



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 7, 2017 – 10:50 AM EST

PDB ID : 5UPH
Title : Lipids bound lysosomal integral membrane protein 2
Authors : Conrad, K.S.; Liu, S.
Deposited on : unknown
Resolution : 3.00 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

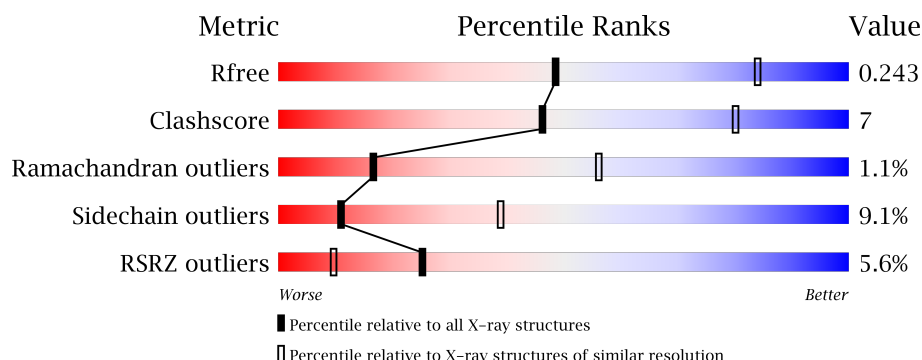
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (3.00-3.00)

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	410	<div> <div>4%</div> <div>58%</div> <div>16%</div> <div>•</div> <div>23%</div> </div>
1	B	410	<div> <div>5%</div> <div>61%</div> <div>16%</div> <div>•</div> <div>21%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	CLR	A	518	-	-	-	X
5	CLR	B	517	-	-	-	X
6	PCW	A	519	-	-	-	X
6	PCW	B	518	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 6066 atoms, of which 271 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 Lysosome membrane protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2566	1672	415	472	7			
1	B	324	Total	C	N	O	S	0	0	0
			2628	1708	427	485	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	432	HIS	-	expression tag	UNP Q14108
A	433	HIS	-	expression tag	UNP Q14108
A	434	HIS	-	expression tag	UNP Q14108
A	435	HIS	-	expression tag	UNP Q14108
A	436	HIS	-	expression tag	UNP Q14108
A	437	HIS	-	expression tag	UNP Q14108
B	432	HIS	-	expression tag	UNP Q14108
B	433	HIS	-	expression tag	UNP Q14108
B	434	HIS	-	expression tag	UNP Q14108
B	435	HIS	-	expression tag	UNP Q14108
B	436	HIS	-	expression tag	UNP Q14108
B	437	HIS	-	expression tag	UNP Q14108

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



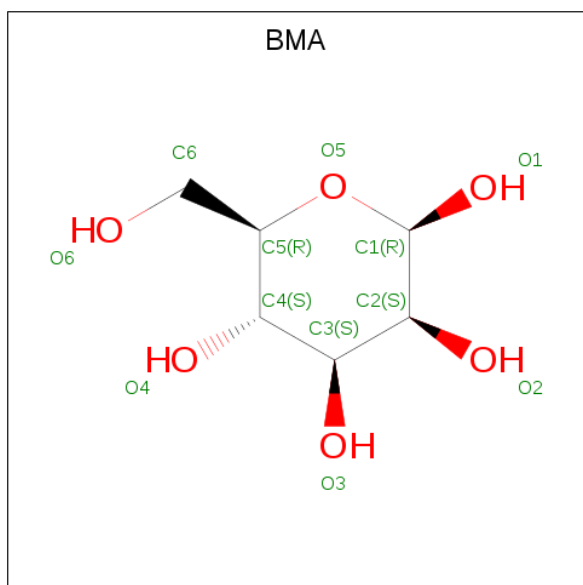
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1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

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		

- Molecule 3 is BETA-D-MANNOSE (three-letter code: BMA) (formula: $C_6H_{12}O_6$).



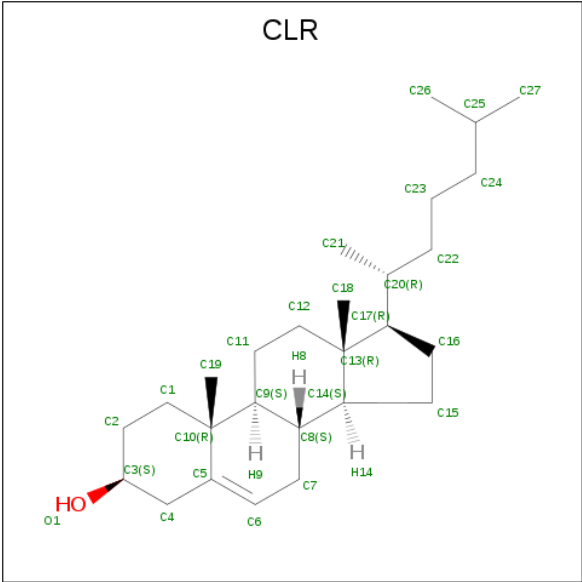
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	A	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: $C_6H_{12}O_6$).



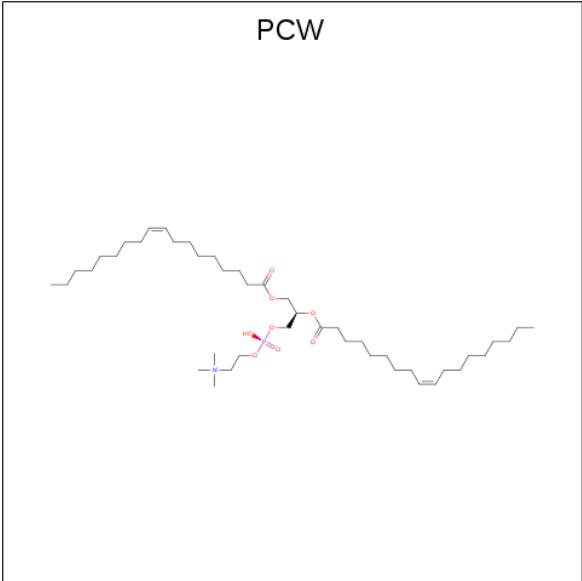
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 11	C 6	O 5	0	0
4	A	1	Total 11	C 6	O 5	0	0
4	A	1	Total 11	C 6	O 5	0	0
4	A	1	Total 11	C 6	O 5	0	0
4	A	1	Total 11	C 6	O 5	0	0
4	A	1	Total 11	C 6	O 5	0	0
4	B	1	Total 11	C 6	O 5	0	0
4	B	1	Total 22	C 6	H 11 O 5	0	0
4	B	1	Total 11	C 6	O 5	0	0
4	B	1	Total 11	C 6	O 5	0	0
4	B	1	Total 11	C 6	O 5	0	0

- Molecule 5 is CHOLESTEROL (three-letter code: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			74	27	46	1		
5	B	1	Total	C	H	O	0	0
			74	27	46	1		

- Molecule 6 is 1,2-DIOLEOYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PCW) (formula: C₄₄H₈₅NO₈P).



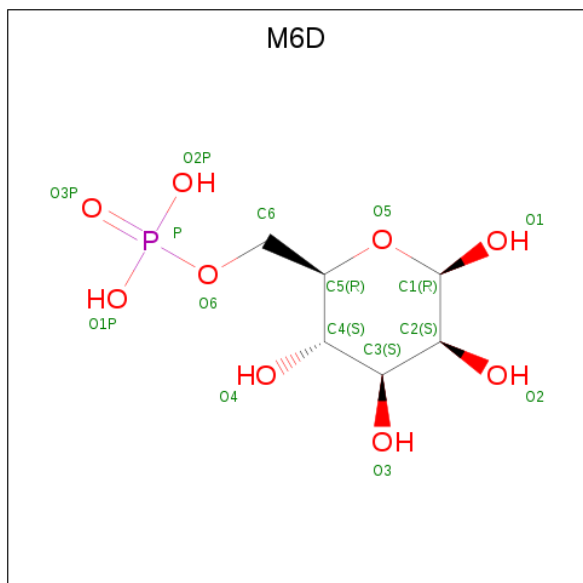
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
6	A	1	Total	C	H	N	O	P	0	0
			138	44	84	1	8	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	B	1	Total	C	H	N	O	P	
			138	44	84	1	8	1	
6	B	1	Total	C					
			11	11					

- Molecule 7 is 6-O-phosphono-beta-D-mannopyranose (three-letter code: M6D) (formula: $C_6H_{13}O_9P$).

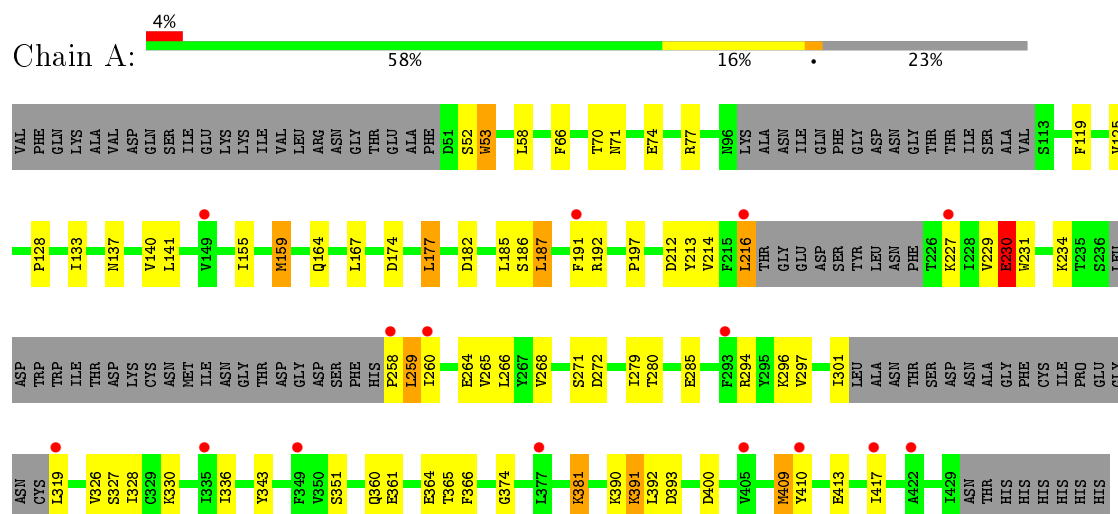


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P		
			15	6	8	1		

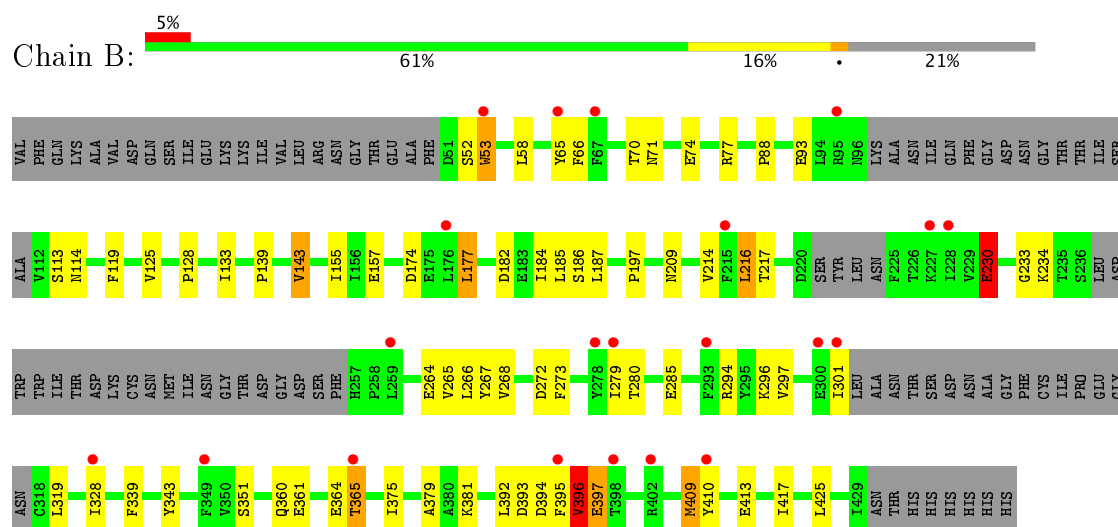
3 Residue-property plots [i](#)

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: Lysosome membrane protein 2



• Molecule 1: Lysosome membrane protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	139.04Å 139.04Å 178.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.61 – 3.00 98.32 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.7 (40.61-3.00) 95.7 (98.32-3.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 3.01Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.193 , 0.228 0.212 , 0.243	Depositor DCC
R_{free} test set	1688 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	103.9	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 122.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6066	wwPDB-VP
Average B, all atoms (Å ²)	130.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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: BMA, NAG, PCW, M6D, CLR, MAN

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	0/2633	0.77	0/3578
1	B	0.55	0/2696	0.78	2/3662 (0.1%)
All	All	0.56	0/5329	0.77	2/7240 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	396	VAL	C-N-CA	6.49	137.92	121.70
1	B	230	GLU	C-N-CA	5.12	134.50	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2566	0	2491	45	0
1	B	2628	0	2548	40	0
2	A	112	0	97	2	0
2	B	112	0	97	1	0
3	A	33	0	25	0	0
3	B	33	0	25	0	0
4	A	66	0	58	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	55	11	50	0	0
5	A	28	46	46	7	0
5	B	28	46	46	6	0
6	A	54	84	84	2	0
6	B	65	84	100	0	0
7	A	15	0	9	0	0
All	All	5795	271	5676	82	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 7.

All (82) 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:268:VAL:HG11	5:B:517:CLR:H151	1.47	0.92
1:B:392:LEU:HD11	1:B:396:VAL:HG23	1.56	0.86
1:B:268:VAL:HG11	5:B:517:CLR:C15	2.10	0.81
1:A:381:LYS:HB2	5:A:518:CLR:H122	1.65	0.79
1:B:396:VAL:HA	1:B:397:GLU:HB2	1.72	0.71
1:A:182:ASP:HB3	1:A:185:LEU:HD12	1.73	0.70
2:A:508:NAG:H83	2:B:509:NAG:O3	1.93	0.68
1:A:229:VAL:O	1:A:230:GLU:HB2	1.93	0.67
1:B:186:SER:HA	1:B:197:PRO:HB3	1.77	0.65
1:A:381:LYS:HB2	5:A:518:CLR:C12	2.26	0.65
1:A:66:PHE:HZ	1:A:177:LEU:HD13	1.62	0.64
1:A:390:LYS:HE2	1:A:392:LEU:HD21	1.79	0.64
1:B:66:PHE:HZ	1:B:177:LEU:HD13	1.63	0.62
1:A:381:LYS:HB3	1:A:413:GLU:HB3	1.85	0.59
1:B:216:LEU:HG	1:B:266:LEU:CD2	2.34	0.57
1:A:268:VAL:HG11	5:A:518:CLR:H161	1.87	0.56
1:A:137:ASN:HB3	1:A:140:VAL:HG22	1.88	0.55
1:A:330:LYS:HZ3	6:A:519:PCW:H62	1.72	0.55
1:B:379:ALA:HB3	5:B:517:CLR:H193	1.87	0.55
1:A:192:ARG:HD3	1:B:272:ASP:O	2.07	0.55
1:B:265:VAL:HG22	1:B:280:THR:HG22	1.89	0.55
1:A:258:PRO:O	1:A:260:ILE:HG13	2.08	0.53
1:A:268:VAL:HG11	5:A:518:CLR:H151	1.91	0.53
1:A:58:LEU:HD22	1:A:417:ILE:HA	1.92	0.51
1:B:409:MET:HG2	1:B:410:TYR:N	2.26	0.51
1:A:214:VAL:HB	1:A:229:VAL:O	2.11	0.51
1:A:192:ARG:NH1	1:B:272:ASP:HB2	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:LEU:HG	1:A:266:LEU:CD2	2.41	0.50
1:A:409:MET:HG2	1:A:410:TYR:N	2.26	0.50
1:B:266:LEU:HB2	1:B:279:ILE:HG13	1.93	0.50
1:B:296:LYS:HE2	1:B:364:GLU:OE1	2.12	0.50
1:B:375:ILE:HD13	1:B:425:LEU:HD11	1.93	0.50
1:A:296:LYS:HE2	1:A:364:GLU:OE1	2.12	0.50
1:A:265:VAL:HG22	1:A:280:THR:HG22	1.93	0.49
1:A:230:GLU:O	1:A:234:LYS:HB2	2.12	0.49
1:A:192:ARG:HH11	1:B:272:ASP:HB2	1.79	0.48
1:A:336:ILE:HD11	2:A:507:NAG:H82	1.94	0.48
1:A:330:LYS:HZ1	6:A:519:PCW:H51	1.78	0.48
1:B:294:ARG:HD3	1:B:296:LYS:HE3	1.96	0.48
1:A:213:TYR:CD2	1:A:231:TRP:HA	2.49	0.48
1:A:266:LEU:HB2	1:A:279:ILE:HG13	1.96	0.47
1:B:381:LYS:HG3	5:B:517:CLR:H213	1.97	0.47
1:B:71:ASN:HB2	1:B:74:GLU:HB2	1.96	0.47
1:B:119:PHE:CZ	1:B:128:PRO:HD3	2.50	0.46
1:B:182:ASP:HB3	1:B:185:LEU:HD12	1.97	0.46
1:B:214:VAL:HG22	1:B:268:VAL:HG13	1.97	0.46
1:B:381:LYS:HB3	1:B:413:GLU:HB3	1.97	0.46
1:A:326:VAL:CG1	1:A:326:VAL:O	2.64	0.46
1:A:391:LYS:HD2	1:A:400:ASP:HA	1.96	0.46
1:B:297:VAL:HG13	1:B:301:ILE:HD12	1.96	0.46
1:B:58:LEU:HD22	1:B:417:ILE:HA	1.98	0.45
1:A:119:PHE:CZ	1:A:128:PRO:HD3	2.50	0.45
1:B:396:VAL:CA	1:B:397:GLU:HB2	2.43	0.45
1:B:230:GLU:HA	1:B:234:LYS:HB2	1.99	0.45
1:A:71:ASN:HB2	1:A:74:GLU:HB2	1.98	0.45
1:A:343:TYR:OH	1:A:360:GLN:HG3	2.17	0.44
1:A:294:ARG:HD2	1:A:366:PHE:HB2	1.99	0.44
1:B:285:GLU:HG3	1:B:294:ARG:HB2	1.99	0.44
1:A:229:VAL:O	1:A:230:GLU:CB	2.64	0.44
1:A:294:ARG:CD	1:A:366:PHE:HB2	2.48	0.44
1:B:139:PRO:O	1:B:143:VAL:HG13	2.18	0.43
1:A:213:TYR:HE1	1:A:271:SER:HA	1.84	0.43
1:A:285:GLU:HG3	1:A:294:ARG:HB2	2.00	0.43
1:B:157:GLU:HG2	1:B:395:PHE:CZ	2.53	0.43
1:B:339:PHE:HE1	1:B:365:THR:HB	1.83	0.43
1:B:343:TYR:OH	1:B:360:GLN:HG3	2.18	0.43
1:B:217:THR:HG21	1:B:267:TYR:HE2	1.84	0.43
1:A:141:LEU:HD21	1:A:167:LEU:CD1	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:381:LYS:HA	5:B:517:CLR:H212	2.01	0.42
1:B:114:ASN:ND2	1:B:209:ASN:HB3	2.34	0.42
1:B:381:LYS:CB	5:B:517:CLR:H122	2.49	0.42
1:A:260:ILE:HD11	1:A:374:GLY:HA2	2.02	0.42
1:A:191:PHE:HD1	1:B:273:PHE:CE2	2.38	0.42
1:B:143:VAL:HG21	1:B:184:ILE:HG21	2.01	0.41
1:A:159:MET:HE2	1:A:187:LEU:HD22	2.01	0.41
1:A:186:SER:HA	1:A:197:PRO:HB3	2.03	0.41
1:A:268:VAL:HG11	5:A:518:CLR:C16	2.49	0.41
1:B:65:TYR:CE2	1:B:88:PRO:HB3	2.55	0.41
1:A:297:VAL:HG13	1:A:301:ILE:HD12	2.02	0.41
1:A:381:LYS:CB	5:A:518:CLR:H122	2.44	0.40
1:B:230:GLU:HG3	1:B:233:GLY:HA2	2.03	0.40
1:A:268:VAL:HG11	5:A:518:CLR:C15	2.52	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	306/410 (75%)	287 (94%)	15 (5%)	4 (1%)	14	51
1	B	314/410 (77%)	291 (93%)	20 (6%)	3 (1%)	18	59
All	All	620/820 (76%)	578 (93%)	35 (6%)	7 (1%)	17	56

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	230	GLU
1	A	259	LEU
1	B	52	SER
1	A	52	SER

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Mol	Chain	Res	Type
1	B	53	TRP
1	A	53	TRP
1	B	230	GLU

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	281/370 (76%)	253 (90%)	28 (10%)	9	33
1	B	288/370 (78%)	264 (92%)	24 (8%)	13	44
All	All	569/740 (77%)	517 (91%)	52 (9%)	11	39

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	TRP
1	A	70	THR
1	A	77	ARG
1	A	125	VAL
1	A	133	ILE
1	A	155	ILE
1	A	159	MET
1	A	164	GLN
1	A	174	ASP
1	A	177	LEU
1	A	187	LEU
1	A	212	ASP
1	A	216	LEU
1	A	227	LYS
1	A	230	GLU
1	A	259	LEU
1	A	264	GLU
1	A	272	ASP
1	A	319	LEU
1	A	327	SER

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Mol	Chain	Res	Type
1	A	328	ILE
1	A	351	SER
1	A	361	GLU
1	A	365	THR
1	A	381	LYS
1	A	391	LYS
1	A	393	ASP
1	A	409	MET
1	B	53	TRP
1	B	70	THR
1	B	77	ARG
1	B	93	GLU
1	B	113	SER
1	B	125	VAL
1	B	133	ILE
1	B	143	VAL
1	B	155	ILE
1	B	174	ASP
1	B	177	LEU
1	B	187	LEU
1	B	216	LEU
1	B	264	GLU
1	B	319	LEU
1	B	328	ILE
1	B	351	SER
1	B	361	GLU
1	B	365	THR
1	B	393	ASP
1	B	394	ASP
1	B	396	VAL
1	B	397	GLU
1	B	409	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	GLN
1	A	148	GLN
1	A	288	GLN
1	B	114	ASN
1	B	288	GLN

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

39 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	$\# Z > 2$
2	NAG	A	501	1,2	14,14,15	0.34	0	15,19,21	0.97	2 (13%)
2	NAG	A	502	3,2	14,14,15	0.27	0	15,19,21	0.68	0
3	BMA	A	503	2,4	11,11,12	0.33	0	13,15,17	0.89	0
4	MAN	A	504	3	11,11,12	0.33	0	13,15,17	1.07	1 (7%)
2	NAG	A	505	1,2	14,14,15	0.30	0	15,19,21	0.69	0
2	NAG	A	506	2	14,14,15	0.30	0	15,19,21	0.57	0
2	NAG	A	507	1,2	14,14,15	0.34	0	15,19,21	1.03	1 (6%)
2	NAG	A	508	3,2	14,14,15	0.30	0	15,19,21	1.42	2 (13%)
3	BMA	A	509	2,4	11,11,12	0.44	0	13,15,17	1.69	1 (7%)
4	MAN	A	510	3,4	11,11,12	0.46	0	13,15,17	0.94	1 (7%)
4	MAN	A	511	4,7	11,11,12	0.50	0	13,15,17	1.51	1 (7%)
4	MAN	A	512	3	11,11,12	0.42	0	13,15,17	0.85	1 (7%)
2	NAG	A	513	1,2	14,14,15	0.35	0	15,19,21	3.12	5 (33%)
2	NAG	A	514	3,2	14,14,15	0.34	0	15,19,21	0.49	0
3	BMA	A	515	2,4	11,11,12	0.29	0	13,15,17	0.87	1 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	MAN	A	516	3	11,11,12	0.33	0	13,15,17	0.95	1 (7%)
4	MAN	A	517	3	11,11,12	0.52	0	13,15,17	1.18	2 (15%)
5	CLR	A	518	-	31,31,31	0.45	0	48,48,48	0.96	5 (10%)
6	PCW	A	519	-	53,53,53	0.45	0	58,61,61	0.53	0
7	M6D	A	520	4	15,15,16	0.72	0	21,22,24	1.45	3 (14%)
2	NAG	B	501	1,2	14,14,15	0.37	0	15,19,21	0.93	1 (6%)
2	NAG	B	502	3,2	14,14,15	0.21	0	15,19,21	0.82	0
3	BMA	B	503	2,4	11,11,12	0.34	0	13,15,17	0.83	0
4	MAN	B	504	3	11,11,12	0.33	0	13,15,17	0.98	1 (7%)
4	MAN	B	505	3	11,11,12	0.40	0	13,15,17	1.13	1 (7%)
2	NAG	B	506	1,2	14,14,15	0.30	0	15,19,21	0.60	0
2	NAG	B	507	2	14,14,15	0.29	0	15,19,21	0.56	0
2	NAG	B	508	1,2	14,14,15	0.44	0	15,19,21	1.28	1 (6%)
2	NAG	B	509	3,2	14,14,15	0.32	0	15,19,21	1.63	2 (13%)
3	BMA	B	510	2,4	11,11,12	0.38	0	13,15,17	0.77	0
4	MAN	B	511	3	11,11,12	0.48	0	13,15,17	1.05	1 (7%)
2	NAG	B	512	1,2	14,14,15	0.33	0	15,19,21	3.27	5 (33%)
2	NAG	B	513	3,2	14,14,15	0.33	0	15,19,21	0.60	0
3	BMA	B	514	2,4	11,11,12	0.30	0	13,15,17	0.78	0
4	MAN	B	515	3	11,11,12	0.38	0	13,15,17	0.93	1 (7%)
4	MAN	B	516	3	11,11,12	0.51	0	13,15,17	1.10	2 (15%)
5	CLR	B	517	-	31,31,31	0.48	0	48,48,48	1.08	5 (10%)
6	PCW	B	518	-	53,53,53	0.43	0	58,61,61	0.55	0
6	PCW	B	519	-	10,10,53	0.41	0	9,9,61	0.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	504	3	-	0/2/19/22	1/1/1/1
2	NAG	A	505	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	506	2	-	0/6/23/26	0/1/1/1
2	NAG	A	507	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	508	3,2	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	A	509	2,4	-	0/2/19/22	1/1/1/1
4	MAN	A	510	3,4	-	0/2/19/22	0/1/1/1
4	MAN	A	511	4,7	-	0/2/19/22	0/1/1/1
4	MAN	A	512	3	-	0/2/19/22	1/1/1/1
2	NAG	A	513	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	514	3,2	-	0/6/23/26	0/1/1/1
3	BMA	A	515	2,4	-	0/2/19/22	0/1/1/1
4	MAN	A	516	3	-	0/2/19/22	0/1/1/1
4	MAN	A	517	3	-	0/2/19/22	0/1/1/1
5	CLR	A	518	-	-	0/10/68/68	0/4/4/4
6	PCW	A	519	-	-	0/57/57/57	0/0/0/0
7	M6D	A	520	4	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	502	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	503	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	504	3	-	0/2/19/22	1/1/1/1
4	MAN	B	505	3	-	0/2/19/22	0/1/1/1
2	NAG	B	506	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	507	2	-	0/6/23/26	0/1/1/1
2	NAG	B	508	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	509	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	510	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	511	3	-	0/2/19/22	0/1/1/1
2	NAG	B	512	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	513	3,2	-	0/6/23/26	0/1/1/1
3	BMA	B	514	2,4	-	0/2/19/22	0/1/1/1
4	MAN	B	515	3	-	0/2/19/22	0/1/1/1
4	MAN	B	516	3	-	0/2/19/22	0/1/1/1
5	CLR	B	517	-	-	0/10/68/68	0/4/4/4
6	PCW	B	518	-	-	0/57/57/57	0/0/0/0
6	PCW	B	519	-	-	0/8/8/57	0/0/0/0

There are no bond length outliers.

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	512	NAG	O5-C1-C2	-8.05	100.27	111.47
2	A	513	NAG	O5-C1-C2	-6.27	102.75	111.47
2	B	508	NAG	C1-C2-N2	-3.99	103.67	110.49
2	B	509	NAG	O5-C1-C2	-3.73	106.29	111.47
2	A	507	NAG	C1-C2-N2	-3.28	104.89	110.49
2	A	508	NAG	O5-C1-C2	-3.25	106.96	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	513	NAG	C4-C3-C2	-2.92	106.74	111.02
2	B	512	NAG	C4-C3-C2	-2.81	106.90	111.02
5	B	517	CLR	C17-C13-C14	-2.80	96.73	100.07
5	A	518	CLR	C11-C9-C8	-2.49	108.14	111.75
5	B	517	CLR	C11-C9-C8	-2.46	108.17	111.75
5	A	518	CLR	C17-C13-C14	-2.32	97.29	100.07
2	A	501	NAG	O5-C1-C2	-2.26	108.33	111.47
5	B	517	CLR	C14-C8-C9	-2.12	106.21	109.09
5	A	518	CLR	C10-C9-C8	2.03	115.86	112.73
4	B	516	MAN	C1-O5-C5	2.10	115.06	112.17
5	A	518	CLR	C11-C12-C13	2.20	116.63	112.80
4	A	512	MAN	C1-O5-C5	2.21	115.22	112.17
3	A	515	BMA	C1-O5-C5	2.22	115.22	112.17
5	A	518	CLR	C13-C17-C20	2.26	123.10	119.47
5	B	517	CLR	C10-C9-C8	2.28	116.24	112.73
4	B	515	MAN	C1-O5-C5	2.38	115.45	112.17
4	A	517	MAN	C1-C2-C3	2.44	112.75	109.65
2	A	501	NAG	C1-C2-N2	2.46	114.68	110.49
2	B	501	NAG	C1-C2-N2	2.49	114.74	110.49
4	A	517	MAN	C1-O5-C5	2.53	115.65	112.17
4	A	516	MAN	C1-O5-C5	2.53	115.66	112.17
4	B	516	MAN	C1-C2-C3	2.54	112.87	109.65
4	A	510	MAN	C1-O5-C5	2.86	116.11	112.17
2	A	513	NAG	C2-N2-C7	2.89	127.16	122.94
7	A	520	M6D	O1P-P-O6	2.95	114.58	106.73
7	A	520	M6D	C1-C2-C3	3.01	113.47	109.65
5	B	517	CLR	C11-C12-C13	3.02	118.07	112.80
2	B	512	NAG	C2-N2-C7	3.16	127.55	122.94
4	B	511	MAN	C1-O5-C5	3.18	116.55	112.17
4	B	504	MAN	C1-O5-C5	3.27	116.67	112.17
4	A	504	MAN	C1-O5-C5	3.41	116.86	112.17
4	B	505	MAN	C1-O5-C5	3.70	117.26	112.17
2	A	508	NAG	C1-O5-C5	3.76	117.34	112.17
2	B	512	NAG	C1-C2-N2	4.06	117.42	110.49
7	A	520	M6D	P-O6-C6	4.28	130.09	118.30
2	B	509	NAG	C1-O5-C5	4.46	118.32	112.17
4	A	511	MAN	C1-O5-C5	4.52	118.40	112.17
3	A	509	BMA	C1-O5-C5	4.81	118.80	112.17
2	A	513	NAG	C1-C2-N2	5.62	120.09	110.49
2	A	513	NAG	C1-O5-C5	7.10	121.95	112.17
2	B	512	NAG	C1-O5-C5	7.24	122.15	112.17

There are no chirality outliers.

There are no torsion outliers.

All (4) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	509	BMA	C1-C2-C3-C4-C5-O5
4	A	512	MAN	C1-C2-C3-C4-C5-O5
4	A	504	MAN	C1-C2-C3-C4-C5-O5
4	B	504	MAN	C1-C2-C3-C4-C5-O5

6 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	507	NAG	1	0
2	A	508	NAG	1	0
5	A	518	CLR	7	0
6	A	519	PCW	2	0
2	B	509	NAG	1	0
5	B	517	CLR	6	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	316/410 (77%)	0.70	15 (4%) 32 13	91, 119, 174, 204	0
1	B	324/410 (79%)	0.63	21 (6%) 20 7	91, 118, 168, 201	0
All	All	640/820 (78%)	0.66	36 (5%) 25 10	91, 119, 171, 204	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	258	PRO	7.3
1	B	53	TRP	4.7
1	B	300	GLU	4.0
1	B	228	ILE	3.5
1	B	410	TYR	3.0
1	B	95	ARG	2.5
1	B	398	THR	2.5
1	A	405	VAL	2.5
1	A	227	LYS	2.5
1	A	149	VAL	2.4
1	A	335	ILE	2.4
1	A	417	ILE	2.4
1	A	410	TYR	2.4
1	A	349	PHE	2.4
1	B	349	PHE	2.3
1	B	67	PHE	2.3
1	B	227	LYS	2.3
1	B	278	TYR	2.3
1	A	191	PHE	2.2
1	B	293	PHE	2.2
1	A	260	ILE	2.2
1	B	301	ILE	2.2
1	B	65	TYR	2.2
1	B	395	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	377	LEU	2.1
1	B	328	ILE	2.1
1	A	293	PHE	2.1
1	B	279	ILE	2.1
1	B	176	LEU	2.1
1	B	365	THR	2.1
1	B	259	LEU	2.1
1	A	422	ALA	2.0
1	A	319	LEU	2.0
1	A	216	LEU	2.0
1	B	215	PHE	2.0
1	B	402	ARG	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
6	PCW	B	518	54/54	0.68	0.82	6.17	115,173,221,225	0
5	CLR	B	517	28/28	0.64	0.70	4.20	128,171,176,177	0
5	CLR	A	518	28/28	0.63	0.58	3.96	123,165,176,177	0
6	PCW	A	519	54/54	0.69	0.68	3.65	122,163,241,248	0
2	NAG	A	507	14/15	0.96	0.32	-0.30	111,118,123,130	0
2	NAG	B	512	14/15	0.91	0.29	-0.51	110,119,129,133	0
2	NAG	B	508	14/15	0.95	0.29	-0.62	120,136,145,153	0
2	NAG	A	513	14/15	0.91	0.23	-0.88	104,120,127,130	0
2	NAG	B	506	14/15	0.93	0.18	-0.99	144,150,154,157	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	PCW	B	519	11/54	0.56	0.30	-1.14	119,130,153,155	0
2	NAG	A	501	14/15	0.93	0.25	-1.46	115,119,125,129	0
2	NAG	A	505	14/15	0.86	0.21	-1.62	135,146,156,163	0
2	NAG	B	501	14/15	0.92	0.28	-1.67	113,118,123,124	0
3	BMA	A	503	11/12	0.70	0.14	-	163,172,181,186	0
3	BMA	B	514	11/12	0.97	0.09	-	155,164,169,172	0
3	BMA	B	510	11/12	0.70	0.45	-	183,190,193,193	0
2	NAG	B	502	14/15	0.94	0.21	-	132,136,146,156	0
4	MAN	B	516	11/12	0.73	0.18	-	171,177,181,181	0
4	MAN	B	511	11/12	0.89	0.12	-	176,188,193,194	0
2	NAG	B	507	14/15	0.85	0.19	-	156,168,174,176	0
4	MAN	A	504	11/12	0.88	0.26	-	187,191,195,197	0
4	MAN	B	515	11/12	0.95	0.17	-	165,167,168,169	0
7	M6D	A	520	15/16	0.75	0.31	-	216,219,224,226	0
4	MAN	A	517	11/12	0.72	0.23	-	181,184,189,190	0
3	BMA	B	503	11/12	0.93	0.19	-	163,175,185,196	0
4	MAN	A	511	11/12	0.58	0.28	-	220,223,225,225	0
2	NAG	A	506	14/15	0.86	0.21	-	164,175,185,188	0
2	NAG	A	508	14/15	0.88	0.36	-	137,146,153,162	0
4	MAN	A	512	11/12	0.53	0.26	-	196,199,204,204	0
3	BMA	A	509	11/12	0.69	0.24	-	175,188,197,204	0
2	NAG	B	509	14/15	0.85	0.34	-	159,167,174,175	0
4	MAN	A	516	11/12	0.91	0.21	-	159,163,174,178	0
3	BMA	A	515	11/12	0.94	0.15	-	154,162,174,178	0
2	NAG	A	514	14/15	0.92	0.25	-	115,134,142,145	0
2	NAG	A	502	14/15	0.92	0.21	-	136,143,148,154	0
2	NAG	B	513	14/15	0.89	0.25	-	115,130,140,144	0
4	MAN	B	504	11/12	0.86	0.19	-	171,182,187,189	0
4	MAN	B	505	11/12	0.76	0.16	-	204,205,207,211	0
4	MAN	A	510	11/12	0.71	0.20	-	208,213,215,217	0

6.5 Other polymers ⓘ

There are no such residues in this entry.