



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:42 PM UTC

PDB ID : 5GKD / pdb_00005gkd
Title : Structure of PL6 family alginate lyase AlyGC
Authors : Zhang, Y.Z.; Wang, P.; Xu, F.
Deposited on : 2016-07-04
Resolution : 2.19 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

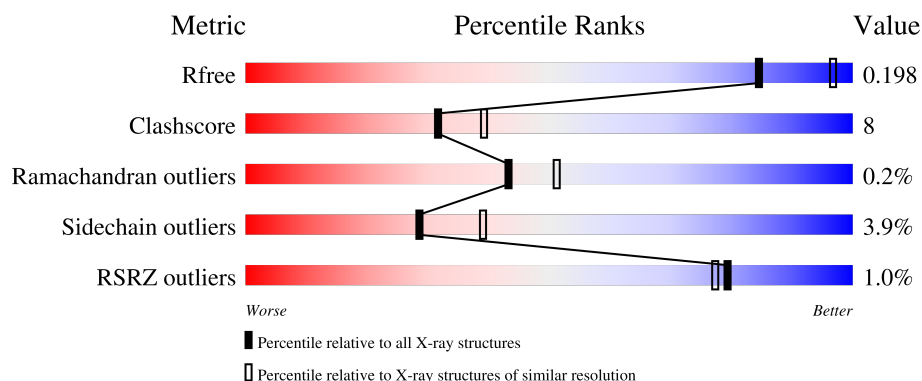
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	726	% 83% 15% .
1	B	726	% 82% 16% .
1	C	726	% 82% 16% .
1	D	726	% 82% 17% .

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
4	PO4	B	803	-	X	X	-
4	PO4	D	803	-	-	X	-
4	PO4	D	805	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 25339 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 AlyGC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	0	0
			5667	3540	1012	1106	9			
1	B	726	Total	C	N	O	S	0	0	0
			5667	3540	1012	1106	9			
1	C	726	Total	C	N	O	S	0	0	0
			5667	3540	1012	1106	9			
1	D	726	Total	C	N	O	S	0	0	0
			5667	3540	1012	1106	9			

- 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 GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



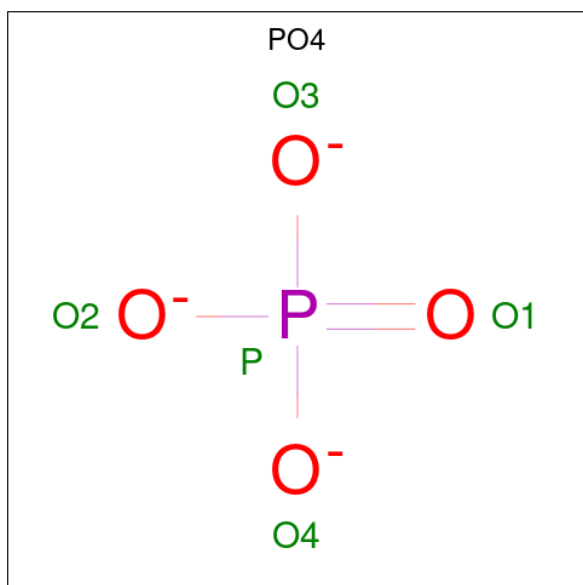
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



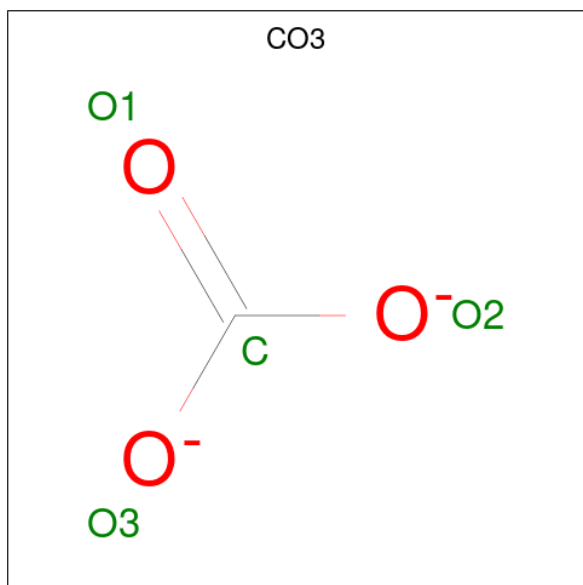
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		
5	B	1	Total	C	O	0	0
			4	1	3		
5	C	1	Total	C	O	0	0
			4	1	3		
5	D	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	646	Total	O	0	0
			646	646		
6	B	693	Total	O	0	0
			693	693		

Continued on next page...

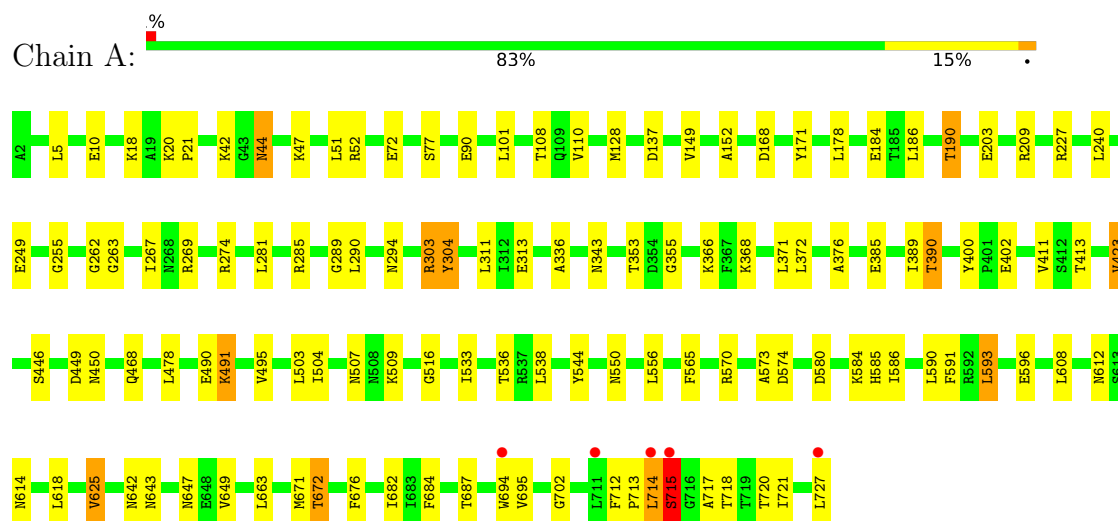
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	C	560	Total 560	O 560	0	0
6	D	596	Total 596	O 596	0	0

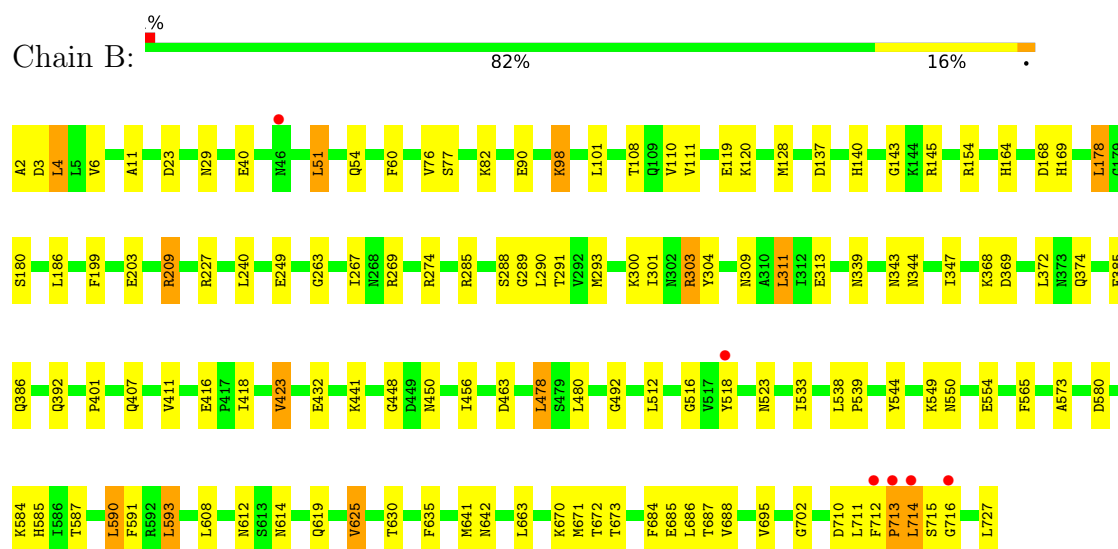
3 Residue-property plots

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

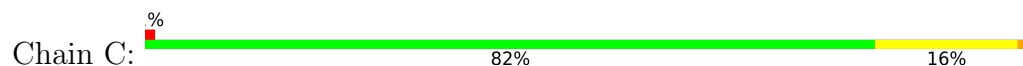
• Molecule 1: AlyGC

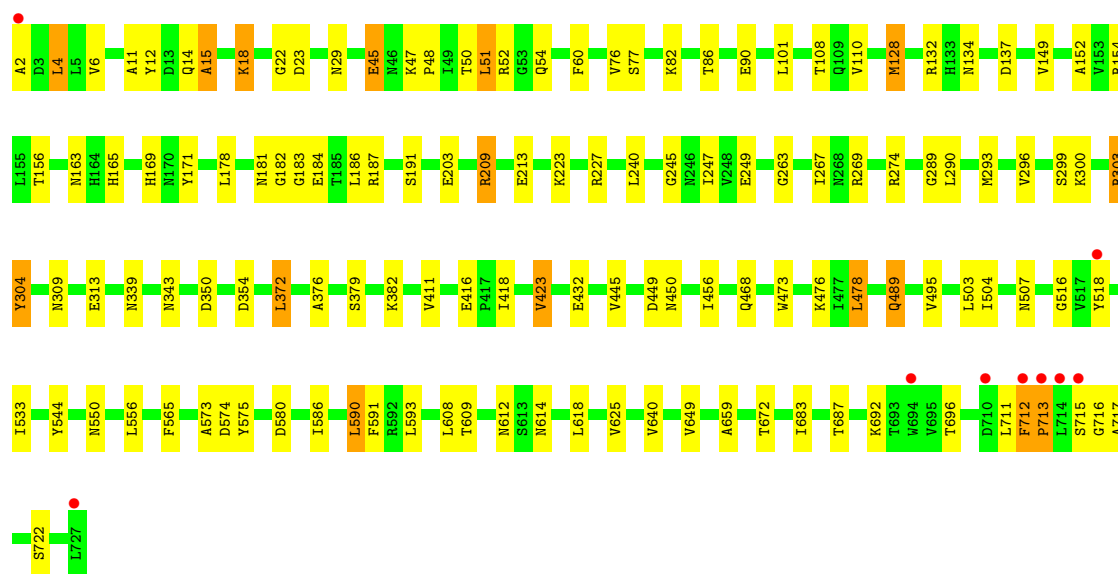


• Molecule 1: AlyGC

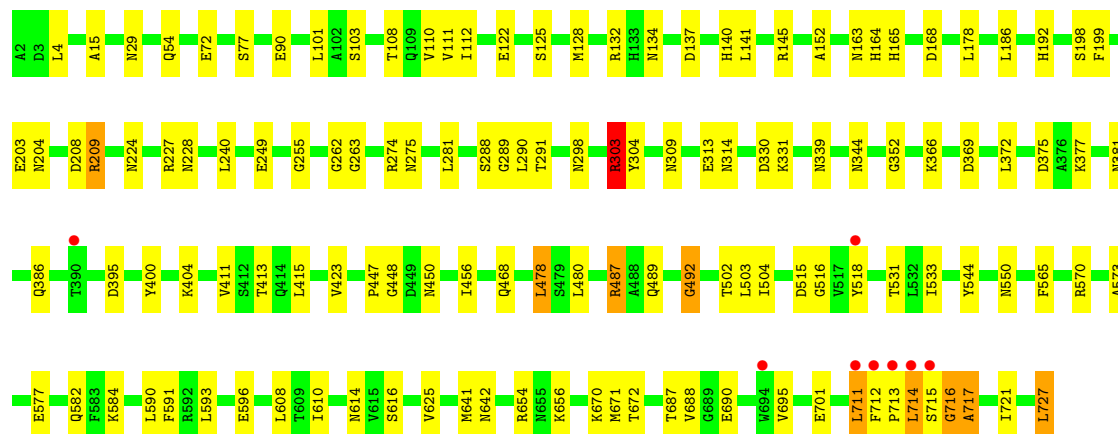
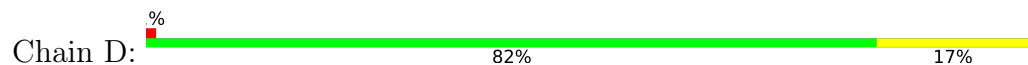


• Molecule 1: AlyGC





• Molecule 1: AlyGC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.61Å 142.84Å 126.28Å 90.00° 111.09° 90.00°	Depositor
Resolution (Å)	34.45 – 2.19 34.45 – 2.19	Depositor EDS
% Data completeness (in resolution range)	98.4 (34.45-2.19) 98.3 (34.45-2.19)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.95 (at 2.20Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.165 , 0.197 0.167 , 0.198	Depositor DCC
R_{free} test set	9768 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	28.7	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.7	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	0.96	EDS
Total number of atoms	25339	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.21% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, CA, CO3, GOL

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	0.56	6/5776 (0.1%)	0.69	9/7830 (0.1%)
1	B	0.51	8/5776 (0.1%)	0.64	7/7830 (0.1%)
1	C	0.52	2/5776 (0.0%)	0.64	4/7830 (0.1%)
1	D	0.46	4/5776 (0.1%)	0.61	4/7830 (0.1%)
All	All	0.51	20/23104 (0.1%)	0.65	24/31320 (0.1%)

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	98	LYS	CE-NZ	-10.60	1.17	1.49
1	B	303	ARG	C-O	-8.40	1.15	1.24
1	A	267	ILE	C-O	-7.13	1.16	1.23
1	B	301	ILE	C-O	-6.49	1.16	1.24
1	B	687	THR	C-O	-6.27	1.16	1.24
1	A	269	ARG	C-O	-6.01	1.16	1.23
1	A	495	VAL	C-O	-5.90	1.17	1.24
1	A	262	GLY	N-CA	5.82	1.49	1.44
1	B	688	VAL	C-O	-5.67	1.17	1.24
1	A	687	THR	C-O	-5.60	1.18	1.24
1	B	267	ILE	C-O	-5.52	1.17	1.23
1	D	487	ARG	CZ-NH2	-5.44	1.26	1.33
1	B	685	GLU	C-O	-5.41	1.17	1.24
1	D	687	THR	C-O	-5.25	1.16	1.24
1	B	686	LEU	C-O	-5.21	1.17	1.23
1	C	15	ALA	C-O	-5.18	1.17	1.24
1	C	267	ILE	C-O	-5.17	1.18	1.23
1	D	688	VAL	C-O	-5.12	1.18	1.24
1	A	304	TYR	C-O	-5.08	1.18	1.23
1	D	145	ARG	CZ-NH2	-5.06	1.26	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	715	SER	N-CA-C	13.96	140.54	110.80
1	A	715	SER	CB-CA-C	-11.74	87.06	110.42
1	C	304	TYR	N-CA-C	8.69	123.40	109.24
1	B	98	LYS	CD-CE-NZ	-8.62	84.31	111.90
1	C	717	ALA	N-CA-C	8.47	122.19	110.24
1	D	303	ARG	N-CA-C	7.88	127.59	110.80
1	B	269	ARG	N-CA-C	7.34	121.52	110.14
1	B	686	LEU	CB-CA-C	7.21	122.72	109.46
1	B	304	TYR	N-CA-C	7.05	120.73	109.24
1	C	269	ARG	N-CA-C	6.71	120.83	110.42
1	A	269	ARG	N-CA-C	6.57	120.61	110.42
1	A	491	LYS	N-CA-C	6.36	120.05	110.64
1	B	303	ARG	N-CA-C	-5.99	100.85	109.29
1	A	712	PHE	O-C-N	5.89	125.49	121.19
1	D	716	GLY	N-CA-C	-5.88	102.62	110.97
1	D	713	PRO	N-CA-C	-5.67	101.59	110.50
1	B	98	LYS	CB-CA-C	-5.60	99.28	110.42
1	A	717	ALA	N-CA-C	5.33	117.42	110.43
1	C	304	TYR	N-CA-CB	-5.33	101.74	110.43
1	B	304	TYR	N-CA-CB	-5.32	101.76	110.43
1	A	712	PHE	CA-C-N	-5.28	114.36	119.90
1	A	712	PHE	C-N-CA	-5.28	114.36	119.90
1	D	492	GLY	N-CA-C	5.21	121.70	114.92
1	A	687	THR	CB-CA-C	-5.02	108.13	114.40

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	5667	0	5529	65	0
1	B	5667	0	5529	102	0
1	C	5667	0	5529	93	0
1	D	5667	0	5529	94	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	24	0	32	3	0
3	B	24	0	32	1	0
3	C	24	0	32	3	0
3	D	24	0	32	0	0
4	A	15	0	0	1	0
4	B	15	0	0	2	0
4	C	15	0	0	0	0
4	D	15	0	0	5	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
6	A	646	0	0	19	2
6	B	693	0	0	20	5
6	C	560	0	0	20	2
6	D	596	0	0	24	1
All	All	25339	0	22244	365	5

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 8.

All (365) 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:A:715:SER:HB2	6:A:913:HOH:O	1.11	1.24
1:A:446:SER:OG	1:A:468:GLN:OE1	1.74	1.04
1:C:712:PHE:O	6:C:902:HOH:O	1.78	1.01
1:B:714:LEU:HG	1:B:715:SER:C	1.89	0.97
1:C:350:ASP:OD2	6:C:903:HOH:O	1.84	0.95
1:B:714:LEU:HD23	1:B:714:LEU:H	1.31	0.94
1:C:692:LYS:NZ	6:C:907:HOH:O	1.99	0.94
1:A:647:ASN:ND2	6:A:903:HOH:O	2.05	0.90
1:A:47:LYS:NZ	6:A:904:HOH:O	2.06	0.87
1:C:574:ASP:OD2	6:C:905:HOH:O	1.93	0.86
1:D:90:GLU:HG2	1:D:128:MET:HG3	1.55	0.86
1:B:372:LEU:HD11	1:B:386:GLN:HG2	1.56	0.86
1:C:711:LEU:HA	6:C:947:HOH:O	1.75	0.85
1:B:714:LEU:N	1:B:715:SER:HA	1.93	0.83
1:D:656:LYS:NZ	6:D:909:HOH:O	2.12	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:808:GOL:O1	6:A:901:HOH:O	1.89	0.83
1:D:654:ARG:NH1	6:D:908:HOH:O	2.11	0.82
1:B:416:GLU:OE1	6:B:901:HOH:O	1.96	0.82
1:D:298:ASN:O	6:D:901:HOH:O	1.96	0.81
4:D:805:PO4:O3	6:D:902:HOH:O	1.98	0.81
1:C:712:PHE:O	1:C:713:PRO:O	1.98	0.81
1:C:14:GLN:OE1	6:C:906:HOH:O	1.98	0.81
1:D:411:VAL:CG1	1:D:415:LEU:HD12	2.11	0.80
1:B:90:GLU:HG2	1:B:128:MET:HG3	1.62	0.80
1:D:468:GLN:OE1	6:D:904:HOH:O	2.01	0.78
1:B:98:LYS:HG2	6:B:954:HOH:O	1.85	0.77
1:A:715:SER:HB3	6:A:1337:HOH:O	1.85	0.76
1:C:614:ASN:ND2	6:C:904:HOH:O	1.90	0.76
1:D:577:GLU:OE1	6:D:905:HOH:O	2.04	0.76
1:A:491:LYS:HE2	1:A:550:ASN:HB3	1.66	0.75
4:D:803:PO4:O4	6:D:906:HOH:O	2.04	0.75
1:B:635:PHE:O	6:B:902:HOH:O	2.03	0.75
1:A:715:SER:O	6:A:902:HOH:O	2.05	0.74
1:C:15:ALA:HA	1:C:18:LYS:HD3	1.70	0.74
1:B:713:PRO:HA	1:B:714:LEU:C	2.10	0.73
1:D:262:GLY:O	6:D:907:HOH:O	2.06	0.72
1:D:717:ALA:N	6:D:903:HOH:O	2.00	0.72
1:D:303:ARG:O	1:D:304:TYR:CG	2.42	0.72
1:B:154:ARG:HH21	4:B:803:PO4:P	2.13	0.72
1:D:134:ASN:H	1:D:165:HIS:HD2	1.36	0.71
1:B:670:LYS:NZ	6:B:914:HOH:O	2.24	0.71
1:A:385:GLU:HG2	6:A:912:HOH:O	1.89	0.71
1:A:614:ASN:OD1	6:A:903:HOH:O	2.08	0.70
1:B:671:MET:HE1	1:B:684:PHE:HZ	1.57	0.69
3:A:808:GOL:O3	6:A:905:HOH:O	2.10	0.69
1:B:712:PHE:O	1:B:715:SER:HB2	1.93	0.69
1:C:209:ARG:NH2	1:C:432:GLU:OE1	2.26	0.69
1:C:90:GLU:HG2	1:C:128:MET:HG3	1.76	0.68
1:D:642:ASN:OD1	1:D:672:THR:HG22	1.93	0.68
1:A:574:ASP:OD2	6:A:906:HOH:O	2.10	0.68
1:D:450:ASN:HA	6:D:1098:HOH:O	1.94	0.68
1:B:374:GLN:OE1	6:B:904:HOH:O	2.12	0.67
4:D:803:PO4:O1	6:D:906:HOH:O	2.13	0.67
1:D:411:VAL:HG11	1:D:415:LEU:HD12	1.76	0.67
1:D:714:LEU:N	1:D:714:LEU:HD12	2.10	0.67
4:D:803:PO4:P	6:D:906:HOH:O	2.53	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:ASN:H	1:C:165:HIS:HD2	1.44	0.66
1:D:670:LYS:NZ	6:D:916:HOH:O	2.22	0.66
1:C:203:GLU:OE2	1:C:227:ARG:NH2	2.28	0.65
1:D:714:LEU:HD12	1:D:714:LEU:H	1.60	0.65
1:C:48:PRO:O	6:C:909:HOH:O	2.14	0.65
1:A:44:ASN:HB3	1:A:47:LYS:H	1.61	0.65
4:D:805:PO4:O4	6:D:910:HOH:O	2.15	0.65
1:B:554:GLU:HG2	1:B:584:LYS:HB3	1.78	0.64
1:C:128:MET:CE	1:C:154:ARG:HG2	2.26	0.64
1:A:190:THR:HG21	6:A:1259:HOH:O	1.96	0.64
1:D:303:ARG:O	1:D:304:TYR:CD2	2.50	0.64
1:A:44:ASN:OD1	6:A:907:HOH:O	2.14	0.64
1:B:587:THR:HA	1:B:619:GLN:HG2	1.79	0.64
1:C:416:GLU:OE1	6:C:910:HOH:O	2.15	0.64
3:A:807:GOL:O1	6:A:908:HOH:O	2.15	0.64
1:B:671:MET:HE2	1:B:695:VAL:HG22	1.80	0.63
1:D:714:LEU:HD13	1:D:714:LEU:O	1.98	0.63
1:B:614:ASN:ND2	6:B:903:HOH:O	2.07	0.62
1:D:716:GLY:CA	6:D:903:HOH:O	2.46	0.62
3:B:809:GOL:O3	6:B:908:HOH:O	2.16	0.62
1:C:274:ARG:NH2	6:C:908:HOH:O	2.12	0.61
1:C:687:THR:HG22	1:C:711:LEU:HD22	1.82	0.61
1:C:171:TYR:HB2	1:C:423:VAL:HG13	1.82	0.60
1:D:447:PRO:O	6:D:912:HOH:O	2.17	0.60
1:A:507:ASN:ND2	1:A:536:THR:HB	2.17	0.60
1:C:128:MET:HE2	1:C:154:ARG:HG2	1.83	0.60
1:B:619:GLN:NE2	6:B:919:HOH:O	2.34	0.60
1:B:538:LEU:O	6:B:907:HOH:O	2.16	0.59
1:B:178:LEU:HD13	1:B:180:SER:HB3	1.85	0.59
1:D:395:ASP:OD2	6:D:911:HOH:O	2.16	0.59
1:C:149:VAL:HG23	1:C:184:GLU:HB2	1.84	0.59
1:B:263:GLY:HA2	1:B:289:GLY:O	2.03	0.59
1:B:285:ARG:HD3	6:B:1335:HOH:O	2.03	0.58
1:B:714:LEU:H	1:B:714:LEU:CD2	2.10	0.58
1:D:366:LYS:HD3	6:D:942:HOH:O	2.04	0.58
1:D:411:VAL:HG13	1:D:415:LEU:HD12	1.86	0.58
1:C:247:ILE:HD11	1:C:274:ARG:NH1	2.19	0.58
1:C:191:SER:OG	3:C:802:GOL:H2	2.04	0.57
1:D:330:ASP:HB2	1:D:331:LYS:NZ	2.19	0.57
1:C:4:LEU:HD11	1:C:23:ASP:HB3	1.86	0.57
1:C:503:LEU:HG	1:C:504:ILE:HG13	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:480:LEU:HD11	1:B:512:LEU:HD13	1.86	0.56
1:C:495:VAL:HG23	1:C:518:TYR:CD1	2.41	0.56
1:C:507:ASN:ND2	6:C:917:HOH:O	2.25	0.56
1:C:533:ILE:O	1:C:565:PHE:HA	2.06	0.56
1:B:401:PRO:O	1:B:407:GLN:NE2	2.39	0.55
1:D:227:ARG:HA	1:D:249:GLU:O	2.06	0.55
1:A:643:ASN:HB3	6:A:917:HOH:O	2.06	0.55
1:B:450:ASN:HA	6:B:1229:HOH:O	2.05	0.55
1:B:227:ARG:HA	1:B:249:GLU:O	2.06	0.55
1:B:671:MET:HE1	1:B:684:PHE:CZ	2.41	0.55
1:C:6:VAL:HG11	1:C:12:TYR:N	2.21	0.55
1:D:309:ASN:HA	1:D:339:ASN:O	2.06	0.55
1:C:6:VAL:HG13	1:C:11:ALA:HB3	1.89	0.55
1:C:60:PHE:CD1	1:C:82:LYS:HE2	2.42	0.55
1:B:712:PHE:O	1:B:715:SER:N	2.41	0.54
1:B:2:ALA:N	1:B:23:ASP:OD1	2.40	0.54
1:B:642:ASN:OD1	1:B:672:THR:OG1	2.25	0.54
1:D:132:ARG:HG2	1:D:163:ASN:HA	1.90	0.54
1:D:122:GLU:OE2	6:D:913:HOH:O	2.18	0.54
1:C:2:ALA:N	1:C:23:ASP:OD1	2.41	0.54
1:A:449:ASP:O	1:A:450:ASN:HB2	2.08	0.54
1:C:712:PHE:N	1:C:712:PHE:CD1	2.76	0.54
1:D:591:PHE:HB3	1:D:593:LEU:CD2	2.37	0.54
1:A:353:THR:HG23	1:A:355:GLY:H	1.73	0.53
1:C:132:ARG:HG2	1:C:163:ASN:HA	1.89	0.53
1:A:90:GLU:HG2	1:A:128:MET:HG3	1.88	0.53
1:B:710:ASP:CG	1:B:714:LEU:O	2.51	0.53
1:C:556:LEU:HB2	1:C:586:ILE:HG12	1.90	0.53
1:B:702:GLY:H	1:B:727:LEU:HD21	1.73	0.53
1:D:714:LEU:N	1:D:714:LEU:CD1	2.72	0.53
1:B:90:GLU:OE1	6:B:909:HOH:O	2.18	0.53
1:D:249:GLU:HG3	1:D:274:ARG:HG3	1.90	0.53
1:A:227:ARG:HA	1:A:249:GLU:O	2.08	0.53
1:D:344:ASN:HA	1:D:369:ASP:O	2.08	0.52
1:B:119:GLU:HG2	1:B:539:PRO:HB2	1.91	0.52
1:A:203:GLU:HA	1:A:227:ARG:O	2.10	0.52
1:A:642:ASN:OD1	1:A:672:THR:HB	2.10	0.52
1:B:143:GLY:O	1:B:145:ARG:HD3	2.10	0.52
1:B:702:GLY:H	1:B:727:LEU:CD2	2.22	0.52
1:C:354:ASP:HB3	1:C:372:LEU:HD11	1.92	0.52
1:D:503:LEU:HG	1:D:504:ILE:HG13	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:803:PO4:O2	6:A:910:HOH:O	2.19	0.52
1:C:263:GLY:HA2	1:C:289:GLY:O	2.10	0.52
1:C:618:LEU:HD23	1:C:649:VAL:HG13	1.91	0.52
1:C:128:MET:HE1	1:C:154:ARG:HG2	1.92	0.51
1:A:503:LEU:HG	1:A:504:ILE:HG13	1.92	0.51
1:A:584:LYS:HG2	1:A:585:HIS:CD2	2.45	0.51
1:D:584:LYS:HA	1:D:616:SER:O	2.11	0.51
1:A:591:PHE:HB3	1:A:593:LEU:HD22	1.91	0.51
1:D:727:LEU:N	1:D:727:LEU:HD12	2.24	0.51
1:B:549:LYS:HE3	6:B:1011:HOH:O	2.11	0.51
1:C:712:PHE:O	1:C:713:PRO:C	2.54	0.51
1:B:40:GLU:O	6:B:910:HOH:O	2.19	0.51
1:B:209:ARG:NH2	1:B:432:GLU:OE1	2.44	0.51
1:D:128:MET:CE	1:D:152:ALA:HB3	2.41	0.50
1:D:288:SER:HB2	1:D:291:THR:OG1	2.12	0.50
1:A:263:GLY:HA2	1:A:289:GLY:O	2.12	0.50
1:C:90:GLU:OE2	6:C:911:HOH:O	2.18	0.50
1:D:168:ASP:HA	1:D:203:GLU:O	2.11	0.50
1:A:533:ILE:O	1:A:565:PHE:HA	2.11	0.50
1:C:450:ASN:ND2	1:C:476:LYS:HE3	2.26	0.50
1:C:22:GLY:O	6:C:912:HOH:O	2.19	0.50
1:B:6:VAL:HG13	1:B:11:ALA:HB3	1.94	0.49
1:B:591:PHE:HB3	1:B:593:LEU:HD22	1.94	0.49
1:C:313:GLU:HA	1:C:343:ASN:O	2.11	0.49
1:B:300:LYS:HG3	6:B:1303:HOH:O	2.13	0.49
1:B:625:VAL:HG13	1:B:663:LEU:CD2	2.42	0.49
1:A:21:PRO:HB3	1:A:44:ASN:HB2	1.93	0.49
1:C:77:SER:HA	1:C:108:THR:O	2.12	0.49
1:B:714:LEU:HG	1:B:716:GLY:N	2.27	0.49
1:C:468:GLN:OE1	1:C:489:GLN:NE2	2.46	0.49
1:B:516:GLY:HA2	1:B:550:ASN:O	2.13	0.49
1:D:487:ARG:NE	1:D:515:ASP:OD2	2.45	0.49
1:A:168:ASP:HA	1:A:203:GLU:O	2.13	0.48
1:C:456:ILE:HD12	1:C:478:LEU:HG	1.95	0.48
1:D:411:VAL:HG13	1:D:415:LEU:CD1	2.42	0.48
1:D:714:LEU:H	1:D:714:LEU:CD1	2.25	0.48
1:C:227:ARG:HA	1:C:249:GLU:O	2.13	0.48
1:D:671:MET:HE2	1:D:695:VAL:HG22	1.95	0.48
1:D:203:GLU:HA	1:D:227:ARG:O	2.13	0.48
1:D:544:TYR:CZ	1:D:573:ALA:HB2	2.49	0.48
1:A:618:LEU:HD23	1:A:649:VAL:HG13	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:203:GLU:HA	1:C:227:ARG:O	2.13	0.48
1:D:90:GLU:HA	1:D:125:SER:O	2.14	0.48
1:D:134:ASN:H	1:D:165:HIS:CD2	2.25	0.48
1:B:584:LYS:HG2	1:B:585:HIS:CD2	2.48	0.48
1:D:331:LYS:HZ2	1:D:715:SER:HA	1.79	0.48
1:C:711:LEU:HB3	1:C:712:PHE:CE1	2.48	0.48
1:B:544:TYR:CZ	1:B:573:ALA:HB2	2.49	0.48
1:B:671:MET:HE2	1:B:671:MET:HB2	1.64	0.47
1:B:714:LEU:HD12	1:B:716:GLY:HA2	1.96	0.47
1:C:4:LEU:N	1:C:4:LEU:HD12	2.29	0.47
1:D:255:GLY:HA3	1:D:281:LEU:HD23	1.96	0.47
1:D:690:GLU:HG2	1:D:716:GLY:HA3	1.96	0.47
1:C:51:LEU:O	1:C:76:VAL:HA	2.15	0.47
1:C:495:VAL:HG23	1:C:518:TYR:HD1	1.79	0.47
1:A:390:THR:O	1:A:402:GLU:HG3	2.15	0.47
1:B:523:ASN:ND2	6:B:946:HOH:O	2.48	0.47
1:D:274:ARG:HA	1:D:313:GLU:O	2.14	0.47
1:D:330:ASP:HB2	1:D:331:LYS:HZ3	1.79	0.47
1:D:411:VAL:CG1	1:D:415:LEU:CD1	2.90	0.47
1:D:533:ILE:O	1:D:565:PHE:HA	2.15	0.47
1:A:149:VAL:HG23	1:A:184:GLU:HB2	1.95	0.47
1:A:509:LYS:HE3	6:A:1314:HOH:O	2.15	0.47
1:B:343:ASN:HA	1:B:368:LYS:O	2.15	0.47
1:D:54:GLN:O	6:D:914:HOH:O	2.20	0.47
1:D:112:ILE:HD12	1:D:141:LEU:HD22	1.97	0.47
1:A:544:TYR:CZ	1:A:573:ALA:HB2	2.49	0.47
1:C:544:TYR:CZ	1:C:573:ALA:HB2	2.49	0.47
1:C:614:ASN:ND2	6:C:942:HOH:O	2.48	0.47
1:B:714:LEU:HG	1:B:715:SER:CA	2.44	0.46
1:D:400:TYR:CZ	1:D:413:THR:HA	2.50	0.46
1:B:590:LEU:HD13	1:B:591:PHE:CE2	2.50	0.46
1:B:108:THR:HA	1:B:137:ASP:O	2.15	0.46
1:D:331:LYS:H	1:D:331:LYS:CE	2.28	0.46
1:C:293:MET:HE1	1:C:304:TYR:CE2	2.50	0.46
1:C:86:THR:HG22	6:C:1149:HOH:O	2.16	0.46
1:A:372:LEU:HD22	1:A:376:ALA:HB3	1.98	0.46
1:C:149:VAL:HG11	1:C:152:ALA:HB2	1.98	0.46
1:A:676:PHE:CZ	1:A:682:ILE:HD11	2.50	0.45
1:D:77:SER:HA	1:D:108:THR:O	2.16	0.45
1:A:18:LYS:O	1:A:20:LYS:HD2	2.16	0.45
1:C:45:GLU:O	1:C:45:GLU:HG3	2.15	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:382:LYS:HB3	1:C:382:LYS:HE2	1.74	0.45
1:D:331:LYS:NZ	1:D:715:SER:CB	2.79	0.45
1:B:311:LEU:HD22	1:B:313:GLU:HG3	1.99	0.45
1:C:29:ASN:OD1	1:C:54:GLN:HB3	2.16	0.45
1:D:108:THR:HA	1:D:137:ASP:O	2.17	0.45
1:A:313:GLU:HA	1:A:343:ASN:O	2.17	0.45
1:B:492:GLY:HA2	1:B:518:TYR:CD1	2.52	0.45
1:D:456:ILE:HD12	1:D:478:LEU:HG	1.99	0.45
1:B:673:THR:HG22	1:B:673:THR:O	2.17	0.45
1:C:4:LEU:HD12	1:C:4:LEU:H	1.82	0.45
1:D:90:GLU:CG	1:D:128:MET:HG3	2.36	0.45
1:D:263:GLY:HA2	1:D:289:GLY:O	2.17	0.45
1:D:372:LEU:O	1:D:386:GLN:HA	2.16	0.45
1:D:487:ARG:NH2	1:D:515:ASP:OD2	2.50	0.45
1:D:582:GLN:OE1	1:D:614:ASN:HB3	2.17	0.45
1:A:108:THR:HA	1:A:137:ASP:O	2.17	0.45
1:B:274:ARG:HA	1:B:313:GLU:O	2.17	0.45
1:C:590:LEU:HD13	1:C:591:PHE:CE2	2.52	0.45
1:D:128:MET:HE1	1:D:152:ALA:HB3	1.98	0.45
1:D:352:GLY:N	6:D:947:HOH:O	2.45	0.45
1:A:516:GLY:HA2	1:A:550:ASN:O	2.17	0.45
1:A:671:MET:HE3	1:A:684:PHE:HZ	1.82	0.45
1:B:614:ASN:ND2	6:B:951:HOH:O	2.50	0.45
1:A:507:ASN:HD22	1:A:536:THR:HB	1.82	0.44
1:A:556:LEU:HB2	1:A:586:ILE:HG12	1.98	0.44
1:B:372:LEU:C	1:B:372:LEU:HD12	2.42	0.44
1:B:533:ILE:O	1:B:565:PHE:HA	2.17	0.44
1:B:29:ASN:OD1	1:B:54:GLN:HB3	2.18	0.44
1:C:50:THR:HG22	1:C:52:ARG:HG2	1.99	0.44
1:A:171:TYR:HB2	1:A:423:VAL:HG12	1.99	0.44
1:B:309:ASN:HA	1:B:339:ASN:O	2.17	0.44
1:B:343:ASN:OD1	1:B:368:LYS:HB3	2.18	0.44
1:C:303:ARG:HD2	1:C:303:ARG:HA	1.52	0.44
1:C:659:ALA:HB2	1:C:683:ILE:HD12	1.98	0.44
1:A:149:VAL:HG11	1:A:152:ALA:HB2	2.00	0.44
1:B:168:ASP:HA	1:B:203:GLU:O	2.17	0.44
1:B:169:HIS:C	1:B:423:VAL:HG22	2.43	0.44
1:B:630:THR:HG22	1:B:712:PHE:CZ	2.53	0.44
1:A:285:ARG:HD3	6:A:1184:HOH:O	2.17	0.44
1:A:371:LEU:HG	1:A:389:ILE:HD11	2.00	0.44
1:D:198:SER:HB3	1:D:224:ASN:OD1	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:ARG:HD2	1:A:303:ARG:HA	1.57	0.44
1:B:4:LEU:CD1	1:B:4:LEU:N	2.81	0.44
1:D:72:GLU:HA	1:D:103:SER:O	2.18	0.44
1:D:125:SER:CB	1:D:128:MET:HE3	2.48	0.44
1:B:441:LYS:NZ	1:B:463:ASP:OD2	2.49	0.44
1:C:274:ARG:HA	1:C:313:GLU:O	2.17	0.44
1:C:445:VAL:O	1:C:468:GLN:HG2	2.18	0.44
1:C:575:TYR:CD2	3:C:809:GOL:H2	2.52	0.44
1:A:52:ARG:NH2	6:A:943:HOH:O	2.50	0.43
1:A:580:ASP:HA	1:A:612:ASN:O	2.18	0.43
1:B:90:GLU:HG2	1:B:128:MET:CG	2.41	0.43
1:C:169:HIS:C	1:C:423:VAL:HG22	2.43	0.43
1:C:300:LYS:CD	1:C:300:LYS:H	2.31	0.43
1:A:570:ARG:HD3	1:A:596:GLU:OE1	2.18	0.43
1:B:203:GLU:HA	1:B:227:ARG:O	2.17	0.43
1:C:580:ASP:HA	1:C:612:ASN:O	2.19	0.43
1:B:344:ASN:HA	1:B:369:ASP:O	2.17	0.43
1:C:6:VAL:HG13	1:C:11:ALA:CB	2.48	0.43
1:D:192:HIS:O	6:D:915:HOH:O	2.21	0.43
1:A:343:ASN:HA	1:A:368:LYS:O	2.19	0.43
1:B:713:PRO:HA	1:B:714:LEU:O	2.17	0.43
1:A:695:VAL:HB	1:A:721:ILE:HG12	2.01	0.43
1:B:111:VAL:HG22	1:B:140:HIS:HB3	2.00	0.43
1:B:154:ARG:NH2	4:B:803:PO4:P	2.87	0.43
1:C:6:VAL:HG11	1:C:12:TYR:CA	2.48	0.43
1:B:288:SER:HB2	1:B:291:THR:OG1	2.19	0.43
1:C:309:ASN:HA	1:C:339:ASN:O	2.18	0.43
1:D:711:LEU:HB3	1:D:712:PHE:CD1	2.54	0.43
1:C:293:MET:HE1	1:C:304:TYR:CD2	2.54	0.42
1:C:296:VAL:HB	1:C:299:SER:HB2	2.00	0.42
1:C:716:GLY:CA	6:C:1318:HOH:O	2.66	0.42
3:C:802:GOL:H31	6:C:940:HOH:O	2.18	0.42
1:D:570:ARG:HD3	1:D:596:GLU:OE1	2.19	0.42
1:A:294:ASN:OD1	1:A:336:ALA:HA	2.19	0.42
1:A:303:ARG:HB3	1:A:304:TYR:H	1.70	0.42
1:A:713:PRO:HA	1:A:714:LEU:HA	1.80	0.42
1:C:223:LYS:HA	1:C:245:GLY:O	2.18	0.42
1:A:274:ARG:HA	1:A:313:GLU:O	2.18	0.42
1:D:4:LEU:HD23	1:D:15:ALA:HB1	2.01	0.42
1:B:492:GLY:HA2	1:B:518:TYR:CE1	2.54	0.42
1:D:377:LYS:HA	1:D:377:LYS:HD3	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:381:ASN:HB3	6:D:1288:HOH:O	2.19	0.42
1:A:702:GLY:H	1:A:727:LEU:HD22	1.85	0.42
1:B:263:GLY:HA2	1:B:289:GLY:HA2	2.01	0.42
1:B:456:ILE:HD12	1:B:478:LEU:HG	2.01	0.42
1:A:694:TRP:CD1	1:A:720:THR:HB	2.54	0.42
1:D:480:LEU:HD12	1:D:480:LEU:HA	1.89	0.42
1:A:42:LYS:HD3	1:A:72:GLU:HG2	2.02	0.42
1:B:274:ARG:NH2	6:B:925:HOH:O	2.45	0.42
1:D:610:ILE:O	1:D:641:MET:HA	2.20	0.42
1:A:52:ARG:HA	1:A:77:SER:O	2.18	0.42
1:B:372:LEU:HD12	1:B:372:LEU:O	2.20	0.42
1:B:372:LEU:CD1	1:B:386:GLN:HG2	2.38	0.42
1:B:727:LEU:HA	1:B:727:LEU:HD22	1.85	0.41
1:D:516:GLY:HA2	1:D:550:ASN:O	2.20	0.41
1:B:51:LEU:O	1:B:76:VAL:HA	2.20	0.41
1:A:538:LEU:O	6:A:911:HOH:O	2.22	0.41
1:B:303:ARG:HD2	1:B:303:ARG:HA	1.87	0.41
1:B:347:ILE:O	1:B:372:LEU:HA	2.20	0.41
1:C:713:PRO:O	6:C:902:HOH:O	2.21	0.41
1:C:274:ARG:NE	6:C:908:HOH:O	2.47	0.41
1:D:204:ASN:HA	1:D:228:ASN:O	2.20	0.41
1:A:625:VAL:HG13	1:A:663:LEU:CD2	2.51	0.41
1:B:3:ASP:C	1:B:4:LEU:HD12	2.46	0.41
1:B:587:THR:HA	1:B:619:GLN:CG	2.48	0.41
1:B:710:ASP:OD1	1:B:714:LEU:O	2.39	0.41
1:C:152:ALA:HA	1:C:187:ARG:O	2.21	0.41
1:C:181:ASN:ND2	1:C:182:GLY:H	2.19	0.41
1:C:183:GLY:C	1:C:213:GLU:HG2	2.45	0.41
1:C:449:ASP:OD1	1:C:473:TRP:HB2	2.21	0.41
1:D:492:GLY:HA2	1:D:518:TYR:CE1	2.55	0.41
1:B:77:SER:HA	1:B:108:THR:O	2.20	0.41
1:C:249:GLU:HA	1:C:274:ARG:O	2.20	0.41
1:C:609:THR:HA	1:C:640:VAL:O	2.21	0.41
1:C:696:THR:HA	1:C:722:SER:O	2.20	0.41
1:B:385:GLU:HG3	6:B:920:HOH:O	2.20	0.41
1:C:372:LEU:HD22	1:C:376:ALA:HB3	2.02	0.41
1:D:111:VAL:HG22	1:D:140:HIS:HB3	2.02	0.41
1:D:208:ASP:OD1	1:D:209:ARG:HD2	2.21	0.41
1:D:591:PHE:HB3	1:D:593:LEU:HD21	2.02	0.41
1:B:641:MET:O	1:B:671:MET:HA	2.21	0.41
1:C:108:THR:HA	1:C:137:ASP:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:LYS:HZ2	1:D:715:SER:CB	2.33	0.41
1:B:60:PHE:CD1	1:B:82:LYS:HE2	2.56	0.41
1:B:128:MET:HE3	1:B:128:MET:HA	2.03	0.41
1:D:502:THR:HA	1:D:531:THR:O	2.21	0.41
1:D:701:GLU:OE1	6:D:917:HOH:O	2.22	0.41
1:A:249:GLU:HA	1:A:274:ARG:O	2.21	0.40
1:B:164:HIS:HA	1:B:199:PHE:O	2.21	0.40
1:B:293:MET:HE2	1:B:293:MET:HB3	1.87	0.40
1:D:137:ASP:HA	1:D:168:ASP:O	2.20	0.40
1:D:164:HIS:HA	1:D:199:PHE:O	2.22	0.40
1:A:255:GLY:HA3	1:A:281:LEU:HD23	2.03	0.40
1:C:516:GLY:HA2	1:C:550:ASN:O	2.20	0.40
1:B:120:LYS:HE2	1:B:120:LYS:HB3	1.91	0.40
1:C:687:THR:HA	1:C:712:PHE:HE1	1.86	0.40
1:D:695:VAL:HB	1:D:721:ILE:HG12	2.04	0.40
1:A:400:TYR:CZ	1:A:413:THR:HA	2.57	0.40
1:B:23:ASP:OD1	6:B:912:HOH:O	2.22	0.40
1:B:711:LEU:O	1:B:712:PHE:CD1	2.74	0.40
1:D:29:ASN:OD1	1:D:54:GLN:HB3	2.21	0.40
1:D:275:ASN:HA	1:D:314:ASN:O	2.22	0.40
1:B:580:ASP:HA	1:B:612:ASN:O	2.21	0.40
1:C:716:GLY:HA2	6:C:1318:HOH:O	2.21	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:1347:HOH:O	6:C:1189:HOH:O[2_647]	1.97	0.23
6:B:1235:HOH:O	6:D:1447:HOH:O[2_647]	2.01	0.19
6:A:1000:HOH:O	6:B:1561:HOH:O[2_556]	2.03	0.17
6:B:1434:HOH:O	6:C:1368:HOH:O[2_647]	2.17	0.03
6:A:1541:HOH:O	6:B:1590:HOH:O[2_556]	2.18	0.02

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	724/726 (100%)	702 (97%)	21 (3%)	1 (0%)	48	57
1	B	724/726 (100%)	707 (98%)	16 (2%)	1 (0%)	48	57
1	C	724/726 (100%)	698 (96%)	24 (3%)	2 (0%)	36	42
1	D	724/726 (100%)	707 (98%)	15 (2%)	2 (0%)	36	42
All	All	2896/2904 (100%)	2814 (97%)	76 (3%)	6 (0%)	43	51

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	713	PRO
1	C	715	SER
1	A	715	SER
1	D	717	ALA
1	D	448	GLY
1	B	448	GLY

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	621/621 (100%)	593 (96%)	28 (4%)	24	33
1	B	621/621 (100%)	600 (97%)	21 (3%)	32	44
1	C	621/621 (100%)	593 (96%)	28 (4%)	24	33
1	D	621/621 (100%)	602 (97%)	19 (3%)	35	48
All	All	2484/2484 (100%)	2388 (96%)	96 (4%)	28	39

All (96) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	10	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	44	ASN
1	A	51	LEU
1	A	101	LEU
1	A	110	VAL
1	A	178	LEU
1	A	186	LEU
1	A	190	THR
1	A	209	ARG
1	A	240	LEU
1	A	290	LEU
1	A	303	ARG
1	A	311	LEU
1	A	366	LYS
1	A	390	THR
1	A	411	VAL
1	A	423	VAL
1	A	478	LEU
1	A	490	GLU
1	A	590	LEU
1	A	593	LEU
1	A	608	LEU
1	A	625	VAL
1	A	672	THR
1	A	714	LEU
1	A	715	SER
1	A	718	THR
1	B	4	LEU
1	B	51	LEU
1	B	101	LEU
1	B	110	VAL
1	B	178	LEU
1	B	186	LEU
1	B	209	ARG
1	B	240	LEU
1	B	290	LEU
1	B	311	LEU
1	B	392	GLN
1	B	411	VAL
1	B	418	ILE
1	B	423	VAL
1	B	478	LEU
1	B	590	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	593	LEU
1	B	608	LEU
1	B	625	VAL
1	B	713	PRO
1	B	714	LEU
1	C	4	LEU
1	C	18	LYS
1	C	45	GLU
1	C	47	LYS
1	C	51	LEU
1	C	101	LEU
1	C	110	VAL
1	C	128	MET
1	C	156	THR
1	C	178	LEU
1	C	186	LEU
1	C	209	ARG
1	C	240	LEU
1	C	290	LEU
1	C	303	ARG
1	C	372	LEU
1	C	379	SER
1	C	411	VAL
1	C	418	ILE
1	C	423	VAL
1	C	478	LEU
1	C	489	GLN
1	C	590	LEU
1	C	593	LEU
1	C	608	LEU
1	C	625	VAL
1	C	672	THR
1	C	712	PHE
1	D	101	LEU
1	D	110	VAL
1	D	178	LEU
1	D	186	LEU
1	D	209	ARG
1	D	240	LEU
1	D	290	LEU
1	D	303	ARG
1	D	375	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	404	LYS
1	D	423	VAL
1	D	478	LEU
1	D	489	GLN
1	D	590	LEU
1	D	608	LEU
1	D	625	VAL
1	D	711	LEU
1	D	714	LEU
1	D	727	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	44	ASN
1	A	164	HIS
1	A	192	HIS
1	A	322	HIS
1	A	343	ASN
1	A	344	ASN
1	A	414	GLN
1	A	450	ASN
1	A	507	ASN
1	A	523	ASN
1	A	550	ASN
1	A	643	ASN
1	A	669	ASN
1	A	678	ASN
1	B	14	GLN
1	B	64	GLN
1	B	73	HIS
1	B	314	ASN
1	B	414	GLN
1	B	499	GLN
1	B	523	ASN
1	B	550	ASN
1	B	604	ASN
1	B	647	ASN
1	B	669	ASN
1	C	73	HIS
1	C	165	HIS
1	C	192	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	204	ASN
1	C	351	GLN
1	C	468	GLN
1	C	489	GLN
1	C	523	ASN
1	C	614	ASN
1	C	619	GLN
1	C	643	ASN
1	C	669	ASN
1	C	678	ASN
1	D	165	HIS
1	D	193	HIS
1	D	339	ASN
1	D	351	GLN
1	D	407	GLN
1	D	414	GLN
1	D	499	GLN
1	D	569	ASN
1	D	643	ASN
1	D	669	ASN
1	D	677	ASN

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 36 ligands modelled in this entry, 4 are monoatomic - leaving 32 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	C	802	-	5,5,5	0.39	0	5,5,5	0.53	0
3	GOL	D	808	-	5,5,5	0.35	0	5,5,5	0.13	0
4	PO4	B	805	-	4,4,4	1.02	0	6,6,6	0.73	0
3	GOL	A	808	-	5,5,5	0.29	0	5,5,5	0.43	0
3	GOL	C	809	-	5,5,5	0.42	0	5,5,5	0.43	0
5	CO3	D	806	-	3,3,3	1.61	1 (33%)	2,3,3	1.96	1 (50%)
3	GOL	B	807	-	5,5,5	0.41	0	5,5,5	0.46	0
3	GOL	B	808	-	5,5,5	0.44	0	5,5,5	0.33	0
3	GOL	D	809	-	5,5,5	0.45	0	5,5,5	0.33	0
3	GOL	D	802	-	5,5,5	0.42	0	5,5,5	0.97	0
4	PO4	C	803	-	4,4,4	0.98	0	6,6,6	0.74	0
4	PO4	D	805	-	4,4,4	0.97	0	6,6,6	0.51	0
4	PO4	C	805	-	4,4,4	0.98	0	6,6,6	0.67	0
4	PO4	C	804	2	4,4,4	1.16	0	6,6,6	1.35	1 (16%)
3	GOL	B	809	-	5,5,5	0.35	0	5,5,5	0.37	0
4	PO4	D	803	-	4,4,4	0.83	0	6,6,6	0.63	0
5	CO3	B	806	-	3,3,3	0.69	0	2,3,3	2.59	2 (100%)
3	GOL	D	807	-	5,5,5	0.39	0	5,5,5	0.25	0
3	GOL	A	802	-	5,5,5	0.39	0	5,5,5	0.95	0
5	CO3	C	806	-	3,3,3	0.65	0	2,3,3	1.62	1 (50%)
3	GOL	C	808	-	5,5,5	0.36	0	5,5,5	0.66	0
4	PO4	A	803	-	4,4,4	0.92	0	6,6,6	0.58	0
5	CO3	A	806	-	3,3,3	0.88	0	2,3,3	2.04	1 (50%)
4	PO4	B	803	-	4,4,4	1.50	1 (25%)	6,6,6	3.14	5 (83%)
4	PO4	A	804	2	4,4,4	1.24	1 (25%)	6,6,6	1.42	1 (16%)
4	PO4	D	804	2	4,4,4	1.10	0	6,6,6	1.66	2 (33%)
4	PO4	B	804	2	4,4,4	1.64	1 (25%)	6,6,6	1.10	1 (16%)
3	GOL	C	807	-	5,5,5	0.40	0	5,5,5	0.18	0
3	GOL	A	809	-	5,5,5	0.49	0	5,5,5	0.51	0
3	GOL	A	807	-	5,5,5	0.51	0	5,5,5	0.77	0
4	PO4	A	805	-	4,4,4	0.99	0	6,6,6	0.48	0
3	GOL	B	802	-	5,5,5	0.43	0	5,5,5	1.09	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	C	802	-	-	2/4/4/4	-
3	GOL	A	802	-	-	2/4/4/4	-
3	GOL	D	807	-	-	2/4/4/4	-
3	GOL	D	802	-	-	3/4/4/4	-
3	GOL	D	808	-	-	4/4/4/4	-
3	GOL	A	809	-	-	3/4/4/4	-
3	GOL	C	808	-	-	2/4/4/4	-
3	GOL	A	808	-	-	2/4/4/4	-
3	GOL	C	809	-	-	4/4/4/4	-
3	GOL	B	807	-	-	4/4/4/4	-
3	GOL	B	809	-	-	4/4/4/4	-
3	GOL	A	807	-	-	2/4/4/4	-
3	GOL	B	808	-	-	2/4/4/4	-
3	GOL	C	807	-	-	2/4/4/4	-
3	GOL	D	809	-	-	0/4/4/4	-
3	GOL	B	802	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	806	CO3	O1-C	2.74	1.35	1.25
4	B	803	PO4	P-O4	-2.53	1.47	1.54
4	A	804	PO4	P-O2	-2.20	1.48	1.54
4	B	804	PO4	P-O1	2.15	1.55	1.50

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	803	PO4	O4-P-O3	-5.53	90.70	107.91
4	B	803	PO4	O3-P-O2	3.47	118.70	107.91
5	A	806	CO3	O2-C-O1	-2.77	112.59	119.68
5	D	806	CO3	O2-C-O1	2.72	126.64	119.68
5	B	806	CO3	O2-C-O1	-2.72	112.72	119.68
4	A	804	PO4	O4-P-O3	2.64	116.11	107.91
5	B	806	CO3	O3-C-O1	2.45	125.94	119.68
4	D	804	PO4	O4-P-O1	2.44	119.56	110.95
4	D	804	PO4	O3-P-O1	-2.39	102.49	110.95
4	B	803	PO4	O3-P-O1	2.31	119.13	110.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	806	CO3	O2-C-O1	-2.26	113.90	119.68
4	B	803	PO4	O4-P-O1	-2.23	103.06	110.95
4	C	804	PO4	O4-P-O3	2.20	114.74	107.91
4	B	803	PO4	O4-P-O2	-2.08	101.43	107.91
4	B	804	PO4	O4-P-O1	2.00	118.03	110.95

There are no chirality outliers.

All (40) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	809	GOL	O1-C1-C2-C3
3	B	807	GOL	O1-C1-C2-C3
3	B	807	GOL	C1-C2-C3-O3
3	B	808	GOL	O1-C1-C2-C3
3	B	809	GOL	C1-C2-C3-O3
3	C	807	GOL	O1-C1-C2-C3
3	C	808	GOL	O1-C1-C2-C3
3	C	809	GOL	O1-C1-C2-C3
3	D	802	GOL	O1-C1-C2-C3
3	D	807	GOL	O1-C1-C2-C3
3	D	808	GOL	O1-C1-C2-C3
3	D	808	GOL	C1-C2-C3-O3
3	B	809	GOL	O2-C2-C3-O3
3	D	807	GOL	O1-C1-C2-O2
3	A	807	GOL	O1-C1-C2-C3
3	A	808	GOL	C1-C2-C3-O3
3	A	809	GOL	C1-C2-C3-O3
3	B	809	GOL	O1-C1-C2-C3
3	C	802	GOL	O1-C1-C2-C3
3	A	807	GOL	O1-C1-C2-O2
3	A	809	GOL	O1-C1-C2-O2
3	B	807	GOL	O1-C1-C2-O2
3	B	809	GOL	O1-C1-C2-O2
3	C	802	GOL	O1-C1-C2-O2
3	C	807	GOL	O1-C1-C2-O2
3	C	808	GOL	O1-C1-C2-O2
3	C	809	GOL	O1-C1-C2-O2
3	D	802	GOL	O1-C1-C2-O2
3	D	808	GOL	O1-C1-C2-O2
3	B	807	GOL	O2-C2-C3-O3
3	D	808	GOL	O2-C2-C3-O3
3	A	802	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	808	GOL	O1-C1-C2-O2
3	C	809	GOL	O2-C2-C3-O3
3	D	802	GOL	O2-C2-C3-O3
3	A	808	GOL	O2-C2-C3-O3
3	B	802	GOL	O1-C1-C2-O2
3	B	802	GOL	O2-C2-C3-O3
3	C	809	GOL	C1-C2-C3-O3
3	A	802	GOL	O1-C1-C2-O2

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	802	GOL	2	0
3	A	808	GOL	2	0
3	C	809	GOL	1	0
4	D	805	PO4	2	0
3	B	809	GOL	1	0
4	D	803	PO4	3	0
4	A	803	PO4	1	0
4	B	803	PO4	2	0
3	A	807	GOL	1	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	726/726 (100%)	-0.47	5 (0%) 84 82	16, 24, 39, 89	0
1	B	726/726 (100%)	-0.50	6 (0%) 82 80	17, 24, 38, 74	0
1	C	726/726 (100%)	-0.33	9 (1%) 76 74	18, 28, 45, 84	0
1	D	726/726 (100%)	-0.28	8 (1%) 78 76	18, 28, 45, 90	0
All	All	2904/2904 (100%)	-0.39	28 (0%) 79 77	16, 26, 43, 90	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	714	LEU	6.1
1	B	714	LEU	5.5
1	D	714	LEU	4.9
1	A	714	LEU	4.2
1	D	715	SER	3.9
1	A	715	SER	3.7
1	B	518	TYR	3.5
1	B	712	PHE	3.5
1	B	716	GLY	3.2
1	A	694	TRP	3.1
1	B	713	PRO	3.0
1	C	715	SER	2.8
1	A	711	LEU	2.7
1	D	711	LEU	2.6
1	C	712	PHE	2.5
1	D	518	TYR	2.5
1	C	2	ALA	2.4
1	C	727	LEU	2.4
1	C	710	ASP	2.4
1	C	713	PRO	2.4
1	D	390	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	518	TYR	2.2
1	C	694	TRP	2.2
1	D	712	PHE	2.1
1	A	727	LEU	2.1
1	D	694	TRP	2.0
1	B	46	ASN	2.0
1	D	713	PRO	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
4	PO4	D	803	5/5	0.56	0.13	65,72,77,88	0
5	CO3	C	806	4/4	0.79	0.16	24,25,28,38	0
3	GOL	D	809	6/6	0.81	0.12	36,40,43,47	0
4	PO4	B	803	5/5	0.82	0.17	43,45,49,51	0
3	GOL	D	808	6/6	0.82	0.13	37,41,48,56	0
5	CO3	A	806	4/4	0.82	0.17	22,23,25,38	0
3	GOL	A	809	6/6	0.82	0.13	34,39,42,43	0
5	CO3	B	806	4/4	0.83	0.14	22,22,23,37	0
3	GOL	B	802	6/6	0.83	0.15	23,34,37,40	0
3	GOL	D	807	6/6	0.84	0.12	34,38,38,48	0
3	GOL	C	809	6/6	0.84	0.10	31,35,38,46	0
3	GOL	C	808	6/6	0.85	0.11	33,37,42,50	0
3	GOL	B	807	6/6	0.85	0.10	30,35,41,51	0
3	GOL	B	809	6/6	0.86	0.10	28,30,39,47	0
3	GOL	C	802	6/6	0.86	0.14	29,43,51,57	0
3	GOL	B	808	6/6	0.86	0.14	38,41,48,49	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CO3	D	806	4/4	0.86	0.12	25,26,27,37	0
3	GOL	C	807	6/6	0.87	0.11	38,46,51,59	0
3	GOL	D	802	6/6	0.90	0.10	31,34,38,39	0
3	GOL	A	808	6/6	0.90	0.10	30,34,36,48	0
4	PO4	C	805	5/5	0.90	0.14	40,51,55,60	0
3	GOL	A	807	6/6	0.90	0.09	23,29,34,36	0
3	GOL	A	802	6/6	0.91	0.10	20,30,35,36	0
4	PO4	B	805	5/5	0.92	0.14	46,50,59,64	0
4	PO4	C	803	5/5	0.92	0.08	42,43,44,45	0
4	PO4	A	803	5/5	0.94	0.11	33,36,45,47	0
4	PO4	D	805	5/5	0.94	0.15	47,48,51,65	0
4	PO4	A	805	5/5	0.95	0.18	35,44,50,50	0
4	PO4	D	804	5/5	0.96	0.07	24,25,27,31	0
4	PO4	C	804	5/5	0.96	0.07	23,24,29,32	0
4	PO4	B	804	5/5	0.97	0.07	20,20,24,31	0
2	CA	C	801	1/1	0.97	0.03	22,22,22,22	0
4	PO4	A	804	5/5	0.97	0.06	17,20,23,27	0
2	CA	D	801	1/1	0.99	0.02	20,20,20,20	0
2	CA	B	801	1/1	0.99	0.03	19,19,19,19	0
2	CA	A	801	1/1	0.99	0.04	22,22,22,22	0

6.5 Other polymers

There are no such residues in this entry.