



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:48 AM GMT

PDB ID : 3CAP
Title : Crystal Structure of Native Opsin: the G Protein-Coupled Receptor Rhodopsin in its Ligand-free State
Authors : Park, J.H.; Scheerer, P.; Hofmann, K.P.; Choe, H.-W.; Ernst, O.P.
Deposited on : 2008-02-20
Resolution : 2.90 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) : 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

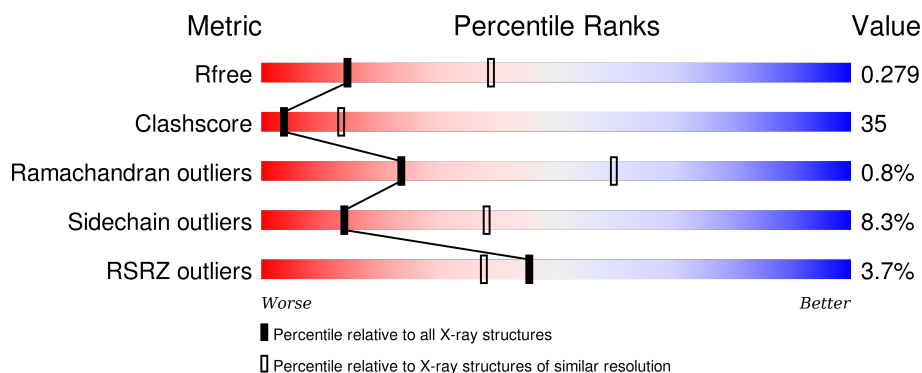
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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.

Mol	Chain	Length	Quality of chain
1	A	348	
1	B	348	

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
3	NAG	A	601	-	-	X	-
3	NAG	B	701	-	-	X	-
4	BGL	A	803	-	-	-	X
4	BGL	A	804	-	-	-	X
4	BGL	B	806	X	-	-	-
5	PLM	A	901	-	-	-	X
5	PLM	B	902	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5504 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	326	Total	C	N	O	S	0	0	0
			2592	1725	400	441	26			
1	B	326	Total	C	N	O	S	0	0	0
			2592	1725	400	441	26			

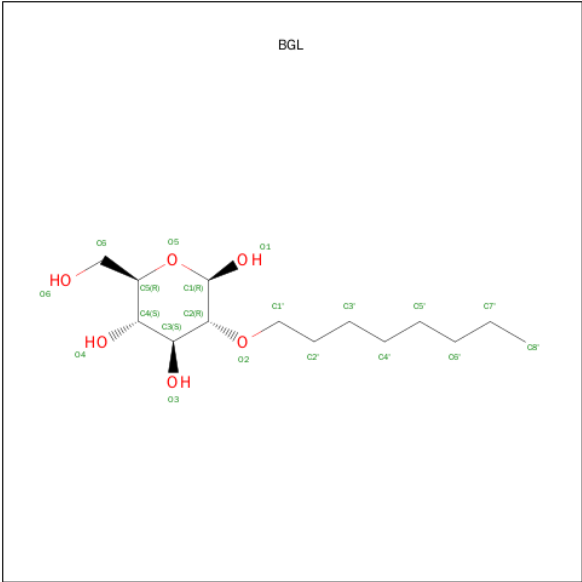
- Molecule 2 is a polymer of unknown type called SUGAR (4-MER).

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

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

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

- Molecule 4 is SUGAR (B-2-OCTYLGLUCOSIDE) (three-letter code: BGL) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



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

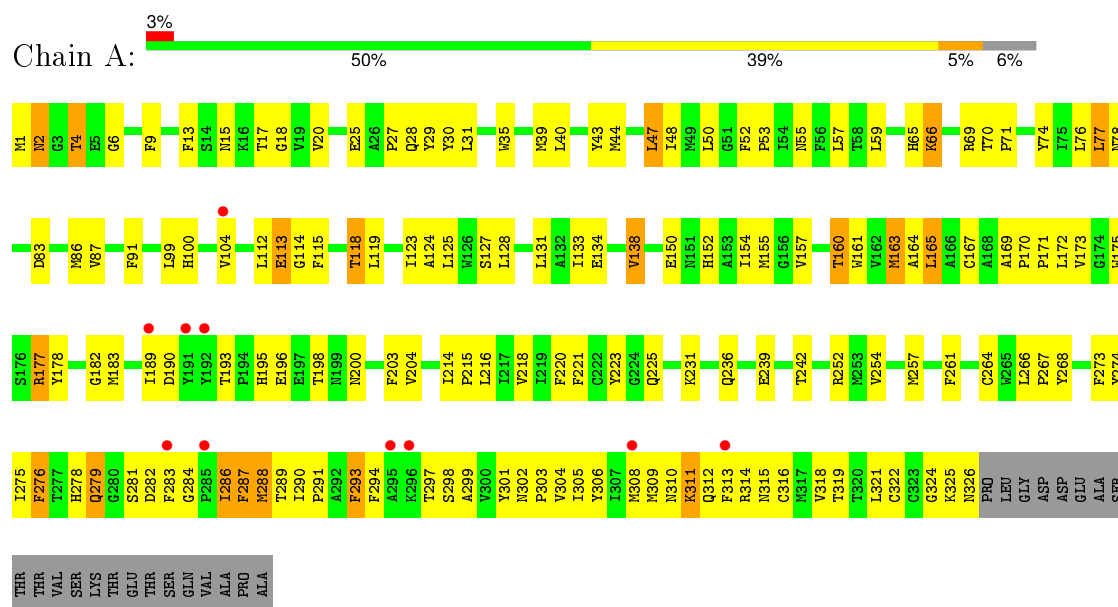
- Molecule 6 is water.

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

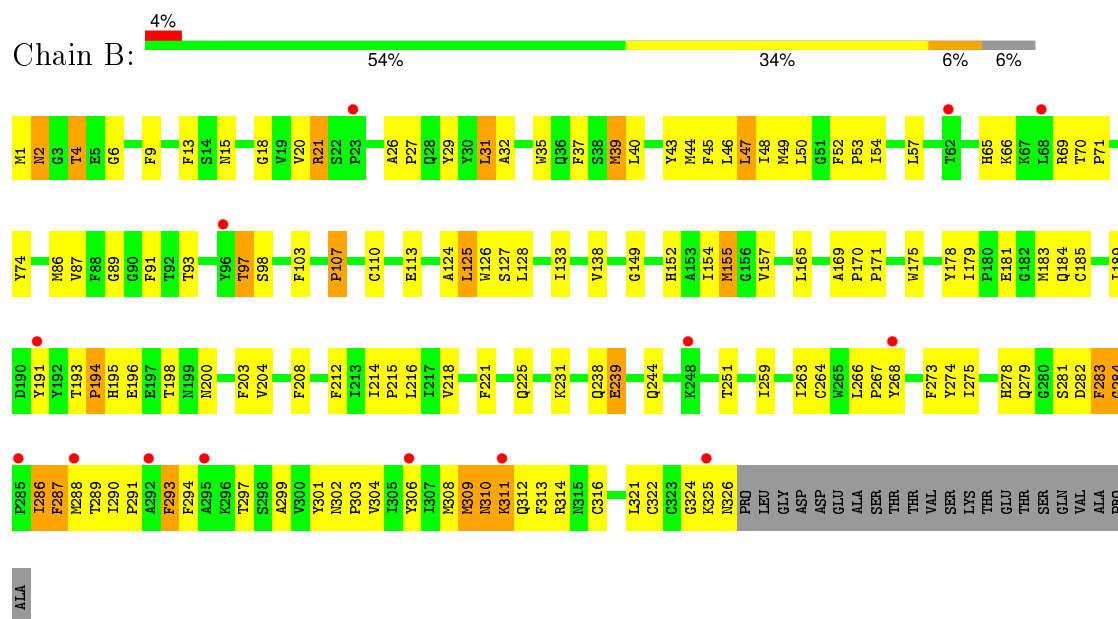
3 Residue-property plots

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

• Molecule 1: Rhodopsin



• Molecule 1: Rhodopsin



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	242.92Å 242.92Å 110.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.90 47.48 – 2.91	Depositor EDS
% Data completeness (in resolution range)	99.1 (50.00-2.90) 99.1 (47.48-2.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.229 , 0.266 0.265 , 0.279	Depositor DCC
R_{free} test set	2691 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 21.2	EDS
Estimated twinning fraction	0.477 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.54$, $\langle L^2 \rangle = 0.38$	Xtriage
Outliers	0 of 52944 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	5504	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.80% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PLM, BMA, BGL, NAG

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	0.45	0/2674	0.59	0/3643
1	B	0.45	0/2674	0.60	0/3643
All	All	0.45	0/5348	0.60	0/7286

There are no bond length outliers.

There are no bond angle outliers.

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	2592	0	2568	188	0
1	B	2592	0	2568	171	0
2	A	50	0	43	4	0
2	B	50	0	43	8	0
3	A	28	0	25	8	0
3	B	28	0	25	7	0
4	A	80	0	112	14	0
4	B	40	0	56	5	0
5	A	17	0	31	6	0
5	B	17	0	31	3	0
6	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	5	0	0	0	0
All	All	5504	0	5502	384	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 35.

All (384) 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:39:MET:CE	1:B:39:MET:HA	1.67	1.23
1:B:155:MET:CE	1:B:155:MET:HA	1.69	1.23
1:A:2:ASN:CB	1:A:282:ASP:HB3	1.69	1.21
1:A:78:ASN:HD21	1:A:160:THR:HG21	1.14	1.12
1:B:155:MET:HE2	1:B:155:MET:HA	1.25	1.10
1:A:311:LYS:HD3	1:A:311:LYS:H	1.20	1.06
1:B:311:LYS:H	1:B:311:LYS:HD3	0.93	1.04
1:B:39:MET:HE2	1:B:39:MET:HA	1.06	1.04
1:A:305:ILE:HA	1:A:309:MET:CE	1.88	1.04
1:A:78:ASN:ND2	1:A:160:THR:HG21	1.72	1.03
1:B:311:LYS:CD	1:B:311:LYS:H	1.70	1.03
1:B:2:ASN:CG	1:B:282:ASP:HB3	1.79	1.02
3:A:601:NAG:O3	3:A:601:NAG:H83	1.59	1.01
1:B:311:LYS:HD3	1:B:311:LYS:N	1.74	1.01
1:A:223:TYR:CZ	1:A:257:MET:HE1	1.96	1.00
1:A:305:ILE:HA	1:A:309:MET:HE2	1.37	1.00
1:A:4:THR:HG22	1:A:13:PHE:O	1.61	1.00
1:A:44:MET:O	1:A:48:ILE:HG13	1.61	1.00
1:B:4:THR:HG22	1:B:13:PHE:O	1.61	0.98
1:A:2:ASN:CG	1:A:282:ASP:HB3	1.83	0.98
1:B:1:MET:HA	3:B:701:NAG:HN2	1.25	0.97
1:B:2:ASN:CB	1:B:282:ASP:HB3	1.95	0.95
1:B:44:MET:CE	1:B:91:PHE:HA	1.96	0.95
1:B:44:MET:O	1:B:48:ILE:HG13	1.68	0.93
1:A:252:ARG:HB2	1:A:252:ARG:NH1	1.82	0.93
1:A:4:THR:HG21	1:A:20:VAL:HG21	1.50	0.93
1:A:123:ILE:HG23	1:A:160:THR:HG23	1.48	0.92
1:B:149:GLY:H	1:B:152:HIS:HD2	1.11	0.91
1:B:39:MET:CE	1:B:39:MET:CA	2.46	0.91
1:A:311:LYS:HD3	1:A:311:LYS:N	1.86	0.90
1:B:325:LYS:O	1:B:326:ASN:HB2	1.69	0.90
1:B:86:MET:HE2	1:B:299:ALA:HB2	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ARG:HB2	1:A:252:ARG:HH11	1.35	0.89
1:B:155:MET:CE	1:B:155:MET:CA	2.48	0.89
1:B:293:PHE:O	1:B:297:THR:HG22	1.73	0.89
1:A:324:GLY:O	1:A:325:LYS:HG3	1.73	0.88
1:A:28:GLN:O	1:A:31:LEU:HD23	1.74	0.88
3:B:701:NAG:H61	3:B:702:NAG:C2	2.04	0.87
1:B:39:MET:HE2	1:B:39:MET:CA	1.99	0.87
1:A:28:GLN:HB3	1:A:31:LEU:HD22	1.56	0.87
1:A:301:TYR:HB3	5:B:902:PLM:HB2	1.56	0.86
1:A:293:PHE:O	1:A:297:THR:HG22	1.75	0.86
1:A:28:GLN:O	1:A:31:LEU:CD2	2.24	0.85
1:A:223:TYR:CZ	1:A:257:MET:CE	2.59	0.85
1:A:2:ASN:CB	1:A:282:ASP:CB	2.52	0.85
1:B:275:ILE:HG12	1:B:283:PHE:CE1	2.12	0.85
1:B:324:GLY:O	1:B:325:LYS:HG3	1.77	0.84
1:A:114:GLY:O	1:A:118:THR:HG23	1.76	0.84
1:B:310:ASN:HD21	1:B:313:PHE:H	1.23	0.84
1:B:155:MET:HE3	1:B:155:MET:HA	1.57	0.84
1:B:4:THR:CG2	1:B:13:PHE:O	2.26	0.83
1:A:2:ASN:HB3	1:A:282:ASP:HB3	1.60	0.83
1:B:4:THR:HG21	1:B:20:VAL:HG21	1.61	0.82
1:B:86:MET:CE	1:B:299:ALA:HB2	2.09	0.81
1:A:70:THR:HG22	1:A:71:PRO:HD2	1.63	0.81
1:B:15:ASN:OD1	1:B:18:GLY:HA2	1.79	0.81
1:A:70:THR:CG2	1:A:71:PRO:HD2	2.11	0.81
4:B:806:BGL:O1	4:B:806:BGL:H1'1	1.76	0.80
1:A:125:LEU:CD1	1:A:261:PHE:HE1	1.95	0.79
1:B:310:ASN:HD21	1:B:313:PHE:N	1.80	0.79
1:A:4:THR:CG2	1:A:13:PHE:O	2.31	0.78
1:B:125:LEU:HD23	1:B:126:TRP:N	1.99	0.78
1:A:66:LYS:CA	1:A:69:ARG:HH11	1.97	0.78
1:A:2:ASN:HB2	1:A:282:ASP:HB3	1.66	0.78
1:A:78:ASN:HD21	1:A:160:THR:CG2	1.97	0.77
1:A:86:MET:HE2	1:A:299:ALA:HB2	1.64	0.77
1:A:322:CYS:HA	5:A:901:PLM:H21	1.67	0.77
1:B:44:MET:HE1	1:B:91:PHE:HA	1.64	0.77
1:B:31:LEU:HD12	1:B:31:LEU:C	2.05	0.77
1:A:252:ARG:CB	1:A:252:ARG:HH11	1.97	0.77
1:B:281:SER:O	1:B:283:PHE:CD2	2.37	0.77
1:A:325:LYS:O	1:A:326:ASN:HB2	1.84	0.76
1:A:52:PHE:HB3	1:A:53:PRO:HD3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:MET:HE3	1:B:155:MET:CA	2.14	0.76
5:A:901:PLM:CB	1:B:301:TYR:HB3	2.15	0.76
1:A:281:SER:O	1:A:283:PHE:CD1	2.39	0.76
1:B:1:MET:HA	3:B:701:NAG:N2	2.00	0.75
1:B:293:PHE:HD1	1:B:294:PHE:N	1.85	0.75
1:A:311:LYS:CD	1:A:311:LYS:H	1.98	0.75
1:A:28:GLN:HB3	1:A:31:LEU:CD2	2.17	0.75
3:A:601:NAG:H83	3:A:601:NAG:HO3	1.48	0.75
1:B:281:SER:O	1:B:283:PHE:CE2	2.39	0.75
1:A:123:ILE:HG23	1:A:160:THR:CG2	2.17	0.74
1:B:97:THR:CG2	1:B:185:CYS:HB3	2.17	0.74
1:B:325:LYS:O	1:B:326:ASN:CB	2.36	0.74
1:A:86:MET:CE	1:A:299:ALA:HB2	2.19	0.73
1:B:149:GLY:H	1:B:152:HIS:CD2	2.00	0.73
1:B:310:ASN:ND2	1:B:313:PHE:HB3	2.03	0.73
3:A:601:NAG:C8	3:A:601:NAG:O3	2.35	0.73
3:B:701:NAG:H61	3:B:702:NAG:N2	2.02	0.73
1:B:149:GLY:N	1:B:152:HIS:HD2	1.87	0.73
1:A:325:LYS:O	1:A:326:ASN:CB	2.35	0.73
2:A:403:BMA:C2	2:A:404:BMA:O2	2.37	0.73
3:B:701:NAG:H61	3:B:702:NAG:H2	1.69	0.72
1:A:163:MET:HA	1:A:163:MET:CE	2.19	0.72
1:B:293:PHE:C	1:B:293:PHE:CD1	2.63	0.72
1:A:264:CYS:HB2	1:A:301:TYR:OH	1.90	0.72
1:B:310:ASN:ND2	1:B:310:ASN:O	2.23	0.71
2:B:503:BMA:H3	2:B:504:BMA:O2	1.90	0.71
1:A:2:ASN:OD1	3:A:601:NAG:H2	1.90	0.70
1:A:163:MET:HE2	1:A:163:MET:HA	1.72	0.70
1:B:302:ASN:HB2	1:B:303:PRO:HD3	1.72	0.70
1:A:150:GLU:O	1:A:154:ILE:HG12	1.92	0.70
1:B:107:PRO:O	1:B:110:CYS:HB3	1.90	0.70
1:B:194:PRO:O	1:B:196:GLU:HG2	1.92	0.70
1:B:310:ASN:OD1	1:B:312:GLN:HB3	1.92	0.69
1:A:113:GLU:OE1	1:A:113:GLU:C	2.30	0.69
2:B:503:BMA:H2	2:B:504:BMA:O2	1.93	0.68
1:B:44:MET:HE2	1:B:91:PHE:HA	1.76	0.68
5:A:901:PLM:HB1	1:B:301:TYR:HB3	1.74	0.67
1:B:6:GLY:HA3	1:B:9:PHE:CZ	2.29	0.67
1:A:221:PHE:O	1:A:225:GLN:HG2	1.94	0.67
1:A:266:LEU:HB3	1:A:267:PRO:HD3	1.77	0.67
2:A:403:BMA:H2	2:A:404:BMA:O2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:802:BGL:H8'2	4:A:802:BGL:H4'1	1.76	0.67
1:A:189:ILE:HD13	1:A:203:PHE:HE2	1.60	0.66
1:A:2:ASN:OD1	1:A:282:ASP:N	2.27	0.66
1:A:171:PRO:HA	1:A:175:TRP:O	1.94	0.66
1:A:57:LEU:HD11	1:A:321:LEU:HD21	1.77	0.66
1:A:66:LYS:HA	1:A:69:ARG:HH11	1.61	0.65
1:B:128:LEU:HD22	1:B:306:TYR:CZ	2.32	0.65
1:B:286:ILE:HG12	1:B:287:PHE:H	1.62	0.65
1:A:70:THR:HG22	1:A:71:PRO:CD	2.27	0.65
1:A:6:GLY:HA3	1:A:9:PHE:CZ	2.32	0.65
2:B:503:BMA:C3	2:B:504:BMA:O2	2.44	0.64
1:B:286:ILE:HD13	1:B:286:ILE:H	1.61	0.64
1:A:290:ILE:H	1:A:291:PRO:HD2	1.61	0.64
1:A:66:LYS:HA	1:A:69:ARG:HE	1.61	0.64
5:A:901:PLM:HB2	1:B:301:TYR:HB3	1.78	0.64
1:A:301:TYR:CB	5:B:902:PLM:HB2	2.27	0.64
1:A:27:PRO:HB3	1:A:29:TYR:CE2	2.33	0.64
1:B:2:ASN:OD1	3:B:701:NAG:C2	2.44	0.64
1:A:281:SER:O	1:A:283:PHE:CE1	2.51	0.64
1:A:128:LEU:HD22	1:A:306:TYR:CZ	2.33	0.63
1:A:2:ASN:HB2	1:A:282:ASP:CB	2.26	0.63
1:B:31:LEU:CD1	1:B:31:LEU:C	2.67	0.63
1:B:15:ASN:OD1	1:B:18:GLY:CA	2.46	0.63
1:B:290:ILE:N	1:B:291:PRO:HD2	2.14	0.63
1:A:133:ILE:HD11	1:A:218:VAL:HG11	1.81	0.63
1:B:266:LEU:HB3	1:B:267:PRO:HD3	1.81	0.63
1:A:290:ILE:N	1:A:291:PRO:HD2	2.14	0.62
4:B:806:BGL:C1'	4:B:806:BGL:O1	2.47	0.62
1:B:169:ALA:HB3	1:B:170:PRO:HD3	1.81	0.62
1:A:293:PHE:HD2	1:A:294:PHE:N	1.97	0.62
1:A:223:TYR:OH	1:A:257:MET:HE1	1.98	0.62
4:A:804:BGL:H1'2	4:A:804:BGL:O1	2.00	0.62
1:B:287:PHE:C	1:B:287:PHE:CD2	2.73	0.62
1:A:310:ASN:OD1	1:A:312:GLN:HB3	2.00	0.61
2:B:503:BMA:C2	2:B:504:BMA:O2	2.48	0.61
1:B:44:MET:CE	1:B:91:PHE:CA	2.77	0.61
1:A:293:PHE:C	1:A:293:PHE:CD2	2.74	0.61
1:A:2:ASN:HB3	1:A:282:ASP:CB	2.26	0.61
1:B:43:TYR:OH	1:B:297:THR:HB	2.01	0.61
1:B:2:ASN:CB	1:B:282:ASP:CB	2.77	0.61
1:A:220:PHE:CE2	4:A:803:BGL:H8'1	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:801:BGL:H6'1	4:A:801:BGL:O1	2.00	0.60
1:A:59:LEU:HD23	1:A:77:LEU:HD12	1.82	0.60
4:B:806:BGL:H3'1	4:B:806:BGL:O1	2.01	0.60
1:B:97:THR:HG21	1:B:185:CYS:O	2.02	0.60
1:A:223:TYR:CE1	1:A:257:MET:CE	2.85	0.60
1:A:275:ILE:HG12	1:A:283:PHE:CE2	2.37	0.59
1:B:133:ILE:HD11	1:B:218:VAL:HG11	1.84	0.59
1:A:311:LYS:HA	1:A:314:ARG:NH2	2.16	0.59
1:B:97:THR:HG23	1:B:185:CYS:HB3	1.85	0.59
1:A:65:HIS:CD2	1:A:316:CYS:HB3	2.37	0.59
1:B:193:THR:C	1:B:195:HIS:H	2.07	0.59
1:A:293:PHE:CD2	1:A:294:PHE:N	2.71	0.58
1:B:66:LYS:HA	1:B:69:ARG:NH2	2.17	0.58
1:A:279:GLN:OE1	1:A:279:GLN:HA	2.03	0.58
1:B:171:PRO:HA	1:B:175:TRP:O	2.03	0.58
1:A:313:PHE:CD2	1:A:313:PHE:C	2.76	0.58
1:B:273:PHE:CD2	1:B:273:PHE:C	2.77	0.58
1:A:216:LEU:C	1:A:216:LEU:HD23	2.24	0.58
1:A:15:ASN:OD1	1:A:18:GLY:HA2	2.02	0.58
1:A:231:LYS:NZ	4:A:803:BGL:H3	2.18	0.58
1:B:293:PHE:CD1	1:B:294:PHE:N	2.69	0.57
1:A:319:THR:HG23	1:A:324:GLY:O	2.03	0.57
1:A:66:LYS:CB	1:A:69:ARG:HH11	2.17	0.57
1:A:2:ASN:OD1	1:A:282:ASP:HB3	2.03	0.57
1:B:52:PHE:HB3	1:B:53:PRO:HD3	1.86	0.57
1:B:154:ILE:O	1:B:155:MET:C	2.42	0.57
1:A:100:HIS:CE1	4:A:804:BGL:H2'1	2.39	0.57
1:B:310:ASN:HD21	1:B:313:PHE:HB3	1.70	0.57
1:B:189:ILE:HD13	1:B:203:PHE:HE2	1.70	0.57
1:B:178:TYR:O	1:B:179:ILE:CG2	2.53	0.57
1:B:2:ASN:OD1	3:B:701:NAG:H2	2.05	0.57
2:A:403:BMA:C2	2:A:404:BMA:HO2	2.17	0.57
1:B:311:LYS:CD	1:B:311:LYS:N	2.50	0.57
1:A:298:SER:HA	1:A:301:TYR:CE2	2.40	0.56
4:A:802:BGL:C1'	4:A:802:BGL:O1	2.52	0.56
1:B:286:ILE:CD1	1:B:286:ILE:H	2.18	0.56
1:B:170:PRO:HB2	1:B:171:PRO:HD3	1.86	0.56
1:A:220:PHE:CD2	4:A:803:BGL:H8'1	2.41	0.56
1:A:275:ILE:HG12	1:A:283:PHE:CZ	2.41	0.56
1:B:71:PRO:HA	1:B:74:TYR:CE1	2.40	0.56
1:A:288:MET:CE	1:A:288:MET:HA	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:284:GLY:HA3	1:B:286:ILE:HD13	1.88	0.56
1:B:31:LEU:HD12	1:B:32:ALA:N	2.22	0.55
1:B:313:PHE:C	1:B:313:PHE:CD2	2.79	0.55
1:A:47:LEU:HB3	1:A:91:PHE:CD2	2.41	0.55
1:A:163:MET:CE	1:A:163:MET:CA	2.84	0.55
1:A:2:ASN:OD1	3:A:601:NAG:C2	2.50	0.55
1:A:35:TRP:CD1	4:B:805:BGL:H4'1	2.41	0.55
1:B:196:GLU:C	1:B:198:THR:H	2.09	0.54
1:B:97:THR:CG2	1:B:98:SER:N	2.70	0.54
1:A:125:LEU:HD13	1:A:261:PHE:HE1	1.72	0.54
1:B:287:PHE:HD2	1:B:288:MET:N	2.06	0.54
1:A:134:GLU:O	1:A:138:VAL:HG13	2.07	0.54
1:A:302:ASN:HB2	1:A:303:PRO:HD3	1.89	0.54
1:A:71:PRO:HA	1:A:74:TYR:CE1	2.43	0.54
1:B:107:PRO:O	1:B:110:CYS:CB	2.56	0.54
1:A:119:LEU:O	1:A:123:ILE:HG13	2.08	0.54
1:A:239:GLU:N	1:A:239:GLU:OE2	2.35	0.54
1:A:223:TYR:OH	1:A:257:MET:CE	2.54	0.54
1:A:28:GLN:CB	1:A:31:LEU:CD2	2.84	0.54
1:B:15:ASN:HD22	2:B:501:NAG:H83	1.72	0.54
1:B:302:ASN:CB	1:B:303:PRO:HD3	2.38	0.53
1:B:283:PHE:N	1:B:283:PHE:CD2	2.76	0.53
1:A:1:MET:HA	3:A:601:NAG:HN2	1.74	0.53
1:A:298:SER:HA	1:A:301:TYR:CZ	2.43	0.53
1:A:314:ARG:O	1:A:318:VAL:HG23	2.09	0.53
1:A:223:TYR:HB3	1:A:254:VAL:CG1	2.39	0.53
1:B:264:CYS:HB2	1:B:301:TYR:OH	2.08	0.53
1:A:40:LEU:HB2	1:A:183:MET:HE2	1.92	0.52
1:A:71:PRO:HA	1:A:74:TYR:CD1	2.44	0.52
1:B:71:PRO:HA	1:B:74:TYR:CD1	2.44	0.52
1:B:97:THR:HG22	1:B:98:SER:N	2.24	0.52
1:A:283:PHE:HD2	1:A:287:PHE:CE2	2.27	0.52
1:A:286:ILE:HD13	1:A:286:ILE:H	1.72	0.52
1:A:193:THR:O	1:A:195:HIS:N	2.39	0.52
1:A:125:LEU:HD11	1:A:261:PHE:HE1	1.70	0.52
1:A:276:PHE:C	1:A:276:PHE:CD2	2.83	0.52
1:A:275:ILE:HD11	1:A:288:MET:HE1	1.91	0.52
1:B:279:GLN:HA	1:B:279:GLN:OE1	2.08	0.52
1:B:27:PRO:HB3	1:B:29:TYR:CE2	2.45	0.51
1:B:214:ILE:HB	1:B:215:PRO:HD3	1.92	0.51
1:B:310:ASN:HD21	1:B:313:PHE:CB	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:LYS:HE2	4:A:803:BGL:H1	1.92	0.51
1:B:194:PRO:O	1:B:196:GLU:CG	2.59	0.51
1:A:196:GLU:C	1:A:198:THR:H	2.14	0.51
2:B:503:BMA:O2	2:B:504:BMA:O5	2.27	0.51
1:B:273:PHE:O	1:B:273:PHE:CD2	2.63	0.51
1:B:290:ILE:H	1:B:291:PRO:HD2	1.75	0.51
1:B:39:MET:N	1:B:39:MET:HE3	2.26	0.50
1:B:193:THR:O	1:B:195:HIS:N	2.44	0.50
1:B:2:ASN:HB2	1:B:282:ASP:HB3	1.86	0.50
1:A:284:GLY:HA3	1:A:286:ILE:HD13	1.94	0.50
1:B:284:GLY:HA3	1:B:286:ILE:CD1	2.42	0.50
4:B:806:BGL:C3'	4:B:806:BGL:O1	2.59	0.50
1:A:66:LYS:CB	1:A:69:ARG:NH1	2.75	0.49
1:A:273:PHE:C	1:A:273:PHE:CD2	2.86	0.49
1:A:76:LEU:HD21	1:A:131:LEU:HD22	1.95	0.49
1:B:286:ILE:HG12	1:B:287:PHE:N	2.27	0.49
1:B:2:ASN:OD1	1:B:282:ASP:HB3	2.12	0.48
1:A:125:LEU:CD1	1:A:261:PHE:CE1	2.85	0.48
1:A:301:TYR:HB3	5:B:902:PLM:CB	2.37	0.48
1:A:216:LEU:HD23	1:A:216:LEU:O	2.14	0.48
1:B:275:ILE:HG12	1:B:283:PHE:CZ	2.49	0.48
1:B:70:THR:HB	1:B:71:PRO:HD2	1.95	0.48
1:A:119:LEU:HD12	1:A:164:ALA:HB1	1.96	0.48
1:A:70:THR:HG23	1:A:71:PRO:HD2	1.93	0.48
1:A:125:LEU:HD11	1:A:261:PHE:CE1	2.48	0.48
3:A:601:NAG:H62	3:A:602:NAG:HN2	1.77	0.47
1:B:125:LEU:C	1:B:125:LEU:HD23	2.34	0.47
1:A:286:ILE:CD1	1:A:286:ILE:H	2.27	0.47
1:B:26:ALA:HB1	1:B:27:PRO:HD2	1.95	0.47
1:B:239:GLU:HG3	1:B:239:GLU:H	1.23	0.47
1:A:59:LEU:CD2	1:A:77:LEU:HD12	2.45	0.47
1:A:154:ILE:O	1:A:155:MET:C	2.53	0.47
1:B:196:GLU:C	1:B:198:THR:N	2.68	0.47
1:A:312:GLN:O	1:A:315:ASN:N	2.48	0.47
1:B:155:MET:HE3	1:B:155:MET:N	2.29	0.47
4:A:804:BGL:H3'1	1:B:35:TRP:CD1	2.50	0.47
1:B:65:HIS:CD2	1:B:316:CYS:HB3	2.49	0.47
1:A:223:TYR:HB3	1:A:254:VAL:HG13	1.97	0.47
1:B:66:LYS:HA	1:B:69:ARG:CZ	2.45	0.47
1:A:231:LYS:HZ1	4:A:803:BGL:H3	1.79	0.46
1:B:238:GLN:HA	1:B:244:GLN:NE2	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:VAL:HA	1:B:308:MET:CG	2.46	0.46
1:B:274:TYR:O	1:B:278:HIS:N	2.46	0.46
1:A:283:PHE:O	1:A:284:GLY:C	2.53	0.46
1:A:57:LEU:HD21	1:A:321:LEU:HD11	1.96	0.46
1:A:66:LYS:HA	1:A:69:ARG:NH1	2.28	0.46
1:A:284:GLY:HA3	1:A:286:ILE:CD1	2.46	0.46
1:B:39:MET:HE3	1:B:39:MET:CA	2.41	0.45
1:B:154:ILE:O	1:B:157:VAL:N	2.49	0.45
1:B:293:PHE:HD1	1:B:294:PHE:CA	2.30	0.45
1:A:133:ILE:HD11	1:A:218:VAL:CG1	2.46	0.45
1:B:178:TYR:C	1:B:179:ILE:HG23	2.37	0.45
1:A:214:ILE:HB	1:A:215:PRO:HD3	1.97	0.45
1:B:32:ALA:HB3	1:B:37:PHE:CE2	2.52	0.44
2:B:501:NAG:H82	2:B:501:NAG:H2	1.71	0.44
1:A:173:VAL:O	1:A:173:VAL:HG23	2.17	0.44
1:A:1:MET:HA	3:A:601:NAG:N2	2.31	0.44
1:A:254:VAL:CG1	4:A:803:BGL:H6'2	2.48	0.44
1:B:86:MET:HE1	1:B:299:ALA:HB2	1.96	0.44
1:B:310:ASN:ND2	1:B:313:PHE:H	2.03	0.44
1:B:259:ILE:O	1:B:263:ILE:HG13	2.18	0.44
1:B:193:THR:C	1:B:195:HIS:N	2.71	0.44
1:B:178:TYR:O	1:B:179:ILE:HG23	2.18	0.44
1:A:284:GLY:CA	1:A:286:ILE:HD13	2.48	0.44
1:B:231:LYS:NZ	1:B:251:THR:HG21	2.33	0.44
1:A:28:GLN:O	1:A:31:LEU:HD22	2.13	0.43
1:A:288:MET:HA	1:A:288:MET:HE3	2.00	0.43
1:B:124:ALA:O	1:B:127:SER:HB2	2.17	0.43
1:A:312:GLN:O	1:A:313:PHE:C	2.57	0.43
1:B:200:ASN:O	1:B:204:VAL:HG23	2.18	0.43
1:A:324:GLY:C	1:A:325:LYS:HG3	2.35	0.43
5:A:901:PLM:HB2	1:B:301:TYR:CB	2.47	0.43
1:A:287:PHE:C	1:A:287:PHE:CD2	2.91	0.43
1:A:15:ASN:OD1	1:A:18:GLY:CA	2.65	0.43
1:A:193:THR:C	1:A:195:HIS:H	2.18	0.43
1:A:66:LYS:HB2	1:A:66:LYS:HE2	1.68	0.43
1:B:178:TYR:O	1:B:179:ILE:HG22	2.18	0.43
1:A:83:ASP:O	1:A:87:VAL:HG23	2.18	0.43
1:A:304:VAL:HA	1:A:308:MET:CG	2.48	0.43
1:A:200:ASN:O	1:A:204:VAL:HG23	2.19	0.43
1:A:302:ASN:CB	1:A:303:PRO:HD3	2.49	0.43
1:B:50:LEU:O	1:B:54:ILE:HD13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:MET:N	1:B:39:MET:CE	2.80	0.43
1:B:170:PRO:CB	1:B:171:PRO:HD3	2.49	0.43
1:A:66:LYS:HA	1:A:69:ARG:NE	2.30	0.43
1:B:37:PHE:HE1	1:B:185:CYS:SG	2.42	0.43
1:B:128:LEU:HD23	1:B:128:LEU:HA	1.67	0.43
1:B:216:LEU:HD12	1:B:216:LEU:HA	1.80	0.43
1:B:57:LEU:HD12	1:B:57:LEU:HA	1.89	0.43
1:A:276:PHE:O	1:A:276:PHE:CD2	2.72	0.43
1:A:196:GLU:C	1:A:198:THR:N	2.72	0.43
1:B:191:TYR:O	1:B:191:TYR:CD1	2.72	0.43
1:A:25:GLU:OE2	1:A:25:GLU:HA	2.19	0.43
1:B:309:MET:O	1:B:314:ARG:NH1	2.52	0.43
1:B:54:ILE:HG21	1:B:303:PRO:HB2	2.00	0.42
1:A:169:ALA:N	1:A:170:PRO:CD	2.82	0.42
1:A:50:LEU:O	1:A:53:PRO:HD2	2.18	0.42
1:A:91:PHE:N	1:A:91:PHE:CD1	2.87	0.42
1:A:124:ALA:O	1:A:127:SER:HB2	2.18	0.42
5:A:901:PLM:CB	1:B:301:TYR:CB	2.93	0.42
1:A:290:ILE:N	1:A:291:PRO:CD	2.81	0.42
2:A:403:BMA:H3	2:A:404:BMA:H2	1.77	0.42
1:B:287:PHE:C	1:B:287:PHE:HD2	2.16	0.42
1:A:214:ILE:O	1:A:215:PRO:C	2.58	0.42
1:B:91:PHE:CD1	1:B:91:PHE:N	2.85	0.42
1:B:47:LEU:HD12	1:B:47:LEU:HA	1.78	0.42
1:B:21:ARG:HH22	2:B:502:NAG:H81	1.83	0.42
1:B:2:ASN:HB2	1:B:282:ASP:CB	2.49	0.42
1:A:125:LEU:HD13	1:A:261:PHE:CE1	2.52	0.42
4:A:802:BGL:O1	4:A:802:BGL:H1'1	2.19	0.42
1:B:208:PHE:O	1:B:212:PHE:HB3	2.20	0.42
1:B:312:GLN:O	1:B:313:PHE:C	2.58	0.42
1:A:165:LEU:C	1:A:167:CYS:H	2.22	0.42
1:A:28:GLN:CB	1:A:31:LEU:HD21	2.49	0.41
1:A:177:ARG:NH1	1:A:190:ASP:OD1	2.53	0.41
1:A:43:TYR:OH	1:A:297:THR:HB	2.19	0.41
1:A:274:TYR:O	1:A:278:HIS:N	2.53	0.41
1:A:115:PHE:CD1	1:A:172:LEU:HD11	2.55	0.41
1:A:152:HIS:HA	1:A:155:MET:HE2	2.03	0.41
1:A:55:ASN:OD1	1:A:83:ASP:HB3	2.20	0.41
1:B:289:THR:O	1:B:289:THR:CG2	2.68	0.41
1:B:89:GLY:O	1:B:113:GLU:HG2	2.21	0.41
1:B:221:PHE:O	1:B:225:GLN:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:GLN:NE2	1:A:30:TYR:OH	2.53	0.41
1:A:171:PRO:HB2	1:A:178:TYR:CE2	2.55	0.41
1:A:128:LEU:HD23	1:A:128:LEU:HA	1.80	0.41
1:A:100:HIS:CG	1:A:104:VAL:HG11	2.56	0.41
1:A:55:ASN:HD21	1:A:303:PRO:HG3	1.85	0.41
1:A:39:MET:O	1:A:40:LEU:C	2.58	0.41
1:B:45:PHE:O	1:B:49:MET:HG2	2.20	0.41
1:B:87:VAL:HA	1:B:91:PHE:CD2	2.55	0.41
1:B:283:PHE:HD2	1:B:283:PHE:H	1.69	0.41
1:A:112:LEU:HA	1:A:112:LEU:HD23	1.94	0.41
1:B:181:GLU:O	1:B:184:GLN:N	2.45	0.41
1:B:286:ILE:CG1	1:B:287:PHE:H	2.31	0.41
1:A:65:HIS:CG	1:A:316:CYS:HB3	2.55	0.41
1:B:57:LEU:HD21	1:B:321:LEU:HD11	2.03	0.41
1:B:324:GLY:C	1:B:325:LYS:HG3	2.38	0.41
1:A:99:LEU:HD13	1:B:35:TRP:HB2	2.03	0.41
1:A:161:TRP:O	1:A:165:LEU:HD22	2.21	0.41
1:B:288:MET:O	1:B:291:PRO:HG2	2.21	0.40
1:B:103:PHE:HD1	1:B:185:CYS:O	2.04	0.40
1:A:154:ILE:O	1:A:157:VAL:N	2.52	0.40
1:A:231:LYS:HZ3	4:A:803:BGL:H3	1.85	0.40
1:B:170:PRO:N	1:B:171:PRO:CD	2.84	0.40
1:A:113:GLU:O	1:A:113:GLU:OE1	2.39	0.40
1:B:40:LEU:HD22	1:B:183:MET:HE3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	324/348 (93%)	284 (88%)	38 (12%)	2 (1%)	30 67

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	324/348 (93%)	277 (86%)	44 (14%)	3 (1%)	21	57
All	All	648/696 (93%)	561 (87%)	82 (13%)	5 (1%)	24	60

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	284	GLY
1	A	279	GLN
1	B	194	PRO
1	A	182	GLY
1	B	107	PRO

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	278/296 (94%)	255 (92%)	23 (8%)	14	38
1	B	278/296 (94%)	255 (92%)	23 (8%)	14	38
All	All	556/592 (94%)	510 (92%)	46 (8%)	14	38

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	4	THR
1	A	17	THR
1	A	47	LEU
1	A	66	LYS
1	A	77	LEU
1	A	113	GLU
1	A	118	THR
1	A	138	VAL
1	A	160	THR
1	A	163	MET

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Mol	Chain	Res	Type
1	A	165	LEU
1	A	177	ARG
1	A	236	GLN
1	A	242	THR
1	A	268	TYR
1	A	276	PHE
1	A	286	ILE
1	A	287	PHE
1	A	288	MET
1	A	289	THR
1	A	293	PHE
1	A	311	LYS
1	B	2	ASN
1	B	4	THR
1	B	21	ARG
1	B	31	LEU
1	B	39	MET
1	B	46	LEU
1	B	47	LEU
1	B	93	THR
1	B	97	THR
1	B	125	LEU
1	B	138	VAL
1	B	155	MET
1	B	165	LEU
1	B	239	GLU
1	B	268	TYR
1	B	283	PHE
1	B	286	ILE
1	B	287	PHE
1	B	293	PHE
1	B	309	MET
1	B	310	ASN
1	B	311	LYS
1	B	322	CYS

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	28	GLN
1	A	55	ASN
1	A	64	GLN

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Mol	Chain	Res	Type
1	A	78	ASN
1	A	184	GLN
1	A	236	GLN
1	A	315	ASN
1	B	28	GLN
1	B	64	GLN
1	B	73	ASN
1	B	152	HIS
1	B	237	GLN
1	B	310	ASN
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 ⓘ

12 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	NAG	A	401	1,2	14,14,15	0.56	0	15,19,21	1.02	1 (6%)
2	NAG	A	402	2	14,14,15	0.44	0	15,19,21	1.03	1 (6%)
2	BMA	A	403	2	11,11,12	0.37	0	14,15,17	1.93	5 (35%)
2	BMA	A	404	2	11,11,12	0.30	0	14,15,17	0.79	0
3	NAG	A	601	1,3	14,14,15	0.51	0	15,19,21	1.57	2 (13%)
3	NAG	A	602	3	14,14,15	0.53	0	15,19,21	0.95	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	501	1,2	14,14,15	0.56	0	15,19,21	2.07	3 (20%)
2	NAG	B	502	2	14,14,15	0.45	0	15,19,21	1.58	2 (13%)
2	BMA	B	503	2	11,11,12	0.73	0	14,15,17	1.76	4 (28%)
2	BMA	B	504	2	11,11,12	0.37	0	14,15,17	0.86	0
3	NAG	B	701	1,3	14,14,15	0.64	0	15,19,21	0.92	1 (6%)
3	NAG	B	702	3	14,14,15	0.62	0	15,19,21	1.16	2 (13%)

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	NAG	A	401	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	402	2	-	0/6/23/26	0/1/1/1
2	BMA	A	403	2	-	0/2/19/22	0/1/1/1
2	BMA	A	404	2	-	0/2/19/22	0/1/1/1
3	NAG	A	601	1,3	-	2/6/23/26	0/1/1/1
3	NAG	A	602	3	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	2	-	0/6/23/26	0/1/1/1
2	BMA	B	503	2	-	0/2/19/22	0/1/1/1
2	BMA	B	504	2	-	0/2/19/22	0/1/1/1
3	NAG	B	701	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	702	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	NAG	C2-N2-C7	-5.78	115.61	123.04
2	B	502	NAG	C2-N2-C7	-4.60	117.13	123.04
2	B	503	BMA	O5-C1-C2	-3.88	104.57	110.86
2	A	403	BMA	O5-C1-C2	-3.21	105.65	110.86
2	B	501	NAG	O7-C7-C8	-2.44	117.59	122.06
3	B	701	NAG	C3-C4-C5	-2.33	106.13	110.20
2	A	402	NAG	C6-C5-C4	-2.27	107.41	113.02
2	A	403	BMA	O2-C2-C3	-2.26	105.57	110.12
2	B	503	BMA	O5-C5-C6	2.01	111.69	107.35
2	B	503	BMA	C1-C2-C3	2.03	111.95	109.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	NAG	C1-O5-C5	2.06	114.86	112.25
3	A	602	NAG	C3-C4-C5	2.11	113.88	110.20
3	B	702	NAG	O5-C5-C6	2.25	112.22	107.35
2	B	502	NAG	C1-O5-C5	2.29	115.16	112.25
2	A	403	BMA	C2-C3-C4	2.65	115.55	111.04
3	B	702	NAG	C4-C3-C2	2.70	115.43	111.23
2	A	403	BMA	C3-C4-C5	2.92	115.29	110.20
2	A	403	BMA	C1-C2-C3	3.32	113.47	109.54
2	B	503	BMA	C3-C4-C5	3.32	115.99	110.20
3	A	601	NAG	C3-C4-C5	3.36	116.05	110.20
2	B	501	NAG	C1-O5-C5	3.92	117.22	112.25
3	A	601	NAG	C1-O5-C5	4.12	117.48	112.25

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	NAG	O7-C7-N2-C2
3	A	601	NAG	C8-C7-N2-C2

There are no ring outliers.

10 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	403	BMA	4	0
2	A	404	BMA	4	0
3	A	601	NAG	8	0
3	A	602	NAG	1	0
2	B	501	NAG	2	0
2	B	502	NAG	1	0
2	B	503	BMA	5	0
2	B	504	BMA	5	0
3	B	701	NAG	7	0
3	B	702	NAG	3	0

5.6 Ligand geometry

8 ligands 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	$\# Z > 2$
4	BGL	A	801	-	19,20,20	0.49	0	23,25,25	0.86	1 (4%)
4	BGL	A	802	-	19,20,20	0.49	0	23,25,25	0.85	0
4	BGL	A	803	-	19,20,20	0.39	0	23,25,25	0.60	0
4	BGL	A	804	-	19,20,20	0.46	0	23,25,25	1.16	2 (8%)
5	PLM	A	901	1	16,16,17	0.42	0	14,15,17	0.55	0
4	BGL	B	805	-	19,20,20	0.43	0	23,25,25	0.69	0
4	BGL	B	806	-	19,20,20	0.50	0	23,25,25	0.84	1 (4%)
5	PLM	B	902	1	16,16,17	0.42	0	14,15,17	0.56	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
4	BGL	A	801	-	-	0/11/31/31	0/1/1/1
4	BGL	A	802	-	-	0/11/31/31	0/1/1/1
4	BGL	A	803	-	-	0/11/31/31	0/1/1/1
4	BGL	A	804	-	-	0/11/31/31	0/1/1/1
5	PLM	A	901	1	-	0/13/14/15	0/0/0/0
4	BGL	B	805	-	-	0/11/31/31	0/1/1/1
4	BGL	B	806	-	1/1/5/5	0/11/31/31	0/1/1/1
5	PLM	B	902	1	-	0/13/14/15	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	804	BGL	C1-C2-C3	-3.35	104.54	110.45
4	A	804	BGL	C4-C3-C2	-2.23	104.69	109.60
4	B	806	BGL	C3-C4-C5	-2.10	106.53	110.20
4	A	801	BGL	C3-C4-C5	2.48	114.52	110.20

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	B	806	BGL	C5

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	BGL	1	0
4	A	802	BGL	3	0
4	A	803	BGL	7	0
4	A	804	BGL	3	0
5	A	901	PLM	6	0
4	B	805	BGL	1	0
4	B	806	BGL	4	0
5	B	902	PLM	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

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, 95th 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 ²)	Q<0.9
1	A	326/348 (93%)	0.65	10 (3%) 52 45	22, 47, 81, 114	1 (0%)
1	B	326/348 (93%)	0.64	14 (4%) 39 32	25, 46, 83, 118	1 (0%)
All	All	652/696 (93%)	0.65	24 (3%) 45 38	22, 47, 83, 118	2 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	191	TYR	4.1
1	B	268	TYR	3.7
1	B	292	ALA	3.7
1	A	189	ILE	3.5
1	B	191	TYR	3.5
1	A	283	PHE	3.3
1	B	325	LYS	3.3
1	B	311	LYS	3.2
1	B	285	PRO	3.0
1	A	295	ALA	2.8
1	A	285	PRO	2.7
1	B	96	TYR	2.7
1	B	288	MET	2.5
1	A	296	LYS	2.5
1	A	313	PHE	2.5
1	B	295	ALA	2.4
1	A	308	MET	2.4
1	B	306	TYR	2.4
1	B	62	THR	2.3
1	B	248	LYS	2.2
1	B	23	PRO	2.2
1	B	68	LEU	2.0
1	A	192	TYR	2.0
1	A	104	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
2	NAG	A	401	14/15	0.98	0.23	0.01	31,43,61,65	0
2	NAG	B	501	14/15	0.94	0.19	-1.28	27,42,74,81	0
3	NAG	A	601	14/15	0.87	0.14	-1.36	63,119,150,170	0
3	NAG	B	701	14/15	0.81	0.13	-1.58	53,139,189,198	0
2	BMA	B	503	11/12	0.82	0.17	-	44,91,135,165	0
2	BMA	A	403	11/12	0.93	0.13	-	60,91,120,146	0
2	BMA	A	404	11/12	0.95	0.13	-	74,115,149,172	0
2	NAG	B	502	14/15	0.96	0.18	-	10,35,56,62	0
3	NAG	A	602	14/15	0.85	0.17	-	85,127,185,193	0
2	BMA	B	504	11/12	0.91	0.12	-	73,114,139,156	0
2	NAG	A	402	14/15	0.97	0.17	-	15,33,54,68	0
3	NAG	B	702	14/15	0.79	0.19	-	50,130,201,220	0

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th 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 ²)	Q<0.9
5	PLM	B	902	17/18	0.77	0.77	8.97	58,82,125,191	0
5	PLM	A	901	17/18	0.83	0.62	5.17	50,87,107,155	0
4	BGL	A	804	20/20	0.72	0.49	4.06	40,80,191,199	0
4	BGL	A	803	20/20	0.88	0.37	3.99	45,94,165,173	0
4	BGL	B	806	20/20	0.77	0.30	1.24	26,91,188,214	0
4	BGL	B	805	20/20	0.70	0.42	-	35,95,194,195	0
4	BGL	A	802	20/20	0.74	0.28	-	36,99,176,177	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	BGL	A	801	20/20	0.69	0.15	-	78,127,206,210	0

6.5 Other polymers [i](#)

There are no such residues in this entry.