Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:40 PM GMT

PDB ID	:	1BOS
Title	:	SHIGA-LIKE TOXIN COMPLEXED WITH ITS RECEPTOR
Authors	:	Ling, H.; Boodhoo, A.; Hazes, B.; Cummings, M.D.; Armstrong, G.D.; Brunton, J.L.; Read, R.J.
Deposited on	:	1998-01-13
Resolution	:	2.80 Å(reported)

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

The following versions of software and data (see references ①) were used in the production of this report:

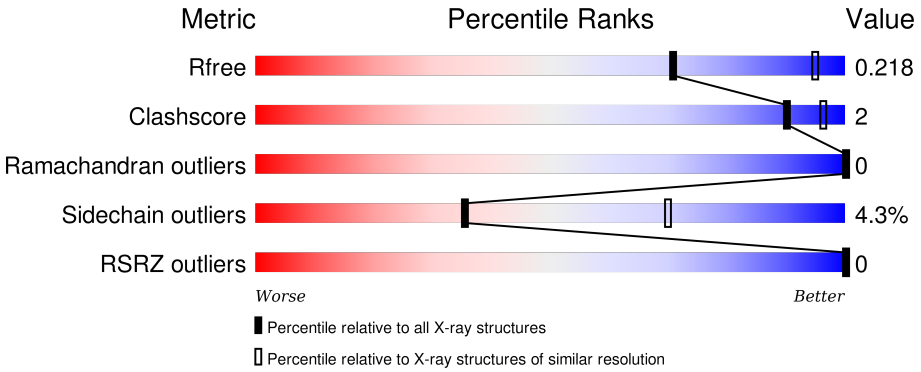
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.80 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	69	90% 9% •
1	B	69	90% 9% •
1	C	69	87% 10% •
1	D	69	90% 7% ••
1	E	69	90% 7% •

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Mol	Chain	Length	Quality of chain
1	F	69	86% 12%
1	G	69	90% 7%
1	H	69	87% 10%
1	I	69	90% 9%
1	J	69	88% 10%
1	K	69	90% 7%
1	L	69	91% 7%
1	M	69	91% 6%
1	N	69	88% 10%
1	O	69	87% 9%
1	P	69	90% 9%
1	Q	69	93% 6%
1	R	69	90% 9%
1	S	69	90% 7%
1	T	69	90% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GLA	J	2580	-	-	-	X
2	GLA	Q	4280	-	-	-	X
3	GLA	B	1270	-	-	-	X
3	GLA	N	3480	-	-	-	X
3	GLA	T	4580	-	-	-	X
4	GAL	C	1370	-	-	-	X
4	GAL	E	1570	-	-	-	X
4	GAL	G	2270	-	-	-	X
4	GAL	I	2470	-	-	-	X
4	GAL	J	2570	-	-	-	X
4	GAL	K	3170	-	-	-	X
4	GAL	L	3270	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GAL	N	3470	-	-	-	X
4	GAL	P	4170	-	-	-	X
4	GAL	R	4370	-	-	-	X
4	GAL	T	4570	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12767 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 SHIGA-LIKE TOXIN I B SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	B	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	C	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	D	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	E	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	F	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	G	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	H	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	I	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	J	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	K	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	L	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	M	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	N	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	O	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	P	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	R	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	S	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			
1	T	69	Total	C	N	O	S	0	0	0
			540	339	90	108	3			

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

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	3	Total	C	O	0	0
			34	18	16		
2	F	3	Total	C	O	0	0
			34	18	16		
2	K	3	Total	C	O	0	0
			34	18	16		
2	P	3	Total	C	O	0	0
			34	18	16		
2	B	3	Total	C	O	0	0
			34	18	16		
2	G	3	Total	C	O	0	0
			34	18	16		
2	L	3	Total	C	O	0	0
			34	18	16		
2	Q	3	Total	C	O	0	0
			34	18	16		
2	C	3	Total	C	O	0	0
			34	18	16		
2	H	3	Total	C	O	0	0
			34	18	16		
2	M	3	Total	C	O	0	0
			34	18	16		
2	R	3	Total	C	O	0	0
			34	18	16		
2	D	3	Total	C	O	0	0
			34	18	16		
2	I	3	Total	C	O	0	0
			34	18	16		
2	N	3	Total	C	O	0	0
			34	18	16		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	S	3	Total C O 34 18 16	0	0
2	E	3	Total C O 34 18 16	0	0
2	J	3	Total C O 34 18 16	0	0
2	O	3	Total C O 34 18 16	0	0
2	T	3	Total C O 34 18 16	0	0
2	F	3	Total C O 34 18 16	11	0
2	Q	3	Total C O 34 18 16	8	0
2	R	3	Total C O 34 18 16	4	0
2	E	3	Total C O 34 18 16	11	0
2	J	3	Total C O 34 18 16	0	0
2	A	3	Total C O 34 18 16	0	0
2	F	3	Total C O 34 18 16	0	0
2	Q	3	Total C O 34 18 16	0	0
2	H	3	Total C O 34 18 16	0	0
2	M	3	Total C O 34 18 16	0	0
2	D	3	Total C O 34 18 16	0	0
2	S	3	Total C O 34 18 16	0	0
2	O	3	Total C O 34 18 16	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total C O 23 12 11	0	0

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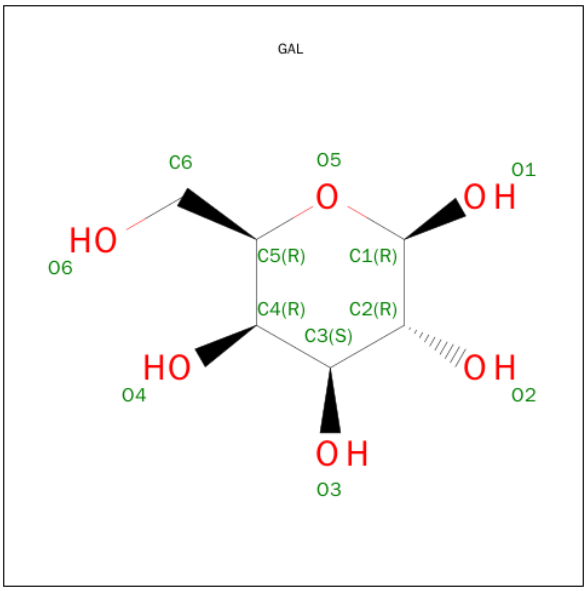
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	K	2	Total C O 23 12 11	0	0
3	P	2	Total C O 23 12 11	0	0
3	B	2	Total C O 23 12 11	0	0
3	G	2	Total C O 23 12 11	0	0
3	L	2	Total C O 23 12 11	0	0
3	C	2	Total C O 23 12 11	0	0
3	H	2	Total C O 23 12 11	0	0
3	M	2	Total C O 23 12 11	0	0
3	D	2	Total C O 23 12 11	0	0
3	I	2	Total C O 23 12 11	0	0
3	N	2	Total C O 23 12 11	0	0
3	S	2	Total C O 23 12 11	0	0
3	O	2	Total C O 23 12 11	0	0
3	T	2	Total C O 23 12 11	0	0
3	B	2	Total C O 23 12 11	0	0

- Molecule 4 is SUGAR (D-GALACTOSE) (three-letter code: GAL) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total C O 12 6 6	0	0
4	C	1	Total C O 12 6 6	0	0
4	E	1	Total C O 12 6 6	0	0
4	G	1	Total C O 12 6 6	0	0
4	I	1	Total C O 12 6 6	0	0
4	J	1	Total C O 12 6 6	0	0
4	K	1	Total C O 12 6 6	0	0
4	L	1	Total C O 12 6 6	0	0
4	N	1	Total C O 12 6 6	0	0
4	R	1	Total C O 12 6 6	0	0
4	T	1	Total C O 12 6 6	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	12	Total O 12 12	0	0

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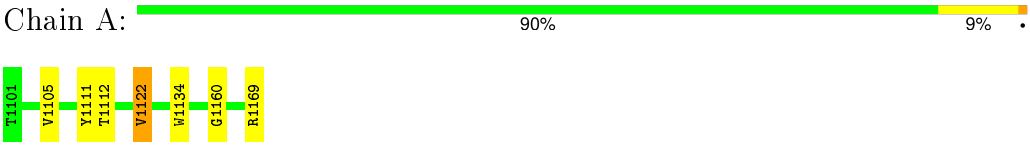
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	27	Total O 27 27	0	0
5	C	19	Total O 19 19	0	0
5	D	16	Total O 16 16	0	0
5	E	18	Total O 18 18	0	0
5	F	15	Total O 15 15	0	0
5	G	21	Total O 21 21	0	0
5	H	17	Total O 17 17	0	0
5	I	17	Total O 17 17	0	0
5	J	15	Total O 15 15	0	0
5	K	21	Total O 21 21	0	0
5	L	23	Total O 23 23	0	0
5	M	24	Total O 24 24	0	0
5	N	14	Total O 14 14	0	0
5	O	23	Total O 23 23	0	0
5	P	17	Total O 17 17	0	0
5	Q	13	Total O 13 13	0	0
5	R	10	Total O 10 10	0	0
5	S	11	Total O 11 11	0	0
5	T	12	Total O 12 12	0	0

3 Residue-property plots (i)

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

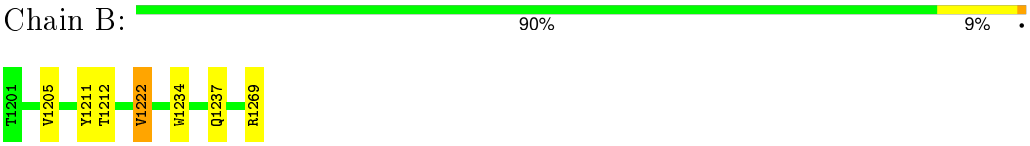
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain A:



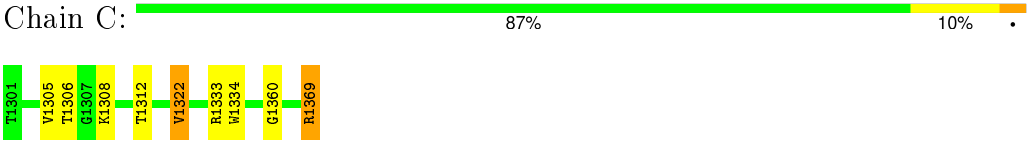
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain B:



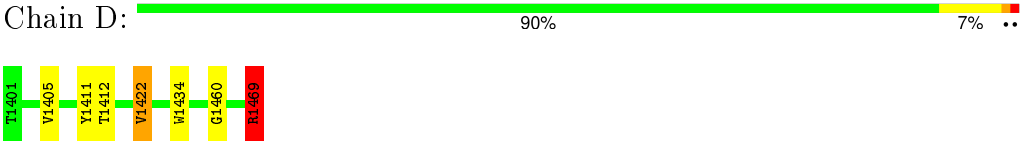
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain C:



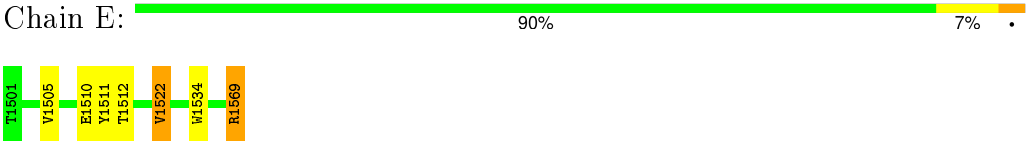
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain D:



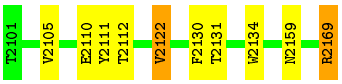
- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain E:



- Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain F:



• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

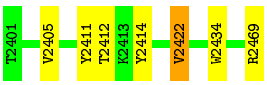
Chain G:

• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain H:

• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain I:



• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

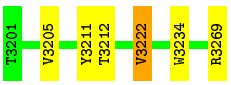
Chain J:

• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain K:

• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain L:

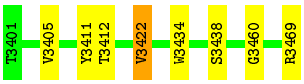


• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain M:

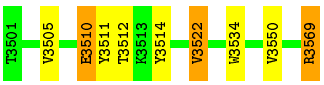
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain N:



• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain O:

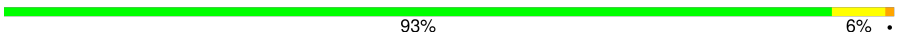


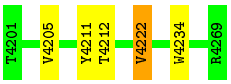
• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain P:

• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain Q:



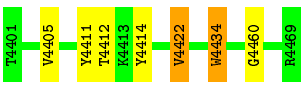


• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain R:

• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain S:



• Molecule 1: SHIGA-LIKE TOXIN I B SUBUNIT

Chain T:


T4501
V4505
E4510
Y4511
T4512
V4522
W4534
G4560
R4569

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	127.50Å 97.70Å 164.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.00 – 2.80 21.05 – 2.75	Depositor EDS
% Data completeness (in resolution range)	81.6 (21.00-2.80) 77.6 (21.05-2.75)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	0.90 (at 2.75Å)	Xtriage
Refinement program	X-PLOR 3.8	Depositor
R, R_{free}	0.170 , 0.226 0.166 , 0.218	Depositor DCC
R_{free} test set	2071 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	22.8	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 39.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 41759 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12767	wwPDB-VP
Average B, all atoms (Å^2)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.85	0/549	1.42	4/742 (0.5%)
1	B	0.85	0/549	1.40	5/742 (0.7%)
1	C	0.88	1/549 (0.2%)	1.44	6/742 (0.8%)
1	D	0.86	0/549	1.33	4/742 (0.5%)
1	E	0.90	0/549	1.35	4/742 (0.5%)
1	F	0.96	1/549 (0.2%)	1.41	7/742 (0.9%)
1	G	0.84	0/549	1.35	5/742 (0.7%)
1	H	0.95	1/549 (0.2%)	1.43	7/742 (0.9%)
1	I	0.88	0/549	1.35	5/742 (0.7%)
1	J	0.76	0/549	1.34	4/742 (0.5%)
1	K	0.85	0/549	1.49	5/742 (0.7%)
1	L	0.84	0/549	1.44	5/742 (0.7%)
1	M	0.86	0/549	1.34	3/742 (0.4%)
1	N	0.88	0/549	1.39	4/742 (0.5%)
1	O	0.88	1/549 (0.2%)	1.46	10/742 (1.3%)
1	P	0.86	0/549	1.33	4/742 (0.5%)
1	Q	0.80	0/549	1.34	3/742 (0.4%)
1	R	0.86	0/549	1.30	4/742 (0.5%)
1	S	0.88	0/549	1.32	5/742 (0.7%)
1	T	0.88	1/549 (0.2%)	1.37	5/742 (0.7%)
All	All	0.87	5/10980 (0.0%)	1.38	99/14840 (0.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	T	4510	GLU	CG-CD	6.03	1.60	1.51
1	O	3510	GLU	CG-CD	5.75	1.60	1.51
1	C	1369	ARG	CZ-NH1	5.41	1.40	1.33
1	F	2169	ARG	NE-CZ	5.20	1.39	1.33
1	H	2369	ARG	NE-CZ	5.04	1.39	1.33

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	3169	ARG	NE-CZ-NH1	16.70	128.65	120.30
1	L	3269	ARG	NE-CZ-NH2	-13.63	113.49	120.30
1	K	3169	ARG	NE-CZ-NH2	-10.11	115.25	120.30
1	T	4569	ARG	NE-CZ-NH1	10.06	125.33	120.30
1	G	2269	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	1169	ARG	NE-CZ-NH1	9.78	125.19	120.30
1	F	2169	ARG	NE-CZ-NH1	9.05	124.83	120.30
1	L	3269	ARG	NE-CZ-NH1	9.03	124.82	120.30
1	B	1269	ARG	NE-CZ-NH1	8.90	124.75	120.30
1	N	3411	TYR	CB-CG-CD2	-8.70	115.78	121.00
1	C	1369	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	H	2369	ARG	CA-CB-CG	8.10	131.22	113.40
1	I	2469	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	O	3569	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	I	2411	TYR	CB-CG-CD2	-7.58	116.45	121.00
1	H	2334	TRP	CD1-CG-CD2	7.54	112.33	106.30
1	C	1334	TRP	CD1-CG-CD2	7.51	112.31	106.30
1	P	4134	TRP	CD1-CG-CD2	7.50	112.30	106.30
1	C	1333	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	T	4569	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	B	1234	TRP	CE2-CD2-CG	-7.36	101.41	107.30
1	R	4311	TYR	CB-CG-CD2	-7.21	116.68	121.00
1	B	1234	TRP	CD1-CG-CD2	7.12	112.00	106.30
1	C	1333	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	Q	4234	TRP	CD1-CG-CD2	7.09	111.97	106.30
1	P	4134	TRP	CE2-CD2-CG	-7.05	101.66	107.30
1	B	1269	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	O	3514	TYR	CB-CG-CD2	-7.02	116.79	121.00
1	F	2169	ARG	CG-CD-NE	7.01	126.52	111.80
1	H	2334	TRP	CE2-CD2-CG	-6.94	101.75	107.30
1	F	2134	TRP	CD1-CG-CD2	6.88	111.81	106.30
1	N	3434	TRP	CE2-CD2-CG	-6.88	101.80	107.30
1	F	2134	TRP	CE2-CD2-CG	-6.87	101.81	107.30
1	C	1334	TRP	CE2-CD2-CG	-6.83	101.83	107.30
1	T	4534	TRP	CE2-CD2-CG	-6.80	101.86	107.30
1	D	1434	TRP	CE2-CD2-CG	-6.78	101.87	107.30
1	J	2511	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	O	3511	TYR	CB-CG-CD2	-6.62	117.03	121.00
1	Q	4234	TRP	CE2-CD2-CG	-6.62	102.00	107.30
1	S	4434	TRP	CD1-CG-CD2	6.61	111.59	106.30
1	R	4334	TRP	CE2-CD2-CG	-6.52	102.08	107.30
1	D	1434	TRP	CD1-CG-CD2	6.48	111.48	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	S	4414	TYR	CB-CG-CD1	-6.44	117.13	121.00
1	L	3234	TRP	CE2-CD2-CG	-6.43	102.15	107.30
1	A	1134	TRP	CE2-CD2-CG	-6.43	102.16	107.30
1	O	3534	TRP	CE2-CD2-CG	-6.39	102.18	107.30
1	O	3534	TRP	CD1-CG-CD2	6.39	111.41	106.30
1	E	1534	TRP	CE2-CD2-CG	-6.37	102.20	107.30
1	J	2569	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	T	4534	TRP	CD1-CG-CD2	6.33	111.37	106.30
1	E	1511	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	L	3211	TYR	CB-CG-CD2	-6.23	117.26	121.00
1	E	1534	TRP	CD1-CG-CD2	6.19	111.25	106.30
1	J	2534	TRP	CD1-CG-CD2	6.18	111.25	106.30
1	S	4434	TRP	CE2-CD2-CG	-6.14	102.39	107.30
1	O	3550	VAL	CG1-CB-CG2	-6.04	101.24	110.90
1	M	3334	TRP	CD1-CG-CD2	6.02	111.11	106.30
1	N	3434	TRP	CD1-CG-CD2	6.00	111.10	106.30
1	L	3234	TRP	CD1-CG-CD2	5.93	111.05	106.30
1	G	2234	TRP	CE2-CD2-CG	-5.93	102.56	107.30
1	F	2169	ARG	CD-NE-CZ	5.90	131.86	123.60
1	H	2311	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	K	3134	TRP	CD1-CG-CD2	5.87	111.00	106.30
1	I	2434	TRP	CE2-CD2-CG	-5.87	102.61	107.30
1	S	4411	TYR	CB-CG-CD2	-5.85	117.49	121.00
1	M	3369	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	P	4111	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	A	1134	TRP	CD1-CG-CD2	5.83	110.96	106.30
1	Q	4211	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	I	2414	TYR	CB-CG-CD1	-5.79	117.52	121.00
1	M	3334	TRP	CE2-CD2-CG	-5.76	102.69	107.30
1	O	3510	GLU	CA-CB-CG	5.74	126.03	113.40
1	K	3134	TRP	CE2-CD2-CG	-5.73	102.72	107.30
1	N	3469	ARG	NE-CZ-NH2	-5.67	117.46	120.30
1	J	2534	TRP	CE2-CD2-CG	-5.63	102.80	107.30
1	A	1111	TYR	CB-CG-CD2	-5.61	117.64	121.00
1	G	2211	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	D	1411	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	R	4334	TRP	NE1-CE2-CD2	5.51	112.81	107.30
1	H	2333	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	H	2334	TRP	CG-CD1-NE1	-5.48	104.62	110.10
1	T	4510	GLU	CA-CB-CG	5.45	125.40	113.40
1	O	3510	GLU	N-CA-CB	-5.41	100.86	110.60
1	O	3569	ARG	NE-CZ-NH1	5.39	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	3111	TYR	CB-CG-CD2	-5.36	117.79	121.00
1	R	4334	TRP	CD1-CG-CD2	5.34	110.57	106.30
1	E	1569	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	C	1369	ARG	CG-CD-NE	-5.31	100.64	111.80
1	B	1211	TYR	CB-CG-CD2	-5.24	117.86	121.00
1	D	1469	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	G	2269	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	G	2234	TRP	CD1-CG-CD2	5.18	110.44	106.30
1	P	4134	TRP	CG-CD1-NE1	-5.16	104.94	110.10
1	F	2169	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
1	I	2434	TRP	CD1-CG-CD2	5.13	110.41	106.30
1	F	2111	TYR	CB-CG-CD2	-5.12	117.92	121.00
1	H	2326	ASP	CB-CG-OD1	5.12	122.91	118.30
1	O	3569	ARG	CB-CA-C	-5.10	100.20	110.40
1	S	4434	TRP	CG-CD1-NE1	-5.00	105.09	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	540	0	524	2	0
1	B	540	0	524	2	0
1	C	540	0	524	5	0
1	D	540	0	524	4	0
1	E	540	0	524	1	0
1	F	540	0	524	4	0
1	G	540	0	524	5	0
1	H	540	0	524	1	0
1	I	540	0	524	1	0
1	J	540	0	524	3	0
1	K	540	0	524	3	0
1	L	540	0	524	1	0
1	M	540	0	524	2	0
1	N	540	0	524	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	540	0	524	2	0
1	P	540	0	524	4	0
1	Q	540	0	524	1	0
1	R	540	0	524	3	0
1	S	540	0	524	3	0
1	T	540	0	524	2	0
2	A	68	0	60	1	0
2	B	34	0	30	0	0
2	C	34	0	30	0	0
2	D	68	0	60	2	0
2	E	68	0	60	0	0
2	F	102	0	90	3	0
2	G	34	0	30	0	0
2	H	68	0	60	0	0
2	I	34	0	30	0	0
2	J	68	0	60	0	0
2	K	34	0	30	0	0
2	L	34	0	30	0	0
2	M	68	0	60	0	0
2	N	34	0	30	0	0
2	O	68	0	60	0	0
2	P	34	0	30	0	0
2	Q	102	0	90	1	0
2	R	68	0	60	1	0
2	S	68	0	60	1	0
2	T	34	0	30	0	0
3	A	23	0	21	0	0
3	B	46	0	42	0	0
3	C	23	0	21	0	0
3	D	23	0	21	0	0
3	G	23	0	21	0	0
3	H	23	0	21	0	0
3	I	23	0	21	0	0
3	K	23	0	21	0	0
3	L	23	0	21	0	0
3	M	23	0	21	0	0
3	N	23	0	21	0	0
3	O	23	0	21	0	0
3	P	23	0	21	0	0
3	S	23	0	21	1	0
3	T	23	0	21	0	0
4	C	12	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	12	0	12	0	0
4	G	12	0	12	2	0
4	I	12	0	12	0	0
4	J	12	0	12	0	0
4	K	12	0	12	0	0
4	L	12	0	12	0	0
4	N	12	0	12	2	0
4	P	12	0	12	3	0
4	R	12	0	12	2	0
4	T	12	0	12	1	0
5	A	12	0	0	0	0
5	B	27	0	0	1	0
5	C	19	0	0	0	0
5	D	16	0	0	0	0
5	E	18	0	0	0	0
5	F	15	0	0	2	0
5	G	21	0	0	0	0
5	H	17	0	0	0	0
5	I	17	0	0	0	0
5	J	15	0	0	2	0
5	K	21	0	0	2	0
5	L	23	0	0	0	0
5	M	24	0	0	2	0
5	N	14	0	0	0	0
5	O	23	0	0	0	0
5	P	17	0	0	0	0
5	Q	13	0	0	0	0
5	R	10	0	0	0	0
5	S	11	0	0	0	0
5	T	12	0	0	0	0
All	All	12767	0	11938	55	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 2.

All (55) 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:R:4360:GLY:HA2	4:R:4370:GAL:H61	1.62	0.81
1:G:2269:ARG:HG2	1:G:2269:ARG:HH11	1.44	0.80
1:P:4112:THR:HG22	1:P:4122:VAL:HG23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:3112:THR:HG22	1:K:3122:VAL:HG23	1.75	0.69
1:I:2412:THR:HG22	1:I:2422:VAL:HG23	1.74	0.68
1:D:1412:THR:HG22	1:D:1422:VAL:HG23	1.76	0.67
1:P:4160:GLY:HA2	4:P:4170:GAL:H61	1.77	0.67
1:M:3312:THR:HG22	1:M:3322:VAL:HG23	1.77	0.66
1:C:1312:THR:HG22	1:C:1322:VAL:HG23	1.78	0.66
1:T:4512:THR:HG22	1:T:4522:VAL:HG23	1.76	0.65
1:A:1112:THR:HG22	1:A:1122:VAL:HG23	1.78	0.65
1:J:2512:THR:HG22	1:J:2522:VAL:HG23	1.78	0.65
1:N:3412:THR:HG22	1:N:3422:VAL:HG23	1.79	0.65
1:F:2112:THR:HG22	1:F:2122:VAL:HG23	1.79	0.64
1:S:4412:THR:HG22	1:S:4422:VAL:HG23	1.79	0.64
1:H:2312:THR:HG22	1:H:2322:VAL:HG23	1.80	0.64
1:O:3512:THR:HG22	1:O:3522:VAL:HG23	1.80	0.63
1:R:4312:THR:HG22	1:R:4322:VAL:HG23	1.80	0.63
1:L:3212:THR:HG22	1:L:3222:VAL:HG23	1.81	0.63
1:Q:4212:THR:HG22	1:Q:4222:VAL:HG23	1.81	0.62
1:K:3169:ARG:HD2	5:K:5224:HOH:O	1.98	0.62
1:E:1512:THR:HG22	1:E:1522:VAL:HG23	1.80	0.62
1:R:4360:GLY:HA2	4:R:4370:GAL:C6	2.30	0.61
1:B:1212:THR:HG22	1:B:1222:VAL:HG23	1.82	0.61
1:J:2537:GLN:HB2	5:J:5179:HOH:O	2.01	0.60
1:G:2212:THR:HG22	1:G:2222:VAL:HG23	1.81	0.60
1:N:3460:GLY:HA2	4:N:3470:GAL:H61	1.83	0.59
1:P:4160:GLY:HA2	4:P:4170:GAL:C6	2.33	0.57
1:S:4460:GLY:HA2	2:S:4470:GLA:O6	2.09	0.53
1:M:3316:ASP:HB3	5:M:5319:HOH:O	2.09	0.52
1:N:3460:GLY:HA2	4:N:3470:GAL:C6	2.42	0.49
1:P:4121:THR:HG1	4:P:4170:GAL:HO4	1.60	0.47
1:T:4560:GLY:HA2	4:T:4570:GAL:H61	1.97	0.47
1:D:1460:GLY:HA2	2:D:1470:GLA:H61	1.97	0.47
5:M:5314:HOH:O	1:N:3438:SER:HB3	2.15	0.47
2:Q:4270:GLA:H5	2:Q:4271:GAL:O3	2.16	0.46
1:D:1460:GLY:HA2	2:D:1470:GLA:C6	2.47	0.45
1:J:2501:THR:HG21	5:J:5104:HOH:O	2.15	0.44
1:S:4434:TRP:CE3	3:S:4481:GAL:H3	2.52	0.44
1:O:3569:ARG:HE	1:O:3569:ARG:HB3	1.72	0.44
1:G:2269:ARG:HG2	1:G:2269:ARG:NH1	2.20	0.44
1:C:1308:LYS:HE2	5:F:5232:HOH:O	2.18	0.43
1:A:1160:GLY:HA2	2:A:1170:GLA:O6	2.18	0.43
1:C:1360:GLY:HA2	4:C:1370:GAL:H61	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1306:THR:HG21	1:F:2159:ASN:HB2	2.01	0.43
1:B:1237:GLN:HB2	5:B:5126:HOH:O	2.19	0.43
1:D:1469:ARG:HH11	1:D:1469:ARG:HG3	1.82	0.43
2:R:4390:GLA:H5	2:R:4391:GAL:O3	2.18	0.43
1:C:1308:LYS:CE	5:F:5232:HOH:O	2.67	0.43
1:F:2130:PHE:CE1	2:F:2171:GAL:H3	2.54	0.42
1:G:2260:GLY:HA2	4:G:2270:GAL:C6	2.50	0.42
2:F:2180:GLA:H5	2:F:2181:GAL:O3	2.19	0.41
1:G:2260:GLY:HA2	4:G:2270:GAL:H61	2.01	0.41
1:K:3119:THR:HG21	5:K:5192:HOH:O	2.22	0.40
1:F:2131:THR:HA	2:F:2190:GLA:O6	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	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	B	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	C	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	D	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	E	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	F	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
1	G	67/69 (97%)	66 (98%)	1 (2%)	0	100	100
1	H	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	I	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	J	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	K	67/69 (97%)	65 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	M	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	N	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	O	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	P	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	Q	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	R	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	S	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
1	T	67/69 (97%)	65 (97%)	2 (3%)	0	100	100
All	All	1340/1380 (97%)	1302 (97%)	38 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	61/61 (100%)	59 (97%)	2 (3%)	45	79
1	B	61/61 (100%)	59 (97%)	2 (3%)	45	79
1	C	61/61 (100%)	58 (95%)	3 (5%)	31	65
1	D	61/61 (100%)	58 (95%)	3 (5%)	31	65
1	E	61/61 (100%)	57 (93%)	4 (7%)	21	51
1	F	61/61 (100%)	57 (93%)	4 (7%)	21	51
1	G	61/61 (100%)	58 (95%)	3 (5%)	31	65
1	H	61/61 (100%)	57 (93%)	4 (7%)	21	51
1	I	61/61 (100%)	59 (97%)	2 (3%)	45	79
1	J	61/61 (100%)	59 (97%)	2 (3%)	45	79
1	K	61/61 (100%)	58 (95%)	3 (5%)	31	65
1	L	61/61 (100%)	59 (97%)	2 (3%)	45	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	M	61/61 (100%)	58 (95%)	3 (5%)	31 65
1	N	61/61 (100%)	59 (97%)	2 (3%)	45 79
1	O	61/61 (100%)	58 (95%)	3 (5%)	31 65
1	P	61/61 (100%)	59 (97%)	2 (3%)	45 79
1	Q	61/61 (100%)	59 (97%)	2 (3%)	45 79
1	R	61/61 (100%)	58 (95%)	3 (5%)	31 65
1	S	61/61 (100%)	59 (97%)	2 (3%)	45 79
1	T	61/61 (100%)	59 (97%)	2 (3%)	45 79
All	All	1220/1220 (100%)	1167 (96%)	53 (4%)	35 70

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1105	VAL
1	A	1122	VAL
1	B	1205	VAL
1	B	1222	VAL
1	C	1305	VAL
1	C	1322	VAL
1	C	1369	ARG
1	D	1405	VAL
1	D	1422	VAL
1	D	1469	ARG
1	E	1505	VAL
1	E	1510	GLU
1	E	1522	VAL
1	E	1569	ARG
1	F	2105	VAL
1	F	2110	GLU
1	F	2122	VAL
1	F	2169	ARG
1	G	2205	VAL
1	G	2222	VAL
1	G	2269	ARG
1	H	2305	VAL
1	H	2310	GLU
1	H	2322	VAL
1	H	2369	ARG
1	I	2405	VAL

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Mol	Chain	Res	Type
1	I	2422	VAL
1	J	2505	VAL
1	J	2522	VAL
1	K	3105	VAL
1	K	3122	VAL
1	K	3169	ARG
1	L	3205	VAL
1	L	3222	VAL
1	M	3305	VAL
1	M	3322	VAL
1	M	3369	ARG
1	N	3405	VAL
1	N	3422	VAL
1	O	3505	VAL
1	O	3510	GLU
1	O	3522	VAL
1	P	4105	VAL
1	P	4122	VAL
1	Q	4205	VAL
1	Q	4222	VAL
1	R	4305	VAL
1	R	4322	VAL
1	R	4369	ARG
1	S	4405	VAL
1	S	4422	VAL
1	T	4505	VAL
1	T	4522	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

131 carbohydrates are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	GLA	A	1170	2	11,11,12	0.40	0	14,15,17	0.78	1 (7%)
2	GAL	A	1171	2	11,11,12	0.71	0	14,15,17	0.83	1 (7%)
2	BGC	A	1172	2	12,12,12	0.54	0	17,17,17	0.60	0
3	GLA	A	1180	3	11,11,12	0.47	0	14,15,17	1.03	1 (7%)
3	GAL	A	1181	3	12,12,12	0.35	0	17,17,17	0.61	0
2	GLA	A	1190	2	11,11,12	0.43	0	14,15,17	0.79	0
2	GAL	A	1191	2	11,11,12	0.45	0	14,15,17	0.65	0
2	BGC	A	1192	2	12,12,12	0.39	0	17,17,17	0.31	0
3	GLA	B	1270	3	11,11,12	0.47	0	14,15,17	0.86	1 (7%)
3	GAL	B	1271	3	12,12,12	0.47	0	17,17,17	0.47	0
3	GLA	B	1280	3	11,11,12	0.43	0	14,15,17	0.93	1 (7%)
3	GAL	B	1281	3	12,12,12	0.33	0	17,17,17	0.44	0
2	GLA	B	1290	2	11,11,12	0.45	0	14,15,17	0.65	0
2	GAL	B	1291	2	11,11,12	0.52	0	14,15,17	0.66	0
2	BGC	B	1292	2	12,12,12	0.35	0	17,17,17	0.58	0
3	GLA	C	1380	3	11,11,12	0.65	0	14,15,17	0.97	1 (7%)
3	GAL	C	1381	3	12,12,12	0.64	0	17,17,17	0.62	0
2	GLA	C	1390	2	11,11,12	0.48	0	14,15,17	0.70	0
2	GAL	C	1391	2	11,11,12	0.55	0	14,15,17	0.56	0
2	BGC	C	1392	2	12,12,12	0.39	0	17,17,17	0.47	0
2	GLA	D	1470	2	11,11,12	0.61	0	14,15,17	0.98	1 (7%)
2	GAL	D	1471	2	11,11,12	0.46	0	14,15,17	0.63	0
2	BGC	D	1472	2	12,12,12	0.50	0	17,17,17	0.52	0
3	GLA	D	1480	3	11,11,12	0.73	0	14,15,17	0.96	1 (7%)
3	GAL	D	1481	3	12,12,12	0.80	0	17,17,17	0.98	1 (5%)
2	GLA	D	1490	2	11,11,12	0.41	0	14,15,17	0.63	0
2	GAL	D	1491	2	11,11,12	0.53	0	14,15,17	0.69	0
2	BGC	D	1492	2	12,12,12	0.35	0	17,17,17	0.55	0
2	GLA	E	1580	2	11,11,12	0.45	0	14,15,17	0.77	0
2	GAL	E	1581	2	11,11,12	0.54	0	14,15,17	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	E	1582	2	12,12,12	0.28	0	17,17,17	0.35	0
2	GLA	E	1590	2	11,11,12	0.51	0	14,15,17	0.66	0
2	GAL	E	1591	2	11,11,12	0.47	0	14,15,17	0.42	0
2	BGC	E	1592	2	12,12,12	0.37	0	17,17,17	0.50	0
2	GLA	F	2170	2	11,11,12	0.34	0	14,15,17	1.33	2 (14%)
2	GAL	F	2171	2	11,11,12	0.47	0	14,15,17	0.81	1 (7%)
2	BGC	F	2172	2	12,12,12	0.24	0	17,17,17	0.53	0
2	GLA	F	2180	2	11,11,12	0.44	0	14,15,17	0.60	0
2	GAL	F	2181	2	11,11,12	0.48	0	14,15,17	0.43	0
2	BGC	F	2182	2	12,12,12	0.37	0	17,17,17	0.35	0
2	GLA	F	2190	2	11,11,12	0.62	0	14,15,17	0.92	1 (7%)
2	GAL	F	2191	2	11,11,12	0.58	0	14,15,17	0.78	0
2	BGC	F	2192	2	12,12,12	0.58	0	17,17,17	0.56	0
3	GLA	G	2280	3	11,11,12	0.59	0	14,15,17	0.56	0
3	GAL	G	2281	3	12,12,12	0.36	0	17,17,17	0.42	0
2	GLA	G	2290	2	11,11,12	0.54	0	14,15,17	0.93	1 (7%)
2	GAL	G	2291	2	11,11,12	0.37	0	14,15,17	0.53	0
2	BGC	G	2292	2	12,12,12	0.28	0	17,17,17	0.45	0
2	GLA	H	2370	2	11,11,12	0.43	0	14,15,17	0.69	0
2	GAL	H	2371	2	11,11,12	0.54	0	14,15,17	0.74	0
2	BGC	H	2372	2	12,12,12	0.49	0	17,17,17	0.97	2 (11%)
3	GLA	H	2380	3	11,11,12	0.60	0	14,15,17	0.72	0
3	GAL	H	2381	3	12,12,12	0.36	0	17,17,17	0.41	0
2	GLA	H	2390	2	11,11,12	0.46	0	14,15,17	0.89	1 (7%)
2	GAL	H	2391	2	11,11,12	0.64	0	14,15,17	0.46	0
2	BGC	H	2392	2	12,12,12	0.61	0	17,17,17	0.43	0
3	GLA	I	2480	3	11,11,12	0.71	0	14,15,17	0.80	0
3	GAL	I	2481	3	12,12,12	0.52	0	17,17,17	0.87	1 (5%)
2	GLA	I	2490	2	11,11,12	0.49	0	14,15,17	0.77	1 (7%)
2	GAL	I	2491	2	11,11,12	0.62	0	14,15,17	0.65	0
2	BGC	I	2492	2	12,12,12	0.53	0	17,17,17	0.59	0
2	GLA	J	2580	2	11,11,12	0.63	0	14,15,17	0.51	0
2	GAL	J	2581	2	11,11,12	0.44	0	14,15,17	0.62	0
2	BGC	J	2582	2	12,12,12	0.33	0	17,17,17	0.36	0
2	GLA	J	2590	2	11,11,12	0.47	0	14,15,17	1.04	2 (14%)
2	GAL	J	2591	2	11,11,12	0.47	0	14,15,17	0.88	0
2	BGC	J	2592	2	12,12,12	0.43	0	17,17,17	0.40	0
3	GLA	K	3180	3	11,11,12	0.52	0	14,15,17	0.51	0
3	GAL	K	3181	3	12,12,12	0.46	0	17,17,17	0.42	0
2	GLA	K	3190	2	11,11,12	0.36	0	14,15,17	0.85	1 (7%)
2	GAL	K	3191	2	11,11,12	0.51	0	14,15,17	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	BGC	K	3192	2	12,12,12	0.40	0	17,17,17	0.46	0
3	GLA	L	3280	3	11,11,12	0.47	0	14,15,17	0.71	0
3	GAL	L	3281	3	12,12,12	0.51	0	17,17,17	0.57	0
2	GLA	L	3290	2	11,11,12	0.39	0	14,15,17	0.66	0
2	GAL	L	3291	2	11,11,12	0.52	0	14,15,17	0.57	0
2	BGC	L	3292	2	12,12,12	0.39	0	17,17,17	0.53	0
2	GLA	M	3370	2	11,11,12	0.60	0	14,15,17	1.14	1 (7%)
2	GAL	M	3371	2	11,11,12	0.54	0	14,15,17	0.60	0
2	BGC	M	3372	2	12,12,12	0.53	0	17,17,17	0.72	0
3	GLA	M	3380	3	11,11,12	0.47	0	14,15,17	0.78	0
3	GAL	M	3381	3	12,12,12	0.21	0	17,17,17	0.60	0
2	GLA	M	3390	2	11,11,12	0.46	0	14,15,17	0.65	0
2	GAL	M	3391	2	11,11,12	0.46	0	14,15,17	0.73	0
2	BGC	M	3392	2	12,12,12	0.39	0	17,17,17	0.37	0
3	GLA	N	3480	3	11,11,12	0.71	0	14,15,17	0.72	0
3	GAL	N	3481	3	12,12,12	0.44	0	17,17,17	0.45	0
2	GLA	N	3490	2	11,11,12	0.38	0	14,15,17	0.77	1 (7%)
2	GAL	N	3491	2	11,11,12	0.59	0	14,15,17	0.88	1 (7%)
2	BGC	N	3492	2	12,12,12	0.50	0	17,17,17	0.38	0
2	GLA	O	3570	2	11,11,12	0.36	0	14,15,17	0.81	1 (7%)
2	GAL	O	3571	2	11,11,12	0.63	0	14,15,17	0.85	0
2	BGC	O	3572	2	12,12,12	0.38	0	17,17,17	0.65	0
3	GLA	O	3580	3	11,11,12	0.56	0	14,15,17	0.56	0
3	GAL	O	3581	3	12,12,12	0.43	0	17,17,17	0.64	0
2	GLA	O	3590	2	11,11,12	0.54	0	14,15,17	0.68	0
2	GAL	O	3591	2	11,11,12	0.49	0	14,15,17	0.84	1 (7%)
2	BGC	O	3592	2	12,12,12	0.50	0	17,17,17	0.38	0
3	GLA	P	4180	3	11,11,12	0.62	0	14,15,17	0.63	0
3	GAL	P	4181	3	12,12,12	0.38	0	17,17,17	0.45	0
2	GLA	P	4190	2	11,11,12	0.41	0	14,15,17	0.67	0
2	GAL	P	4191	2	11,11,12	0.63	0	14,15,17	0.80	0
2	BGC	P	4192	2	12,12,12	0.43	0	17,17,17	0.40	0
2	GLA	Q	4270	2	11,11,12	0.70	0	14,15,17	0.70	1 (7%)
2	GAL	Q	4271	2	11,11,12	0.64	0	14,15,17	0.51	0
2	BGC	Q	4272	2	12,12,12	0.35	0	17,17,17	0.66	0
2	GLA	Q	4280	2	11,11,12	0.66	0	14,15,17	0.80	0
2	GAL	Q	4281	2	11,11,12	0.62	0	14,15,17	0.57	0
2	BGC	Q	4282	2	12,12,12	0.41	0	17,17,17	0.35	0
2	GLA	Q	4290	2	11,11,12	0.45	0	14,15,17	0.72	0
2	GAL	Q	4291	2	11,11,12	0.64	0	14,15,17	0.62	0
2	BGC	Q	4292	2	12,12,12	0.37	0	17,17,17	0.54	0
2	GLA	R	4380	2	11,11,12	0.74	0	14,15,17	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GAL	R	4381	2	11,11,12	0.49	0	14,15,17	0.46	0
2	BGC	R	4382	2	12,12,12	0.65	0	17,17,17	0.44	0
2	GLA	R	4390	2	11,11,12	0.49	0	14,15,17	0.92	1 (7%)
2	GAL	R	4391	2	11,11,12	0.59	0	14,15,17	0.63	0
2	BGC	R	4392	2	12,12,12	0.41	0	17,17,17	0.51	0
2	GLA	S	4470	2	11,11,12	0.46	0	14,15,17	0.89	1 (7%)
2	GAL	S	4471	2	11,11,12	0.51	0	14,15,17	0.62	0
2	BGC	S	4472	2	12,12,12	0.33	0	17,17,17	0.43	0
3	GLA	S	4480	3	11,11,12	0.53	0	14,15,17	0.70	0
3	GAL	S	4481	3	12,12,12	0.43	0	17,17,17	0.42	0
2	GLA	S	4490	2	11,11,12	0.44	0	14,15,17	0.76	1 (7%)
2	GAL	S	4491	2	11,11,12	0.64	0	14,15,17	0.45	0
2	BGC	S	4492	2	12,12,12	0.36	0	17,17,17	0.41	0
3	GLA	T	4580	3	11,11,12	0.64	0	14,15,17	0.80	1 (7%)
3	GAL	T	4581	3	12,12,12	0.44	0	17,17,17	0.54	0
2	GLA	T	4590	2	11,11,12	0.39	0	14,15,17	0.76	0
2	GAL	T	4591	2	11,11,12	0.47	0	14,15,17	0.49	0
2	BGC	T	4592	2	12,12,12	0.27	0	17,17,17	0.36	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	A	1170	2	-	0/2/19/22	0/1/1/1
2	GAL	A	1171	2	-	0/2/19/22	0/1/1/1
2	BGC	A	1172	2	-	0/2/22/22	0/1/1/1
3	GLA	A	1180	3	-	0/2/19/22	0/1/1/1
3	GAL	A	1181	3	-	0/2/22/22	0/1/1/1
2	GLA	A	1190	2	-	0/2/19/22	0/1/1/1
2	GAL	A	1191	2	-	0/2/19/22	0/1/1/1
2	BGC	A	1192	2	-	0/2/22/22	0/1/1/1
3	GLA	B	1270	3	-	0/2/19/22	0/1/1/1
3	GAL	B	1271	3	-	0/2/22/22	0/1/1/1
3	GLA	B	1280	3	-	0/2/19/22	0/1/1/1
3	GAL	B	1281	3	-	0/2/22/22	0/1/1/1
2	GLA	B	1290	2	-	0/2/19/22	0/1/1/1
2	GAL	B	1291	2	-	0/2/19/22	0/1/1/1
2	BGC	B	1292	2	-	0/2/22/22	0/1/1/1
3	GLA	C	1380	3	-	0/2/19/22	0/1/1/1
3	GAL	C	1381	3	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GLA	C	1390	2	-	0/2/19/22	0/1/1/1
2	GAL	C	1391	2	-	0/2/19/22	0/1/1/1
2	BGC	C	1392	2	-	0/2/22/22	0/1/1/1
2	GLA	D	1470	2	-	0/2/19/22	0/1/1/1
2	GAL	D	1471	2	-	0/2/19/22	0/1/1/1
2	BGC	D	1472	2	-	0/2/22/22	0/1/1/1
3	GLA	D	1480	3	-	0/2/19/22	0/1/1/1
3	GAL	D	1481	3	-	0/2/22/22	0/1/1/1
2	GLA	D	1490	2	-	0/2/19/22	0/1/1/1
2	GAL	D	1491	2	-	0/2/19/22	0/1/1/1
2	BGC	D	1492	2	-	0/2/22/22	0/1/1/1
2	GLA	E	1580	2	-	0/2/19/22	0/1/1/1
2	GAL	E	1581	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1582	2	-	0/2/22/22	0/1/1/1
2	GLA	E	1590	2	-	0/2/19/22	0/1/1/1
2	GAL	E	1591	2	-	0/2/19/22	0/1/1/1
2	BGC	E	1592	2	-	0/2/22/22	0/1/1/1
2	GLA	F	2170	2	-	0/2/19/22	0/1/1/1
2	GAL	F	2171	2	-	0/2/19/22	0/1/1/1
2	BGC	F	2172	2	-	0/2/22/22	0/1/1/1
2	GLA	F	2180	2	-	0/2/19/22	0/1/1/1
2	GAL	F	2181	2	-	0/2/19/22	0/1/1/1
2	BGC	F	2182	2	-	0/2/22/22	0/1/1/1
2	GLA	F	2190	2	-	0/2/19/22	0/1/1/1
2	GAL	F	2191	2	-	0/2/19/22	0/1/1/1
2	BGC	F	2192	2	-	0/2/22/22	0/1/1/1
3	GLA	G	2280	3	-	0/2/19/22	0/1/1/1
3	GAL	G	2281	3	-	0/2/22/22	0/1/1/1
2	GLA	G	2290	2	-	0/2/19/22	0/1/1/1
2	GAL	G	2291	2	-	0/2/19/22	0/1/1/1
2	BGC	G	2292	2	-	0/2/22/22	0/1/1/1
2	GLA	H	2370	2	-	0/2/19/22	0/1/1/1
2	GAL	H	2371	2	-	0/2/19/22	0/1/1/1
2	BGC	H	2372	2	-	0/2/22/22	0/1/1/1
3	GLA	H	2380	3	-	0/2/19/22	0/1/1/1
3	GAL	H	2381	3	-	0/2/22/22	0/1/1/1
2	GLA	H	2390	2	-	0/2/19/22	0/1/1/1
2	GAL	H	2391	2	-	0/2/19/22	0/1/1/1
2	BGC	H	2392	2	-	0/2/22/22	0/1/1/1
3	GLA	I	2480	3	-	0/2/19/22	0/1/1/1
3	GAL	I	2481	3	-	0/2/22/22	0/1/1/1
2	GLA	I	2490	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	I	2491	2	-	0/2/19/22	0/1/1/1
2	BGC	I	2492	2	-	0/2/22/22	0/1/1/1
2	GLA	J	2580	2	-	0/2/19/22	0/1/1/1
2	GAL	J	2581	2	-	0/2/19/22	0/1/1/1
2	BGC	J	2582	2	-	0/2/22/22	0/1/1/1
2	GLA	J	2590	2	-	0/2/19/22	0/1/1/1
2	GAL	J	2591	2	-	0/2/19/22	0/1/1/1
2	BGC	J	2592	2	-	0/2/22/22	0/1/1/1
3	GLA	K	3180	3	-	0/2/19/22	0/1/1/1
3	GAL	K	3181	3	-	0/2/22/22	0/1/1/1
2	GLA	K	3190	2	-	0/2/19/22	0/1/1/1
2	GAL	K	3191	2	-	0/2/19/22	0/1/1/1
2	BGC	K	3192	2	-	0/2/22/22	0/1/1/1
3	GLA	L	3280	3	-	0/2/19/22	0/1/1/1
3	GAL	L	3281	3	-	0/2/22/22	0/1/1/1
2	GLA	L	3290	2	-	0/2/19/22	0/1/1/1
2	GAL	L	3291	2	-	0/2/19/22	0/1/1/1
2	BGC	L	3292	2	-	0/2/22/22	0/1/1/1
2	GLA	M	3370	2	-	0/2/19/22	0/1/1/1
2	GAL	M	3371	2	-	0/2/19/22	0/1/1/1
2	BGC	M	3372	2	-	0/2/22/22	0/1/1/1
3	GLA	M	3380	3	-	0/2/19/22	0/1/1/1
3	GAL	M	3381	3	-	0/2/22/22	0/1/1/1
2	GLA	M	3390	2	-	0/2/19/22	0/1/1/1
2	GAL	M	3391	2	-	0/2/19/22	0/1/1/1
2	BGC	M	3392	2	-	0/2/22/22	0/1/1/1
3	GLA	N	3480	3	-	0/2/19/22	0/1/1/1
3	GAL	N	3481	3	-	0/2/22/22	0/1/1/1
2	GLA	N	3490	2	-	0/2/19/22	0/1/1/1
2	GAL	N	3491	2	-	0/2/19/22	0/1/1/1
2	BGC	N	3492	2	-	0/2/22/22	0/1/1/1
2	GLA	O	3570	2	-	0/2/19/22	0/1/1/1
2	GAL	O	3571	2	-	0/2/19/22	0/1/1/1
2	BGC	O	3572	2	-	0/2/22/22	0/1/1/1
3	GLA	O	3580	3	-	0/2/19/22	0/1/1/1
3	GAL	O	3581	3	-	0/2/22/22	0/1/1/1
2	GLA	O	3590	2	-	0/2/19/22	0/1/1/1
2	GAL	O	3591	2	-	0/2/19/22	0/1/1/1
2	BGC	O	3592	2	-	0/2/22/22	0/1/1/1
3	GLA	P	4180	3	-	0/2/19/22	0/1/1/1
3	GAL	P	4181	3	-	0/2/22/22	0/1/1/1
2	GLA	P	4190	2	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GAL	P	4191	2	-	0/2/19/22	0/1/1/1
2	BGC	P	4192	2	-	0/2/22/22	0/1/1/1
2	GLA	Q	4270	2	-	0/2/19/22	0/1/1/1
2	GAL	Q	4271	2	-	0/2/19/22	0/1/1/1
2	BGC	Q	4272	2	-	0/2/22/22	0/1/1/1
2	GLA	Q	4280	2	-	0/2/19/22	0/1/1/1
2	GAL	Q	4281	2	-	0/2/19/22	0/1/1/1
2	BGC	Q	4282	2	-	0/2/22/22	0/1/1/1
2	GLA	Q	4290	2	-	0/2/19/22	0/1/1/1
2	GAL	Q	4291	2	-	0/2/19/22	0/1/1/1
2	BGC	Q	4292	2	-	0/2/22/22	0/1/1/1
2	GLA	R	4380	2	-	0/2/19/22	0/1/1/1
2	GAL	R	4381	2	-	0/2/19/22	0/1/1/1
2	BGC	R	4382	2	-	0/2/22/22	0/1/1/1
2	GLA	R	4390	2	-	0/2/19/22	0/1/1/1
2	GAL	R	4391	2	-	0/2/19/22	0/1/1/1
2	BGC	R	4392	2	-	0/2/22/22	0/1/1/1
2	GLA	S	4470	2	-	0/2/19/22	0/1/1/1
2	GAL	S	4471	2	-	0/2/19/22	0/1/1/1
2	BGC	S	4472	2	-	0/2/22/22	0/1/1/1
3	GLA	S	4480	3	-	0/2/19/22	0/1/1/1
3	GAL	S	4481	3	-	0/2/22/22	0/1/1/1
2	GLA	S	4490	2	-	0/2/19/22	0/1/1/1
2	GAL	S	4491	2	-	0/2/19/22	0/1/1/1
2	BGC	S	4492	2	-	0/2/22/22	0/1/1/1
3	GLA	T	4580	3	-	0/2/19/22	0/1/1/1
3	GAL	T	4581	3	-	0/2/22/22	0/1/1/1
2	GLA	T	4590	2	-	0/2/19/22	0/1/1/1
2	GAL	T	4591	2	-	0/2/19/22	0/1/1/1
2	BGC	T	4592	2	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	2481	GAL	C1-C2-C3	-2.48	106.75	110.43
2	N	3491	GAL	C3-C4-C5	-2.30	106.19	110.20
2	F	2190	GLA	C2-C3-C4	-2.05	107.55	111.04
3	D	1481	GAL	C3-C4-C5	-2.01	106.69	110.20
2	S	4490	GLA	C1-O5-C5	2.01	114.81	112.25
2	N	3490	GLA	C1-O5-C5	2.02	114.81	112.25
2	I	2490	GLA	C1-O5-C5	2.04	114.83	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	3591	GAL	C1-C2-C3	2.04	111.96	109.54
2	Q	4270	GLA	C1-O5-C5	2.07	114.88	112.25
2	O	3570	GLA	C1-O5-C5	2.08	114.88	112.25
3	B	1280	GLA	C1-O5-C5	2.10	114.91	112.25
2	A	1170	GLA	C1-O5-C5	2.12	114.94	112.25
3	T	4580	GLA	C1-C2-C3	2.14	112.07	109.54
2	H	2372	BGC	C1-C2-C3	2.19	113.68	110.43
2	H	2372	BGC	C4-C3-C2	2.19	114.88	110.79
2	G	2290	GLA	C1-C2-C3	2.20	112.15	109.54
2	J	2590	GLA	C1-C2-C3	2.22	112.16	109.54
2	H	2390	GLA	C1-O5-C5	2.23	115.08	112.25
2	K	3190	GLA	C1-O5-C5	2.26	115.12	112.25
2	F	2171	GAL	C1-C2-C3	2.28	112.23	109.54
2	J	2590	GLA	C1-O5-C5	2.28	115.14	112.25
3	B	1270	GLA	C1-C2-C3	2.32	112.29	109.54
2	A	1171	GAL	C1-C2-C3	2.33	112.30	109.54
2	S	4470	GLA	C1-C2-C3	2.42	112.41	109.54
2	R	4390	GLA	C1-O5-C5	2.59	115.54	112.25
3	D	1480	GLA	C1-C2-C3	2.89	112.96	109.54
2	D	1470	GLA	C1-C2-C3	2.90	112.97	109.54
2	M	3370	GLA	C1-O5-C5	2.90	115.92	112.25
2	F	2170	GLA	C1-C2-C3	2.96	113.05	109.54
3	C	1380	GLA	C1-O5-C5	3.01	116.07	112.25
3	A	1180	GLA	C1-C2-C3	3.06	113.17	109.54
2	F	2170	GLA	C1-O5-C5	3.50	116.69	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1170	GLA	1	0
2	D	1470	GLA	2	0
2	F	2171	GAL	1	0
2	F	2180	GLA	1	0
2	F	2181	GAL	1	0
2	F	2190	GLA	1	0
2	Q	4270	GLA	1	0
2	Q	4271	GAL	1	0
2	R	4390	GLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	R	4391	GAL	1	0
2	S	4470	GLA	1	0
3	S	4481	GAL	1	0

5.6 Ligand geometry (i)

11 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GAL	C	1370	-	12,12,12	0.46	0	17,17,17	0.42	0
4	GAL	E	1570	-	12,12,12	0.40	0	17,17,17	0.42	0
4	GAL	G	2270	-	12,12,12	0.48	0	17,17,17	0.53	0
4	GAL	I	2470	-	12,12,12	0.40	0	17,17,17	0.51	0
4	GAL	J	2570	-	12,12,12	0.40	0	17,17,17	0.41	0
4	GAL	K	3170	-	12,12,12	0.38	0	17,17,17	0.47	0
4	GAL	L	3270	-	12,12,12	0.40	0	17,17,17	0.42	0
4	GAL	N	3470	-	12,12,12	0.43	0	17,17,17	0.36	0
4	GAL	P	4170	-	12,12,12	0.37	0	17,17,17	0.78	1 (5%)
4	GAL	R	4370	-	12,12,12	0.43	0	17,17,17	0.52	0
4	GAL	T	4570	-	12,12,12	0.58	0	17,17,17	0.64	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	C	1370	-	-	0/2/22/22	0/1/1/1
4	GAL	E	1570	-	-	0/2/22/22	0/1/1/1
4	GAL	G	2270	-	-	0/2/22/22	0/1/1/1
4	GAL	I	2470	-	-	0/2/22/22	0/1/1/1
4	GAL	J	2570	-	-	0/2/22/22	0/1/1/1
4	GAL	K	3170	-	-	0/2/22/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GAL	L	3270	-	-	0/2/22/22	0/1/1/1
4	GAL	N	3470	-	-	0/2/22/22	0/1/1/1
4	GAL	P	4170	-	-	0/2/22/22	0/1/1/1
4	GAL	R	4370	-	-	0/2/22/22	0/1/1/1
4	GAL	T	4570	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	P	4170	GAL	C3-C4-C5	2.51	114.57	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1370	GAL	1	0
4	G	2270	GAL	2	0
4	N	3470	GAL	2	0
4	P	4170	GAL	3	0
4	R	4370	GAL	2	0
4	T	4570	GAL	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	69/69 (100%)	-0.71	0	100	100	8, 17, 30, 34	0
1	B	69/69 (100%)	-0.73	0	100	100	8, 17, 28, 36	0
1	C	69/69 (100%)	-0.69	0	100	100	7, 16, 29, 36	0
1	D	69/69 (100%)	-0.71	0	100	100	5, 16, 29, 34	0
1	E	69/69 (100%)	-0.69	0	100	100	8, 19, 31, 39	0
1	F	69/69 (100%)	-0.72	0	100	100	7, 15, 26, 40	0
1	G	69/69 (100%)	-0.83	0	100	100	4, 14, 26, 34	0
1	H	69/69 (100%)	-0.81	0	100	100	4, 14, 23, 34	0
1	I	69/69 (100%)	-0.66	0	100	100	7, 17, 30, 42	0
1	J	69/69 (100%)	-0.58	0	100	100	7, 22, 33, 42	0
1	K	69/69 (100%)	-0.68	0	100	100	7, 18, 30, 34	0
1	L	69/69 (100%)	-0.78	0	100	100	7, 15, 26, 34	0
1	M	69/69 (100%)	-0.77	0	100	100	5, 13, 24, 32	0
1	N	69/69 (100%)	-0.75	0	100	100	6, 16, 29, 36	0
1	O	69/69 (100%)	-0.73	0	100	100	5, 15, 27, 41	0
1	P	69/69 (100%)	-0.67	0	100	100	8, 19, 30, 40	0
1	Q	69/69 (100%)	-0.68	0	100	100	11, 18, 29, 43	0
1	R	69/69 (100%)	-0.52	0	100	100	11, 25, 38, 44	0
1	S	69/69 (100%)	-0.58	0	100	100	12, 25, 34, 45	0
1	T	69/69 (100%)	-0.57	0	100	100	12, 25, 37, 47	0
All	All	1380/1380 (100%)	-0.69	0	100	100	4, 18, 32, 47	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GLA	B	1270	11/12	0.88	0.36	8.71	72,74,77,78	0
3	GLA	N	3480	11/12	0.95	0.17	4.39	23,24,27,28	0
2	GLA	Q	4280	11/12	0.96	0.17	3.06	15,25,28,32	0
2	GLA	J	2580	11/12	0.95	0.19	2.15	19,29,30,31	0
3	GLA	T	4580	11/12	0.94	0.17	2.05	19,22,24,25	0
3	GLA	I	2480	11/12	0.95	0.17	1.84	15,21,25,29	0
2	GLA	E	1580	11/12	0.95	0.16	1.72	14,22,23,24	0
3	GLA	D	1480	11/12	0.95	0.16	1.55	14,20,26,27	0
3	GLA	B	1280	11/12	0.97	0.15	1.44	15,18,20,22	0
3	GLA	L	3280	11/12	0.95	0.16	1.39	7,18,19,21	0
2	GLA	A	1170	11/12	0.93	0.17	1.27	4,12,17,25	0
3	GLA	P	4180	11/12	0.91	0.17	1.16	18,21,26,27	0
2	GAL	O	3591	11/12	0.91	0.19	1.13	27,31,34,36	0
2	GAL	H	2371	11/12	0.93	0.15	1.05	21,29,33,38	0
2	GAL	O	3571	11/12	0.96	0.15	1.04	14,24,32,36	0
3	GLA	M	3380	11/12	0.95	0.15	0.79	5,15,22,22	0
3	GLA	C	1380	11/12	0.96	0.15	0.68	17,19,22,30	0
3	GLA	O	3580	11/12	0.96	0.15	0.65	24,27,28,29	0
2	GAL	J	2591	11/12	0.91	0.18	0.60	27,35,40,44	0
2	GAL	I	2491	11/12	0.94	0.17	0.48	21,27,37,40	0
3	GLA	K	3180	11/12	0.95	0.14	0.47	7,18,25,26	0
2	GAL	P	4191	11/12	0.97	0.15	0.25	15,26,28,30	0
2	GAL	Q	4271	11/12	0.94	0.14	0.17	2,5,9,11	0
2	GAL	G	2291	11/12	0.95	0.13	0.16	8,15,20,20	0
2	GAL	A	1171	11/12	0.95	0.14	-0.01	8,13,22,23	0
2	GAL	K	3191	11/12	0.90	0.16	-0.04	30,32,38,39	0
2	GLA	F	2180	11/12	0.95	0.14	-0.04	20,22,27,27	0
3	GLA	A	1180	11/12	0.95	0.14	-0.09	11,23,28,29	0
2	GLA	N	3490	11/12	0.95	0.14	-0.14	10,16,23,26	0
2	GLA	Q	4290	11/12	0.96	0.13	-0.20	13,15,18,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	GLA	R	4390	11/12	0.93	0.16	-0.26	21,28,30,31	0
2	GLA	H	2370	11/12	0.95	0.12	-0.28	8,14,17,21	0
2	GAL	R	4391	11/12	0.92	0.17	-0.29	30,41,44,44	0
2	GLA	H	2390	11/12	0.96	0.13	-0.36	7,10,16,20	0
2	GLA	F	2170	11/12	0.96	0.14	-0.37	17,19,21,27	0
2	GAL	C	1391	11/12	0.94	0.14	-0.42	15,19,26,27	0
2	GAL	F	2171	11/12	0.97	0.13	-0.43	18,25,29,30	0
2	GLA	P	4190	11/12	0.94	0.14	-0.43	13,20,24,28	0
2	GAL	N	3491	11/12	0.95	0.14	-0.46	25,29,34,36	0
2	GAL	F	2191	11/12	0.94	0.12	-0.47	14,21,29,30	0
2	GAL	L	3291	11/12	0.94	0.12	-0.52	17,21,24,25	0
2	GLA	F	2190	11/12	0.97	0.11	-0.52	4,7,14,15	0
3	GLA	S	4480	11/12	0.95	0.14	-0.53	18,22,29,30	0
2	GLA	I	2490	11/12	0.94	0.13	-0.57	10,12,17,18	0
2	GAL	M	3391	11/12	0.96	0.12	-0.61	17,22,25,25	0
2	GLA	S	4490	11/12	0.95	0.13	-0.61	26,29,31,31	0
2	GLA	A	1190	11/12	0.95	0.13	-0.62	8,15,20,20	0
2	GLA	R	4380	11/12	0.96	0.14	-0.68	19,22,29,30	0
2	GAL	Q	4291	11/12	0.95	0.13	-0.73	15,20,28,29	0
2	GLA	K	3190	11/12	0.94	0.13	-0.75	14,16,25,28	0
2	GAL	D	1471	11/12	0.97	0.11	-0.76	10,14,18,18	0
2	GAL	S	4471	11/12	0.93	0.13	-0.79	26,30,34,34	0
2	GAL	M	3371	11/12	0.96	0.11	-0.80	5,8,10,12	0
2	GLA	S	4470	11/12	0.94	0.14	-0.82	14,25,30,31	0
2	GAL	D	1491	11/12	0.95	0.12	-0.95	18,22,28,35	0
2	GLA	Q	4270	11/12	0.96	0.11	-0.96	2,9,13,17	0
2	GLA	J	2590	11/12	0.96	0.12	-0.97	21,25,27,30	0
2	GLA	D	1470	11/12	0.94	0.11	-1.00	5,9,13,15	0
3	GLA	H	2380	11/12	0.96	0.12	-1.01	14,17,21,25	0
2	GLA	G	2290	11/12	0.96	0.12	-1.03	2,9,12,14	0
2	GLA	T	4590	11/12	0.94	0.13	-1.03	28,30,33,36	0
2	GAL	A	1191	11/12	0.94	0.12	-1.11	21,29,34,34	0
2	GLA	O	3570	11/12	0.97	0.11	-1.11	20,22,30,35	0
2	GLA	D	1490	11/12	0.96	0.11	-1.12	9,11,14,14	0
2	GLA	B	1290	11/12	0.96	0.12	-1.13	9,12,16,19	0
2	GLA	C	1390	11/12	0.95	0.12	-1.15	2,10,15,20	0
2	GAL	S	4491	11/12	0.95	0.12	-1.18	27,33,37,37	0
2	GAL	H	2391	11/12	0.95	0.10	-1.33	10,20,23,23	0
2	GLA	E	1590	11/12	0.96	0.11	-1.57	16,20,24,24	0
2	GLA	L	3290	11/12	0.96	0.09	-1.62	5,10,16,16	0
2	GAL	T	4591	11/12	0.90	0.14	-1.63	38,41,45,47	0
2	GLA	M	3390	11/12	0.97	0.10	-1.74	9,14,18,22	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GLA	G	2280	11/12	0.96	0.12	-1.81	14,16,20,22	0
2	GAL	E	1591	11/12	0.96	0.12	-1.83	21,27,34,34	0
2	GLA	M	3370	11/12	0.97	0.10	-1.92	2,3,15,18	0
2	GLA	O	3590	11/12	0.96	0.12	-2.01	6,10,14,16	0
2	GAL	B	1291	11/12	0.96	0.09	-2.40	10,20,23,25	0
2	BGC	S	4492	12/12	0.91	0.28	-	40,52,56,59	0
2	BGC	N	3492	12/12	0.89	0.20	-	40,49,54,54	0
2	BGC	S	4472	12/12	0.94	0.18	-	19,26,38,44	0
2	BGC	F	2182	12/12	0.85	0.25	-	43,48,48,48	11
3	GAL	G	2281	12/12	0.95	0.16	-	23,26,32,34	0
2	BGC	E	1582	12/12	0.60	0.21	-	36,41,42,42	11
2	BGC	P	4192	12/12	0.91	0.24	-	36,46,49,53	0
2	BGC	H	2392	12/12	0.89	0.24	-	27,39,43,44	0
2	BGC	H	2372	12/12	0.94	0.16	-	14,23,29,29	0
2	BGC	Q	4272	12/12	0.95	0.18	-	19,28,32,38	0
2	BGC	M	3392	12/12	0.80	0.23	-	33,47,49,52	0
2	BGC	A	1172	12/12	0.88	0.22	-	22,30,39,45	0
3	GAL	C	1381	12/12	0.93	0.17	-	22,26,30,35	0
2	BGC	O	3572	12/12	0.93	0.16	-	25,31,36,42	0
2	BGC	F	2172	12/12	0.91	0.20	-	28,31,36,38	0
3	GAL	H	2381	12/12	0.93	0.14	-	18,28,31,32	0
2	BGC	J	2592	12/12	0.82	0.31	-	51,55,61,62	0
2	GAL	F	2181	11/12	0.91	0.16	-	27,37,40,40	0
2	BGC	Q	4292	12/12	0.92	0.16	-	31,39,43,45	0
3	GAL	B	1271	12/12	0.84	0.36	-	60,67,69,73	0
2	GAL	R	4381	11/12	0.93	0.16	-	32,34,39,39	0
2	BGC	D	1492	12/12	0.93	0.16	-	29,36,38,40	0
2	BGC	J	2582	12/12	0.84	0.31	-	47,67,73,74	0
3	GAL	B	1281	12/12	0.96	0.15	-	22,28,29,31	0
2	BGC	F	2192	12/12	0.85	0.29	-	36,49,53,53	0
2	GAL	J	2581	11/12	0.91	0.19	-	25,33,41,45	0
2	BGC	O	3592	12/12	0.81	0.30	-	44,51,54,55	0
2	BGC	K	3192	12/12	0.91	0.24	-	40,51,53,55	0
3	GAL	S	4481	12/12	0.93	0.19	-	29,32,35,36	0
2	GAL	Q	4281	11/12	0.92	0.17	-	22,28,33,33	0
3	GAL	D	1481	12/12	0.91	0.18	-	23,28,30,34	0
2	BGC	G	2292	12/12	0.91	0.17	-	26,38,40,43	0
2	BGC	I	2492	12/12	0.89	0.23	-	36,42,47,51	0
3	GAL	P	4181	12/12	0.94	0.21	-	25,31,38,38	0
2	BGC	L	3292	12/12	0.89	0.22	-	29,41,45,49	0
3	GAL	N	3481	12/12	0.94	0.20	-	22,27,37,42	0
2	BGC	B	1292	12/12	0.89	0.20	-	28,39,43,46	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	GAL	O	3581	12/12	0.93	0.19	-	25,31,38,42	0
3	GAL	T	4581	12/12	0.95	0.14	-	21,27,32,34	0
2	GAL	E	1581	11/12	0.93	0.14	-	25,26,31,35	0
2	BGC	T	4592	12/12	0.88	0.32	-	49,56,61,62	0
2	BGC	C	1392	12/12	0.94	0.22	-	31,36,43,43	0
3	GAL	K	3181	12/12	0.89	0.21	-	28,37,41,44	0
2	BGC	E	1592	12/12	0.90	0.19	-	38,42,44,44	0
2	BGC	R	4392	12/12	0.86	0.22	-	47,55,59,61	0
3	GAL	M	3381	12/12	0.95	0.16	-	20,24,29,29	0
2	BGC	Q	4282	12/12	0.89	0.16	-	35,40,40,41	8
3	GAL	L	3281	12/12	0.94	0.18	-	20,27,31,33	0
2	BGC	R	4382	12/12	0.84	0.23	-	46,58,61,62	4
2	BGC	M	3372	12/12	0.94	0.15	-	2,8,12,15	0
2	BGC	D	1472	12/12	0.91	0.16	-	20,25,32,33	0
3	GAL	I	2481	12/12	0.93	0.15	-	18,23,26,27	0
3	GAL	A	1181	12/12	0.93	0.17	-	29,32,35,38	0
2	BGC	A	1192	12/12	0.81	0.26	-	37,50,54,56	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	GAL	G	2270	12/12	0.79	0.42	20.26	79,88,90,93	0
4	GAL	J	2570	12/12	0.77	0.58	15.94	84,89,91,91	0
4	GAL	C	1370	12/12	0.72	0.54	15.01	67,74,77,77	0
4	GAL	N	3470	12/12	0.63	0.58	13.30	81,85,86,87	0
4	GAL	I	2470	12/12	0.82	0.44	12.13	79,81,83,83	0
4	GAL	R	4370	12/12	0.73	0.52	10.80	81,88,90,91	0
4	GAL	K	3170	12/12	0.75	0.51	9.62	72,84,87,87	0
4	GAL	E	1570	12/12	0.71	0.45	9.20	85,88,90,90	0
4	GAL	T	4570	12/12	0.63	0.42	8.84	65,74,76,77	0
4	GAL	P	4170	12/12	0.79	0.37	8.08	68,81,83,83	0
4	GAL	L	3270	12/12	0.81	0.37	7.63	55,65,68,71	0

6.5 Other polymers (i)

There are no such residues in this entry.