



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:53 AM UTC

PDB ID : 3UL2 / pdb_00003ul2
Title : Galactose-specific lectin from Dolichos lablab in P6522 space group
Authors : Shetty, K.N.; Latha, V.L.; Rao, R.N.; Nadimpalli, S.K.; Suguna, K.
Deposited on : 2011-11-10
Resolution : 2.50 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

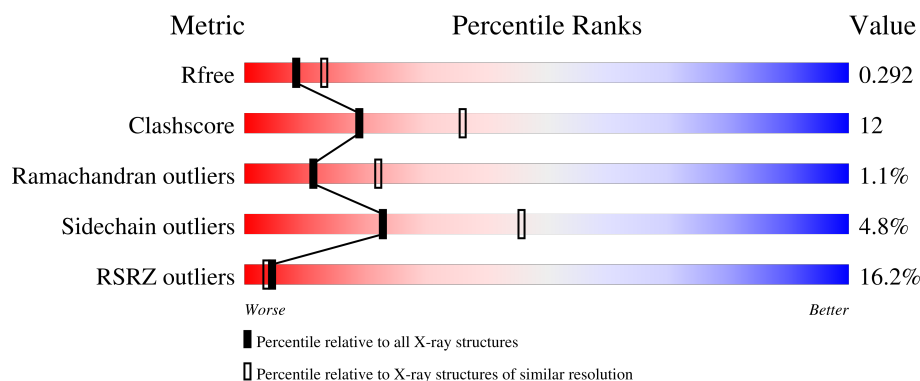
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	281	15% 69% 18% • 12%
1	B	281	11% 73% 14% • 12%
1	C	281	17% 68% 17% • 12%
1	D	281	14% 72% 15% • 12%

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
5	EDO	A	307	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7829 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 Legume lectin.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	248	Total	C	N	O	0	0	0
			1890	1205	312	373			
1	B	248	Total	C	N	O	0	0	0
			1890	1205	312	373			
1	C	248	Total	C	N	O	0	0	0
			1890	1205	312	373			
1	D	248	Total	C	N	O	0	0	0
			1890	1205	312	373			

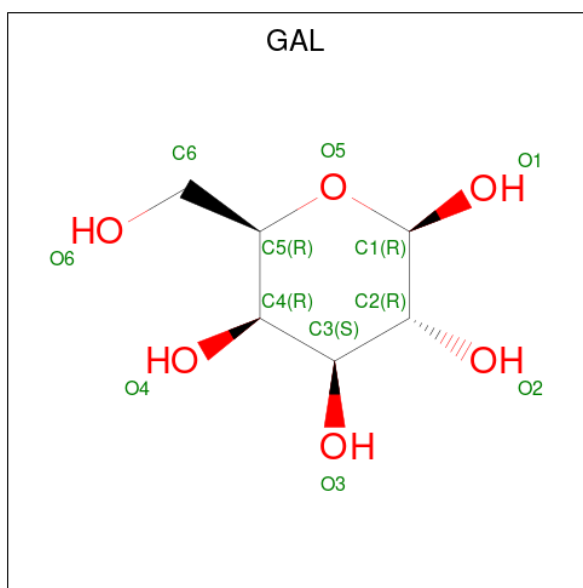
- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

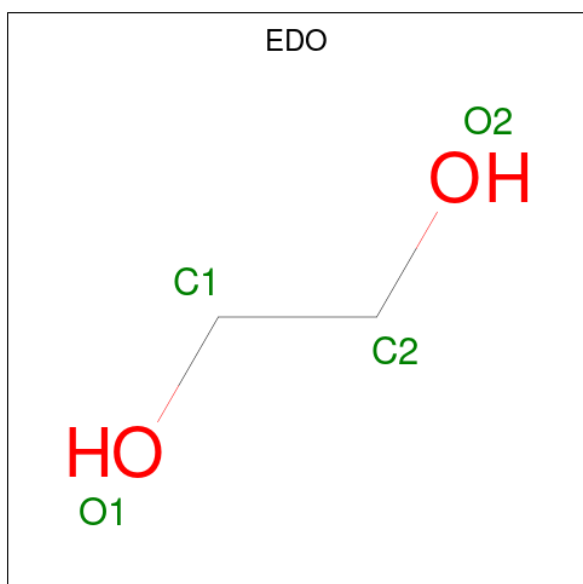
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		
3	B	1	Total	Mn	0	0
			1	1		
3	C	1	Total	Mn	0	0
			1	1		
3	D	1	Total	Mn	0	0
			1	1		

- Molecule 4 is beta-D-galactopyranose (CCD ID: GAL) (formula: $C_6H_{12}O_6$).



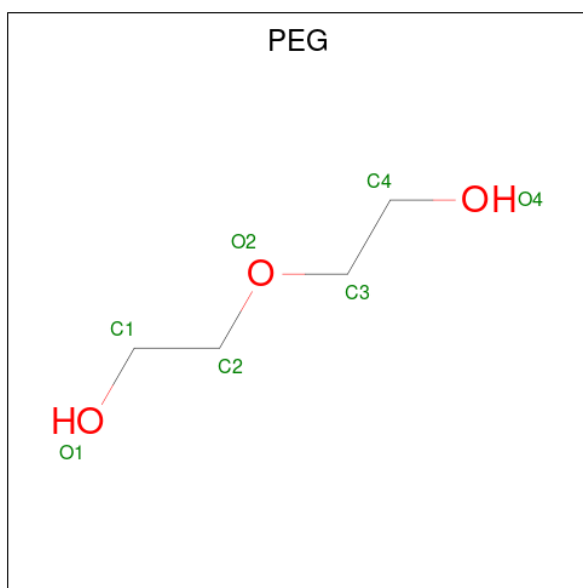
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			12	6	6		
4	B	1	Total	C	O	0	1
			12	6	6		
4	C	1	Total	C	O	0	1
			12	6	6		
4	D	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C O 7 4 3	0	0
6	C	1	Total C O 7 4 3	0	0

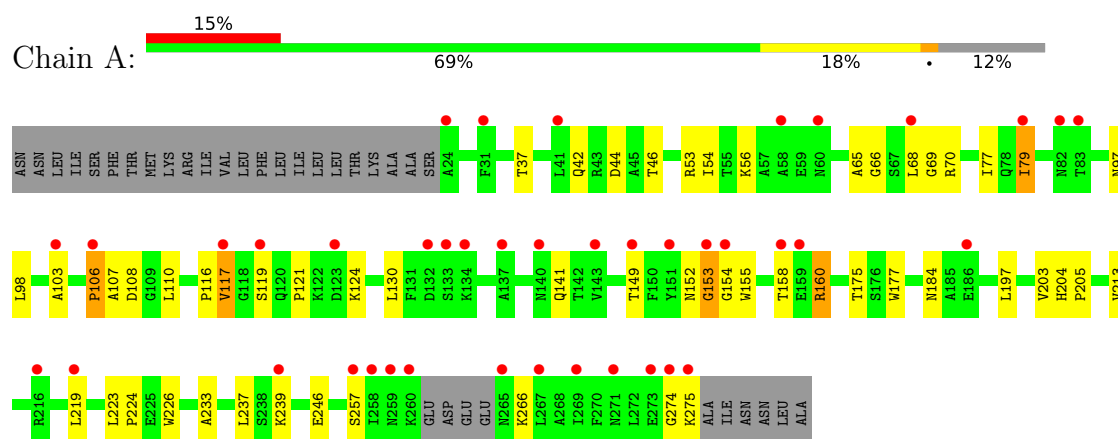
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	45	Total 45	O 45	0	0
7	B	40	Total 40	O 40	0	0
7	C	45	Total 45	O 45	0	0
7	D	37	Total 37	O 37	0	0

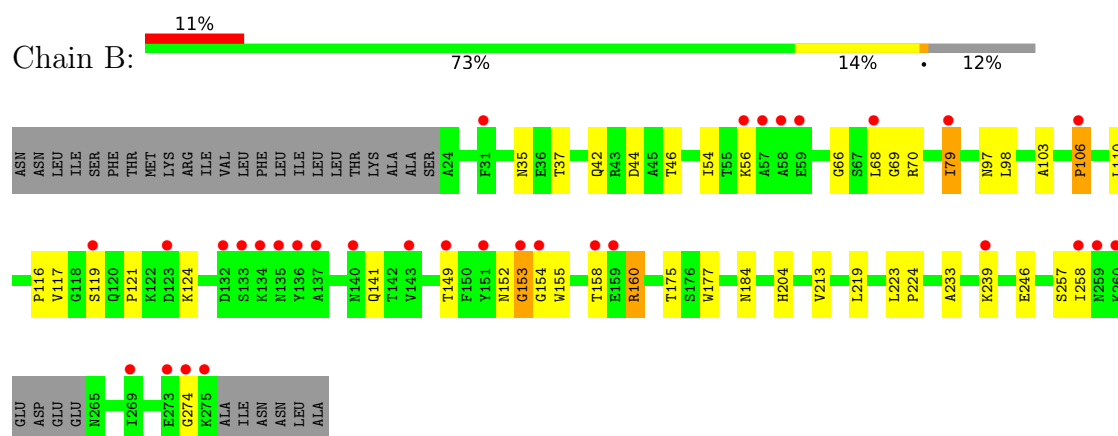
3 Residue-property plots [i](#)

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.

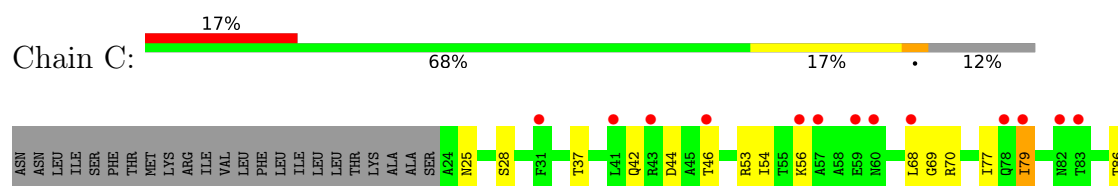
• Molecule 1: Legume lectin

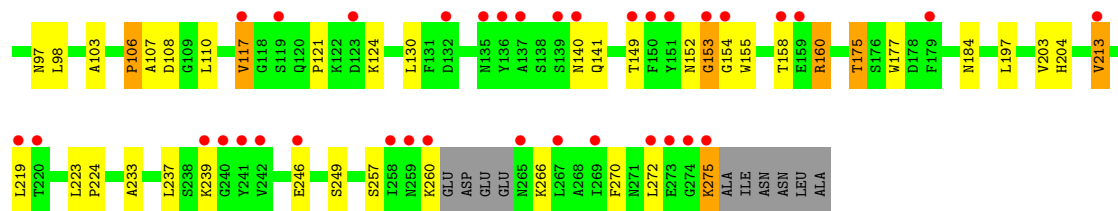


• Molecule 1: Legume lectin

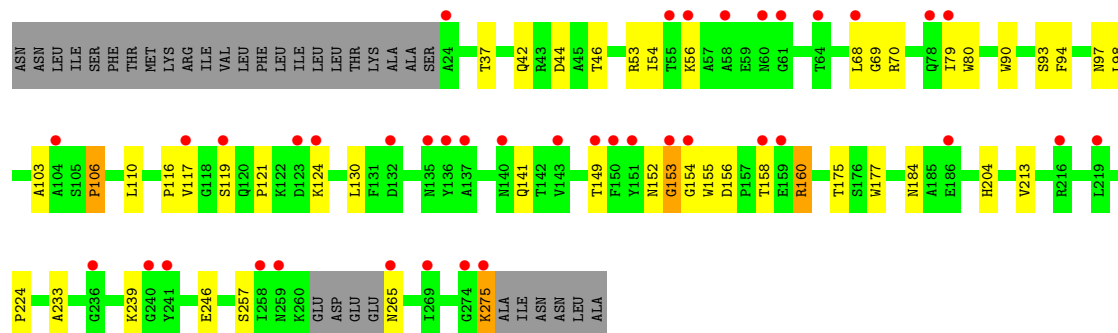
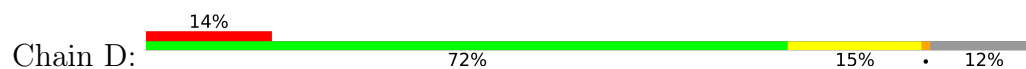


• Molecule 1: Legume lectin





● Molecule 1: Legume lectin



4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.50Å 90.50Å 514.24Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.50 50.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.0 (50.00-2.50) 95.1 (50.00-2.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.273 , 0.296 0.270 , 0.292	Depositor DCC
R_{free} test set	2154 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 30.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7829	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	0.45	0/1932	0.74	1/2630 (0.0%)
1	B	0.45	0/1932	0.73	1/2630 (0.0%)
1	C	0.45	0/1932	0.76	3/2630 (0.1%)
1	D	0.44	0/1932	0.76	2/2630 (0.1%)
All	All	0.45	0/7728	0.75	7/10520 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	270	PHE	N-CA-C	6.55	118.50	111.36
1	A	117	VAL	N-CA-C	6.10	116.77	110.36
1	C	272	LEU	CB-CA-C	6.08	121.19	110.85
1	D	117	VAL	N-CA-C	5.86	116.05	110.42
1	B	117	VAL	N-CA-C	5.77	116.42	110.36
1	D	265	ASN	CB-CA-C	5.39	120.35	110.10
1	C	117	VAL	N-CA-C	5.14	115.75	110.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1890	0	1839	51	0
1	B	1890	0	1847	38	0
1	C	1890	0	1840	51	0
1	D	1890	0	1847	43	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	12	0	0
4	B	12	0	12	0	0
4	C	12	0	12	0	0
4	D	12	0	12	0	0
5	A	16	0	24	6	0
5	B	4	0	6	1	0
5	C	8	0	12	1	0
5	D	4	0	6	0	0
6	C	14	0	20	2	0
7	A	45	0	0	2	0
7	B	40	0	0	3	0
7	C	45	0	0	3	0
7	D	37	0	0	2	0
All	All	7829	0	7489	178	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 12.

All (178) 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:160:ARG:HH11	1:B:160:ARG:HG3	1.27	1.00
1:D:160:ARG:HH11	1:D:160:ARG:HG3	1.27	1.00
1:C:160:ARG:HH11	1:C:160:ARG:HG3	1.27	0.98
1:A:160:ARG:HH11	1:A:160:ARG:HG3	1.26	0.98
1:D:79:ILE:HD11	1:D:90:TRP:NE1	1.85	0.91
1:C:160:ARG:HH11	1:C:160:ARG:CG	1.86	0.89
1:A:160:ARG:HH11	1:A:160:ARG:CG	1.87	0.87
1:B:160:ARG:HH11	1:B:160:ARG:CG	1.88	0.87
1:D:160:ARG:HH11	1:D:160:ARG:CG	1.87	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:ILE:HD11	1:D:90:TRP:HE1	1.40	0.84
1:C:54:ILE:HG21	1:C:233:ALA:HB3	1.62	0.81
1:D:54:ILE:HG21	1:D:233:ALA:HB3	1.61	0.80
1:A:54:ILE:HG21	1:A:233:ALA:HB3	1.62	0.79
1:B:54:ILE:HG21	1:B:233:ALA:HB3	1.63	0.79
1:C:79:ILE:CD1	1:C:223:LEU:HD12	2.16	0.75
1:A:79:ILE:CD1	1:A:223:LEU:HD12	2.17	0.74
1:C:79:ILE:HD11	1:C:219:LEU:HD13	1.69	0.73
1:B:246:GLU:OE1	7:B:424:HOH:O	2.06	0.72
1:B:79:ILE:CD1	1:B:223:LEU:HD12	2.19	0.72
1:B:79:ILE:HD11	1:B:219:LEU:HD13	1.72	0.72
1:C:117:VAL:O	7:C:435:HOH:O	2.08	0.72
1:A:79:ILE:HD11	1:A:219:LEU:HD13	1.72	0.70
1:A:226:TRP:HZ3	5:A:304:EDO:H21	1.55	0.70
1:D:79:ILE:HG23	1:D:80:TRP:HD1	1.57	0.70
1:A:54:ILE:CG2	1:A:233:ALA:HB3	2.21	0.70
1:D:54:ILE:CG2	1:D:233:ALA:HB3	2.21	0.70
1:B:54:ILE:CG2	1:B:233:ALA:HB3	2.22	0.69
1:D:152:ASN:O	1:D:154:GLY:N	2.26	0.69
1:A:66:GLY:HA3	5:A:307:EDO:H12	1.73	0.68
1:C:152:ASN:O	1:C:154:GLY:N	2.26	0.68
1:C:54:ILE:CG2	1:C:233:ALA:HB3	2.23	0.68
1:B:152:ASN:O	1:B:154:GLY:N	2.25	0.67
1:A:152:ASN:O	1:A:154:GLY:N	2.26	0.67
1:B:79:ILE:HD11	1:B:219:LEU:HB3	1.77	0.66
1:A:160:ARG:HG3	1:A:160:ARG:NH1	2.05	0.66
1:A:79:ILE:HD11	1:A:219:LEU:HB3	1.78	0.65
1:D:79:ILE:HD11	1:D:90:TRP:CD1	2.32	0.65
1:B:160:ARG:HG3	1:B:160:ARG:NH1	2.06	0.65
1:C:79:ILE:HD11	1:C:219:LEU:HB3	1.77	0.65
1:C:140:ASN:ND2	7:C:427:HOH:O	2.29	0.65
1:A:226:TRP:CZ3	5:A:304:EDO:H21	2.33	0.63
1:A:266:LYS:HZ3	1:C:28:SER:HB2	1.62	0.63
1:C:160:ARG:HG3	1:C:160:ARG:NH1	2.05	0.62
1:D:79:ILE:CD1	7:D:423:HOH:O	2.47	0.62
1:C:97:ASN:HD22	1:C:184:ASN:HD22	1.49	0.61
1:C:79:ILE:CD1	1:C:219:LEU:HD13	2.30	0.61
1:D:160:ARG:HG3	1:D:160:ARG:NH1	2.05	0.61
1:C:79:ILE:HG13	7:C:410:HOH:O	2.02	0.60
1:A:97:ASN:HD22	1:A:184:ASN:HD22	1.50	0.59
1:A:68:LEU:HD12	1:A:124:LYS:HG2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:SER:HB2	1:D:275:LYS:HG2	1.82	0.59
1:A:237:LEU:O	1:A:237:LEU:HG	2.02	0.59
1:D:79:ILE:CD1	1:D:90:TRP:CD1	2.85	0.59
1:A:79:ILE:CD1	1:A:219:LEU:HD13	2.33	0.59
1:B:68:LEU:HD12	1:B:124:LYS:HG2	1.84	0.59
1:B:97:ASN:HD22	1:B:184:ASN:HD22	1.50	0.58
1:C:160:ARG:CG	1:C:160:ARG:NH1	2.56	0.58
1:C:68:LEU:HD12	1:C:124:LYS:HG2	1.85	0.58
1:D:68:LEU:HD12	1:D:124:LYS:HG2	1.85	0.58
1:B:79:ILE:CD1	1:B:219:LEU:HD13	2.33	0.58
1:C:42:GLN:HB2	1:C:70:ARG:HB2	1.87	0.57
1:C:79:ILE:HD13	1:C:223:LEU:HD12	1.87	0.57
1:A:42:GLN:HB2	1:A:70:ARG:HB2	1.87	0.56
1:B:149:THR:HG22	1:B:149:THR:O	2.05	0.56
1:C:97:ASN:HD22	1:C:184:ASN:ND2	2.03	0.56
1:A:266:LYS:NZ	1:C:28:SER:HB2	2.20	0.56
1:C:103:ALA:O	1:C:106:PRO:HD3	2.05	0.56
1:A:149:THR:HG22	1:A:149:THR:O	2.06	0.56
1:D:97:ASN:HD22	1:D:184:ASN:HD22	1.53	0.56
1:B:42:GLN:HB2	1:B:70:ARG:HB2	1.88	0.56
1:B:97:ASN:HD22	1:B:184:ASN:ND2	2.04	0.56
1:A:103:ALA:HB1	7:A:442:HOH:O	2.06	0.55
1:A:117:VAL:O	7:A:428:HOH:O	2.18	0.55
1:C:149:THR:HG22	1:C:149:THR:O	2.06	0.55
1:D:54:ILE:O	1:D:69:GLY:HA3	2.06	0.55
1:C:237:LEU:HD21	6:C:304:PEG:O2	2.07	0.55
1:D:42:GLN:HB2	1:D:70:ARG:HB2	1.89	0.54
1:B:103:ALA:O	1:B:106:PRO:HD3	2.07	0.54
1:D:79:ILE:CD1	1:D:90:TRP:NE1	2.67	0.54
1:A:97:ASN:HD22	1:A:184:ASN:ND2	2.05	0.54
1:D:98:LEU:HD21	1:D:110:LEU:HD23	1.89	0.54
1:B:98:LEU:HD21	1:B:110:LEU:HD23	1.88	0.54
1:A:66:GLY:HA3	5:A:307:EDO:C1	2.39	0.53
1:A:103:ALA:O	1:A:106:PRO:HD3	2.08	0.53
1:C:79:ILE:HD13	1:C:223:LEU:CD1	2.39	0.53
1:D:103:ALA:O	1:D:106:PRO:HD3	2.09	0.53
1:D:149:THR:O	1:D:149:THR:HG22	2.08	0.53
1:D:97:ASN:HD22	1:D:184:ASN:ND2	2.07	0.53
1:A:79:ILE:HD13	1:A:223:LEU:HD12	1.91	0.52
1:C:184:ASN:H	6:C:305:PEG:H31	1.73	0.52
1:A:98:LEU:HD21	1:A:110:LEU:HD23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:ILE:CD1	1:C:223:LEU:CD1	2.87	0.52
1:B:66:GLY:HA3	5:B:304:EDO:O1	2.10	0.52
1:B:79:ILE:CD1	1:B:223:LEU:CD1	2.88	0.52
1:A:54:ILE:O	1:A:69:GLY:HA3	2.10	0.51
1:C:98:LEU:HD21	1:C:110:LEU:HD23	1.91	0.51
1:B:54:ILE:O	1:B:69:GLY:HA3	2.11	0.51
1:B:79:ILE:HD13	1:B:223:LEU:HD12	1.92	0.51
1:C:54:ILE:O	1:C:69:GLY:HA3	2.11	0.50
1:A:160:ARG:CG	1:A:160:ARG:NH1	2.57	0.50
1:B:160:ARG:CG	1:B:160:ARG:NH1	2.57	0.50
1:D:153:GLY:C	1:D:155:TRP:N	2.67	0.50
1:A:65:ALA:HB3	5:A:307:EDO:O2	2.12	0.49
1:A:79:ILE:CD1	1:A:223:LEU:CD1	2.88	0.49
1:A:153:GLY:C	1:A:155:TRP:N	2.70	0.49
1:B:79:ILE:HD13	1:B:223:LEU:CD1	2.42	0.49
1:C:153:GLY:C	1:C:155:TRP:N	2.69	0.49
1:C:249:SER:OG	1:C:275:LYS:CE	2.60	0.49
1:D:141:GLN:HB3	1:D:224:PRO:HD3	1.95	0.49
1:A:79:ILE:HD13	1:A:223:LEU:CD1	2.43	0.48
1:C:86:THR:HG22	1:C:260:LYS:C	2.38	0.48
1:B:153:GLY:C	1:B:155:TRP:N	2.70	0.48
1:D:160:ARG:CG	1:D:160:ARG:NH1	2.57	0.48
1:B:44:ASP:HB3	1:B:56:LYS:HG3	1.96	0.48
1:A:44:ASP:HB3	1:A:56:LYS:HG3	1.97	0.47
1:D:79:ILE:HD11	7:D:423:HOH:O	2.11	0.47
1:C:44:ASP:HB3	1:C:56:LYS:HG3	1.97	0.47
1:A:141:GLN:HB3	1:A:224:PRO:HD3	1.97	0.47
1:B:54:ILE:HG21	1:B:233:ALA:CB	2.40	0.47
1:C:54:ILE:HG21	1:C:233:ALA:CB	2.40	0.47
1:B:141:GLN:HB3	1:B:224:PRO:HD3	1.97	0.46
1:C:141:GLN:HB3	1:C:224:PRO:HD3	1.97	0.46
1:C:184:ASN:O	1:C:204:HIS:HD2	1.98	0.46
1:A:54:ILE:HG21	1:A:233:ALA:CB	2.39	0.46
1:D:54:ILE:HG21	1:D:233:ALA:CB	2.38	0.46
1:B:68:LEU:HD23	1:B:69:GLY:N	2.31	0.46
1:D:94:PHE:N	1:D:275:LYS:HE2	2.31	0.46
1:C:70:ARG:HD2	1:C:121:PRO:HG3	1.98	0.46
1:B:70:ARG:HD2	1:B:121:PRO:HG3	1.97	0.46
1:B:177:TRP:HE1	1:B:204:HIS:CE1	2.34	0.45
1:C:68:LEU:CD1	1:C:124:LYS:HG2	2.47	0.45
1:B:258:ILE:CG2	7:B:440:HOH:O	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:SER:C	1:D:275:LYS:HE2	2.41	0.45
1:A:68:LEU:CD1	1:A:124:LYS:HG2	2.47	0.45
1:A:70:ARG:HD2	1:A:121:PRO:HG3	1.99	0.45
1:D:44:ASP:HB3	1:D:56:LYS:HG3	1.97	0.45
1:C:68:LEU:HD23	1:C:69:GLY:N	2.31	0.44
1:D:94:PHE:HA	1:D:275:LYS:CE	2.48	0.44
1:A:197:LEU:HD21	1:C:203:VAL:HG11	1.99	0.44
1:B:116:PRO:O	1:B:119:SER:HB2	2.17	0.44
1:A:184:ASN:O	1:A:204:HIS:HD2	2.00	0.44
1:A:68:LEU:HD23	1:A:69:GLY:N	2.33	0.44
1:D:70:ARG:HH21	1:D:130:LEU:HD23	1.83	0.44
1:D:70:ARG:HD2	1:D:121:PRO:HG3	1.99	0.43
1:C:42:GLN:OE1	1:C:70:ARG:HD3	2.18	0.43
1:A:116:PRO:O	1:A:119:SER:HB2	2.19	0.43
1:B:68:LEU:CD1	1:B:124:LYS:HG2	2.48	0.43
1:C:177:TRP:HE1	1:C:204:HIS:CE1	2.37	0.43
1:A:70:ARG:HH21	1:A:130:LEU:HD23	1.83	0.43
1:B:42:GLN:OE1	1:B:70:ARG:HD3	2.19	0.43
1:B:177:TRP:HE1	1:B:204:HIS:HE1	1.67	0.43
1:A:205:PRO:HA	1:C:197:LEU:HD22	1.99	0.43
1:D:68:LEU:HD23	1:D:69:GLY:N	2.34	0.43
1:B:184:ASN:O	1:B:204:HIS:HD2	2.02	0.42
1:C:249:SER:OG	1:C:275:LYS:HE2	2.20	0.42
1:A:107:ALA:HA	1:A:108:ASP:HA	1.89	0.42
1:A:42:GLN:OE1	1:A:70:ARG:HD3	2.20	0.42
1:C:25:ASN:HD22	5:C:306:EDO:H12	1.85	0.42
1:D:42:GLN:OE1	1:D:70:ARG:HD3	2.20	0.42
1:A:149:THR:O	1:A:149:THR:CG2	2.68	0.42
1:D:116:PRO:O	1:D:119:SER:HB2	2.20	0.41
1:A:65:ALA:CB	5:A:307:EDO:O2	2.69	0.41
1:C:175:THR:HG22	1:C:213:VAL:HG22	2.02	0.41
1:A:53:ARG:HD2	1:A:246:GLU:HG2	2.03	0.41
1:A:177:TRP:HE1	1:A:204:HIS:CE1	2.39	0.41
1:C:70:ARG:HH21	1:C:130:LEU:HD23	1.84	0.41
1:D:177:TRP:HE1	1:D:204:HIS:CE1	2.37	0.41
1:C:53:ARG:HD2	1:C:246:GLU:HG2	2.03	0.41
1:D:94:PHE:CA	1:D:275:LYS:HE2	2.51	0.41
1:D:184:ASN:O	1:D:204:HIS:HD2	2.03	0.41
1:B:35:ASN:HB3	7:B:439:HOH:O	2.21	0.40
1:D:153:GLY:C	1:D:155:TRP:H	2.28	0.40
1:D:153:GLY:H	1:D:156:ASP:HB2	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:ALA:HA	1:C:108:ASP:HA	1.88	0.40
1:D:53:ARG:HD2	1:D:246:GLU:HG2	2.02	0.40
1:D:68:LEU:CD1	1:D:124:LYS:HG2	2.48	0.40
1:A:203:VAL:HG11	1:C:197:LEU:CD2	2.51	0.40
1:C:107:ALA:HB1	1:C:108:ASP:CG	2.46	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	244/281 (87%)	232 (95%)	9 (4%)	3 (1%)	10	20
1	B	244/281 (87%)	230 (94%)	11 (4%)	3 (1%)	10	20
1	C	244/281 (87%)	233 (96%)	8 (3%)	3 (1%)	10	20
1	D	244/281 (87%)	233 (96%)	9 (4%)	2 (1%)	16	31
All	All	976/1124 (87%)	928 (95%)	37 (4%)	11 (1%)	11	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	106	PRO
1	A	153	GLY
1	A	274	GLY
1	B	153	GLY
1	B	274	GLY
1	C	153	GLY
1	C	266	LYS
1	D	153	GLY
1	B	106	PRO
1	C	106	PRO

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Mol	Chain	Res	Type
1	D	106	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	207/237 (87%)	196 (95%)	11 (5%)	20	42
1	B	207/237 (87%)	198 (96%)	9 (4%)	26	51
1	C	207/237 (87%)	196 (95%)	11 (5%)	20	42
1	D	207/237 (87%)	198 (96%)	9 (4%)	26	51
All	All	828/948 (87%)	788 (95%)	40 (5%)	23	46

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	THR
1	A	46	THR
1	A	77	ILE
1	A	79	ILE
1	A	158	THR
1	A	160	ARG
1	A	175	THR
1	A	213	VAL
1	A	239	LYS
1	A	257	SER
1	A	275	LYS
1	B	37	THR
1	B	46	THR
1	B	79	ILE
1	B	158	THR
1	B	160	ARG
1	B	175	THR
1	B	213	VAL
1	B	239	LYS
1	B	257	SER

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Mol	Chain	Res	Type
1	C	37	THR
1	C	46	THR
1	C	77	ILE
1	C	79	ILE
1	C	158	THR
1	C	160	ARG
1	C	175	THR
1	C	213	VAL
1	C	239	LYS
1	C	257	SER
1	C	275	LYS
1	D	37	THR
1	D	46	THR
1	D	158	THR
1	D	160	ARG
1	D	175	THR
1	D	213	VAL
1	D	239	LYS
1	D	257	SER
1	D	275	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	99	GLN
1	A	102	ASN
1	A	141	GLN
1	A	184	ASN
1	A	204	HIS
1	A	271	ASN
1	B	78	GLN
1	B	99	GLN
1	B	184	ASN
1	B	204	HIS
1	C	25	ASN
1	C	78	GLN
1	C	99	GLN
1	C	184	ASN
1	C	204	HIS
1	C	207	GLN
1	D	78	GLN

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Mol	Chain	Res	Type
1	D	99	GLN
1	D	184	ASN
1	D	204	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 8 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	$\# Z > 2$
5	EDO	A	306	-	3,3,3	0.43	0	2,2,2	0.35	0
6	PEG	C	304	-	6,6,6	0.45	0	5,5,5	0.27	0
5	EDO	B	304	-	3,3,3	0.43	0	2,2,2	0.35	0
5	EDO	D	304	-	3,3,3	0.41	0	2,2,2	0.46	0
5	EDO	A	304	-	3,3,3	0.41	0	2,2,2	0.28	0
4	GAL	A	303[B]	-	12,12,12	0.55	0	17,17,17	0.53	0
5	EDO	C	307	-	3,3,3	0.45	0	2,2,2	0.34	0
4	GAL	D	303[B]	-	12,12,12	0.56	0	17,17,17	0.69	0
4	GAL	C	303[B]	-	12,12,12	0.55	0	17,17,17	0.58	0
5	EDO	A	305	-	3,3,3	0.48	0	2,2,2	0.23	0
5	EDO	C	306	-	3,3,3	0.41	0	2,2,2	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GAL	B	303[B]	-	12,12,12	0.50	0	17,17,17	0.71	0
6	PEG	C	305	-	6,6,6	0.48	0	5,5,5	0.24	0
5	EDO	A	307	-	3,3,3	0.42	0	2,2,2	0.39	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
5	EDO	A	306	-	-	0/1/1/1	-
6	PEG	C	304	-	-	3/4/4/4	-
5	EDO	B	304	-	-	1/1/1/1	-
5	EDO	D	304	-	-	1/1/1/1	-
5	EDO	A	304	-	-	1/1/1/1	-
4	GAL	A	303[B]	-	-	0/2/22/22	0/1/1/1
5	EDO	C	307	-	-	1/1/1/1	-
4	GAL	D	303[B]	-	-	0/2/22/22	0/1/1/1
4	GAL	C	303[B]	-	-	0/2/22/22	0/1/1/1
5	EDO	A	305	-	-	0/1/1/1	-
5	EDO	C	306	-	-	1/1/1/1	-
4	GAL	B	303[B]	-	-	2/2/22/22	0/1/1/1
6	PEG	C	305	-	-	2/4/4/4	-
5	EDO	A	307	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	303[B]	GAL	O5-C5-C6-O6
6	C	304	PEG	O1-C1-C2-O2
4	B	303[B]	GAL	C4-C5-C6-O6
6	C	305	PEG	O2-C3-C4-O4
5	C	306	EDO	O1-C1-C2-O2
5	D	304	EDO	O1-C1-C2-O2
6	C	304	PEG	O2-C3-C4-O4
6	C	305	PEG	C4-C3-O2-C2
6	C	304	PEG	C1-C2-O2-C3

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Mol	Chain	Res	Type	Atoms
5	B	304	EDO	O1-C1-C2-O2
5	A	304	EDO	O1-C1-C2-O2
5	C	307	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	304	PEG	1	0
5	B	304	EDO	1	0
5	A	304	EDO	2	0
5	C	306	EDO	1	0
6	C	305	PEG	1	0
5	A	307	EDO	4	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	248/281 (88%)	0.98	41 (16%)	4 3	17, 36, 51, 64	12 (4%)
1	B	248/281 (88%)	0.96	32 (12%)	7 6	16, 36, 51, 64	11 (4%)
1	C	248/281 (88%)	1.06	48 (19%)	3 2	14, 36, 51, 63	12 (4%)
1	D	248/281 (88%)	0.96	40 (16%)	4 4	16, 36, 51, 63	12 (4%)
All	All	992/1124 (88%)	0.99	161 (16%)	4 3	14, 36, 52, 64	47 (4%)

All (161) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	275	LYS	7.7
1	B	275	LYS	7.1
1	D	153	GLY	6.8
1	A	151	TYR	6.5
1	C	123	ASP	6.2
1	D	274	GLY	5.7
1	A	275	LYS	5.7
1	C	154	GLY	5.6
1	D	151	TYR	5.5
1	D	275	LYS	5.5
1	C	258	ILE	5.4
1	A	154	GLY	5.2
1	B	151	TYR	5.1
1	D	154	GLY	5.0
1	B	153	GLY	5.0
1	B	154	GLY	4.9
1	A	269	ILE	4.8
1	B	258	ILE	4.8
1	B	158	THR	4.7
1	A	158	THR	4.7
1	C	132	ASP	4.6

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Mol	Chain	Res	Type	RSRZ
1	B	274	GLY	4.6
1	B	136	TYR	4.5
1	D	123	ASP	4.5
1	C	151	TYR	4.4
1	C	219	LEU	4.4
1	C	158	THR	4.3
1	C	59	GLU	4.3
1	D	140	ASN	4.3
1	D	259	ASN	4.3
1	A	259	ASN	4.2
1	B	140	ASN	4.2
1	C	159	GLU	4.2
1	B	132	ASP	4.1
1	A	153	GLY	4.1
1	D	258	ILE	4.1
1	D	219	LEU	4.0
1	C	140	ASN	4.0
1	C	265	ASN	4.0
1	C	269	ILE	4.0
1	C	259	ASN	4.0
1	C	273	GLU	3.9
1	D	269	ILE	3.9
1	A	258	ILE	3.9
1	A	274	GLY	3.9
1	C	153	GLY	3.8
1	A	119	SER	3.7
1	C	272	LEU	3.6
1	C	79	ILE	3.6
1	D	158	THR	3.6
1	B	259	ASN	3.5
1	B	57	ALA	3.5
1	D	58	ALA	3.5
1	A	60	ASN	3.5
1	D	60	ASN	3.5
1	C	274	GLY	3.5
1	C	239	LYS	3.4
1	B	269	ILE	3.4
1	A	159	GLU	3.4
1	A	265	ASN	3.3
1	B	260	LYS	3.3
1	B	106	PRO	3.3
1	A	260	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	271	ASN	3.2
1	A	132	ASP	3.2
1	B	123	ASP	3.2
1	A	24	ALA	3.2
1	B	79	ILE	3.2
1	C	31	PHE	3.1
1	C	57	ALA	3.0
1	D	68	LEU	3.0
1	A	140	ASN	3.0
1	D	149	THR	2.9
1	C	46	THR	2.9
1	D	159	GLU	2.9
1	A	117	VAL	2.9
1	B	133	SER	2.8
1	C	135	ASN	2.8
1	B	134	LYS	2.8
1	D	104	ALA	2.8
1	B	68	LEU	2.8
1	C	41	LEU	2.7
1	D	136	TYR	2.7
1	A	68	LEU	2.7
1	C	149	THR	2.7
1	C	82	ASN	2.7
1	D	117	VAL	2.7
1	A	219	LEU	2.7
1	C	136	TYR	2.7
1	C	137	ALA	2.7
1	D	132	ASP	2.6
1	C	60	ASN	2.6
1	D	241	TYR	2.6
1	D	240	GLY	2.6
1	C	213	VAL	2.6
1	D	79	ILE	2.6
1	A	267	LEU	2.6
1	B	159	GLU	2.6
1	C	68	LEU	2.6
1	B	149	THR	2.6
1	A	79	ILE	2.5
1	B	31	PHE	2.5
1	D	135	ASN	2.5
1	C	220	THR	2.5
1	D	64	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	150	PHE	2.5
1	A	239	LYS	2.5
1	A	133	SER	2.5
1	B	273	GLU	2.5
1	C	117	VAL	2.5
1	A	58	ALA	2.5
1	B	58	ALA	2.5
1	A	82	ASN	2.5
1	D	24	ALA	2.5
1	D	137	ALA	2.4
1	C	56	LYS	2.4
1	D	150	PHE	2.4
1	A	257	SER	2.4
1	D	186	GLU	2.4
1	D	61	GLY	2.4
1	D	216	ARG	2.4
1	C	260	LYS	2.4
1	C	119	SER	2.4
1	A	123	ASP	2.4
1	A	134	LYS	2.4
1	B	239	LYS	2.4
1	D	78	GLN	2.3
1	A	143	VAL	2.3
1	D	143	VAL	2.3
1	A	31	PHE	2.3
1	D	124	LYS	2.3
1	A	137	ALA	2.3
1	A	41	LEU	2.3
1	D	56	LYS	2.3
1	C	242	VAL	2.3
1	A	103	ALA	2.2
1	B	137	ALA	2.2
1	C	241	TYR	2.3
1	C	83	THR	2.2
1	A	273	GLU	2.2
1	A	106	PRO	2.2
1	A	83	THR	2.2
1	D	265	ASN	2.2
1	B	119	SER	2.2
1	C	246	GLU	2.2
1	B	135	ASN	2.1
1	B	143	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	139	SER	2.1
1	C	267	LEU	2.1
1	A	216	ARG	2.1
1	D	119	SER	2.1
1	C	43	ARG	2.1
1	B	59	GLU	2.1
1	D	55	THR	2.1
1	B	56	LYS	2.1
1	C	179	PHE	2.0
1	A	186	GLU	2.0
1	C	240	GLY	2.0
1	C	78	GLN	2.0
1	D	236	GLY	2.0
1	A	149	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
5	EDO	A	307	4/4	0.56	0.25	20,20,20,20	0
6	PEG	C	304	7/7	0.59	0.34	43,44,45,45	7
6	PEG	C	305	7/7	0.67	0.33	47,47,48,48	7
5	EDO	A	305	4/4	0.77	0.17	48,48,48,49	0
5	EDO	D	304	4/4	0.77	0.20	45,45,46,46	0
5	EDO	B	304	4/4	0.81	0.20	49,49,49,49	0
5	EDO	A	306	4/4	0.82	0.29	20,20,20,20	0
5	EDO	C	306	4/4	0.84	0.17	46,46,46,47	0
5	EDO	A	304	4/4	0.84	0.21	29,30,30,30	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GAL	C	303[B]	12/12	0.86	0.15	22,22,23,24	12
5	EDO	C	307	4/4	0.87	0.15	49,49,49,50	0
4	GAL	A	303[B]	12/12	0.88	0.15	28,29,30,32	12
4	GAL	D	303[B]	12/12	0.88	0.15	30,30,32,32	12
4	GAL	B	303[B]	12/12	0.89	0.16	25,26,27,27	12
2	CA	C	301	1/1	0.95	0.10	36,36,36,36	0
2	CA	B	301	1/1	0.98	0.03	39,39,39,39	0
3	MN	A	302	1/1	0.99	0.05	44,44,44,44	0
3	MN	B	302	1/1	0.99	0.07	52,52,52,52	0
3	MN	C	302	1/1	0.99	0.05	46,46,46,46	0
3	MN	D	302	1/1	0.99	0.06	51,51,51,51	0
2	CA	A	301	1/1	0.99	0.02	34,34,34,34	0
2	CA	D	301	1/1	0.99	0.06	36,36,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.