



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 01:12 pm BST

PDB ID : 9S8X / pdb\_00009s8x  
Title : Amuc0953\_S1\_20 in complex with D-Galactose  
Authors : Dey, D.; Cartmell, A.  
Deposited on : 2025-08-05  
Resolution : 2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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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 : 1.8.4, CSD as541be (2020)  
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

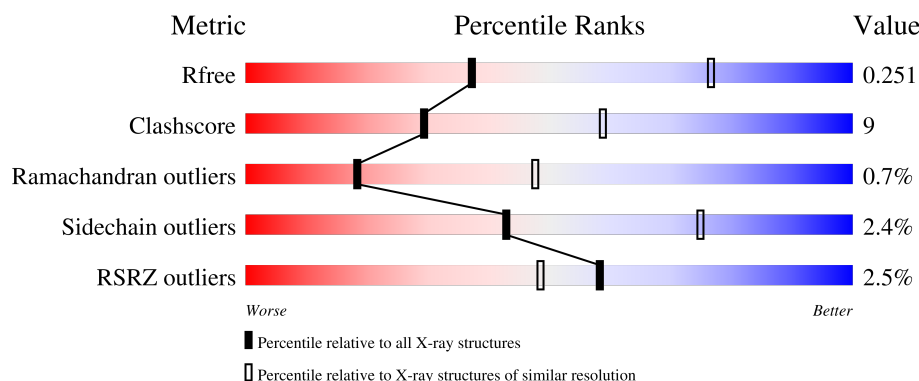
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	1263	
1	B	1263	

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	IOD	A	1303	-	-	X	-
3	IOD	B	1303	-	-	X	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 19074 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.

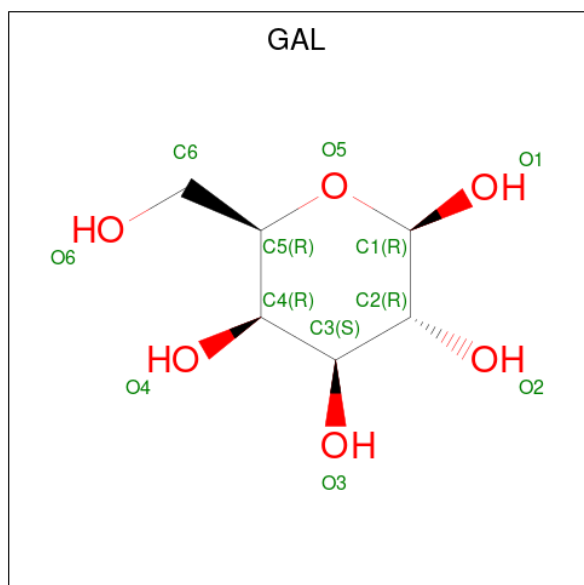
- Molecule 1 is a protein called Sulfatase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1263	Total	C	N	O	S	0	0	0
			9522	5938	1670	1879	35			
1	B	1263	Total	C	N	O	S	0	0	0
			9522	5938	1670	1879	35			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	66	ASN	THR	conflict	UNP B2UQQ0
A	67	ALA	ASN	conflict	UNP B2UQQ0
B	66	ASN	THR	conflict	UNP B2UQQ0
B	67	ALA	ASN	conflict	UNP B2UQQ0

- Molecule 2 is beta-D-galactopyranose (CCD ID: GAL) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 3 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total I 2 2	0	0
3	B	2	Total I 2 2	0	0

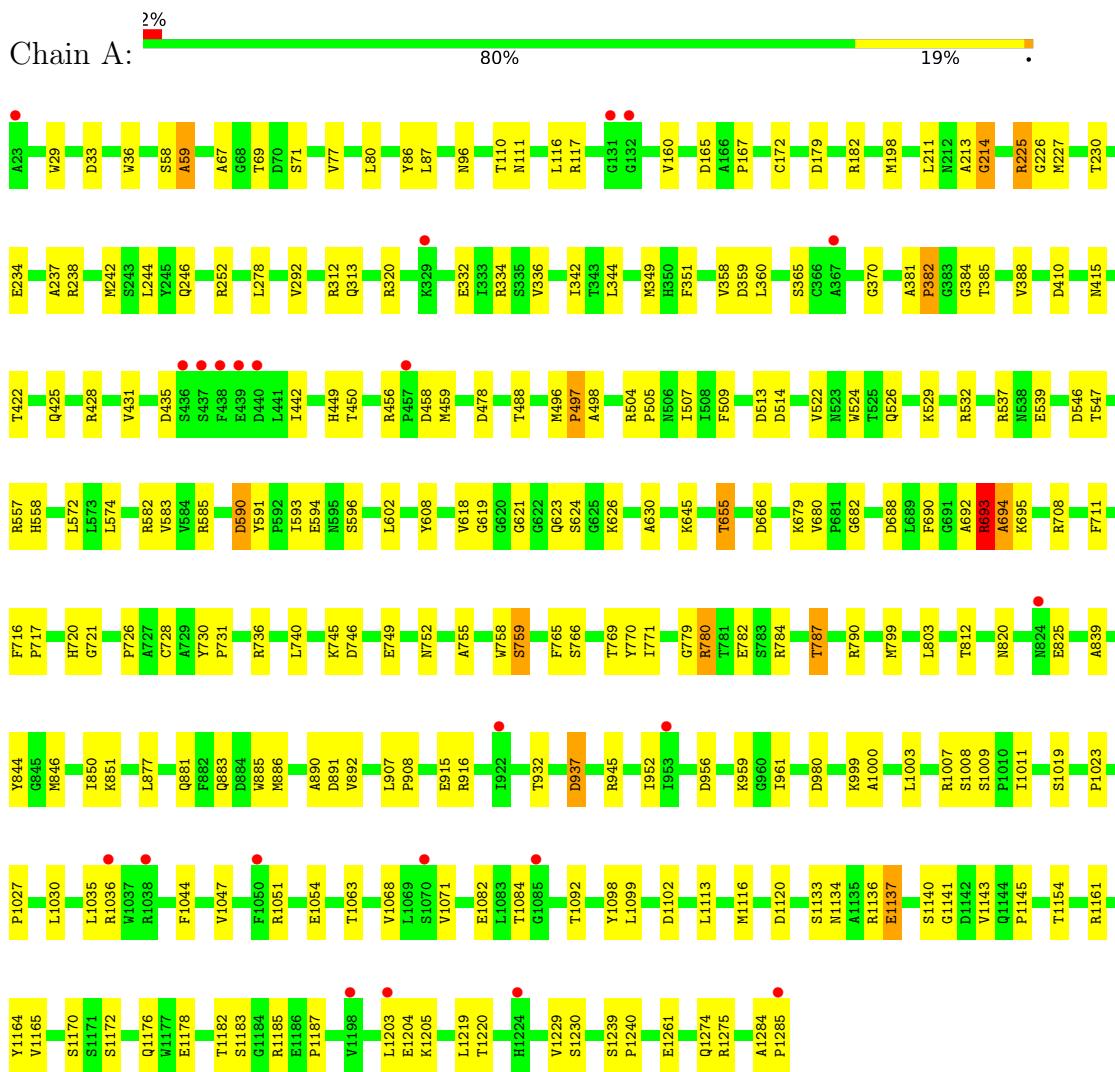
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Ca 1 1	0	0
4	B	1	Total Ca 1 1	0	0

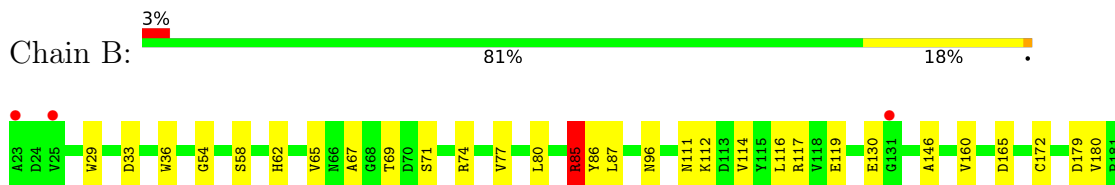
### 3 Residue-property plots

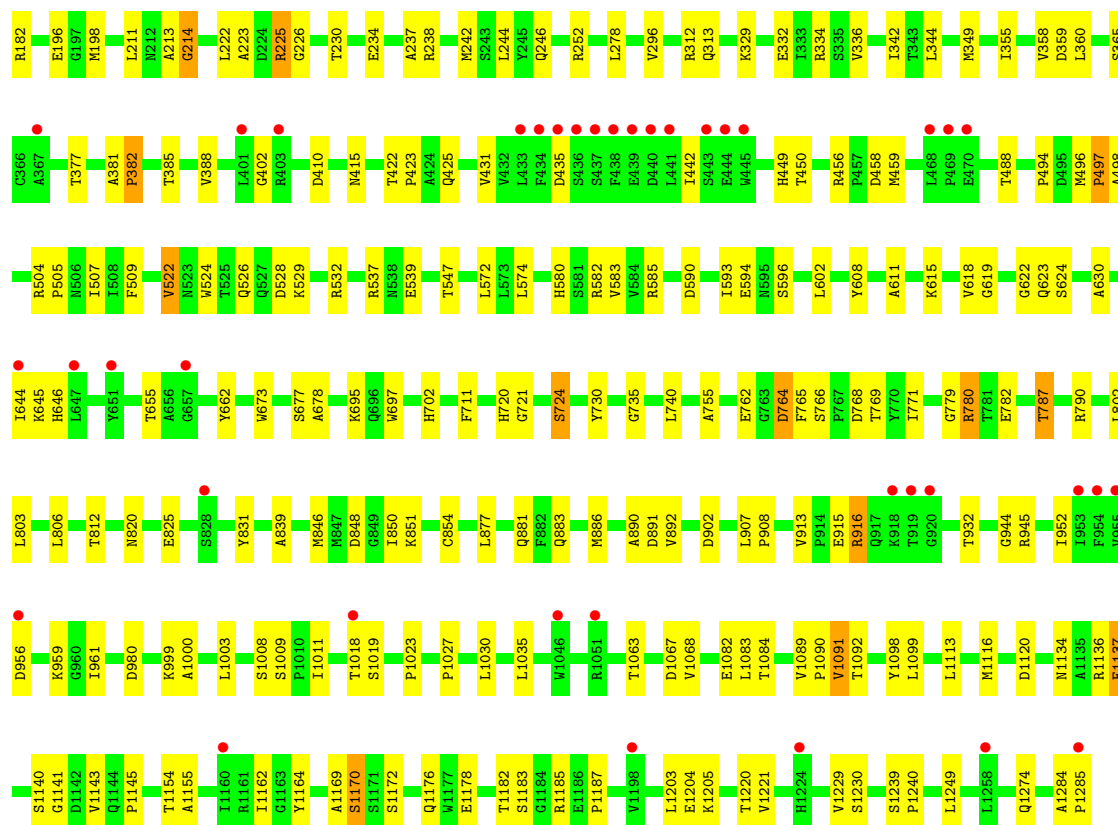
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



#### • Molecule 1: Sulfatase





## 4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	187.28Å 187.28Å 221.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.48 – 2.90 78.48 – 2.90	Depositor EDS
% Data completeness (in resolution range)	100.0 (78.48-2.90) 100.0 (78.48-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.71 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0430 (refmacat 0.4.105)	Depositor
R, $R_{free}$	0.212 , 0.257 0.209 , 0.251	Depositor DCC
$R_{free}$ test set	4384 reflections (5.20%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.7	Xtriage
Anisotropy	0.527	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 47.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19074	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.51 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.3790e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GAL, IOD

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	0.60	0/9743	1.12	25/13265 (0.2%)
1	B	0.61	0/9743	1.13	26/13265 (0.2%)
All	All	0.60	0/19486	1.13	51/26530 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	11
1	B	0	6
All	All	0	17

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1169	ALA	N-CA-C	-8.47	95.40	109.46
1	A	693	ARG	NE-CZ-NH1	-8.41	113.09	121.50
1	B	85	ARG	NE-CZ-NH1	-7.97	113.53	121.50
1	A	1274	GLN	CB-CA-C	-7.32	99.93	110.62
1	B	1274	GLN	CB-CA-C	-7.11	100.23	110.62
1	B	172	CYS	CB-CA-C	6.94	120.99	109.53
1	B	762	GLU	CB-CG-CD	6.80	124.16	112.60
1	A	693	ARG	N-CA-C	-6.73	101.61	110.43
1	A	172	CYS	CB-CA-C	6.52	120.44	109.48
1	A	915	GLU	CB-CG-CD	6.51	123.67	112.60
1	B	787	THR	CA-CB-OG1	-6.51	99.83	109.60
1	B	85	ARG	NE-CZ-NH2	6.51	125.06	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	787	THR	CA-CB-OG1	-6.40	100.00	109.60
1	B	415	ASN	CB-CA-C	6.23	119.81	109.53
1	B	528	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	415	ASN	CB-CA-C	6.03	119.71	109.53
1	B	956	ASP	CA-CB-CG	6.02	118.62	112.60
1	B	547	THR	CA-CB-OG1	-5.94	100.69	109.60
1	B	77	VAL	N-CA-CB	5.85	117.51	110.31
1	B	450	THR	CA-CB-OG1	-5.82	100.88	109.60
1	A	431	VAL	N-CA-CB	5.81	116.86	110.53
1	A	77	VAL	N-CA-CB	5.78	117.42	110.31
1	B	768	ASP	CA-CB-CG	5.78	118.38	112.60
1	B	431	VAL	N-CA-CB	5.74	116.79	110.53
1	A	547	THR	CA-CB-OG1	-5.74	101.00	109.60
1	A	450	THR	CA-CB-OG1	-5.73	101.01	109.60
1	A	179	ASP	CB-CA-C	5.59	119.36	111.86
1	B	230	THR	CA-CB-OG1	-5.57	101.24	109.60
1	A	1054	GLU	CB-CG-CD	5.53	122.00	112.60
1	A	230	THR	CA-CB-OG1	-5.50	101.34	109.60
1	B	179	ASP	CB-CA-C	5.48	119.21	111.86
1	B	1170	SER	N-CA-CB	5.48	119.75	110.49
1	A	655	THR	CA-CB-OG1	-5.44	101.44	109.60
1	B	1120	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	165	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	980	ASP	CA-CB-CG	5.42	118.02	112.60
1	A	956	ASP	CA-CB-CG	5.35	117.95	112.60
1	A	590	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	932	THR	CA-CB-OG1	-5.28	101.69	109.60
1	B	180	VAL	N-CA-CB	-5.26	107.19	111.67
1	A	666	ASP	CA-CB-CG	5.19	117.79	112.60
1	B	848	ASP	CA-CB-CG	5.13	117.73	112.60
1	A	1120	ASP	CA-CB-CG	5.12	117.72	112.60
1	B	522	VAL	N-CA-CB	5.11	120.02	110.77
1	A	937	ASP	CA-CB-CG	5.08	117.68	112.60
1	B	377	THR	CA-CB-OG1	-5.07	102.00	109.60
1	A	1261	GLU	N-CA-CB	-5.05	103.47	110.38
1	B	980	ASP	CA-CB-CG	5.05	117.65	112.60
1	A	478	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	165	ASP	CA-CB-CG	5.03	117.63	112.60
1	B	1018	THR	CA-CB-OG1	-5.02	102.07	109.60

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1036	ARG	Sidechain
1	A	1275	ARG	Sidechain
1	A	225	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	320	ARG	Sidechain
1	A	428	ARG	Sidechain
1	A	693	ARG	Sidechain
1	A	708	ARG	Sidechain
1	A	736	ARG	Sidechain
1	A	780	ARG	Sidechain
1	A	790	ARG	Sidechain
1	B	225	ARG	Sidechain
1	B	238	ARG	Sidechain
1	B	780	ARG	Sidechain
1	B	790	ARG	Sidechain
1	B	85	ARG	Sidechain
1	B	945	ARG	Sidechain

## 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	9522	0	9119	165	0
1	B	9522	0	9118	157	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	2	0	0	3	0
3	B	2	0	0	3	0
4	A	1	0	0	1	0
4	B	1	0	0	0	0
All	All	19074	0	18261	322	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 9.

All (322) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:959:LYS:HE2	1:B:961:ILE:HD11	1.25	1.14
1:B:111:ASN:ND2	3:B:1302:IOD:I	2.49	1.14
1:A:959:LYS:HE2	1:A:961:ILE:HD11	1.25	1.13
1:B:952:ILE:HG12	1:B:961:ILE:CD1	1.80	1.12
1:A:952:ILE:HG12	1:A:961:ILE:CD1	1.79	1.11
1:B:952:ILE:HG12	1:B:961:ILE:HD12	1.34	1.08
1:A:952:ILE:HG12	1:A:961:ILE:HD12	1.35	1.02
1:A:959:LYS:HE2	1:A:961:ILE:CD1	1.92	0.98
1:B:959:LYS:HE2	1:B:961:ILE:CD1	1.93	0.98
1:B:644:ILE:HD11	1:B:673:TRP:HZ2	1.36	0.88
1:B:644:ILE:HD12	1:B:662:TYR:CE2	2.09	0.88
1:A:590:ASP:OD2	1:A:645:LYS:HG3	1.74	0.87
1:B:590:ASP:OD2	1:B:645:LYS:HG3	1.75	0.86
1:A:1071:VAL:HG11	1:A:1164:TYR:CD1	2.11	0.85
1:B:529:LYS:O	1:B:877:LEU:HD11	1.80	0.82
1:A:505:PRO:CD	1:A:892:VAL:CG1	2.59	0.81
1:A:505:PRO:HD2	1:A:892:VAL:CG1	2.10	0.81
1:A:959:LYS:CE	1:A:961:ILE:HD11	2.09	0.81
1:B:505:PRO:CD	1:B:892:VAL:CG1	2.59	0.81
1:B:644:ILE:HD11	1:B:673:TRP:CZ2	2.16	0.80
1:B:959:LYS:CE	1:B:961:ILE:HD11	2.09	0.80
1:B:422:THR:HG21	1:B:458:ASP:OD1	1.82	0.79
1:B:505:PRO:HD2	1:B:892:VAL:CG1	2.12	0.79
1:A:342:ILE:HG21	1:A:349:MET:HE1	1.64	0.78
1:A:529:LYS:O	1:A:877:LEU:HD11	1.83	0.78
1:A:422:THR:HG21	1:A:458:ASP:OD1	1.83	0.78
1:A:505:PRO:HD2	1:A:892:VAL:HG12	1.63	0.78
1:B:342:ILE:HG21	1:B:349:MET:HE1	1.64	0.76
1:B:505:PRO:HD2	1:B:892:VAL:HG12	1.65	0.76
1:A:1071:VAL:HG11	1:A:1164:TYR:CG	2.20	0.75
1:A:513:ASP:OD1	1:A:514:ASP:OD1	2.05	0.74
1:B:891:ASP:CG	1:B:907:LEU:HD12	2.12	0.74
1:A:693:ARG:O	1:A:694:ALA:HB3	1.88	0.73
1:A:891:ASP:CG	1:A:907:LEU:HD12	2.14	0.71
1:A:312:ARG:HD2	1:A:334:ARG:NH2	2.06	0.70
1:B:494:PRO:HG2	1:B:913:VAL:HG13	1.73	0.70
1:B:1035:LEU:H	1:B:1063:THR:HG22	1.56	0.69
1:B:505:PRO:CD	1:B:892:VAL:HG11	2.22	0.69
1:A:1035:LEU:H	1:A:1063:THR:HG22	1.56	0.69
1:B:312:ARG:HD2	1:B:334:ARG:NH2	2.08	0.69
1:A:422:THR:HG23	1:A:456:ARG:HD3	1.75	0.68
1:B:422:THR:HG23	1:B:456:ARG:HD3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:537:ARG:NH1	1:A:839:ALA:O	2.25	0.68
1:A:505:PRO:CD	1:A:892:VAL:HG11	2.24	0.67
1:B:720:HIS:CG	1:B:721:GLY:N	2.62	0.67
1:A:1071:VAL:HG12	1:A:1071:VAL:O	1.93	0.67
1:A:1044:PHE:HB2	1:A:1165:VAL:CG1	2.25	0.66
1:A:679:LYS:HD3	1:A:749:GLU:HG3	1.78	0.66
1:B:1203:LEU:CD2	1:B:1221:VAL:HG22	2.26	0.65
1:A:529:LYS:O	1:A:877:LEU:CD1	2.44	0.64
1:A:87:LEU:HD12	1:A:116:LEU:HD11	1.79	0.64
1:A:720:HIS:CG	1:A:721:GLY:N	2.66	0.64
1:A:1134:ASN:O	1:A:1136:ARG:HG2	1.98	0.63
1:B:999:LYS:O	1:B:1000:ALA:HB3	1.98	0.63
1:A:582:ARG:O	1:A:1136:ARG:NH2	2.29	0.63
1:A:999:LYS:O	1:A:1000:ALA:HB3	1.99	0.63
1:A:720:HIS:CG	1:A:721:GLY:H	2.15	0.63
1:B:529:LYS:O	1:B:877:LEU:CD1	2.46	0.62
1:B:1134:ASN:O	1:B:1136:ARG:HG2	2.00	0.62
1:B:1011:ILE:HD12	3:B:1303:IOD:I	2.70	0.61
1:A:514:ASP:OD1	4:A:1304:CA:CA	1.77	0.61
1:B:505:PRO:CD	1:B:892:VAL:HG12	2.30	0.61
1:B:87:LEU:HD12	1:B:116:LEU:HD11	1.83	0.60
1:A:36:TRP:CE3	1:A:80:LEU:CD2	2.85	0.60
1:A:585:ARG:HH11	1:A:1009:SER:HB2	1.65	0.60
1:B:582:ARG:O	1:B:1136:ARG:NH2	2.29	0.60
1:B:755:ALA:HA	1:B:765:PHE:CZ	2.37	0.60
1:B:644:ILE:CD1	1:B:662:TYR:CE2	2.85	0.59
1:A:1011:ILE:HD12	3:A:1303:IOD:I	2.73	0.59
1:A:1044:PHE:HB2	1:A:1165:VAL:HG11	1.83	0.59
1:A:336:VAL:HG11	1:A:358:VAL:CG2	2.32	0.59
1:A:952:ILE:CG1	1:A:961:ILE:CD1	2.70	0.59
1:B:29:TRP:O	1:B:71:SER:HB3	2.02	0.59
1:B:36:TRP:CE3	1:B:80:LEU:CD2	2.85	0.59
1:A:234:GLU:HA	1:A:252:ARG:HG3	1.85	0.59
1:A:29:TRP:O	1:A:71:SER:HB3	2.02	0.58
1:A:1102:ASP:HB3	1:A:1172:SER:OG	2.04	0.58
1:B:505:PRO:HD3	1:B:892:VAL:CG1	2.32	0.58
1:A:752:ASN:HB2	1:A:759:SER:O	2.03	0.58
1:A:619:GLY:HA2	1:A:630:ALA:HB3	1.86	0.57
1:B:336:VAL:HG11	1:B:358:VAL:CG2	2.34	0.57
1:A:655:THR:HG21	1:A:680:VAL:HB	1.87	0.57
1:A:771:ILE:HA	1:A:787:THR:HG21	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:THR:HG21	1:A:1068:VAL:O	2.04	0.57
1:B:771:ILE:HA	1:B:787:THR:HG21	1.86	0.57
1:B:585:ARG:HH11	1:B:1009:SER:HB2	1.69	0.57
1:B:234:GLU:HA	1:B:252:ARG:HG3	1.87	0.57
1:A:694:ALA:O	1:A:695:LYS:C	2.47	0.57
1:A:952:ILE:HG12	1:A:961:ILE:HD13	1.81	0.57
1:B:402:GLY:HA2	1:B:435:ASP:OD1	2.05	0.57
1:B:952:ILE:HG12	1:B:961:ILE:HD13	1.83	0.56
1:A:505:PRO:HD3	1:A:892:VAL:CG1	2.33	0.56
1:A:1113:LEU:O	1:A:1116:MET:HG3	2.05	0.56
1:B:196:GLU:O	1:B:225:ARG:NH2	2.37	0.56
1:B:1063:THR:HG21	1:B:1068:VAL:O	2.06	0.55
1:A:755:ALA:HA	1:A:765:PHE:CZ	2.41	0.55
1:B:58:SER:HB2	1:B:62:HIS:CD2	2.42	0.55
1:A:505:PRO:CD	1:A:892:VAL:HG12	2.30	0.55
1:B:913:VAL:HG12	1:B:916:ARG:HB2	1.87	0.55
1:B:952:ILE:CG1	1:B:961:ILE:CD1	2.71	0.55
1:B:1239:SER:HA	1:B:1240:PRO:C	2.31	0.55
1:A:1239:SER:HA	1:A:1240:PRO:C	2.31	0.55
1:B:312:ARG:HD2	1:B:334:ARG:CZ	2.37	0.55
1:A:766:SER:HB3	1:A:769:THR:HG21	1.89	0.54
1:B:952:ILE:CG1	1:B:961:ILE:HD12	2.24	0.54
1:A:1082:GLU:HG2	1:A:1084:THR:HG23	1.89	0.54
1:B:1082:GLU:HG2	1:B:1084:THR:HG23	1.89	0.54
1:A:312:ARG:HD2	1:A:334:ARG:CZ	2.37	0.54
1:B:720:HIS:CG	1:B:721:GLY:H	2.24	0.54
1:A:679:LYS:HD3	1:A:749:GLU:CG	2.37	0.54
1:A:110:THR:HG21	1:A:167:PRO:HG2	1.88	0.54
1:A:745:LYS:HE3	1:A:758:TRP:HA	1.90	0.54
1:B:505:PRO:HD2	1:B:892:VAL:HG11	1.87	0.54
1:A:558:HIS:HE2	1:A:885:TRP:HE1	1.56	0.53
1:B:226:GLY:HA2	1:B:244:LEU:O	2.08	0.53
1:B:779:GLY:O	1:B:780:ARG:C	2.51	0.53
1:A:693:ARG:O	1:A:694:ALA:CB	2.48	0.53
1:B:1182:THR:O	1:B:1183:SER:C	2.52	0.53
1:A:1047:VAL:HA	1:A:1165:VAL:HG21	1.91	0.53
1:A:1178:GLU:HB2	1:A:1185:ARG:HG3	1.91	0.53
1:B:422:THR:HG23	1:B:456:ARG:CD	2.37	0.53
1:A:655:THR:OG1	1:A:682:GLY:HA2	2.08	0.53
1:B:1113:LEU:O	1:B:1116:MET:HG3	2.08	0.53
1:B:1203:LEU:HD21	1:B:1221:VAL:HG22	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:497:PRO:O	1:B:498:ALA:HB3	2.09	0.53
1:A:892:VAL:CG2	1:A:907:LEU:HD21	2.39	0.52
1:A:1071:VAL:CG1	1:A:1164:TYR:CD1	2.90	0.52
1:A:211:LEU:HD23	1:A:237:ALA:HB1	1.90	0.52
1:A:226:GLY:HA2	1:A:244:LEU:O	2.08	0.52
1:A:779:GLY:O	1:A:780:ARG:C	2.52	0.52
1:B:537:ARG:NH1	1:B:839:ALA:O	2.27	0.52
1:A:1011:ILE:CD1	1:A:1143:VAL:HG13	2.40	0.52
1:A:1143:VAL:HG12	1:A:1143:VAL:O	2.09	0.52
1:A:1182:THR:O	1:A:1183:SER:C	2.53	0.52
1:A:1044:PHE:HB2	1:A:1165:VAL:HG13	1.90	0.52
1:B:1090:PRO:O	1:B:1091:VAL:HB	2.09	0.52
1:B:1178:GLU:HB2	1:B:1185:ARG:HG3	1.90	0.52
1:A:422:THR:HG23	1:A:456:ARG:CD	2.39	0.51
1:B:497:PRO:HD3	1:B:913:VAL:HG21	1.93	0.51
1:B:850:ILE:O	1:B:851:LYS:C	2.54	0.51
1:A:58:SER:O	1:A:59:ALA:C	2.53	0.51
1:A:225:ARG:HA	1:A:225:ARG:NE	2.26	0.51
1:A:381:ALA:O	1:A:382:PRO:C	2.54	0.51
1:A:497:PRO:O	1:A:498:ALA:HB3	2.10	0.51
1:B:358:VAL:HG12	1:B:359:ASP:N	2.26	0.51
1:B:1011:ILE:CD1	3:B:1303:IOD:I	3.29	0.51
1:A:850:ILE:O	1:A:851:LYS:C	2.54	0.50
1:A:358:VAL:HG12	1:A:359:ASP:N	2.25	0.50
1:A:111:ASN:HB2	3:A:1302:IOD:I	2.81	0.50
1:B:522:VAL:C	1:B:524:TRP:H	2.20	0.50
1:B:1027:PRO:HD2	1:B:1030:LEU:HG	1.94	0.50
1:B:1143:VAL:HG12	1:B:1143:VAL:O	2.11	0.50
1:B:582:ARG:HB2	1:B:594:GLU:HG2	1.93	0.50
1:B:160:VAL:HG12	1:B:198:MET:HE3	1.92	0.50
1:A:336:VAL:HG11	1:A:358:VAL:HG22	1.94	0.49
1:B:422:THR:CG2	1:B:456:ARG:HD3	2.43	0.49
1:A:1035:LEU:N	1:A:1063:THR:HG22	2.27	0.49
1:B:381:ALA:O	1:B:382:PRO:C	2.55	0.49
1:B:892:VAL:CG2	1:B:907:LEU:HD21	2.42	0.49
1:B:1284:ALA:HB1	1:B:1285:PRO:HD2	1.93	0.49
1:A:458:ASP:O	1:A:459:MET:C	2.56	0.49
1:B:522:VAL:C	1:B:524:TRP:N	2.70	0.49
1:B:1098:TYR:CE1	1:B:1185:ARG:HD2	2.47	0.49
1:A:505:PRO:HD2	1:A:892:VAL:HG11	1.87	0.49
1:B:509:PHE:CE1	1:B:572:LEU:HD21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:602:LEU:HD21	1:B:890:ALA:HB2	1.95	0.49
1:B:1011:ILE:CD1	1:B:1143:VAL:HG13	2.43	0.49
1:A:86:TYR:CD2	1:A:117:ARG:HD2	2.48	0.48
1:B:388:VAL:HG11	1:B:425:GLN:OE1	2.12	0.48
1:A:213:ALA:O	1:A:214:GLY:C	2.56	0.48
1:A:1141:GLY:HA2	1:A:1145:PRO:HG3	1.94	0.48
1:B:1003:LEU:HD13	1:B:1019:SER:OG	2.14	0.48
1:A:522:VAL:C	1:A:524:TRP:N	2.70	0.48
1:A:1011:ILE:CD1	3:A:1303:IOD:I	3.31	0.48
1:A:1098:TYR:CE1	1:A:1185:ARG:HD2	2.48	0.48
1:B:582:ARG:HB2	1:B:594:GLU:CG	2.43	0.48
1:B:766:SER:HB3	1:B:769:THR:HG21	1.95	0.48
1:B:496:MET:HE1	1:B:908:PRO:HG3	1.96	0.48
1:A:952:ILE:CG1	1:A:961:ILE:HD12	2.25	0.48
1:A:623:GLN:O	1:A:624:SER:C	2.57	0.47
1:A:509:PHE:CE1	1:A:572:LEU:HD21	2.49	0.47
1:A:422:THR:CG2	1:A:456:ARG:HD3	2.43	0.47
1:A:602:LEU:HD21	1:A:890:ALA:HB2	1.95	0.47
1:B:112:LYS:O	1:B:114:VAL:HG23	2.14	0.47
1:A:522:VAL:C	1:A:524:TRP:H	2.21	0.47
1:A:410:ASP:OD2	1:A:449:HIS:ND1	2.39	0.47
1:A:999:LYS:O	1:A:1000:ALA:CB	2.62	0.47
1:A:1027:PRO:HD2	1:A:1030:LEU:HG	1.96	0.47
1:B:458:ASP:O	1:B:459:MET:C	2.56	0.47
1:B:615:LYS:HE2	1:B:646:HIS:CD2	2.49	0.47
1:B:1176:GLN:HA	1:B:1187:PRO:HA	1.96	0.47
1:A:593:ILE:HG23	1:A:618:VAL:HB	1.96	0.47
1:A:1003:LEU:HD13	1:A:1019:SER:OG	2.14	0.47
1:B:1204:GLU:HG3	1:B:1205:LYS:HG2	1.96	0.47
1:A:344:LEU:HG	1:A:360:LEU:HD11	1.96	0.47
1:B:1035:LEU:N	1:B:1063:THR:HG22	2.27	0.47
1:B:623:GLN:O	1:B:624:SER:C	2.58	0.47
1:A:388:VAL:HG11	1:A:425:GLN:OE1	2.15	0.46
1:A:591:TYR:CE2	1:A:626:LYS:HE3	2.50	0.46
1:B:410:ASP:OD2	1:B:449:HIS:ND1	2.41	0.46
1:A:959:LYS:HE2	1:A:961:ILE:CG1	2.45	0.46
1:A:160:VAL:HG12	1:A:198:MET:HE3	1.97	0.46
1:A:278:LEU:HD11	1:A:292:VAL:HG11	1.97	0.46
1:B:86:TYR:CD2	1:B:117:ARG:HD2	2.51	0.46
1:B:211:LEU:HD23	1:B:237:ALA:HB1	1.96	0.46
1:B:730:TYR:OH	1:B:740:LEU:HD12	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:999:LYS:O	1:B:1000:ALA:CB	2.63	0.46
1:A:507:ILE:O	1:A:711:PHE:HA	2.16	0.46
1:B:1141:GLY:HA2	1:B:1145:PRO:HG3	1.98	0.46
1:B:365:SER:HA	1:B:385:THR:OG1	2.16	0.45
1:B:907:LEU:N	1:B:908:PRO:CD	2.79	0.45
1:A:496:MET:HE1	1:A:908:PRO:HG3	1.98	0.45
1:B:36:TRP:HB2	1:B:80:LEU:HD23	1.98	0.45
1:B:344:LEU:HG	1:B:360:LEU:HD11	1.97	0.45
1:B:336:VAL:HG11	1:B:358:VAL:HG22	1.97	0.45
1:B:959:LYS:HE2	1:B:961:ILE:CG1	2.47	0.45
1:A:1204:GLU:HG3	1:A:1205:LYS:HG2	1.99	0.45
1:B:1137:GLU:H	1:B:1137:GLU:HG2	1.58	0.45
1:A:86:TYR:CE2	1:A:117:ARG:HD2	2.51	0.45
1:A:1182:THR:O	1:A:1182:THR:OG1	2.32	0.45
1:B:213:ALA:O	1:B:214:GLY:C	2.59	0.45
1:A:582:ARG:HB2	1:A:594:GLU:HG2	1.99	0.45
1:A:692:ALA:C	1:A:693:ARG:O	2.57	0.45
1:B:1229:VAL:HG12	1:B:1230:SER:N	2.32	0.45
1:A:582:ARG:HB2	1:A:594:GLU:CG	2.47	0.45
1:A:621:GLY:O	1:A:624:SER:OG	2.25	0.45
1:B:1023:PRO:HD3	1:B:1154:THR:HB	1.99	0.45
1:A:803:LEU:HD13	1:A:812:THR:HG21	1.99	0.45
1:B:574:LEU:HD11	1:B:593:ILE:HB	1.98	0.45
1:B:724:SER:HB3	1:B:831:TYR:O	2.16	0.45
1:A:1229:VAL:HG12	1:A:1230:SER:N	2.33	0.44
1:A:1137:GLU:H	1:A:1137:GLU:HG2	1.56	0.44
1:B:611:ALA:HB2	1:B:697:TRP:CZ2	2.53	0.44
1:A:36:TRP:HB2	1:A:80:LEU:HD23	1.99	0.44
1:A:907:LEU:N	1:A:908:PRO:CD	2.81	0.44
1:A:574:LEU:HD11	1:A:593:ILE:HB	1.99	0.44
1:A:1092:THR:HG23	1:A:1154:THR:HA	2.00	0.43
1:A:881:GLN:HB3	1:A:883:GLN:NE2	2.32	0.43
1:B:618:VAL:HG23	1:B:618:VAL:O	2.17	0.43
1:A:96:ASN:OD1	1:A:96:ASN:C	2.61	0.43
1:B:54:GLY:H	1:B:62:HIS:HD2	1.65	0.43
1:A:679:LYS:HB3	1:A:749:GLU:H	1.83	0.43
1:A:1176:GLN:HA	1:A:1187:PRO:HA	2.01	0.43
1:B:86:TYR:CE2	1:B:117:ARG:HD2	2.53	0.43
1:A:358:VAL:CG1	1:A:359:ASP:N	2.81	0.43
1:A:583:VAL:HG22	1:A:1143:VAL:HG11	2.00	0.43
1:B:583:VAL:HG22	1:B:1143:VAL:HG11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1284:ALA:HB1	1:A:1285:PRO:HD2	2.00	0.43
1:A:1205:LYS:HE2	1:A:1219:LEU:HB3	2.01	0.43
1:B:119:GLU:HG2	1:B:146:ALA:HB2	2.01	0.43
1:B:507:ILE:O	1:B:711:PHE:HA	2.18	0.43
1:A:351:PHE:O	1:A:370:GLY:HA3	2.19	0.42
1:A:690:PHE:O	1:A:693:ARG:O	2.36	0.42
1:B:313:GLN:NE2	1:B:332:GLU:OE2	2.52	0.42
1:B:1030:LEU:HD23	1:B:1030:LEU:HA	1.93	0.42
1:A:182:ARG:HG2	1:A:182:ARG:HH11	1.84	0.42
1:A:1164:TYR:CD1	1:A:1164:TYR:C	2.97	0.42
1:B:358:VAL:CG1	1:B:359:ASP:N	2.81	0.42
1:B:442:ILE:HG23	1:B:488:THR:HG21	2.01	0.42
1:A:1007:ARG:NH2	1:A:1133:SER:O	2.52	0.42
1:B:96:ASN:C	1:B:96:ASN:OD1	2.62	0.42
1:B:1182:THR:O	1:B:1182:THR:OG1	2.31	0.42
1:A:1051:ARG:HH21	1:A:1161:ARG:NH2	2.18	0.42
1:B:1204:GLU:HG2	1:B:1220:THR:H	1.84	0.42
1:A:692:ALA:HB2	1:A:740:LEU:HD22	2.01	0.42
1:B:803:LEU:HD13	1:B:812:THR:HG21	2.01	0.42
1:B:1092:THR:HG23	1:B:1154:THR:HA	2.01	0.42
1:B:1229:VAL:HG21	1:B:1249:LEU:HD13	2.02	0.42
1:A:442:ILE:HG23	1:A:488:THR:HG21	2.01	0.42
1:A:1030:LEU:HD23	1:A:1030:LEU:HA	1.94	0.42
1:B:222:LEU:O	1:B:223:ALA:C	2.62	0.42
1:B:1099:LEU:C	1:B:1099:LEU:HD23	2.45	0.42
1:A:313:GLN:NE2	1:A:332:GLU:OE2	2.53	0.42
1:A:799:MET:HE2	1:A:799:MET:HB3	1.85	0.41
1:A:1204:GLU:HG2	1:A:1220:THR:H	1.84	0.41
1:B:67:ALA:C	1:B:69:THR:H	2.28	0.41
1:A:522:VAL:HG13	1:A:546:ASP:HA	2.01	0.41
1:A:886:MET:HB2	1:A:886:MET:HE3	1.73	0.41
1:A:1047:VAL:HA	1:A:1165:VAL:CG2	2.48	0.41
1:A:1023:PRO:HD3	1:A:1154:THR:HB	2.03	0.41
1:B:87:LEU:CD1	1:B:116:LEU:HD11	2.49	0.41
1:B:242:MET:HE3	1:B:242:MET:HB3	1.91	0.41
1:B:695:LYS:NZ	1:B:735:GLY:O	2.53	0.41
1:B:702:HIS:CD2	1:B:806:LEU:HB3	2.55	0.41
1:B:1089:VAL:HG12	1:B:1155:ALA:HA	2.02	0.41
1:A:388:VAL:CG1	1:A:425:GLN:OE1	2.68	0.41
1:A:688:ASP:HA	1:A:740:LEU:HD11	2.02	0.41
1:B:764:ASP:OD1	1:B:764:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ALA:C	1:A:69:THR:H	2.28	0.41
1:A:1099:LEU:HD23	1:A:1099:LEU:C	2.46	0.41
1:B:388:VAL:CG1	1:B:425:GLN:OE1	2.69	0.41
1:A:242:MET:HE3	1:A:242:MET:HB3	1.90	0.41
1:A:365:SER:HA	1:A:385:THR:OG1	2.21	0.41
1:B:881:GLN:HB3	1:B:883:GLN:NE2	2.35	0.41
1:B:907:LEU:HB2	1:B:908:PRO:HD3	2.02	0.41
1:B:1067:ASP:OD1	1:B:1067:ASP:N	2.52	0.41
1:B:1164:TYR:CD1	1:B:1164:TYR:C	2.99	0.41
1:A:730:TYR:O	1:A:731:PRO:C	2.64	0.41
1:A:885:TRP:O	1:A:886:MET:C	2.63	0.41
1:B:619:GLY:HA2	1:B:630:ALA:HB3	2.03	0.41
1:B:802:LEU:O	1:B:806:LEU:HG	2.21	0.41
1:A:225:ARG:NH2	1:A:226:GLY:H	2.19	0.41
1:B:36:TRP:CE3	1:B:80:LEU:HD21	2.55	0.41
1:B:182:ARG:HH11	1:B:182:ARG:HG2	1.86	0.41
1:B:932:THR:O	1:B:944:GLY:HA2	2.21	0.41
1:B:198:MET:O	1:B:225:ARG:NE	2.54	0.41
1:B:622:GLY:HA2	1:B:645:LYS:HD3	2.01	0.41
1:B:913:VAL:HG12	1:B:913:VAL:O	2.21	0.41
1:B:1083:LEU:HB2	1:B:1162:ILE:HB	2.02	0.41
1:B:422:THR:HA	1:B:423:PRO:HD3	1.92	0.40
1:A:716:PHE:HA	1:A:717:PRO:HD3	1.90	0.40
1:A:907:LEU:HB2	1:A:908:PRO:HD3	2.03	0.40
1:A:693:ARG:HA	1:A:693:ARG:HD3	1.85	0.40
1:A:726:PRO:HG2	1:A:770:TYR:HB3	2.03	0.40
1:A:844:TYR:OH	1:A:937:ASP:OD2	2.26	0.40
1:A:1011:ILE:HD11	1:A:1143:VAL:HG13	2.02	0.40
1:B:644:ILE:CD1	1:B:662:TYR:CD2	3.04	0.40
1:A:504:ARG:HA	1:A:608:TYR:OH	2.20	0.40
1:B:504:ARG:HA	1:B:608:TYR:OH	2.22	0.40
1:B:580:HIS:HD1	1:B:902:ASP:CG	2.29	0.40
1:B:854:CYS:HB3	1:B:952:ILE:HD11	2.03	0.40
1:B:278:LEU:O	1:B:296:VAL:HA	2.21	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	1261/1263 (100%)	1137 (90%)	114 (9%)	10 (1%)	16	44
1	B	1261/1263 (100%)	1143 (91%)	111 (9%)	7 (1%)	21	51
All	All	2522/2526 (100%)	2280 (90%)	225 (9%)	17 (1%)	18	48

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	59	ALA
1	A	382	PRO
1	B	382	PRO
1	B	1170	SER
1	A	246	GLN
1	A	759	SER
1	B	246	GLN
1	A	1170	SER
1	B	1091	VAL
1	A	694	ALA
1	A	746	ASP
1	B	130	GLU
1	B	678	ALA
1	A	384	GLY
1	A	214	GLY
1	A	497	PRO
1	B	214	GLY

### 5.3.2 Protein sidechains [i](#)

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	993/993 (100%)	972 (98%)	21 (2%)	47	77
1	B	993/993 (100%)	967 (97%)	26 (3%)	40	73
All	All	1986/1986 (100%)	1939 (98%)	47 (2%)	43	75

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	ASP
1	A	227	MET
1	A	435	ASP
1	A	526	GLN
1	A	532	ARG
1	A	539	GLU
1	A	557	ARG
1	A	596	SER
1	A	693	ARG
1	A	728	CYS
1	A	782	GLU
1	A	784	ARG
1	A	820	ASN
1	A	825	GLU
1	A	846	MET
1	A	916	ARG
1	A	945	ARG
1	A	1008	SER
1	A	1137	GLU
1	A	1140	SER
1	A	1203	LEU
1	B	33	ASP
1	B	65	VAL
1	B	74	ARG
1	B	85	ARG
1	B	329	LYS
1	B	355	ILE
1	B	497	PRO
1	B	526	GLN
1	B	532	ARG
1	B	539	GLU
1	B	596	SER
1	B	655	THR
1	B	677	SER

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Mol	Chain	Res	Type
1	B	724	SER
1	B	764	ASP
1	B	782	GLU
1	B	820	ASN
1	B	825	GLU
1	B	846	MET
1	B	886	MET
1	B	915	GLU
1	B	916	ARG
1	B	1008	SER
1	B	1137	GLU
1	B	1140	SER
1	B	1172	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	269	GLN
1	A	587	ASN
1	A	836	GLN
1	A	1001	GLN
1	A	1117	GLN
1	B	141	GLN
1	B	269	GLN
1	B	350	HIS
1	B	587	ASN
1	B	646	HIS
1	B	836	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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
2	GAL	A	1301	-	12,12,12	0.66	0	17,17,17	0.93	2 (11%)
2	GAL	B	1301	-	12,12,12	0.86	1 (8%)	17,17,17	1.09	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	A	1301	-	-	0/2/22/22	0/1/1/1
2	GAL	B	1301	-	-	0/2/22/22	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	GAL	C4-C5	2.17	1.57	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1301	GAL	C1-O5-C5	-2.91	108.18	113.66
2	A	1301	GAL	C1-O5-C5	-2.11	109.68	113.66
2	A	1301	GAL	O5-C1-C2	-2.01	106.69	110.28

There are no chirality outliers.

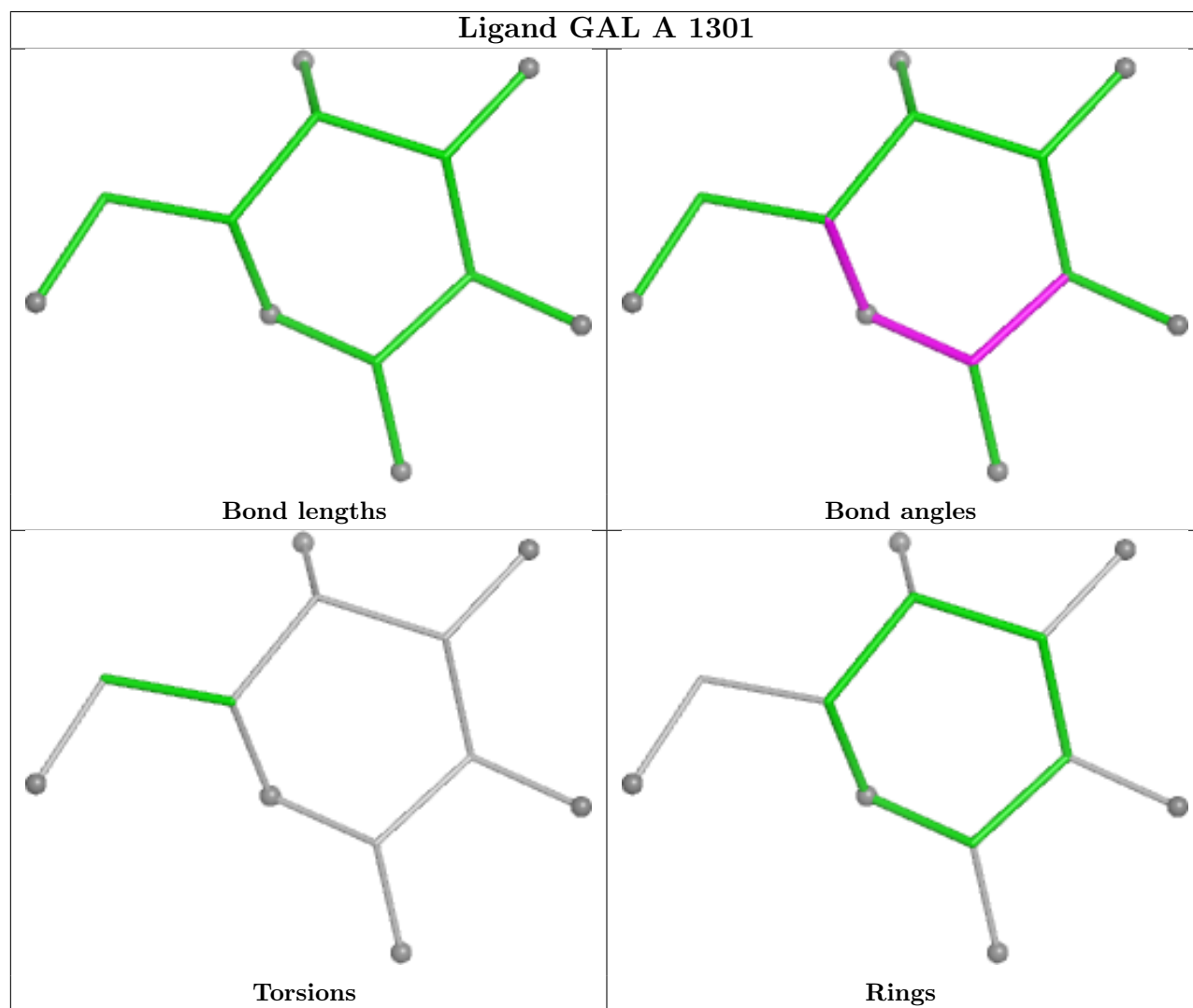
There are no torsion outliers.

There are no ring outliers.

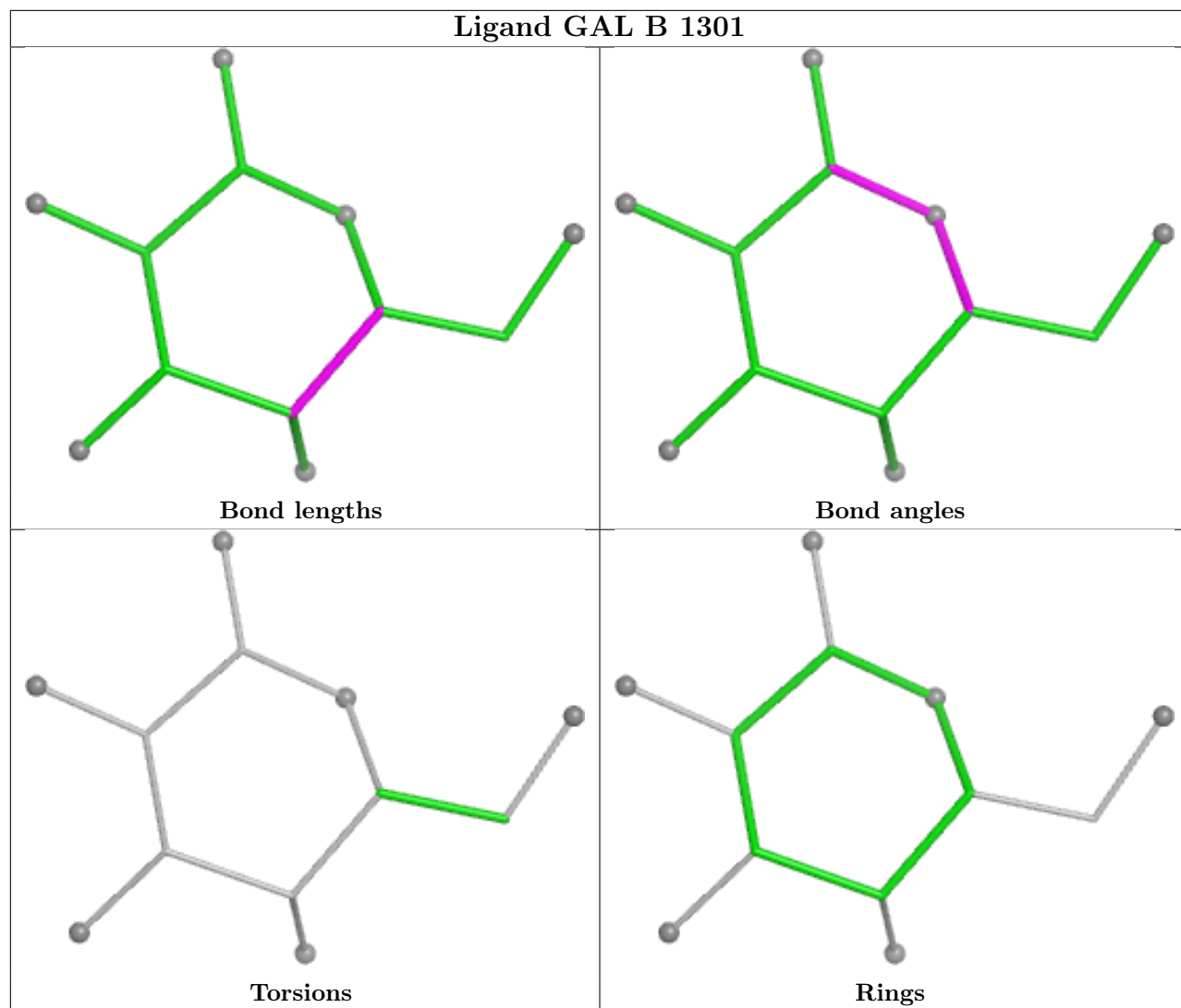
No monomer is involved in short contacts.

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.







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1263/1263 (100%)	-0.10	23 (1%) 67 59	58, 88, 132, 190	0
1	B	1263/1263 (100%)	-0.01	41 (3%) 50 41	55, 87, 134, 194	0
All	All	2526/2526 (100%)	-0.06	64 (2%) 58 48	55, 88, 133, 194	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	438	PHE	5.3
1	A	440	ASP	5.1
1	B	956	ASP	4.4
1	B	434	PHE	4.1
1	B	1198	VAL	4.0
1	B	470	GLU	3.9
1	A	1036	ARG	3.9
1	A	23	ALA	3.8
1	B	440	ASP	3.7
1	A	1198	VAL	3.7
1	B	443	SER	3.7
1	B	1285	PRO	3.7
1	B	23	ALA	3.7
1	A	1285	PRO	3.5
1	B	439	GLU	3.5
1	B	401	LEU	3.5
1	B	444	GLU	3.5
1	B	367	ALA	3.4
1	B	828	SER	3.3
1	B	441	LEU	3.3
1	A	436	SER	3.2
1	B	954	PHE	3.2
1	A	1085	GLY	3.0
1	B	955	VAL	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	1224	HIS	3.0
1	A	329	LYS	2.9
1	A	922	ILE	2.8
1	B	1051	ARG	2.8
1	B	436	SER	2.7
1	B	647	LEU	2.7
1	B	918	LYS	2.7
1	B	651	TYR	2.6
1	B	1046	TRP	2.6
1	B	403	ARG	2.6
1	B	657	GLY	2.6
1	A	1203	LEU	2.6
1	A	953	ILE	2.6
1	B	953	ILE	2.5
1	A	1224	HIS	2.5
1	B	468	LEU	2.5
1	B	437	SER	2.5
1	B	1258	LEU	2.4
1	A	1038	ARG	2.4
1	A	367	ALA	2.4
1	A	131	GLY	2.4
1	B	433	LEU	2.3
1	B	25	VAL	2.3
1	B	920	GLY	2.3
1	A	824	ASN	2.2
1	A	1070	SER	2.2
1	B	469	PRO	2.2
1	A	1050	PHE	2.2
1	B	445	TRP	2.2
1	A	437	SER	2.2
1	B	435	ASP	2.2
1	B	131	GLY	2.2
1	A	439	GLU	2.2
1	A	132	GLY	2.1
1	B	644	ILE	2.1
1	B	1160	ILE	2.1
1	A	457	PRO	2.0
1	B	919	THR	2.0
1	A	438	PHE	2.0
1	B	1018	THR	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

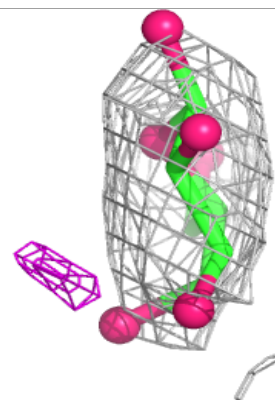
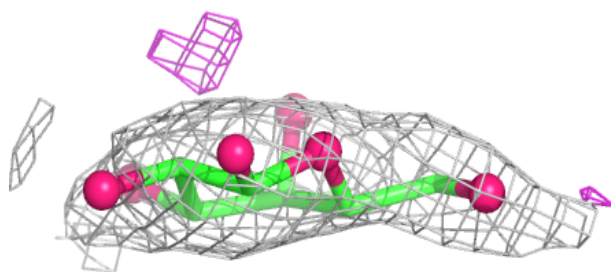
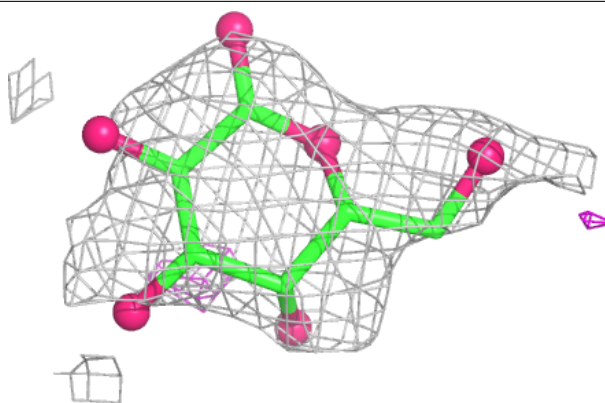
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
2	GAL	B	1301	12/12	0.89	0.11	82,112,123,129	0
2	GAL	A	1301	12/12	0.94	0.08	85,89,97,99	0
3	IOD	A	1302	1/1	0.99	0.05	89,89,89,89	0
3	IOD	A	1303	1/1	0.99	0.03	89,89,89,89	1
3	IOD	B	1302	1/1	0.99	0.06	87,87,87,87	0
3	IOD	B	1303	1/1	0.99	0.03	89,89,89,89	1
4	CA	A	1304	1/1	1.00	0.05	30,30,30,30	1
4	CA	B	1304	1/1	1.00	0.02	26,26,26,26	1

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.

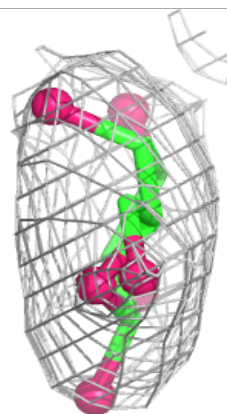
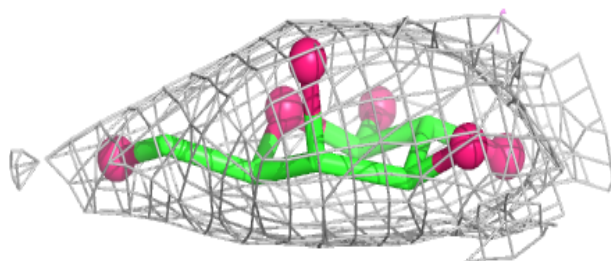
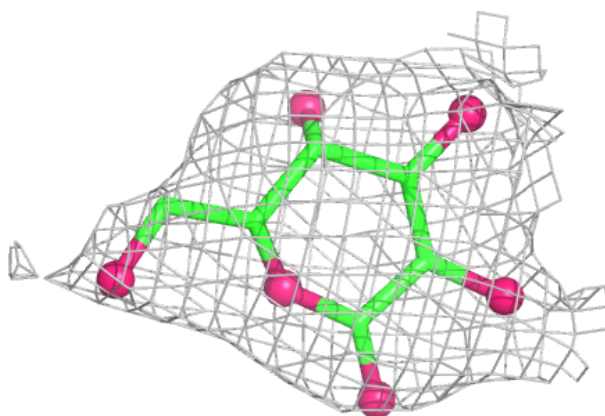
**Electron density around GAL B 1301:**

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



**Electron density around GAL A 1301:**

$2mF_o-DF_c$  (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.