Full wwPDB X-ray Structure Validation Report (i)

Apr 27, 2024 – 06:19 pm BST

PDB ID	:	1QM5
Title	:	Phosphorylase recognition and phosphorylysis of its oligosaccharide substrate: answers to a long outstanding question
Authors	:	Watson, K.A.; McCleverty, C.; Geremia, S.; Cottaz, S.; Driguez, H.; Johnson, L.N.
Deposited on	:	1999-09-20
Resolution	:	2.00 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

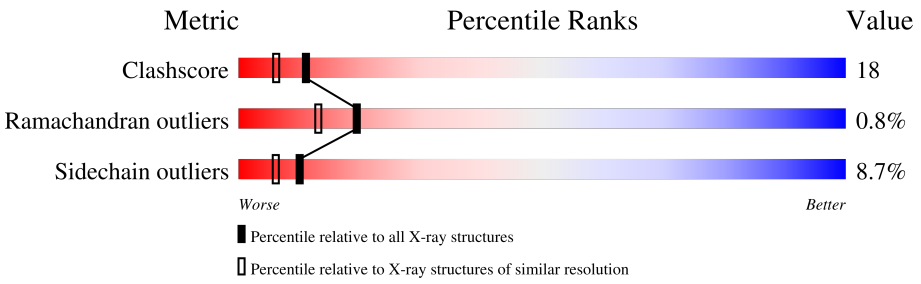
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. 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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	796	68% 27% .
1	B	796	67% 28% 5%
2	C	4	25% 25% 50%
2	D	4	25% 25% 50%

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
2	GLC	C	1	X	-	-	-
2	SGC	C	4	X	-	-	-
2	GLC	D	1	X	-	-	-
2	SGC	D	4	X	-	-	-
3	PO4	A	900	-	X	X	-
3	PO4	B	900	-	X	X	-
5	PLP	A	999	-	X	-	-
5	PLP	B	999	-	X	-	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 13662 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.

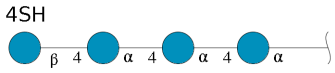
- Molecule 1 is a protein called MALTODEXTRIN PHOSPHORYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	796	6378	4068	1127	1163	20	0	0	0
1	B	796	6378	4068	1127	1163	20	0	0	0

There are 16 discrepancies between the modelled and reference sequences:

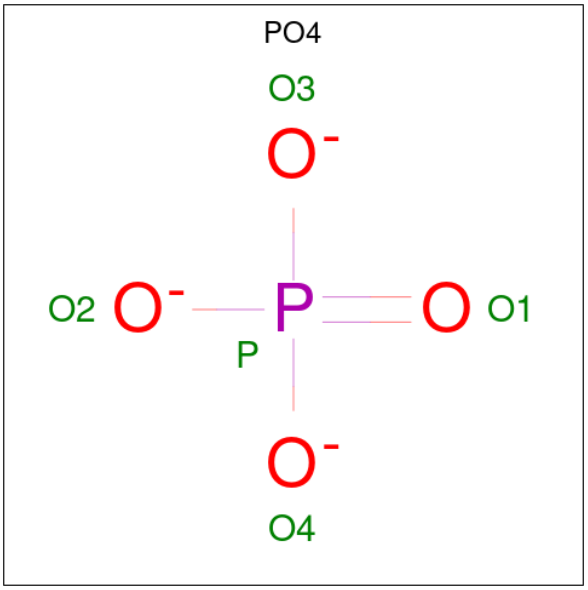
Chain	Residue	Modelled	Actual	Comment	Reference
A	293	LYS	GLU	conflict	UNP P00490
A	487	GLU	VAL	conflict	UNP P00490
A	489	PHE	LEU	conflict	UNP P00490
A	497	ASP	GLN	conflict	UNP P00490
A	498	GLN	LEU	conflict	UNP P00490
A	501	GLU	VAL	conflict	UNP P00490
A	521	GLU	ASP	conflict	UNP P00490
A	547	HIS	ARG	conflict	UNP P00490
B	293	LYS	GLU	conflict	UNP P00490
B	487	GLU	VAL	conflict	UNP P00490
B	489	PHE	LEU	conflict	UNP P00490
B	497	ASP	GLN	conflict	UNP P00490
B	498	GLN	LEU	conflict	UNP P00490
B	501	GLU	VAL	conflict	UNP P00490
B	521	GLU	ASP	conflict	UNP P00490
B	547	HIS	ARG	conflict	UNP P00490

- Molecule 2 is an oligosaccharide called 4-thio-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose.



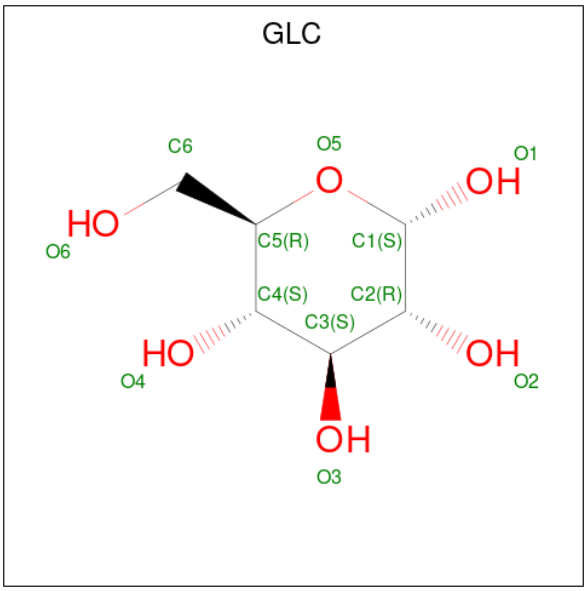
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	O	S			
2	C	4	45	24	20	1	0	0	0
			Total	C	O	S			
2	D	4	45	24	20	1	0	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



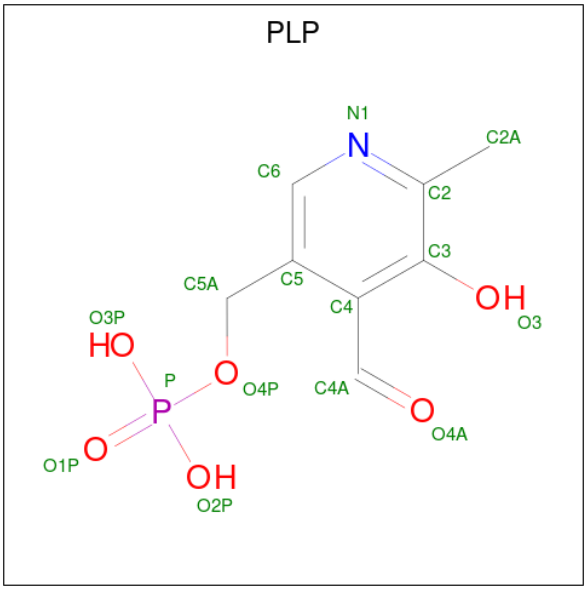
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0
			Total	O	P		
3	B	1	5	4	1	0	0

- Molecule 4 is alpha-D-glucopyranose (three-letter code: GLC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O		0	0
			11	6	5			
4	B	1	Total	C	O		0	0
			11	6	5			

- Molecule 5 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
5	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	377	377	377	0	0
			Total	O		
6	B	377	377	377	0	0

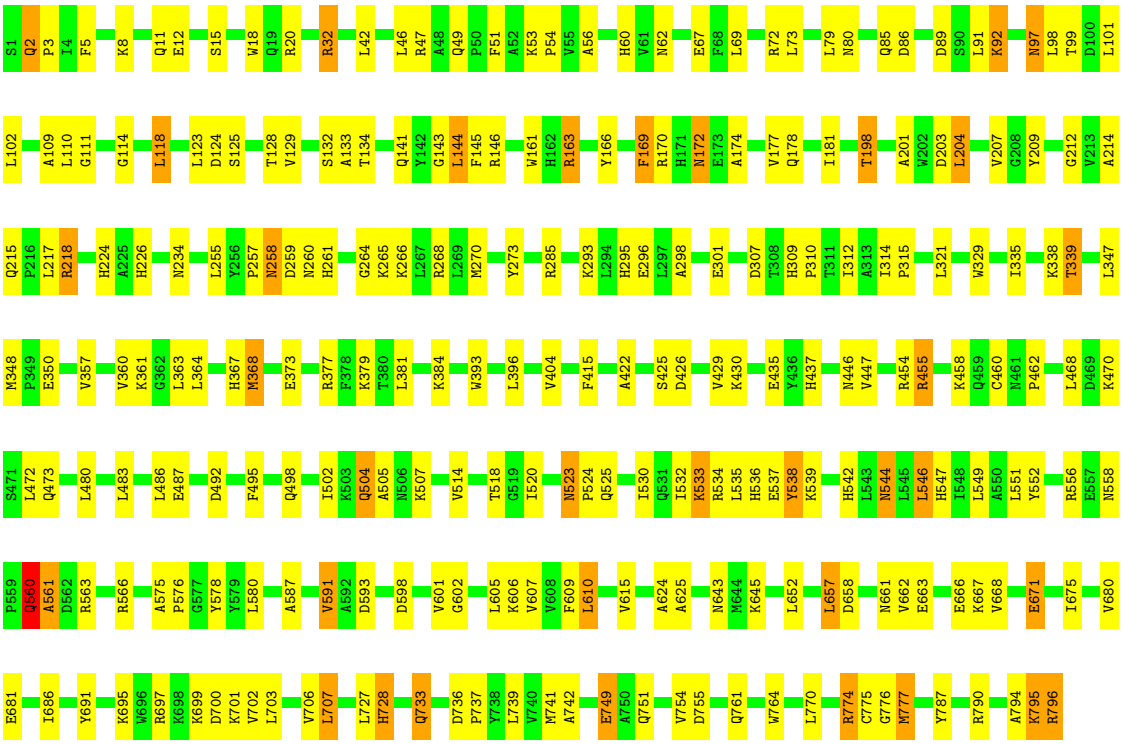
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

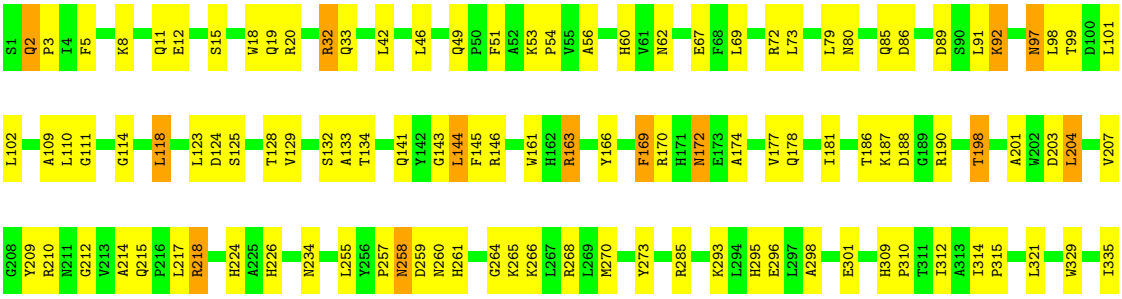
• Molecule 1: MALTODEXTRIN PHOSPHORYLASE

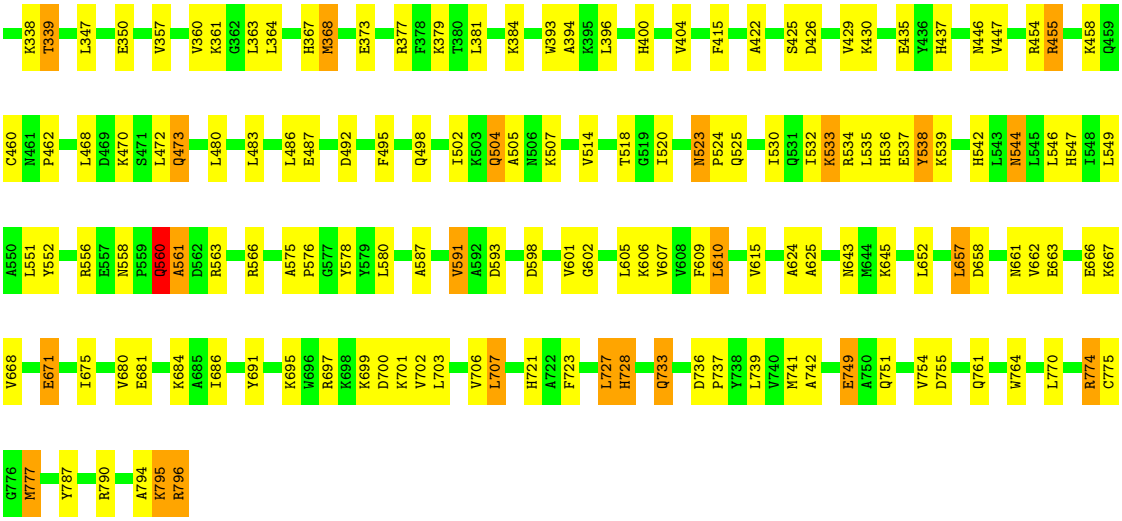
Chain A: 68% 27% •



• Molecule 1: MALTODEXTRIN PHOSPHORYLASE

Chain B: 67% 28% 5%





• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain C:

• Molecule 2: 4-thio-beta-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose-(1-4)-alpha-D-glucopyranose

Chain D:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	107.41Å 61.50Å 132.38Å 90.00° 105.03° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00	Depositor
% Data completeness (in resolution range)	80.0 (50.00-2.00)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.5	Depositor
R, R_{free}	0.228 , 0.261	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13662	wwPDB-VP
Average B, all atoms (Å^2)	26.0	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: SGC, PLP, GLC, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| >5$	RMSZ	$\#\|Z\| >5$
1	A	0.37	0/6528	0.60	0/8853
1	B	0.37	0/6528	0.60	0/8853
All	All	0.37	0/13056	0.60	0/17706

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 (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	6378	0	6308	227	0
1	B	6378	0	6308	238	0
2	C	45	0	38	2	0
2	D	45	0	38	2	0
3	A	5	0	0	2	0
3	B	5	0	0	2	0
4	A	11	0	10	0	0
4	B	11	0	10	0	0
5	A	15	0	7	2	0
5	B	15	0	7	2	0
6	A	377	0	0	20	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	377	0	0	26	0
All	All	13662	0	12726	461	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 18.

All (461) 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:473:GLN:CG	6:B:2227:HOH:O	1.91	1.15
1:A:728:HIS:HB3	1:A:733:GLN:NE2	1.72	1.04
1:B:657:LEU:HD13	1:B:662:VAL:HG12	1.41	1.03
1:B:728:HIS:HB3	1:B:733:GLN:NE2	1.72	1.02
1:A:657:LEU:HD13	1:A:662:VAL:HG12	1.41	1.01
1:A:796:ARG:HA	1:A:796:ARG:NE	1.77	0.99
1:A:794:ALA:C	1:A:796:ARG:H	1.62	0.98
1:B:796:ARG:HA	1:B:796:ARG:NE	1.77	0.98
1:B:794:ALA:C	1:B:796:ARG:H	1.62	0.97
1:B:473:GLN:CD	6:B:2227:HOH:O	2.04	0.94
1:A:132:SER:HA	1:A:215:GLN:HE22	1.34	0.93
1:B:2:GLN:HB3	1:B:3:PRO:HD3	1.52	0.92
1:A:547:HIS:CE1	1:A:751:GLN:HG2	2.04	0.92
1:B:547:HIS:CE1	1:B:751:GLN:HG2	2.04	0.92
1:A:2:GLN:HB3	1:A:3:PRO:HD3	1.52	0.91
1:B:132:SER:HA	1:B:215:GLN:HE22	1.34	0.91
1:A:170:ARG:HG3	1:B:20:ARG:O	1.72	0.90
1:A:794:ALA:O	1:A:796:ARG:N	2.07	0.88
1:B:794:ALA:O	1:B:796:ARG:N	2.07	0.88
1:A:697:ARG:HB2	1:A:741:MET:HE2	1.57	0.86
1:B:697:ARG:HB2	1:B:741:MET:HE2	1.58	0.86
1:B:396:LEU:HD21	1:B:435:GLU:HB2	1.61	0.83
1:B:566:ARG:HH12	1:B:751:GLN:NE2	1.76	0.83
1:A:396:LEU:HD21	1:A:435:GLU:HB2	1.60	0.83
1:A:20:ARG:O	1:B:170:ARG:HG3	1.79	0.83
1:A:566:ARG:HH12	1:A:751:GLN:NE2	1.76	0.82
1:B:46:LEU:O	1:B:49:GLN:HG2	1.83	0.78
1:B:224:HIS:HD2	1:B:226:HIS:H	1.31	0.78
1:B:794:ALA:C	1:B:796:ARG:N	2.38	0.77
1:B:201:ALA:HB1	1:B:218:ARG:HD2	1.66	0.77
1:A:46:LEU:O	1:A:49:GLN:HG2	1.83	0.77
1:A:224:HIS:HD2	1:A:226:HIS:H	1.31	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:ALA:HB1	1:A:218:ARG:HD2	1.66	0.76
1:A:51:PHE:HE1	1:A:214:ALA:H	1.33	0.76
1:A:794:ALA:C	1:A:796:ARG:N	2.38	0.76
1:B:770:LEU:O	1:B:774:ARG:HG2	1.86	0.76
1:A:770:LEU:O	1:A:774:ARG:HG2	1.86	0.75
1:B:51:PHE:HE1	1:B:214:ALA:H	1.33	0.75
1:A:749:GLU:HG3	6:A:2352:HOH:O	1.87	0.75
1:B:217:LEU:HD12	1:B:217:LEU:O	1.87	0.75
1:B:314:ILE:HB	1:B:315:PRO:HD3	1.69	0.75
1:A:657:LEU:HD13	1:A:662:VAL:CG1	2.17	0.75
1:A:132:SER:HA	1:A:215:GLN:NE2	2.02	0.74
1:B:749:GLU:HG3	6:B:2350:HOH:O	1.87	0.74
1:A:217:LEU:HD12	1:A:217:LEU:O	1.87	0.73
1:A:314:ILE:HB	1:A:315:PRO:HD3	1.69	0.73
1:B:298:ALA:HB2	1:B:339:THR:HG22	1.71	0.73
1:B:518:THR:HG22	1:B:520:ILE:HG13	1.70	0.73
1:B:132:SER:HA	1:B:215:GLN:NE2	2.02	0.72
1:A:518:THR:HG22	1:A:520:ILE:HG13	1.70	0.72
1:A:203:ASP:OD2	1:A:218:ARG:HD3	1.90	0.72
1:B:203:ASP:OD2	1:B:218:ARG:HD3	1.90	0.72
1:B:728:HIS:HB3	1:B:733:GLN:HE22	1.54	0.72
1:B:657:LEU:HD13	1:B:662:VAL:CG1	2.17	0.71
1:A:298:ALA:HB2	1:A:339:THR:HG22	1.71	0.71
1:A:728:HIS:HB3	1:A:733:GLN:HE22	1.54	0.71
1:A:533:LYS:HG3	1:A:539:LYS:HG2	1.72	0.71
1:A:224:HIS:CD2	1:A:226:HIS:H	2.07	0.71
1:B:224:HIS:CD2	1:B:226:HIS:H	2.07	0.71
1:A:666:GLU:HG2	6:A:2319:HOH:O	1.91	0.71
1:B:533:LYS:HG3	1:B:539:LYS:HG2	1.72	0.71
1:B:796:ARG:CZ	1:B:796:ARG:OXT	2.39	0.71
1:A:124:ASP:O	1:A:128:THR:HG23	1.92	0.70
1:B:666:GLU:HG2	6:B:2314:HOH:O	1.91	0.70
1:B:124:ASP:O	1:B:128:THR:HG23	1.92	0.70
1:A:796:ARG:NE	1:A:796:ARG:CA	2.51	0.69
1:A:796:ARG:CZ	1:A:796:ARG:OXT	2.39	0.69
1:A:667:LYS:HG3	1:A:777:MET:HE2	1.76	0.68
1:B:373:GLU:OE1	1:B:377:ARG:HD2	1.95	0.67
1:B:667:LYS:HG3	1:B:777:MET:HE2	1.77	0.67
1:A:373:GLU:OE1	1:A:377:ARG:HD2	1.95	0.67
1:B:796:ARG:NE	1:B:796:ARG:CA	2.51	0.67
1:A:128:THR:HG22	1:A:209:TYR:H	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:PHE:CE2	1:A:796:ARG:OXT	2.48	0.67
1:B:128:THR:HG22	1:B:209:TYR:H	1.59	0.66
1:B:309:HIS:HB2	1:B:310:PRO:HD3	1.78	0.66
1:B:415:PHE:CE2	1:B:796:ARG:OXT	2.48	0.66
1:B:261:HIS:CD2	1:B:264:GLY:H	2.14	0.66
1:B:728:HIS:HB3	1:B:733:GLN:HE21	1.61	0.66
1:A:266:LYS:HG3	1:A:363:LEU:HD11	1.78	0.66
1:B:796:ARG:CZ	1:B:796:ARG:CA	2.74	0.65
1:A:796:ARG:CA	1:A:796:ARG:CZ	2.74	0.65
1:A:261:HIS:HE1	1:B:234:ASN:O	1.79	0.65
1:B:146:ARG:HH11	1:B:146:ARG:HG3	1.61	0.65
1:B:266:LYS:HG3	1:B:363:LEU:HD11	1.78	0.65
1:A:261:HIS:CD2	1:A:264:GLY:H	2.14	0.65
1:A:146:ARG:HG3	1:A:146:ARG:HH11	1.61	0.64
1:A:309:HIS:HB2	1:A:310:PRO:HD3	1.78	0.64
1:B:563:ARG:O	6:B:2264:HOH:O	2.15	0.64
1:B:188:ASP:OD1	6:B:2102:HOH:O	2.15	0.64
1:A:728:HIS:HB3	1:A:733:GLN:HE21	1.61	0.64
1:A:60:HIS:HD2	1:A:132:SER:OG	1.79	0.64
1:B:60:HIS:HD2	1:B:132:SER:OG	1.80	0.64
1:B:473:GLN:HG3	6:B:2227:HOH:O	1.73	0.63
1:B:335:ILE:O	1:B:339:THR:HG23	1.99	0.63
1:A:587:ALA:O	1:A:591:VAL:HG13	1.99	0.62
1:A:335:ILE:O	1:A:339:THR:HG23	1.98	0.62
1:B:587:ALA:O	1:B:591:VAL:HG13	1.99	0.62
1:A:523:ASN:HD22	1:A:524:PRO:HD2	1.65	0.62
1:B:368:MET:HE3	1:B:404:VAL:HG21	1.82	0.62
1:A:60:HIS:HE1	1:A:134:THR:OG1	1.83	0.61
1:A:662:VAL:HG21	6:A:2210:HOH:O	1.99	0.61
1:B:169:PHE:CD2	1:B:204:LEU:HD13	2.36	0.61
1:B:523:ASN:HD22	1:B:524:PRO:HD2	1.65	0.61
1:B:662:VAL:HG21	6:B:2206:HOH:O	1.99	0.61
1:A:169:PHE:CD2	1:A:204:LEU:HD13	2.36	0.60
1:A:487:GLU:OE2	1:A:774:ARG:NH1	2.34	0.60
1:A:739:LEU:HB3	1:A:742:ALA:HB3	1.82	0.60
1:B:60:HIS:HE1	1:B:134:THR:OG1	1.83	0.60
1:B:487:GLU:OE2	1:B:774:ARG:NH1	2.34	0.60
1:A:514:VAL:HG22	1:A:610:LEU:HD21	1.83	0.60
1:B:739:LEU:HB3	1:B:742:ALA:HB3	1.82	0.60
1:B:514:VAL:HG22	1:B:610:LEU:HD21	1.84	0.60
1:A:234:ASN:O	1:B:261:HIS:HE1	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:796:ARG:HA	1:B:796:ARG:CZ	2.32	0.59
1:A:796:ARG:HA	1:A:796:ARG:CZ	2.32	0.59
1:A:563:ARG:O	6:A:2269:HOH:O	2.15	0.59
1:B:109:ALA:HB1	1:B:143:GLY:HA3	1.84	0.59
1:A:109:ALA:HB1	1:A:143:GLY:HA3	1.84	0.59
1:B:796:ARG:OXT	1:B:796:ARG:NH2	2.36	0.59
1:A:268:ARG:NH1	6:A:2159:HOH:O	2.33	0.58
1:A:796:ARG:OXT	1:A:796:ARG:NH2	2.36	0.58
1:B:132:SER:CA	1:B:215:GLN:HE22	2.13	0.58
1:A:2:GLN:CB	1:A:3:PRO:HD3	2.31	0.58
1:B:268:ARG:NH1	6:B:2155:HOH:O	2.33	0.58
1:B:396:LEU:HD21	1:B:435:GLU:CB	2.32	0.58
1:B:470:LYS:NZ	1:B:498:GLN:HE22	2.02	0.58
1:A:429:VAL:HG13	1:A:437:HIS:CG	2.39	0.58
1:A:198:THR:HG21	6:A:2110:HOH:O	2.05	0.57
1:B:429:VAL:HG13	1:B:437:HIS:CG	2.39	0.57
1:A:226:HIS:HD2	6:A:2043:HOH:O	1.88	0.57
1:A:598:ASP:O	1:A:601:VAL:HG12	2.05	0.57
1:A:368:MET:HE3	1:A:404:VAL:HG21	1.87	0.56
1:A:470:LYS:NZ	1:A:498:GLN:HE22	2.02	0.56
3:B:900:PO4:O4	2:D:4:SGC:H62	2.05	0.56
1:B:473:GLN:NE2	6:B:2227:HOH:O	2.31	0.56
1:B:598:ASP:O	1:B:601:VAL:HG12	2.05	0.56
1:B:198:THR:HG21	6:B:2107:HOH:O	2.05	0.56
1:B:560:GLN:CD	1:B:561:ALA:H	2.09	0.56
1:B:796:ARG:CZ	1:B:796:ARG:C	2.73	0.56
1:A:560:GLN:CD	1:A:561:ALA:H	2.09	0.56
1:A:700:ASP:HB3	1:A:703:LEU:HB3	1.87	0.56
1:A:796:ARG:CZ	1:A:796:ARG:C	2.73	0.56
1:B:258:ASN:ND2	1:B:260:ASN:H	2.04	0.56
1:B:700:ASP:HB3	1:B:703:LEU:HB3	1.87	0.56
1:A:62:ASN:HD21	1:A:301:GLU:HG3	1.71	0.56
3:A:900:PO4:O4	2:C:4:SGC:H62	2.05	0.56
1:B:133:ALA:H	1:B:215:GLN:NE2	2.03	0.56
1:B:523:ASN:HD22	1:B:524:PRO:CD	2.18	0.56
1:A:396:LEU:HD21	1:A:435:GLU:CB	2.32	0.56
1:A:258:ASN:ND2	1:A:260:ASN:H	2.04	0.55
1:A:468:LEU:CD2	1:A:486:LEU:HD11	2.36	0.55
6:A:2022:HOH:O	1:B:226:HIS:HD2	1.88	0.55
1:B:62:ASN:HD21	1:B:301:GLU:HG3	1.71	0.55
1:A:426:ASP:O	1:A:430:LYS:HG2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:ASN:HD22	1:A:524:PRO:CD	2.18	0.55
1:A:132:SER:CA	1:A:215:GLN:HE22	2.13	0.55
1:A:671:GLU:CD	1:A:671:GLU:H	2.10	0.55
1:B:468:LEU:CD2	1:B:486:LEU:HD11	2.37	0.55
1:B:379:LYS:HD3	1:B:393:TRP:CD2	2.42	0.55
1:A:645:LYS:NZ	5:A:999:PLP:C4A	2.70	0.55
1:A:703:LEU:HD21	1:A:741:MET:HE3	1.89	0.55
1:B:671:GLU:CD	1:B:671:GLU:H	2.10	0.55
1:A:379:LYS:HD3	1:A:393:TRP:CD2	2.42	0.54
1:A:736:ASP:N	1:A:737:PRO:HD3	2.23	0.54
1:B:560:GLN:CD	1:B:561:ALA:N	2.61	0.54
1:B:601:VAL:HG21	1:B:605:LEU:HB3	1.89	0.54
1:A:133:ALA:H	1:A:215:GLN:NE2	2.03	0.54
1:B:426:ASP:O	1:B:430:LYS:HG2	2.06	0.54
1:B:645:LYS:NZ	5:B:999:PLP:C4A	2.70	0.54
1:A:601:VAL:HG21	1:A:605:LEU:HB3	1.89	0.54
1:B:643:ASN:HD22	1:B:661:ASN:ND2	2.05	0.54
1:B:668:VAL:HA	1:B:774:ARG:HG3	1.88	0.54
1:A:8:LYS:O	1:A:12:GLU:HG3	2.08	0.54
1:B:8:LYS:O	1:B:12:GLU:HG3	2.08	0.54
1:B:3:PRO:HB3	1:B:49:GLN:OE1	2.08	0.54
1:B:598:ASP:HB3	1:B:601:VAL:HG12	1.90	0.54
1:A:560:GLN:CD	1:A:561:ALA:N	2.61	0.54
1:B:15:SER:HA	1:B:18:TRP:NE1	2.23	0.53
1:A:146:ARG:NH1	6:A:2077:HOH:O	2.42	0.53
1:A:668:VAL:HA	1:A:774:ARG:HG3	1.88	0.53
1:B:62:ASN:ND2	1:B:301:GLU:HG3	2.23	0.53
1:A:643:ASN:HD22	1:A:661:ASN:ND2	2.05	0.53
1:A:697:ARG:HB2	1:A:741:MET:CE	2.34	0.53
1:B:60:HIS:HB3	1:B:301:GLU:OE2	2.09	0.53
1:A:62:ASN:ND2	1:A:301:GLU:HG3	2.23	0.53
1:A:598:ASP:HB3	1:A:601:VAL:HG12	1.90	0.53
1:B:736:ASP:N	1:B:737:PRO:HD3	2.23	0.53
1:A:3:PRO:HB3	1:A:49:GLN:OE1	2.08	0.53
1:B:2:GLN:CB	1:B:3:PRO:HD3	2.31	0.53
1:B:146:ARG:NH1	6:B:2073:HOH:O	2.42	0.53
1:B:350:GLU:HG2	2:D:2:GLC:H5	1.90	0.53
1:A:15:SER:HA	1:A:18:TRP:NE1	2.23	0.53
1:B:697:ARG:HB2	1:B:741:MET:CE	2.34	0.52
1:A:60:HIS:HB3	1:A:301:GLU:OE2	2.09	0.52
1:A:114:GLY:O	1:A:118:LEU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:GLU:HG2	2:C:2:GLC:H5	1.90	0.52
1:A:796:ARG:OXT	1:A:796:ARG:NH1	2.42	0.52
1:A:686:ILE:HG22	1:A:691:TYR:HB2	1.91	0.52
1:B:796:ARG:OXT	1:B:796:ARG:NH1	2.42	0.52
1:B:523:ASN:ND2	1:B:525:GLN:H	2.08	0.52
1:A:523:ASN:ND2	1:A:525:GLN:H	2.08	0.52
1:A:368:MET:CE	1:A:404:VAL:HG21	2.39	0.52
1:A:422:ALA:HB3	6:A:2210:HOH:O	2.10	0.52
1:A:381:LEU:C	1:A:381:LEU:HD13	2.31	0.51
1:A:536:HIS:HB3	1:A:539:LYS:HD3	1.92	0.51
1:B:32:ARG:HD2	6:B:2052:HOH:O	2.11	0.51
1:B:114:GLY:O	1:B:118:LEU:HB2	2.10	0.51
1:B:470:LYS:HZ1	1:B:498:GLN:HE22	1.57	0.51
1:B:504:GLN:HG2	1:B:505:ALA:N	2.24	0.51
1:A:181:ILE:HD11	1:A:270:MET:HG2	1.91	0.51
1:B:181:ILE:HD11	1:B:270:MET:HG2	1.91	0.51
1:B:368:MET:CE	1:B:404:VAL:HG21	2.39	0.51
1:B:381:LEU:HD13	1:B:381:LEU:C	2.31	0.51
1:B:544:ASN:HD22	1:B:544:ASN:C	2.14	0.51
1:B:686:ILE:HG22	1:B:691:TYR:HB2	1.91	0.51
1:B:795:LYS:O	1:B:796:ARG:HG2	2.11	0.51
1:A:361:LYS:HG3	1:A:368:MET:HG3	1.93	0.51
1:A:357:VAL:O	1:A:361:LYS:HB2	2.11	0.51
1:A:544:ASN:C	1:A:544:ASN:HD22	2.14	0.51
1:A:795:LYS:O	1:A:796:ARG:HG2	2.11	0.51
1:A:796:ARG:HA	1:A:796:ARG:HE	1.73	0.51
1:A:447:VAL:HG11	1:A:787:TYR:CD2	2.46	0.51
1:B:2:GLN:HG2	1:B:212:GLY:HA3	1.93	0.51
1:B:101:LEU:C	1:B:101:LEU:HD23	2.31	0.51
1:A:101:LEU:C	1:A:101:LEU:HD23	2.31	0.50
1:A:796:ARG:C	6:A:2374:HOH:O	2.49	0.50
1:B:209:TYR:OH	1:B:458:LYS:HE3	2.11	0.50
1:B:536:HIS:HB3	1:B:539:LYS:HD3	1.92	0.50
1:A:209:TYR:OH	1:A:458:LYS:HE3	2.11	0.50
1:A:5:PHE:CD2	1:A:86:ASP:HB3	2.46	0.50
1:B:5:PHE:CD2	1:B:86:ASP:HB3	2.46	0.50
1:B:187:LYS:HG3	6:B:2102:HOH:O	2.12	0.50
1:A:504:GLN:HG2	1:A:505:ALA:N	2.24	0.50
1:B:796:ARG:C	6:B:2374:HOH:O	2.49	0.50
1:B:422:ALA:HB3	6:B:2206:HOH:O	2.11	0.50
1:B:796:ARG:NH2	1:B:796:ARG:C	2.65	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ARG:HD2	6:A:2055:HOH:O	2.11	0.50
1:B:357:VAL:O	1:B:361:LYS:HB2	2.11	0.50
1:B:447:VAL:HG11	1:B:787:TYR:CD2	2.46	0.50
1:A:796:ARG:NH2	1:A:796:ARG:C	2.65	0.50
1:A:2:GLN:HG2	1:A:212:GLY:HA3	1.93	0.49
1:B:361:LYS:HG3	1:B:368:MET:HG3	1.93	0.49
1:A:172:ASN:ND2	1:A:174:ALA:H	2.11	0.49
1:A:695:LYS:O	1:A:699:LYS:HG2	2.12	0.49
1:B:257:PRO:O	1:B:268:ARG:NH1	2.43	0.49
1:B:695:LYS:O	1:B:699:LYS:HG2	2.12	0.49
1:B:11:GLN:OE1	1:B:11:GLN:HA	2.13	0.49
1:B:657:LEU:HD23	1:B:675:ILE:HG21	1.94	0.49
1:A:364:LEU:HB3	1:A:367:HIS:CD2	2.48	0.49
1:B:60:HIS:CE1	1:B:134:THR:OG1	2.65	0.49
1:B:172:ASN:ND2	1:B:174:ALA:H	2.11	0.49
1:A:60:HIS:CE1	1:A:134:THR:OG1	2.65	0.49
1:A:169:PHE:CE2	1:A:204:LEU:HD13	2.47	0.49
1:B:169:PHE:CE2	1:B:204:LEU:HD13	2.47	0.49
1:A:11:GLN:HA	1:A:11:GLN:OE1	2.13	0.49
1:A:97:ASN:HD22	1:A:97:ASN:C	2.16	0.49
1:A:480:LEU:O	1:A:483:LEU:HB2	2.13	0.49
1:B:312:ILE:O	1:B:315:PRO:HD2	2.13	0.49
1:B:97:ASN:C	1:B:97:ASN:HD22	2.16	0.48
1:B:518:THR:HG21	1:B:520:ILE:HD12	1.95	0.48
1:A:447:VAL:HG11	1:A:787:TYR:CE2	2.48	0.48
1:B:364:LEU:HB3	1:B:367:HIS:CD2	2.48	0.48
1:B:447:VAL:HG11	1:B:787:TYR:CE2	2.48	0.48
1:A:312:ILE:O	1:A:315:PRO:HD2	2.13	0.48
1:A:580:LEU:HD23	1:A:580:LEU:O	2.14	0.48
1:B:534:ARG:HE	3:B:900:PO4:P	2.36	0.48
1:B:721:HIS:CD2	6:B:2339:HOH:O	2.66	0.48
1:A:518:THR:HG21	1:A:520:ILE:HD12	1.96	0.48
1:A:657:LEU:HD23	1:A:675:ILE:HG21	1.94	0.48
1:B:480:LEU:O	1:B:483:LEU:HB2	2.13	0.48
1:B:552:TYR:O	1:B:556:ARG:HB2	2.14	0.48
1:B:703:LEU:HD21	1:B:741:MET:HE3	1.95	0.48
1:A:172:ASN:ND2	1:B:33:GLN:HE22	2.12	0.47
1:B:285:ARG:HD2	6:B:2162:HOH:O	2.14	0.47
1:B:580:LEU:O	1:B:580:LEU:HD23	2.14	0.47
1:A:534:ARG:HE	3:A:900:PO4:P	2.36	0.47
1:B:210:ARG:HD2	6:B:2001:HOH:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:733:GLN:HE21	1:B:733:GLN:HB3	1.52	0.47
1:A:658:ASP:O	1:A:661:ASN:HB2	2.15	0.47
1:A:141:GLN:HB2	1:A:163:ARG:CZ	2.45	0.47
1:A:691:TYR:CE2	1:A:739:LEU:HD23	2.50	0.47
1:A:79:LEU:HD23	1:A:80:ASN:HD22	1.80	0.47
1:A:425:SER:CB	1:A:446:ASN:HB2	2.44	0.47
1:A:285:ARG:HD2	6:A:2166:HOH:O	2.14	0.47
1:B:538:TYR:CZ	1:B:539:LYS:HD2	2.50	0.47
1:A:72:ARG:O	1:A:455:ARG:NH2	2.34	0.46
1:A:552:TYR:O	1:A:556:ARG:HB2	2.14	0.46
1:B:425:SER:CB	1:B:446:ASN:HB2	2.44	0.46
1:B:703:LEU:HD21	1:B:741:MET:CE	2.45	0.46
1:B:141:GLN:HB2	1:B:163:ARG:CZ	2.45	0.46
1:B:379:LYS:HD3	1:B:393:TRP:CE2	2.50	0.46
1:B:645:LYS:HZ1	5:B:999:PLP:C4A	2.27	0.46
1:A:97:ASN:HD21	1:A:99:THR:HB	1.81	0.46
1:B:507:LYS:HA	1:B:624:ALA:HB1	1.98	0.46
1:A:538:TYR:CZ	1:A:539:LYS:HD2	2.50	0.46
1:B:97:ASN:HD21	1:B:99:THR:HB	1.81	0.46
1:A:790:ARG:HG2	6:A:2220:HOH:O	2.15	0.46
1:A:379:LYS:HD3	1:A:393:TRP:CE2	2.50	0.46
1:B:658:ASP:O	1:B:661:ASN:HB2	2.15	0.46
1:B:691:TYR:CE2	1:B:739:LEU:HD23	2.50	0.46
1:B:79:LEU:HD23	1:B:80:ASN:HD22	1.80	0.46
1:B:680:VAL:HG13	1:B:681:GLU:CD	2.36	0.46
1:A:680:VAL:HG13	1:A:681:GLU:CD	2.36	0.46
1:A:468:LEU:HD21	1:A:486:LEU:HD11	1.98	0.46
1:A:163:ARG:HD2	6:A:2092:HOH:O	2.16	0.45
1:A:751:GLN:NE2	1:A:754:VAL:HG21	2.32	0.45
1:B:163:ARG:HD2	6:B:2086:HOH:O	2.16	0.45
1:B:790:ARG:HG2	6:B:2216:HOH:O	2.15	0.45
1:A:51:PHE:HE1	1:A:214:ALA:N	2.08	0.45
1:B:530:ILE:HD12	1:B:625:ALA:HB2	1.99	0.45
1:A:360:VAL:HG11	1:A:368:MET:CE	2.47	0.45
1:A:652:LEU:HD12	1:A:764:TRP:CZ3	2.52	0.45
1:A:703:LEU:HD21	1:A:741:MET:CE	2.45	0.45
1:B:652:LEU:HD12	1:B:764:TRP:CZ3	2.52	0.45
1:B:360:VAL:HG11	1:B:368:MET:CE	2.47	0.45
1:B:51:PHE:HE1	1:B:214:ALA:N	2.08	0.45
1:B:67:GLU:HB2	1:B:111:GLY:HA2	1.99	0.45
1:B:217:LEU:O	1:B:217:LEU:CD1	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:60:HIS:CD2	1:B:132:SER:OG	2.67	0.45
1:B:751:GLN:NE2	1:B:754:VAL:HG21	2.31	0.45
1:A:507:LYS:HA	1:A:624:ALA:HB1	1.98	0.45
1:A:67:GLU:HB2	1:A:111:GLY:HA2	1.99	0.44
1:B:146:ARG:HG3	1:B:146:ARG:NH1	2.30	0.44
1:B:468:LEU:HD21	1:B:486:LEU:HD11	1.98	0.44
1:A:98:LEU:O	1:A:102:LEU:HG	2.18	0.44
1:A:172:ASN:HD22	1:A:172:ASN:C	2.20	0.44
1:A:530:ILE:HD12	1:A:625:ALA:HB2	1.99	0.44
1:A:645:LYS:HZ2	5:A:999:PLP:C4A	2.30	0.44
1:A:662:VAL:CG2	1:A:663:GLU:N	2.80	0.44
1:A:774:ARG:O	1:A:775:CYS:HB2	2.18	0.44
1:B:53:LYS:HG2	1:B:54:PRO:HD2	2.00	0.44
1:B:777:MET:SD	6:B:2310:HOH:O	2.62	0.44
1:A:368:MET:HE2	1:A:368:MET:HA	1.99	0.44
1:B:98:LEU:O	1:B:102:LEU:HG	2.17	0.44
1:A:80:ASN:HD21	1:A:454:ARG:HG2	1.82	0.44
1:A:109:ALA:HB3	1:A:161:TRP:CD1	2.53	0.44
1:A:523:ASN:HD22	1:A:524:PRO:N	2.15	0.44
1:A:703:LEU:O	1:A:707:LEU:HD22	2.18	0.44
1:B:72:ARG:O	1:B:455:ARG:NH2	2.34	0.44
1:B:178:GLN:NE2	1:B:178:GLN:HA	2.32	0.44
1:B:364:LEU:HB3	1:B:367:HIS:HB2	2.00	0.44
1:B:662:VAL:CG2	1:B:663:GLU:N	2.80	0.44
1:A:777:MET:SD	6:A:2315:HOH:O	2.62	0.44
1:B:363:LEU:HB3	1:B:364:LEU:HD22	2.00	0.44
1:B:523:ASN:HD22	1:B:524:PRO:N	2.15	0.44
1:B:549:LEU:HB3	1:B:706:VAL:HG22	2.00	0.44
1:A:178:GLN:HA	1:A:178:GLN:NE2	2.32	0.43
1:B:172:ASN:C	1:B:172:ASN:HD22	2.20	0.43
1:B:312:ILE:C	1:B:315:PRO:HD2	2.38	0.43
1:A:144:LEU:HD13	1:A:145:PHE:CE2	2.54	0.43
1:A:312:ILE:C	1:A:315:PRO:HD2	2.38	0.43
1:B:80:ASN:HD21	1:B:454:ARG:HG2	1.82	0.43
1:B:774:ARG:O	1:B:775:CYS:HB2	2.18	0.43
1:A:204:LEU:HD12	1:A:204:LEU:HA	1.81	0.43
1:A:360:VAL:HG12	1:A:368:MET:HG2	2.01	0.43
1:B:109:ALA:HB3	1:B:161:TRP:CD1	2.53	0.43
1:B:293:LYS:HB2	1:B:296:GLU:HG3	2.01	0.43
1:A:364:LEU:HB3	1:A:367:HIS:HB2	2.00	0.43
1:A:379:LYS:HB2	1:A:393:TRP:CH2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:TYR:HA	1:B:312:ILE:HG21	2.00	0.43
1:B:363:LEU:CB	1:B:364:LEU:HD22	2.49	0.43
1:B:379:LYS:HB2	1:B:393:TRP:CH2	2.53	0.43
1:A:133:ALA:H	1:A:215:GLN:HE22	1.67	0.43
1:A:257:PRO:O	1:A:268:ARG:NH1	2.43	0.43
1:B:360:VAL:HG12	1:B:368:MET:HG2	2.01	0.43
1:A:89:ASP:O	1:A:92:LYS:HB3	2.19	0.43
1:A:363:LEU:CB	1:A:364:LEU:HD22	2.49	0.43
1:A:794:ALA:HB3	1:A:796:ARG:O	2.19	0.43
1:B:89:ASP:O	1:B:92:LYS:HB3	2.19	0.43
1:B:703:LEU:O	1:B:707:LEU:HD22	2.18	0.43
1:A:53:LYS:HG2	1:A:54:PRO:HD2	2.00	0.42
1:A:273:TYR:HA	1:A:312:ILE:HG21	2.00	0.42
1:A:293:LYS:HB2	1:A:296:GLU:HG3	2.01	0.42
1:B:128:THR:HG22	1:B:209:TYR:N	2.32	0.42
1:B:794:ALA:HB3	1:B:796:ARG:O	2.19	0.42
1:A:146:ARG:HG3	1:A:146:ARG:NH1	2.30	0.42
1:A:363:LEU:HB3	1:A:364:LEU:HD22	1.99	0.42
1:B:133:ALA:H	1:B:215:GLN:HE22	1.67	0.42
1:B:537:GLU:CD	1:B:580:LEU:HD13	2.40	0.42
1:A:47:ARG:HD2	1:B:19:GLN:O	2.19	0.42
1:A:217:LEU:O	1:A:217:LEU:CD1	2.60	0.42
1:A:338:LYS:HD2	1:A:796:ARG:HD3	2.02	0.42
1:A:558:ASN:OD1	1:A:560:GLN:N	2.52	0.42
1:A:537:GLU:CD	1:A:580:LEU:HD13	2.40	0.42
1:A:549:LEU:HB3	1:A:706:VAL:HG22	2.00	0.42
1:B:144:LEU:HD13	1:B:145:PHE:CE2	2.54	0.42
1:B:558:ASN:OD1	1:B:560:GLN:N	2.52	0.42
1:A:2:GLN:HB3	1:A:3:PRO:CD	2.37	0.42
1:A:125:SER:O	1:A:129:VAL:HB	2.19	0.42
1:B:125:SER:O	1:B:129:VAL:HB	2.19	0.42
1:B:460:CYS:C	1:B:462:PRO:HD3	2.40	0.42
1:B:532:ILE:O	1:B:532:ILE:HG13	2.20	0.42
1:B:796:ARG:HA	1:B:796:ARG:HE	1.73	0.42
1:A:601:VAL:HG13	1:A:602:GLY:N	2.35	0.42
1:B:69:LEU:HG	1:B:615:VAL:CG2	2.50	0.42
1:B:204:LEU:HD12	1:B:204:LEU:HA	1.81	0.42
1:B:667:LYS:CE	1:B:777:MET:HE1	2.50	0.42
1:B:727:LEU:HD12	1:B:727:LEU:HA	1.91	0.42
1:A:470:LYS:HZ1	1:A:498:GLN:HE22	1.67	0.42
1:A:537:GLU:OE2	1:A:580:LEU:HD13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:360:VAL:HG11	1:B:368:MET:HE2	2.02	0.42
1:B:188:ASP:OD2	1:B:190:ARG:NH1	2.49	0.41
1:B:368:MET:HE2	1:B:368:MET:HA	2.01	0.41
1:A:329:TRP:CZ3	1:A:373:GLU:HG2	2.55	0.41
1:A:348:MET:HE1	6:A:2302:HOH:O	2.20	0.41
1:B:186:THR:HB	6:B:2102:HOH:O	2.19	0.41
1:B:293:LYS:HD3	1:B:295:HIS:NE2	2.35	0.41
1:A:69:LEU:HG	1:A:615:VAL:CG2	2.50	0.41
1:A:460:CYS:C	1:A:462:PRO:HD3	2.40	0.41
1:A:662:VAL:HG23	1:A:663:GLU:N	2.35	0.41
1:B:795:LYS:HA	6:B:2029:HOH:O	2.21	0.41
1:A:492:ASP:HB3	1:A:495:PHE:HB3	2.02	0.41
1:A:695:LYS:HE2	1:A:695:LYS:HB2	1.92	0.41
1:A:384:LYS:HE2	1:A:384:LYS:HB2	1.94	0.41
1:A:532:ILE:O	1:A:532:ILE:HG13	2.20	0.41
1:B:3:PRO:HG3	1:B:49:GLN:NE2	2.36	0.41
1:B:537:GLU:OE2	1:B:580:LEU:HD13	2.19	0.41
1:B:662:VAL:HG23	1:B:663:GLU:N	2.35	0.41
1:B:680:VAL:O	1:B:684:LYS:HG3	2.21	0.41
1:B:146:ARG:HH11	1:B:146:ARG:CG	2.31	0.41
1:B:415:PHE:CG	1:B:796:ARG:NH1	2.88	0.41
1:B:601:VAL:HG13	1:B:602:GLY:N	2.35	0.41
1:A:258:ASN:HD22	1:A:259:ASP:N	2.19	0.41
1:A:733:GLN:HE21	1:A:733:GLN:HB3	1.52	0.41
1:B:5:PHE:CE2	1:B:86:ASP:HB3	2.56	0.41
1:B:329:TRP:CZ3	1:B:373:GLU:HG2	2.55	0.41
1:B:338:LYS:HD2	1:B:796:ARG:HD3	2.02	0.41
1:B:384:LYS:HE2	1:B:384:LYS:HB2	1.94	0.41
1:A:686:ILE:HG13	6:A:2330:HOH:O	2.21	0.41
1:B:166:TYR:HB3	1:B:169:PHE:CD1	2.56	0.41
1:B:394:ALA:HA	1:B:400:HIS:CD2	2.56	0.41
1:B:473:GLN:HG2	6:B:2227:HOH:O	1.86	0.41
1:B:796:ARG:CB	6:B:2374:HOH:O	2.68	0.41
1:A:166:TYR:HB3	1:A:169:PHE:CD1	2.56	0.41
1:A:796:ARG:NH1	1:A:796:ARG:HB3	2.36	0.41
1:A:796:ARG:CB	6:A:2374:HOH:O	2.68	0.41
1:A:667:LYS:CE	1:A:777:MET:HE1	2.51	0.40
1:B:261:HIS:O	1:B:265:LYS:HG3	2.22	0.40
1:B:295:HIS:HA	1:B:335:ILE:HD11	2.03	0.40
1:B:498:GLN:O	1:B:502:ILE:HG13	2.21	0.40
1:A:261:HIS:O	1:A:265:LYS:HG3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:795:LYS:HA	6:A:2031:HOH:O	2.21	0.40
1:B:258:ASN:HD22	1:B:259:ASP:N	2.19	0.40
1:B:575:ALA:HA	1:B:576:PRO:HD3	1.94	0.40
1:A:60:HIS:CD2	1:A:132:SER:OG	2.67	0.40
1:A:69:LEU:HG	1:A:615:VAL:HG23	2.03	0.40
1:A:480:LEU:HG	1:A:776:GLY:HA2	2.03	0.40
1:A:538:TYR:CE1	1:A:539:LYS:HD2	2.56	0.40
1:B:224:HIS:HD2	1:B:226:HIS:N	2.10	0.40
1:A:295:HIS:HA	1:A:335:ILE:HD11	2.03	0.40
1:A:415:PHE:CG	1:A:796:ARG:NH1	2.88	0.40
1:A:498:GLN:O	1:A:502:ILE:HG13	2.21	0.40
1:A:546:LEU:HA	1:A:546:LEU:HD12	1.87	0.40
1:B:796:ARG:NH1	1:B:796:ARG:HB3	2.36	0.40
1:A:146:ARG:HH11	1:A:146:ARG:CG	2.31	0.40
1:A:293:LYS:HD3	1:A:295:HIS:NE2	2.35	0.40
1:A:307:ASP:O	1:A:310:PRO:HD2	2.22	0.40
1:A:575:ALA:HA	1:A:576:PRO:HD3	1.94	0.40
1:B:492:ASP:HB3	1:B:495:PHE:HB3	2.02	0.40
1:B:587:ALA:HA	1:B:723:PHE:CE2	2.57	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	794/796 (100%)	753 (95%)	35 (4%)	6 (1%)	19	13
1	B	794/796 (100%)	753 (95%)	35 (4%)	6 (1%)	19	13
All	All	1588/1592 (100%)	1506 (95%)	70 (4%)	12 (1%)	19	13

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	218	ARG
1	A	795	LYS
1	B	795	LYS
1	A	2	GLN
1	B	2	GLN
1	B	218	ARG
1	A	561	ALA
1	B	561	ALA
1	A	56	ALA
1	A	560	GLN
1	B	56	ALA
1	B	560	GLN

5.3.2 Protein sidechains (i)

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	665/667 (100%)	607 (91%)	58 (9%)	10 6
1	B	665/667 (100%)	607 (91%)	58 (9%)	10 6
All	All	1330/1334 (100%)	1214 (91%)	116 (9%)	10 6

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	42	LEU
1	A	73	LEU
1	A	85	GLN
1	A	91	LEU
1	A	92	LYS
1	A	97	ASN
1	A	110	LEU
1	A	118	LEU
1	A	123	LEU
1	A	144	LEU
1	A	163	ARG

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Mol	Chain	Res	Type
1	A	169	PHE
1	A	172	ASN
1	A	177	VAL
1	A	198	THR
1	A	204	LEU
1	A	207	VAL
1	A	255	LEU
1	A	258	ASN
1	A	321	LEU
1	A	339	THR
1	A	347	LEU
1	A	368	MET
1	A	455	ARG
1	A	472	LEU
1	A	473	GLN
1	A	504	GLN
1	A	523	ASN
1	A	533	LYS
1	A	535	LEU
1	A	538	TYR
1	A	542	HIS
1	A	544	ASN
1	A	546	LEU
1	A	551	LEU
1	A	560	GLN
1	A	578	TYR
1	A	591	VAL
1	A	593	ASP
1	A	606	LYS
1	A	607	VAL
1	A	609	PHE
1	A	610	LEU
1	A	657	LEU
1	A	671	GLU
1	A	701	LYS
1	A	702	VAL
1	A	707	LEU
1	A	727	LEU
1	A	728	HIS
1	A	733	GLN
1	A	749	GLU
1	A	755	ASP

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Mol	Chain	Res	Type
1	A	761	GLN
1	A	774	ARG
1	A	777	MET
1	A	796	ARG
1	B	32	ARG
1	B	42	LEU
1	B	73	LEU
1	B	85	GLN
1	B	91	LEU
1	B	92	LYS
1	B	97	ASN
1	B	110	LEU
1	B	118	LEU
1	B	123	LEU
1	B	144	LEU
1	B	163	ARG
1	B	169	PHE
1	B	172	ASN
1	B	177	VAL
1	B	198	THR
1	B	204	LEU
1	B	207	VAL
1	B	255	LEU
1	B	258	ASN
1	B	321	LEU
1	B	339	THR
1	B	347	LEU
1	B	368	MET
1	B	455	ARG
1	B	472	LEU
1	B	473	GLN
1	B	504	GLN
1	B	523	ASN
1	B	533	LYS
1	B	535	LEU
1	B	538	TYR
1	B	542	HIS
1	B	544	ASN
1	B	546	LEU
1	B	551	LEU
1	B	560	GLN
1	B	578	TYR

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Mol	Chain	Res	Type
1	B	591	VAL
1	B	593	ASP
1	B	606	LYS
1	B	607	VAL
1	B	609	PHE
1	B	610	LEU
1	B	657	LEU
1	B	671	GLU
1	B	701	LYS
1	B	702	VAL
1	B	707	LEU
1	B	727	LEU
1	B	728	HIS
1	B	733	GLN
1	B	749	GLU
1	B	755	ASP
1	B	761	GLN
1	B	774	ARG
1	B	777	MET
1	B	796	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	GLN
1	A	6	ASN
1	A	58	GLN
1	A	60	HIS
1	A	80	ASN
1	A	88	GLN
1	A	97	ASN
1	A	112	ASN
1	A	162	HIS
1	A	172	ASN
1	A	178	GLN
1	A	215	GLN
1	A	224	HIS
1	A	226	HIS
1	A	244	GLN
1	A	258	ASN
1	A	261	HIS
1	A	306	ASN

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Mol	Chain	Res	Type
1	A	326	GLN
1	A	367	HIS
1	A	408	ASN
1	A	446	ASN
1	A	498	GLN
1	A	523	ASN
1	A	531	GLN
1	A	544	ASN
1	A	597	ASN
1	A	661	ASN
1	A	678	HIS
1	A	733	GLN
1	A	751	GLN
1	B	2	GLN
1	B	6	ASN
1	B	58	GLN
1	B	60	HIS
1	B	80	ASN
1	B	88	GLN
1	B	97	ASN
1	B	112	ASN
1	B	162	HIS
1	B	172	ASN
1	B	178	GLN
1	B	215	GLN
1	B	224	HIS
1	B	226	HIS
1	B	244	GLN
1	B	258	ASN
1	B	261	HIS
1	B	306	ASN
1	B	326	GLN
1	B	367	HIS
1	B	408	ASN
1	B	446	ASN
1	B	498	GLN
1	B	523	ASN
1	B	531	GLN
1	B	544	ASN
1	B	597	ASN
1	B	661	ASN
1	B	678	HIS

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Mol	Chain	Res	Type
1	B	733	GLN
1	B	751	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

8 monosaccharides 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	GLC	C	1	2	12,12,12	0.42	0	17,17,17	0.33	0
2	GLC	C	2	2	11,11,12	0.51	0	15,15,17	0.69	1 (6%)
2	GLC	C	3	2	11,11,12	0.46	0	15,15,17	0.64	1 (6%)
2	SGC	C	4	3,2	10,11,12	0.86	1 (10%)	12,15,17	0.84	0
2	GLC	D	1	2	12,12,12	0.43	0	17,17,17	0.34	0
2	GLC	D	2	2	11,11,12	0.51	0	15,15,17	0.69	1 (6%)
2	GLC	D	3	2	11,11,12	0.46	0	15,15,17	0.64	1 (6%)
2	SGC	D	4	3,2	10,11,12	0.87	1 (10%)	12,15,17	0.84	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	GLC	C	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	C	2	2	-	0/2/19/22	0/1/1/1
2	GLC	C	3	2	-	0/2/19/22	0/1/1/1
2	SGC	C	4	3,2	1/1/4/5	0/2/19/22	0/1/1/1
2	GLC	D	1	2	1/1/5/5	0/2/22/22	0/1/1/1
2	GLC	D	2	2	-	0/2/19/22	0/1/1/1
2	GLC	D	3	2	-	0/2/19/22	0/1/1/1
2	SGC	D	4	3,2	1/1/4/5	0/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	SGC	C5-C4	2.11	1.54	1.53
2	C	4	SGC	C5-C4	2.04	1.54	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	2	GLC	C1-O5-C5	2.47	115.54	112.19
2	C	2	GLC	C1-O5-C5	2.47	115.53	112.19
2	C	3	GLC	C1-O5-C5	2.07	114.99	112.19
2	D	3	GLC	C1-O5-C5	2.04	114.96	112.19

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1	GLC	C1
2	C	4	SGC	C1
2	D	1	GLC	C1
2	D	4	SGC	C1

There are no torsion outliers.

There are no ring outliers.

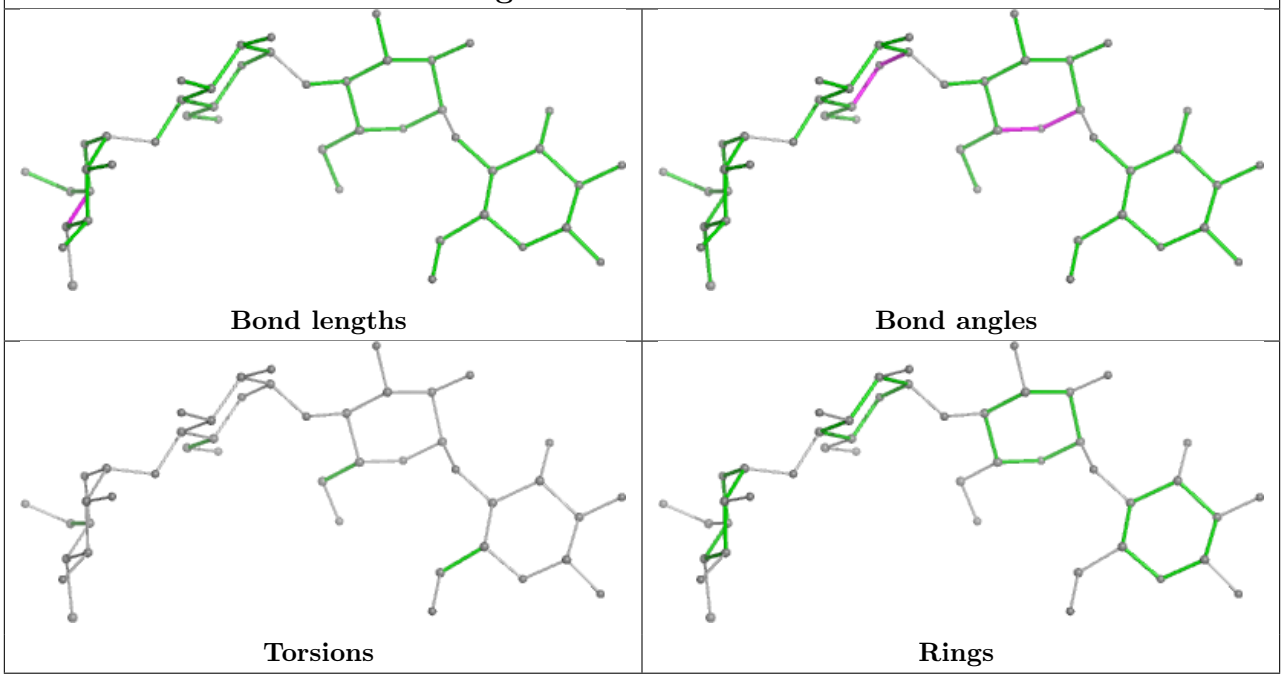
4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	4	SGC	1	0
2	D	2	GLC	1	0
2	C	2	GLC	1	0
2	C	4	SGC	1	0

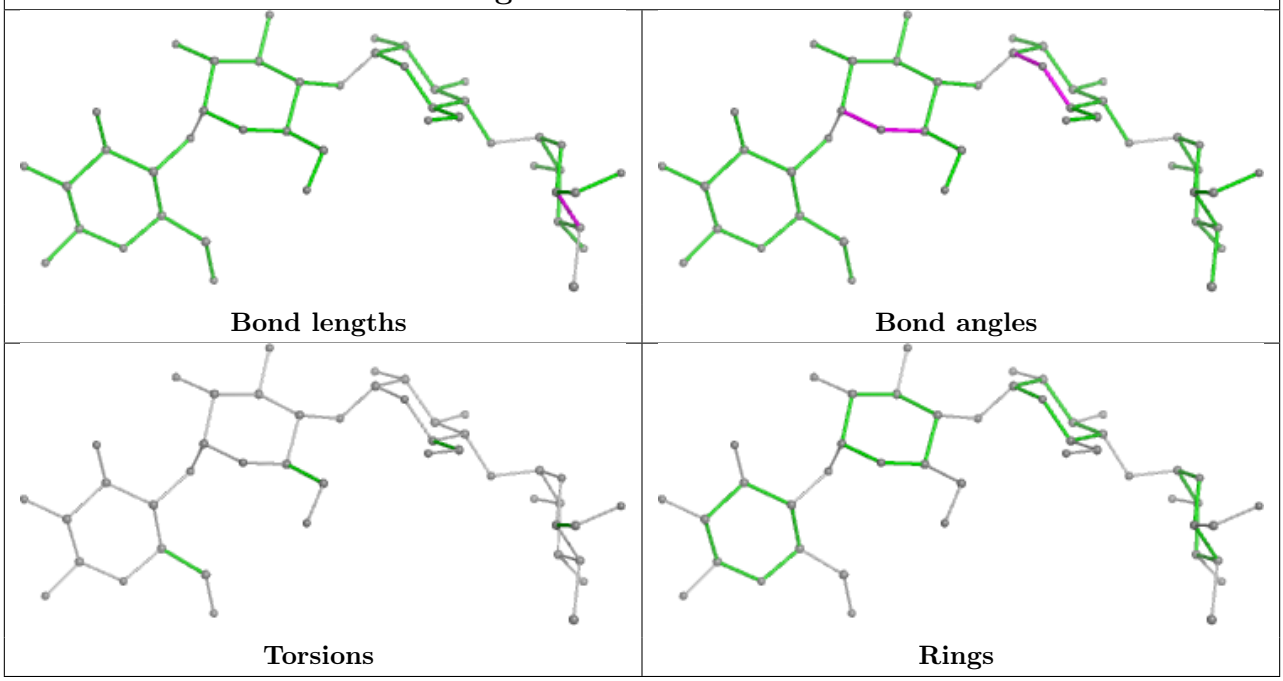
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

bond angles, torsion angles, and ring geometry for oligosaccharide.

Oligosaccharide Chain C



Oligosaccharide Chain D



5.6 Ligand geometry (i)

6 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	$\#\|Z\| > 2$
5	PLP	B	999	-	15,15,16	2.27	7 (46%)	20,22,23	3.38	11 (55%)
4	GLC	B	998	-	11,11,12	0.48	0	15,15,17	1.04	2 (13%)
3	PO4	B	900	2	4,4,4	2.92	3 (75%)	6,6,6	2.20	4 (66%)
4	GLC	A	998	-	11,11,12	0.48	0	15,15,17	1.04	2 (13%)
3	PO4	A	900	2	4,4,4	2.92	3 (75%)	6,6,6	2.20	4 (66%)
5	PLP	A	999	-	15,15,16	2.27	7 (46%)	20,22,23	3.38	11 (55%)

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
5	PLP	B	999	-	-	1/6/6/8	0/1/1/1
5	PLP	A	999	-	-	1/6/6/8	0/1/1/1
4	GLC	B	998	-	-	0/2/19/22	0/1/1/1
4	GLC	A	998	-	-	0/2/19/22	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	999	PLP	C4A-C4	-4.88	1.41	1.51
5	A	999	PLP	C4A-C4	-4.88	1.41	1.51
5	A	999	PLP	P-O4P	-3.98	1.47	1.60
5	B	999	PLP	P-O4P	-3.97	1.47	1.60
3	A	900	PO4	P-O1	3.54	1.59	1.50
3	B	900	PO4	P-O1	3.53	1.59	1.50
3	B	900	PO4	P-O2	-3.30	1.44	1.54
3	A	900	PO4	P-O2	-3.30	1.44	1.54
3	A	900	PO4	P-O3	-3.06	1.45	1.54
5	A	999	PLP	C3-C2	3.05	1.44	1.40
3	B	900	PO4	P-O3	-3.05	1.45	1.54
5	B	999	PLP	C3-C2	3.04	1.43	1.40
5	B	999	PLP	P-O1P	2.64	1.59	1.50
5	A	999	PLP	P-O1P	2.64	1.59	1.50
5	B	999	PLP	C6-N1	2.46	1.39	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	999	PLP	C6-N1	2.45	1.39	1.34
5	B	999	PLP	C2-N1	2.28	1.38	1.33
5	A	999	PLP	C2-N1	2.24	1.38	1.33
5	A	999	PLP	C6-C5	2.24	1.42	1.37
5	B	999	PLP	C6-C5	2.22	1.42	1.37

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	999	PLP	C3-C4-C5	7.24	126.56	118.74
5	B	999	PLP	C3-C4-C5	7.23	126.55	118.74
5	B	999	PLP	C4A-C4-C5	-6.64	114.10	120.94
5	A	999	PLP	C4A-C4-C5	-6.60	114.13	120.94
5	A	999	PLP	C4A-C4-C3	-6.28	109.86	120.50
5	B	999	PLP	C4A-C4-C3	-6.23	109.93	120.50
5	A	999	PLP	C6-C5-C4	-4.13	114.91	118.16
5	B	999	PLP	C6-C5-C4	-4.11	114.92	118.16
5	B	999	PLP	C3-C2-N1	-3.79	115.87	120.77
5	A	999	PLP	C3-C2-N1	-3.75	115.92	120.77
5	A	999	PLP	C6-N1-C2	3.54	125.72	119.17
5	B	999	PLP	C6-N1-C2	3.53	125.71	119.17
5	B	999	PLP	C2A-C2-C3	3.06	124.67	120.89
5	A	999	PLP	C2A-C2-C3	3.00	124.59	120.89
5	A	999	PLP	O4P-C5A-C5	2.92	114.91	109.35
5	B	999	PLP	O4P-C5A-C5	2.90	114.89	109.35
5	B	999	PLP	C5-C6-N1	-2.83	119.11	123.82
5	A	999	PLP	C5-C6-N1	-2.82	119.12	123.82
3	B	900	PO4	O2-P-O1	-2.81	100.60	110.89
3	A	900	PO4	O2-P-O1	-2.81	100.61	110.89
4	B	998	GLC	C1-O5-C5	2.71	115.87	112.19
4	A	998	GLC	C1-O5-C5	2.71	115.86	112.19
3	A	900	PO4	O4-P-O2	2.44	115.79	107.97
3	B	900	PO4	O4-P-O2	2.43	115.77	107.97
4	B	998	GLC	C1-C2-C3	2.32	112.52	109.67
3	B	900	PO4	O4-P-O3	2.32	115.42	107.97
4	A	998	GLC	C1-C2-C3	2.32	112.51	109.67
3	A	900	PO4	O4-P-O3	2.31	115.37	107.97
3	A	900	PO4	O4-P-O1	-2.26	102.64	110.89
3	B	900	PO4	O4-P-O1	-2.25	102.67	110.89
5	B	999	PLP	C5A-C5-C6	-2.18	115.78	119.37
5	A	999	PLP	C5A-C5-C6	-2.15	115.83	119.37
5	B	999	PLP	O2P-P-O4P	2.04	112.17	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	999	PLP	O2P-P-O4P	2.03	112.14	106.73

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	999	PLP	C6-C5-C5A-O4P
5	B	999	PLP	C6-C5-C5A-O4P

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	999	PLP	2	0
3	B	900	PO4	2	0
3	A	900	PO4	2	0
5	A	999	PLP	2	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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.