



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:02 PM BST

PDB ID : 5XNP
Title : Crystal structures of human SALM5 in complex with human PTPdelta
Authors : Liu, H.; Lin, Z.; Xu, F.
Deposited on : 2017-05-24
Resolution : 3.73 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

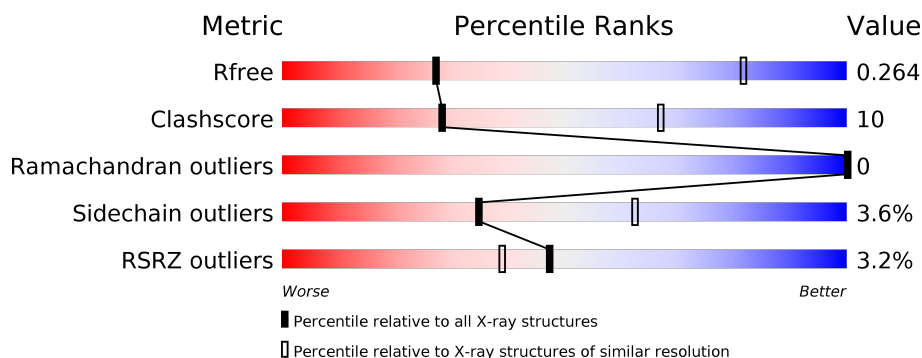
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.73 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.90-3.54)
Clashscore	141614	1012 (3.88-3.56)
Ramachandran outliers	138981	1114 (3.90-3.54)
Sidechain outliers	138945	1110 (3.90-3.54)
RSRZ outliers	127900	1020 (3.90-3.54)

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 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	361	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>26%</div> <div></div> </div> <div></div> </div>
1	B	361	<div> <div>3%</div> <div> <div></div> <div>70%</div> <div>28%</div> <div></div> </div> <div></div> </div>
2	D	291	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>20%</div> <div></div> </div> <div></div> </div>
2	E	291	<div> <div>3%</div> <div> <div></div> <div>81%</div> <div>18%</div> <div></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	NAG	A	401	-	-	-	X
3	NAG	B	401	-	-	-	X
7	SO4	A	415	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 10418 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 Leucine-rich repeat and fibronectin type-III domain-containing protein 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	0	0
			2839	1793	500	530	16			
1	B	361	Total	C	N	O	S	0	0	0
			2839	1793	500	530	16			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	PRO	-	expression tag	UNP Q96NI6
A	15	GLY	-	expression tag	UNP Q96NI6
A	16	ASP	-	expression tag	UNP Q96NI6
A	17	PRO	-	expression tag	UNP Q96NI6
B	14	PRO	-	expression tag	UNP Q96NI6
B	15	GLY	-	expression tag	UNP Q96NI6
B	16	ASP	-	expression tag	UNP Q96NI6
B	17	PRO	-	expression tag	UNP Q96NI6

- Molecule 2 is a protein called Receptor-type tyrosine-protein phosphatase delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	291	Total	C	N	O	S	0	0	0
			2244	1394	400	437	13			
2	E	291	Total	C	N	O	S	0	0	0
			2244	1394	400	437	13			

There are 18 discrepancies between the modelled and reference sequences:

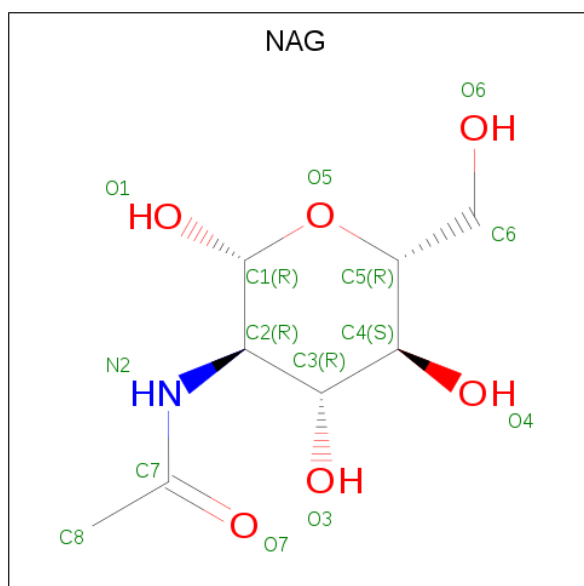
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLU	deletion	UNP P23468
D	?	-	SER	deletion	UNP P23468
D	?	-	ILE	deletion	UNP P23468

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Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLY	deletion	UNP P23468
D	?	-	GLY	deletion	UNP P23468
D	?	-	THR	deletion	UNP P23468
D	?	-	PRO	deletion	UNP P23468
D	?	-	ILE	deletion	UNP P23468
D	?	-	ARG	deletion	UNP P23468
E	?	-	GLU	deletion	UNP P23468
E	?	-	SER	deletion	UNP P23468
E	?	-	ILE	deletion	UNP P23468
E	?	-	GLY	deletion	UNP P23468
E	?	-	GLY	deletion	UNP P23468
E	?	-	THR	deletion	UNP P23468
E	?	-	PRO	deletion	UNP P23468
E	?	-	ILE	deletion	UNP P23468
E	?	-	ARG	deletion	UNP P23468

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	A	1	Total	Na	0	0
			1	1		

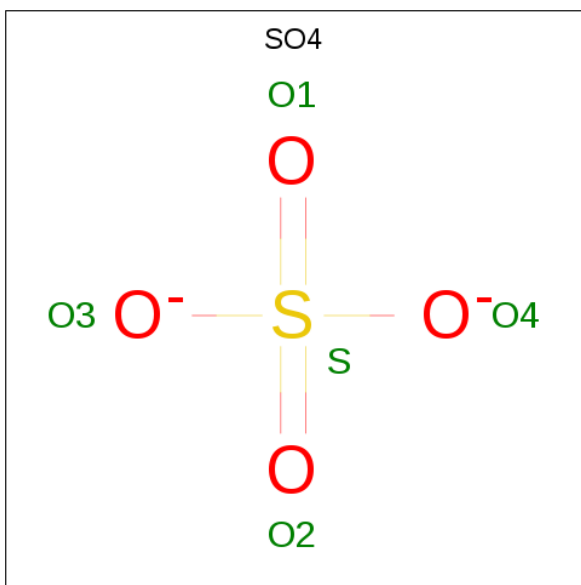
- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	6	Total	Ca	0	0
			6	6		
5	A	6	Total	Ca	0	0
			6	6		

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	3	Total	Cl	0	0
			3	3		
6	A	3	Total	Cl	0	0
			3	3		
6	D	3	Total	Cl	0	0
			3	3		
6	E	3	Total	Cl	0	0
			3	3		

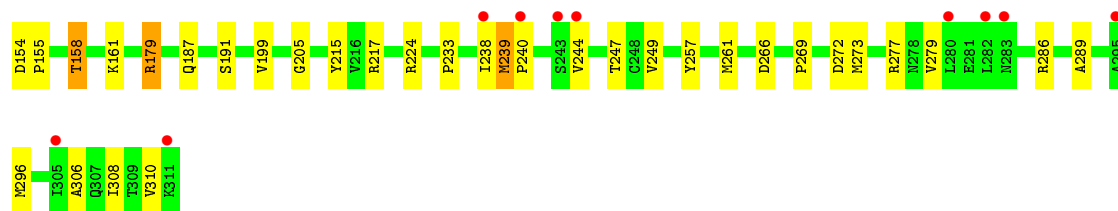
- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



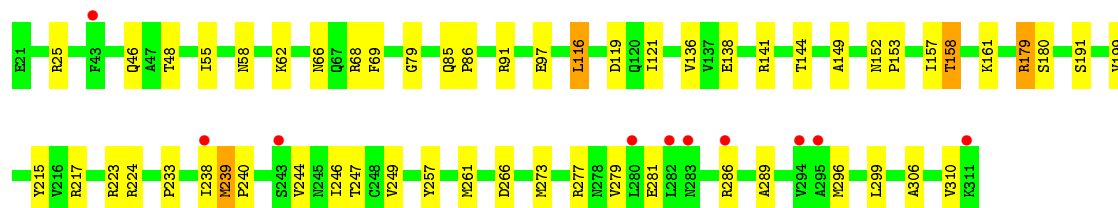
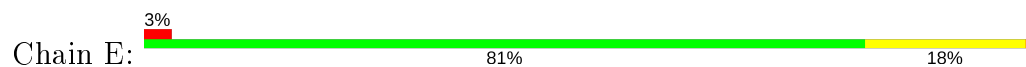
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	O	S	0	0
			5	4	1		
7	A	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		
7	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	32	Total	O	0	0
			32	32		
8	B	35	Total	O	0	0
			35	35		
8	D	14	Total	O	0	0
			14	14		
8	E	13	Total	O	0	0
			13	13		



- Molecule 2: Receptor-type tyrosine-protein phosphatase delta



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 3	Depositor
Cell constants a, b, c, α , β , γ	249.38Å 249.38Å 249.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.91 – 3.73 48.91 – 3.73	Depositor EDS
% Data completeness (in resolution range)	99.1 (48.91-3.73) 99.1 (48.91-3.73)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.32 (at 3.77Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.232 , 0.264 0.232 , 0.264	Depositor DCC
R_{free} test set	1318 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å ²)	122.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 89.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.440 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10418	wwPDB-VP
Average B, all atoms (Å ²)	133.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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: SO4, NA, CA, NAG, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.27	1/2900 (0.0%)	0.48	0/3947
1	B	0.28	0/2900	0.52	0/3947
2	D	0.25	0/2287	0.46	0/3109
2	E	0.25	0/2287	0.46	0/3109
All	All	0.27	1/10374 (0.0%)	0.48	0/14112

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	ASN	C-N	5.59	1.44	1.34

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2839	0	2847	68	0
1	B	2839	0	2847	69	0
2	D	2244	0	2228	38	0
2	E	2244	0	2228	36	0
3	A	42	0	39	0	0
3	B	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	14	0	13	0	0
3	E	14	0	13	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	6	0	0	0	0
5	B	6	0	0	0	0
6	A	3	0	0	0	0
6	B	3	0	0	0	0
6	D	3	0	0	0	0
6	E	3	0	0	0	0
7	A	10	0	0	4	0
7	B	10	0	0	0	0
8	A	32	0	0	1	0
8	B	35	0	0	0	0
8	D	14	0	0	3	0
8	E	13	0	0	2	0
All	All	10418	0	10254	201	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 10.

All (201) 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:292:HIS:CE1	1:A:368:GLN:HE22	1.75	1.05
1:B:292:HIS:CE1	1:B:368:GLN:HE22	1.78	1.01
2:E:25:ARG:HG2	2:E:48:THR:HG22	1.56	0.88
2:D:25:ARG:HG2	2:D:48:THR:HG22	1.56	0.87
1:A:292:HIS:CE1	1:A:368:GLN:NE2	2.45	0.85
1:B:292:HIS:CG	1:B:368:GLN:HE22	1.95	0.83
1:B:292:HIS:CE1	1:B:368:GLN:NE2	2.48	0.82
1:A:96:ALA:HA	1:A:121:GLY:HA3	1.62	0.81
2:E:233:PRO:HB2	2:E:306:ALA:HB2	1.64	0.80
1:A:292:HIS:CG	1:A:368:GLN:HE22	1.99	0.80
1:A:59:ALA:HB2	1:A:81:THR:HG22	1.63	0.79
1:A:204:SER:H	1:A:239:GLY:HA3	1.50	0.77
2:D:257:TYR:HB3	2:D:273:MET:HG2	1.65	0.77
2:D:25:ARG:HG2	2:D:48:THR:CG2	2.14	0.77
1:A:290:THR:HG22	1:A:291:ARG:HG3	1.67	0.76
1:B:96:ALA:HA	1:B:121:GLY:HA3	1.68	0.76
1:A:292:HIS:CD2	1:A:368:GLN:HE22	2.04	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:HIS:CD2	1:B:368:GLN:HE22	2.04	0.75
2:D:233:PRO:HB2	2:D:306:ALA:HB2	1.68	0.74
1:B:59:ALA:HB2	1:B:81:THR:HG22	1.69	0.74
1:A:28:ILE:HD12	1:A:29:LEU:HD23	1.70	0.74
2:E:25:ARG:HG2	2:E:48:THR:CG2	2.17	0.74
1:B:290:THR:HG22	1:B:291:ARG:HG3	1.70	0.73
2:E:257:TYR:HB3	2:E:273:MET:HG2	1.69	0.73
2:E:158:THR:HG23	2:E:199:VAL:HB	1.71	0.72
1:B:101:LEU:HD23	1:B:122:LEU:HD11	1.72	0.71
1:B:191:PHE:HA	1:B:194:LEU:HD23	1.72	0.71
1:A:101:LEU:HD23	1:A:122:LEU:HD11	1.71	0.71
1:B:204:SER:H	1:B:239:GLY:HA3	1.56	0.70
2:D:158:THR:HG23	2:D:199:VAL:HB	1.72	0.69
2:D:289:ALA:O	8:D:501:HOH:O	2.10	0.68
1:B:238:GLY:HA2	1:B:261:GLU:HB3	1.77	0.67
2:E:224:ARG:HB2	2:E:299:LEU:HD21	1.76	0.67
2:D:240:PRO:HG3	2:D:310:VAL:HB	1.76	0.67
2:E:240:PRO:HG3	2:E:310:VAL:HB	1.75	0.67
1:A:292:HIS:CD2	7:A:415:SO4:O4	2.48	0.66
2:E:138:GLU:HB2	2:E:141:ARG:HD2	1.77	0.66
2:D:138:GLU:HB2	2:D:141:ARG:HD2	1.78	0.66
1:B:287:PRO:HG3	1:B:361:ASN:HB2	1.78	0.65
1:A:73:ASN:N	1:A:97:ASP:OD2	2.21	0.65
1:B:292:HIS:ND1	1:B:368:GLN:NE2	2.45	0.64
1:A:287:PRO:HG3	1:A:361:ASN:HB2	1.79	0.64
2:E:247:THR:HA	2:E:279:VAL:HG12	1.80	0.63
2:D:66:ASN:HB3	2:D:69:PHE:HD2	1.64	0.63
2:E:62:LYS:HD2	8:E:506:HOH:O	1.99	0.63
1:A:292:HIS:ND1	1:A:368:GLN:NE2	2.45	0.63
2:E:244:VAL:O	2:E:281:GLU:HA	2.00	0.61
1:B:73:ASN:N	1:B:97:ASP:OD2	2.22	0.61
2:E:238:ILE:HD13	2:E:244:VAL:HB	1.81	0.61
1:A:122:LEU:HG	1:A:125:LEU:HD22	1.83	0.61
2:D:238:ILE:HD13	2:D:244:VAL:HB	1.83	0.61
2:E:66:ASN:HB3	2:E:69:PHE:HD2	1.65	0.60
1:B:292:HIS:CG	1:B:368:GLN:NE2	2.68	0.60
2:E:136:VAL:HG22	2:E:215:TYR:HB2	1.84	0.59
1:B:222:LEU:HB3	1:B:255:SER:HB3	1.85	0.59
1:B:98:LEU:H	1:B:98:LEU:HD22	1.68	0.59
2:D:136:VAL:HG22	2:D:215:TYR:HB2	1.84	0.59
1:A:238:GLY:HA2	1:A:261:GLU:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:289:ILE:HD13	1:B:310:ALA:HB2	1.85	0.59
2:E:249:VAL:HG22	2:E:277:ARG:HG3	1.85	0.59
1:B:21:PRO:HG3	1:B:49:ILE:HG12	1.84	0.58
1:A:289:ILE:HD13	1:A:310:ALA:HB2	1.85	0.58
1:B:221:VAL:HG13	1:B:229:SER:HB2	1.85	0.58
1:A:292:HIS:CG	1:A:368:GLN:NE2	2.71	0.58
1:B:338:ASP:N	1:B:338:ASP:OD1	2.37	0.57
1:A:21:PRO:HG3	1:A:49:ILE:HG12	1.87	0.57
1:B:60:ASP:OD2	1:B:84:ARG:NH1	2.38	0.57
1:B:321:ILE:HB	1:B:356:THR:HB	1.86	0.56
1:A:321:ILE:HB	1:A:356:THR:HB	1.85	0.56
1:B:285:GLU:N	1:B:313:ASP:O	2.38	0.56
1:B:285:GLU:O	1:B:361:ASN:ND2	2.39	0.56
1:A:36:LEU:HD22	1:A:57:ARG:HD2	1.87	0.56
2:E:246:ILE:O	2:E:279:VAL:HA	2.05	0.55
1:A:139:SER:HB2	1:A:142:ALA:HB2	1.89	0.55
1:A:292:HIS:HD2	7:A:415:SO4:O4	1.87	0.55
1:A:59:ALA:HB2	1:A:81:THR:CG2	2.34	0.55
2:E:161:LYS:NZ	2:E:191:SER:O	2.40	0.55
1:A:269:LEU:HD22	1:A:277:ILE:HD13	1.87	0.55
2:D:249:VAL:HG22	2:D:277:ARG:HG3	1.88	0.55
1:A:285:GLU:O	1:A:361:ASN:ND2	2.41	0.54
1:A:278:PRO:HG2	1:A:281:GLU:HG3	1.90	0.54
1:B:59:ALA:HB2	1:B:81:THR:CG2	2.36	0.54
2:D:308:ILE:N	8:D:501:HOH:O	2.28	0.54
1:A:221:VAL:HG23	1:A:231:SER:HB2	1.89	0.54
1:A:235:LEU:O	1:A:256:ARG:NH2	2.41	0.54
1:A:279:GLU:O	2:D:217:ARG:NH2	2.41	0.53
1:A:300:GLU:HG3	1:A:347:THR:O	2.09	0.53
2:D:68:ARG:HH21	2:D:91:ARG:HH21	1.56	0.53
1:B:82:LEU:O	1:B:85:ASN:ND2	2.42	0.52
1:B:300:GLU:HG3	1:B:347:THR:O	2.09	0.52
1:B:279:GLU:O	2:E:217:ARG:NH2	2.42	0.52
1:B:269:LEU:HD22	1:B:277:ILE:HD13	1.92	0.52
1:B:278:PRO:HG2	1:B:281:GLU:HG3	1.91	0.52
1:B:122:LEU:HG	1:B:125:LEU:HD22	1.92	0.52
1:B:235:LEU:O	1:B:256:ARG:NH2	2.43	0.52
1:B:139:SER:HB2	1:B:142:ALA:HB2	1.92	0.51
1:A:288:LEU:HD11	2:D:296:MET:HB3	1.91	0.51
2:E:261:MET:HG2	2:E:266:ASP:HA	1.93	0.51
2:D:55:ILE:HG13	2:D:79:GLY:HA2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:251:LEU:HD12	1:B:254:LEU:HD12	1.93	0.50
1:A:60:ASP:OD2	1:A:84:ARG:NH1	2.45	0.50
2:D:179:ARG:H	2:D:179:ARG:HD2	1.76	0.50
1:A:116:ASN:HA	1:A:142:ALA:HA	1.94	0.49
1:B:32:ASN:HB3	1:B:54:VAL:HB	1.93	0.49
1:B:327:LEU:HD23	1:B:328:ILE:H	1.78	0.49
1:A:327:LEU:HD11	2:D:130:MET:CE	2.42	0.49
2:E:46:GLN:HA	2:E:79:GLY:HA3	1.95	0.49
1:A:27:GLN:HB3	1:A:29:LEU:HG	1.93	0.49
2:D:46:GLN:HA	2:D:79:GLY:HA3	1.93	0.49
1:B:92:PRO:HB3	1:B:117:ASP:HB2	1.94	0.49
1:B:37:CYS:HB2	1:B:58:LEU:HD23	1.94	0.49
2:E:55:ILE:HG13	2:E:79:GLY:HA2	1.95	0.49
1:A:181:ASN:O	1:A:205:ASN:HA	2.13	0.48
2:D:247:THR:HA	2:D:279:VAL:HG12	1.94	0.48
1:A:32:ASN:HB3	1:A:54:VAL:HB	1.95	0.48
1:A:45:VAL:HG11	1:A:70:ASP:HB3	1.96	0.48
2:D:161:LYS:NZ	2:D:191:SER:O	2.46	0.48
2:D:116:LEU:HD12	2:D:121:ILE:HD13	1.94	0.48
1:A:175:THR:HG22	1:A:199:ARG:HB3	1.95	0.48
2:E:289:ALA:O	8:E:501:HOH:O	2.20	0.47
2:E:116:LEU:HD12	2:E:121:ILE:HD13	1.96	0.47
2:E:68:ARG:HH21	2:E:91:ARG:HH21	1.63	0.47
1:B:168:GLU:HA	1:B:194:LEU:HD21	1.96	0.47
2:E:58:ASN:HB2	2:E:97:GLU:HB3	1.97	0.47
1:A:62:PHE:CE2	1:B:239:GLY:HA2	2.50	0.46
1:B:126:HIS:ND1	1:B:150:GLU:OE2	2.48	0.46
1:A:239:GLY:HA2	1:B:62:PHE:CE2	2.51	0.46
1:B:175:THR:HG22	1:B:199:ARG:HB3	1.96	0.46
1:A:251:LEU:HD12	1:A:254:LEU:HD12	1.98	0.46
2:E:179:ARG:HH21	2:E:179:ARG:HB3	1.80	0.46
1:A:78:VAL:O	1:A:101:LEU:HD12	2.16	0.46
1:A:92:PRO:HB3	1:A:117:ASP:HB2	1.97	0.46
1:B:181:ASN:O	1:B:205:ASN:HA	2.16	0.46
2:D:56:VAL:HG13	2:D:63:LYS:HD3	1.98	0.45
1:A:222:LEU:HB3	1:A:255:SER:HB3	1.97	0.45
2:D:239:MET:H	2:D:239:MET:HG2	1.61	0.45
1:A:37:CYS:HB2	1:A:58:LEU:HD23	1.99	0.45
1:B:51:ARG:HB3	1:B:73:ASN:O	2.15	0.45
2:D:58:ASN:HB2	2:D:97:GLU:HB3	1.97	0.45
1:A:285:GLU:N	1:A:313:ASP:O	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:ARG:NH1	8:A:501:HOH:O	2.31	0.45
1:A:327:LEU:HD11	2:D:130:MET:HE2	1.99	0.45
2:E:179:ARG:NH2	2:E:179:ARG:HB3	2.31	0.45
1:A:328:ILE:HG22	1:A:329:SER:H	1.82	0.45
1:A:292:HIS:NE2	7:A:415:SO4:S	2.89	0.45
1:A:23:ARG:NH1	1:B:271:GLY:O	2.50	0.45
2:D:240:PRO:HB3	2:D:286:ARG:HA	1.99	0.45
1:B:220:GLN:HA	1:B:256:ARG:HG2	1.98	0.45
2:D:89:THR:HA	2:D:90:PRO:HA	1.83	0.45
1:B:223:ALA:HB2	1:B:229:SER:OG	2.17	0.44
2:E:240:PRO:HB3	2:E:286:ARG:HA	1.99	0.44
2:D:261:MET:HG2	2:D:266:ASP:HA	1.98	0.44
1:B:291:ARG:C	1:B:292:HIS:ND1	2.71	0.44
1:A:160:GLU:O	1:A:183:ILE:HA	2.18	0.44
1:A:214:PRO:O	1:A:218:ARG:HG3	2.18	0.43
1:B:23:ARG:HE	1:B:42:LEU:HD23	1.83	0.43
2:E:149:ALA:HB3	2:E:157:ILE:HD11	2.00	0.43
1:B:28:ILE:HD12	1:B:29:LEU:HD23	2.00	0.43
2:E:152:ASN:HA	2:E:153:PRO:HA	1.92	0.43
1:A:328:ILE:HD12	1:A:342:LEU:HD11	1.99	0.43
1:A:61:ASN:O	1:A:85:ASN:HA	2.18	0.43
2:D:34:THR:HB	2:D:205:GLY:HA2	2.01	0.43
1:A:293:THR:HG23	1:A:307:ARG:HB2	2.00	0.43
1:B:46:PRO:HA	1:B:47:PRO:HD3	1.91	0.43
1:B:61:ASN:O	1:B:85:ASN:HA	2.18	0.43
1:B:288:LEU:HD11	2:E:296:MET:HB3	2.01	0.43
2:E:179:ARG:HG2	2:E:180:SER:H	1.83	0.43
1:A:292:HIS:CD2	7:A:415:SO4:S	3.12	0.42
1:A:291:ARG:C	1:A:292:HIS:ND1	2.73	0.42
1:A:116:ASN:HB2	1:A:141:THR:OG1	2.19	0.42
1:A:332:THR:HG23	1:A:333:ARG:HG3	2.02	0.42
1:A:352:THR:HG23	1:A:373:HIS:HA	2.01	0.42
1:B:160:GLU:O	1:B:183:ILE:HA	2.19	0.42
2:D:62:LYS:HD2	8:D:510:HOH:O	2.19	0.42
1:B:206:LYS:HD3	1:B:206:LYS:HA	1.80	0.42
1:B:45:VAL:HG11	1:B:70:ASP:HB3	2.02	0.42
1:B:368:GLN:HG2	1:B:369:ILE:H	1.84	0.42
2:E:239:MET:HG2	2:E:239:MET:H	1.62	0.42
1:A:146:VAL:HB	1:A:149:LEU:HD21	2.02	0.42
1:B:40:LYS:HA	1:B:40:LYS:HD3	1.74	0.42
1:B:293:THR:HG23	1:B:307:ARG:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:328:ILE:HG22	1:B:329:SER:H	1.85	0.41
2:D:140:THR:HA	2:D:187:GLN:HA	2.02	0.41
1:A:185:ASN:HA	1:A:207:LEU:HD22	2.02	0.41
1:A:40:LYS:HA	1:A:40:LYS:HD3	1.76	0.41
1:B:119:PHE:HA	1:B:122:LEU:HD23	2.02	0.41
1:B:185:ASN:HA	1:B:207:LEU:HD22	2.01	0.41
2:D:269:PRO:HG2	2:D:272:ASP:OD1	2.20	0.41
2:D:119:ASP:OD1	2:D:119:ASP:N	2.48	0.41
2:E:66:ASN:HA	2:E:66:ASN:HD22	1.75	0.41
2:D:56:VAL:HB	2:D:99:VAL:HB	2.02	0.41
1:B:292:HIS:CD2	1:B:368:GLN:NE2	2.83	0.41
2:D:154:ASP:HA	2:D:155:PRO:HD3	1.95	0.41
2:E:119:ASP:N	2:E:119:ASP:OD1	2.46	0.40
1:B:188:LYS:HG3	1:B:189:GLY:N	2.36	0.40
1:B:347:THR:HB	1:B:374:ILE:HD13	2.03	0.40
1:A:271:GLY:O	1:B:23:ARG:NH1	2.54	0.40
1:A:338:ASP:OD1	1:A:338:ASP:N	2.54	0.40
1:B:116:ASN:HA	1:B:142:ALA:HA	2.04	0.40
2:D:29:THR:HB	2:D:109:VAL:HG11	2.03	0.40
2:E:85:GLN:HA	2:E:86:PRO:HA	1.86	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	359/361 (99%)	349 (97%)	10 (3%)	0	100	100
1	B	359/361 (99%)	352 (98%)	7 (2%)	0	100	100
2	D	289/291 (99%)	283 (98%)	6 (2%)	0	100	100
2	E	289/291 (99%)	283 (98%)	6 (2%)	0	100	100
All	All	1296/1304 (99%)	1267 (98%)	29 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	325/325 (100%)	311 (96%)	14 (4%)	29	58
1	B	325/325 (100%)	309 (95%)	16 (5%)	25	55
2	D	252/252 (100%)	246 (98%)	6 (2%)	49	70
2	E	252/252 (100%)	246 (98%)	6 (2%)	49	70
All	All	1154/1154 (100%)	1112 (96%)	42 (4%)	35	62

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ARG
1	A	57	ARG
1	A	98	LEU
1	A	122	LEU
1	A	145	ASP
1	A	146	VAL
1	A	147	PHE
1	A	213	ASP
1	A	292	HIS
1	A	299	LEU
1	A	327	LEU
1	A	332	THR
1	A	342	LEU
1	A	370	VAL
1	B	98	LEU
1	B	122	LEU
1	B	131	ASN
1	B	145	ASP
1	B	146	VAL
1	B	147	PHE
1	B	213	ASP
1	B	232	THR

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Mol	Chain	Res	Type
1	B	292	HIS
1	B	299	LEU
1	B	327	LEU
1	B	328	ILE
1	B	332	THR
1	B	338	ASP
1	B	342	LEU
1	B	370	VAL
2	D	116	LEU
2	D	144	THR
2	D	158	THR
2	D	179	ARG
2	D	224	ARG
2	D	239	MET
2	E	116	LEU
2	E	144	THR
2	E	158	THR
2	E	179	ARG
2	E	223	ARG
2	E	239	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	B	368	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 38 ligands modelled in this entry, 26 are monoatomic - leaving 12 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	NAG	A	402	1	14,14,15	0.35	0	17,19,21	0.49	0
3	NAG	B	403	1	14,14,15	0.22	0	17,19,21	0.46	0
7	SO4	B	415	-	4,4,4	0.81	0	6,6,6	1.38	1 (16%)
7	SO4	B	414	-	4,4,4	0.13	0	6,6,6	0.07	0
3	NAG	A	401	1	14,14,15	0.20	0	17,19,21	0.41	0
3	NAG	B	401	1	14,14,15	0.18	0	17,19,21	0.43	0
7	SO4	A	414	-	4,4,4	0.14	0	6,6,6	0.07	0
3	NAG	D	401	2	14,14,15	0.26	0	17,19,21	0.44	0
3	NAG	E	401	2	14,14,15	0.26	0	17,19,21	0.39	0
3	NAG	B	402	1	14,14,15	0.32	0	17,19,21	0.41	0
7	SO4	A	415	-	4,4,4	0.81	0	6,6,6	1.38	1 (16%)
3	NAG	A	403	1	14,14,15	0.28	0	17,19,21	0.44	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	NAG	A	402	1	-	2/6/23/26	0/1/1/1
3	NAG	B	403	1	-	2/6/23/26	0/1/1/1
3	NAG	D	401	2	-	2/6/23/26	0/1/1/1
3	NAG	A	401	1	-	2/6/23/26	0/1/1/1
3	NAG	B	401	1	-	2/6/23/26	0/1/1/1
3	NAG	E	401	2	-	2/6/23/26	0/1/1/1
3	NAG	B	402	1	-	2/6/23/26	0/1/1/1
3	NAG	A	403	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	415	SO4	O4-S-O2	3.08	125.38	109.31
7	B	415	SO4	O4-S-O1	3.08	125.38	109.31

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	NAG	O5-C5-C6-O6
3	D	401	NAG	O5-C5-C6-O6
3	B	401	NAG	O5-C5-C6-O6
3	A	401	NAG	O5-C5-C6-O6
3	B	403	NAG	O5-C5-C6-O6
3	B	402	NAG	C4-C5-C6-O6
3	D	401	NAG	C4-C5-C6-O6
3	A	403	NAG	O5-C5-C6-O6
3	B	401	NAG	C4-C5-C6-O6
3	A	403	NAG	C4-C5-C6-O6
3	B	403	NAG	C4-C5-C6-O6
3	E	401	NAG	O5-C5-C6-O6
3	A	401	NAG	C4-C5-C6-O6
3	E	401	NAG	C4-C5-C6-O6
3	A	402	NAG	O5-C5-C6-O6
3	A	402	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	415	SO4	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	361/361 (100%)	0.23	8 (2%) 62 55	77, 118, 196, 250	0
1	B	361/361 (100%)	0.26	11 (3%) 50 40	78, 119, 201, 263	0
2	D	291/291 (100%)	0.29	13 (4%) 33 28	100, 132, 209, 228	0
2	E	291/291 (100%)	0.23	10 (3%) 45 37	98, 132, 212, 235	0
All	All	1304/1304 (100%)	0.25	42 (3%) 47 39	77, 127, 203, 263	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	282	LEU	6.0
2	E	282	LEU	5.1
1	B	225	SER	4.6
1	B	226	GLY	4.2
2	D	311	LYS	4.0
2	E	311	LYS	3.9
2	D	243	SER	3.5
2	D	280	LEU	3.5
2	D	240	PRO	3.3
1	B	227	ILE	3.2
2	D	283	ASN	3.2
1	A	297	ARG	3.2
1	B	303	ARG	3.1
1	B	297	ARG	3.1
2	E	238	ILE	3.1
1	B	224	THR	3.0
2	D	244	VAL	2.9
2	E	243	SER	2.9
1	A	305	THR	2.8
1	B	228	ILE	2.8
2	D	295	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	306	LEU	2.7
1	A	226	GLY	2.6
2	D	36	VAL	2.6
2	E	286	ARG	2.5
2	E	43	PHE	2.5
2	E	280	LEU	2.4
2	E	283	ASN	2.3
1	B	305	THR	2.3
1	A	58	LEU	2.3
2	D	305	ILE	2.3
1	A	225	SER	2.2
2	D	238	ILE	2.2
2	E	295	ALA	2.2
2	D	43	PHE	2.2
1	B	304	ALA	2.2
2	E	294	VAL	2.2
2	D	146	LEU	2.1
1	B	345	LEU	2.1
1	A	303	ARG	2.0
1	A	152	LEU	2.0
1	B	58	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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(\AA^2)	Q<0.9
5	CA	A	407	1/1	0.43	0.20	162,162,162,162	0
6	CL	E	404	1/1	0.45	0.19	158,158,158,158	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	CA	B	410	1/1	0.50	0.20	152,152,152,152	0
5	CA	B	407	1/1	0.62	0.16	154,154,154,154	0
5	CA	A	406	1/1	0.66	0.12	162,162,162,162	0
6	CL	A	413	1/1	0.67	0.24	112,112,112,112	0
6	CL	B	413	1/1	0.67	0.26	111,111,111,111	0
3	NAG	E	401	14/15	0.69	0.32	192,209,216,222	0
6	CL	B	412	1/1	0.69	0.26	174,174,174,174	0
3	NAG	B	401	14/15	0.71	0.50	176,198,207,216	0
7	SO4	A	414	5/5	0.74	0.24	125,131,150,152	0
3	NAG	A	401	14/15	0.75	0.41	179,201,209,217	0
6	CL	D	402	1/1	0.77	0.22	152,152,152,152	0
3	NAG	B	402	14/15	0.77	0.31	172,189,195,202	0
7	SO4	A	415	5/5	0.77	0.19	179,188,196,207	0
3	NAG	A	402	14/15	0.78	0.21	171,200,209,210	0
3	NAG	D	401	14/15	0.79	0.23	188,208,216,218	0
7	SO4	B	414	5/5	0.79	0.23	128,139,158,160	0
5	CA	B	406	1/1	0.79	0.17	147,147,147,147	0
5	CA	A	409	1/1	0.80	0.26	114,114,114,114	0
7	SO4	B	415	5/5	0.81	0.17	185,188,191,210	0
6	CL	A	412	1/1	0.81	0.24	128,128,128,128	0
5	CA	B	408	1/1	0.82	0.22	144,144,144,144	0
3	NAG	B	403	14/15	0.82	0.28	184,192,201,210	0
5	CA	B	409	1/1	0.83	0.27	111,111,111,111	0
6	CL	D	404	1/1	0.85	0.18	141,141,141,141	0
6	CL	E	403	1/1	0.85	0.17	146,146,146,146	0
6	CL	E	402	1/1	0.86	0.19	157,157,157,157	0
5	CA	A	408	1/1	0.87	0.10	146,146,146,146	0
3	NAG	A	403	14/15	0.88	0.24	177,183,187,188	0
5	CA	B	405	1/1	0.88	0.17	98,98,98,98	0
6	CL	B	411	1/1	0.89	0.33	97,97,97,97	0
6	CL	D	403	1/1	0.91	0.10	152,152,152,152	0
5	CA	A	410	1/1	0.91	0.12	148,148,148,148	0
6	CL	A	411	1/1	0.94	0.47	98,98,98,98	0
4	NA	A	404	1/1	0.94	0.99	107,107,107,107	0
5	CA	A	405	1/1	0.94	0.11	95,95,95,95	0
4	NA	B	404	1/1	0.96	1.49	107,107,107,107	0

6.5 Other polymers ⓘ

There are no such residues in this entry.