Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 03:07 AM EDT

PDB ID	:	2XCI
Title	:	Membrane-embedded monofunctional glycosyltransferase WaaA of Aquifex aeolicus, substrate-free form
Authors	:	Schmidt, H.; Hansen, G.; Hilgenfeld, R.; Mamat, U.; Mesters, J.R.
Deposited on	:	2010-04-26
Resolution	:	2.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

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

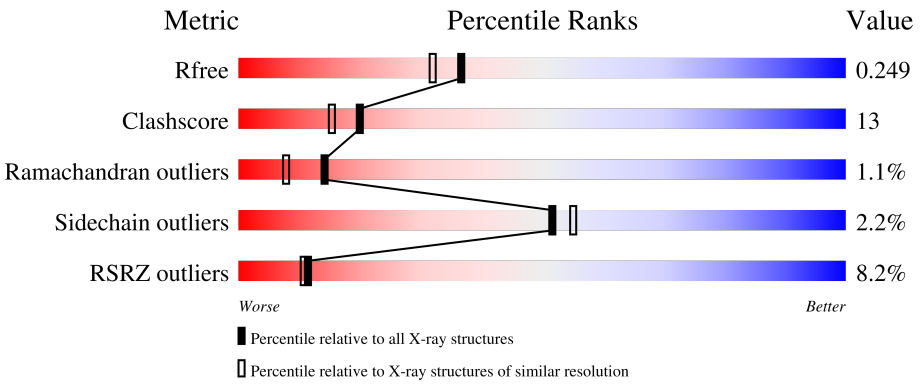
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	374	7% 70% 23% • 5%
1	B	374	6% 73% 19% • 6%
1	C	374	10% 70% 22% • 6%
1	D	374	8% 78% 15% • 6%

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	PG4	D	1353	-	-	X	-
3	GOL	A	1356	-	-	X	-
3	GOL	A	1357	-	-	X	-
3	GOL	C	1353	-	-	X	-
3	GOL	C	1354	-	-	X	-
6	BME	C	1356	-	-	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 11857 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 3-DEOXY-D-MANNO-2-OCTULOSONIC ACID TRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	354	2888	1899	482	499	8	0	0	0
1	B	352	2867	1887	475	497	8	0	0	0
1	C	353	2877	1893	478	498	8	0	0	0
1	D	352	2867	1887	475	497	8	0	0	0

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP O66663
A	-19	GLY	-	expression tag	UNP O66663
A	-18	HIS	-	expression tag	UNP O66663
A	-17	HIS	-	expression tag	UNP O66663
A	-16	HIS	-	expression tag	UNP O66663
A	-15	HIS	-	expression tag	UNP O66663
A	-14	HIS	-	expression tag	UNP O66663
A	-13	HIS	-	expression tag	UNP O66663
A	-12	HIS	-	expression tag	UNP O66663
A	-11	HIS	-	expression tag	UNP O66663
A	-10	HIS	-	expression tag	UNP O66663
A	-9	HIS	-	expression tag	UNP O66663
A	-8	SER	-	expression tag	UNP O66663
A	-7	SER	-	expression tag	UNP O66663
A	-6	GLY	-	expression tag	UNP O66663
A	-5	HIS	-	expression tag	UNP O66663
A	-4	ILE	-	expression tag	UNP O66663
A	-3	GLU	-	expression tag	UNP O66663
A	-2	GLY	-	expression tag	UNP O66663
A	-1	ARG	-	expression tag	UNP O66663

Continued on next page...

Continued from previous page...

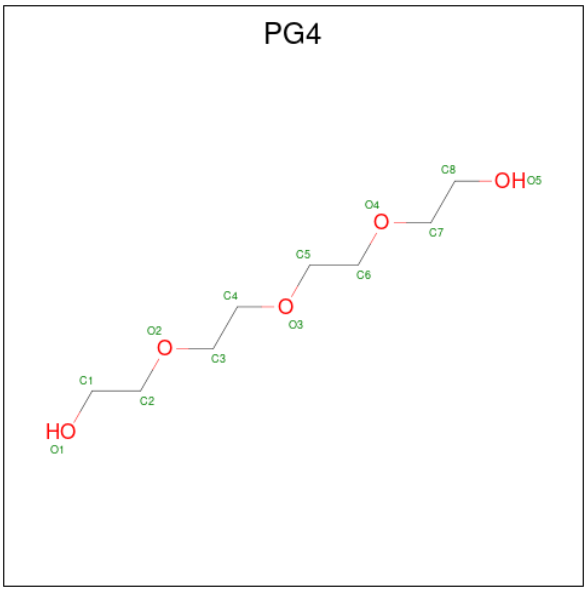
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP O66663
B	-20	MET	-	expression tag	UNP O66663
B	-19	GLY	-	expression tag	UNP O66663
B	-18	HIS	-	expression tag	UNP O66663
B	-17	HIS	-	expression tag	UNP O66663
B	-16	HIS	-	expression tag	UNP O66663
B	-15	HIS	-	expression tag	UNP O66663
B	-14	HIS	-	expression tag	UNP O66663
B	-13	HIS	-	expression tag	UNP O66663
B	-12	HIS	-	expression tag	UNP O66663
B	-11	HIS	-	expression tag	UNP O66663
B	-10	HIS	-	expression tag	UNP O66663
B	-9	HIS	-	expression tag	UNP O66663
B	-8	SER	-	expression tag	UNP O66663
B	-7	SER	-	expression tag	UNP O66663
B	-6	GLY	-	expression tag	UNP O66663
B	-5	HIS	-	expression tag	UNP O66663
B	-4	ILE	-	expression tag	UNP O66663
B	-3	GLU	-	expression tag	UNP O66663
B	-2	GLY	-	expression tag	UNP O66663
B	-1	ARG	-	expression tag	UNP O66663
B	0	HIS	-	expression tag	UNP O66663
C	-20	MET	-	expression tag	UNP O66663
C	-19	GLY	-	expression tag	UNP O66663
C	-18	HIS	-	expression tag	UNP O66663
C	-17	HIS	-	expression tag	UNP O66663
C	-16	HIS	-	expression tag	UNP O66663
C	-15	HIS	-	expression tag	UNP O66663
C	-14	HIS	-	expression tag	UNP O66663
C	-13	HIS	-	expression tag	UNP O66663
C	-12	HIS	-	expression tag	UNP O66663
C	-11	HIS	-	expression tag	UNP O66663
C	-10	HIS	-	expression tag	UNP O66663
C	-9	HIS	-	expression tag	UNP O66663
C	-8	SER	-	expression tag	UNP O66663
C	-7	SER	-	expression tag	UNP O66663
C	-6	GLY	-	expression tag	UNP O66663
C	-5	HIS	-	expression tag	UNP O66663
C	-4	ILE	-	expression tag	UNP O66663
C	-3	GLU	-	expression tag	UNP O66663
C	-2	GLY	-	expression tag	UNP O66663
C	-1	ARG	-	expression tag	UNP O66663

Continued on next page...

Continued from previous page...

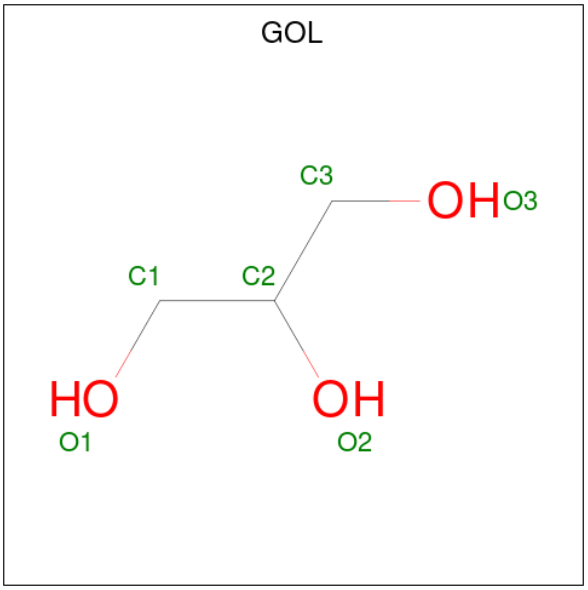
Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP O66663
D	-20	MET	-	expression tag	UNP O66663
D	-19	GLY	-	expression tag	UNP O66663
D	-18	HIS	-	expression tag	UNP O66663
D	-17	HIS	-	expression tag	UNP O66663
D	-16	HIS	-	expression tag	UNP O66663
D	-15	HIS	-	expression tag	UNP O66663
D	-14	HIS	-	expression tag	UNP O66663
D	-13	HIS	-	expression tag	UNP O66663
D	-12	HIS	-	expression tag	UNP O66663
D	-11	HIS	-	expression tag	UNP O66663
D	-10	HIS	-	expression tag	UNP O66663
D	-9	HIS	-	expression tag	UNP O66663
D	-8	SER	-	expression tag	UNP O66663
D	-7	SER	-	expression tag	UNP O66663
D	-6	GLY	-	expression tag	UNP O66663
D	-5	HIS	-	expression tag	UNP O66663
D	-4	ILE	-	expression tag	UNP O66663
D	-3	GLU	-	expression tag	UNP O66663
D	-2	GLY	-	expression tag	UNP O66663
D	-1	ARG	-	expression tag	UNP O66663
D	0	HIS	-	expression tag	UNP O66663

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 7	C 4	O 3	0	0
2	A	1	Total 12	C 8	O 4	0	0
2	D	1	Total 13	C 8	O 5	0	0
2	D	1	Total 10	C 6	O 4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

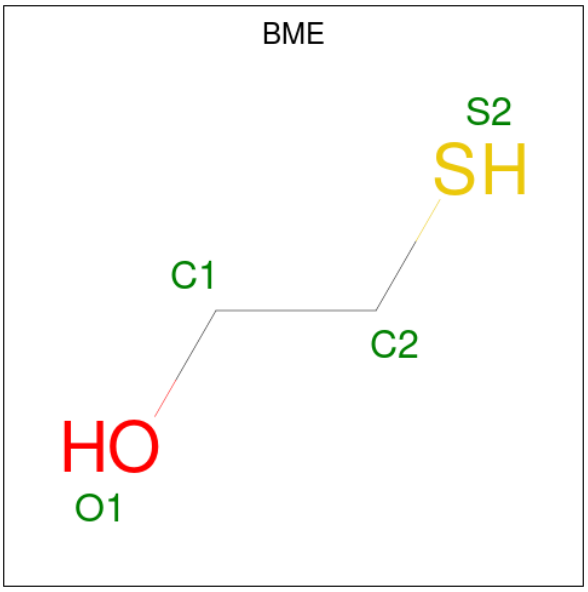
- Molecule 4 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ni		
4	A	1	1	1	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	1	1	1	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
5	A	3	3	3	0	0
5	B	2	2	2	0	0
5	C	1	1	1	0	0
5	D	2	2	2	0	0

- Molecule 6 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
6	C	1	4	2	1	1	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
6	C	1	4	2	1	1	0	0

- Molecule 7 is water.

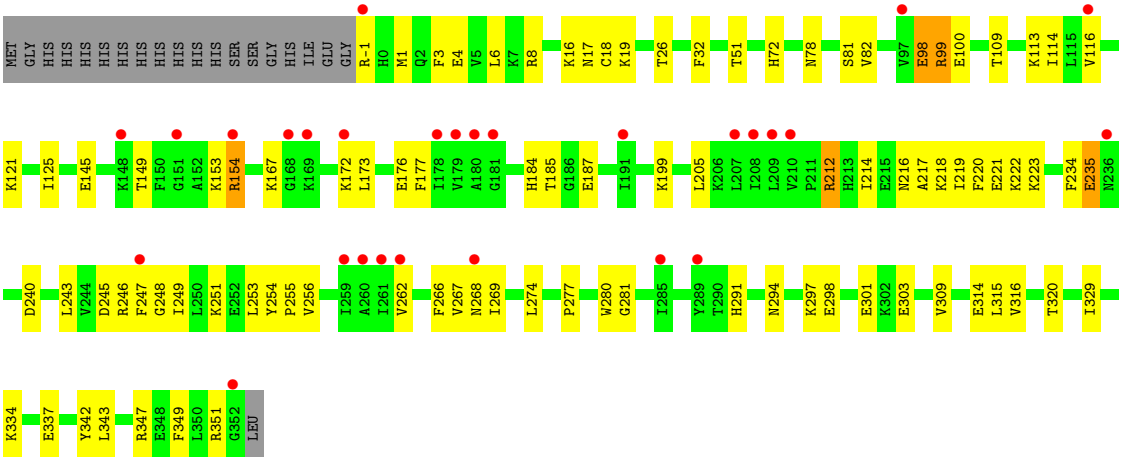
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
7	A	57	57	57	0	0
			Total	O		
7	B	69	69	69	0	0
			Total	O		
7	C	58	58	58	0	0
			Total	O		
7	D	64	64	64	0	0

3 Residue-property plots (i)

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

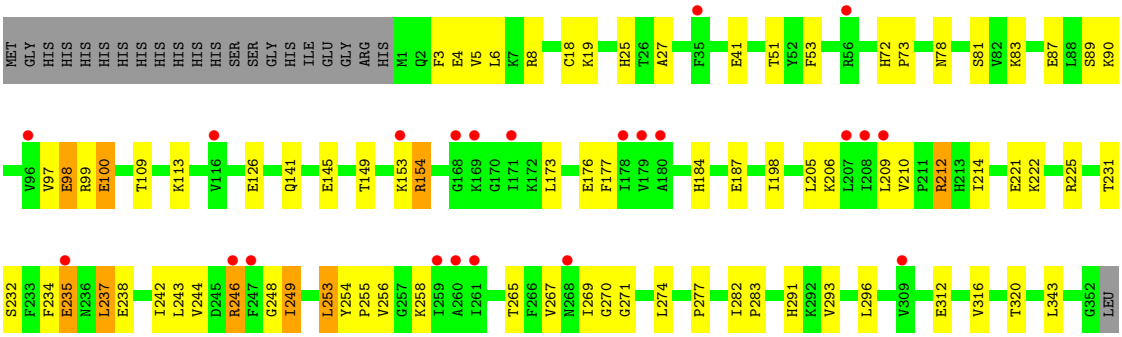
• Molecule 1: 3-DEOXY-D-MANNO-2-OCTULOSONIC ACID TRANSFERASE

Chain A:



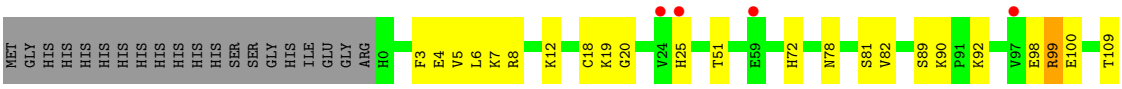
• Molecule 1: 3-DEOXY-D-MANNO-2-OCTULOSONIC ACID TRANSFERASE

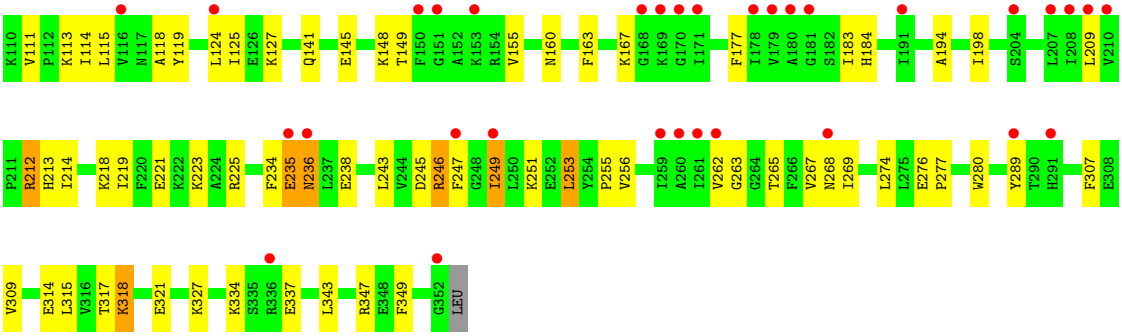
Chain B:



• Molecule 1: 3-DEOXY-D-MANNO-2-OCTULOSONIC ACID TRANSFERASE

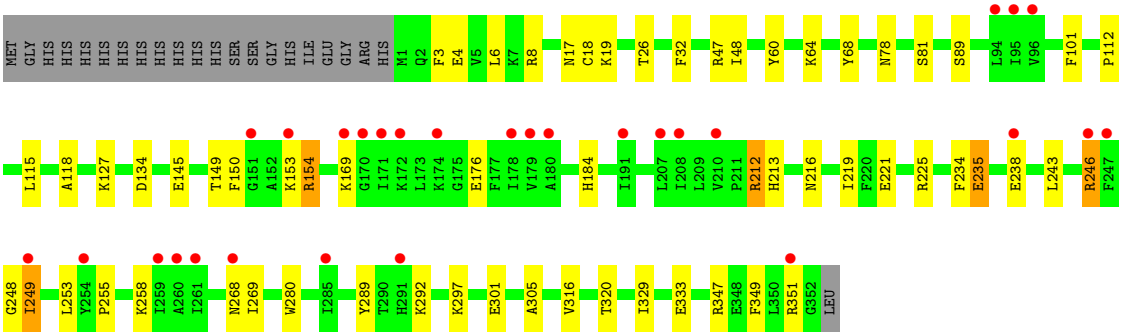
Chain C:





- Molecule 1: 3-DEOXY-D-MANNO-2-OCTULOSONIC ACID TRANSFERASE

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	132.50Å 45.82Å 144.07Å 90.00° 97.23° 90.00°	Depositor
Resolution (Å)	29.85 – 2.00 29.85 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.9 (29.85-2.00) 98.9 (29.85-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.25 (at 2.00Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.207 , 0.254 0.203 , 0.249	Depositor DCC
R_{free} test set	5821 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.712	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	11857	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.23% 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, 0.333 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: GOL, BME, PG4, NI, CL

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	0.40	0/2952	0.55	0/3960
1	B	0.41	0/2930	0.55	0/3931
1	C	0.39	0/2941	0.55	0/3946
1	D	0.39	0/2930	0.54	0/3931
All	All	0.39	0/11753	0.55	0/15768

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2888	0	3028	87	0
1	B	2867	0	3008	75	0
1	C	2877	0	3015	84	0
1	D	2867	0	3008	52	0
2	A	19	0	24	3	0
2	D	23	0	31	10	0
3	A	18	0	24	10	0
3	B	6	0	8	3	0
3	C	12	0	16	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	12	0	16	4	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
5	C	1	0	0	0	0
5	D	2	0	0	0	0
6	C	8	0	12	8	0
7	A	57	0	0	2	0
7	B	69	0	0	1	0
7	C	58	0	0	2	0
7	D	64	0	0	5	0
All	All	11857	0	12190	299	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 13.

All (299) 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:221:GLU:HG2	1:B:231:THR:HG21	1.37	1.03
3:A:1357:GOL:H12	6:C:1356:BME:S2	2.02	0.99
3:B:1353:GOL:H11	7:B:2004:HOH:O	1.73	0.88
1:B:5:VAL:HG21	2:D:1353:PG4:H81	1.56	0.88
3:D:1355:GOL:H11	7:D:2001:HOH:O	1.75	0.85
1:B:176:GLU:HG2	1:B:205:LEU:HD23	1.56	0.85
1:D:219:ILE:HD12	1:D:219:ILE:H	1.41	0.85
1:C:6:LEU:HB2	3:C:1354:GOL:H32	1.56	0.85
1:A:-1:ARG:HD2	1:C:119:TYR:OH	1.77	0.84
1:A:185:THR:H	3:A:1357:GOL:H32	1.41	0.84
1:A:219:ILE:H	1:A:219:ILE:HD12	1.42	0.84
1:C:209:LEU:HD23	1:C:243:LEU:HD21	1.61	0.83
1:B:248:GLY:O	1:B:249:ILE:HG22	1.77	0.83
1:A:6:LEU:H	3:A:1356:GOL:H2	1.42	0.82
1:D:184:HIS:CE1	1:D:269:ILE:HD13	2.17	0.80
1:D:6:LEU:H	3:D:1355:GOL:H2	1.46	0.80
1:B:19:LYS:HE3	1:B:90:LYS:HD2	1.65	0.79
1:D:216:ASN:HA	1:D:219:ILE:HD13	1.63	0.79
1:B:5:VAL:HG22	2:D:1353:PG4:H42	1.64	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:153:LYS:O	1:D:154:ARG:HB2	1.82	0.78
1:A:216:ASN:HA	1:A:219:ILE:HD13	1.65	0.76
1:B:246:ARG:HH22	1:B:249:ILE:HD13	1.51	0.76
1:B:5:VAL:CG2	2:D:1353:PG4:H81	2.15	0.76
1:A:212:ARG:HD3	1:A:212:ARG:C	2.06	0.74
1:C:307:PHE:CD1	1:C:318:LYS:HE2	2.22	0.74
3:A:1356:GOL:H11	1:C:125:ILE:HB	1.70	0.73
1:A:297:LYS:HE2	1:A:301:GLU:OE2	1.89	0.72
1:B:6:LEU:H	3:B:1353:GOL:H2	1.56	0.71
1:A:262:VAL:HG21	1:A:274:LEU:HD22	1.72	0.70
1:C:6:LEU:CB	3:C:1354:GOL:H32	2.20	0.70
1:B:246:ARG:HH11	1:B:246:ARG:H	1.39	0.70
1:C:6:LEU:HB2	3:C:1354:GOL:C3	2.22	0.69
1:C:262:VAL:HG21	1:C:274:LEU:HD23	1.73	0.69
1:B:109:THR:OG1	1:B:113:LYS:HE3	1.93	0.69
3:A:1357:GOL:C1	6:C:1356:BME:S2	2.80	0.69
1:A:116:VAL:HG13	1:A:342:TYR:CE1	2.28	0.69
1:A:212:ARG:HD3	1:A:212:ARG:O	1.93	0.69
1:A:116:VAL:HG13	1:A:342:TYR:HE1	1.59	0.68
1:A:125:ILE:HB	3:C:1354:GOL:H31	1.74	0.68
1:C:246:ARG:HH11	1:C:246:ARG:HB2	1.58	0.68
1:D:234:PHE:O	1:D:235:GLU:HB2	1.91	0.68
1:A:262:VAL:HG21	1:A:274:LEU:CD2	2.24	0.67
1:C:124:LEU:HA	1:C:127:LYS:HE3	1.77	0.67
1:B:25:HIS:NE2	1:B:100:GLU:OE1	2.28	0.67
1:B:153:LYS:O	1:B:154:ARG:HB2	1.94	0.66
1:C:255:PRO:HG3	1:C:280:TRP:CD2	2.30	0.66
1:C:262:VAL:HG21	1:C:274:LEU:CD2	2.25	0.65
1:D:18:CYS:HA	1:D:47:ARG:NH2	2.12	0.65
1:C:267:VAL:HG23	1:C:269:ILE:HG12	1.78	0.64
1:C:255:PRO:HG3	1:C:280:TRP:CE2	2.33	0.64
1:A:219:ILE:O	1:A:222:LYS:HG3	1.97	0.64
1:A:255:PRO:HG3	1:A:280:TRP:CE2	2.33	0.63
1:B:41:GLU:HG3	1:B:343:LEU:HD11	1.79	0.63
1:D:101:PHE:H	2:D:1353:PG4:H72	1.64	0.63
1:C:98:GLU:O	1:C:99:ARG:HB2	1.98	0.62
1:A:220:PHE:HB2	1:A:243:LEU:HD21	1.80	0.62
1:C:78:ASN:ND2	1:C:81:SER:H	1.97	0.62
1:B:209:LEU:HB3	1:B:243:LEU:HD23	1.81	0.62
1:B:293:VAL:HG22	1:B:296:LEU:HB3	1.80	0.61
1:C:99:ARG:O	1:C:99:ARG:HG2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:PHE:O	1:C:235:GLU:HB2	1.99	0.61
1:A:-1:ARG:HD3	1:A:3:PHE:HE2	1.66	0.61
1:B:234:PHE:O	1:B:235:GLU:HG2	2.01	0.61
1:A:255:PRO:HG3	1:A:280:TRP:CD2	2.37	0.60
1:A:303:GLU:HG3	7:A:2055:HOH:O	2.00	0.59
1:A:218:LYS:O	1:A:222:LYS:HG2	2.02	0.59
1:D:219:ILE:HD12	1:D:219:ILE:N	2.13	0.59
1:B:25:HIS:CD2	1:B:100:GLU:OE1	2.56	0.59
1:B:254:TYR:N	1:B:255:PRO:HD2	2.18	0.59
1:D:219:ILE:H	1:D:219:ILE:CD1	2.13	0.59
1:C:221:GLU:HB2	1:C:243:LEU:HD12	1.84	0.59
1:C:4:GLU:HA	3:C:1354:GOL:H12	1.85	0.59
1:D:127:LYS:HG2	1:D:150:PHE:CE1	2.38	0.58
1:A:219:ILE:HG23	1:C:223:LYS:NZ	2.18	0.58
1:C:19:LYS:HA	1:C:89:SER:O	2.03	0.58
1:D:316:VAL:O	1:D:320:THR:HG23	2.03	0.58
3:A:1356:GOL:H11	1:C:125:ILE:CB	2.33	0.58
1:B:316:VAL:O	1:B:320:THR:HG23	2.04	0.58
3:A:1356:GOL:H11	1:C:125:ILE:CG2	2.34	0.57
1:D:213:HIS:ND1	3:D:1356:GOL:H31	2.19	0.57
1:D:154:ARG:HG3	7:D:2024:HOH:O	2.05	0.57
1:A:248:GLY:O	1:A:249:ILE:HB	2.04	0.57
1:B:209:LEU:HD23	1:B:243:LEU:HD21	1.87	0.57
1:C:213:HIS:ND1	6:C:1356:BME:H21	2.20	0.57
1:A:82:VAL:CG1	1:A:109:THR:HG23	2.35	0.57
1:A:234:PHE:O	1:A:235:GLU:HB2	2.05	0.57
1:C:219:ILE:HD12	7:C:2038:HOH:O	2.05	0.56
1:A:281:GLY:HA2	1:A:329:ILE:HB	1.88	0.56
1:A:262:VAL:CG2	1:A:274:LEU:HD22	2.36	0.56
1:B:209:LEU:HB3	1:B:243:LEU:CD2	2.36	0.56
1:C:109:THR:OG1	1:C:113:LYS:HE3	2.05	0.56
1:D:248:GLY:O	1:D:249:ILE:HB	2.06	0.56
1:A:121:LYS:NZ	3:C:1353:GOL:C3	2.68	0.56
1:A:184:HIS:CE1	1:A:269:ILE:HD12	2.40	0.56
1:B:267:VAL:HG23	1:B:269:ILE:HG12	1.88	0.55
1:C:209:LEU:HB3	1:C:243:LEU:HD23	1.88	0.55
1:B:221:GLU:HB2	1:B:243:LEU:HD12	1.87	0.55
1:C:274:LEU:O	1:C:277:PRO:HD2	2.07	0.55
1:D:184:HIS:CE1	1:D:269:ILE:CD1	2.89	0.55
1:D:297:LYS:HE2	1:D:301:GLU:OE2	2.06	0.55
1:A:153:LYS:O	1:A:154:ARG:HB2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:NZ	3:C:1353:GOL:H31	2.21	0.54
1:C:7:LYS:HG2	1:C:12:LYS:HG3	1.88	0.54
1:A:234:PHE:CD2	1:A:235:GLU:N	2.76	0.54
3:C:1353:GOL:H2	3:C:1354:GOL:O2	2.08	0.54
1:A:184:HIS:HB3	3:A:1357:GOL:H31	1.89	0.54
1:B:141:GLN:O	1:B:145:GLU:HG2	2.06	0.54
1:B:19:LYS:HE3	1:B:90:LYS:CD	2.36	0.54
1:D:212:ARG:HD3	1:D:212:ARG:C	2.28	0.54
1:B:222:LYS:HG2	1:B:225:ARG:NH2	2.23	0.54
1:B:72:HIS:ND1	1:B:73:PRO:HD2	2.23	0.54
1:B:176:GLU:HG3	1:B:258:LYS:HD2	1.89	0.54
1:B:3:PHE:CD1	2:D:1353:PG4:H62	2.43	0.53
1:B:3:PHE:HB2	2:D:1353:PG4:H82	1.89	0.53
1:A:268:ASN:OD1	1:A:291:HIS:HE1	1.91	0.53
1:A:267:VAL:HB	6:C:1355:BME:H12	1.91	0.53
1:D:212:ARG:HD3	1:D:212:ARG:O	2.09	0.53
1:D:19:LYS:HA	1:D:89:SER:O	2.08	0.52
1:A:221:GLU:HB2	1:A:243:LEU:HD22	1.90	0.52
1:C:78:ASN:HD21	1:C:81:SER:H	1.58	0.52
1:C:213:HIS:ND1	6:C:1356:BME:C2	2.73	0.52
1:B:153:LYS:O	1:B:154:ARG:CB	2.58	0.52
1:C:268:ASN:HA	1:C:289:TYR:CD1	2.45	0.52
1:A:114:ILE:HD11	1:A:349:PHE:CD1	2.45	0.52
1:C:214:ILE:HG13	1:C:245:ASP:HA	1.91	0.51
1:C:218:LYS:HG3	7:C:2039:HOH:O	2.09	0.51
1:D:176:GLU:HG3	1:D:258:LYS:CE	2.40	0.51
1:D:255:PRO:HG3	1:D:280:TRP:CD2	2.45	0.51
1:D:18:CYS:HA	1:D:47:ARG:HH21	1.74	0.51
1:B:184:HIS:NE2	1:B:212:ARG:HG3	2.25	0.51
1:D:213:HIS:CE1	3:D:1356:GOL:H31	2.45	0.51
1:A:4:GLU:O	1:A:8:ARG:HG3	2.11	0.51
1:A:16:LYS:O	1:A:19:LYS:HG3	2.11	0.51
1:A:-1:ARG:HD3	1:A:3:PHE:CE2	2.46	0.51
1:B:83:LYS:O	1:B:87:GLU:HG2	2.11	0.51
1:D:255:PRO:HG3	1:D:280:TRP:CE2	2.45	0.50
1:A:309:VAL:HG11	1:A:315:LEU:HB2	1.94	0.50
2:A:1354:PG4:H52	1:C:5:VAL:HG22	1.93	0.50
1:B:78:ASN:ND2	1:B:81:SER:H	2.09	0.50
1:C:309:VAL:HG13	1:C:314:GLU:HB2	1.93	0.50
1:B:25:HIS:HE2	1:B:100:GLU:CD	2.15	0.50
1:C:114:ILE:HD11	1:C:349:PHE:CE1	2.47	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:351:ARG:HB3	7:D:2064:HOH:O	2.11	0.50
1:A:109:THR:OG1	1:A:113:LYS:HE3	2.12	0.50
1:C:184:HIS:HA	6:C:1356:BME:H11	1.93	0.50
1:A:26:THR:HG21	1:A:32:PHE:HA	1.93	0.49
1:A:351:ARG:HD2	7:A:2057:HOH:O	2.11	0.49
1:C:25:HIS:CD2	1:C:100:GLU:HG3	2.47	0.49
1:A:-1:ARG:HD2	1:C:119:TYR:HH	1.78	0.49
1:C:82:VAL:CG1	1:C:109:THR:HG23	2.41	0.49
1:C:141:GLN:O	1:C:145:GLU:HG2	2.13	0.49
1:A:267:VAL:HG23	1:A:269:ILE:HG13	1.93	0.49
1:D:101:PHE:H	2:D:1353:PG4:C7	2.26	0.49
1:B:5:VAL:N	3:B:1353:GOL:H2	2.27	0.48
1:C:209:LEU:HB3	1:C:243:LEU:CD2	2.43	0.48
1:B:246:ARG:HB2	1:B:246:ARG:CZ	2.43	0.48
1:C:114:ILE:HD11	1:C:349:PHE:CD1	2.47	0.48
1:C:234:PHE:O	1:C:235:GLU:CB	2.61	0.48
1:D:246:ARG:HB3	1:D:246:ARG:NH1	2.29	0.48
1:A:172:LYS:O	1:A:173:LEU:HD23	2.14	0.48
1:C:317:THR:O	1:C:321:GLU:HG3	2.14	0.48
1:A:316:VAL:O	1:A:320:THR:HG23	2.14	0.48
1:C:145:GLU:O	1:C:149:THR:HG23	2.13	0.48
1:A:184:HIS:CE1	1:A:212:ARG:HG3	2.48	0.47
1:D:246:ARG:HB3	1:D:246:ARG:CZ	2.44	0.47
1:D:234:PHE:O	1:D:235:GLU:CB	2.61	0.47
1:A:262:VAL:CG2	1:A:274:LEU:CD2	2.92	0.47
1:B:27:ALA:HB2	1:B:100:GLU:CD	2.35	0.47
1:C:51:THR:HA	1:C:72:HIS:O	2.15	0.47
1:C:309:VAL:HG11	1:C:315:LEU:HB2	1.95	0.47
1:B:253:LEU:O	1:B:256:VAL:HB	2.15	0.47
1:C:4:GLU:O	1:C:8:ARG:HG3	2.14	0.47
1:C:253:LEU:O	1:C:256:VAL:HB	2.15	0.47
1:C:262:VAL:CG2	1:C:274:LEU:HD23	2.44	0.47
1:A:145:GLU:O	1:A:149:THR:HG23	2.14	0.47
1:A:199:LYS:HE3	1:A:205:LEU:O	2.14	0.47
1:B:97:VAL:HG12	1:B:98:GLU:CG	2.45	0.47
1:B:265:THR:HG22	1:B:271:GLY:HA2	1.97	0.47
1:C:109:THR:HB	1:C:111:VAL:HG12	1.97	0.47
1:A:219:ILE:HG23	1:C:223:LYS:HZ1	1.78	0.47
1:C:167:LYS:O	1:C:251:LYS:HE2	2.15	0.47
1:A:254:TYR:N	1:A:255:PRO:CD	2.78	0.47
1:C:249:ILE:HG22	1:C:253:LEU:HD22	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:LYS:HZ2	3:C:1353:GOL:H31	1.80	0.47
1:A:274:LEU:O	1:A:277:PRO:HD2	2.15	0.47
1:B:19:LYS:HA	1:B:89:SER:O	2.14	0.46
1:A:262:VAL:O	1:A:262:VAL:HG23	2.16	0.46
3:A:1356:GOL:H11	1:C:125:ILE:HG22	1.97	0.46
1:A:121:LYS:NZ	3:C:1353:GOL:H32	2.31	0.46
1:C:20:GLY:O	1:C:92:LYS:HE2	2.16	0.46
1:B:267:VAL:HG23	1:B:269:ILE:CG1	2.46	0.46
1:B:293:VAL:CG2	1:B:296:LEU:HD23	2.46	0.46
1:C:343:LEU:HG	1:C:347:ARG:CZ	2.46	0.46
1:A:214:ILE:HG21	1:A:245:ASP:O	2.16	0.46
1:A:187:GLU:HG2	1:A:266:PHE:HB2	1.98	0.46
1:D:4:GLU:O	1:D:8:ARG:HG3	2.16	0.46
1:B:244:VAL:HG11	1:B:249:ILE:HG21	1.98	0.46
3:A:1355:GOL:H11	3:A:1356:GOL:H12	1.98	0.46
1:B:187:GLU:HG2	1:B:267:VAL:HG13	1.98	0.46
1:C:183:ILE:O	6:C:1356:BME:H11	2.16	0.46
1:D:221:GLU:HA	1:D:243:LEU:HD11	1.97	0.46
1:D:268:ASN:HA	1:D:289:TYR:CG	2.51	0.46
1:B:265:THR:CG2	1:B:271:GLY:HA2	2.46	0.45
1:A:234:PHE:O	1:A:235:GLU:CB	2.63	0.45
1:B:198:ILE:HD12	1:B:316:VAL:HG13	1.98	0.45
1:B:221:GLU:N	1:B:243:LEU:HD11	2.32	0.45
1:B:312:GLU:O	1:B:316:VAL:HG23	2.17	0.45
1:C:262:VAL:CG2	1:C:274:LEU:CD2	2.95	0.45
1:B:234:PHE:O	1:B:235:GLU:CB	2.63	0.45
1:D:60:TYR:CZ	1:D:64:LYS:HE3	2.52	0.45
1:D:249:ILE:HG23	1:D:253:LEU:CD2	2.46	0.45
1:A:176:GLU:HG3	1:A:205:LEU:HA	1.98	0.45
1:C:212:ARG:HB3	6:C:1356:BME:H21	1.99	0.45
1:A:177:PHE:CD2	1:A:256:VAL:HG12	2.52	0.45
1:C:115:LEU:HG	1:C:118:ALA:HB2	1.98	0.45
1:A:219:ILE:H	1:A:219:ILE:CD1	2.16	0.45
1:B:3:PHE:CB	2:D:1353:PG4:H82	2.47	0.45
1:C:3:PHE:HB2	3:C:1353:GOL:O3	2.17	0.45
1:C:263:GLY:O	1:C:265:THR:HG23	2.17	0.45
1:C:148:LYS:HG3	1:C:155:VAL:HG11	1.99	0.44
1:A:334:LYS:O	1:A:337:GLU:HB3	2.17	0.44
1:B:97:VAL:HG12	1:B:98:GLU:HG2	1.99	0.44
1:B:210:VAL:HG22	1:B:244:VAL:HG21	1.99	0.44
1:D:112:PRO:HA	1:D:134:ASP:OD2	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:THR:HA	1:A:72:HIS:O	2.18	0.44
1:B:109:THR:OG1	1:B:113:LYS:CE	2.65	0.44
1:D:153:LYS:O	1:D:154:ARG:CB	2.55	0.44
1:A:343:LEU:O	1:A:347:ARG:HG3	2.18	0.44
1:B:244:VAL:CG1	1:B:249:ILE:HG21	2.47	0.44
1:B:231:THR:HG22	1:B:232:SER:N	2.33	0.44
1:C:243:LEU:HD23	1:C:243:LEU:HA	1.65	0.44
1:B:177:PHE:CD1	1:B:206:LYS:HB2	2.53	0.44
1:B:246:ARG:HH22	1:B:249:ILE:CD1	2.25	0.44
1:A:217:ALA:O	1:A:243:LEU:CD2	2.66	0.43
2:A:1354:PG4:H52	1:C:5:VAL:CG2	2.48	0.43
1:B:53:PHE:CZ	2:D:1353:PG4:H21	2.53	0.43
1:A:294:ASN:O	1:A:298:GLU:HG3	2.18	0.43
1:D:176:GLU:HG3	1:D:258:LYS:HE2	2.01	0.43
1:A:16:LYS:C	1:A:18:CYS:H	2.22	0.43
1:B:51:THR:HA	1:B:72:HIS:O	2.19	0.43
1:A:78:ASN:ND2	1:A:81:SER:H	2.16	0.43
1:A:167:LYS:O	1:A:251:LYS:HE2	2.19	0.43
1:B:274:LEU:O	1:B:277:PRO:HD2	2.18	0.43
1:A:121:LYS:HZ3	3:C:1353:GOL:C3	2.31	0.43
1:C:148:LYS:HG3	1:C:155:VAL:CG1	2.48	0.43
1:A:184:HIS:CE1	1:A:269:ILE:CD1	3.01	0.43
1:D:17:ASN:O	1:D:47:ARG:NH2	2.52	0.42
1:D:48:ILE:HB	1:D:68:TYR:HA	2.01	0.42
1:D:221:GLU:HB2	1:D:243:LEU:HD13	2.01	0.42
1:C:184:HIS:NE2	1:C:212:ARG:HG3	2.33	0.42
1:C:194:ALA:O	1:C:198:ILE:HG12	2.19	0.42
1:A:121:LYS:HZ3	3:C:1353:GOL:H32	1.84	0.42
1:A:220:PHE:CB	1:A:243:LEU:HD21	2.47	0.42
1:D:47:ARG:HG3	1:D:47:ARG:HH11	1.83	0.42
1:B:258:LYS:HE2	1:B:258:LYS:HB3	1.77	0.42
1:C:262:VAL:HG21	1:C:274:LEU:HD22	2.00	0.42
1:A:153:LYS:O	1:A:154:ARG:CB	2.66	0.42
1:C:334:LYS:O	1:C:337:GLU:HB3	2.20	0.42
1:A:99:ARG:O	1:A:100:GLU:C	2.58	0.42
1:A:249:ILE:HG22	1:A:253:LEU:HD22	2.01	0.42
1:A:262:VAL:HG21	1:A:274:LEU:HD23	1.99	0.42
1:B:4:GLU:O	1:B:8:ARG:HG3	2.20	0.42
1:A:121:LYS:HZ2	3:C:1353:GOL:C3	2.32	0.42
1:A:309:VAL:HG13	1:A:314:GLU:HB2	2.01	0.42
1:B:234:PHE:O	1:B:235:GLU:CG	2.68	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:219:ILE:HD12	1:C:219:ILE:H	1.85	0.42
1:D:292:LYS:HD3	7:D:2046:HOH:O	2.19	0.42
1:A:218:LYS:HG2	1:A:222:LYS:NZ	2.35	0.41
1:B:255:PRO:HA	1:B:282:ILE:HD11	2.01	0.41
1:D:78:ASN:ND2	1:D:81:SER:H	2.18	0.41
1:D:347:ARG:HG2	7:D:2006:HOH:O	2.19	0.41
1:C:177:PHE:CD2	1:C:256:VAL:HG13	2.55	0.41
1:A:199:LYS:NZ	1:A:240:ASP:OD2	2.52	0.41
1:D:3:PHE:HD1	2:D:1354:PG4:H32	1.84	0.41
1:C:7:LYS:HD3	1:C:12:LYS:CD	2.50	0.41
1:C:89:SER:O	1:C:90:LYS:C	2.58	0.41
1:A:-1:ARG:C	1:A:1:MET:H	2.22	0.41
1:B:255:PRO:HA	1:B:282:ILE:CD1	2.50	0.41
1:B:221:GLU:CA	1:B:243:LEU:HD11	2.50	0.41
1:B:99:ARG:NH1	1:B:126:GLU:OE1	2.48	0.41
1:B:237:LEU:HA	1:B:242:ILE:HG12	2.03	0.41
1:B:237:LEU:N	1:B:237:LEU:HD23	2.36	0.41
1:C:236:ASN:HD22	1:C:236:ASN:HA	1.68	0.41
1:D:145:GLU:O	1:D:149:THR:HG23	2.21	0.41
1:A:153:LYS:HE2	1:A:153:LYS:HB3	1.94	0.41
1:A:219:ILE:HG23	1:C:223:LYS:HZ2	1.86	0.41
1:B:173:LEU:HD12	1:B:256:VAL:HG11	2.02	0.41
1:D:154:ARG:HH11	1:D:349:PHE:HD2	1.67	0.41
1:D:221:GLU:OE2	1:D:225:ARG:NH1	2.54	0.41
1:D:305:ALA:HB2	1:D:329:ILE:HD12	2.03	0.41
1:C:4:GLU:HA	3:C:1354:GOL:C1	2.51	0.41
1:C:160:ASN:HB3	1:C:163:PHE:CD2	2.56	0.40
1:C:236:ASN:HB3	1:C:238:GLU:OE1	2.21	0.40
1:D:115:LEU:HG	1:D:118:ALA:HB2	2.03	0.40
1:D:26:THR:HG21	1:D:32:PHE:HA	2.03	0.40
1:A:114:ILE:HD11	1:A:349:PHE:CE1	2.56	0.40
2:A:1354:PG4:H32	1:C:8:ARG:CZ	2.51	0.40
1:B:145:GLU:O	1:B:149:THR:HG23	2.21	0.40
1:B:270:GLY:HA2	1:B:291:HIS:CE1	2.55	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	352/374 (94%)	336 (96%)	11 (3%)	5 (1%)	11 5
1	B	350/374 (94%)	333 (95%)	12 (3%)	5 (1%)	11 5
1	C	351/374 (94%)	340 (97%)	8 (2%)	3 (1%)	17 11
1	D	350/374 (94%)	341 (97%)	6 (2%)	3 (1%)	17 11
All	All	1403/1496 (94%)	1350 (96%)	37 (3%)	16 (1%)	14 8

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	100	GLU
1	B	235	GLU
1	C	99	ARG
1	D	154	ARG
1	D	235	GLU
1	A	154	ARG
1	A	235	GLU
1	B	154	ARG
1	C	235	GLU
1	D	249	ILE
1	A	17	ASN
1	B	98	GLU
1	A	98	GLU
1	A	99	ARG
1	C	249	ILE
1	B	249	ILE

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	317/334 (95%)	312 (98%)	5 (2%)	62	67
1	B	315/334 (94%)	307 (98%)	8 (2%)	47	49
1	C	316/334 (95%)	306 (97%)	10 (3%)	39	38
1	D	315/334 (94%)	310 (98%)	5 (2%)	62	67
All	All	1263/1336 (94%)	1235 (98%)	28 (2%)	52	55

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	GLU
1	A	212	ARG
1	A	223	LYS
1	A	246	ARG
1	A	247	PHE
1	B	18	CYS
1	B	212	ARG
1	B	214	ILE
1	B	237	LEU
1	B	238	GLU
1	B	246	ARG
1	B	253	LEU
1	B	283	PRO
1	C	18	CYS
1	C	212	ARG
1	C	225	ARG
1	C	236	ASN
1	C	246	ARG
1	C	247	PHE
1	C	253	LEU
1	C	276	GLU
1	C	318	LYS
1	C	327	LYS
1	D	169	LYS
1	D	212	ARG
1	D	238	GLU
1	D	246	ARG
1	D	333	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	141	GLN
1	A	216	ASN
1	A	291	HIS
1	B	78	ASN
1	B	216	ASN
1	B	291	HIS
1	C	78	ASN
1	C	141	GLN
1	C	216	ASN
1	C	236	ASN
1	C	291	HIS
1	D	78	ASN
1	D	216	ASN
1	D	291	HIS

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)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 12 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	A	1357	-	5,5,5	0.40	0	5,5,5	0.47	0
3	GOL	C	1354	-	5,5,5	0.37	0	5,5,5	0.88	0
3	GOL	D	1355	-	5,5,5	0.45	0	5,5,5	0.61	0
2	PG4	D	1354	-	9,9,12	0.52	0	8,8,11	1.46	0
6	BME	C	1356	-	3,3,3	0.36	0	2,2,2	0.62	0
3	GOL	A	1355	-	5,5,5	0.36	0	5,5,5	0.55	0
2	PG4	A	1354	-	11,11,12	0.54	0	10,10,11	1.28	0
3	GOL	A	1356	-	5,5,5	0.45	0	5,5,5	0.70	0
3	GOL	C	1353	-	5,5,5	0.36	0	5,5,5	0.45	0
3	GOL	B	1353	-	5,5,5	0.42	0	5,5,5	0.35	0
6	BME	C	1355	-	3,3,3	0.38	0	2,2,2	0.34	0
2	PG4	D	1353	-	12,12,12	0.50	0	11,11,11	1.82	4 (36%)
3	GOL	D	1356	-	5,5,5	0.61	0	5,5,5	0.48	0
2	PG4	A	1353	-	6,6,12	0.52	0	5,5,11	1.41	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	1357	-	-	4/4/4/4	-
3	GOL	C	1354	-	-	3/4/4/4	-
3	GOL	D	1355	-	-	4/4/4/4	-
2	PG4	D	1354	-	-	3/7/7/10	-
6	BME	C	1356	-	-	0/1/1/1	-
3	GOL	A	1355	-	-	2/4/4/4	-
2	PG4	A	1354	-	-	6/9/9/10	-
3	GOL	A	1356	-	-	2/4/4/4	-
3	GOL	C	1353	-	-	2/4/4/4	-
3	GOL	B	1353	-	-	4/4/4/4	-
6	BME	C	1355	-	-	1/1/1/1	-
2	PG4	D	1353	-	-	6/10/10/10	-
3	GOL	D	1356	-	-	0/4/4/4	-
2	PG4	A	1353	-	-	3/4/4/10	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1353	PG4	O4-C7-C8	2.25	120.02	110.11
2	D	1353	PG4	C5-O3-C4	2.18	122.81	113.26
2	D	1353	PG4	O2-C3-C4	2.17	120.23	110.35
2	D	1353	PG4	O3-C5-C6	2.10	119.92	110.35

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1355	GOL	C1-C2-C3-O3
3	A	1356	GOL	C1-C2-C3-O3
3	A	1357	GOL	C1-C2-C3-O3
3	A	1357	GOL	O2-C2-C3-O3
3	B	1353	GOL	O1-C1-C2-C3
3	B	1353	GOL	C1-C2-C3-O3
3	C	1353	GOL	C1-C2-C3-O3
3	C	1354	GOL	C1-C2-C3-O3
3	D	1355	GOL	O1-C1-C2-C3
3	D	1355	GOL	C1-C2-C3-O3
3	D	1355	GOL	O2-C2-C3-O3
2	D	1353	PG4	C8-C7-O4-C6
2	D	1354	PG4	O2-C3-C4-O3
2	D	1353	PG4	O3-C5-C6-O4
3	C	1353	GOL	O2-C2-C3-O3
3	C	1354	GOL	O2-C2-C3-O3
2	A	1353	PG4	O2-C3-C4-O3
2	D	1353	PG4	C6-C5-O3-C4
3	A	1357	GOL	O1-C1-C2-C3
3	A	1355	GOL	O2-C2-C3-O3
3	A	1356	GOL	O2-C2-C3-O3
3	A	1357	GOL	O1-C1-C2-O2
3	B	1353	GOL	O1-C1-C2-O2
3	B	1353	GOL	O2-C2-C3-O3
3	D	1355	GOL	O1-C1-C2-O2
2	A	1354	PG4	O3-C5-C6-O4
2	D	1354	PG4	O3-C5-C6-O4
2	D	1353	PG4	C3-C4-O3-C5
6	C	1355	BME	O1-C1-C2-S2
2	A	1354	PG4	O1-C1-C2-O2
2	A	1354	PG4	C5-C6-O4-C7
2	D	1353	PG4	O4-C7-C8-O5
2	A	1354	PG4	C6-C5-O3-C4
2	A	1353	PG4	C4-C3-O2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	1354	PG4	C4-C3-O2-C2
2	D	1354	PG4	C4-C3-O2-C2
3	C	1354	GOL	O1-C1-C2-O2
2	A	1353	PG4	C1-C2-O2-C3
2	D	1353	PG4	C4-C3-O2-C2
2	A	1354	PG4	C8-C7-O4-C6

There are no ring outliers.

13 monomers are involved in 51 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1357	GOL	4	0
3	C	1354	GOL	7	0
3	D	1355	GOL	2	0
2	D	1354	PG4	1	0
6	C	1356	BME	7	0
3	A	1355	GOL	1	0
2	A	1354	PG4	3	0
3	A	1356	GOL	6	0
3	C	1353	GOL	9	0
3	B	1353	GOL	3	0
6	C	1355	BME	1	0
2	D	1353	PG4	9	0
3	D	1356	GOL	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	354/374 (94%)	0.29	28 (7%)	12	11	28, 54, 85, 133	0
1	B	352/374 (94%)	0.32	22 (6%)	20	19	27, 56, 91, 117	0
1	C	353/374 (94%)	0.35	36 (10%)	6	6	28, 56, 90, 112	0
1	D	352/374 (94%)	0.33	29 (8%)	11	11	28, 56, 94, 123	0
All	All	1411/1496 (94%)	0.33	115 (8%)	11	11	27, 55, 91, 133	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	247	PHE	6.3
1	A	247	PHE	6.0
1	D	247	PHE	5.8
1	A	352	GLY	4.9
1	D	261	ILE	4.8
1	D	180	ALA	4.8
1	C	179	VAL	4.7
1	C	169	LYS	4.5
1	A	-1	ARG	4.5
1	B	169	LYS	4.3
1	C	247	PHE	4.3
1	D	179	VAL	4.2
1	C	178	ILE	4.2
1	A	261	ILE	4.1
1	C	261	ILE	4.1
1	C	289	TYR	4.0
1	A	179	VAL	4.0
1	B	153	LYS	4.0
1	D	208	ILE	3.8
1	D	178	ILE	3.8
1	C	180	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	153	LYS	3.6
1	D	246	ARG	3.5
1	C	170	GLY	3.5
1	D	260	ALA	3.5
1	A	169	LYS	3.5
1	C	207	LEU	3.5
1	B	178	ILE	3.4
1	B	261	ILE	3.4
1	A	207	LEU	3.4
1	B	260	ALA	3.3
1	C	171	ILE	3.3
1	C	260	ALA	3.2
1	A	178	ILE	3.2
1	C	259	ILE	3.2
1	C	352	GLY	3.2
1	B	246	ARG	3.1
1	D	96	VAL	3.1
1	B	179	VAL	3.1
1	C	249	ILE	3.1
1	A	260	ALA	3.0
1	D	351	ARG	3.0
1	B	209	LEU	3.0
1	A	180	ALA	3.0
1	D	259	ILE	2.9
1	D	95	ILE	2.9
1	C	262	VAL	2.8
1	A	172	LYS	2.8
1	C	97	VAL	2.8
1	B	208	ILE	2.8
1	D	249	ILE	2.8
1	D	238	GLU	2.8
1	A	236	ASN	2.8
1	A	151	GLY	2.7
1	A	191	ILE	2.7
1	C	208	ILE	2.7
1	C	181	GLY	2.7
1	A	208	ILE	2.6
1	D	169	LYS	2.6
1	A	262	VAL	2.6
1	D	94	LEU	2.6
1	C	209	LEU	2.5
1	D	254	TYR	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	235	GLU	2.5
1	B	180	ALA	2.5
1	D	268	ASN	2.5
1	D	191	ILE	2.5
1	C	336	ARG	2.4
1	C	291	HIS	2.4
1	C	151	GLY	2.4
1	B	171	ILE	2.4
1	C	191	ILE	2.4
1	B	207	LEU	2.4
1	D	170	GLY	2.4
1	B	35	PHE	2.3
1	D	207	LEU	2.3
1	A	97	VAL	2.3
1	A	181	GLY	2.3
1	D	171	ILE	2.3
1	D	174	LYS	2.3
1	C	116	VAL	2.3
1	C	210	VAL	2.3
1	D	291	HIS	2.3
1	A	268	ASN	2.3
1	A	209	LEU	2.3
1	B	235	GLU	2.3
1	B	259	ILE	2.2
1	B	309	VAL	2.2
1	C	124	LEU	2.2
1	C	150	PHE	2.2
1	D	210	VAL	2.2
1	D	285	ILE	2.2
1	A	116	VAL	2.2
1	D	151	GLY	2.2
1	A	154	ARG	2.2
1	A	289	TYR	2.2
1	C	204	SER	2.2
1	A	148	LYS	2.1
1	A	210	VAL	2.1
1	A	259	ILE	2.1
1	B	268	ASN	2.1
1	C	59	GLU	2.1
1	D	172	LYS	2.1
1	A	285	ILE	2.1
1	B	96	VAL	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	25	HIS	2.1
1	B	168	GLY	2.1
1	C	236	ASN	2.0
1	C	24	VAL	2.0
1	B	56	ARG	2.0
1	C	268	ASN	2.0
1	C	153	LYS	2.0
1	B	116	VAL	2.0
1	A	168	GLY	2.0
1	C	168	GLY	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 monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	A	1356	6/6	0.66	0.27	48,56,60,64	0
3	GOL	C	1354	6/6	0.70	0.27	55,61,65,66	0
5	CL	D	1359	1/1	0.70	0.17	74,74,74,74	0
5	CL	B	1356	1/1	0.76	0.30	93,93,93,93	0
3	GOL	D	1356	6/6	0.79	0.13	40,53,56,57	0
5	CL	A	1359	1/1	0.82	0.33	84,84,84,84	0
2	PG4	D	1354	10/13	0.82	0.23	51,57,71,72	0
3	GOL	A	1357	6/6	0.82	0.12	49,50,56,56	0
2	PG4	D	1353	13/13	0.84	0.18	43,58,61,66	0
6	BME	C	1356	4/4	0.84	0.23	44,45,51,67	0
2	PG4	A	1354	12/13	0.85	0.25	41,58,69,71	0
3	GOL	A	1355	6/6	0.85	0.18	42,51,66,71	0
3	GOL	C	1353	6/6	0.85	0.11	47,54,56,57	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	GOL	D	1355	6/6	0.87	0.20	49,55,59,59	0
2	PG4	A	1353	7/13	0.87	0.30	49,50,55,61	0
6	BME	C	1355	4/4	0.89	0.11	66,67,67,68	0
5	CL	C	1358	1/1	0.89	0.31	93,93,93,93	0
3	GOL	B	1353	6/6	0.90	0.19	45,53,56,59	0
5	CL	D	1357	1/1	0.91	0.23	80,80,80,80	0
4	NI	D	1358	1/1	0.92	0.04	59,59,59,59	1
5	CL	A	1361	1/1	0.92	0.27	77,77,77,77	0
4	NI	B	1354	1/1	0.93	0.05	61,61,61,61	1
4	NI	C	1357	1/1	0.94	0.05	60,60,60,60	1
4	NI	A	1358	1/1	0.95	0.04	64,64,64,64	1
5	CL	B	1355	1/1	0.96	0.08	50,50,50,50	0
5	CL	A	1360	1/1	0.98	0.27	86,86,86,86	0

6.5 Other polymers (i)

There are no such residues in this entry.