



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 15, 2017 – 04:25 PM EDT

PDB ID : 2RL7
Title : Crystal Structure cation-dependent mannose 6-phosphate receptor at pH 4.8
Authors : Olson, L.J.; Hindsgaul, O.; Kim, J.-J.P.; Dahms, N.M.
Deposited on : unknown
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

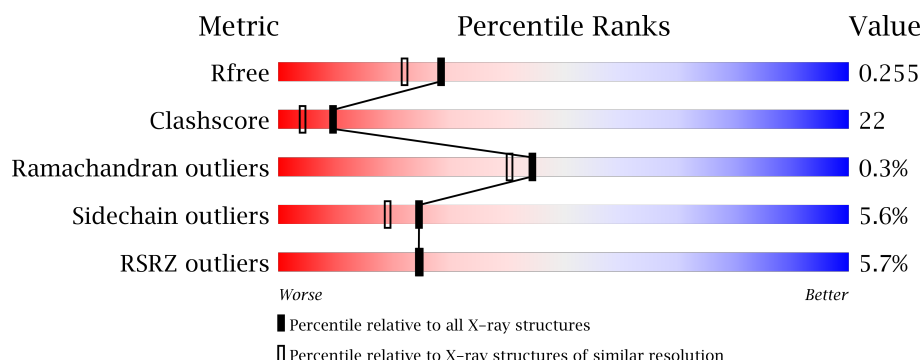
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	100719	6609 (2.00-2.00)
Clashscore	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	154	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>30%</div> <div>..</div> </div> </div>
1	B	154	<div> <div>8%</div> <div> <div></div> <div>62%</div> <div>26%</div> <div>6%</div> <div>5%</div> </div> </div>
1	C	154	<div> <div>3%</div> <div> <div></div> <div>69%</div> <div>22%</div> <div>5%</div> <div>5%</div> </div> </div>
1	D	154	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>32%</div> <div>6%</div> <div>..</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	A	155	-	-	-	X
4	ACT	B	318	-	-	-	X
4	ACT	C	156	-	-	-	X
5	CAC	B	317	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5329 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 Cation-dependent mannose-6-phosphate receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	148	Total	C	N	O	S	0	0	0
			1171	726	206	229	10			
1	B	147	Total	C	N	O	S	0	0	0
			1162	721	205	226	10			
1	C	147	Total	C	N	O	S	0	0	0
			1162	721	205	226	10			
1	D	152	Total	C	N	O	S	0	0	0
			1203	745	212	236	10			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	31	GLN	ASN	ENGINEERED	UNP P11456
A	57	GLN	ASN	ENGINEERED	UNP P11456
A	68	GLN	ASN	ENGINEERED	UNP P11456
A	87	GLN	ASN	ENGINEERED	UNP P11456
B	31	GLN	ASN	ENGINEERED	UNP P11456
B	57	GLN	ASN	ENGINEERED	UNP P11456
B	68	GLN	ASN	ENGINEERED	UNP P11456
B	87	GLN	ASN	ENGINEERED	UNP P11456
C	31	GLN	ASN	ENGINEERED	UNP P11456
C	57	GLN	ASN	ENGINEERED	UNP P11456
C	68	GLN	ASN	ENGINEERED	UNP P11456
C	87	GLN	ASN	ENGINEERED	UNP P11456
D	31	GLN	ASN	ENGINEERED	UNP P11456
D	57	GLN	ASN	ENGINEERED	UNP P11456
D	68	GLN	ASN	ENGINEERED	UNP P11456
D	87	GLN	ASN	ENGINEERED	UNP P11456

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



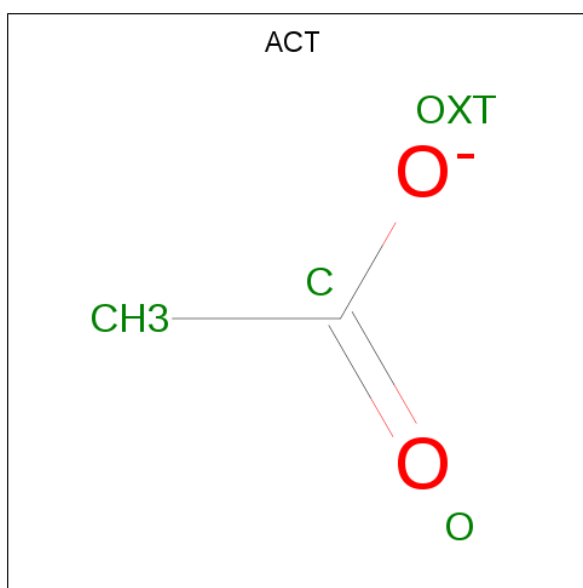
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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



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

- Molecule 4 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



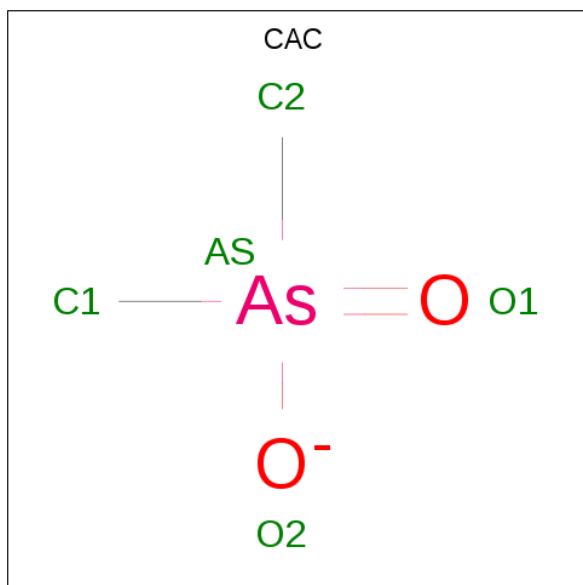
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			4	2	2		
4	B	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 5 is CACODYLATE ION (three-letter code: CAC) (formula: $C_2H_6AsO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	As	C	O	0	0
			5	1	2	2		

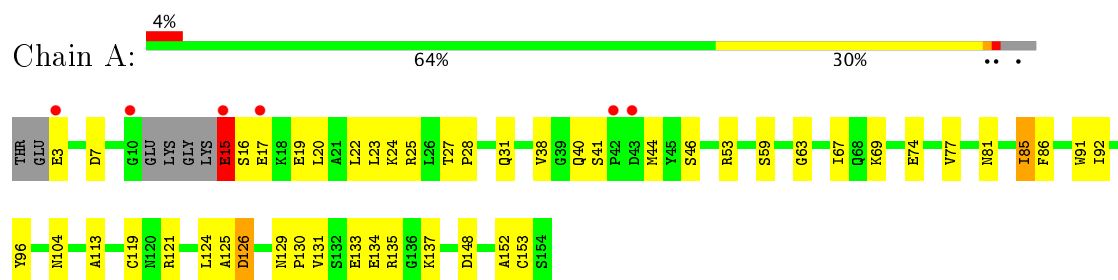
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	120	Total	O	0	0
			120	120		
6	B	122	Total	O	0	0
			122	122		
6	C	118	Total	O	0	0
			118	118		
6	D	122	Total	O	0	0
			122	122		

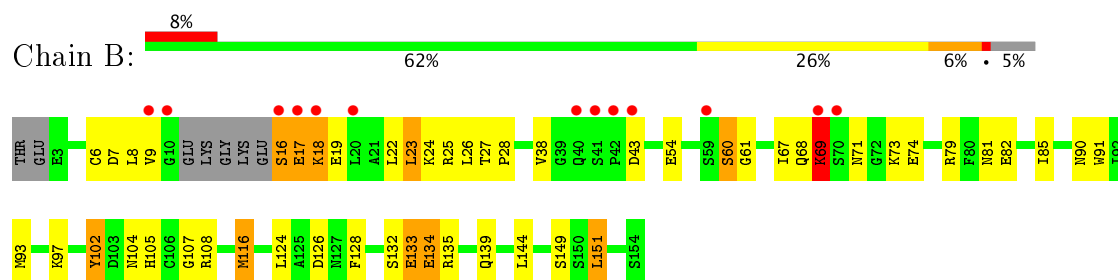
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

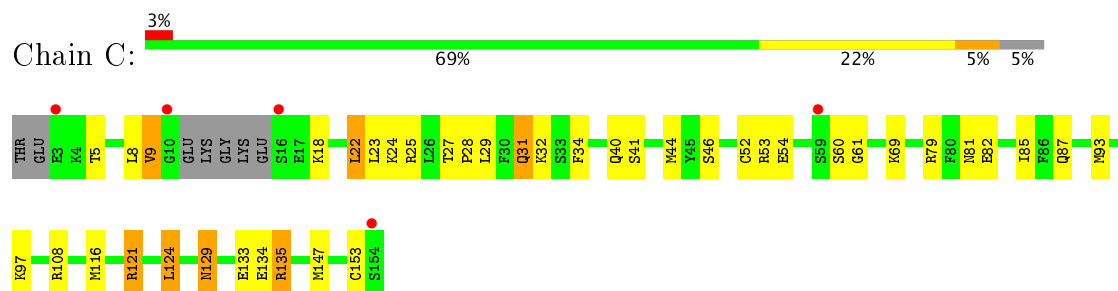
- Molecule 1: Cation-dependent mannose-6-phosphate receptor



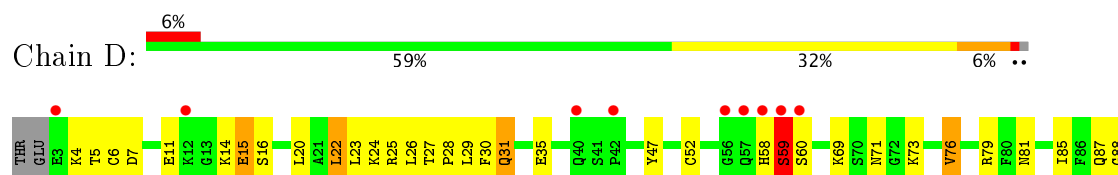
- Molecule 1: Cation-dependent mannose-6-phosphate receptor

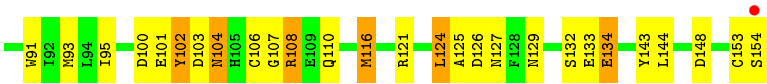


- Molecule 1: Cation-dependent mannose-6-phosphate receptor



- Molecule 1: Cation-dependent mannose-6-phosphate receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	50.84Å 123.03Å 53.09Å 90.00° 92.46° 90.00°	Depositor
Resolution (Å)	27.67 – 2.00 27.67 – 2.00	Depositor EDS
% Data completeness (in resolution range)	86.0 (27.67-2.00) 85.7 (27.67-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	10.21 (at 1.99Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.211 , 0.257 0.211 , 0.255	Depositor DCC
R_{free} test set	3047 reflections (8.77%)	DCC
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 57.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.009 for l,k,-h 0.039 for h,-k,-l 0.027 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	5329	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% 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: CAC, GOL, NAG, ACT

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	0.44	1/1190 (0.1%)	0.67	2/1596 (0.1%)
1	B	0.40	0/1181	0.73	6/1584 (0.4%)
1	C	0.35	0/1181	0.61	1/1584 (0.1%)
1	D	0.43	1/1223 (0.1%)	0.98	6/1638 (0.4%)
All	All	0.41	2/4775 (0.0%)	0.76	15/6402 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	3
1	C	0	1
1	D	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	59	SER	C-N	9.32	1.55	1.34
1	A	7	ASP	C-N	-8.69	1.14	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	59	SER	O-C-N	-24.71	83.16	122.70
1	D	59	SER	CA-C-N	16.18	152.79	117.20
1	A	126	ASP	N-CA-CB	10.45	129.41	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	CYS	O-C-N	8.08	135.63	122.70
1	B	6	CYS	CA-C-N	-6.39	103.14	117.20
1	A	134	GLU	N-CA-C	-6.35	93.86	111.00
1	B	102	TYR	N-CA-C	-6.20	94.27	111.00
1	D	104	ASN	CB-CA-C	-6.18	98.05	110.40
1	B	69	LYS	O-C-N	-5.79	113.44	122.70
1	B	134	GLU	N-CA-C	-5.60	95.88	111.00
1	D	102	TYR	N-CA-C	-5.54	96.04	111.00
1	B	6	CYS	C-N-CA	-5.50	107.95	121.70
1	D	59	SER	C-N-CA	-5.40	108.20	121.70
1	C	134	GLU	N-CA-C	-5.25	96.81	111.00
1	D	134	GLU	N-CA-C	-5.10	97.23	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	GLU	Peptide
1	B	16	SER	Peptide
1	B	17	GLU	Peptide
1	B	69	LYS	Mainchain
1	C	9	VAL	Peptide
1	D	59	SER	Mainchain

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	1171	0	1120	48	0
1	B	1162	0	1115	44	0
1	C	1162	0	1115	44	0
1	D	1203	0	1157	70	0
2	A	28	0	24	3	0
2	B	28	0	24	3	0
2	C	28	0	24	3	0
2	D	28	0	24	1	0
3	A	6	0	8	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	6	0	8	2	0
4	B	8	0	6	1	0
4	C	8	0	6	0	0
4	D	4	0	3	0	0
5	B	5	0	0	1	0
6	A	120	0	0	3	0
6	B	122	0	0	7	0
6	C	118	0	0	5	0
6	D	122	0	0	5	0
All	All	5329	0	4634	205	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 22.

All (205) 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:D:95:ILE:HD13	6:D:4443:HOH:O	1.37	1.21
1:D:5:THR:HG22	1:D:6:CYS:H	1.00	1.08
1:D:5:THR:HG23	1:D:52:CYS:HB3	1.34	1.06
1:D:60:SER:HB2	1:D:79:ARG:HH12	1.10	1.04
1:B:8:LEU:HD11	1:B:23:LEU:HD22	1.40	1.03
1:D:104:ASN:OD1	1:D:106:CYS:N	1.94	1.00
1:D:5:THR:HG22	1:D:6:CYS:N	1.79	0.98
1:D:60:SER:HB2	1:D:79:ARG:NH1	1.79	0.96
1:D:5:THR:CG2	1:D:52:CYS:HB3	1.95	0.96
1:A:31:GLN:HE22	1:A:53:ARG:HH12	1.17	0.92
1:D:5:THR:CG2	1:D:6:CYS:H	1.84	0.90
1:D:102:TYR:O	1:D:108:ARG:HA	1.72	0.89
1:B:8:LEU:HD11	1:B:23:LEU:CD2	2.03	0.89
1:D:5:THR:HG23	1:D:52:CYS:CB	2.04	0.87
1:D:60:SER:CB	1:D:79:ARG:NH1	2.38	0.86
1:A:3:GLU:N	1:C:121:ARG:HE	1.74	0.85
1:B:69:LYS:HE2	1:B:69:LYS:HA	1.57	0.85
1:D:60:SER:CB	1:D:79:ARG:HH12	1.89	0.85
1:B:25:ARG:HH11	1:B:25:ARG:HG3	1.45	0.81
1:A:17:GLU:O	1:A:17:GLU:OE2	1.97	0.81
1:A:131:VAL:HG13	6:B:4220:HOH:O	1.80	0.80
1:D:15:GLU:HG3	1:D:20:LEU:HD21	1.65	0.78
1:D:71:ASN:ND2	1:D:73:LYS:HB2	2.01	0.76
1:B:81:ASN:HD21	2:B:202:NAG:C1	1.99	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASN:HD21	2:A:201:NAG:C1	2.00	0.73
1:D:81:ASN:HD21	2:D:204:NAG:C1	2.01	0.73
1:B:16:SER:N	1:B:17:GLU:OE2	2.22	0.72
1:C:5:THR:HG21	6:C:4314:HOH:O	1.89	0.72
1:A:91:TRP:C	1:A:92:ILE:HD12	2.09	0.72
1:B:104:ASN:HB2	6:B:4387:HOH:O	1.89	0.72
1:B:9:VAL:HG21	1:B:97:LYS:HE2	1.72	0.71
1:A:85:ILE:HD11	1:A:92:ILE:HG23	1.71	0.71
1:A:27:THR:OG1	1:A:28:PRO:HD3	1.92	0.70
1:A:22:LEU:HG	1:A:85:ILE:HD12	1.74	0.69
1:C:5:THR:HG22	1:C:53:ARG:HH21	1.57	0.69
1:A:17:GLU:HA	1:A:20:LEU:HB2	1.74	0.68
1:D:15:GLU:CG	1:D:20:LEU:HD21	2.24	0.67
1:D:25:ARG:HH12	1:D:87:GLN:HE22	1.44	0.66
1:C:18:LYS:HE3	6:C:4018:HOH:O	1.95	0.65
1:A:59:SER:HB3	3:A:155:GOL:H2	1.77	0.65
1:C:108:ARG:HD2	6:C:4397:HOH:O	1.96	0.65
1:B:27:THR:OG1	1:B:28:PRO:HD3	1.96	0.65
1:D:15:GLU:HB2	1:D:20:LEU:HD21	1.78	0.64
1:C:18:LYS:HE2	6:C:4330:HOH:O	1.97	0.64
1:A:92:ILE:HD13	1:A:152:ALA:HA	1.79	0.64
1:A:31:GLN:NE2	1:A:53:ARG:HH12	1.93	0.64
1:D:71:ASN:HD21	1:D:73:LYS:HB2	1.62	0.64
1:C:9:VAL:HG21	1:C:97:LYS:HE2	1.78	0.63
1:D:153:CYS:O	1:D:154:SER:HB2	1.99	0.63
1:A:31:GLN:HE22	1:A:53:ARG:NH1	1.94	0.62
1:C:54:GLU:OE2	1:C:60:SER:HA	1.99	0.62
1:D:16:SER:O	1:D:20:LEU:HD23	1.99	0.62
1:C:31:GLN:H	1:C:31:GLN:NE2	1.98	0.62
1:B:60:SER:O	1:B:79:ARG:NH1	2.33	0.62
1:C:32:LYS:HE3	1:C:124:LEU:HD13	1.81	0.61
1:B:126:ASP:OD2	4:B:319:ACT:H1	2.01	0.61
1:B:69:LYS:CE	1:B:69:LYS:HA	2.28	0.60
1:B:7:ASP:HB2	1:B:81:ASN:HA	1.84	0.59
1:C:24:LYS:O	1:C:27:THR:HG23	2.01	0.59
1:A:67:ILE:HG12	1:A:74:GLU:HG2	1.85	0.59
1:D:27:THR:OG1	1:D:28:PRO:HD3	2.02	0.59
1:B:25:ARG:NH1	1:B:25:ARG:HG3	2.15	0.59
1:C:9:VAL:HG21	1:C:97:LYS:CE	2.33	0.59
1:A:38:VAL:HG21	1:A:135:ARG:HH11	1.67	0.59
1:D:22:LEU:O	1:D:26:LEU:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:SER:HB2	1:A:69:LYS:HE2	1.86	0.58
1:C:27:THR:OG1	1:C:28:PRO:HD3	2.03	0.58
1:D:11:GLU:HB2	1:D:14:LYS:HB2	1.86	0.58
1:D:25:ARG:HH12	1:D:87:GLN:NE2	2.00	0.58
1:D:29:LEU:HD21	1:D:124:LEU:HD22	1.85	0.57
1:A:85:ILE:HD13	1:A:86:PHE:N	2.18	0.57
1:D:69:LYS:NZ	1:D:69:LYS:HB3	2.19	0.57
1:D:95:ILE:CD1	6:D:4443:HOH:O	2.18	0.57
1:A:31:GLN:HG2	6:A:4218:HOH:O	2.04	0.57
1:B:102:TYR:O	1:B:108:ARG:HA	2.04	0.57
1:C:9:VAL:HG11	1:C:97:LYS:NZ	2.20	0.57
1:D:91:TRP:CE3	1:D:116:MET:HE1	2.40	0.56
1:C:46:SER:HB2	1:C:69:LYS:NZ	2.20	0.56
1:C:29:LEU:HD21	1:C:124:LEU:HD22	1.88	0.56
1:C:22:LEU:HB3	1:C:85:ILE:HD13	1.87	0.56
1:C:40:GLN:HG3	3:C:157:GOL:H2	1.88	0.56
1:B:93:MET:HB2	1:B:116:MET:HE2	1.88	0.55
1:D:23:LEU:HD22	1:D:85:ILE:HG21	1.89	0.55
1:A:24:LYS:O	1:A:27:THR:HG23	2.07	0.55
1:B:73:LYS:HE2	6:B:4242:HOH:O	2.07	0.55
1:D:101:GLU:HA	1:D:110:GLN:HA	1.89	0.55
1:D:15:GLU:CB	1:D:20:LEU:HD21	2.37	0.54
1:C:46:SER:HB2	1:C:69:LYS:HZ3	1.73	0.54
1:B:67:ILE:HG12	1:B:74:GLU:HG2	1.90	0.54
1:D:22:LEU:HD13	6:D:4058:HOH:O	2.08	0.54
1:D:60:SER:HB3	1:D:79:ARG:NH1	2.20	0.53
1:A:137:LYS:HG2	6:A:4445:HOH:O	2.09	0.53
1:A:15:GLU:HB3	1:A:17:GLU:HB3	1.90	0.53
1:C:23:LEU:CD2	1:C:85:ILE:HG21	2.38	0.53
1:C:133:GLU:OE1	1:C:135:ARG:HD3	2.09	0.53
1:D:24:LYS:O	1:D:27:THR:HG23	2.09	0.52
1:B:22:LEU:HD23	1:B:85:ILE:HG12	1.90	0.52
1:A:91:TRP:O	1:A:92:ILE:HD12	2.09	0.52
1:B:24:LYS:O	1:B:27:THR:HG23	2.10	0.52
1:C:5:THR:CG2	1:C:53:ARG:HH21	2.23	0.52
1:A:133:GLU:OE1	1:A:135:ARG:HD3	2.10	0.52
1:D:60:SER:CB	1:D:79:ARG:CZ	2.89	0.51
1:C:32:LYS:CE	1:C:124:LEU:HD13	2.40	0.51
1:A:119:CYS:HB2	1:A:153:CYS:HA	1.94	0.50
1:A:23:LEU:O	1:A:23:LEU:HD13	2.11	0.50
1:D:104:ASN:C	1:D:104:ASN:OD1	2.49	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PHE:CE2	1:C:147:MET:HE1	2.47	0.50
1:D:5:THR:CG2	1:D:52:CYS:CB	2.75	0.50
1:D:15:GLU:HB2	1:D:20:LEU:CD2	2.42	0.49
1:D:102:TYR:O	1:D:107:GLY:O	2.31	0.49
1:A:81:ASN:ND2	2:A:201:NAG:C1	2.74	0.49
1:C:82:GLU:HG2	2:C:203:NAG:H82	1.93	0.49
1:A:41:SER:N	1:A:44:MET:HE2	2.27	0.49
1:C:121:ARG:HD3	6:C:4168:HOH:O	2.12	0.49
1:D:76:VAL:HG13	1:D:100:ASP:CG	2.33	0.49
1:B:38:VAL:HG23	1:B:135:ARG:HD2	1.95	0.48
1:A:15:GLU:HA	1:A:16:SER:C	2.33	0.48
1:B:105:HIS:CE1	1:B:139:GLN:HB3	2.48	0.48
1:B:133:GLU:OE1	1:B:135:ARG:HD3	2.14	0.48
1:B:128:PHE:O	5:B:317:CAC:C2	2.62	0.48
1:D:11:GLU:HG3	1:D:14:LYS:HD3	1.95	0.48
1:B:18:LYS:HD3	6:B:4279:HOH:O	2.13	0.48
1:C:44:MET:HB2	1:C:69:LYS:HD2	1.94	0.47
1:D:153:CYS:O	1:D:154:SER:CB	2.61	0.47
1:D:76:VAL:HG13	1:D:100:ASP:OD1	2.14	0.47
1:C:54:GLU:OE2	1:C:61:GLY:N	2.39	0.47
1:B:19:GLU:HG2	1:B:85:ILE:CG2	2.44	0.47
1:B:82:GLU:HG2	2:B:202:NAG:H82	1.96	0.47
1:B:19:GLU:HG2	1:B:85:ILE:HG22	1.94	0.47
1:A:85:ILE:C	1:A:85:ILE:HD13	2.35	0.47
1:D:4:LYS:HE3	6:D:4413:HOH:O	2.15	0.47
1:C:121:ARG:HD2	1:C:153:CYS:SG	2.55	0.47
1:A:25:ARG:HG2	1:A:25:ARG:HH11	1.80	0.47
1:C:121:ARG:H	1:C:121:ARG:HD3	1.79	0.47
1:B:8:LEU:HD23	1:B:19:GLU:HB3	1.96	0.47
1:D:125:ALA:HA	1:D:148:ASP:O	2.15	0.47
1:D:58:HIS:CG	1:D:59:SER:H	2.31	0.47
1:D:7:ASP:HB2	1:D:81:ASN:HA	1.96	0.47
1:D:88:GLY:HA3	1:D:91:TRP:CE2	2.50	0.46
1:D:60:SER:HB3	1:D:79:ARG:CZ	2.46	0.46
1:C:116:MET:HE3	1:C:116:MET:HB2	1.63	0.46
1:A:81:ASN:HD21	2:A:201:NAG:C2	2.28	0.46
1:C:81:ASN:ND2	2:C:203:NAG:C1	2.79	0.46
1:A:38:VAL:CG2	1:A:135:ARG:HH11	2.28	0.46
1:B:90:ASN:HB2	6:B:4350:HOH:O	2.15	0.46
1:D:22:LEU:HB3	1:D:85:ILE:HD13	1.98	0.46
1:D:103:ASP:OD2	1:D:108:ARG:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:SER:HB2	1:D:79:ARG:CZ	2.44	0.45
1:A:38:VAL:HG11	1:A:130:PRO:HG3	1.97	0.45
1:A:17:GLU:O	1:A:17:GLU:CD	2.54	0.45
1:A:19:GLU:O	1:A:23:LEU:HB2	2.17	0.45
1:D:5:THR:HG22	1:D:52:CYS:HB3	1.87	0.45
1:A:31:GLN:NE2	1:A:53:ARG:NH1	2.59	0.45
2:C:203:NAG:H4	2:C:207:NAG:N2	2.32	0.45
1:D:58:HIS:HB3	6:D:4088:HOH:O	2.17	0.45
1:D:58:HIS:ND1	1:D:59:SER:N	2.48	0.44
1:B:104:ASN:ND2	6:B:4512:HOH:O	2.51	0.44
1:B:149:SER:OG	1:B:151:LEU:HB2	2.18	0.44
1:B:22:LEU:HB3	1:B:85:ILE:HD13	1.99	0.44
1:C:93:MET:HE3	1:C:116:MET:HE1	1.99	0.44
1:D:93:MET:HB2	1:D:116:MET:HE1	2.00	0.44
1:D:35:GLU:HA	1:D:47:TYR:O	2.18	0.44
1:D:126:ASP:CG	1:D:127:ASN:H	2.22	0.43
1:C:23:LEU:HD12	1:C:52:CYS:SG	2.58	0.43
1:D:27:THR:HA	1:D:30:PHE:CE1	2.53	0.43
1:C:60:SER:O	1:C:79:ARG:NH1	2.50	0.43
1:C:44:MET:CB	1:C:69:LYS:HD2	2.48	0.43
1:D:11:GLU:CG	1:D:14:LYS:HD3	2.49	0.43
1:D:28:PRO:O	1:D:31:GLN:NE2	2.52	0.43
1:C:29:LEU:CD2	1:C:124:LEU:HD22	2.48	0.42
1:C:9:VAL:HG11	1:C:97:LYS:HZ3	1.80	0.42
1:D:121:ARG:HG2	1:D:121:ARG:HH11	1.83	0.42
1:C:41:SER:O	3:C:157:GOL:O3	2.37	0.42
1:A:38:VAL:HB	1:A:135:ARG:NH1	2.34	0.42
1:A:104:ASN:HB2	6:A:4340:HOH:O	2.19	0.42
1:A:3:GLU:N	1:C:121:ARG:NE	2.55	0.42
1:B:91:TRP:CE3	1:B:116:MET:HE1	2.54	0.42
1:A:22:LEU:CG	1:A:85:ILE:HD12	2.46	0.42
1:B:25:ARG:NH1	1:B:25:ARG:CG	2.80	0.42
1:D:126:ASP:OD2	1:D:127:ASN:ND2	2.53	0.42
1:D:27:THR:N	1:D:28:PRO:CD	2.83	0.42
1:B:54:GLU:OE2	1:B:61:GLY:N	2.53	0.42
1:B:81:ASN:HD21	2:B:202:NAG:C2	2.33	0.42
1:B:79:ARG:HH11	1:B:79:ARG:HG2	1.85	0.42
1:C:129:ASN:HD22	1:C:129:ASN:C	2.23	0.42
1:D:69:LYS:HZ3	1:D:69:LYS:HB3	1.85	0.42
1:D:134:GLU:HB3	1:D:143:TYR:OH	2.20	0.41
1:C:25:ARG:NH1	1:C:87:GLN:OE1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HG12	1:A:113:ALA:HB2	2.02	0.41
1:A:15:GLU:CA	1:A:16:SER:C	2.89	0.41
1:C:53:ARG:HD3	1:C:53:ARG:HA	1.87	0.41
1:B:60:SER:HB2	1:B:79:ARG:HH12	1.84	0.41
1:A:63:GLY:HA3	1:A:96:TYR:CE1	2.56	0.41
1:B:68:GLN:NE2	1:B:71:ASN:HD21	2.19	0.41
1:B:8:LEU:CD1	1:B:23:LEU:CD2	2.87	0.41
1:A:129:ASN:HB2	1:A:130:PRO:HD2	2.03	0.41
1:D:134:GLU:HB3	1:D:143:TYR:CZ	2.55	0.41
1:A:125:ALA:HA	1:A:148:ASP:O	2.21	0.40
1:A:41:SER:H	1:A:44:MET:HE2	1.86	0.40
1:B:102:TYR:CE1	1:B:134:GLU:HG2	2.56	0.40
1:B:132:SER:HB3	1:B:144:LEU:HB3	2.03	0.40
1:C:124:LEU:HD23	1:C:124:LEU:O	2.21	0.40
1:A:121:ARG:HH11	1:A:121:ARG:HG2	1.86	0.40
1:B:107:GLY:HA3	6:B:4252:HOH:O	2.22	0.40
1:D:132:SER:HB3	1:D:144:LEU:HB3	2.03	0.40

There are no symmetry-related clashes.

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	144/154 (94%)	133 (92%)	11 (8%)	0	100	100
1	B	143/154 (93%)	127 (89%)	14 (10%)	2 (1%)	13	6
1	C	143/154 (93%)	135 (94%)	8 (6%)	0	100	100
1	D	150/154 (97%)	138 (92%)	12 (8%)	0	100	100
All	All	580/616 (94%)	533 (92%)	45 (8%)	2 (0%)	44	40

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	18	LYS
1	B	43	ASP

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	130/135 (96%)	125 (96%)	5 (4%)	38	35
1	B	129/135 (96%)	121 (94%)	8 (6%)	21	16
1	C	129/135 (96%)	122 (95%)	7 (5%)	26	20
1	D	133/135 (98%)	124 (93%)	9 (7%)	18	13
All	All	521/540 (96%)	492 (94%)	29 (6%)	25	19

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	40	GLN
1	A	85	ILE
1	A	124	LEU
1	A	126	ASP
1	B	23	LEU
1	B	26	LEU
1	B	60	SER
1	B	69	LYS
1	B	116	MET
1	B	124	LEU
1	B	133	GLU
1	B	151	LEU
1	C	8	LEU
1	C	22	LEU
1	C	31	GLN
1	C	121	ARG
1	C	124	LEU
1	C	129	ASN
1	C	135	ARG

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Mol	Chain	Res	Type
1	D	15	GLU
1	D	22	LEU
1	D	31	GLN
1	D	76	VAL
1	D	108	ARG
1	D	116	MET
1	D	124	LEU
1	D	129	ASN
1	D	133	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	68	GLN
1	A	81	ASN
1	A	87	GLN
1	B	31	GLN
1	B	66	GLN
1	B	68	GLN
1	B	81	ASN
1	B	127	ASN
1	C	31	GLN
1	C	40	GLN
1	C	81	ASN
1	C	90	ASN
1	C	129	ASN
1	D	81	ASN
1	D	87	GLN
1	D	122	HIS
1	D	127	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

16 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	A	155	-	5,5,5	0.47	0	5,5,5	0.40	0
2	NAG	A	201	2	14,14,15	0.99	0	15,19,21	0.69	0
2	NAG	A	205	2	14,14,15	1.64	2 (14%)	15,19,21	2.23	4 (26%)
2	NAG	B	202	2	14,14,15	0.96	0	15,19,21	0.75	0
2	NAG	B	206	2	14,14,15	1.60	2 (14%)	15,19,21	2.28	4 (26%)
5	CAC	B	317	-	0,4,4	0.00	-	0,6,6	0.00	-
4	ACT	B	318	-	1,3,3	4.79	1 (100%)	0,3,3	0.00	-
4	ACT	B	319	-	1,3,3	4.10	1 (100%)	0,3,3	0.00	-
4	ACT	C	155	-	1,3,3	3.13	1 (100%)	0,3,3	0.00	-
4	ACT	C	156	-	1,3,3	3.07	1 (100%)	0,3,3	0.00	-
3	GOL	C	157	-	5,5,5	0.32	0	5,5,5	0.59	0
2	NAG	C	203	2	14,14,15	1.11	0	15,19,21	0.86	0
2	NAG	C	207	2	14,14,15	1.82	3 (21%)	15,19,21	2.32	4 (26%)
4	ACT	D	202	-	1,3,3	3.27	1 (100%)	0,3,3	0.00	-
2	NAG	D	204	2	14,14,15	1.16	1 (7%)	15,19,21	0.85	0
2	NAG	D	208	2	14,14,15	1.64	2 (14%)	15,19,21	2.32	4 (26%)

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	155	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	201	2	-	0/6/23/26	0/1/1/1
2	NAG	A	205	2	-	0/6/23/26	0/1/1/1
2	NAG	B	202	2	-	0/6/23/26	0/1/1/1
2	NAG	B	206	2	-	0/6/23/26	0/1/1/1
5	CAC	B	317	-	-	0/0/0/0	0/0/0/0
4	ACT	B	318	-	-	0/0/0/0	0/0/0/0
4	ACT	B	319	-	-	0/0/0/0	0/0/0/0
4	ACT	C	155	-	-	0/0/0/0	0/0/0/0
4	ACT	C	156	-	-	0/0/0/0	0/0/0/0
3	GOL	C	157	-	-	0/4/4/4	0/0/0/0
2	NAG	C	203	2	-	0/6/23/26	0/1/1/1
2	NAG	C	207	2	-	0/6/23/26	0/1/1/1
4	ACT	D	202	-	-	0/0/0/0	0/0/0/0
2	NAG	D	204	2	-	0/6/23/26	0/1/1/1
2	NAG	D	208	2	-	0/6/23/26	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	207	NAG	O5-C5	2.09	1.47	1.43
2	D	204	NAG	O4-C4	2.52	1.48	1.43
2	A	205	NAG	O5-C1	2.74	1.48	1.43
2	B	206	NAG	O5-C1	2.76	1.48	1.43
2	C	207	NAG	O5-C1	2.77	1.48	1.43
2	D	208	NAG	O5-C1	2.87	1.48	1.43
4	C	156	ACT	CH3-C	3.07	1.52	1.48
4	C	155	ACT	CH3-C	3.13	1.52	1.48
4	D	202	ACT	CH3-C	3.27	1.53	1.48
4	B	319	ACT	CH3-C	4.10	1.54	1.48
2	B	206	NAG	C1-C2	4.54	1.58	1.52
2	D	208	NAG	C1-C2	4.67	1.58	1.52
4	B	318	ACT	CH3-C	4.79	1.54	1.48
2	A	205	NAG	C1-C2	4.80	1.59	1.52
2	C	207	NAG	C1-C2	5.49	1.60	1.52

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	207	NAG	O5-C1-C2	-6.53	102.39	111.47
2	D	208	NAG	O5-C1-C2	-6.42	102.54	111.47
2	B	206	NAG	O5-C1-C2	-6.18	102.87	111.47
2	A	205	NAG	O5-C1-C2	-6.08	103.01	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	206	NAG	C1-C2-N2	-3.89	103.84	110.49
2	D	208	NAG	C1-C2-N2	-3.87	103.87	110.49
2	A	205	NAG	C1-C2-N2	-3.61	104.32	110.49
2	C	207	NAG	C1-C2-N2	-3.60	104.34	110.49
2	D	208	NAG	O4-C4-C5	2.19	114.81	109.28
2	B	206	NAG	O4-C4-C5	2.24	114.93	109.28
2	C	207	NAG	O4-C4-C5	2.26	114.98	109.28
2	A	205	NAG	O4-C4-C5	2.31	115.10	109.28
2	A	205	NAG	C1-O5-C5	2.44	115.53	112.17
2	B	206	NAG	C1-O5-C5	2.73	115.94	112.17
2	D	208	NAG	C1-O5-C5	2.80	116.03	112.17
2	C	207	NAG	C1-O5-C5	2.83	116.06	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	155	GOL	1	0
2	A	201	NAG	3	0
2	B	202	NAG	3	0
5	B	317	CAC	1	0
4	B	319	ACT	1	0
3	C	157	GOL	2	0
2	C	203	NAG	3	0
2	C	207	NAG	1	0
2	D	204	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	7:ASP	C	8:LEU	N	1.14

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	148/154 (96%)	0.31	6 (4%) 38 38	7, 21, 39, 65	0
1	B	147/154 (95%)	0.27	13 (8%) 11 11	7, 18, 41, 58	0
1	C	147/154 (95%)	0.05	5 (3%) 46 46	6, 16, 36, 50	0
1	D	152/154 (98%)	0.38	10 (6%) 19 19	10, 23, 42, 53	0
All	All	594/616 (96%)	0.25	34 (5%) 24 25	6, 20, 41, 65	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	GLU	7.3
1	D	57	GLN	6.0
1	C	10	GLY	4.8
1	A	10	GLY	4.5
1	B	43	ASP	4.4
1	D	12	LYS	4.3
1	B	17	GLU	4.1
1	B	16	SER	4.1
1	A	3	GLU	4.0
1	D	59	SER	4.0
1	D	40	GLN	3.8
1	C	16	SER	3.7
1	A	17	GLU	3.6
1	D	42	PRO	3.6
1	D	154	SER	3.5
1	D	58	HIS	3.3
1	B	42	PRO	3.3
1	D	60	SER	3.0
1	C	59	SER	3.0
1	B	10	GLY	2.9
1	D	56	GLY	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	69	LYS	2.8
1	B	70	SER	2.7
1	B	18	LYS	2.5
1	C	3	GLU	2.5
1	B	59	SER	2.5
1	B	20	LEU	2.4
1	B	40	GLN	2.4
1	C	154	SER	2.3
1	A	42	PRO	2.3
1	B	41	SER	2.2
1	D	3	GLU	2.2
1	A	43	ASP	2.1
1	B	9	VAL	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	GOL	A	155	6/6	0.72	0.38	14.51	37,38,39,41	0
5	CAC	B	317	5/5	0.66	0.48	12.29	18,45,66,83	0
4	ACT	B	318	4/4	0.73	0.24	7.33	31,34,34,34	0
4	ACT	C	156	4/4	0.69	0.27	2.72	21,25,26,27	0
3	GOL	C	157	6/6	0.88	0.18	0.49	14,25,27,29	0
4	ACT	C	155	4/4	0.86	0.11	-0.29	25,25,26,27	0
2	NAG	D	204	14/15	0.61	0.27	-	55,59,60,63	0
2	NAG	B	202	14/15	0.75	0.22	-	58,59,61,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	ACT	B	319	4/4	0.81	0.20	-	29,30,31,31	0
2	NAG	A	201	14/15	0.74	0.20	-	46,48,50,53	0
2	NAG	B	206	14/15	0.62	0.58	-	69,72,75,75	0
2	NAG	D	208	14/15	0.62	0.41	-	63,65,66,67	0
2	NAG	A	205	14/15	0.68	0.28	-	56,58,60,61	0
2	NAG	C	203	14/15	0.72	0.18	-	54,58,59,62	0
4	ACT	D	202	4/4	0.82	0.24	-	17,20,21,22	0
2	NAG	C	207	14/15	0.51	0.43	-	65,67,70,71	0

6.5 Other polymers [i](#)

There are no such residues in this entry.