER:HB3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	347/349 (99%)	292 (84%)	39 (11%)	16 (5%)	3	3
1	B	347/349 (99%)	287 (83%)	40 (12%)	20 (6%)	2	2
All	All	694/698 (99%)	579 (83%)	79 (11%)	36 (5%)	2	3

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	HIS
1	A	212	PHE
1	A	240	SER
1	A	241	ALA
1	A	323	CYS
1	A	341	GLU
1	B	237	GLN
1	B	240	SER
1	B	241	ALA
1	B	331	ASP
1	B	337	VAL
1	B	347	PRO
1	A	324	GLY
1	A	328	LEU
1	A	329	GLY
1	A	347	PRO
1	B	195	HIS
1	B	229	THR
1	B	323	CYS
1	B	328	LEU
1	B	341	GLU
1	A	335	THR
1	A	338	SER
1	B	238	GLN
1	A	145	ASN
1	A	322	CYS
1	B	235	ALA
1	B	324	GLY
1	A	229	THR
1	B	66	LYS
1	B	141	LYS
1	B	212	PHE
1	B	333	ALA
1	A	141	LYS
1	B	106	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	197	GLU

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%)	278 (94%)	18 (6%)	23	46
1	B	296/296 (100%)	273 (92%)	23 (8%)	16	30
All	All	592/592 (100%)	551 (93%)	41 (7%)	19	38

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	57	LEU
1	A	76	LEU
1	A	79	LEU
1	A	94	THR
1	A	119	LEU
1	A	134	GLU
1	A	135	ARG
1	A	143	MET
1	A	237	GLN
1	A	239	GLU
1	A	244	GLN
1	A	245	LYS
1	A	252	ARG
1	A	266	LEU
1	A	331	ASP
1	A	332	GLU
1	A	336	THR
1	B	8	ASN
1	B	38	SER
1	B	50	LEU
1	B	94	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	104	VAL
1	B	119	LEU
1	B	134	GLU
1	B	135	ARG
1	B	143	MET
1	B	148	PHE
1	B	167	CYS
1	B	222	CYS
1	B	229	THR
1	B	231	LYS
1	B	236	GLN
1	B	237	GLN
1	B	244	GLN
1	B	245	LYS
1	B	249	GLU
1	B	264	CYS
1	B	308	MET
1	B	330	ASP
1	B	332	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	64	GLN
1	A	73	ASN
1	A	100	HIS
1	A	111	ASN
1	A	225	GLN
1	A	237	GLN
1	A	326	ASN
1	B	8	ASN
1	B	64	GLN
1	B	73	ASN
1	B	111	ASN
1	B	151	ASN
1	B	237	GLN
1	B	244	GLN

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	0.92	0	14,15,17	0.83	0
2	NAG	A	504	2	14,14,15	0.81	0	15,19,21	0.84	1 (6%)
2	NAG	A	505	1,2	14,14,15	0.59	0	15,19,21	0.80	0
4	NAG	A	704	4	14,14,15	0.59	0	15,19,21	0.88	1 (6%)
4	NAG	A	705	1,4	14,14,15	0.76	0	15,19,21	0.78	0
3	BMA	B	602	3	11,11,12	0.90	0	14,15,17	0.99	1 (7%)
3	BMA	B	603	3	11,11,12	0.81	0	14,15,17	0.73	0
3	NAG	B	604	3	14,14,15	0.41	0	15,19,21	1.24	1 (6%)
3	NAG	B	605	1,3	14,14,15	0.55	0	15,19,21	0.68	0
4	NAG	B	804	4	14,14,15	0.71	0	15,19,21	0.76	1 (6%)
4	NAG	B	805	1,4	14,14,15	0.60	0	15,19,21	0.84	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

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	604	NAG	C2-N2-C7	-4.18	117.67	123.04
4	A	704	NAG	C2-N2-C7	-2.93	119.27	123.04
4	B	804	NAG	C2-N2-C7	-2.35	120.02	123.04
4	B	805	NAG	C2-N2-C7	-2.20	120.21	123.04
2	A	504	NAG	C8-C7-N2	2.04	120.02	116.11
3	B	602	BMA	C1-O5-C5	2.19	115.03	112.25

There are no chirality outliers.

All (1) torsion outliers are listed below:

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

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	504	NAG	1	0
2	A	505	NAG	1	0
4	A	704	NAG	1	0
4	A	705	NAG	1	0
3	B	605	NAG	2	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	1.99	2 (10%)	27,27,28	1.97	8 (29%)
8	PLM	A	1322	1	16,16,17	0.92	1 (6%)	15,15,17	0.62	0
8	PLM	A	1323	1	16,16,17	0.93	1 (6%)	15,15,17	0.54	0
8	PLM	A	1410	-	15,15,17	1.91	3 (20%)	14,14,17	3.27	6 (42%)
10	HTG	A	1507	-	19,19,19	2.82	8 (42%)	22,24,24	2.83	1 (4%)
7	RET	B	1296	1	19,20,21	2.13	3 (15%)	27,27,28	1.96	6 (22%)
8	PLM	B	1322	1	16,16,17	1.01	1 (6%)	15,15,17	0.42	0
8	PLM	B	1323	1	16,16,17	0.93	1 (6%)	15,15,17	0.49	0
9	HTO	B	1401	-	9,9,9	1.96	2 (22%)	8,10,10	1.17	1 (12%)
8	PLM	B	1407	-	15,15,17	1.71	3 (20%)	14,14,17	3.32	6 (42%)
10	HTG	B	1506	-	19,19,19	2.73	8 (42%)	22,24,24	2.62	1 (4%)
10	HTG	B	1508	-	19,19,19	2.26	8 (42%)	22,24,24	3.58	2 (9%)
10	HTG	B	1509	-	19,19,19	2.93	8 (42%)	22,24,24	2.97	2 (9%)

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
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	1508	-	-	0/10/30/30	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	-5.00	1.22	1.51
8	B	1407	PLM	CC-CB	-4.41	1.26	1.51
8	A	1410	PLM	CB-CA	-3.61	1.30	1.51
8	B	1322	PLM	O1-C1	-3.59	1.22	1.42
8	A	1322	PLM	O1-C1	-3.53	1.23	1.42
8	A	1323	PLM	O1-C1	-3.46	1.23	1.42
8	B	1323	PLM	O1-C1	-3.32	1.24	1.42
8	A	1410	PLM	CD-CC	-3.24	1.32	1.51
8	B	1407	PLM	CB-CA	-3.00	1.34	1.51
8	B	1407	PLM	CD-CC	-2.69	1.36	1.51
10	B	1508	HTG	C1'-S1	2.15	1.84	1.81
7	B	1296	RET	C17-C1	2.26	1.58	1.53
9	B	1401	HTO	C4-C3	2.29	1.57	1.52
10	B	1508	HTG	C4-C3	2.32	1.58	1.52
10	B	1508	HTG	C1-S1	2.45	1.84	1.80
10	B	1509	HTG	C6-C5	2.55	1.61	1.51
10	A	1507	HTG	C1'-S1	2.84	1.85	1.81
10	B	1508	HTG	C3-C2	2.84	1.59	1.52
10	B	1506	HTG	C1'-S1	2.92	1.85	1.81
10	B	1506	HTG	O5-C5	2.93	1.51	1.44
10	B	1508	HTG	C1-C2	2.96	1.59	1.53
10	B	1506	HTG	C3-C2	3.04	1.60	1.52
10	B	1506	HTG	C4-C3	3.04	1.60	1.52
10	B	1509	HTG	C3-C2	3.11	1.60	1.52
10	A	1507	HTG	C3-C2	3.18	1.60	1.52
10	B	1509	HTG	C4-C3	3.23	1.60	1.52
10	A	1507	HTG	O5-C5	3.30	1.52	1.44
10	A	1507	HTG	C4-C5	3.33	1.60	1.53
10	A	1507	HTG	C4-C3	3.37	1.61	1.52
10	B	1508	HTG	O5-C5	3.38	1.52	1.44
10	A	1507	HTG	C1-C2	3.53	1.60	1.53
10	B	1506	HTG	C1-C2	3.56	1.60	1.53
10	B	1506	HTG	C1-S1	3.56	1.86	1.80
10	B	1509	HTG	O5-C5	3.63	1.53	1.44
10	B	1508	HTG	C4-C5	3.85	1.61	1.53
10	B	1509	HTG	C1-S1	3.87	1.86	1.80
7	A	1296	RET	C1-C6	4.09	1.59	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	1509	HTG	C1-C2	4.24	1.61	1.53
10	A	1507	HTG	C1-S1	4.41	1.87	1.80
10	B	1506	HTG	C4-C5	4.56	1.62	1.53
9	B	1401	HTO	C3-C2	4.68	1.65	1.52
7	B	1296	RET	C1-C6	4.96	1.60	1.53
10	B	1509	HTG	C4-C5	5.13	1.64	1.53
10	B	1508	HTG	O5-C1	5.78	1.52	1.42
7	B	1296	RET	C5-C6	6.71	1.45	1.34
7	A	1296	RET	C5-C6	6.93	1.45	1.34
10	B	1506	HTG	O5-C1	7.53	1.55	1.42
10	B	1509	HTG	O5-C1	7.77	1.55	1.42
10	A	1507	HTG	O5-C1	7.99	1.56	1.42

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1296	RET	C8-C9-C10	-5.30	110.45	118.98
7	A	1296	RET	C8-C9-C10	-4.20	112.22	118.98
7	A	1296	RET	C18-C5-C4	-2.74	108.23	113.43
7	B	1296	RET	C18-C5-C4	-2.58	108.55	113.43
9	B	1401	HTO	O3-C3-C4	-2.40	104.01	109.35
7	B	1296	RET	C10-C11-C12	-2.32	116.05	123.13
7	A	1296	RET	C10-C11-C12	-2.25	116.28	123.13
7	A	1296	RET	C1-C6-C5	-2.11	119.56	122.66
8	A	1410	PLM	CF-CE-CD	-2.07	94.70	115.51
10	B	1509	HTG	O5-C5-C6	2.03	111.50	106.36
10	B	1508	HTG	O5-C5-C6	2.05	111.55	106.36
8	B	1407	PLM	C9-C8-C7	2.20	125.87	114.53
8	A	1410	PLM	CE-CD-CC	2.21	125.96	114.53
7	B	1296	RET	C2-C1-C6	2.25	113.92	110.36
8	B	1407	PLM	C5-C4-C3	2.34	126.60	114.53
8	B	1407	PLM	CE-CD-CC	2.47	127.31	114.53
8	A	1410	PLM	C5-C4-C3	2.53	127.57	114.53
7	A	1296	RET	C2-C1-C6	2.54	114.39	110.36
7	A	1296	RET	C7-C8-C9	2.94	130.70	126.22
8	A	1410	PLM	CC-CB-CA	3.07	130.36	114.53
8	B	1407	PLM	CC-CB-CA	3.31	131.61	114.53
7	A	1296	RET	C19-C9-C10	3.77	128.47	122.90
7	B	1296	RET	C19-C9-C10	3.98	128.78	122.90
7	B	1296	RET	C18-C5-C6	4.91	129.43	124.61
7	A	1296	RET	C18-C5-C6	5.44	129.95	124.61
8	B	1407	PLM	CA-C9-C8	7.22	151.83	114.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	A	1410	PLM	CA-C9-C8	7.24	151.91	114.53
8	A	1410	PLM	CD-CC-CB	8.00	155.84	114.53
8	B	1407	PLM	CD-CC-CB	8.10	156.34	114.53
10	B	1506	HTG	C1'-S1-C1	11.84	116.62	100.30
10	A	1507	HTG	C1'-S1-C1	12.66	117.75	100.30
10	B	1509	HTG	C1'-S1-C1	13.36	118.72	100.30
10	B	1508	HTG	C1'-S1-C1	16.23	122.68	100.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1296	RET	3	0
8	A	1322	PLM	3	0
8	A	1410	PLM	1	0
7	B	1296	RET	4	0
8	B	1322	PLM	2	0
8	B	1323	PLM	3	0
9	B	1401	HTO	1	0
8	B	1407	PLM	1	0
10	B	1508	HTG	2	0
10	B	1509	HTG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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.