



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:43 PM GMT

PDB ID : 3RT1
Title : Maltodextarn bound activated state form of yeast glycogen synthase isoform 2
Authors : Baskaran, S.; Hurley, T.D.
Deposited on : 2011-05-02
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

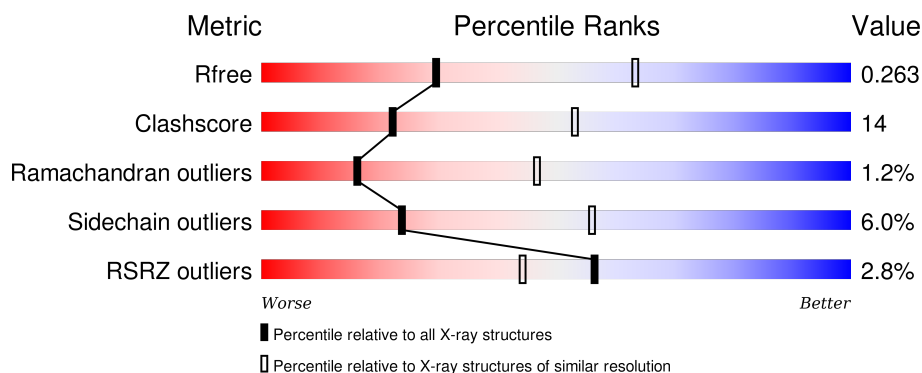
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	725	<div> <div>0%</div> <div> <div></div> <div>64%</div> <div>22%</div> <div>•</div> <div>12%</div> </div> </div>
1	B	725	<div> <div>2%</div> <div> <div></div> <div>60%</div> <div>26%</div> <div>•</div> <div>12%</div> </div> </div>
1	C	725	<div> <div>3%</div> <div> <div></div> <div>64%</div> <div>23%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	725	<div> <div>3%</div> <div> <div></div> <div>57%</div> <div>27%</div> <div>•</div> <div>12%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GLC	A	801	-	-	-	X
4	GLC	A	809	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 20951 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 PROTEIN (Glycogen [starch] synthase isoform 2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	B	638	Total	C	N	O	S	0	0	0
			5145	3286	896	944	19			
1	C	646	Total	C	N	O	S	0	0	0
			5200	3322	907	952	19			
1	D	636	Total	C	N	O	S	0	0	0
			5128	3274	894	941	19			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP P27472
A	-18	GLY	-	EXPRESSION TAG	UNP P27472
A	-17	SER	-	EXPRESSION TAG	UNP P27472
A	-16	SER	-	EXPRESSION TAG	UNP P27472
A	-15	HIS	-	EXPRESSION TAG	UNP P27472
A	-14	HIS	-	EXPRESSION TAG	UNP P27472
A	-13	HIS	-	EXPRESSION TAG	UNP P27472
A	-12	HIS	-	EXPRESSION TAG	UNP P27472
A	-11	HIS	-	EXPRESSION TAG	UNP P27472
A	-10	HIS	-	EXPRESSION TAG	UNP P27472
A	-9	SER	-	EXPRESSION TAG	UNP P27472
A	-8	SER	-	EXPRESSION TAG	UNP P27472
A	-7	GLY	-	EXPRESSION TAG	UNP P27472
A	-6	LEU	-	EXPRESSION TAG	UNP P27472
A	-5	VAL	-	EXPRESSION TAG	UNP P27472
A	-4	PRO	-	EXPRESSION TAG	UNP P27472
A	-3	ARG	-	EXPRESSION TAG	UNP P27472
A	-2	GLY	-	EXPRESSION TAG	UNP P27472
A	-1	SER	-	EXPRESSION TAG	UNP P27472
A	0	HIS	-	EXPRESSION TAG	UNP P27472
A	535	SER	ALA	SEE REMARK 999	UNP P27472

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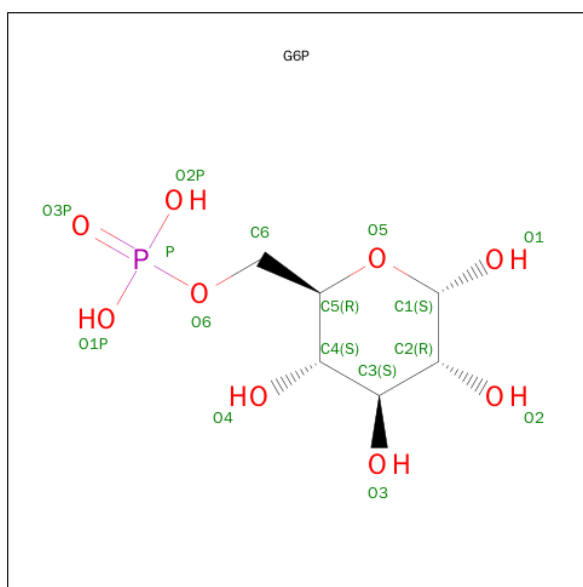
Chain	Residue	Modelled	Actual	Comment	Reference
A	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
A	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	-19	MET	-	EXPRESSION TAG	UNP P27472
B	-18	GLY	-	EXPRESSION TAG	UNP P27472
B	-17	SER	-	EXPRESSION TAG	UNP P27472
B	-16	SER	-	EXPRESSION TAG	UNP P27472
B	-15	HIS	-	EXPRESSION TAG	UNP P27472
B	-14	HIS	-	EXPRESSION TAG	UNP P27472
B	-13	HIS	-	EXPRESSION TAG	UNP P27472
B	-12	HIS	-	EXPRESSION TAG	UNP P27472
B	-11	HIS	-	EXPRESSION TAG	UNP P27472
B	-10	HIS	-	EXPRESSION TAG	UNP P27472
B	-9	SER	-	EXPRESSION TAG	UNP P27472
B	-8	SER	-	EXPRESSION TAG	UNP P27472
B	-7	GLY	-	EXPRESSION TAG	UNP P27472
B	-6	LEU	-	EXPRESSION TAG	UNP P27472
B	-5	VAL	-	EXPRESSION TAG	UNP P27472
B	-4	PRO	-	EXPRESSION TAG	UNP P27472
B	-3	ARG	-	EXPRESSION TAG	UNP P27472
B	-2	GLY	-	EXPRESSION TAG	UNP P27472
B	-1	SER	-	EXPRESSION TAG	UNP P27472
B	0	HIS	-	EXPRESSION TAG	UNP P27472
B	535	SER	ALA	SEE REMARK 999	UNP P27472
B	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
B	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	-19	MET	-	EXPRESSION TAG	UNP P27472
C	-18	GLY	-	EXPRESSION TAG	UNP P27472
C	-17	SER	-	EXPRESSION TAG	UNP P27472
C	-16	SER	-	EXPRESSION TAG	UNP P27472
C	-15	HIS	-	EXPRESSION TAG	UNP P27472
C	-14	HIS	-	EXPRESSION TAG	UNP P27472
C	-13	HIS	-	EXPRESSION TAG	UNP P27472
C	-12	HIS	-	EXPRESSION TAG	UNP P27472
C	-11	HIS	-	EXPRESSION TAG	UNP P27472
C	-10	HIS	-	EXPRESSION TAG	UNP P27472
C	-9	SER	-	EXPRESSION TAG	UNP P27472
C	-8	SER	-	EXPRESSION TAG	UNP P27472
C	-7	GLY	-	EXPRESSION TAG	UNP P27472
C	-6	LEU	-	EXPRESSION TAG	UNP P27472
C	-5	VAL	-	EXPRESSION TAG	UNP P27472
C	-4	PRO	-	EXPRESSION TAG	UNP P27472
C	-3	ARG	-	EXPRESSION TAG	UNP P27472

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	EXPRESSION TAG	UNP P27472
C	-1	SER	-	EXPRESSION TAG	UNP P27472
C	0	HIS	-	EXPRESSION TAG	UNP P27472
C	535	SER	ALA	SEE REMARK 999	UNP P27472
C	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
C	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	-19	MET	-	EXPRESSION TAG	UNP P27472
D	-18	GLY	-	EXPRESSION TAG	UNP P27472
D	-17	SER	-	EXPRESSION TAG	UNP P27472
D	-16	SER	-	EXPRESSION TAG	UNP P27472
D	-15	HIS	-	EXPRESSION TAG	UNP P27472
D	-14	HIS	-	EXPRESSION TAG	UNP P27472
D	-13	HIS	-	EXPRESSION TAG	UNP P27472
D	-12	HIS	-	EXPRESSION TAG	UNP P27472
D	-11	HIS	-	EXPRESSION TAG	UNP P27472
D	-10	HIS	-	EXPRESSION TAG	UNP P27472
D	-9	SER	-	EXPRESSION TAG	UNP P27472
D	-8	SER	-	EXPRESSION TAG	UNP P27472
D	-7	GLY	-	EXPRESSION TAG	UNP P27472
D	-6	LEU	-	EXPRESSION TAG	UNP P27472
D	-5	VAL	-	EXPRESSION TAG	UNP P27472
D	-4	PRO	-	EXPRESSION TAG	UNP P27472
D	-3	ARG	-	EXPRESSION TAG	UNP P27472
D	-2	GLY	-	EXPRESSION TAG	UNP P27472
D	-1	SER	-	EXPRESSION TAG	UNP P27472
D	0	HIS	-	EXPRESSION TAG	UNP P27472
D	535	SER	ALA	SEE REMARK 999	UNP P27472
D	589	ALA	ARG	ENGINEERED MUTATION	UNP P27472
D	592	ALA	ARG	ENGINEERED MUTATION	UNP P27472

- Molecule 2 is SUGAR (ALPHA-D-GLUCOSE-6-PHOSPHATE) (three-letter code: G6P) (formula: C₆H₁₃O₉P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	B	1	Total	C	O	P	0	0
			16	6	9	1		
2	C	1	Total	C	O	P	0	0
			16	6	9	1		
2	D	1	Total	C	O	P	0	0
			16	6	9	1		

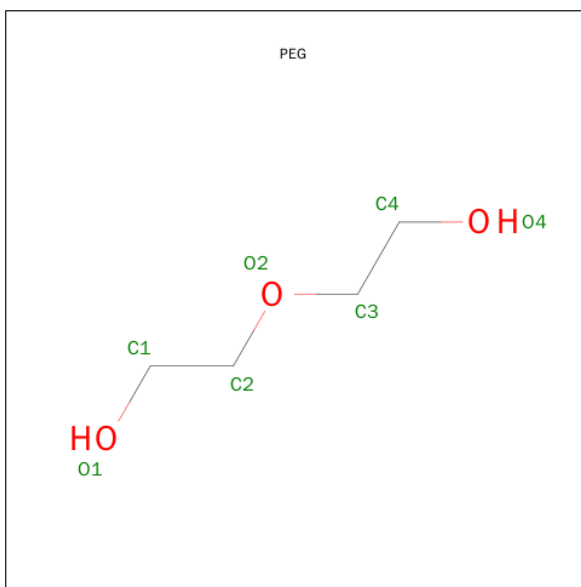
- Molecule 3 is a polymer of unknown type called SUGAR (8-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	8	Total	C	O	0	0
			78	42	36		

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	3	Total	C	O	0	0
			23	12	11		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		
5	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	4	Total	C	O	0	0
			34	18	16		

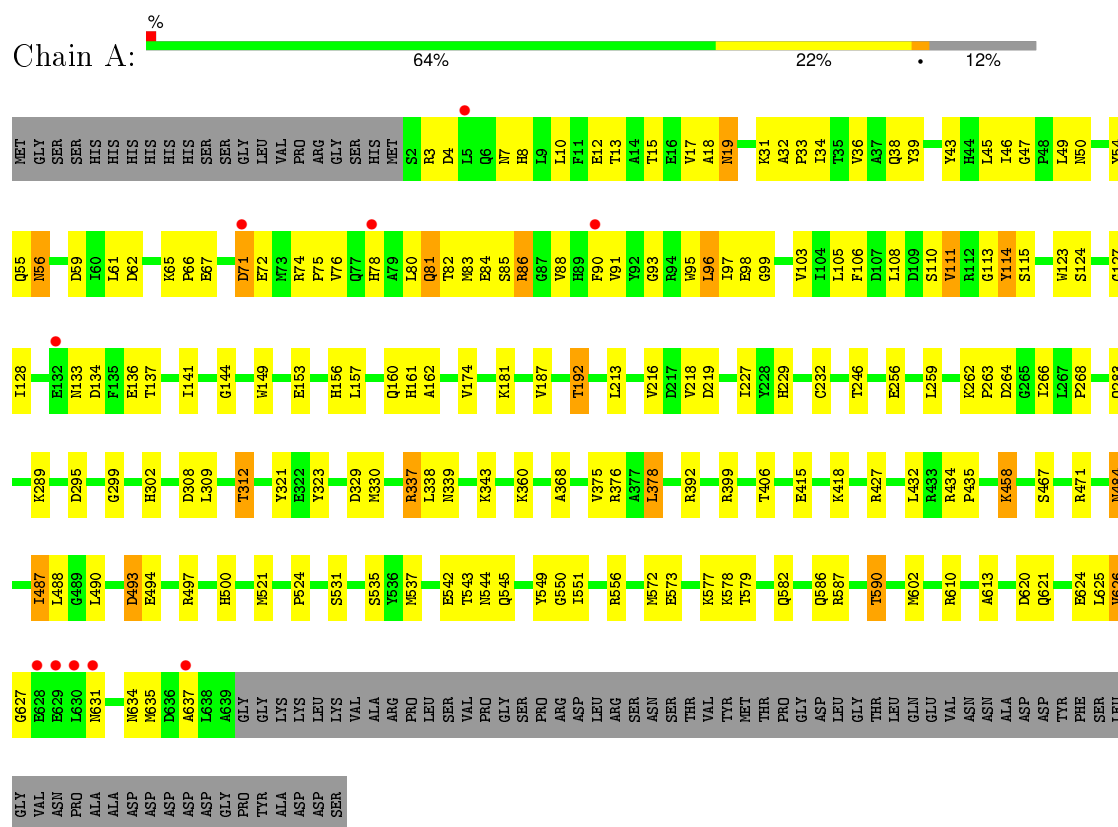
- Molecule 7 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	5	Total	C	O	0	0
			45	24	21		
7	D	5	Total	C	O	0	0
			45	24	21		

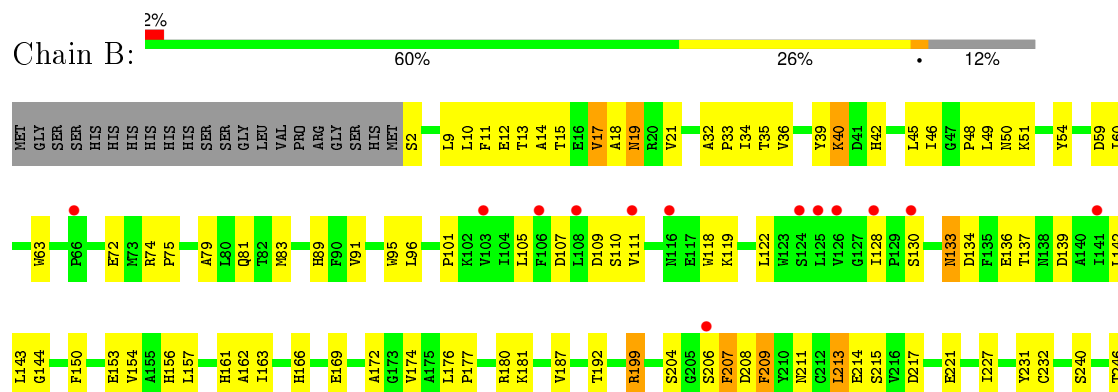
3 Residue-property plots [i](#)

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: PROTEIN (Glycogen [starch] synthase isoform 2)



- Molecule 1: PROTEIN (Glycogen [starch] synthase isoform 2)







4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	193.44Å 205.33Å 206.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.58 – 2.80 48.58 – 2.79	Depositor EDS
% Data completeness (in resolution range)	95.1 (48.58-2.80) 99.7 (48.58-2.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.81Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.211 , 0.261 0.215 , 0.263	Depositor DCC
R_{free} test set	5042 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	63.0	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.1	EDS
Estimated twinning fraction	0.009 for -h,-l,-k	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 101270 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	20951	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GLC, G6P, PEG

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	0.39	0/5270	0.52	0/7141
1	B	0.35	0/5270	0.49	0/7141
1	C	0.35	1/5325 (0.0%)	0.49	1/7212 (0.0%)
1	D	0.38	0/5251	0.51	1/7114 (0.0%)
All	All	0.37	1/21116 (0.0%)	0.51	2/28608 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	434	ARG	C-N	-5.21	1.24	1.34

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	39	TYR	CB-CA-C	-5.88	98.64	110.40
1	C	435	PRO	O-C-N	5.20	131.02	122.70

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	5145	0	5054	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5145	0	5054	133	0
1	C	5200	0	5124	148	0
1	D	5128	0	5039	180	0
2	A	16	0	11	1	0
2	B	32	0	22	1	0
2	C	16	0	11	1	0
2	D	16	0	11	2	0
3	A	78	0	64	2	0
4	A	23	0	19	2	0
5	A	7	0	10	0	0
5	B	14	0	20	2	0
5	C	7	0	10	0	0
6	C	34	0	28	3	0
7	D	90	0	74	2	0
All	All	20951	0	20551	573	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 14.

All (573) 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:C:399:ARG:HD3	1:C:403:ASN:HD22	1.20	1.07
1:D:579:THR:H	1:D:582:GLN:HE21	1.17	0.93
1:B:48:PRO:HG3	1:B:143:LEU:HD22	1.53	0.90
1:A:110:SER:O	1:A:111:VAL:HG13	1.78	0.84
1:B:19:ASN:OD1	1:B:21:VAL:HG23	1.79	0.83
1:A:108:LEU:O	1:A:111:VAL:HG22	1.80	0.81
1:B:312:THR:HG22	1:B:350:THR:HB	1.62	0.81
1:D:586:GLN:O	1:D:590:THR:HG22	1.82	0.80
1:D:144:GLY:HA3	1:D:174:VAL:HB	1.64	0.80
1:A:542:GLU:OE2	1:A:544:ASN:HB2	1.82	0.79
1:B:192:THR:HG22	1:B:246:THR:HG22	1.65	0.78
1:B:368:ALA:HB1	1:B:487:ILE:HD11	1.65	0.77
1:D:213:LEU:HD21	1:D:253:PHE:HE1	1.49	0.77
1:C:61:LEU:HB2	1:C:93:GLY:HA2	1.69	0.75
1:D:66:PRO:HA	1:D:74:ARG:HH12	1.51	0.75
1:B:17:VAL:HG21	1:B:46:ILE:O	1.87	0.75
1:D:507:TYR:HB2	1:D:556:ARG:NH2	2.01	0.75
1:A:283:GLN:HG2	1:B:280:HIS:CE1	2.22	0.75
1:C:168:HIS:HD2	1:C:193:HIS:NE2	1.85	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HB2	1:A:93:GLY:HA2	1.69	0.74
1:D:292:LYS:HD3	1:D:490:LEU:HD21	1.69	0.74
1:A:49:LEU:CD1	1:A:105:LEU:HB3	2.17	0.73
1:C:284:ASN:HD21	1:D:284:ASN:HD21	1.34	0.73
1:D:264:ASP:O	1:D:635:MET:HG3	1.88	0.73
1:C:200:TYR:CE1	1:C:227:ILE:HD11	2.23	0.73
1:D:482:ASN:HD22	1:D:484:ASN:H	1.37	0.72
1:A:578:LYS:HA	1:A:582:GLN:NE2	2.05	0.71
1:D:579:THR:H	1:D:582:GLN:NE2	1.89	0.71
1:D:456:LEU:O	1:D:460:ARG:HG3	1.90	0.71
1:A:17:VAL:HG21	1:A:47:GLY:HA3	1.73	0.70
1:D:399:ARG:HD3	1:D:403:ASN:HD22	1.56	0.70
1:B:513:TYR:O	1:B:517:GLU:HG2	1.92	0.70
1:D:213:LEU:HD21	1:D:253:PHE:CE1	2.26	0.70
1:B:431:ALA:HB2	1:C:484:ASN:HD21	1.57	0.70
1:C:399:ARG:HD3	1:C:403:ASN:ND2	2.03	0.69
1:D:121:ASP:O	1:D:125:LEU:HB2	1.92	0.69
1:B:579:THR:H	1:B:582:GLN:HE21	1.36	0.69
1:C:283:GLN:HG3	2:C:901:G6P:O1	1.93	0.69
1:D:32:ALA:HB3	1:D:33:PRO:HD3	1.74	0.69
1:C:482:ASN:C	1:C:484:ASN:H	1.96	0.69
1:C:378:LEU:O	1:C:382:VAL:HG23	1.93	0.69
1:A:49:LEU:HD11	1:A:105:LEU:HB3	1.74	0.68
1:C:283:GLN:HG2	1:D:280:HIS:CE1	2.28	0.68
1:A:59:ASP:HB2	1:A:96:LEU:HD21	1.76	0.68
1:B:542:GLU:OE1	1:B:544:ASN:HB3	1.93	0.68
1:B:307:PHE:HD1	1:B:312:THR:HG21	1.59	0.67
1:C:323:TYR:CZ	1:C:329:ASP:HB3	2.30	0.67
1:C:200:TYR:CD1	1:C:227:ILE:HD11	2.30	0.67
1:C:305:PHE:HZ	1:C:309:LEU:HG	1.59	0.67
1:B:579:THR:H	1:B:582:GLN:NE2	1.93	0.67
1:A:192:THR:HG22	1:A:246:THR:HG22	1.76	0.67
1:B:192:THR:CG2	1:B:246:THR:HG22	2.24	0.67
1:D:14:ALA:HB2	1:D:168:HIS:HB2	1.76	0.66
1:C:176:LEU:HD12	1:C:237:ALA:HB1	1.78	0.66
1:A:8:HIS:HB2	1:A:162:ALA:O	1.96	0.66
1:A:110:SER:O	1:A:111:VAL:CG1	2.43	0.66
1:B:431:ALA:HB2	1:C:484:ASN:ND2	2.11	0.65
1:B:254:GLU:HG3	1:B:258:LEU:HD12	1.78	0.65
1:A:339:ASN:O	1:A:343:LYS:HG3	1.96	0.65
1:B:17:VAL:HG21	1:B:46:ILE:C	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:586:GLN:O	1:C:590:THR:HG22	1.96	0.65
1:B:14:ALA:O	1:B:17:VAL:HG23	1.97	0.65
1:C:192:THR:HG22	1:C:246:THR:HG22	1.79	0.64
1:D:140:ALA:O	1:D:174:VAL:HG21	1.96	0.64
1:C:634:ASN:HB2	1:C:637:ALA:CB	2.28	0.64
1:C:482:ASN:O	1:C:484:ASN:N	2.31	0.64
1:A:49:LEU:HD11	1:A:105:LEU:C	2.18	0.64
1:B:497:ARG:CZ	1:B:521:MET:HG2	2.26	0.64
1:A:392:ARG:NH2	1:A:418:LYS:HG2	2.12	0.64
1:A:76:VAL:O	1:A:80:LEU:HG	1.98	0.64
1:A:586:GLN:O	1:A:590:THR:HG22	1.96	0.64
1:B:307:PHE:CD1	1:B:312:THR:HG21	2.32	0.64
1:B:17:VAL:HG12	1:B:18:ALA:N	2.12	0.64
1:B:50:ASN:O	1:B:54:TYR:HB3	1.98	0.64
1:A:49:LEU:HD13	1:A:106:PHE:C	2.18	0.63
1:A:490:LEU:HD22	1:A:494:GLU:HB3	1.79	0.63
1:B:331:PHE:CZ	1:B:335:LEU:HD11	2.34	0.63
1:A:83:MET:HE3	1:A:88:VAL:HG21	1.79	0.63
1:B:379:GLU:HG3	1:D:394:PHE:CE1	2.34	0.63
1:C:626:VAL:HG11	1:C:630:LEU:HD11	1.81	0.63
1:C:50:ASN:O	1:C:54:TYR:HB3	1.99	0.63
1:B:174:VAL:O	1:B:177:PRO:HD2	1.99	0.63
1:A:62:ASP:HB3	1:A:65:LYS:HE3	1.80	0.63
1:B:323:TYR:CZ	1:B:329:ASP:HB3	2.32	0.63
1:D:19:ASN:HD22	1:D:19:ASN:H	1.46	0.63
1:A:309:LEU:HA	1:A:312:THR:HG23	1.81	0.63
1:A:213:LEU:HA	1:A:216:VAL:HG23	1.82	0.62
1:C:399:ARG:HH11	1:C:403:ASN:ND2	1.97	0.62
1:D:210:TYR:CZ	1:D:530:VAL:HG13	2.34	0.62
1:D:153:GLU:O	1:D:157:LEU:HG	2.00	0.62
1:D:12:GLU:HG3	1:D:166:HIS:HB3	1.82	0.62
1:A:17:VAL:CG2	1:A:47:GLY:HA3	2.29	0.62
1:B:512:GLY:O	1:B:515:PRO:HD2	1.99	0.62
1:B:450:ASP:OD1	1:B:460:ARG:NH2	2.33	0.62
1:B:51:LYS:HE3	1:B:107:ASP:OD1	1.99	0.62
1:C:150:PHE:O	1:C:154:VAL:HG23	2.00	0.61
1:D:74:ARG:N	1:D:75:PRO:HD2	2.16	0.61
1:A:19:ASN:N	1:A:19:ASN:HD22	1.98	0.61
1:C:31:LYS:O	1:C:35:THR:HG22	2.01	0.61
1:C:111:VAL:HG12	1:C:111:VAL:O	2.00	0.61
1:A:137:THR:O	1:A:141:ILE:HG13	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:ASN:HB2	1:B:511:TRP:CD1	2.36	0.61
1:B:176:LEU:HB2	1:B:177:PRO:HD3	1.83	0.61
1:A:302:HIS:HB2	1:A:432:LEU:HD22	1.83	0.60
1:A:330:MET:CG	3:A:801:GLC:H61	2.31	0.60
1:D:72:GLU:O	1:D:161:HIS:HE1	1.83	0.60
1:B:227:ILE:O	1:B:227:ILE:HG22	2.01	0.60
1:A:549:TYR:O	1:A:590:THR:HB	2.02	0.60
1:A:12:GLU:HB3	1:A:45:LEU:HD23	1.83	0.59
1:D:110:SER:O	1:D:111:VAL:HG23	2.03	0.59
1:B:308:ASP:O	1:B:312:THR:HG23	2.02	0.59
1:C:169:GLU:O	1:C:190:PHE:HE1	1.85	0.59
1:A:634:ASN:HB2	1:A:637:ALA:H	1.68	0.59
1:D:19:ASN:HD22	1:D:19:ASN:N	2.00	0.59
1:B:89:HIS:CD2	1:B:110:SER:HB3	2.37	0.58
1:B:153:GLU:O	1:B:157:LEU:HG	2.03	0.58
1:D:217:ASP:O	1:D:221:GLU:HG2	2.03	0.58
1:C:447:MET:HG3	1:C:456:LEU:HD11	1.85	0.58
1:D:125:LEU:HD21	1:D:181:LYS:HZ2	1.68	0.58
1:A:7:ASN:O	1:A:161:HIS:HD2	1.85	0.58
1:C:59:ASP:HB2	1:C:96:LEU:HD21	1.84	0.58
1:A:299:GLY:HA2	1:A:375:VAL:HG21	1.86	0.58
1:D:170:TRP:NE1	1:D:196:LEU:HD21	2.19	0.58
1:C:399:ARG:CD	1:C:403:ASN:HD22	2.06	0.58
1:B:144:GLY:HA3	1:B:174:VAL:HB	1.85	0.58
1:A:72:GLU:HB2	1:A:161:HIS:HE1	1.68	0.58
1:A:86:ARG:HB3	1:A:86:ARG:HH11	1.68	0.58
1:B:206:SER:O	1:B:207:PHE:HB3	2.04	0.58
1:D:177:PRO:HA	1:D:240:SER:CB	2.33	0.58
1:B:278:ALA:HB1	1:B:280:HIS:CE1	2.39	0.58
1:C:169:GLU:HA	1:C:169:GLU:OE2	2.03	0.58
6:C:802:GLC:H5	6:C:803:GLC:H62	1.86	0.58
1:C:399:ARG:HH11	1:C:403:ASN:HD21	1.52	0.57
1:C:280:HIS:CE1	1:D:283:GLN:HG2	2.39	0.57
1:B:504:PHE:CE1	1:B:514:THR:HG22	2.39	0.57
1:B:537:MET:HG2	1:B:551:ILE:HD13	1.87	0.57
1:C:199:ARG:HG2	1:C:508:TYR:CE2	2.40	0.57
1:B:368:ALA:HB1	1:B:487:ILE:CD1	2.34	0.57
1:A:49:LEU:HD11	1:A:105:LEU:CB	2.33	0.57
1:D:183:ARG:HG3	1:D:183:ARG:O	2.05	0.57
1:B:249:GLN:OE1	1:B:266:ILE:HD11	2.04	0.57
1:D:447:MET:HB2	1:D:450:ASP:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:634:ASN:HB2	1:C:637:ALA:H	1.70	0.56
1:A:587:ARG:HA	1:A:590:THR:HG23	1.86	0.56
1:A:13:THR:HG23	1:A:46:ILE:HB	1.86	0.56
1:C:91:VAL:HG12	1:C:92:TYR:N	2.19	0.56
1:C:509:GLU:HB3	1:C:531:SER:HB2	1.87	0.56
1:C:19:ASN:N	1:C:19:ASN:HD22	2.02	0.56
1:D:593:LEU:O	1:D:596:LEU:HB3	2.05	0.56
1:D:402:HIS:O	1:D:404:GLY:N	2.38	0.56
1:D:32:ALA:HB1	1:D:101:PRO:HG3	1.88	0.56
1:D:180:ARG:HD2	1:D:240:SER:HA	1.86	0.56
1:D:400:TYR:CD2	1:D:401:PRO:HA	2.41	0.56
1:B:274:ILE:HG13	1:B:274:ILE:O	2.04	0.56
1:D:170:TRP:HE1	1:D:196:LEU:HD21	1.70	0.56
1:C:196:LEU:O	1:C:200:TYR:HD2	1.88	0.56
1:C:634:ASN:CB	1:C:637:ALA:H	2.19	0.56
1:C:528:THR:HG21	1:C:556:ARG:HG3	1.87	0.56
1:A:264:ASP:O	1:A:635:MET:HG3	2.06	0.56
1:B:9:LEU:HD21	1:B:161:HIS:ND1	2.20	0.56
1:B:79:ALA:O	1:B:83:MET:HG2	2.06	0.56
1:D:227:ILE:HG22	1:D:227:ILE:O	2.05	0.56
1:D:80:LEU:HD22	1:D:90:PHE:CE1	2.40	0.56
1:D:48:PRO:HG3	1:D:143:LEU:HD22	1.88	0.56
1:D:14:ALA:O	1:D:17:VAL:HG23	2.06	0.55
1:D:75:PRO:HB3	1:D:158:ASP:HB2	1.89	0.55
1:C:383:HIS:O	1:C:387:THR:HG23	2.06	0.55
1:B:54:TYR:HE1	1:B:60:ILE:HD11	1.70	0.55
1:A:85:SER:HB2	1:A:86:ARG:HD3	1.89	0.55
1:D:292:LYS:CD	1:D:490:LEU:HD21	2.37	0.55
1:A:578:LYS:HA	1:A:582:GLN:HE21	1.70	0.55
1:A:80:LEU:HD22	1:A:90:PHE:CE1	2.42	0.55
1:B:299:GLY:HA2	1:B:375:VAL:HG21	1.89	0.55
1:D:434:ARG:HB2	1:D:435:PRO:HD2	1.88	0.55
1:D:150:PHE:O	1:D:154:VAL:HG23	2.07	0.55
1:D:541:ILE:HG22	1:D:545:GLN:HB3	1.89	0.55
1:A:74:ARG:N	1:A:75:PRO:CD	2.70	0.54
1:D:144:GLY:O	1:D:175:ALA:HB2	2.06	0.54
1:C:193:HIS:HD1	1:C:247:VAL:HG11	1.72	0.54
1:D:275:LYS:NZ	1:D:279:PHE:HD1	2.05	0.54
1:B:634:ASN:HB2	1:B:637:ALA:CB	2.38	0.54
1:C:507:TYR:HB2	1:C:556:ARG:NH2	2.23	0.54
1:A:266:ILE:HG22	1:A:268:PRO:HD3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:536:TYR:O	1:B:540:LEU:HD23	2.08	0.54
1:A:153:GLU:O	1:A:157:LEU:HG	2.08	0.54
1:D:168:HIS:HD2	1:D:193:HIS:NE2	2.06	0.54
1:D:192:THR:HG22	1:D:246:THR:HG22	1.90	0.54
1:C:581:ARG:NH2	1:D:275:LYS:HD3	2.23	0.54
1:D:187:VAL:HG11	1:D:613:ALA:O	2.08	0.54
1:C:299:GLY:HA2	1:C:375:VAL:HG21	1.90	0.54
1:A:32:ALA:HB3	1:A:33:PRO:HD3	1.90	0.54
1:B:330:MET:HG3	1:B:565:VAL:HG22	1.90	0.53
1:D:19:ASN:ND2	1:D:19:ASN:H	2.05	0.53
1:B:463:GLN:HA	1:B:465:PHE:CE2	2.44	0.53
1:A:19:ASN:N	1:A:19:ASN:ND2	2.56	0.53
1:D:59:ASP:O	1:D:61:LEU:HG	2.08	0.53
1:A:192:THR:CG2	1:A:246:THR:HG22	2.39	0.53
1:D:176:LEU:N	1:D:177:PRO:HD2	2.24	0.53
1:A:84:GLU:OE2	1:A:84:GLU:HA	2.08	0.53
1:B:458:LYS:O	1:B:462:VAL:HG22	2.07	0.53
1:C:170:TRP:CH2	1:C:230:ARG:HG2	2.44	0.53
1:C:482:ASN:C	1:C:484:ASN:N	2.63	0.53
1:A:368:ALA:HB1	1:A:487:ILE:CD1	2.38	0.53
1:D:17:VAL:HG21	1:D:46:ILE:O	2.08	0.52
1:D:86:ARG:HB3	1:D:86:ARG:HH11	1.74	0.52
1:B:162:ALA:C	1:B:163:ILE:HG13	2.29	0.52
1:A:434:ARG:HB2	1:A:435:PRO:HD2	1.91	0.52
1:D:292:LYS:HD3	1:D:490:LEU:CD2	2.38	0.52
1:D:21:VAL:HG12	1:D:21:VAL:O	2.09	0.52
1:B:488:LEU:O	1:B:490:LEU:N	2.41	0.52
1:C:284:ASN:ND2	1:D:284:ASN:HD21	2.06	0.52
1:D:514:THR:HB	1:D:515:PRO:HD3	1.91	0.52
1:C:634:ASN:HB2	1:C:637:ALA:HB3	1.91	0.52
1:C:447:MET:HG3	1:C:456:LEU:CD1	2.40	0.52
1:B:279:PHE:CD1	1:B:279:PHE:N	2.77	0.52
1:D:164:VAL:HA	1:D:187:VAL:HG23	1.92	0.52
1:D:537:MET:HG2	1:D:551:ILE:HD13	1.91	0.52
1:C:492:TYR:O	1:C:496:VAL:HG23	2.10	0.52
1:C:227:ILE:O	1:C:230:ARG:HB2	2.10	0.52
1:A:80:LEU:HD22	1:A:90:PHE:HE1	1.75	0.52
1:C:278:ALA:HB1	1:C:280:HIS:CE1	2.44	0.51
1:D:278:ALA:HB1	1:D:280:HIS:CE1	2.45	0.51
1:D:368:ALA:HB1	1:D:487:ILE:CD1	2.40	0.51
1:C:269:ASN:HB2	1:C:511:TRP:NE1	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:THR:HG21	1:A:229:HIS:HD2	1.75	0.51
1:D:31:LYS:NZ	1:D:35:THR:HG21	2.25	0.51
1:D:167:PHE:HB2	1:D:176:LEU:HD11	1.92	0.51
1:C:12:GLU:OE2	1:C:168:HIS:HE1	1.93	0.51
1:A:256:GLU:OE2	1:A:262:LYS:HG3	2.10	0.51
1:D:594:SER:C	1:D:596:LEU:H	2.13	0.51
1:C:30:SER:O	1:C:272:ASN:ND2	2.44	0.51
1:B:249:GLN:HG2	1:B:266:ILE:CD1	2.40	0.51
1:D:620:ASP:HA	1:D:623:ARG:NH1	2.26	0.51
1:B:42:HIS:CE1	1:B:72:GLU:OE2	2.64	0.51
1:A:283:GLN:HG3	2:A:901:G6P:O1	2.11	0.51
1:A:33:PRO:HG3	1:A:98:GLU:HG2	1.92	0.51
1:A:31:LYS:O	1:A:34:ILE:HG22	2.11	0.50
1:B:607:VAL:O	1:B:611:GLN:HG2	2.12	0.50
1:B:374:GLU:HB3	1:B:432:LEU:CD2	2.40	0.50
1:D:86:ARG:HB3	1:D:86:ARG:NH1	2.26	0.50
1:A:187:VAL:HG11	1:A:613:ALA:O	2.12	0.50
1:B:133:ASN:ND2	1:B:133:ASN:H	2.07	0.50
1:B:95:TRP:HB3	1:B:101:PRO:HD2	1.94	0.50
1:D:612:LEU:O	1:D:612:LEU:HG	2.11	0.50
1:C:17:VAL:HG12	1:C:18:ALA:N	2.27	0.50
1:A:542:GLU:OE1	1:A:545:GLN:HB2	2.12	0.50
1:D:113:GLY:C	1:D:115:SER:H	2.15	0.50
1:D:543:THR:CG2	1:D:543:THR:O	2.60	0.50
1:B:323:TYR:CE1	1:B:329:ASP:HB3	2.47	0.50
1:A:537:MET:HG2	1:A:551:ILE:HD12	1.94	0.50
1:B:368:ALA:CB	1:B:487:ILE:HD11	2.39	0.49
1:C:510:PRO:O	1:C:532:GLY:HA3	2.12	0.49
1:B:111:VAL:CG1	1:B:118:TRP:CH2	2.95	0.49
1:C:200:TYR:CE2	1:C:227:ILE:HD13	2.48	0.49
1:A:427:ARG:HH21	1:D:482:ASN:HD21	1.60	0.49
1:D:150:PHE:CE2	1:D:154:VAL:HG21	2.47	0.49
1:D:122:LEU:CD2	1:D:128:ILE:HD12	2.41	0.49
1:B:199:ARG:HB3	1:B:508:TYR:CE2	2.48	0.49
1:A:330:MET:HG2	3:A:801:GLC:H61	1.94	0.49
1:B:32:ALA:HB3	1:B:33:PRO:HD3	1.94	0.49
1:D:74:ARG:N	1:D:75:PRO:CD	2.75	0.49
1:B:391:LYS:HD3	5:B:1001:PEG:H41	1.94	0.49
1:D:141:ILE:HA	1:D:174:VAL:HG11	1.94	0.49
1:C:18:ALA:HB2	1:C:105:LEU:HD11	1.95	0.49
1:B:150:PHE:O	1:B:154:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:6:GLN:NE2	1:D:625:LEU:HD23	2.27	0.49
1:B:13:THR:HG22	1:B:172:ALA:HB1	1.95	0.49
1:B:279:PHE:HD1	1:B:279:PHE:H	1.60	0.49
1:C:533:PHE:O	1:C:537:MET:HB2	2.13	0.49
1:A:110:SER:C	1:A:111:VAL:HG13	2.32	0.49
1:D:368:ALA:HB1	1:D:487:ILE:HD13	1.95	0.49
1:B:323:TYR:OH	1:B:458:LYS:HG3	2.13	0.49
1:D:19:ASN:ND2	1:D:19:ASN:N	2.61	0.49
1:A:493:ASP:O	1:A:497:ARG:HG3	2.13	0.49
1:D:176:LEU:HD13	1:D:190:PHE:HB2	1.95	0.48
1:D:208:ASP:OD1	1:D:209:PHE:N	2.46	0.48
1:B:304:CYS:SG	1:B:434:ARG:HD3	2.53	0.48
1:C:537:MET:HG2	1:C:551:ILE:HG21	1.96	0.48
1:B:34:ILE:HD13	1:B:599:TRP:HB3	1.95	0.48
1:B:227:ILE:O	1:B:227:ILE:CG2	2.61	0.48
1:A:218:VAL:HG23	1:A:219:ASP:N	2.29	0.48
1:C:179:CYS:HA	1:C:184:ILE:HD12	1.95	0.48
1:C:196:LEU:HD13	1:C:227:ILE:CG2	2.43	0.48
1:D:163:ILE:HB	1:D:186:VAL:HG12	1.96	0.48
1:C:14:ALA:HB3	1:C:28:LEU:HD11	1.96	0.48
1:D:289:LYS:HE3	1:D:494:GLU:HG2	1.95	0.48
1:A:108:LEU:O	1:A:111:VAL:CG2	2.56	0.48
1:A:302:HIS:O	1:A:434:ARG:HD2	2.13	0.48
1:C:442:ILE:HD11	1:C:465:PHE:HA	1.95	0.48
1:B:319:GLY:O	1:B:357:MET:HG2	2.13	0.48
1:A:626:VAL:HG12	1:A:627:GLY:N	2.28	0.48
1:B:15:THR:O	1:B:15:THR:CG2	2.62	0.48
1:D:580:ARG:HE	2:D:901:G6P:H62	1.79	0.48
1:C:328:ALA:O	1:C:332:ILE:HG13	2.13	0.48
1:A:323:TYR:CZ	1:A:329:ASP:HB3	2.48	0.48
1:C:227:ILE:O	1:C:230:ARG:N	2.45	0.48
1:D:128:ILE:HG12	1:D:232:CYS:HB3	1.95	0.48
1:D:510:PRO:O	1:D:532:GLY:HA3	2.13	0.48
1:B:600:LYS:HE3	1:B:600:LYS:O	2.14	0.48
1:B:312:THR:CG2	1:B:350:THR:HB	2.40	0.47
1:A:3:ARG:H	1:A:621:GLN:HE22	1.62	0.47
1:B:89:HIS:HD2	1:B:110:SER:HB3	1.78	0.47
1:C:200:TYR:CZ	1:C:227:ILE:HD11	2.49	0.47
1:A:624:GLU:C	1:A:626:VAL:H	2.17	0.47
1:D:238:ALA:O	1:D:261:ARG:HD3	2.15	0.47
4:A:808:GLC:O5	4:A:809:GLC:H62	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:275:LYS:HZ1	1:D:279:PHE:HD1	1.60	0.47
1:B:634:ASN:HB2	1:B:637:ALA:HB3	1.96	0.47
1:A:537:MET:HG2	1:A:551:ILE:HG21	1.95	0.47
1:D:606:TYR:O	1:D:610:ARG:HG3	2.14	0.47
1:B:513:TYR:HD1	1:B:514:THR:N	2.12	0.47
1:D:19:ASN:O	1:D:21:VAL:HG23	2.15	0.47
1:A:19:ASN:ND2	1:A:19:ASN:H	2.13	0.47
1:D:620:ASP:HA	1:D:623:ARG:HH12	1.80	0.47
1:C:228:TYR:O	1:C:230:ARG:N	2.48	0.47
1:C:31:LYS:HB2	1:C:599:TRP:CZ2	2.50	0.47
1:D:130:SER:O	1:D:132:GLU:N	2.48	0.47
1:A:95:TRP:O	1:A:97:ILE:N	2.47	0.47
1:A:392:ARG:CZ	1:A:418:LYS:HG2	2.43	0.47
1:A:83:MET:CE	1:A:88:VAL:HG11	2.45	0.47
1:C:235:ARG:HA	1:C:259:LEU:HD22	1.96	0.47
1:C:357:MET:O	1:C:478:PRO:HA	2.14	0.47
1:D:344:VAL:C	1:D:346:GLY:H	2.18	0.47
1:A:19:ASN:HD22	1:A:19:ASN:H	1.62	0.47
1:C:19:ASN:O	1:C:21:VAL:HG23	2.14	0.47
1:A:378:LEU:HD13	1:C:394:PHE:CD1	2.50	0.47
1:A:378:LEU:HD13	1:C:394:PHE:CE1	2.50	0.47
1:D:222:ALA:HB1	1:D:228:TYR:HA	1.97	0.47
1:C:269:ASN:O	1:C:602:MET:HE3	2.14	0.46
1:C:611:GLN:HA	1:C:611:GLN:HE21	1.80	0.46
1:C:213:LEU:HD21	1:C:253:PHE:HE1	1.81	0.46
1:A:83:MET:HE2	1:A:88:VAL:HG11	1.97	0.46
1:D:500:HIS:O	1:D:524:PRO:HD2	2.15	0.46
1:A:579:THR:H	1:A:582:GLN:NE2	2.13	0.46
1:D:176:LEU:CD2	1:D:188:THR:HB	2.45	0.46
1:C:482:ASN:C	1:C:490:LEU:O	2.53	0.46
1:C:176:LEU:HB2	1:C:177:PRO:HD2	1.98	0.46
1:A:103:VAL:HG13	1:A:103:VAL:O	2.16	0.46
1:C:385:VAL:O	1:C:389:ILE:HG13	2.15	0.46
1:A:268:PRO:HB2	1:A:602:MET:HE1	1.97	0.46
1:C:269:ASN:HB2	1:C:511:TRP:CE2	2.49	0.46
1:C:526:ILE:HG12	1:C:552:TYR:HB2	1.96	0.46
1:C:482:ASN:OD1	1:C:483:ALA:N	2.48	0.46
1:D:279:PHE:CE1	1:D:591:GLU:OE1	2.69	0.46
1:C:371:GLY:O	1:C:375:VAL:HG23	2.15	0.46
1:C:10:LEU:HD12	1:C:11:PHE:N	2.31	0.46
1:D:331:PHE:CZ	1:D:335:LEU:HD11	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:114:TYR:H	1:D:114:TYR:HD1	1.62	0.46
1:B:134:ASP:OD2	1:B:137:THR:HG23	2.16	0.46
1:C:200:TYR:CD2	1:C:227:ILE:HD13	2.50	0.46
1:D:549:TYR:O	1:D:590:THR:HB	2.16	0.46
1:A:74:ARG:N	1:A:75:PRO:HD2	2.31	0.46
1:D:59:ASP:HB2	1:D:96:LEU:HD21	1.97	0.46
1:D:378:LEU:HD22	1:D:382:VAL:HG23	1.97	0.46
1:C:388:SER:HB3	1:C:392:ARG:NH2	2.30	0.46
1:B:139:ASP:HA	1:B:142:LEU:HD12	1.97	0.46
1:C:74:ARG:HB2	1:C:75:PRO:HD3	1.98	0.46
1:D:47:GLY:O	1:D:105:LEU:HA	2.16	0.46
1:B:32:ALA:O	1:B:36:VAL:HG23	2.15	0.46
1:D:114:TYR:CD1	1:D:114:TYR:N	2.84	0.46
1:D:13:THR:HB	1:D:167:PHE:CD1	2.51	0.46
1:A:17:VAL:HG23	1:A:18:ALA:N	2.30	0.46
1:D:122:LEU:HD21	1:D:128:ILE:HD12	1.96	0.46
1:D:167:PHE:CD2	1:D:176:LEU:HD21	2.51	0.45
1:A:587:ARG:HA	1:A:590:THR:CG2	2.44	0.45
1:A:134:ASP:OD1	1:A:137:THR:HG23	2.16	0.45
1:A:50:ASN:O	1:A:54:TYR:HB3	2.16	0.45
1:D:123:TRP:CE3	1:D:123:TRP:O	2.69	0.45
1:D:487:ILE:HG22	1:D:488:LEU:N	2.32	0.45
1:C:333:GLU:HG3	1:C:337:ARG:HD2	1.98	0.45
1:C:112:ARG:HG2	1:C:112:ARG:O	2.16	0.45
1:C:227:ILE:HG22	1:C:227:ILE:O	2.16	0.45
1:D:540:LEU:C	1:D:541:ILE:HG13	2.36	0.45
1:D:81:GLN:HA	1:D:84:GLU:HB3	1.99	0.45
1:A:71:ASP:O	1:A:74:ARG:HG2	2.17	0.45
1:C:487:ILE:HG23	1:C:488:LEU:N	2.31	0.45
1:C:485:ASN:HB2	1:C:488:LEU:O	2.17	0.45
1:C:168:HIS:CD2	1:C:193:HIS:NE2	2.75	0.45
1:C:509:GLU:O	1:C:531:SER:HA	2.17	0.45
1:C:547:LYS:HG2	1:C:552:TYR:CE1	2.52	0.45
1:D:16:GLU:OE2	1:D:24:ILE:HD12	2.17	0.45
1:C:425:LEU:HD23	1:C:425:LEU:HA	1.86	0.45
1:D:200:TYR:CE2	1:D:227:ILE:HD13	2.52	0.45
1:D:164:VAL:HG13	1:D:187:VAL:HG23	1.98	0.45
1:B:510:PRO:O	1:B:532:GLY:HA3	2.16	0.45
1:D:92:TYR:OH	1:D:102:LYS:HD3	2.16	0.45
1:A:114:TYR:CD1	1:A:114:TYR:N	2.84	0.45
1:A:83:MET:O	1:A:88:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:279:PHE:HE1	1:D:591:GLU:OE1	2.00	0.45
1:A:4:ASP:HB2	1:A:160:GLN:O	2.17	0.45
1:D:615:ARG:HD3	1:D:622:PHE:CD1	2.52	0.45
1:C:387:THR:O	1:C:391:LYS:HG3	2.17	0.45
1:C:463:GLN:HG2	1:C:465:PHE:HE2	1.82	0.45
1:A:550:GLY:HA2	1:A:586:GLN:NE2	2.32	0.45
1:D:540:LEU:C	1:D:541:ILE:CG1	2.86	0.45
1:A:268:PRO:HB2	1:A:602:MET:CE	2.46	0.45
1:B:561:PRO:O	1:B:565:VAL:HG23	2.17	0.45
1:B:283:GLN:O	2:B:901:G6P:H1	2.17	0.45
1:B:180:ARG:HD2	1:B:240:SER:O	2.17	0.45
1:D:512:GLY:O	1:D:515:PRO:HD2	2.17	0.44
1:B:32:ALA:HB1	1:B:101:PRO:HG3	1.99	0.44
1:A:113:GLY:C	1:A:115:SER:H	2.20	0.44
1:A:418:LYS:HA	1:A:418:LYS:HD3	1.47	0.44
1:D:543:THR:HG22	1:D:543:THR:O	2.17	0.44
1:A:54:TYR:CE1	1:A:91:VAL:HG21	2.52	0.44
1:A:39:TYR:CB	1:A:43:TYR:HB2	2.47	0.44
1:D:441:PRO:HA	7:D:803:GLC:H62	1.98	0.44
1:D:54:TYR:O	1:D:58:VAL:HG23	2.18	0.44
1:D:618:TYR:CD1	1:D:618:TYR:N	2.86	0.44
1:D:557:ARG:HD3	1:D:558:PHE:CZ	2.52	0.44
1:D:144:GLY:HA3	1:D:174:VAL:CB	2.42	0.44
1:D:66:PRO:O	1:D:74:ARG:NH2	2.50	0.44
1:C:91:VAL:CG1	1:C:92:TYR:N	2.79	0.44
1:B:12:GLU:HG3	1:B:166:HIS:HB3	1.98	0.44
1:B:577:LYS:HA	1:B:577:LYS:HD3	1.80	0.44
1:B:49:LEU:HA	1:B:105:LEU:HB3	1.98	0.44
1:B:273:VAL:HG13	1:B:520:VAL:HG13	1.99	0.44
1:C:581:ARG:HH22	1:D:275:LYS:HD3	1.83	0.44
1:A:114:TYR:HD1	1:A:114:TYR:N	2.16	0.44
1:C:152:GLY:CA	6:C:801:GLC:H61	2.48	0.44
1:D:283:GLN:HG3	2:D:901:G6P:O1	2.18	0.44
1:D:507:TYR:HB2	1:D:556:ARG:HH21	1.78	0.44
1:D:200:TYR:CE1	1:D:227:ILE:HD11	2.53	0.44
1:C:547:LYS:HB2	1:C:547:LYS:HE3	1.73	0.44
1:D:422:LYS:O	1:D:426:LYS:HG3	2.17	0.44
1:C:315:PHE:CD1	1:C:315:PHE:N	2.84	0.44
1:B:181:LYS:HD3	1:B:181:LYS:O	2.18	0.44
1:D:174:VAL:O	1:D:177:PRO:HD2	2.18	0.43
1:B:422:LYS:O	1:B:426:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:428:ARG:HD2	1:C:428:ARG:HA	1.42	0.43
1:C:31:LYS:O	1:C:35:THR:CG2	2.66	0.43
1:D:617:GLY:C	1:D:619:PRO:HD3	2.38	0.43
1:B:249:GLN:HG2	1:B:266:ILE:HD11	1.98	0.43
1:C:169:GLU:CA	1:C:169:GLU:OE2	2.65	0.43
1:B:374:GLU:HB3	1:B:432:LEU:HD23	2.00	0.43
1:B:133:ASN:ND2	1:B:133:ASN:N	2.66	0.43
1:C:422:LYS:O	1:C:426:LYS:HD3	2.18	0.43
1:D:266:ILE:O	1:D:267:LEU:HD23	2.19	0.43
1:A:432:LEU:HD13	1:C:398:ILE:HD12	2.00	0.43
1:C:364:PHE:CE1	1:C:487:ILE:HG21	2.53	0.43
1:B:587:ARG:HA	1:B:590:THR:HG23	2.00	0.43
1:D:125:LEU:HD21	1:D:181:LYS:NZ	2.34	0.43
1:B:391:LYS:CD	5:B:1001:PEG:H41	2.48	0.43
1:B:394:PHE:CE1	1:D:378:LEU:HD13	2.53	0.43
1:B:18:ALA:HB3	1:B:105:LEU:HD11	2.01	0.43
1:C:169:GLU:O	1:C:190:PHE:CE1	2.68	0.43
1:D:321:TYR:OH	1:D:455:ILE:HG12	2.19	0.43
1:C:118:TRP:HE1	6:C:803:GLC:HO3	1.67	0.43
1:D:209:PHE:O	1:D:213:LEU:HB3	2.18	0.43
1:A:213:LEU:HA	1:A:216:VAL:CG2	2.48	0.43
1:B:425:LEU:O	1:B:429:ILE:HG13	2.19	0.43
1:C:92:TYR:OH	1:C:102:LYS:HD3	2.19	0.42
1:D:163:ILE:O	1:D:187:VAL:HG22	2.19	0.42
1:D:523:VAL:HA	1:D:524:PRO:HD3	1.84	0.42
1:A:114:TYR:H	1:A:114:TYR:HD1	1.66	0.42
1:B:526:ILE:HG12	1:B:552:TYR:HB2	2.01	0.42
1:A:308:ASP:O	1:A:312:THR:HG23	2.19	0.42
1:D:108:LEU:HD22	1:D:142:LEU:HB3	2.01	0.42
1:C:458:LYS:O	1:C:462:VAL:HG22	2.19	0.42
1:C:326:LYS:HA	1:C:326:LYS:HD3	1.74	0.42
1:B:370:LYS:HE2	1:B:370:LYS:HB3	1.82	0.42
1:B:458:LYS:HD3	1:B:458:LYS:O	2.19	0.42
1:B:217:ASP:O	1:B:221:GLU:HB2	2.19	0.42
1:C:14:ALA:CB	1:C:28:LEU:HD11	2.50	0.42
1:D:439:LEU:HD12	7:D:802:GLC:H61	2.01	0.42
1:B:63:TRP:HZ3	1:B:81:GLN:HG3	1.84	0.42
1:D:218:VAL:HG11	1:D:260:LYS:HE2	2.02	0.42
1:A:338:LEU:HD22	1:A:572:MET:HB3	2.01	0.42
1:D:587:ARG:HA	1:D:590:THR:CG2	2.50	0.42
1:B:465:PHE:O	1:B:466:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:ASP:C	1:B:111:VAL:H	2.23	0.42
1:B:34:ILE:HG13	1:B:35:THR:N	2.35	0.42
1:C:289:LYS:HD2	1:C:289:LYS:HA	1.72	0.42
1:C:73:MET:HE3	1:C:76:VAL:HG21	2.01	0.42
1:D:520:VAL:HA	1:D:594:SER:HB2	2.02	0.42
1:D:192:THR:O	1:D:192:THR:HG23	2.19	0.42
1:D:82:THR:HG22	1:D:82:THR:O	2.20	0.42
1:B:208:ASP:OD2	1:B:211:ASN:HB2	2.20	0.42
1:D:107:ASP:OD1	1:D:109:ASP:HB2	2.20	0.42
1:D:176:LEU:H	1:D:177:PRO:HD2	1.84	0.42
1:C:228:TYR:C	1:C:230:ARG:N	2.72	0.42
1:D:30:SER:O	1:D:33:PRO:HD2	2.20	0.42
1:A:65:LYS:HA	1:A:66:PRO:HD3	1.79	0.42
1:B:250:ILE:HD12	1:B:535:SER:HB3	2.02	0.42
1:D:257:HIS:O	1:D:258:LEU:HD23	2.19	0.42
1:B:615:ARG:HD2	1:B:615:ARG:O	2.20	0.42
1:D:482:ASN:ND2	1:D:484:ASN:H	2.12	0.42
1:C:56:ASN:N	1:C:56:ASN:OD1	2.52	0.42
1:A:10:LEU:HD21	1:A:610:ARG:HE	1.85	0.42
1:B:187:VAL:HG11	1:B:613:ALA:O	2.20	0.42
1:D:70:SER:O	1:D:74:ARG:HG2	2.20	0.41
1:A:86:ARG:HG3	1:A:149:TRP:CH2	2.55	0.41
1:D:3:ARG:NH2	1:D:155:ALA:O	2.52	0.41
1:B:17:VAL:CG2	1:B:46:ILE:O	2.62	0.41
1:C:408:GLU:O	1:C:409:LEU:HD23	2.20	0.41
1:D:383:HIS:O	1:D:387:THR:HG23	2.20	0.41
1:D:283:GLN:HE22	1:D:587:ARG:HE	1.66	0.41
1:D:3:ARG:NH2	1:D:158:ASP:O	2.53	0.41
1:C:483:ALA:N	1:C:491:ASP:OD1	2.29	0.41
1:C:18:ALA:CB	1:C:105:LEU:HD11	2.50	0.41
1:C:611:GLN:HA	1:C:611:GLN:NE2	2.35	0.41
1:B:255:ALA:O	1:B:259:LEU:HB2	2.21	0.41
1:B:10:LEU:HD12	1:B:11:PHE:N	2.35	0.41
1:C:80:LEU:HD23	1:C:80:LEU:HA	1.93	0.41
1:D:74:ARG:O	1:D:77:GLN:N	2.53	0.41
1:A:7:ASN:O	1:A:161:HIS:CD2	2.71	0.41
1:C:372:GLN:HG3	1:C:487:ILE:HD12	2.02	0.41
1:C:400:TYR:CD1	1:C:408:GLU:HA	2.55	0.41
1:B:39:TYR:O	1:B:40:LYS:HB2	2.21	0.41
1:D:191:THR:HA	1:D:245:THR:O	2.20	0.41
1:A:56:ASN:N	1:A:56:ASN:OD1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:227:ILE:O	1:C:228:TYR:C	2.57	0.41
1:A:54:TYR:CE2	1:A:55:GLN:HG3	2.55	0.41
1:A:128:ILE:HG12	1:A:232:CYS:HB3	2.02	0.41
1:B:74:ARG:N	1:B:75:PRO:CD	2.83	0.41
1:B:122:LEU:HG	1:B:128:ILE:HB	2.01	0.41
1:B:59:ASP:HB2	1:B:96:LEU:HD21	2.02	0.41
1:A:550:GLY:HA2	1:A:586:GLN:HE21	1.85	0.41
1:D:435:PRO:HD2	1:D:438:GLN:NE2	2.35	0.41
1:C:327:GLY:HA3	1:C:505:PRO:O	2.21	0.41
1:A:484:ASN:HB3	1:D:428:ARG:NH1	2.35	0.41
1:A:259:LEU:HD23	1:A:259:LEU:HA	1.84	0.41
1:B:134:ASP:OD1	1:B:136:GLU:HB2	2.21	0.41
1:C:128:ILE:HA	1:C:129:PRO:HD3	1.77	0.41
1:C:358:PRO:HG2	1:C:480:PHE:CE2	2.55	0.41
1:D:459:ILE:HG22	1:D:459:ILE:O	2.20	0.41
1:D:125:LEU:HD11	1:D:181:LYS:NZ	2.36	0.41
1:C:31:LYS:HG2	1:C:35:THR:HG22	2.03	0.41
1:C:143:LEU:O	1:C:147:VAL:HG23	2.21	0.41
1:C:644:LEU:C	1:C:644:LEU:HD13	2.40	0.41
1:C:513:TYR:CD2	1:C:513:TYR:N	2.85	0.41
1:C:200:TYR:CE2	1:C:227:ILE:CD1	3.04	0.41
1:C:176:LEU:HB2	1:C:177:PRO:CD	2.51	0.41
1:A:86:ARG:HB3	1:A:86:ARG:NH1	2.36	0.41
1:D:31:LYS:HZ3	1:D:35:THR:HG21	1.85	0.41
1:A:620:ASP:O	1:A:624:GLU:HG2	2.21	0.41
1:A:133:ASN:OD1	1:A:133:ASN:N	2.42	0.41
1:A:144:GLY:HA3	1:A:174:VAL:HB	2.03	0.41
1:D:337:ARG:HE	1:D:565:VAL:HG11	1.85	0.41
1:A:458:LYS:HD3	1:A:458:LYS:O	2.21	0.41
1:C:228:TYR:O	1:C:231:TYR:N	2.53	0.41
1:A:123:TRP:O	1:A:127:GLY:HA2	2.21	0.41
1:D:409:LEU:HA	1:D:409:LEU:HD12	1.78	0.41
1:B:394:PHE:CD1	1:D:378:LEU:HD13	2.55	0.40
1:D:49:LEU:HD11	1:D:54:TYR:CG	2.55	0.40
1:A:500:HIS:O	1:A:524:PRO:HD2	2.20	0.40
1:A:36:VAL:HG21	1:A:99:GLY:O	2.21	0.40
1:C:264:ASP:OD2	1:C:616:ARG:NH1	2.54	0.40
1:D:417:LEU:HA	1:D:417:LEU:HD23	1.52	0.40
1:D:485:ASN:HA	1:D:486:PRO:HD3	1.84	0.40
1:C:54:TYR:CD1	1:C:54:TYR:O	2.74	0.40
1:A:573:GLU:O	1:A:577:LYS:HG3	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:513:TYR:CD2	1:D:513:TYR:N	2.90	0.40
1:A:78:HIS:O	1:A:81:GLN:HB2	2.21	0.40
1:C:301:PHE:HE1	1:C:473:LYS:HD2	1.86	0.40
1:B:49:LEU:HD22	1:B:91:VAL:HG23	2.04	0.40
1:A:337:ARG:HG3	4:A:808:GLC:O2	2.22	0.40
1:D:459:ILE:CG2	1:D:459:ILE:O	2.67	0.40
1:C:40:LYS:HB3	1:C:41:ASP:H	1.44	0.40
1:B:119:LYS:NZ	1:B:130:SER:HB2	2.36	0.40
1:C:200:TYR:CZ	1:C:227:ILE:CD1	3.05	0.40
1:B:513:TYR:CD1	1:B:514:THR:N	2.89	0.40
1:B:493:ASP:O	1:B:497:ARG:HG3	2.22	0.40
1:A:262:LYS:HA	1:A:263:PRO:HD3	1.83	0.40
1:B:627:GLY:C	1:B:628:GLU:HG2	2.40	0.40
1:D:140:ALA:C	1:D:174:VAL:HG21	2.42	0.40
1:C:372:GLN:CG	1:C:487:ILE:HD12	2.51	0.40
1:B:547:LYS:HE3	1:B:574:GLU:OE1	2.21	0.40
1:C:543:THR:HB	1:C:544:ASN:H	1.77	0.40
1:B:386:THR:HG21	1:D:390:GLY:CA	2.51	0.40
1:A:227:ILE:HD13	1:A:227:ILE:HA	1.67	0.40
1:B:209:PHE:O	1:B:213:LEU:HB3	2.22	0.40
1:B:410:PRO:HG2	1:B:416:LEU:HD21	2.02	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	636/725 (88%)	586 (92%)	44 (7%)	6 (1%)	21	55
1	B	636/725 (88%)	581 (91%)	48 (8%)	7 (1%)	17	50
1	C	644/725 (89%)	598 (93%)	38 (6%)	8 (1%)	16	47
1	D	632/725 (87%)	556 (88%)	67 (11%)	9 (1%)	14	42

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2548/2900 (88%)	2321 (91%)	197 (8%)	30 (1%)	16	47

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	204	SER
1	C	483	ALA
1	C	543	THR
1	D	132	GLU
1	D	204	SER
1	D	403	ASN
1	A	38	GLN
1	A	111	VAL
1	B	209	PHE
1	B	489	GLY
1	C	17	VAL
1	D	107	ASP
1	D	111	VAL
1	D	115	SER
1	D	131	PRO
1	A	96	LEU
1	A	625	LEU
1	B	17	VAL
1	C	19	ASN
1	C	229	HIS
1	D	40	LYS
1	B	169	GLU
1	B	215	SER
1	A	631	ASN
1	B	543	THR
1	C	228	TYR
1	C	641	GLY
1	D	402	HIS
1	C	205	GLY
1	A	626	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	551/623 (88%)	513 (93%)	38 (7%)	19	48
1	B	551/623 (88%)	518 (94%)	33 (6%)	24	56
1	C	556/623 (89%)	527 (95%)	29 (5%)	29	62
1	D	549/623 (88%)	517 (94%)	32 (6%)	25	57
All	All	2207/2492 (89%)	2075 (94%)	132 (6%)	24	56

All (132) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	19	ASN
1	A	56	ASN
1	A	67	GLU
1	A	71	ASP
1	A	81	GLN
1	A	82	THR
1	A	86	ARG
1	A	114	TYR
1	A	124	SER
1	A	136	GLU
1	A	156	HIS
1	A	181	LYS
1	A	192	THR
1	A	289	LYS
1	A	295	ASP
1	A	312	THR
1	A	321	TYR
1	A	337	ARG
1	A	360	LYS
1	A	376	ARG
1	A	378	LEU
1	A	399	ARG
1	A	406	THR
1	A	415	GLU
1	A	458	LYS
1	A	467	SER
1	A	471	ARG
1	A	484	ASN
1	A	487	ILE

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Mol	Chain	Res	Type
1	A	488	LEU
1	A	493	ASP
1	A	521	MET
1	A	531	SER
1	A	535	SER
1	A	543	THR
1	A	556	ARG
1	A	590	THR
1	B	2	SER
1	B	19	ASN
1	B	40	LYS
1	B	45	LEU
1	B	133	ASN
1	B	156	HIS
1	B	199	ARG
1	B	207	PHE
1	B	213	LEU
1	B	214	GLU
1	B	231	TYR
1	B	232	CYS
1	B	289	LYS
1	B	310	ASP
1	B	320	ARG
1	B	321	TYR
1	B	376	ARG
1	B	417	LEU
1	B	458	LYS
1	B	471	ARG
1	B	484	ASN
1	B	488	LEU
1	B	513	TYR
1	B	520	VAL
1	B	525	SER
1	B	539	ASP
1	B	540	LEU
1	B	568	LEU
1	B	590	THR
1	B	593	LEU
1	B	600	LYS
1	B	628	GLU
1	B	632	ASP
1	C	2	SER

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Mol	Chain	Res	Type
1	C	19	ASN
1	C	35	THR
1	C	41	ASP
1	C	56	ASN
1	C	116	ASN
1	C	124	SER
1	C	169	GLU
1	C	181	LYS
1	C	199	ARG
1	C	289	LYS
1	C	295	ASP
1	C	321	TYR
1	C	348	LYS
1	C	376	ARG
1	C	387	THR
1	C	426	LYS
1	C	428	ARG
1	C	436	GLU
1	C	461	GLN
1	C	471	ARG
1	C	472	VAL
1	C	520	VAL
1	C	543	THR
1	C	545	GLN
1	C	556	ARG
1	C	568	LEU
1	C	590	THR
1	C	643	LYS
1	D	6	GLN
1	D	19	ASN
1	D	42	HIS
1	D	71	ASP
1	D	86	ARG
1	D	109	ASP
1	D	114	TYR
1	D	122	LEU
1	D	132	GLU
1	D	181	LYS
1	D	213	LEU
1	D	289	LYS
1	D	310	ASP
1	D	321	TYR

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Mol	Chain	Res	Type
1	D	324	LYS
1	D	337	ARG
1	D	376	ARG
1	D	378	LEU
1	D	409	LEU
1	D	412	ASP
1	D	436	GLU
1	D	450	ASP
1	D	457	ASN
1	D	461	GLN
1	D	482	ASN
1	D	487	ILE
1	D	488	LEU
1	D	525	SER
1	D	542	GLU
1	D	557	ARG
1	D	590	THR
1	D	591	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	19	ASN
1	A	81	GLN
1	A	89	HIS
1	A	161	HIS
1	A	168	HIS
1	A	239	HIS
1	A	403	ASN
1	A	582	GLN
1	A	621	GLN
1	B	78	HIS
1	B	81	GLN
1	B	89	HIS
1	B	133	ASN
1	B	484	ASN
1	B	582	GLN
1	C	8	HIS
1	C	19	ASN
1	C	81	GLN
1	C	168	HIS

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Mol	Chain	Res	Type
1	C	249	GLN
1	C	272	ASN
1	C	277	GLN
1	C	284	ASN
1	C	403	ASN
1	C	484	ASN
1	C	611	GLN
1	D	6	GLN
1	D	19	ASN
1	D	50	ASN
1	D	55	GLN
1	D	89	HIS
1	D	161	HIS
1	D	168	HIS
1	D	239	HIS
1	D	257	HIS
1	D	283	GLN
1	D	403	ASN
1	D	482	ASN
1	D	582	GLN
1	D	621	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](#)

Of 25 carbohydrates modelled in this entry, 5 are modelled with single atom - leaving 20 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
3	GLC	A	801	3	11,11,12	0.81	0	14,15,17	1.27	1 (7%)
3	GLC	A	802	3	11,11,12	0.55	0	14,15,17	1.36	3 (21%)
3	GLC	A	803	3	11,11,12	0.28	0	14,15,17	1.33	2 (14%)
3	GLC	A	804	3	11,11,12	0.35	0	14,15,17	0.96	1 (7%)
3	GLC	A	805	3	11,11,12	0.53	0	14,15,17	0.83	0
3	GLC	A	806	3	11,11,12	0.83	0	14,15,17	1.25	1 (7%)
3	GLC	A	807	3	11,11,12	0.82	0	14,15,17	1.71	2 (14%)
4	GLC	A	808	4	11,11,12	0.72	0	14,15,17	0.99	1 (7%)
4	GLC	A	809	4	11,11,12	0.58	0	14,15,17	2.02	4 (28%)
6	GLC	C	801	6	11,11,12	0.38	0	14,15,17	1.19	2 (14%)
6	GLC	C	802	6	11,11,12	0.39	0	14,15,17	0.82	0
6	GLC	C	803	6	11,11,12	0.26	0	14,15,17	0.89	1 (7%)
7	GLC	D	801	7	11,11,12	0.55	0	14,15,17	0.99	0
7	GLC	D	802	7	11,11,12	0.34	0	14,15,17	1.27	1 (7%)
7	GLC	D	803	7	11,11,12	0.36	0	14,15,17	1.02	0
7	GLC	D	804	7	11,11,12	0.82	0	14,15,17	2.19	3 (21%)
7	GLC	D	806	7	11,11,12	0.67	0	14,15,17	1.87	2 (14%)
7	GLC	D	807	7	11,11,12	0.60	0	14,15,17	1.27	2 (14%)
7	GLC	D	808	7	11,11,12	0.35	0	14,15,17	1.51	1 (7%)
7	GLC	D	809	7	11,11,12	0.62	0	14,15,17	1.53	1 (7%)

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
3	GLC	A	801	3	-	0/2/19/22	0/1/1/1
3	GLC	A	802	3	-	0/2/19/22	0/1/1/1
3	GLC	A	803	3	-	0/2/19/22	0/1/1/1
3	GLC	A	804	3	-	0/2/19/22	0/1/1/1
3	GLC	A	805	3	-	0/2/19/22	0/1/1/1
3	GLC	A	806	3	-	0/2/19/22	0/1/1/1
3	GLC	A	807	3	-	0/2/19/22	0/1/1/1
4	GLC	A	808	4	-	0/2/19/22	0/1/1/1
4	GLC	A	809	4	-	0/2/19/22	0/1/1/1
6	GLC	C	801	6	-	0/2/19/22	0/1/1/1
6	GLC	C	802	6	-	0/2/19/22	0/1/1/1
6	GLC	C	803	6	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GLC	D	801	7	-	0/2/19/22	0/1/1/1
7	GLC	D	802	7	-	0/2/19/22	0/1/1/1
7	GLC	D	803	7	-	0/2/19/22	0/1/1/1
7	GLC	D	804	7	-	0/2/19/22	0/1/1/1
7	GLC	D	806	7	-	0/2/19/22	0/1/1/1
7	GLC	D	807	7	-	0/2/19/22	0/1/1/1
7	GLC	D	808	7	-	0/2/19/22	0/1/1/1
7	GLC	D	809	7	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	GLC	C2-C3-C4	-2.75	106.37	111.04
7	D	804	GLC	C2-C3-C4	-2.52	106.77	111.04
4	A	809	GLC	O4-C4-C3	-2.09	105.63	110.34
3	A	802	GLC	O5-C1-C2	-2.08	107.49	110.86
4	A	809	GLC	C3-C4-C5	2.01	113.71	110.20
6	C	803	GLC	C1-C2-C3	2.14	112.08	109.54
7	D	807	GLC	C2-C3-C4	2.16	114.71	111.04
3	A	804	GLC	C1-O5-C5	2.27	115.13	112.25
3	A	803	GLC	C1-O5-C5	2.34	115.22	112.25
3	A	801	GLC	C1-O5-C5	2.39	115.28	112.25
3	A	802	GLC	C1-C2-C3	2.49	112.48	109.54
7	D	806	GLC	C1-O5-C5	2.54	115.47	112.25
4	A	809	GLC	O2-C2-C1	2.63	114.47	109.21
7	D	804	GLC	O2-C2-C1	2.65	114.52	109.21
4	A	808	GLC	C1-C2-C3	2.80	112.85	109.54
6	C	801	GLC	C1-O5-C5	2.87	115.90	112.25
6	C	801	GLC	C1-C2-C3	2.90	112.97	109.54
3	A	807	GLC	C1-C2-C3	2.90	112.97	109.54
7	D	807	GLC	C1-C2-C3	3.13	113.24	109.54
7	D	802	GLC	C1-C2-C3	3.53	113.72	109.54
3	A	802	GLC	C1-O5-C5	3.66	116.89	112.25
3	A	806	GLC	C1-O5-C5	3.72	116.97	112.25
7	D	809	GLC	C1-O5-C5	4.22	117.60	112.25
3	A	807	GLC	C1-O5-C5	4.52	117.99	112.25
7	D	808	GLC	C1-O5-C5	4.77	118.30	112.25
7	D	806	GLC	C1-C2-C3	5.59	116.16	109.54
4	A	809	GLC	C1-O5-C5	6.00	119.86	112.25
7	D	804	GLC	C1-O5-C5	6.59	120.62	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	GLC	2	0
4	A	808	GLC	2	0
4	A	809	GLC	1	0
6	C	801	GLC	1	0
6	C	802	GLC	1	0
6	C	803	GLC	2	0
7	D	802	GLC	1	0
7	D	803	GLC	1	0

5.6 Ligand geometry

9 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	PEG	A	1009	-	6,6,6	0.52	0	5,5,5	0.25	0
2	G6P	A	901	-	16,16,16	0.55	0	23,24,24	0.95	1 (4%)
5	PEG	B	1001	-	6,6,6	0.53	0	5,5,5	0.21	0
5	PEG	B	706	-	6,6,6	0.54	0	5,5,5	0.21	0
2	G6P	B	901	-	16,16,16	0.55	0	23,24,24	1.16	3 (13%)
2	G6P	B	902	-	16,16,16	0.68	0	23,24,24	1.56	3 (13%)
5	PEG	C	1004	-	6,6,6	0.55	0	5,5,5	0.14	0
2	G6P	C	901	-	16,16,16	0.53	0	23,24,24	0.94	1 (4%)
2	G6P	D	901	-	16,16,16	0.45	0	23,24,24	1.00	1 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PEG	A	1009	-	-	0/4/4/4	0/0/0/0
2	G6P	A	901	-	-	0/6/26/26	0/1/1/1
5	PEG	B	1001	-	-	0/4/4/4	0/0/0/0
5	PEG	B	706	-	-	0/4/4/4	0/0/0/0
2	G6P	B	901	-	-	0/6/26/26	0/1/1/1
2	G6P	B	902	-	-	0/6/26/26	0/1/1/1
5	PEG	C	1004	-	-	0/4/4/4	0/0/0/0
2	G6P	C	901	-	-	0/6/26/26	0/1/1/1
2	G6P	D	901	-	-	0/6/26/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	902	G6P	C3-C4-C5	-3.61	103.90	110.20
2	B	902	G6P	C4-C3-C2	-2.93	105.33	110.79
2	B	901	G6P	C1-C2-C3	-2.65	106.48	110.43
2	A	901	G6P	C1-C2-C3	-2.31	107.00	110.43
2	D	901	G6P	O6-P-O3P	-2.25	101.42	107.14
2	C	901	G6P	O6-P-O3P	-2.18	101.60	107.14
2	B	901	G6P	O6-P-O3P	-2.04	101.94	107.14
2	B	901	G6P	O5-C5-C6	2.39	111.50	106.61
2	B	902	G6P	O5-C5-C6	3.84	114.46	106.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	G6P	1	0
5	B	1001	PEG	2	0
2	B	901	G6P	1	0
2	C	901	G6P	1	0
2	D	901	G6P	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	638/725 (88%)	-0.00	10 (1%) 74 66	27, 58, 110, 124	0
1	B	638/725 (88%)	0.09	16 (2%) 61 48	38, 65, 110, 123	0
1	C	646/725 (89%)	0.16	22 (3%) 49 36	42, 70, 111, 126	0
1	D	636/725 (87%)	0.16	23 (3%) 46 34	32, 76, 127, 136	0
All	All	2558/2900 (88%)	0.10	71 (2%) 56 44	27, 66, 118, 136	0

All (71) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	627	GLY	6.3
1	D	624	GLU	5.1
1	D	625	LEU	4.1
1	D	630	LEU	4.1
1	C	62	ASP	3.8
1	A	71	ASP	3.6
1	B	125	LEU	3.6
1	C	206	SER	3.5
1	D	126	VAL	3.5
1	B	128	ILE	3.5
1	C	66	PRO	3.5
1	A	132	GLU	3.5
1	D	124	SER	3.4
1	D	636	ASP	3.4
1	A	631	ASN	3.3
1	D	629	GLU	3.2
1	C	79	ALA	3.2
1	C	69	PHE	3.1
1	B	111	VAL	3.1
1	A	637	ALA	3.1
1	B	124	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	106	PHE	3.0
1	C	647	ALA	3.0
1	C	159	SER	3.0
1	D	626	VAL	2.9
1	C	61	LEU	2.9
1	A	78	HIS	2.8
1	D	638	LEU	2.8
1	A	5	LEU	2.8
1	C	76	VAL	2.8
1	C	646	VAL	2.8
1	D	128	ILE	2.7
1	C	543	THR	2.7
1	A	90	PHE	2.7
1	D	122	LEU	2.7
1	C	483	ALA	2.6
1	B	126	VAL	2.6
1	B	130	SER	2.6
1	D	622	PHE	2.5
1	C	63	TRP	2.5
1	B	544	ASN	2.5
1	D	119	LYS	2.5
1	B	106	PHE	2.5
1	A	630	LEU	2.4
1	B	436	GLU	2.4
1	B	206	SER	2.4
1	C	227	ILE	2.4
1	C	92	TYR	2.4
1	A	628	GLU	2.4
1	D	628	GLU	2.4
1	C	78	HIS	2.4
1	D	225	PHE	2.4
1	B	108	LEU	2.3
1	D	226	GLY	2.3
1	C	67	GLU	2.3
1	D	633	SER	2.3
1	A	629	GLU	2.3
1	D	227	ILE	2.3
1	C	68	ALA	2.2
1	C	83	MET	2.2
1	D	6	GLN	2.2
1	D	67	GLU	2.2
1	B	141	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	103	VAL	2.1
1	B	545	GLN	2.1
1	B	116	ASN	2.1
1	C	157	LEU	2.1
1	D	621	GLN	2.0
1	D	631	ASN	2.0
1	C	545	GLN	2.0
1	B	66	PRO	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
3	GLC	A	801	11/12	0.84	0.32	6.80	61,70,74,76	0
4	GLC	A	809	11/12	0.85	0.25	3.05	60,62,69,69	0
6	GLC	C	802	11/12	0.91	0.23	0.12	108,110,113,113	0
7	GLC	D	804	11/12	0.91	0.20	0.09	46,56,60,63	0
3	GLC	A	802	11/12	0.92	0.18	-0.04	54,61,66,67	0
7	GLC	D	802	11/12	0.93	0.16	-0.04	58,63,69,75	0
6	GLC	C	801	11/12	0.70	0.23	-0.11	111,113,115,116	0
3	GLC	A	804	11/12	0.94	0.16	-0.84	64,65,71,75	0
3	GLC	A	803	11/12	0.96	0.15	-1.40	53,60,63,66	0
7	GLC	D	803	11/12	0.98	0.12	-1.64	49,53,56,56	0
7	GLC	D	809	11/12	0.90	0.18	-	66,71,75,77	0
7	GLC	D	807	11/12	0.91	0.23	-	65,71,75,80	0
7	GLC	D	808	11/12	0.94	0.20	-	57,60,65,69	0
3	GLC	A	800	1/12	0.57	0.47	-	76,76,76,76	0
7	GLC	D	806	11/12	0.82	0.36	-	84,94,99,99	0
3	GLC	A	805	11/12	0.92	0.21	-	68,77,83,86	0
7	GLC	D	805	1/12	0.82	0.18	-	52,52,52,52	0
7	GLC	D	801	11/12	0.89	0.31	-	78,85,87,87	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	GLC	D	810	1/12	0.73	0.27	-	78,78,78,78	0
4	GLC	A	808	11/12	0.86	0.32	-	66,71,75,75	0
3	GLC	A	807	11/12	0.83	0.23	-	70,80,85,86	0
3	GLC	A	806	11/12	0.92	0.23	-	76,82,87,88	0
4	GLC	A	810	1/12	0.85	0.28	-	64,64,64,64	0
6	GLC	C	804	1/12	0.96	0.18	-	105,105,105,105	0
6	GLC	C	803	11/12	0.86	0.18	-	103,106,109,110	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(\AA^2)	Q<0.9
2	G6P	B	902	16/16	0.90	0.19	0.59	78,83,88,89	0
5	PEG	B	706	7/7	0.89	0.21	0.48	51,56,63,63	0
2	G6P	C	901	16/16	0.97	0.19	0.46	46,50,52,52	0
2	G6P	A	901	16/16	0.99	0.18	0.22	34,36,41,43	0
5	PEG	A	1009	7/7	0.93	0.18	-0.66	58,60,62,62	0
2	G6P	B	901	16/16	0.98	0.17	-0.66	42,45,48,50	0
2	G6P	D	901	16/16	0.99	0.15	-1.11	35,37,40,41	0
5	PEG	C	1004	7/7	0.94	0.16	-2.06	48,51,58,60	0
5	PEG	B	1001	7/7	0.90	0.14	-2.13	50,52,55,55	0

6.5 Other polymers [i](#)

There are no such residues in this entry.