



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:00 AM UTC

PDB ID : 8R4G / pdb_00008r4g
Title : Plastidial phosphorylase Pho1 from Solanum tuberosum in complex with α-D-glucose
Authors : Koulas, S.M.; Leonidas, D.D.
Deposited on : 2023-11-13
Resolution : 3.10 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

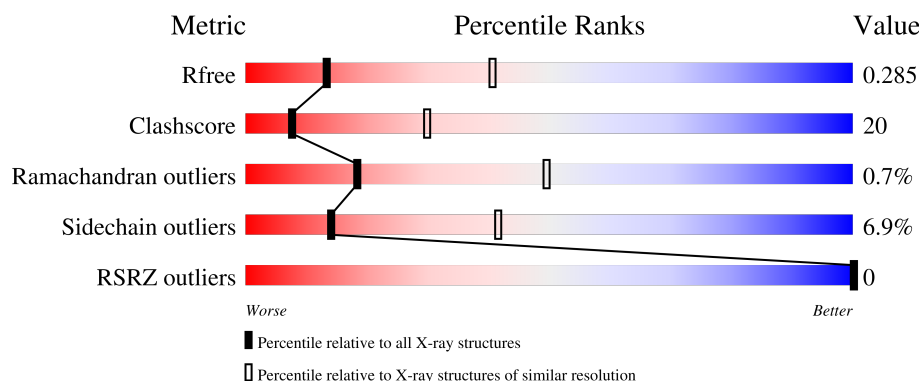
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. 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	916	
1	B	916	
1	C	916	

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	GOL	C	1002	-	-	X	-

2 Entry composition [i](#)

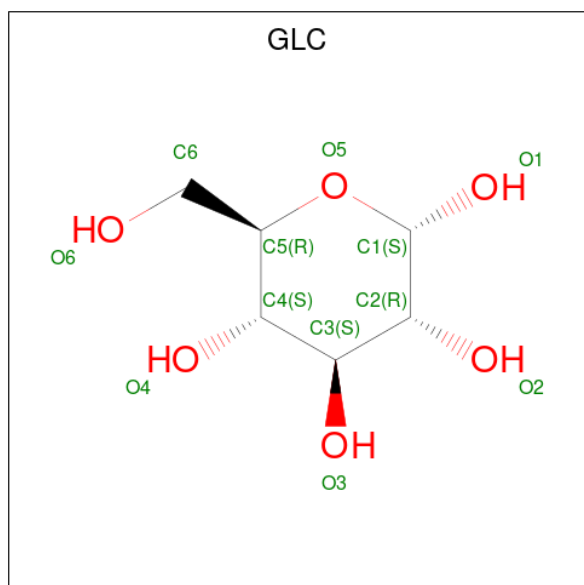
There are 4 unique types of molecules in this entry. The entry contains 20212 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/a myloplastic.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	830	Total	C	N	O	P	S	0	0	0
			6664	4258	1116	1264	1	25			
1	B	830	Total	C	N	O	P	S	0	0	0
			6664	4258	1116	1264	1	25			
1	C	830	Total	C	N	O	P	S	0	0	0
			6664	4258	1116	1264	1	25			

- Molecule 2 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



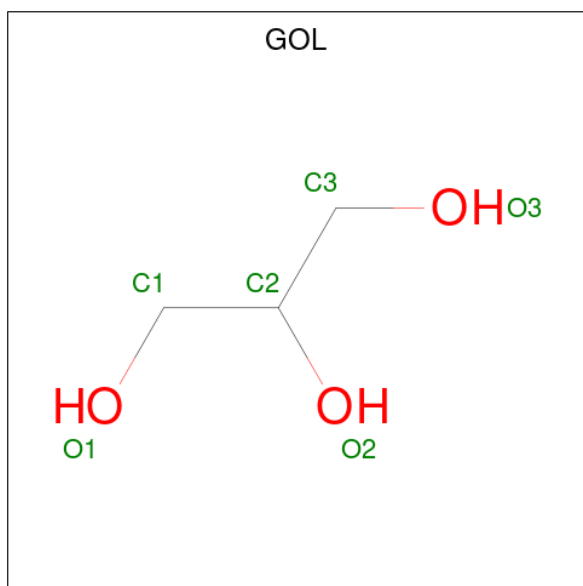
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

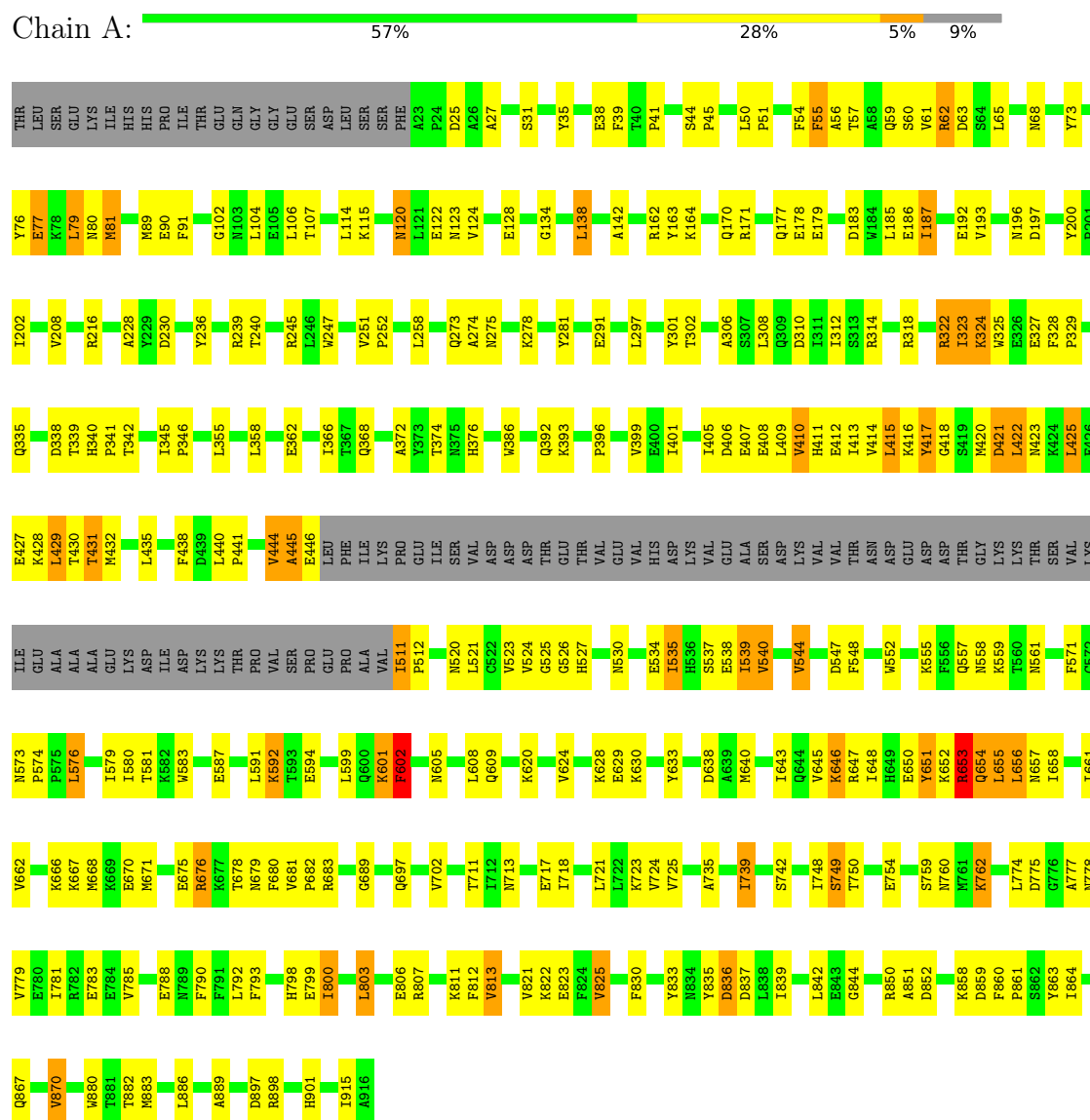
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	53	Total 53	O 53	0	0
4	B	36	Total 36	O 36	0	0
4	C	41	Total 41	O 41	0	0

3 Residue-property plots

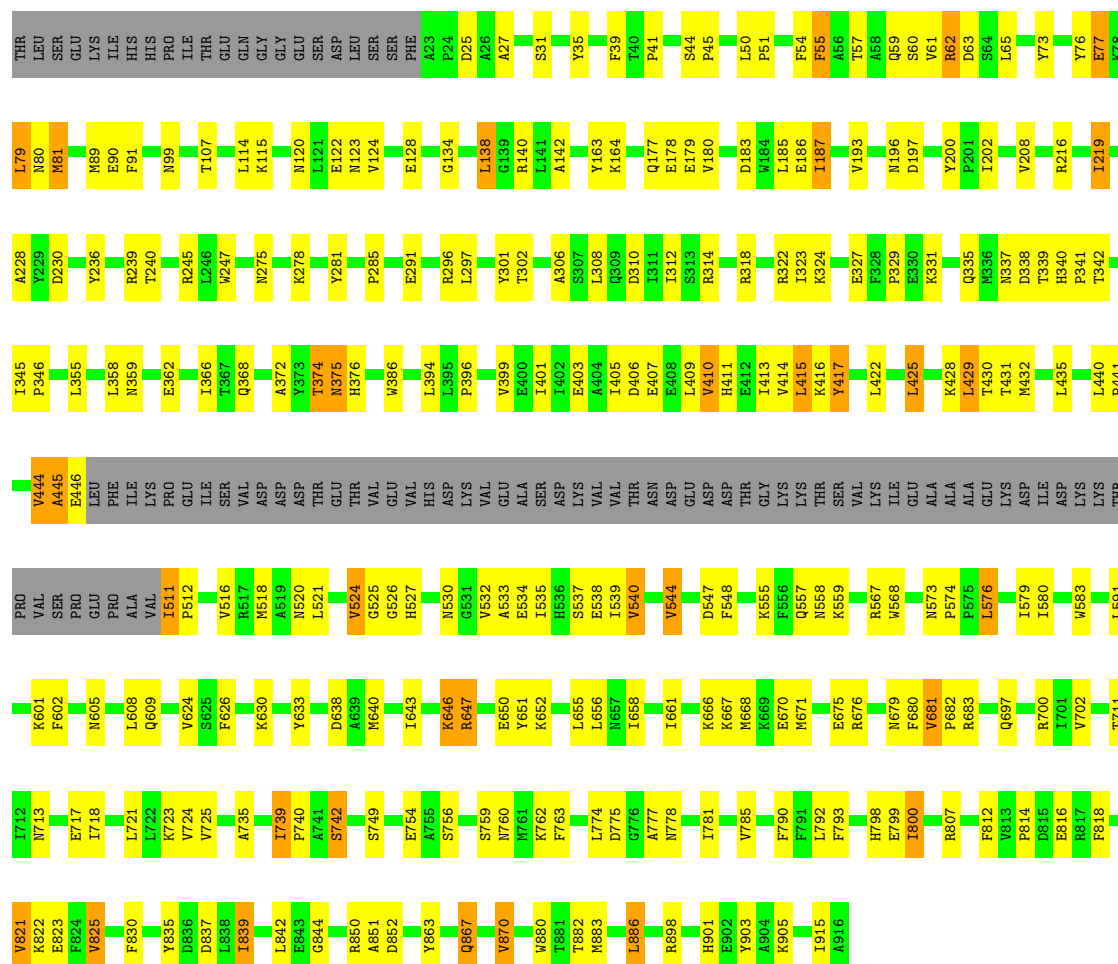
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/amyloplastic



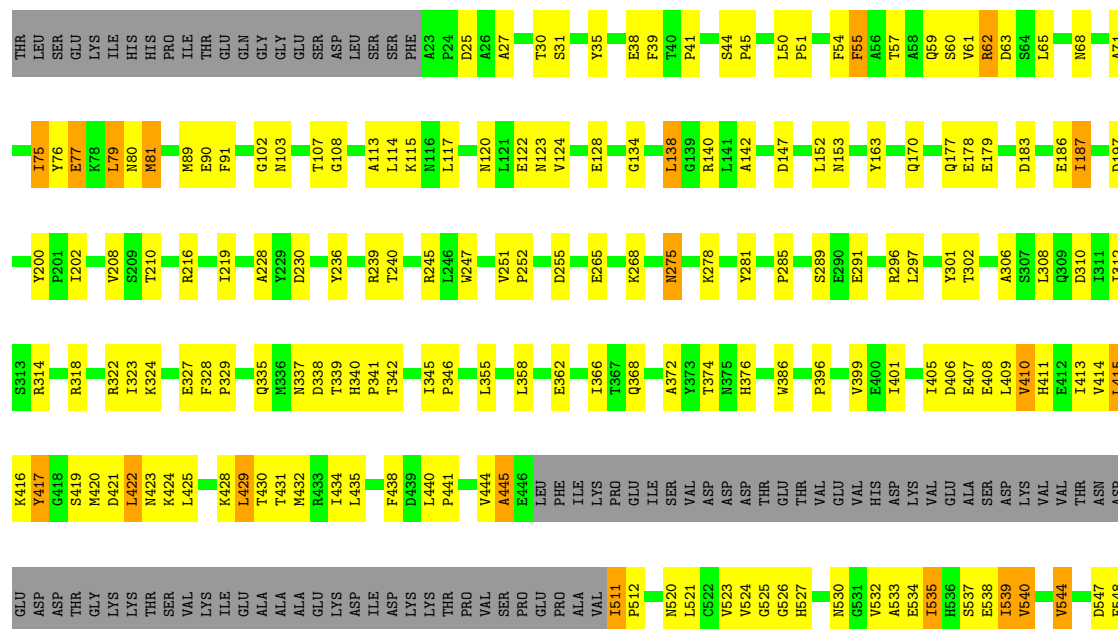
- Molecule 1: Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/amyloplastic

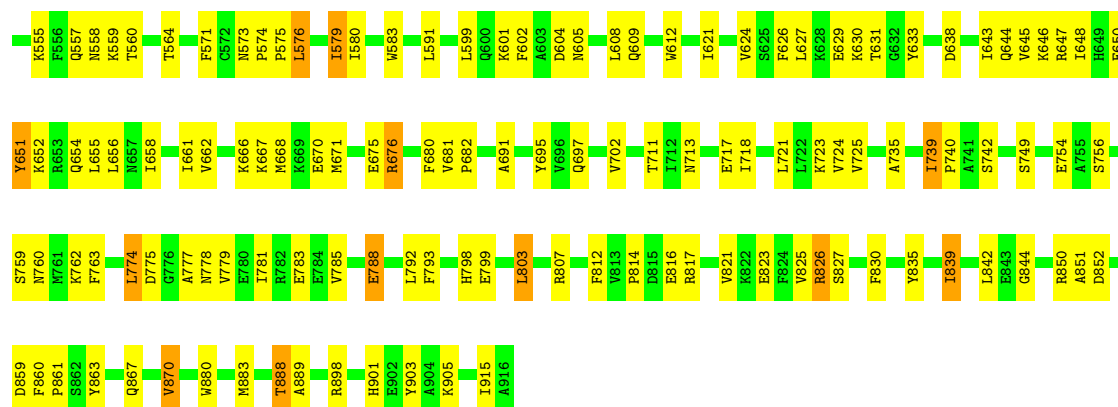




- Molecule 1: Alpha-1,4 glucan phosphorylase L-1 isozyme, chloroplastic/amyloplastic

Chain C: 58% 29% 9%





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	218.23Å 125.91Å 117.08Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	117.07 – 3.10 117.07 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.3 (117.07-3.10) 95.0 (117.07-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.235 , 0.286 0.236 , 0.285	Depositor DCC
R_{free} test set	2611 reflections (4.53%)	wwPDB-VP
Wilson B-factor (Å ²)	75.6	Xtriage
Anisotropy	0.044	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.008 for -1/2*h-3/2*k,-1/2*h+1/2*k,-l 0.002 for -1/2*h+3/2*k,1/2*h+1/2*k,-l 0.380 for 1/2*h-3/2*k,-1/2*h-1/2*k,-l 0.399 for 1/2*h+3/2*k,1/2*h-1/2*k,-l 0.009 for -h,-k,l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	20212	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.95% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.55	0/6790	1.11	10/9188 (0.1%)
1	B	0.55	0/6790	1.08	4/9188 (0.0%)
1	C	0.54	0/6790	1.09	5/9188 (0.1%)
All	All	0.55	0/20370	1.09	19/27564 (0.1%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	LYS	N-CA-C	-9.41	103.89	114.62
1	A	655	LEU	CA-C-N	-7.46	110.75	120.44
1	A	655	LEU	C-N-CA	-7.46	110.75	120.44
1	A	656	LEU	N-CA-C	-6.18	104.46	111.07
1	B	647	ARG	CB-CA-C	5.75	118.47	109.84
1	A	574	PRO	N-CA-C	5.64	117.58	110.70
1	C	574	PRO	N-CA-C	5.50	117.41	110.70
1	C	788	GLU	CB-CG-CD	5.41	121.79	112.60
1	B	816	GLU	CB-CG-CD	5.30	121.62	112.60
1	C	816	GLU	CB-CG-CD	5.30	121.61	112.60
1	C	275	ASN	CB-CA-C	5.19	119.61	110.37
1	A	788	GLU	CB-CG-CD	5.17	121.39	112.60
1	A	602	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	680	PHE	CB-CA-C	5.12	118.20	109.75
1	C	680	PHE	CB-CA-C	5.09	118.15	109.75
1	B	574	PRO	N-CA-C	5.04	116.85	110.70
1	A	421	ASP	CB-CA-C	5.03	119.12	111.02
1	A	680	PHE	CB-CA-C	5.03	118.33	110.19
1	A	689	GLY	CA-C-O	-5.00	118.72	122.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6664	0	6538	286	0
1	B	6664	0	6538	258	0
1	C	6664	0	6538	265	0
2	A	12	0	12	2	0
2	B	12	0	12	2	0
2	C	12	0	12	1	0
3	A	18	0	24	3	0
3	B	12	0	16	2	0
3	C	24	0	32	9	0
4	A	53	0	0	1	0
4	B	36	0	0	0	0
4	C	41	0	0	1	0
All	All	20212	0	19722	798	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 20.

All (798) 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:76:TYR:HA	1:C:81:MET:CE	1.66	1.26
1:B:76:TYR:HA	1:B:81:MET:CE	1.65	1.25
1:A:76:TYR:HA	1:A:81:MET:CE	1.66	1.24
1:B:432:MET:CE	1:B:547:ASP:HB3	1.68	1.22
1:C:432:MET:CE	1:C:547:ASP:HB3	1.68	1.22
1:A:432:MET:CE	1:A:547:ASP:HB3	1.70	1.20
1:A:655:LEU:HA	1:A:658:ILE:HG22	1.20	1.13
1:B:432:MET:HE3	1:B:547:ASP:HB3	1.25	1.12
1:C:108:GLY:H	3:C:1002:GOL:H12	1.09	1.11
1:C:108:GLY:H	3:C:1002:GOL:C1	1.62	1.11
1:C:432:MET:HE3	1:C:547:ASP:HB3	1.23	1.10
1:B:76:TYR:HA	1:B:81:MET:HE1	1.34	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:108:GLY:N	3:C:1002:GOL:H12	1.66	1.09
1:C:76:TYR:HA	1:C:81:MET:HE1	1.36	1.08
1:A:432:MET:HE3	1:A:547:ASP:HB3	1.26	1.05
1:A:76:TYR:HA	1:A:81:MET:HE1	1.36	1.04
1:B:671:MET:HE2	1:B:675:GLU:C	1.84	1.01
1:B:671:MET:HE2	1:B:676:ARG:N	1.76	0.99
1:B:76:TYR:CA	1:B:81:MET:HE1	1.97	0.94
1:C:108:GLY:CA	3:C:1002:GOL:H12	1.97	0.94
1:C:76:TYR:CA	1:C:81:MET:HE1	1.98	0.92
1:A:76:TYR:CA	1:A:81:MET:HE1	2.00	0.92
1:B:187:ILE:HD13	1:B:187:ILE:H	1.33	0.92
1:A:657:ASN:OD1	1:A:661:ILE:HD13	1.69	0.92
1:B:432:MET:HE2	1:B:547:ASP:HB3	1.52	0.91
1:A:187:ILE:HD12	1:A:187:ILE:H	1.33	0.89
1:A:432:MET:HE2	1:A:547:ASP:HB3	1.54	0.89
1:A:392:GLN:HB2	1:A:399:VAL:HG21	1.55	0.89
1:C:432:MET:HE2	1:C:547:ASP:HB3	1.53	0.88
1:B:668:MET:HE3	1:B:721:LEU:HD23	1.55	0.88
1:C:177:GLN:HE22	1:C:691:ALA:H	1.14	0.88
1:A:653:ARG:NH1	1:A:748:ILE:O	2.07	0.87
1:C:774:LEU:HD22	1:C:779:VAL:HG22	1.57	0.87
1:B:425:LEU:CD1	1:B:429:LEU:CD2	2.52	0.87
1:C:668:MET:HE3	1:C:721:LEU:HD23	1.56	0.87
1:C:652:LYS:HE2	1:C:754:GLU:OE2	1.75	0.87
1:C:76:TYR:CA	1:C:81:MET:CE	2.53	0.86
1:A:657:ASN:OD1	1:A:661:ILE:CD1	2.24	0.85
1:A:236:TYR:HD2	1:A:591:LEU:HD11	1.39	0.85
1:A:374:THR:HG22	1:A:376:HIS:CE1	2.11	0.85
1:A:432:MET:CE	1:A:547:ASP:CB	2.54	0.85
1:C:187:ILE:HD13	1:C:187:ILE:H	1.42	0.85
1:C:621:ILE:O	1:C:624:VAL:HG22	1.76	0.84
1:C:432:MET:CE	1:C:547:ASP:CB	2.54	0.84
1:A:432:MET:HE2	1:A:547:ASP:CB	2.07	0.84
1:A:676:ARG:HH12	1:A:717:GLU:HG2	1.41	0.84
1:A:374:THR:CG2	1:A:376:HIS:CE1	2.61	0.83
1:B:652:LYS:HE2	1:B:754:GLU:OE2	1.78	0.83
1:B:671:MET:CE	1:B:675:GLU:C	2.50	0.83
1:C:108:GLY:HA3	3:C:1002:GOL:H12	1.60	0.83
1:B:432:MET:CE	1:B:547:ASP:CB	2.55	0.82
1:B:425:LEU:CD1	1:B:429:LEU:HD21	2.10	0.82
1:A:76:TYR:CA	1:A:81:MET:CE	2.54	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:76:TYR:CA	1:B:81:MET:CE	2.53	0.82
1:A:656:LEU:HD21	1:A:863:TYR:CG	2.15	0.81
1:B:432:MET:HE2	1:B:547:ASP:CB	2.09	0.81
1:A:652:LYS:HE2	1:A:754:GLU:OE2	1.79	0.81
1:A:671:MET:HB2	1:A:675:GLU:HG3	1.63	0.81
1:C:826:ARG:HG2	1:C:826:ARG:HH11	1.46	0.80
1:A:668:MET:HE3	1:A:721:LEU:HD23	1.64	0.79
1:C:30:THR:HG23	1:C:117:LEU:HD21	1.63	0.79
1:C:671:MET:HB2	1:C:675:GLU:HG3	1.64	0.79
1:A:648:ILE:HD13	1:A:654:GLN:NE2	1.98	0.79
1:C:71:ALA:O	1:C:75:ILE:HD13	1.83	0.79
1:C:432:MET:HE2	1:C:547:ASP:CB	2.10	0.78
1:A:392:GLN:HG3	1:A:392:GLN:O	1.82	0.78
1:B:671:MET:HB2	1:B:675:GLU:HG3	1.66	0.78
1:B:297:LEU:HD12	1:B:394:LEU:HD23	1.66	0.77
1:C:170:GLN:HE21	1:C:177:GLN:HE21	1.30	0.77
1:B:425:LEU:HD13	1:B:429:LEU:CD2	2.14	0.76
1:C:76:TYR:CB	1:C:81:MET:HE1	2.16	0.76
1:C:77:GLU:OE1	1:C:77:GLU:HA	1.84	0.76
1:B:406:ASP:CG	1:B:435:LEU:HD12	2.10	0.76
1:B:583:TRP:HE3	1:B:602:PHE:CD2	2.04	0.76
1:C:406:ASP:CG	1:C:435:LEU:HD12	2.11	0.75
1:A:77:GLU:OE1	1:A:77:GLU:HA	1.87	0.75
1:A:678:THR:HG22	1:A:679:ASN:H	1.51	0.75
1:B:76:TYR:CB	1:B:81:MET:HE1	2.16	0.75
1:B:77:GLU:HA	1:B:77:GLU:OE1	1.87	0.75
1:C:656:LEU:HD21	1:C:863:TYR:CG	2.23	0.74
1:B:650:GLU:OE2	1:B:697:GLN:HG2	1.87	0.74
1:A:656:LEU:HD21	1:A:863:TYR:CD2	2.23	0.74
1:A:236:TYR:CD2	1:A:591:LEU:HD11	2.22	0.73
1:A:421:ASP:O	1:A:423:ASN:N	2.21	0.73
1:B:656:LEU:HD21	1:B:863:TYR:CG	2.23	0.73
1:C:650:GLU:OE2	1:C:697:GLN:HG2	1.87	0.73
1:A:650:GLU:OE2	1:A:697:GLN:HG2	1.88	0.73
1:B:374:THR:HG22	1:B:376:HIS:CD2	2.23	0.73
1:A:76:TYR:CB	1:A:81:MET:HE1	2.18	0.73
1:C:345:ILE:HB	1:C:346:PRO:HD3	1.71	0.72
1:C:421:ASP:O	1:C:423:ASN:N	2.22	0.72
1:B:511:ILE:HG12	1:B:512:PRO:HD2	1.71	0.72
1:B:583:TRP:HE3	1:B:602:PHE:HD2	1.37	0.72
1:A:39:PHE:C	1:A:41:PRO:HD3	2.15	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:ARG:HH12	3:A:1002:GOL:H2	1.53	0.72
1:B:867:GLN:HE21	1:B:867:GLN:HA	1.53	0.72
1:A:655:LEU:HA	1:A:658:ILE:CG2	2.11	0.71
1:C:39:PHE:C	1:C:41:PRO:HD3	2.14	0.71
1:C:411:HIS:O	1:C:415:LEU:HD22	1.90	0.71
1:A:646:LYS:HD3	1:A:652:LYS:HD2	1.72	0.71
1:B:230:ASP:OD1	1:B:245:ARG:HG2	1.91	0.71
1:C:230:ASP:OD1	1:C:245:ARG:HG2	1.91	0.71
1:C:187:ILE:H	1:C:187:ILE:CD1	2.02	0.70
1:B:39:PHE:C	1:B:41:PRO:HD3	2.16	0.70
1:A:76:TYR:HA	1:A:81:MET:HE2	1.73	0.70
1:C:374:THR:HG22	1:C:376:HIS:CD2	2.27	0.70
1:A:230:ASP:OD1	1:A:245:ARG:HG2	1.92	0.70
1:A:535:ILE:O	1:A:539:ILE:HD12	1.92	0.69
1:C:612:TRP:HH2	1:C:888:THR:HG21	1.56	0.69
1:C:627:LEU:O	1:C:631:THR:CG2	2.41	0.69
1:C:108:GLY:H	3:C:1002:GOL:H11	1.52	0.69
1:A:427:GLU:OE2	1:A:431:THR:HG21	1.93	0.68
1:A:628:LYS:HG3	1:C:788:GLU:HG3	1.75	0.68
1:B:652:LYS:CE	1:B:754:GLU:OE2	2.41	0.68
1:A:683:ARG:NH1	1:A:867:GLN:OE1	2.25	0.68
1:A:656:LEU:CD2	1:A:863:TYR:CD2	2.77	0.68
1:B:76:TYR:HA	1:B:81:MET:HE2	1.73	0.68
1:A:322:ARG:O	1:A:322:ARG:HG3	1.92	0.68
1:C:535:ILE:O	1:C:539:ILE:HD12	1.93	0.68
1:C:652:LYS:CE	1:C:754:GLU:OE2	2.41	0.68
1:C:792:LEU:HD23	1:C:793:PHE:N	2.09	0.68
1:C:76:TYR:HA	1:C:81:MET:HE2	1.72	0.68
1:A:792:LEU:HD23	1:A:793:PHE:N	2.08	0.68
1:A:652:LYS:CE	1:A:754:GLU:OE2	2.41	0.67
1:A:882:THR:O	1:A:886:LEU:HD23	1.95	0.67
1:A:411:HIS:O	1:A:415:LEU:HD22	1.95	0.67
1:A:196:ASN:CG	1:B:187:ILE:HG22	2.20	0.66
1:B:656:LEU:C	1:B:656:LEU:HD23	2.20	0.66
1:B:792:LEU:HD23	1:B:793:PHE:N	2.09	0.66
1:B:410:VAL:HG12	1:B:429:LEU:HD12	1.78	0.66
1:B:540:VAL:HA	1:B:544:VAL:HG23	1.78	0.66
1:B:342:THR:HG22	1:B:521:LEU:HD23	1.77	0.66
1:B:432:MET:HE2	1:B:547:ASP:C	2.20	0.66
1:C:656:LEU:HD23	1:C:656:LEU:C	2.20	0.66
1:A:432:MET:HE2	1:A:547:ASP:C	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:882:THR:O	1:A:886:LEU:CD2	2.44	0.66
1:B:89:MET:HE3	1:B:163:TYR:OH	1.96	0.66
1:B:676:ARG:HH12	1:B:717:GLU:HG2	1.61	0.65
1:B:411:HIS:O	1:B:415:LEU:HD22	1.96	0.65
1:A:656:LEU:C	1:A:656:LEU:HD23	2.21	0.65
1:C:676:ARG:HH12	1:C:717:GLU:HG2	1.61	0.65
1:C:35:TYR:CD1	1:C:39:PHE:HD2	2.14	0.65
1:C:89:MET:HE3	1:C:163:TYR:OH	1.97	0.65
1:A:89:MET:HE3	1:A:163:TYR:OH	1.96	0.65
1:A:374:THR:CG2	1:A:376:HIS:HE1	2.09	0.65
1:A:668:MET:HE2	1:A:718:ILE:HD12	1.78	0.65
1:B:219:ILE:HD13	1:B:219:ILE:H	1.61	0.65
1:C:601:LYS:HE2	1:C:602:PHE:CE2	2.31	0.65
1:C:432:MET:HE2	1:C:547:ASP:C	2.22	0.65
1:A:540:VAL:HA	1:A:544:VAL:HG23	1.79	0.64
1:C:342:THR:HG22	1:C:521:LEU:HD23	1.79	0.64
1:C:627:LEU:O	1:C:631:THR:HG23	1.97	0.64
1:A:735:ALA:O	1:A:739:ILE:HG13	1.98	0.64
1:B:77:GLU:OE1	1:B:318:ARG:HG2	1.96	0.64
1:B:425:LEU:HD12	1:B:429:LEU:CD2	2.28	0.64
1:C:210:THR:H	3:C:1004:GOL:H31	1.62	0.64
1:A:35:TYR:CD1	1:A:39:PHE:HD2	2.15	0.64
1:A:432:MET:HB3	1:A:548:PHE:CZ	2.32	0.64
1:B:882:THR:O	1:B:886:LEU:HD23	1.98	0.64
1:C:774:LEU:HD13	1:C:774:LEU:C	2.23	0.64
1:B:187:ILE:HD13	1:B:187:ILE:N	2.10	0.64
1:B:882:THR:O	1:B:886:LEU:CD2	2.45	0.64
1:B:520:ASN:O	1:B:524:VAL:HG13	1.96	0.64
1:A:77:GLU:OE1	1:A:318:ARG:HG2	1.96	0.64
1:C:410:VAL:HG12	1:C:429:LEU:HD12	1.80	0.64
1:B:432:MET:HB3	1:B:548:PHE:CZ	2.33	0.64
1:B:35:TYR:CD1	1:B:39:PHE:HD2	2.16	0.63
1:B:99:ASN:ND2	1:B:567:ARG:NH1	2.46	0.63
1:C:432:MET:HB3	1:C:548:PHE:CZ	2.33	0.63
1:A:821:VAL:O	1:A:825:VAL:HG12	1.98	0.63
1:B:410:VAL:HG12	1:B:429:LEU:CD1	2.29	0.63
1:C:668:MET:HE2	1:C:718:ILE:HD12	1.79	0.63
1:A:342:THR:HG22	1:A:521:LEU:HD23	1.78	0.63
1:B:583:TRP:CE3	1:B:602:PHE:HD2	2.15	0.63
1:C:540:VAL:HA	1:C:544:VAL:HG23	1.81	0.63
1:C:77:GLU:OE1	1:C:318:ARG:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:671:MET:HE2	1:B:676:ARG:CA	2.28	0.63
1:B:821:VAL:O	1:B:825:VAL:HG12	1.99	0.62
1:C:575:PRO:O	1:C:579:ILE:HD12	1.98	0.62
1:C:612:TRP:CH2	1:C:888:THR:HG21	2.34	0.62
1:A:410:VAL:HG12	1:A:429:LEU:CD1	2.29	0.62
1:A:652:LYS:O	1:A:653:ARG:HB2	1.99	0.62
1:A:410:VAL:HG12	1:A:429:LEU:HD12	1.80	0.62
1:C:177:GLN:HB2	1:C:702:VAL:HG11	1.81	0.62
1:C:648:ILE:HA	1:C:654:GLN:NE2	2.15	0.62
1:A:104:LEU:O	1:A:106:LEU:HD13	1.99	0.61
1:A:407:GLU:HG3	1:A:441:PRO:HG2	1.83	0.61
1:B:668:MET:HE2	1:B:718:ILE:HD12	1.81	0.61
1:C:410:VAL:HG12	1:C:429:LEU:CD1	2.30	0.61
1:A:89:MET:HG2	1:A:340:HIS:CB	2.30	0.61
1:B:425:LEU:HD12	1:B:429:LEU:HD23	1.82	0.61
1:B:516:VAL:HG12	1:B:518:MET:HE3	1.82	0.61
1:A:676:ARG:HH12	1:A:717:GLU:CG	2.13	0.61
1:B:240:THR:OG1	1:B:915:ILE:HD13	2.01	0.61
1:A:208:VAL:HG12	1:A:216:ARG:CZ	2.31	0.60
1:B:89:MET:HG2	1:B:340:HIS:CB	2.31	0.60
1:C:89:MET:HG2	1:C:340:HIS:CB	2.31	0.60
1:C:560:THR:O	1:C:898:ARG:NH2	2.34	0.60
1:B:407:GLU:HG3	1:B:441:PRO:HG2	1.82	0.60
1:B:425:LEU:CD1	1:B:429:LEU:HD23	2.30	0.60
1:B:177:GLN:HB2	1:B:702:VAL:HG11	1.84	0.60
1:B:573:ASN:CG	1:B:576:LEU:HB2	2.27	0.60
1:A:104:LEU:O	1:A:106:LEU:CD1	2.50	0.60
1:B:345:ILE:HD13	1:B:525:GLY:HA3	1.83	0.60
1:C:177:GLN:NE2	1:C:691:ALA:H	1.93	0.60
1:C:345:ILE:HD13	1:C:525:GLY:HA3	1.83	0.60
1:A:240:THR:OG1	1:A:915:ILE:HD13	2.02	0.60
1:A:653:ARG:NH1	1:A:749:SER:C	2.59	0.60
1:B:208:VAL:HG12	1:B:216:ARG:CZ	2.32	0.60
1:A:345:ILE:HD13	1:A:525:GLY:HA3	1.84	0.60
1:A:620:LYS:O	1:A:624:VAL:HG23	2.01	0.60
1:C:208:VAL:HG12	1:C:216:ARG:CZ	2.31	0.60
1:C:240:THR:OG1	1:C:915:ILE:HD13	2.02	0.60
1:B:526:GLY:O	1:B:555:LYS:HE3	2.02	0.60
1:B:668:MET:HE3	1:B:721:LEU:CD2	2.30	0.59
1:A:573:ASN:CG	1:A:576:LEU:HB2	2.27	0.59
1:C:573:ASN:CG	1:C:576:LEU:HB2	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:526:GLY:O	1:A:555:LYS:HE3	2.02	0.59
1:A:653:ARG:HH11	1:A:653:ARG:CG	2.15	0.59
1:B:120:ASN:HD21	1:B:122:GLU:HG2	1.67	0.59
1:B:867:GLN:HA	1:B:867:GLN:NE2	2.18	0.59
1:B:183:ASP:HB2	1:B:186:GLU:HG3	1.83	0.59
1:B:671:MET:HE1	1:B:675:GLU:O	2.02	0.59
1:C:526:GLY:O	1:C:555:LYS:HE3	2.03	0.59
1:C:668:MET:HE3	1:C:721:LEU:CD2	2.31	0.59
1:B:375:ASN:O	1:B:376:HIS:HB2	2.01	0.59
1:B:683:ARG:HH12	1:B:867:GLN:NE2	2.00	0.59
1:C:676:ARG:NH1	1:C:717:GLU:HG2	2.17	0.59
1:B:568:TRP:CE3	1:B:762:LLP:HG3	2.37	0.58
1:B:676:ARG:NH1	1:B:717:GLU:HG2	2.18	0.58
1:C:645:VAL:C	1:C:646:LYS:HG3	2.28	0.58
1:B:54:PHE:HA	1:B:124:VAL:HG13	1.86	0.58
1:B:285:PRO:O	1:B:296:ARG:NH1	2.36	0.58
1:B:322:ARG:HG3	1:B:322:ARG:O	2.04	0.58
1:B:425:LEU:O	1:B:429:LEU:HD23	2.03	0.58
1:C:407:GLU:HG3	1:C:441:PRO:HG2	1.86	0.58
1:C:774:LEU:HD13	1:C:774:LEU:O	2.04	0.58
1:C:844:GLY:O	1:C:851:ALA:HA	2.03	0.58
1:B:671:MET:CE	1:B:675:GLU:O	2.51	0.58
1:A:323:ILE:HD13	1:A:323:ILE:C	2.29	0.58
1:A:62:ARG:O	1:A:65:LEU:N	2.37	0.58
1:A:183:ASP:HB2	1:A:186:GLU:HG3	1.85	0.58
1:B:62:ARG:O	1:B:65:LEU:N	2.36	0.58
1:B:583:TRP:CE3	1:B:602:PHE:CD2	2.89	0.58
1:B:682:PRO:HA	1:B:721:LEU:O	2.04	0.58
1:A:653:ARG:NH1	1:A:653:ARG:HG3	2.18	0.58
1:A:653:ARG:HG3	1:A:748:ILE:O	2.04	0.58
1:A:643:ILE:HD12	1:A:742:SER:HB3	1.87	0.57
1:A:844:GLY:O	1:A:851:ALA:HA	2.03	0.57
1:C:62:ARG:O	1:C:65:LEU:N	2.37	0.57
1:B:844:GLY:O	1:B:851:ALA:HA	2.04	0.57
1:C:682:PRO:HA	1:C:721:LEU:O	2.04	0.57
1:A:236:TYR:CD2	1:A:591:LEU:CD1	2.87	0.57
1:A:417:TYR:CE2	1:A:428:LYS:HD2	2.39	0.57
1:A:592:LYS:HD2	1:A:594:GLU:OE1	2.05	0.57
1:A:676:ARG:NH1	1:A:717:GLU:HG2	2.16	0.57
1:B:759:SER:HA	1:B:762:LLP:HE3	1.85	0.57
1:C:511:ILE:HG12	1:C:512:PRO:HD2	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:PHE:HA	1:A:124:VAL:HG13	1.86	0.57
1:A:177:GLN:HB2	1:A:702:VAL:HG11	1.87	0.57
1:B:76:TYR:HA	1:B:81:MET:HE3	1.78	0.57
1:C:322:ARG:O	1:C:322:ARG:HG3	2.05	0.57
1:A:90:GLU:OE2	1:A:138:LEU:HD23	2.04	0.57
1:B:90:GLU:OE2	1:B:138:LEU:HD23	2.05	0.57
1:B:822:LYS:O	1:B:825:VAL:HG13	2.05	0.57
1:C:90:GLU:OE2	1:C:138:LEU:HD23	2.05	0.57
1:C:647:ARG:NH2	2:C:1001:GLC:O1	2.37	0.57
1:C:120:ASN:HD21	1:C:122:GLU:HG2	1.69	0.56
1:C:285:PRO:O	1:C:296:ARG:NH1	2.37	0.56
1:A:557:GLN:HE21	1:A:559:LYS:HE2	1.69	0.56
1:A:629:GLU:HG3	1:A:630:LYS:HG2	1.86	0.56
1:C:152:LEU:HD13	1:C:901:HIS:CD2	2.40	0.56
1:A:76:TYR:HA	1:A:81:MET:HE3	1.78	0.56
1:A:682:PRO:HA	1:A:721:LEU:O	2.05	0.56
1:A:401:ILE:O	1:A:405:ILE:HG13	2.06	0.56
1:B:867:GLN:O	1:B:870:VAL:HG22	2.06	0.56
1:C:54:PHE:HA	1:C:124:VAL:HG13	1.87	0.56
1:C:643:ILE:HD12	1:C:742:SER:HB3	1.88	0.56
1:A:441:PRO:HB2	4:A:1102:HOH:O	2.05	0.56
1:C:68:ASN:ND2	1:C:239:ARG:CZ	2.69	0.56
1:C:425:LEU:O	1:C:429:LEU:HD23	2.06	0.56
1:A:44:SER:HB2	1:A:45:PRO:HD2	1.87	0.56
1:B:446:GLU:N	1:B:446:GLU:OE1	2.37	0.56
1:A:68:ASN:ND2	1:A:239:ARG:CZ	2.69	0.56
1:C:401:ILE:O	1:C:405:ILE:HG13	2.06	0.56
1:C:523:VAL:O	1:C:555:LYS:NZ	2.27	0.56
1:A:374:THR:HG21	1:A:376:HIS:CE1	2.41	0.55
1:A:867:GLN:O	1:A:870:VAL:HG22	2.06	0.55
1:B:401:ILE:O	1:B:405:ILE:HG13	2.06	0.55
1:B:867:GLN:HE21	1:B:867:GLN:CA	2.12	0.55
1:C:114:LEU:HD22	1:C:124:VAL:HG21	1.88	0.55
1:C:297:LEU:HD13	1:C:386:TRP:CE2	2.42	0.55
1:C:627:LEU:O	1:C:631:THR:HG22	2.07	0.55
1:A:425:LEU:O	1:A:429:LEU:HD23	2.06	0.55
1:C:80:ASN:ND2	1:C:318:ARG:HB3	2.22	0.55
1:A:602:PHE:O	1:A:608:LEU:HD23	2.05	0.55
1:C:867:GLN:O	1:C:870:VAL:HG22	2.07	0.55
1:B:114:LEU:HD22	1:B:124:VAL:HG21	1.89	0.55
1:C:90:GLU:CD	1:C:138:LEU:HD23	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:LEU:HD13	1:A:386:TRP:CE2	2.42	0.55
1:A:520:ASN:ND2	1:A:548:PHE:HE2	2.05	0.55
1:C:803:LEU:N	1:C:803:LEU:HD23	2.22	0.55
1:A:138:LEU:HD12	1:A:376:HIS:HD2	1.71	0.54
1:B:44:SER:HB2	1:B:45:PRO:HD2	1.88	0.54
1:B:739:ILE:HD13	1:B:763:PHE:CE1	2.42	0.54
1:A:114:LEU:HD22	1:A:124:VAL:HG21	1.88	0.54
1:B:538:GLU:OE1	1:B:538:GLU:HA	2.08	0.54
1:A:41:PRO:HG2	1:B:193:VAL:CG1	2.38	0.54
1:A:374:THR:HG21	1:A:376:HIS:HE1	1.72	0.54
1:A:668:MET:HE3	1:A:721:LEU:CD2	2.37	0.54
1:B:90:GLU:CD	1:B:138:LEU:HD23	2.32	0.54
1:A:230:ASP:OD1	1:A:245:ARG:CG	2.56	0.54
1:A:193:VAL:HG13	1:B:41:PRO:HG2	1.88	0.54
1:A:822:LYS:O	1:A:825:VAL:HG13	2.07	0.54
1:B:335:GLN:OE1	1:B:372:ALA:HB3	2.08	0.54
1:B:359:ASN:OD1	1:B:359:ASN:C	2.50	0.54
1:A:897:ASP:O	1:A:901:HIS:HD2	1.90	0.54
1:A:511:ILE:HG12	1:A:512:PRO:HD2	1.90	0.54
1:A:335:GLN:OE1	1:A:372:ALA:HB3	2.08	0.54
1:A:601:LYS:O	1:A:602:PHE:CG	2.60	0.54
1:A:835:TYR:O	1:A:836:ASP:C	2.50	0.54
1:B:342:THR:CG2	1:B:521:LEU:HD23	2.38	0.53
1:C:170:GLN:NE2	1:C:177:GLN:HE21	2.02	0.53
1:C:579:ILE:O	1:C:583:TRP:HD1	1.91	0.53
1:B:200:TYR:OH	1:B:310:ASP:HA	2.09	0.53
1:C:739:ILE:HB	1:C:740:PRO:HD3	1.90	0.53
1:A:193:VAL:CG1	1:B:41:PRO:HG2	2.38	0.53
1:A:200:TYR:OH	1:A:310:ASP:HA	2.09	0.53
1:C:335:GLN:OE1	1:C:372:ALA:HB3	2.09	0.53
1:C:668:MET:CE	1:C:721:LEU:HD23	2.34	0.53
1:A:523:VAL:O	1:A:555:LYS:NZ	2.27	0.53
1:B:668:MET:CE	1:B:721:LEU:HD23	2.35	0.53
1:C:538:GLU:OE1	1:C:538:GLU:HA	2.08	0.53
1:B:76:TYR:CG	1:B:81:MET:HE1	2.44	0.53
1:A:413:ILE:O	1:A:416:LYS:O	2.25	0.53
1:A:538:GLU:OE1	1:A:538:GLU:HA	2.09	0.53
1:C:557:GLN:HE21	1:C:559:LYS:HE2	1.73	0.53
1:C:739:ILE:HD13	1:C:763:PHE:CE1	2.44	0.53
1:A:187:ILE:H	1:A:187:ILE:CD1	2.11	0.53
1:A:446:GLU:OE1	1:A:446:GLU:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:PRO:HG2	1:B:193:VAL:HG13	1.90	0.53
1:A:342:THR:CG2	1:A:521:LEU:HD23	2.38	0.53
1:A:803:LEU:N	1:A:803:LEU:HD23	2.23	0.53
1:B:230:ASP:OD1	1:B:245:ARG:CG	2.56	0.53
1:C:183:ASP:HB2	1:C:186:GLU:HG3	1.90	0.53
1:C:200:TYR:OH	1:C:310:ASP:HA	2.08	0.53
1:A:653:ARG:NH1	1:A:653:ARG:CG	2.72	0.52
1:C:76:TYR:HA	1:C:81:MET:HE3	1.78	0.52
1:B:236:TYR:HD2	1:B:591:LEU:HD21	1.74	0.52
1:C:413:ILE:O	1:C:416:LYS:O	2.28	0.52
1:C:775:ASP:O	1:C:778:ASN:HB2	2.09	0.52
1:A:573:ASN:HD21	1:A:576:LEU:HD23	1.74	0.52
1:B:643:ILE:HD12	1:B:742:SER:HB3	1.91	0.52
1:C:230:ASP:OD1	1:C:245:ARG:CG	2.56	0.52
1:A:656:LEU:CD2	1:A:863:TYR:CG	2.90	0.52
1:A:80:ASN:ND2	1:A:318:ARG:HB3	2.24	0.52
1:B:425:LEU:O	1:B:429:LEU:CD2	2.58	0.52
1:C:342:THR:CG2	1:C:521:LEU:HD23	2.39	0.52
1:C:76:TYR:CG	1:C:81:MET:HE1	2.45	0.52
1:A:407:GLU:HA	1:A:410:VAL:HG22	1.91	0.52
1:B:573:ASN:HD21	1:B:576:LEU:HD23	1.75	0.52
1:C:50:LEU:HD11	1:C:123:ASN:HB3	1.92	0.52
1:C:626:PHE:CE1	1:C:630:LYS:HG3	2.45	0.52
1:A:417:TYR:CE2	1:A:428:LYS:CD	2.93	0.52
1:A:668:MET:CE	1:A:721:LEU:HD23	2.36	0.52
1:A:798:HIS:CE1	1:A:799:GLU:HG3	2.45	0.52
1:C:417:TYR:CE2	1:C:428:LYS:CD	2.92	0.52
1:C:425:LEU:O	1:C:429:LEU:CD2	2.58	0.52
1:A:775:ASP:O	1:A:778:ASN:HB2	2.10	0.52
1:C:251:VAL:HG22	1:C:252:PRO:HD2	1.92	0.52
1:A:50:LEU:HD11	1:A:123:ASN:HB3	1.91	0.51
1:B:413:ILE:O	1:B:416:LYS:O	2.28	0.51
1:B:579:ILE:O	1:B:583:TRP:HD1	1.92	0.51
1:B:775:ASP:O	1:B:778:ASN:HB2	2.09	0.51
1:A:601:LYS:O	1:A:602:PHE:CB	2.58	0.51
1:A:803:LEU:HD13	1:A:858:LYS:HE3	1.92	0.51
1:B:842:LEU:HA	1:B:852:ASP:HB2	1.90	0.51
1:A:444:VAL:O	1:A:445:ALA:HB2	2.10	0.51
1:B:50:LEU:HD11	1:B:123:ASN:HB3	1.92	0.51
1:B:407:GLU:HA	1:B:410:VAL:HG22	1.91	0.51
1:A:579:ILE:O	1:A:583:TRP:HD1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:ILE:CD1	1:A:654:GLN:NE2	2.70	0.51
1:B:711:THR:HG21	1:B:830:PHE:HA	1.92	0.51
1:C:605:ASN:O	1:C:609:GLN:HG3	2.11	0.51
1:A:368:GLN:O	1:A:527:HIS:HB3	2.11	0.51
1:A:520:ASN:O	1:A:524:VAL:HG23	2.11	0.51
1:A:605:ASN:O	1:A:609:GLN:HG3	2.10	0.51
1:C:573:ASN:HD21	1:C:576:LEU:HD23	1.74	0.51
1:A:520:ASN:ND2	1:A:548:PHE:CE2	2.79	0.51
1:B:417:TYR:CE2	1:B:428:LYS:CD	2.93	0.51
1:C:711:THR:HG21	1:C:830:PHE:HA	1.93	0.51
1:A:120:ASN:HD21	1:A:122:GLU:HG2	1.75	0.51
1:A:251:VAL:HG22	1:A:252:PRO:HD2	1.93	0.51
1:B:297:LEU:HD23	1:B:386:TRP:CE2	2.45	0.51
1:C:44:SER:HB2	1:C:45:PRO:HD2	1.91	0.51
1:B:605:ASN:O	1:B:609:GLN:HG3	2.11	0.51
1:A:76:TYR:CG	1:A:81:MET:HE1	2.45	0.51
1:A:425:LEU:O	1:A:429:LEU:CD2	2.59	0.51
1:C:520:ASN:O	1:C:524:VAL:HG23	2.11	0.51
1:B:297:LEU:HD12	1:B:394:LEU:CD2	2.39	0.50
1:C:798:HIS:CE1	1:C:799:GLU:HG3	2.46	0.50
1:B:539:ILE:HG22	1:B:544:VAL:CG2	2.40	0.50
1:C:30:THR:HG23	1:C:117:LEU:CD2	2.35	0.50
1:C:50:LEU:N	1:C:51:PRO:HD2	2.25	0.50
1:C:103:ASN:HD22	1:C:236:TYR:HD1	1.59	0.50
1:B:602:PHE:O	1:B:608:LEU:HD23	2.11	0.50
1:B:798:HIS:CE1	1:B:799:GLU:HG3	2.46	0.50
1:C:434:ILE:HD12	1:C:521:LEU:HA	1.94	0.50
1:B:739:ILE:HB	1:B:740:PRO:HD3	1.92	0.50
1:A:651:TYR:CZ	1:A:652:LYS:HE3	2.47	0.50
1:C:236:TYR:HD2	1:C:591:LEU:HD21	1.77	0.50
1:A:322:ARG:O	1:A:322:ARG:CG	2.60	0.50
1:B:626:PHE:CE1	1:B:630:LYS:HG3	2.47	0.50
1:B:818:PHE:O	1:B:821:VAL:CG2	2.59	0.50
1:A:50:LEU:N	1:A:51:PRO:HD2	2.27	0.50
1:B:633:TYR:HD2	1:B:725:VAL:HG12	1.76	0.50
1:A:656:LEU:CD2	1:A:656:LEU:C	2.85	0.50
1:A:676:ARG:NH1	1:A:717:GLU:O	2.45	0.50
1:A:806:GLU:HG2	1:A:811:LYS:HB2	1.94	0.50
1:B:406:ASP:CB	1:B:435:LEU:CD1	2.89	0.50
1:B:406:ASP:CB	1:B:435:LEU:HD12	2.42	0.50
1:B:50:LEU:N	1:B:51:PRO:HD2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:516:VAL:HG12	1:B:518:MET:CE	2.42	0.50
1:C:407:GLU:HA	1:C:410:VAL:HG22	1.93	0.49
1:C:860:PHE:N	1:C:861:PRO:HD2	2.26	0.49
1:A:812:PHE:O	1:A:813:VAL:HG22	2.12	0.49
1:B:882:THR:O	1:B:886:LEU:HD22	2.12	0.49
1:C:91:PHE:CE1	1:C:142:ALA:HB1	2.47	0.49
1:C:842:LEU:HA	1:C:852:ASP:HB2	1.93	0.49
1:B:651:TYR:CZ	1:B:652:LYS:HE3	2.47	0.49
1:C:113:ALA:O	1:C:117:LEU:HD22	2.12	0.49
1:C:651:TYR:CZ	1:C:652:LYS:HE3	2.47	0.49
1:B:601:LYS:HE2	1:B:602:PHE:CE1	2.47	0.49
1:C:374:THR:HG22	1:C:376:HIS:NE2	2.28	0.49
1:C:417:TYR:HE2	1:C:428:LYS:HD3	1.78	0.49
1:A:648:ILE:HD13	1:A:654:GLN:HE22	1.76	0.49
1:A:860:PHE:N	1:A:861:PRO:HD2	2.27	0.49
1:C:434:ILE:HD13	1:C:520:ASN:HB3	1.94	0.49
1:C:539:ILE:HG22	1:C:544:VAL:CG2	2.42	0.49
1:A:91:PHE:CE1	1:A:142:ALA:HB1	2.47	0.49
1:B:818:PHE:O	1:B:821:VAL:HG22	2.13	0.49
1:C:406:ASP:CB	1:C:435:LEU:CD1	2.90	0.49
1:B:91:PHE:CE1	1:B:142:ALA:HB1	2.48	0.49
1:B:239:ARG:O	1:B:240:THR:C	2.56	0.49
1:A:57:THR:O	1:A:60:SER:HB2	2.13	0.49
1:A:711:THR:HG21	1:A:830:PHE:HA	1.93	0.49
1:A:56:ALA:HA	1:A:59:GLN:HE21	1.77	0.49
1:A:114:LEU:O	1:A:115:LYS:C	2.56	0.49
1:A:187:ILE:HG22	1:B:196:ASN:CG	2.38	0.49
1:C:57:THR:O	1:C:60:SER:HB2	2.13	0.49
1:C:406:ASP:CB	1:C:435:LEU:HD12	2.42	0.49
1:C:774:LEU:HD21	1:C:779:VAL:HG13	1.95	0.49
1:C:75:ILE:CD1	1:C:75:ILE:N	2.75	0.49
1:B:57:THR:O	1:B:60:SER:HB2	2.13	0.48
1:B:314:ARG:HD3	1:B:318:ARG:NH2	2.28	0.48
1:B:368:GLN:O	1:B:527:HIS:HB3	2.13	0.48
1:C:314:ARG:HD3	1:C:318:ARG:NH2	2.28	0.48
1:A:25:ASP:OD1	1:A:27:ALA:HB3	2.12	0.48
1:C:25:ASP:OD1	1:C:27:ALA:HB3	2.12	0.48
1:B:25:ASP:OD1	1:B:27:ALA:HB3	2.12	0.48
1:C:228:ALA:HB2	1:C:247:TRP:CZ3	2.49	0.48
1:A:633:TYR:HD2	1:A:725:VAL:HG12	1.77	0.48
1:A:760:ASN:HD21	1:A:777:ALA:HB3	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:228:ALA:HB2	1:B:247:TRP:CZ3	2.48	0.48
1:C:759:SER:CB	1:C:762:LLP:OP1	2.61	0.48
1:A:89:MET:HG2	1:A:340:HIS:HB3	1.95	0.48
1:B:187:ILE:H	1:B:187:ILE:CD1	2.12	0.48
1:B:537:SER:CB	1:B:558:ASN:HB2	2.44	0.48
1:C:202:ILE:HD11	1:C:306:ALA:HB2	1.96	0.48
1:A:842:LEU:HA	1:A:852:ASP:HB2	1.94	0.48
1:B:444:VAL:O	1:B:445:ALA:HB2	2.11	0.48
1:C:368:GLN:O	1:C:527:HIS:HB3	2.13	0.48
1:A:314:ARG:HD3	1:A:318:ARG:NH2	2.28	0.48
1:B:576:LEU:HD12	1:B:580:ILE:HD11	1.96	0.48
1:C:533:ALA:C	1:C:558:ASN:HD21	2.21	0.48
1:A:239:ARG:O	1:A:240:THR:C	2.56	0.48
1:A:539:ILE:HG22	1:A:544:VAL:CG2	2.44	0.48
1:B:774:LEU:HD23	1:B:774:LEU:O	2.14	0.48
1:B:823:GLU:OE1	1:B:823:GLU:HA	2.12	0.48
1:C:792:LEU:HD23	1:C:792:LEU:C	2.39	0.48
1:A:54:PHE:CE1	1:A:128:GLU:HB2	2.49	0.48
1:A:537:SER:CB	1:A:558:ASN:HB2	2.44	0.48
1:A:882:THR:O	1:A:886:LEU:HD22	2.13	0.48
1:B:54:PHE:CE1	1:B:128:GLU:HB2	2.49	0.48
1:B:647:ARG:NH2	2:B:1001:GLC:O2	2.46	0.48
1:C:114:LEU:O	1:C:115:LYS:C	2.56	0.48
1:C:644:GLN:HE21	1:C:646:LYS:HE2	1.78	0.48
1:A:202:ILE:HD11	1:A:306:ALA:HB2	1.96	0.48
1:C:90:GLU:HB2	1:C:134:GLY:HA2	1.95	0.48
1:A:312:ILE:HD13	1:A:328:PHE:CE2	2.49	0.47
1:A:396:PRO:O	1:A:399:VAL:HG22	2.13	0.47
1:A:656:LEU:HD23	1:A:656:LEU:O	2.14	0.47
1:A:823:GLU:HA	1:A:823:GLU:OE1	2.13	0.47
1:C:396:PRO:O	1:C:399:VAL:HG22	2.14	0.47
1:C:417:TYR:HE2	1:C:428:LYS:CD	2.27	0.47
1:C:633:TYR:HD2	1:C:725:VAL:HG12	1.79	0.47
1:A:576:LEU:HD12	1:A:580:ILE:HD11	1.96	0.47
1:A:601:LYS:O	1:A:601:LYS:HG3	2.14	0.47
1:B:89:MET:HG2	1:B:340:HIS:HB3	1.95	0.47
1:B:114:LEU:O	1:B:115:LYS:C	2.57	0.47
1:C:537:SER:CB	1:C:558:ASN:HB2	2.44	0.47
1:C:602:PHE:O	1:C:608:LEU:HD23	2.14	0.47
1:A:45:PRO:HG2	1:B:73:TYR:CD2	2.50	0.47
1:A:645:VAL:C	1:A:646:LYS:HG2	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ILE:HG21	1:A:724:VAL:HG21	1.97	0.47
1:B:90:GLU:HB2	1:B:134:GLY:HA2	1.96	0.47
1:A:592:LYS:NZ	1:A:594:GLU:OE1	2.47	0.47
1:B:760:ASN:HD21	1:B:777:ALA:HB3	1.79	0.47
1:C:62:ARG:O	1:C:63:ASP:C	2.56	0.47
1:C:576:LEU:HD12	1:C:580:ILE:HD11	1.96	0.47
1:B:62:ARG:O	1:B:63:ASP:C	2.57	0.47
1:B:792:LEU:HD23	1:B:792:LEU:C	2.39	0.47
1:A:228:ALA:HB2	1:A:247:TRP:CZ3	2.49	0.47
1:A:792:LEU:HD23	1:A:792:LEU:C	2.39	0.47
1:B:202:ILE:HD11	1:B:306:ALA:HB2	1.97	0.47
1:B:396:PRO:O	1:B:399:VAL:HG22	2.14	0.47
1:B:568:TRP:CE2	1:B:762:LLP:HD3	2.49	0.47
1:C:80:ASN:HD22	1:C:318:ARG:HB3	1.79	0.47
1:C:147:ASP:OD2	1:C:564:THR:OG1	2.27	0.47
1:C:662:VAL:HG12	1:C:821:VAL:HG13	1.96	0.47
1:C:774:LEU:O	1:C:774:LEU:CD1	2.62	0.47
1:A:833:TYR:HD2	1:A:835:TYR:CE1	2.32	0.47
1:B:735:ALA:O	1:B:739:ILE:CG1	2.63	0.47
1:C:374:THR:CG2	1:C:376:HIS:NE2	2.78	0.47
1:A:62:ARG:O	1:A:63:ASP:C	2.57	0.47
1:A:640:MET:HE1	1:A:870:VAL:HG23	1.97	0.47
1:B:44:SER:HB2	1:B:45:PRO:CD	2.45	0.47
1:B:374:THR:HG22	1:B:376:HIS:NE2	2.30	0.47
1:B:417:TYR:HE2	1:B:428:LYS:CD	2.28	0.47
1:A:410:VAL:O	1:A:414:VAL:HG23	2.15	0.47
1:A:774:LEU:O	1:A:774:LEU:HD23	2.14	0.47
1:C:760:ASN:HD21	1:C:777:ALA:HB3	1.79	0.47
1:C:807:ARG:NH2	1:C:842:LEU:O	2.47	0.47
1:B:410:VAL:O	1:B:414:VAL:HG23	2.14	0.46
1:C:239:ARG:O	1:C:240:THR:C	2.56	0.46
1:C:417:TYR:O	1:C:420:MET:HG3	2.16	0.46
1:A:581:THR:HG21	1:A:587:GLU:HG2	1.97	0.46
1:A:667:LYS:O	1:A:671:MET:HG2	2.15	0.46
1:B:533:ALA:C	1:B:558:ASN:HD21	2.22	0.46
1:B:655:LEU:HA	1:B:658:ILE:HG22	1.97	0.46
1:C:54:PHE:CE1	1:C:128:GLU:HB2	2.50	0.46
1:C:89:MET:HG2	1:C:340:HIS:HB3	1.96	0.46
1:C:312:ILE:HD13	1:C:328:PHE:CE2	2.51	0.46
1:C:826:ARG:HG2	1:C:826:ARG:NH1	2.22	0.46
1:A:44:SER:HB2	1:A:45:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:TYR:O	1:C:81:MET:HE3	2.16	0.46
1:C:177:GLN:HG2	1:C:178:GLU:N	2.30	0.46
1:B:79:LEU:O	1:B:80:ASN:C	2.59	0.46
1:C:358:LEU:HD22	1:C:362:GLU:OE1	2.16	0.46
1:A:90:GLU:HB2	1:A:134:GLY:HA2	1.97	0.46
1:A:800:ILE:CD1	1:A:800:ILE:N	2.79	0.46
1:B:57:THR:O	1:B:61:VAL:HG23	2.16	0.46
1:B:89:MET:HG2	1:B:340:HIS:HB2	1.98	0.46
1:B:656:LEU:HD23	1:B:656:LEU:O	2.16	0.46
1:B:682:PRO:HG3	1:B:721:LEU:HD12	1.97	0.46
1:B:739:ILE:HD13	1:B:763:PHE:CZ	2.51	0.46
1:B:807:ARG:NH2	1:B:842:LEU:O	2.48	0.46
1:C:645:VAL:C	1:C:646:LYS:CG	2.89	0.46
1:A:76:TYR:O	1:A:81:MET:HE3	2.16	0.46
1:A:79:LEU:O	1:A:80:ASN:C	2.59	0.46
1:A:358:LEU:HD22	1:A:362:GLU:OE1	2.15	0.46
1:B:557:GLN:HE21	1:B:559:LYS:HE2	1.80	0.46
1:C:406:ASP:O	1:C:409:LEU:HB3	2.16	0.46
1:C:735:ALA:O	1:C:739:ILE:CG1	2.63	0.46
1:C:859:ASP:C	1:C:861:PRO:HD2	2.41	0.46
1:C:880:TRP:HA	1:C:883:MET:HE2	1.98	0.46
1:A:653:ARG:HH11	1:A:749:SER:C	2.23	0.46
1:A:807:ARG:NH2	1:A:842:LEU:O	2.49	0.46
1:B:428:LYS:HE3	1:B:432:MET:HE3	1.96	0.46
1:C:57:THR:O	1:C:61:VAL:HG23	2.16	0.46
1:A:73:TYR:CD2	1:B:45:PRO:HG2	2.51	0.46
1:A:258:LEU:HD11	1:B:180:VAL:C	2.41	0.46
1:B:322:ARG:O	1:B:322:ARG:CG	2.64	0.46
1:C:656:LEU:HD23	1:C:656:LEU:O	2.16	0.46
1:A:392:GLN:CB	1:A:399:VAL:HG21	2.38	0.45
1:B:297:LEU:HD13	1:B:297:LEU:C	2.40	0.45
1:B:530:ASN:HA	1:B:557:GLN:O	2.16	0.45
1:C:68:ASN:HD21	1:C:239:ARG:NH1	2.14	0.45
1:C:410:VAL:O	1:C:414:VAL:HG23	2.16	0.45
1:C:428:LYS:HE3	1:C:432:MET:HE3	1.97	0.45
1:C:533:ALA:C	1:C:558:ASN:ND2	2.74	0.45
1:A:57:THR:O	1:A:61:VAL:HG23	2.16	0.45
1:A:89:MET:HG2	1:A:340:HIS:HB2	1.98	0.45
1:A:530:ASN:HA	1:A:557:GLN:O	2.17	0.45
1:A:583:TRP:CD2	1:A:608:LEU:HD13	2.51	0.45
1:B:759:SER:CB	1:B:762:LLP:OP1	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:530:ASN:HA	1:C:557:GLN:O	2.16	0.45
1:B:417:TYR:HE2	1:B:428:LYS:HD3	1.81	0.45
1:B:835:TYR:O	1:B:839:ILE:HD12	2.15	0.45
1:C:559:LYS:HB3	1:C:903:TYR:CE1	2.52	0.45
1:A:80:ASN:HD22	1:A:318:ARG:HB3	1.81	0.45
1:A:850:ARG:O	1:A:851:ALA:HB3	2.17	0.45
1:B:358:LEU:HD22	1:B:362:GLU:OE1	2.17	0.45
1:C:79:LEU:O	1:C:80:ASN:C	2.59	0.45
1:B:297:LEU:HD13	1:B:297:LEU:O	2.16	0.45
1:B:583:TRP:CD2	1:B:608:LEU:HD13	2.52	0.45
1:B:651:TYR:OH	1:B:652:LYS:HE3	2.17	0.45
1:A:68:ASN:HD21	1:A:239:ARG:NH1	2.15	0.45
1:C:655:LEU:HA	1:C:658:ILE:HG22	1.99	0.45
1:C:656:LEU:C	1:C:656:LEU:CD2	2.89	0.45
1:A:197:ASP:C	1:A:197:ASP:OD1	2.60	0.45
1:A:651:TYR:OH	1:A:652:LYS:HE3	2.17	0.45
1:C:322:ARG:O	1:C:322:ARG:CG	2.64	0.45
1:C:817:ARG:O	1:C:821:VAL:HG23	2.17	0.45
1:A:654:GLN:O	1:A:657:ASN:HB3	2.17	0.45
1:B:850:ARG:O	1:B:851:ALA:HB3	2.16	0.45
1:C:337:ASN:OD1	1:C:376:HIS:CE1	2.70	0.45
1:B:429:LEU:HD13	1:B:429:LEU:HA	1.84	0.45
1:C:667:LYS:O	1:C:671:MET:HG2	2.17	0.45
1:C:682:PRO:HG3	1:C:721:LEU:HD12	1.99	0.45
1:C:739:ILE:HD13	1:C:763:PHE:CZ	2.51	0.45
1:A:324:LYS:O	1:A:327:GLU:HB2	2.16	0.45
1:A:859:ASP:C	1:A:861:PRO:HD2	2.42	0.45
1:B:882:THR:HG22	1:B:886:LEU:HD23	1.98	0.45
1:C:781:ILE:O	1:C:785:VAL:HG22	2.17	0.45
1:C:835:TYR:O	1:C:839:ILE:HD12	2.17	0.45
1:A:177:GLN:HG2	1:A:178:GLU:N	2.31	0.44
1:A:647:ARG:NH2	2:A:1001:GLC:O1	2.51	0.44
1:A:662:VAL:HG12	1:A:821:VAL:HG13	1.97	0.44
1:B:197:ASP:OD1	1:B:197:ASP:C	2.60	0.44
1:B:656:LEU:HD21	1:B:863:TYR:CD2	2.52	0.44
1:C:265:GLU:HB3	1:C:268:LYS:HB3	1.99	0.44
1:C:329:PRO:HD3	1:C:366:ILE:HG23	1.99	0.44
1:A:406:ASP:O	1:A:409:LEU:HB3	2.17	0.44
1:B:374:THR:CG2	1:B:376:HIS:CD2	2.99	0.44
1:B:559:LYS:HB3	1:B:903:TYR:CE1	2.52	0.44
1:C:197:ASP:C	1:C:197:ASP:OD1	2.60	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:646:LYS:O	1:C:647:ARG:C	2.60	0.44
1:C:648:ILE:HG23	1:C:654:GLN:HE21	1.83	0.44
1:C:661:ILE:HG21	1:C:724:VAL:HG21	1.99	0.44
1:C:823:GLU:HA	1:C:823:GLU:OE1	2.16	0.44
1:A:323:ILE:HD13	1:A:323:ILE:O	2.17	0.44
1:B:646:LYS:O	1:B:647:ARG:C	2.60	0.44
1:B:661:ILE:HG21	1:B:724:VAL:HG21	1.99	0.44
1:B:800:ILE:N	1:B:800:ILE:CD1	2.79	0.44
1:C:89:MET:HG2	1:C:340:HIS:HB2	1.99	0.44
1:C:444:VAL:HG23	1:C:445:ALA:N	2.32	0.44
1:C:583:TRP:CD2	1:C:608:LEU:HD13	2.53	0.44
1:C:651:TYR:OH	1:C:652:LYS:HE3	2.18	0.44
1:B:324:LYS:O	1:B:327:GLU:HB2	2.18	0.44
1:B:374:THR:CG2	1:B:376:HIS:NE2	2.81	0.44
1:B:416:LYS:O	1:B:417:TYR:CB	2.65	0.44
1:B:533:ALA:C	1:B:558:ASN:ND2	2.75	0.44
1:C:671:MET:SD	1:C:676:ARG:HA	2.57	0.44
1:A:90:GLU:CD	1:A:138:LEU:HD23	2.42	0.44
1:A:652:LYS:O	1:A:653:ARG:CB	2.65	0.44
1:C:416:LYS:O	1:C:417:TYR:CB	2.65	0.44
1:A:273:GLN:HG3	1:A:274:ALA:N	2.33	0.44
1:A:323:ILE:HD11	1:A:325:TRP:NE1	2.33	0.44
1:B:656:LEU:C	1:B:656:LEU:CD2	2.90	0.44
1:B:329:PRO:HD3	1:B:366:ILE:HG23	1.99	0.44
1:C:850:ARG:O	1:C:851:ALA:HB3	2.18	0.44
1:A:882:THR:HG22	1:A:886:LEU:HD23	1.99	0.43
1:C:759:SER:HB2	1:C:762:LLP:OP1	2.18	0.43
1:B:79:LEU:HB3	1:B:81:MET:HG3	2.00	0.43
1:B:187:ILE:N	1:B:187:ILE:CD1	2.78	0.43
1:B:375:ASN:O	1:B:376:HIS:CB	2.67	0.43
1:B:601:LYS:HG3	1:B:602:PHE:CD1	2.53	0.43
1:C:179:GLU:N	1:C:179:GLU:OE1	2.51	0.43
1:A:179:GLU:N	1:A:179:GLU:OE1	2.52	0.43
1:A:329:PRO:HD3	1:A:366:ILE:HG23	1.99	0.43
1:A:561:ASN:ND2	2:A:1001:GLC:O6	2.48	0.43
1:A:880:TRP:HA	1:A:883:MET:HE2	1.99	0.43
1:B:179:GLU:N	1:B:179:GLU:OE1	2.52	0.43
1:C:419:SER:HA	1:C:425:LEU:HD22	1.99	0.43
1:C:656:LEU:HD21	1:C:863:TYR:CD2	2.53	0.43
1:A:138:LEU:CD1	1:A:376:HIS:HD2	2.31	0.43
1:A:162:ARG:HH12	3:A:1002:GOL:C2	2.25	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:667:LYS:O	1:B:671:MET:HG2	2.18	0.43
1:B:671:MET:HE3	1:B:675:GLU:HB2	2.01	0.43
1:B:781:ILE:O	1:B:785:VAL:HG22	2.18	0.43
1:A:666:LYS:NZ	1:A:670:GLU:OE2	2.51	0.43
1:B:880:TRP:HA	1:B:883:MET:HE2	1.99	0.43
1:A:55:PHE:O	1:A:59:GLN:HG3	2.19	0.43
1:A:628:LYS:HG3	1:C:788:GLU:CG	2.47	0.43
1:A:653:ARG:NH1	1:A:750:THR:N	2.66	0.43
1:B:532:VAL:HG23	1:B:756:SER:HB2	1.99	0.43
1:C:573:ASN:OD1	1:C:576:LEU:HB2	2.18	0.43
1:B:177:GLN:HG2	1:B:178:GLU:N	2.32	0.43
1:B:640:MET:HE1	1:B:870:VAL:HG23	2.00	0.43
1:C:825:VAL:HG22	1:C:830:PHE:HE2	1.84	0.43
1:A:138:LEU:HD12	1:A:376:HIS:CD2	2.52	0.43
1:B:297:LEU:HD23	1:B:386:TRP:CZ2	2.52	0.43
1:C:79:LEU:HB3	1:C:81:MET:HG3	2.01	0.43
1:A:345:ILE:HB	1:A:346:PRO:CD	2.48	0.43
1:A:682:PRO:HG3	1:A:721:LEU:HD12	2.00	0.43
1:B:406:ASP:CG	1:B:435:LEU:CD1	2.88	0.43
1:A:392:GLN:OE1	1:A:399:VAL:CG2	2.67	0.42
1:A:657:ASN:OD1	1:A:661:ILE:HD11	2.16	0.42
1:B:76:TYR:O	1:B:81:MET:HE3	2.18	0.42
1:B:713:ASN:OD1	1:B:723:LYS:HA	2.19	0.42
1:C:170:GLN:HE21	1:C:177:GLN:NE2	2.06	0.42
1:C:297:LEU:HD13	1:C:386:TRP:CZ2	2.54	0.42
1:C:416:LYS:O	1:C:417:TYR:CG	2.72	0.42
1:C:735:ALA:O	1:C:739:ILE:HG12	2.19	0.42
1:A:392:GLN:OE1	1:A:399:VAL:HG21	2.18	0.42
1:A:713:ASN:OD1	1:A:723:LYS:HA	2.19	0.42
1:B:55:PHE:O	1:B:59:GLN:HG3	2.19	0.42
1:C:275:ASN:HA	1:C:278:LYS:HG2	2.01	0.42
1:C:340:HIS:N	1:C:341:PRO:CD	2.83	0.42
1:C:532:VAL:HG23	1:C:756:SER:HB2	2.01	0.42
1:C:713:ASN:OD1	1:C:723:LYS:HA	2.20	0.42
1:B:573:ASN:OD1	1:B:576:LEU:HB2	2.18	0.42
1:C:55:PHE:O	1:C:59:GLN:HG3	2.20	0.42
1:A:646:LYS:O	1:A:647:ARG:C	2.60	0.42
1:A:278:LYS:HA	1:A:281:TYR:CD2	2.54	0.42
1:B:301:TYR:O	1:B:302:THR:C	2.62	0.42
1:B:416:LYS:O	1:B:417:TYR:CG	2.72	0.42
1:A:573:ASN:OD1	1:A:576:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:HIS:N	1:B:341:PRO:CD	2.83	0.42
1:A:406:ASP:CG	1:A:435:LEU:HD23	2.45	0.42
1:A:806:GLU:CG	1:A:811:LYS:HB2	2.50	0.42
1:C:666:LYS:NZ	1:C:670:GLU:OE2	2.51	0.42
1:C:826:ARG:NH1	1:C:826:ARG:CG	2.79	0.42
1:A:759:SER:CB	1:A:762:LLP:OP1	2.68	0.42
1:B:278:LYS:HA	1:B:281:TYR:CD2	2.54	0.42
1:B:345:ILE:HB	1:B:346:PRO:CD	2.50	0.42
3:B:1003:GOL:O3	3:B:1003:GOL:O1	2.34	0.42
1:C:113:ALA:O	1:C:117:LEU:CD2	2.68	0.42
1:A:345:ILE:HB	1:A:346:PRO:HD3	2.02	0.42
1:A:662:VAL:CG1	1:A:821:VAL:HG13	2.50	0.42
1:A:836:ASP:O	1:A:839:ILE:N	2.52	0.42
1:C:278:LYS:HA	1:C:281:TYR:CD2	2.55	0.42
1:A:412:GLU:OE1	1:A:552:TRP:HZ2	2.03	0.42
1:C:324:LYS:O	1:C:327:GLU:HB2	2.20	0.42
1:A:781:ILE:O	1:A:785:VAL:HG22	2.19	0.41
1:B:331:LYS:NZ	3:B:1003:GOL:H31	2.35	0.41
1:B:671:MET:HE2	1:B:676:ARG:HA	1.99	0.41
1:C:108:GLY:N	3:C:1002:GOL:C1	2.42	0.41
1:C:644:GLN:HE21	1:C:646:LYS:CE	2.33	0.41
1:A:653:ARG:HH11	1:A:653:ARG:HG3	1.79	0.41
1:C:867:GLN:OE1	1:C:867:GLN:HA	2.20	0.41
1:B:308:LEU:O	1:B:312:ILE:HG12	2.20	0.41
1:C:301:TYR:O	1:C:302:THR:C	2.63	0.41
1:C:779:VAL:O	1:C:783:GLU:HG3	2.20	0.41
1:A:162:ARG:NH1	3:A:1002:GOL:H2	2.29	0.41
1:A:678:THR:HG22	1:A:679:ASN:N	2.25	0.41
1:B:337:ASN:OD1	1:B:376:HIS:CE1	2.73	0.41
1:B:867:GLN:HE22	1:B:870:VAL:HG21	1.85	0.41
1:A:79:LEU:HB3	1:A:81:MET:HG3	2.02	0.41
1:A:301:TYR:O	1:A:302:THR:C	2.63	0.41
1:B:120:ASN:ND2	1:B:122:GLU:HG2	2.34	0.41
1:B:647:ARG:NH2	2:B:1001:GLC:O1	2.53	0.41
1:B:812:PHE:CZ	1:B:814:PRO:HA	2.56	0.41
1:C:599:LEU:HB2	1:C:889:ALA:HB2	2.02	0.41
1:A:308:LEU:O	1:A:312:ILE:HG12	2.19	0.41
1:C:38:GLU:OE1	1:C:39:PHE:CZ	2.74	0.41
1:C:444:VAL:HG23	1:C:445:ALA:H	1.86	0.41
1:C:760:ASN:ND2	1:C:781:ILE:HD12	2.35	0.41
1:A:392:GLN:CD	1:A:399:VAL:HG21	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:416:LYS:O	1:A:417:TYR:CB	2.69	0.41
1:A:416:LYS:O	1:A:417:TYR:CG	2.73	0.41
1:A:275:ASN:HA	1:A:278:LYS:HG2	2.02	0.41
1:A:171:ARG:NH1	1:C:604:ASP:OD2	2.54	0.41
1:A:779:VAL:O	1:A:783:GLU:HG3	2.21	0.41
1:A:860:PHE:CE1	1:A:864:ILE:HD13	2.56	0.41
1:B:368:GLN:HA	1:B:525:GLY:O	2.21	0.41
1:B:666:LYS:NZ	1:B:670:GLU:OE2	2.52	0.41
1:B:681:VAL:HG12	1:B:682:PRO:HD2	2.03	0.41
1:B:882:THR:HG22	1:B:886:LEU:CD2	2.51	0.41
1:C:103:ASN:ND2	1:C:236:TYR:HD1	2.17	0.41
1:C:140:ARG:HD2	1:C:140:ARG:HA	1.80	0.41
1:C:153:ASN:ND2	1:C:240:THR:OG1	2.50	0.41
1:C:429:LEU:HD13	1:C:429:LEU:HA	1.84	0.41
1:C:656:LEU:HD21	1:C:863:TYR:CD1	2.56	0.41
1:A:839:ILE:H	1:A:839:ILE:HD12	1.85	0.41
1:B:671:MET:HE1	1:B:679:ASN:OD1	2.21	0.41
1:B:700:ARG:CZ	1:B:837:ASP:HB3	2.51	0.41
1:A:164:LYS:HA	1:A:185:LEU:HD12	2.04	0.40
1:A:882:THR:HG22	1:A:886:LEU:CD2	2.52	0.40
1:B:164:LYS:HA	1:B:185:LEU:HD12	2.03	0.40
1:B:762:LLP:H4'1	1:B:762:LLP:H5'1	1.94	0.40
1:C:187:ILE:HD13	1:C:187:ILE:N	2.20	0.40
1:C:200:TYR:CZ	1:C:310:ASP:HA	2.56	0.40
1:C:812:PHE:CZ	1:C:814:PRO:HA	2.57	0.40
1:A:89:MET:CE	1:A:163:TYR:OH	2.68	0.40
1:A:162:ARG:NH2	1:A:192:GLU:OE2	2.49	0.40
1:A:297:LEU:HD13	1:A:386:TRP:CZ2	2.55	0.40
1:A:340:HIS:N	1:A:341:PRO:CD	2.84	0.40
1:A:418:GLY:C	1:A:420:MET:H	2.28	0.40
1:A:790:PHE:CD1	1:A:790:PHE:C	2.99	0.40
1:B:200:TYR:CZ	1:B:310:ASP:HA	2.56	0.40
1:C:901:HIS:O	1:C:905:LYS:HG2	2.22	0.40
1:A:187:ILE:HD12	1:A:187:ILE:N	2.15	0.40
1:A:599:LEU:HB2	1:A:889:ALA:HB2	2.02	0.40
1:B:275:ASN:HA	1:B:278:LYS:HG2	2.04	0.40
1:B:399:VAL:O	1:B:403:GLU:HG3	2.22	0.40
1:C:210:THR:H	3:C:1004:GOL:C3	2.31	0.40
1:C:308:LEU:O	1:C:312:ILE:HG12	2.21	0.40
1:B:140:ARG:HD2	1:B:140:ARG:HA	1.81	0.40
1:B:345:ILE:HB	1:B:346:PRO:HD3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:790:PHE:CD1	1:B:790:PHE:C	2.99	0.40
1:B:901:HIS:O	1:B:905:LYS:HG2	2.21	0.40
1:C:102:GLY:HA3	1:C:571:PHE:CZ	2.56	0.40
1:A:38:GLU:OE1	1:A:39:PHE:CZ	2.75	0.40
1:A:102:GLY:HA3	1:A:571:PHE:CZ	2.56	0.40
1:A:170:GLN:HG3	1:A:177:GLN:HG3	2.03	0.40
1:C:695:TYR:HA	4:C:1108:HOH:O	2.22	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	825/916 (90%)	763 (92%)	53 (6%)	9 (1%)	11	39
1	B	825/916 (90%)	765 (93%)	56 (7%)	4 (0%)	24	57
1	C	825/916 (90%)	768 (93%)	53 (6%)	4 (0%)	24	57
All	All	2475/2748 (90%)	2296 (93%)	162 (6%)	17 (1%)	18	49

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	LEU
1	A	445	ALA
1	A	602	PHE
1	A	836	ASP
1	A	837	ASP
1	B	417	TYR
1	B	445	ALA
1	C	417	TYR
1	C	422	LEU
1	B	375	ASN

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Mol	Chain	Res	Type
1	C	445	ALA
1	A	338	ASP
1	A	653	ARG
1	B	338	ASP
1	C	338	ASP
1	A	417	TYR
1	A	813	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	707/786 (90%)	657 (93%)	50 (7%)	13	41
1	B	707/786 (90%)	660 (93%)	47 (7%)	15	43
1	C	707/786 (90%)	658 (93%)	49 (7%)	14	41
All	All	2121/2358 (90%)	1975 (93%)	146 (7%)	14	41

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	55	PHE
1	A	62	ARG
1	A	77	GLU
1	A	79	LEU
1	A	81	MET
1	A	107	THR
1	A	120	ASN
1	A	138	LEU
1	A	187	ILE
1	A	291	GLU
1	A	322	ARG
1	A	323	ILE
1	A	324	LYS
1	A	339	THR

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Mol	Chain	Res	Type
1	A	355	LEU
1	A	408	GLU
1	A	410	VAL
1	A	415	LEU
1	A	422	LEU
1	A	425	LEU
1	A	429	LEU
1	A	430	THR
1	A	431	THR
1	A	438	PHE
1	A	440	LEU
1	A	444	VAL
1	A	511	ILE
1	A	534	GLU
1	A	535	ILE
1	A	539	ILE
1	A	540	VAL
1	A	544	VAL
1	A	576	LEU
1	A	592	LYS
1	A	601	LYS
1	A	638	ASP
1	A	646	LYS
1	A	651	TYR
1	A	653	ARG
1	A	654	GLN
1	A	676	ARG
1	A	681	VAL
1	A	739	ILE
1	A	749	SER
1	A	800	ILE
1	A	803	LEU
1	A	825	VAL
1	A	870	VAL
1	A	898	ARG
1	B	31	SER
1	B	55	PHE
1	B	62	ARG
1	B	77	GLU
1	B	79	LEU
1	B	81	MET
1	B	107	THR

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Mol	Chain	Res	Type
1	B	138	LEU
1	B	187	ILE
1	B	219	ILE
1	B	291	GLU
1	B	323	ILE
1	B	339	THR
1	B	355	LEU
1	B	374	THR
1	B	409	LEU
1	B	410	VAL
1	B	415	LEU
1	B	422	LEU
1	B	425	LEU
1	B	429	LEU
1	B	430	THR
1	B	431	THR
1	B	440	LEU
1	B	444	VAL
1	B	511	ILE
1	B	524	VAL
1	B	534	GLU
1	B	535	ILE
1	B	540	VAL
1	B	544	VAL
1	B	576	LEU
1	B	624	VAL
1	B	638	ASP
1	B	646	LYS
1	B	681	VAL
1	B	739	ILE
1	B	742	SER
1	B	749	SER
1	B	800	ILE
1	B	821	VAL
1	B	825	VAL
1	B	839	ILE
1	B	867	GLN
1	B	870	VAL
1	B	886	LEU
1	B	898	ARG
1	C	31	SER
1	C	55	PHE

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Mol	Chain	Res	Type
1	C	62	ARG
1	C	75	ILE
1	C	77	GLU
1	C	79	LEU
1	C	81	MET
1	C	107	THR
1	C	138	LEU
1	C	187	ILE
1	C	219	ILE
1	C	255	ASP
1	C	289	SER
1	C	291	GLU
1	C	323	ILE
1	C	339	THR
1	C	355	LEU
1	C	408	GLU
1	C	410	VAL
1	C	415	LEU
1	C	422	LEU
1	C	424	LYS
1	C	429	LEU
1	C	430	THR
1	C	431	THR
1	C	438	PHE
1	C	440	LEU
1	C	511	ILE
1	C	534	GLU
1	C	535	ILE
1	C	539	ILE
1	C	540	VAL
1	C	544	VAL
1	C	576	LEU
1	C	579	ILE
1	C	629	GLU
1	C	638	ASP
1	C	651	TYR
1	C	676	ARG
1	C	681	VAL
1	C	739	ILE
1	C	749	SER
1	C	774	LEU
1	C	803	LEU

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Mol	Chain	Res	Type
1	C	826	ARG
1	C	827	SER
1	C	839	ILE
1	C	870	VAL
1	C	888	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	GLN
1	A	68	ASN
1	A	80	ASN
1	A	93	GLN
1	A	153	ASN
1	A	250	GLN
1	A	530	ASN
1	A	557	GLN
1	A	561	ASN
1	A	654	GLN
1	A	760	ASN
1	A	789	ASN
1	A	834	ASN
1	A	887	ASN
1	A	901	HIS
1	B	93	GLN
1	B	153	ASN
1	B	376	HIS
1	B	557	GLN
1	B	558	ASN
1	B	644	GLN
1	B	657	ASN
1	B	760	ASN
1	B	789	ASN
1	B	845	ASN
1	B	867	GLN
1	C	68	ASN
1	C	80	ASN
1	C	93	GLN
1	C	103	ASN
1	C	153	ASN
1	C	177	GLN
1	C	376	HIS

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Mol	Chain	Res	Type
1	C	392	GLN
1	C	557	GLN
1	C	558	ASN
1	C	644	GLN
1	C	654	GLN
1	C	657	ASN
1	C	747	HIS
1	C	760	ASN
1	C	789	ASN
1	C	845	ASN
1	C	887	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	LLP	B	762	1	23,24,25	0.53	0	25,32,34	0.73	0
1	LLP	C	762	1	23,24,25	0.46	0	25,32,34	0.69	0
1	LLP	A	762	1	23,24,25	0.50	0	25,32,34	0.81	2 (8%)

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
1	LLP	B	762	1	-	9/16/17/19	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	C	762	1	-	7/16/17/19	0/1/1/1
1	LLP	A	762	1	-	7/16/17/19	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	762	LLP	OP3-P-OP2	2.25	116.23	107.80
1	A	762	LLP	OP4-P-OP1	-2.21	100.47	106.44

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	762	LLP	C5'-OP4-P-OP2
1	A	762	LLP	N-CA-CB-CG
1	A	762	LLP	C-CA-CB-CG
1	B	762	LLP	C5'-OP4-P-OP2
1	B	762	LLP	C5'-OP4-P-OP3
1	B	762	LLP	C-CA-CB-CG
1	B	762	LLP	CG-CD-CE-NZ
1	C	762	LLP	C5'-OP4-P-OP2
1	C	762	LLP	C5'-OP4-P-OP3
1	C	762	LLP	N-CA-CB-CG
1	C	762	LLP	C-CA-CB-CG
1	B	762	LLP	C4-C4'-NZ-CE
1	A	762	LLP	CG-CD-CE-NZ
1	C	762	LLP	CG-CD-CE-NZ
1	B	762	LLP	CA-CB-CG-CD
1	B	762	LLP	C5'-OP4-P-OP1
1	C	762	LLP	C5'-OP4-P-OP1
1	B	762	LLP	CE-CD-CG-CB
1	B	762	LLP	N-CA-CB-CG
1	A	762	LLP	C5'-OP4-P-OP1
1	A	762	LLP	C5'-OP4-P-OP3
1	A	762	LLP	CD-CE-NZ-C4'
1	C	762	LLP	CD-CE-NZ-C4'

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	762	LLP	5	0
1	C	762	LLP	2	0
1	A	762	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 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	$\# Z > 2$
3	GOL	B	1002	-	5,5,5	0.12	0	5,5,5	0.22	0
3	GOL	C	1003	-	5,5,5	0.08	0	5,5,5	0.41	0
2	GLC	A	1001	-	12,12,12	0.94	1 (8%)	17,17,17	1.26	2 (11%)
3	GOL	C	1004	-	5,5,5	0.18	0	5,5,5	0.23	0
2	GLC	B	1001	-	12,12,12	0.95	0	17,17,17	2.32	6 (35%)
3	GOL	C	1002	-	5,5,5	0.21	0	5,5,5	0.22	0
3	GOL	A	1002	-	5,5,5	0.10	0	5,5,5	0.48	0
3	GOL	A	1004	-	5,5,5	0.25	0	5,5,5	0.93	0
3	GOL	A	1003	-	5,5,5	0.15	0	5,5,5	0.42	0
3	GOL	B	1003	-	5,5,5	0.11	0	5,5,5	0.46	0
2	GLC	C	1001	-	12,12,12	0.81	1 (8%)	17,17,17	1.57	3 (17%)
3	GOL	C	1005	-	5,5,5	0.09	0	5,5,5	0.43	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
3	GOL	B	1002	-	-	1/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	1003	-	-	2/4/4/4	-
2	GLC	A	1001	-	-	2/2/22/22	0/1/1/1
3	GOL	C	1004	-	-	0/4/4/4	-
2	GLC	B	1001	-	-	0/2/22/22	0/1/1/1
3	GOL	C	1002	-	-	1/4/4/4	-
3	GOL	A	1002	-	-	2/4/4/4	-
3	GOL	A	1004	-	-	4/4/4/4	-
3	GOL	A	1003	-	-	2/4/4/4	-
3	GOL	B	1003	-	-	2/4/4/4	-
2	GLC	C	1001	-	-	0/2/22/22	0/1/1/1
3	GOL	C	1005	-	-	4/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	GLC	O1-C1	2.18	1.46	1.39
2	C	1001	GLC	O1-C1	2.13	1.46	1.39

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1001	GLC	C4-C3-C2	4.67	119.03	110.83
2	B	1001	GLC	C1-O5-C5	4.50	122.36	113.65
2	C	1001	GLC	C4-C3-C2	3.81	117.52	110.83
2	B	1001	GLC	C1-C2-C3	3.59	117.68	110.36
2	B	1001	GLC	O5-C5-C4	2.80	114.74	109.70
2	B	1001	GLC	O5-C1-C2	2.46	114.63	110.30
2	C	1001	GLC	O5-C5-C6	2.43	112.45	106.44
2	A	1001	GLC	C1-C2-C3	2.39	115.23	110.36
2	C	1001	GLC	O4-C4-C5	-2.33	103.58	109.32
2	A	1001	GLC	C4-C3-C2	2.32	114.91	110.83
2	B	1001	GLC	O5-C5-C6	2.14	111.75	106.44

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1004	GOL	O1-C1-C2-O2
3	A	1004	GOL	O1-C1-C2-C3
3	A	1004	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
3	A	1004	GOL	O2-C2-C3-O3
2	A	1001	GLC	C4-C5-C6-O6
2	A	1001	GLC	O5-C5-C6-O6
3	A	1002	GOL	C1-C2-C3-O3
3	A	1003	GOL	O1-C1-C2-C3
3	B	1003	GOL	O1-C1-C2-C3
3	C	1002	GOL	O1-C1-C2-C3
3	C	1003	GOL	O1-C1-C2-C3
3	C	1005	GOL	O1-C1-C2-C3
3	C	1005	GOL	C1-C2-C3-O3
3	A	1002	GOL	O2-C2-C3-O3
3	B	1003	GOL	O1-C1-C2-O2
3	C	1005	GOL	O1-C1-C2-O2
3	A	1003	GOL	O1-C1-C2-O2
3	B	1002	GOL	O1-C1-C2-C3
3	C	1005	GOL	O2-C2-C3-O3
3	C	1003	GOL	O1-C1-C2-O2

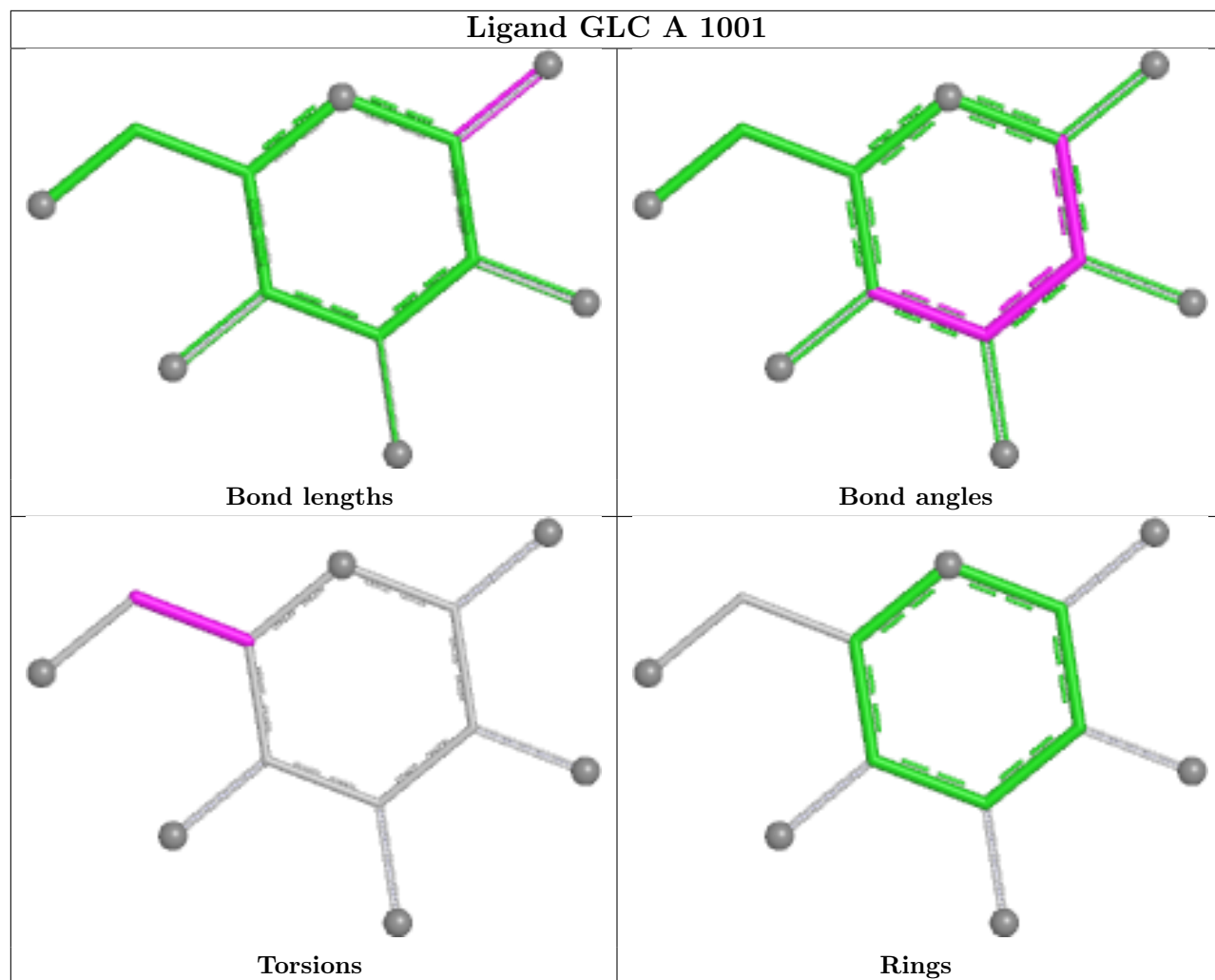
There are no ring outliers.

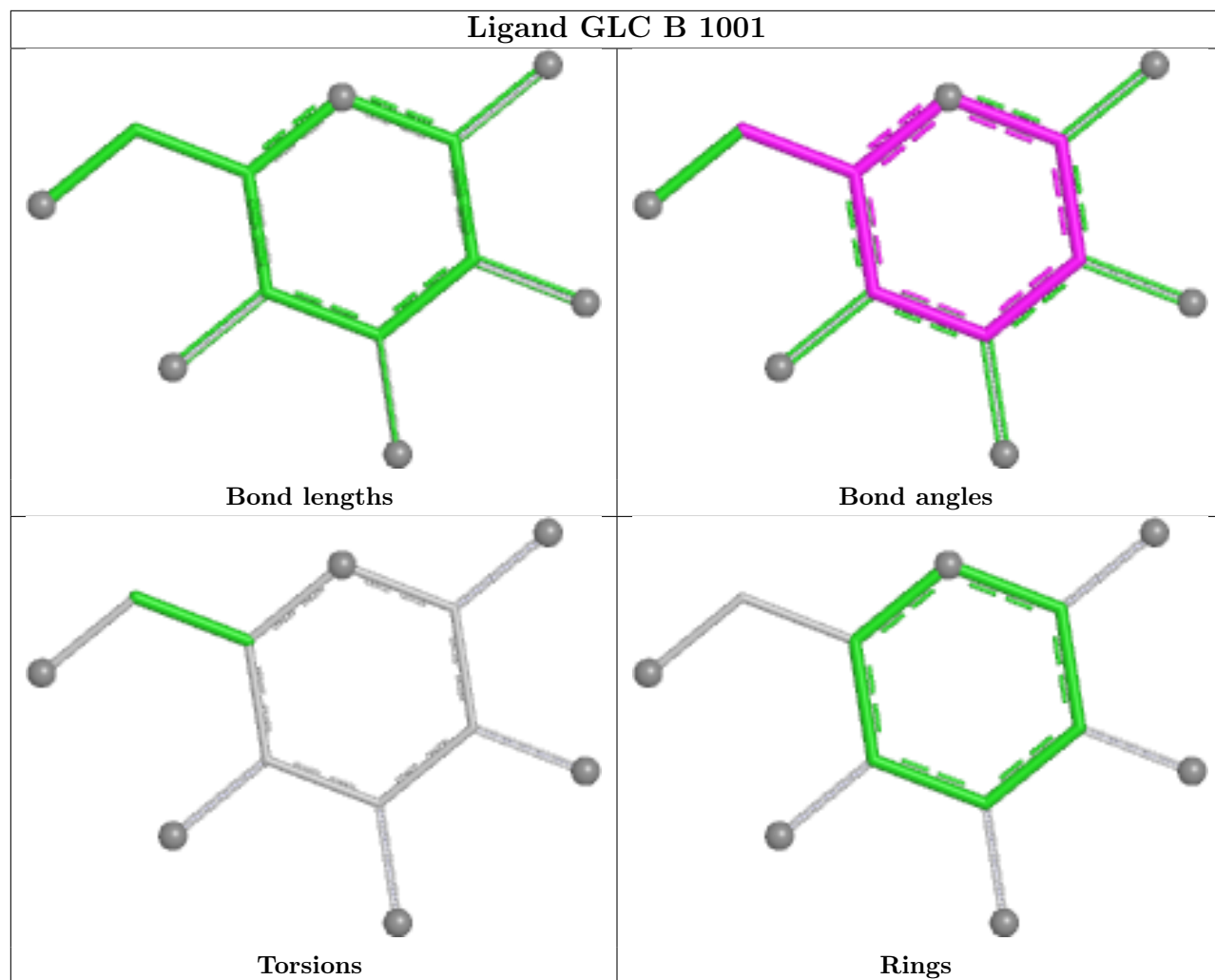
7 monomers are involved in 19 short contacts:

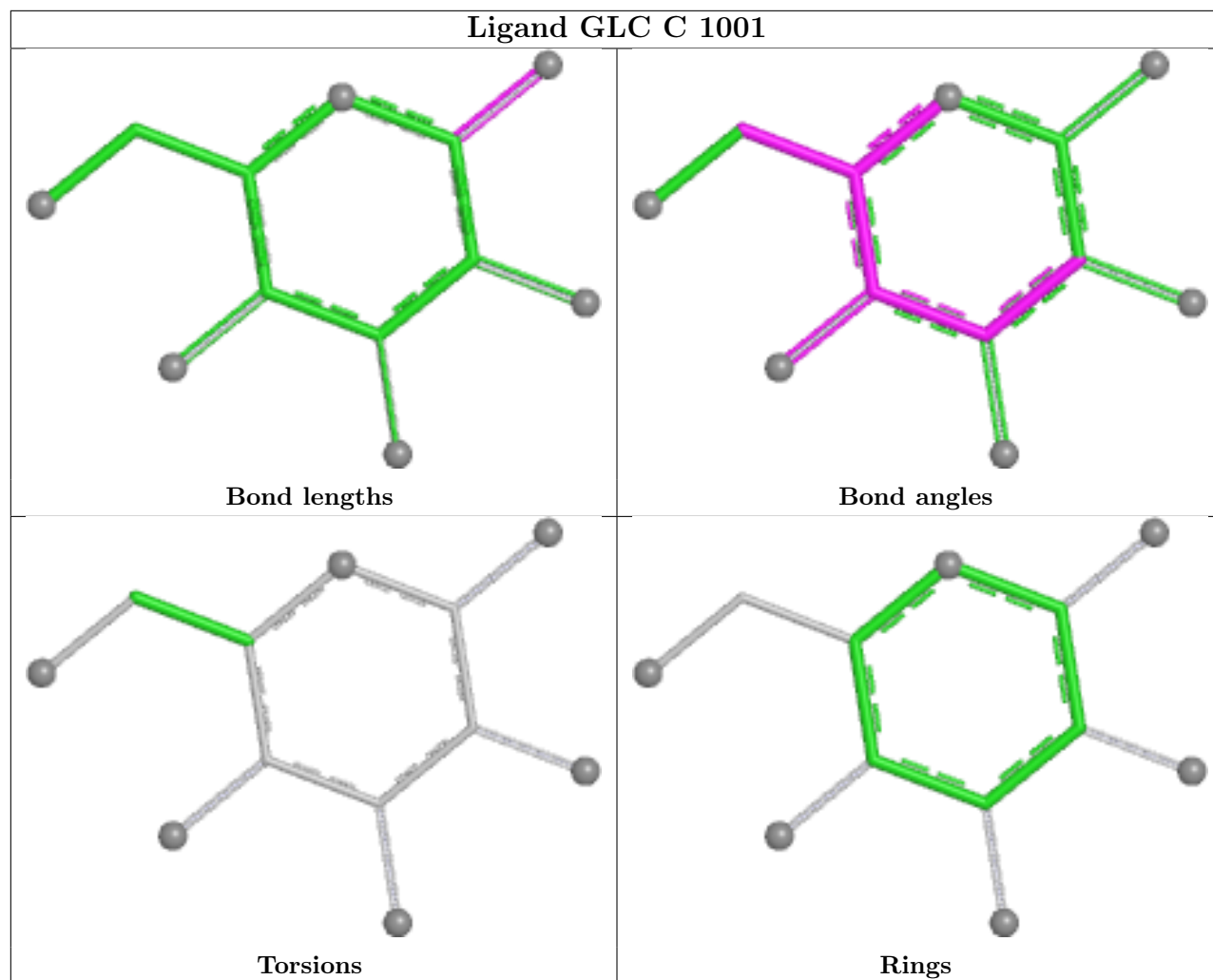
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	GLC	2	0
3	C	1004	GOL	2	0
2	B	1001	GLC	2	0
3	C	1002	GOL	7	0
3	A	1002	GOL	3	0
3	B	1003	GOL	2	0
2	C	1001	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GLC A 1001







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](#)

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	829/916 (90%)	-1.53	0 100 100	33, 33, 33, 33	0
1	B	829/916 (90%)	-1.52	0 100 100	33, 33, 33, 33	0
1	C	829/916 (90%)	-1.51	0 100 100	33, 33, 33, 33	0
All	All	2487/2748 (90%)	-1.52	0 100 100	33, 33, 33, 33	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
1	LLP	A	762	24/25	0.99	0.04	33,33,33,33	0
1	LLP	C	762	24/25	0.99	0.03	33,33,33,33	0
1	LLP	B	762	24/25	1.00	0.03	33,33,33,33	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

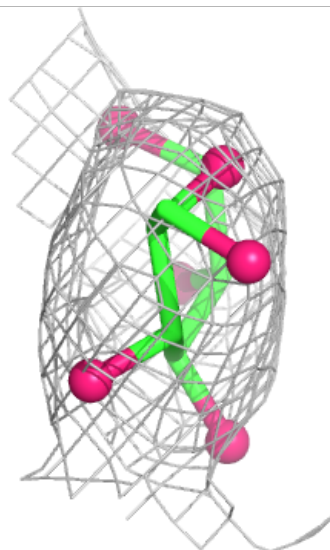
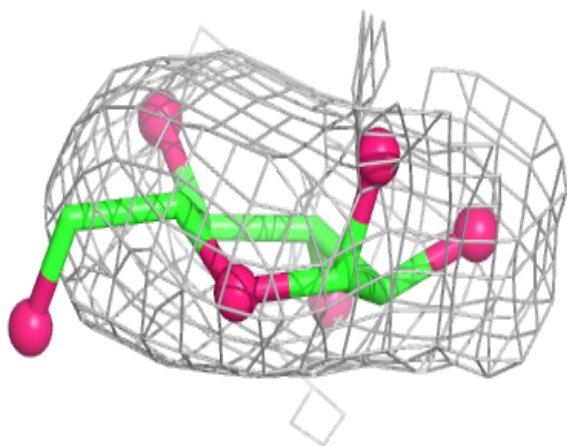
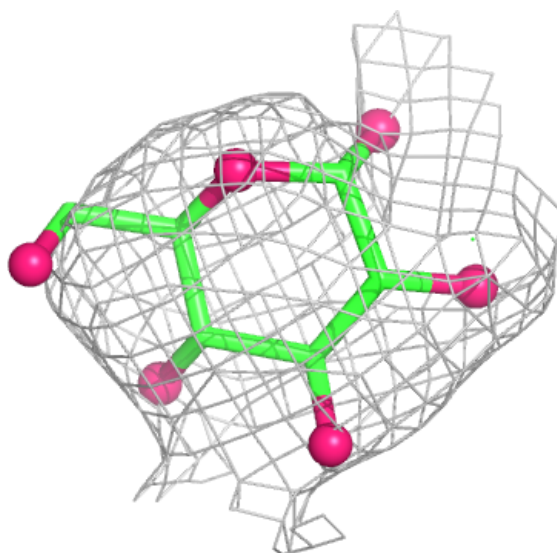
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	B	1003	6/6	0.95	0.06	50,50,50,50	0
3	GOL	C	1005	6/6	0.97	0.05	50,50,50,50	0
3	GOL	A	1003	6/6	0.98	0.08	50,50,50,50	0
3	GOL	C	1002	6/6	0.98	0.07	50,50,50,50	0
3	GOL	C	1004	6/6	0.98	0.06	50,50,50,50	0
3	GOL	A	1004	6/6	0.98	0.04	20,20,20,20	0
3	GOL	B	1002	6/6	0.99	0.05	50,50,50,50	0
2	GLC	C	1001	12/12	0.99	0.04	50,50,50,50	0
3	GOL	A	1002	6/6	0.99	0.06	50,50,50,50	0
2	GLC	A	1001	12/12	0.99	0.05	50,50,50,50	0
2	GLC	B	1001	12/12	0.99	0.05	50,50,50,50	0
3	GOL	C	1003	6/6	1.00	0.04	50,50,50,50	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

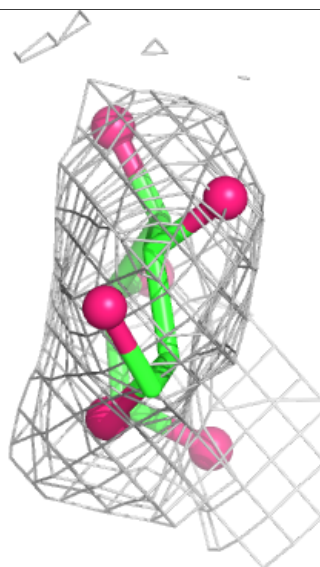
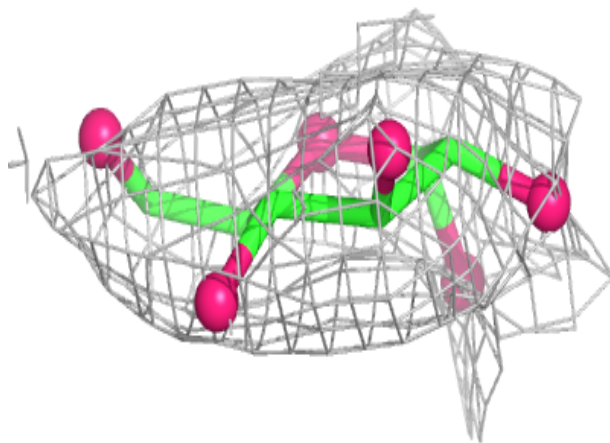
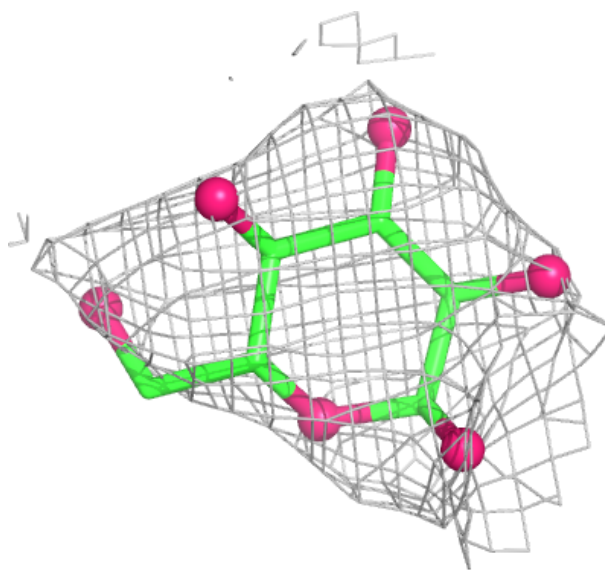
Electron density around GLC C 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



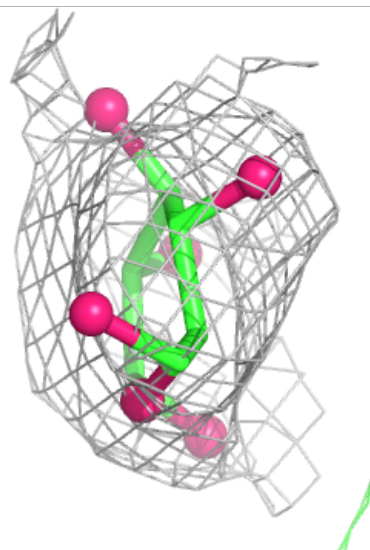
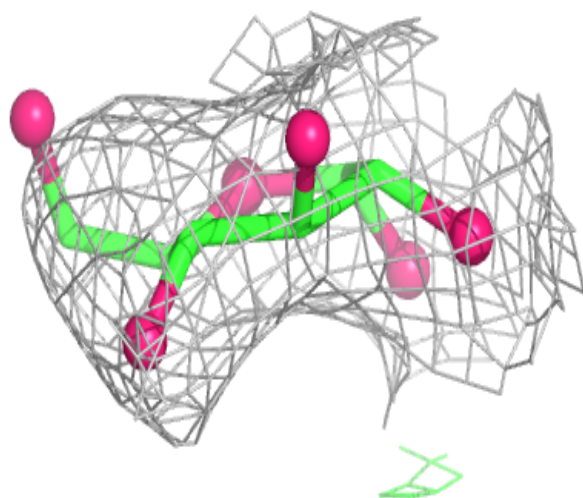
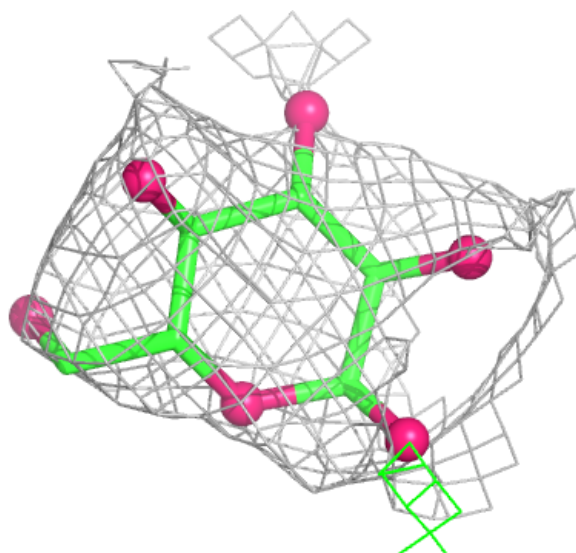
Electron density around GLC A 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around GLC B 1001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.