



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:04 PM GMT

PDB ID : 1N9E
Title : Crystal structure of Pichia pastoris Lysyl Oxidase PPLO
Authors : Guss, J.M.; Duff, A.P.
Deposited on : 2002-11-24
Resolution : 1.65 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

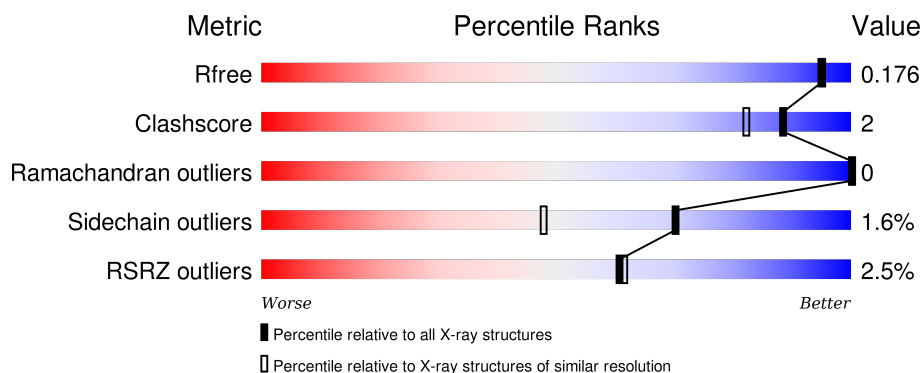
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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}	91344	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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	787	<div> <div>2%</div> <div>85%</div> <div>8% • 7%</div> </div>
1	B	787	<div> <div>3%</div> <div>87%</div> <div>6% • 7%</div> </div>
1	C	787	<div> <div>3%</div> <div>86%</div> <div>7% 7%</div> </div>
1	D	787	<div> <div>2%</div> <div>85%</div> <div>8% • 7%</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
6	SO4	A	810	-	-	-	X
6	SO4	A	812	-	-	-	X
6	SO4	A	815	-	-	-	X
6	SO4	A	816	-	-	-	X
6	SO4	B	820	-	-	-	X
6	SO4	B	822	-	-	-	X
6	SO4	B	825	-	-	-	X
6	SO4	B	826	-	-	-	X
6	SO4	C	830	-	-	-	X
6	SO4	C	832	-	-	-	X
6	SO4	C	835	-	-	-	X
6	SO4	D	840	-	-	-	X
6	SO4	D	842	-	-	-	X
6	SO4	D	845	-	-	-	X
6	SO4	D	846	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 28271 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 LYSYL OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	5	8	0
			5951	3772	962	1201	16			
1	B	735	Total	C	N	O	S	4	7	0
			5950	3772	962	1200	16			
1	C	735	Total	C	N	O	S	5	7	0
			5950	3772	962	1200	16			
1	D	735	Total	C	N	O	S	5	8	0
			5951	3772	962	1201	16			

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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		

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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	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	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		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		
3	B	2	Total	C	N	O	0	0
			28	16	2	10		
3	C	2	Total	C	N	O	0	0
			28	16	2	10		
3	D	2	Total	C	N	O	0	0
			28	16	2	10		

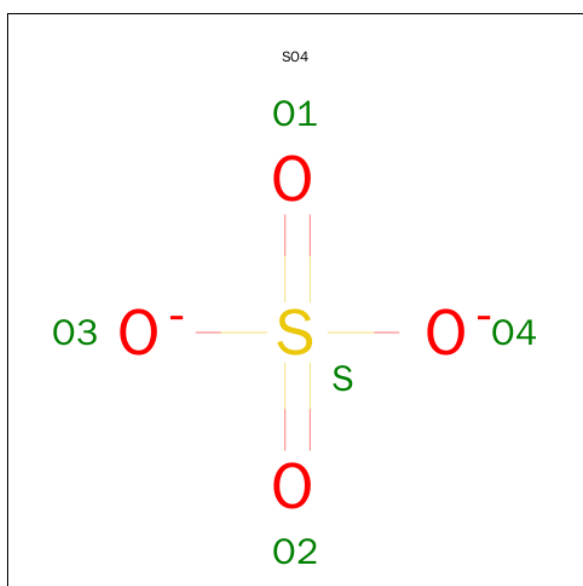
- Molecule 4 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cu 1 1	0	0
4	A	1	Total Cu 1 1	0	0
4	D	1	Total Cu 1 1	0	0
4	C	1	Total Cu 1 1	0	0

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

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

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

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

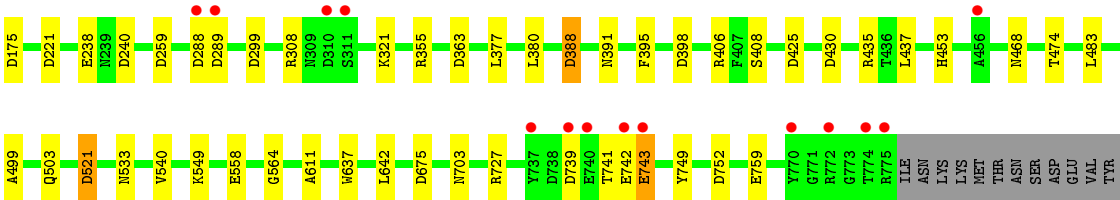
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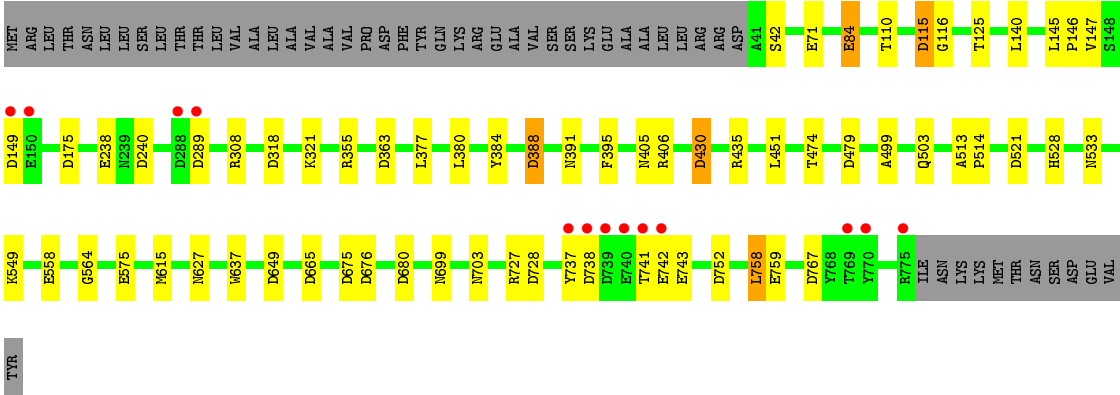
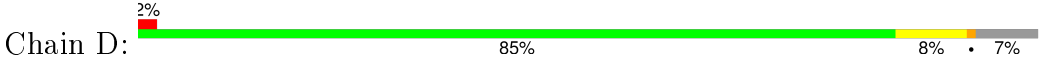
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	961	Total	O	0	0
			961	961		
7	B	1048	Total	O	0	0
			1048	1048		
7	C	1036	Total	O	0	0
			1036	1036		
7	D	936	Total	O	0	0
			936	936		



• Molecule 1: LYSYL OXIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	248.44Å 121.12Å 151.84Å 90.00° 124.64° 90.00°	Depositor
Resolution (Å)	24.60 – 1.65 24.60 – 1.65	Depositor EDS
% Data completeness (in resolution range)	94.7 (24.60-1.65) 90.5 (24.60-1.65)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.65Å)	Xtriage
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.161 , 0.187 0.170 , 0.176	Depositor DCC
R_{free} test set	20061 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 47.5	EDS
Estimated twinning fraction	0.010 for -h-2*k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 781518 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	28271	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CA, CU, NAG, TPQ, SO4

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	0.49	0/6132	0.86	20/8355 (0.2%)
1	B	0.51	0/6126	0.86	12/8347 (0.1%)
1	C	0.51	0/6126	0.86	15/8347 (0.2%)
1	D	0.48	0/6132	0.86	18/8355 (0.2%)
All	All	0.50	0/24516	0.86	65/33404 (0.2%)

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	388	ASP	CB-CG-OD2	7.16	124.74	118.30
1	B	521	ASP	CB-CG-OD2	6.95	124.56	118.30
1	D	388	ASP	CB-CG-OD2	6.58	124.22	118.30
1	C	240	ASP	CB-CG-OD2	6.53	124.17	118.30
1	D	240	ASP	CB-CG-OD2	6.50	124.15	118.30
1	D	680	ASP	CB-CG-OD2	6.47	124.12	118.30
1	B	665	ASP	CB-CG-OD2	6.42	124.07	118.30
1	C	521	ASP	CB-CG-OD2	6.29	123.96	118.30
1	A	240	ASP	CB-CG-OD2	6.29	123.96	118.30
1	D	479	ASP	CB-CG-OD2	6.26	123.93	118.30
1	D	675	ASP	CB-CG-OD2	6.22	123.90	118.30
1	C	175	ASP	CB-CG-OD2	6.17	123.85	118.30
1	B	221	ASP	CB-CG-OD2	6.06	123.75	118.30
1	D	738	ASP	CB-CG-OD2	6.04	123.73	118.30
1	D	318	ASP	CB-CG-OD2	5.98	123.68	118.30
1	D	728	ASP	CB-CG-OD2	5.91	123.62	118.30
1	D	175	ASP	CB-CG-OD2	5.82	123.53	118.30
1	C	221	ASP	CB-CG-OD2	5.76	123.49	118.30
1	B	115	ASP	CB-CG-OD2	5.75	123.47	118.30
1	C	388	ASP	CB-CG-OD2	5.68	123.41	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	642	LEU	CA-CB-CG	5.66	128.31	115.30
1	C	259	ASP	CB-CG-OD2	5.65	123.39	118.30
1	C	675	ASP	CB-CG-OD2	5.62	123.36	118.30
1	B	240	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	297	ASP	CB-CG-OD2	5.55	123.30	118.30
1	C	288	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	675	ASP	CB-CG-OD2	5.52	123.26	118.30
1	B	680	ASP	CB-CG-OD2	5.51	123.26	118.30
1	A	676	ASP	CB-CG-OD2	5.51	123.25	118.30
1	A	387	ASP	CB-CG-OD2	5.50	123.25	118.30
1	C	642	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	728	ASP	CB-CG-OD2	5.47	123.22	118.30
1	D	363	ASP	CB-CG-OD2	5.42	123.17	118.30
1	A	175	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	388	ASP	CB-CG-OD2	5.39	123.15	118.30
1	B	289	ASP	CB-CG-OD2	5.37	123.13	118.30
1	B	430	ASP	CB-CG-OD2	5.36	123.12	118.30
1	D	665	ASP	CB-CG-OD2	5.35	123.11	118.30
1	C	299	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	479	ASP	CB-CG-OD2	5.33	123.09	118.30
1	D	115	ASP	CB-CG-OD2	5.33	123.09	118.30
1	C	289	ASP	CB-CG-OD2	5.32	123.09	118.30
1	D	149	ASP	CB-CG-OD2	5.32	123.09	118.30
1	C	739	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	363	ASP	CB-CG-OD2	5.30	123.07	118.30
1	D	289	ASP	CB-CG-OD2	5.26	123.04	118.30
1	A	665	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	115	ASP	CB-CG-OD2	5.24	123.02	118.30
1	D	767	ASP	CB-CG-OD2	5.23	123.00	118.30
1	B	319	ASP	CB-CG-OD2	5.23	123.00	118.30
1	A	319	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	767	ASP	CB-CG-OD2	5.18	122.96	118.30
1	D	676	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	425	ASP	CB-CG-OD2	5.16	122.95	118.30
1	C	398	ASP	CB-CG-OD2	5.16	122.94	118.30
1	A	289	ASP	CB-CG-OD2	5.15	122.93	118.30
1	B	676	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	546	ARG	CG-CD-NE	-5.11	101.07	111.80
1	D	649	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	149	ASP	CB-CG-OD2	5.10	122.89	118.30
1	A	299	ASP	CB-CG-OD2	5.04	122.83	118.30
1	A	738	ASP	CB-CG-OD2	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	308	ARG	CG-CD-NE	-5.01	101.27	111.80
1	B	149	ASP	CB-CG-OD2	5.01	122.81	118.30
1	D	430	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5951	0	5497	35	0
1	B	5950	0	5495	29	0
1	C	5950	0	5495	26	0
1	D	5951	0	5496	34	0
2	A	56	0	52	0	0
2	B	56	0	52	0	0
2	C	56	0	52	0	0
2	D	56	0	52	0	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	A	35	0	0	0	0
6	B	35	0	0	0	0
6	C	35	0	0	0	0
6	D	35	0	0	0	0
7	A	961	0	0	5	0
7	B	1048	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	1036	0	0	6	0
7	D	936	0	0	3	0
All	All	28271	0	22291	114	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 2.

All (114) 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:435:ARG:HD2	7:A:2718:HOH:O	0.97	1.15
1:C:435:ARG:HD2	7:C:6718:HOH:O	0.96	1.13
1:B:435:ARG:HD2	7:B:4718:HOH:O	0.88	1.04
1:A:764:ASN:HD22	1:A:764:ASN:H	1.16	0.90
1:C:743:GLU:HA	1:C:743:GLU:OE2	1.71	0.90
1:A:549:LYS:NZ	1:A:575:GLU:OE1	2.06	0.88
1:A:499:ALA:HB1	7:A:2670:HOH:O	1.74	0.85
1:B:239:ASN:H	1:B:239:ASN:HD22	1.24	0.84
1:C:499:ALA:HB1	7:C:6670:HOH:O	1.86	0.74
1:B:759:GLU:HA	1:B:759:GLU:OE2	1.87	0.73
1:B:499:ALA:HB1	7:B:4670:HOH:O	1.88	0.73
1:A:239:ASN:HD22	1:A:239:ASN:H	1.37	0.72
1:A:764:ASN:H	1:A:764:ASN:ND2	1.89	0.70
1:C:435:ARG:CD	7:C:6718:HOH:O	1.74	0.70
1:B:435:ARG:CD	7:B:4718:HOH:O	1.64	0.67
1:B:738:ASP:C	1:B:738:ASP:OD1	2.33	0.67
1:B:738:ASP:OD1	1:B:740:GLU:N	2.27	0.66
1:B:239:ASN:N	1:B:239:ASN:HD22	1.94	0.66
1:D:741:THR:O	1:D:742:GLU:HB2	1.97	0.64
1:D:391:ASN:ND2	1:D:503:GLN:HE21	1.94	0.64
1:D:549:LYS:NZ	1:D:575:GLU:OE1	2.31	0.64
1:D:499:ALA:HB1	7:D:8670:HOH:O	1.97	0.63
1:C:391:ASN:ND2	1:C:503:GLN:HE21	1.99	0.61
1:D:627:ASN:ND2	7:D:9062:HOH:O	2.35	0.59
1:C:42:SER:OG	1:D:759:GLU:OE2	2.20	0.57
1:D:84:GLU:OE2	1:D:84:GLU:CA	2.52	0.57
1:A:377:LEU:HD21	1:A:380:LEU:HD11	1.87	0.56
1:B:741:THR:O	1:B:742:GLU:HB2	2.06	0.56
1:D:110:THR:HG22	1:D:116:GLY:HA3	1.88	0.55
1:A:613:ASN:ND2	1:A:615[B]:MET:HG3	2.22	0.54
1:B:463:GLN:NE2	7:B:2441:HOH:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558[B]:GLU:CD	1:A:564:GLY:H	2.11	0.54
1:C:741:THR:O	1:C:742:GLU:HB2	2.08	0.54
1:A:435:ARG:CD	7:A:2718:HOH:O	1.86	0.53
1:B:558[B]:GLU:CD	1:B:564:GLY:H	2.12	0.53
1:D:84:GLU:OE2	1:D:84:GLU:N	2.43	0.52
1:C:558[B]:GLU:CD	1:C:564:GLY:H	2.12	0.52
1:D:84:GLU:OE2	1:D:84:GLU:HA	2.11	0.51
7:C:8739:HOH:O	1:D:615[A]:MET:HE3	2.11	0.51
1:A:741:THR:O	1:A:742:GLU:HB2	2.11	0.51
1:A:239:ASN:N	1:A:239:ASN:HD22	2.03	0.51
1:A:737:TYR:CZ	1:A:742:GLU:HA	2.45	0.50
7:C:8739:HOH:O	1:D:615[A]:MET:CE	2.59	0.50
1:A:558[B]:GLU:OE1	7:A:2647:HOH:O	2.20	0.50
1:B:727:ARG:HA	1:B:727:ARG:CZ	2.42	0.50
1:D:558[B]:GLU:CD	1:D:564:GLY:H	2.14	0.50
1:D:405:ASN:HA	1:D:435:ARG:CZ	2.42	0.49
1:B:58:THR:HG21	7:B:5161:HOH:O	2.12	0.49
1:B:758:LEU:HD12	1:B:758:LEU:C	2.33	0.49
1:A:739:ASP:OD1	1:A:739:ASP:N	2.45	0.49
1:D:377:LEU:HD21	1:D:380:LEU:HD11	1.95	0.48
1:C:321:LYS:HE2	1:D:752:ASP:O	2.12	0.48
1:C:377:LEU:HD21	1:C:380:LEU:HD11	1.94	0.48
1:A:456:ALA:HB2	1:B:240:ASP:HB2	1.95	0.48
1:C:238:GLU:HA	1:C:238:GLU:OE1	2.13	0.48
1:D:125[B]:THR:CG2	1:D:140:LEU:HB2	2.44	0.48
1:C:743:GLU:OE2	1:C:743:GLU:CA	2.54	0.47
1:A:125[B]:THR:HG22	1:A:140:LEU:O	2.14	0.47
1:A:703:ASN:HD21	1:B:453:HIS:HB2	1.79	0.47
1:C:145:LEU:HA	1:C:146:PRO:C	2.35	0.47
1:A:451:LEU:C	1:A:451:LEU:HD12	2.35	0.47
1:C:533:ASN:HB2	1:C:637:TRP:CE3	2.50	0.47
1:D:758:LEU:C	1:D:758:LEU:HD12	2.34	0.47
1:B:533:ASN:HB2	1:B:637:TRP:CE3	2.50	0.47
1:A:757:GLY:HA2	1:B:759:GLU:OE2	2.14	0.46
1:A:533:ASN:HB2	1:A:637:TRP:CE3	2.51	0.46
1:C:453:HIS:HB2	1:D:703:ASN:HD21	1.80	0.46
1:D:451:LEU:C	1:D:451:LEU:HD12	2.36	0.46
1:B:125[B]:THR:CG2	1:B:140:LEU:HB2	2.46	0.46
1:D:533:ASN:HB2	1:D:637:TRP:CE3	2.51	0.46
1:B:145:LEU:HA	1:B:146:PRO:C	2.37	0.45
1:D:741:THR:OG1	1:D:743:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:125[B]:THR:HG22	1:C:140:LEU:HB2	1.99	0.45
1:A:145:LEU:HA	1:A:146:PRO:C	2.37	0.45
1:C:749:TYR:CE2	1:D:308:ARG:HB3	2.52	0.45
1:D:238:GLU:HG2	1:D:238:GLU:H	1.66	0.45
1:D:727:ARG:CZ	1:D:727:ARG:HA	2.47	0.45
1:A:321:LYS:HE2	1:B:752:ASP:O	2.17	0.45
1:D:145:LEU:HA	1:D:146:PRO:C	2.38	0.44
1:C:727:ARG:HA	1:C:727:ARG:CZ	2.48	0.44
1:A:314:ILE:HG23	1:A:318:ASP:HB3	1.99	0.44
1:A:737:TYR:OH	1:A:742:GLU:HA	2.18	0.44
1:A:540:VAL:HG11	1:A:611:ALA:HA	1.98	0.44
1:C:430:ASP:N	7:C:6516:HOH:O	2.36	0.43
1:A:254:ASP:HB2	1:A:266:LEU:HD11	2.00	0.43
1:C:125[B]:THR:CG2	1:C:140:LEU:HB2	2.48	0.43
1:D:384:TYR:CD2	1:D:528:HIS:HB3	2.54	0.43
1:A:615[B]:MET:HE2	1:A:714:MET:HB2	2.00	0.43
1:C:540:VAL:HG11	1:C:611:ALA:HA	2.00	0.43
1:D:513:ALA:N	1:D:514:PRO:CD	2.82	0.43
1:C:406:ARG:HD2	1:C:474:THR:O	2.18	0.43
1:C:468:ASN:HB3	1:C:483:LEU:HD11	2.01	0.42
1:B:134:GLU:HA	1:B:134:GLU:OE2	2.17	0.42
1:B:243:ASN:HA	1:B:243:ASN:HD22	1.61	0.42
1:B:250:PHE:HB2	1:B:269:ILE:HB	2.02	0.42
1:D:737:TYR:CZ	1:D:742:GLU:HA	2.54	0.42
1:C:408:SER:HB3	1:C:437:LEU:HB2	2.02	0.42
1:C:752:ASP:O	1:D:321:LYS:HE2	2.19	0.42
1:B:75:LEU:HG	1:B:153:ILE:HD11	2.02	0.41
1:D:125[B]:THR:HG22	1:D:140:LEU:O	2.20	0.41
1:D:406:ARG:HD2	1:D:474:THR:O	2.20	0.41
1:B:758:LEU:HD12	1:B:758:LEU:O	2.21	0.41
1:B:549:LYS:NZ	1:B:575:GLU:OE1	2.54	0.41
1:A:338:GLU:HG2	7:A:3127:HOH:O	2.20	0.41
1:A:613:ASN:ND2	1:A:615[B]:MET:CG	2.84	0.41
1:A:525[A]:GLY:O	1:A:696:PRO:HD2	2.20	0.41
1:D:71:GLU:HB3	1:D:147:VAL:CG2	2.51	0.41
1:B:468:ASN:HB3	1:B:483:LEU:HD11	2.02	0.41
1:A:752:ASP:O	1:B:321:LYS:HE2	2.21	0.41
1:A:134:GLU:HA	1:A:134:GLU:OE2	2.19	0.41
1:C:110:THR:HG22	1:C:116:GLY:HA3	2.03	0.41
1:A:429:TYR:O	1:A:430:ASP:HB2	2.22	0.40
1:D:430:ASP:N	7:D:8516:HOH:O	2.44	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ILE:HG22	1:A:315:ARG:O	2.22	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	740/787 (94%)	716 (97%)	24 (3%)	0	100	100
1	B	739/787 (94%)	717 (97%)	22 (3%)	0	100	100
1	C	739/787 (94%)	715 (97%)	24 (3%)	0	100	100
1	D	740/787 (94%)	715 (97%)	25 (3%)	0	100	100
All	All	2958/3148 (94%)	2863 (97%)	95 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	652/692 (94%)	641 (98%)	11 (2%)	68	45
1	B	651/692 (94%)	641 (98%)	10 (2%)	72	51
1	C	651/692 (94%)	641 (98%)	10 (2%)	72	51
1	D	652/692 (94%)	643 (99%)	9 (1%)	74	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2606/2768 (94%)	2566 (98%)	40 (2%)	70 51

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

Mol	Chain	Res	Type
1	A	134	GLU
1	A	239	ASN
1	A	243	ASN
1	A	355	ARG
1	A	388	ASP
1	A	395	PHE
1	A	521	ASP
1	A	627	ASN
1	A	725	ASN
1	A	739	ASP
1	A	764	ASN
1	B	134	GLU
1	B	239	ASN
1	B	355	ARG
1	B	388	ASP
1	B	395	PHE
1	B	425	ASP
1	B	521	ASP
1	B	703	ASN
1	B	738	ASP
1	B	743	GLU
1	C	115	ASP
1	C	355	ARG
1	C	388	ASP
1	C	395	PHE
1	C	425	ASP
1	C	521	ASP
1	C	549	LYS
1	C	703	ASN
1	C	743	GLU
1	C	759	GLU
1	D	42	SER
1	D	84	GLU
1	D	115	ASP
1	D	355	ARG
1	D	388	ASP
1	D	395	PHE

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Mol	Chain	Res	Type
1	D	521	ASP
1	D	699	ASN
1	D	758	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	239	ASN
1	A	243	ASN
1	A	272	ASN
1	A	613	ASN
1	A	627	ASN
1	A	703	ASN
1	A	764	ASN
1	B	77	HIS
1	B	187	ASN
1	B	239	ASN
1	B	243	ASN
1	C	77	HIS
1	C	187	ASN
1	C	262	GLN
1	C	271	ASN
1	C	391	ASN
1	C	571	GLN
1	C	583	ASN
1	D	50	ASN
1	D	243	ASN
1	D	271	ASN
1	D	272	ASN
1	D	391	ASN
1	D	627	ASN
1	D	703	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	TPQ	A	478	1,4	13,14,15	1.57	2 (15%)	15,19,21	1.62	5 (33%)
1	TPQ	B	478	1,4	13,14,15	1.46	2 (15%)	15,19,21	1.90	4 (26%)
1	TPQ	C	478	1,4	13,14,15	1.49	2 (15%)	15,19,21	2.02	4 (26%)
1	TPQ	D	478	1,4	13,14,15	1.48	3 (23%)	15,19,21	1.88	3 (20%)

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
1	TPQ	A	478	1,4	-	0/4/22/24	0/1/1/1
1	TPQ	B	478	1,4	-	0/4/22/24	0/1/1/1
1	TPQ	C	478	1,4	-	0/4/22/24	0/1/1/1
1	TPQ	D	478	1,4	-	0/4/22/24	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	478	TPQ	O4-C4	-3.66	1.24	1.34
1	D	478	TPQ	O4-C4	-3.61	1.24	1.34
1	C	478	TPQ	O4-C4	-3.36	1.25	1.34
1	B	478	TPQ	O4-C4	-3.33	1.25	1.34
1	D	478	TPQ	C3-C4	2.01	1.38	1.35
1	D	478	TPQ	C6-C1	2.07	1.40	1.34
1	A	478	TPQ	C3-C4	2.30	1.39	1.35
1	B	478	TPQ	C3-C4	2.32	1.39	1.35
1	C	478	TPQ	C3-C4	2.54	1.39	1.35

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	478	TPQ	C1-C6-C5	-5.08	119.88	122.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	478	TPQ	C1-C6-C5	-4.89	119.99	122.97
1	B	478	TPQ	C1-C6-C5	-4.56	120.19	122.97
1	C	478	TPQ	CA-CB-C1	-3.36	106.90	113.63
1	A	478	TPQ	C1-C6-C5	-3.16	121.05	122.97
1	D	478	TPQ	CA-CB-C1	-2.51	108.60	113.63
1	A	478	TPQ	O2-C2-C1	-2.30	118.84	120.85
1	B	478	TPQ	CA-CB-C1	-2.19	109.23	113.63
1	A	478	TPQ	O-C-CA	-2.15	119.90	125.49
1	B	478	TPQ	O-C-CA	-2.13	119.95	125.49
1	A	478	TPQ	CA-CB-C1	-2.06	109.50	113.63
1	C	478	TPQ	O-C-CA	-2.01	120.26	125.49
1	D	478	TPQ	C3-C2-C1	2.90	120.47	118.30
1	C	478	TPQ	C3-C2-C1	3.10	120.62	118.30
1	A	478	TPQ	C3-C2-C1	3.34	120.80	118.30
1	B	478	TPQ	C3-C2-C1	3.60	120.99	118.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates ⓘ

8 carbohydrates 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	NAG	A	1104	1,3	14,14,15	0.61	0	15,19,21	1.09	1 (6%)
3	NAG	A	1105	3	14,14,15	0.57	0	15,19,21	0.80	0
3	NAG	B	1104	1,3	14,14,15	0.74	1 (7%)	15,19,21	1.15	2 (13%)
3	NAG	B	1105	3	14,14,15	0.65	0	15,19,21	1.12	1 (6%)
3	NAG	C	1104	1,3	14,14,15	0.71	1 (7%)	15,19,21	1.34	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	C	1105	3	14,14,15	0.48	0	15,19,21	2.90	3 (20%)
3	NAG	D	1104	1,3	14,14,15	0.77	1 (7%)	15,19,21	0.95	1 (6%)
3	NAG	D	1105	3	14,14,15	0.48	0	15,19,21	1.08	1 (6%)

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	1104	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1105	3	-	0/6/23/26	0/1/1/1
3	NAG	B	1104	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	1105	3	-	0/6/23/26	0/1/1/1
3	NAG	C	1104	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	1105	3	-	0/6/23/26	0/1/1/1
3	NAG	D	1104	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	1105	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1104	NAG	O5-C1	-2.21	1.40	1.43
3	C	1104	NAG	O5-C1	-2.15	1.40	1.43
3	D	1104	NAG	O5-C1	-2.04	1.40	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1105	NAG	C2-N2-C7	-8.07	112.67	123.04
3	C	1105	NAG	C4-C3-C2	-5.49	102.69	111.23
3	C	1104	NAG	C2-N2-C7	-3.42	118.65	123.04
3	B	1104	NAG	C3-C4-C5	-2.75	105.41	110.20
3	D	1104	NAG	C2-N2-C7	-2.71	119.55	123.04
3	C	1104	NAG	C3-C4-C5	-2.67	105.54	110.20
3	B	1104	NAG	C2-N2-C7	-2.67	119.61	123.04
3	A	1104	NAG	C2-N2-C7	-2.02	120.44	123.04
3	D	1105	NAG	C1-O5-C5	2.81	115.82	112.25
3	B	1105	NAG	C1-O5-C5	2.90	115.92	112.25
3	C	1105	NAG	C1-O5-C5	4.67	118.17	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry

Of 56 ligands modelled in this entry, 12 are monoatomic - leaving 44 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	$\# Z > 2$
2	NAG	A	1081	1	14,14,15	0.62	0	15,19,21	0.98	1 (6%)
2	NAG	A	1191	1	14,14,15	0.68	0	15,19,21	1.01	0
2	NAG	A	1309	1	14,14,15	0.54	0	15,19,21	0.80	0
2	NAG	A	1434	1	14,14,15	0.51	0	15,19,21	1.07	1 (6%)
6	SO4	A	810	-	4,4,4	0.29	0	6,6,6	0.23	0
6	SO4	A	811	-	4,4,4	0.86	0	6,6,6	0.77	0
6	SO4	A	812	-	4,4,4	0.16	0	6,6,6	0.17	0
6	SO4	A	813	-	4,4,4	0.12	0	6,6,6	0.28	0
6	SO4	A	814	-	4,4,4	0.13	0	6,6,6	0.23	0
6	SO4	A	815	-	4,4,4	0.26	0	6,6,6	0.34	0
6	SO4	A	816	-	4,4,4	0.11	0	6,6,6	0.13	0
2	NAG	B	1081	1	14,14,15	0.46	0	15,19,21	0.93	0
2	NAG	B	1191	1	14,14,15	0.53	0	15,19,21	0.88	1 (6%)
2	NAG	B	1309	1	14,14,15	0.55	0	15,19,21	0.66	0
2	NAG	B	1434	1	14,14,15	0.55	0	15,19,21	0.77	1 (6%)
6	SO4	B	820	-	4,4,4	0.27	0	6,6,6	0.22	0
6	SO4	B	821	-	4,4,4	0.94	0	6,6,6	0.87	0
6	SO4	B	822	-	4,4,4	0.15	0	6,6,6	0.13	0
6	SO4	B	823	-	4,4,4	0.36	0	6,6,6	0.42	0
6	SO4	B	824	-	4,4,4	0.11	0	6,6,6	0.19	0
6	SO4	B	825	-	4,4,4	0.10	0	6,6,6	0.09	0
6	SO4	B	826	-	4,4,4	0.16	0	6,6,6	0.09	0
2	NAG	C	1081	1	14,14,15	0.51	0	15,19,21	1.19	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1191	1	14,14,15	0.54	0	15,19,21	1.04	1 (6%)
2	NAG	C	1309	1	14,14,15	0.59	0	15,19,21	0.97	1 (6%)
2	NAG	C	1434	1	14,14,15	0.52	0	15,19,21	0.74	0
6	SO4	C	830	-	4,4,4	0.23	0	6,6,6	0.12	0
6	SO4	C	831	-	4,4,4	0.67	0	6,6,6	0.37	0
6	SO4	C	832	-	4,4,4	0.11	0	6,6,6	0.21	0
6	SO4	C	833	-	4,4,4	0.16	0	6,6,6	0.20	0
6	SO4	C	834	-	4,4,4	0.18	0	6,6,6	0.28	0
6	SO4	C	835	-	4,4,4	0.15	0	6,6,6	0.09	0
6	SO4	C	836	-	4,4,4	0.13	0	6,6,6	0.18	0
2	NAG	D	1081	1	14,14,15	0.69	0	15,19,21	0.99	1 (6%)
2	NAG	D	1191	1	14,14,15	0.48	0	15,19,21	0.72	0
2	NAG	D	1309	1	14,14,15	0.60	0	15,19,21	0.94	0
2	NAG	D	1434	1	14,14,15	0.53	0	15,19,21	0.95	1 (6%)
6	SO4	D	840	-	4,4,4	0.17	0	6,6,6	0.22	0
6	SO4	D	841	-	4,4,4	0.38	0	6,6,6	0.61	0
6	SO4	D	842	-	4,4,4	0.13	0	6,6,6	0.23	0
6	SO4	D	843	-	4,4,4	0.18	0	6,6,6	0.37	0
6	SO4	D	844	-	4,4,4	0.16	0	6,6,6	0.22	0
6	SO4	D	845	-	4,4,4	0.09	0	6,6,6	0.12	0
6	SO4	D	846	-	4,4,4	0.13	0	6,6,6	0.11	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	1081	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1191	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1434	1	-	0/6/23/26	0/1/1/1
6	SO4	A	810	-	-	0/0/0/0	0/0/0/0
6	SO4	A	811	-	-	0/0/0/0	0/0/0/0
6	SO4	A	812	-	-	0/0/0/0	0/0/0/0
6	SO4	A	813	-	-	0/0/0/0	0/0/0/0
6	SO4	A	814	-	-	0/0/0/0	0/0/0/0
6	SO4	A	815	-	-	0/0/0/0	0/0/0/0
6	SO4	A	816	-	-	0/0/0/0	0/0/0/0
2	NAG	B	1081	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1191	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1434	1	-	0/6/23/26	0/1/1/1
6	SO4	B	820	-	-	0/0/0/0	0/0/0/0
6	SO4	B	821	-	-	0/0/0/0	0/0/0/0
6	SO4	B	822	-	-	0/0/0/0	0/0/0/0
6	SO4	B	823	-	-	0/0/0/0	0/0/0/0
6	SO4	B	824	-	-	0/0/0/0	0/0/0/0
6	SO4	B	825	-	-	0/0/0/0	0/0/0/0
6	SO4	B	826	-	-	0/0/0/0	0/0/0/0
2	NAG	C	1081	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1191	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1434	1	-	0/6/23/26	0/1/1/1
6	SO4	C	830	-	-	0/0/0/0	0/0/0/0
6	SO4	C	831	-	-	0/0/0/0	0/0/0/0
6	SO4	C	832	-	-	0/0/0/0	0/0/0/0
6	SO4	C	833	-	-	0/0/0/0	0/0/0/0
6	SO4	C	834	-	-	0/0/0/0	0/0/0/0
6	SO4	C	835	-	-	0/0/0/0	0/0/0/0
6	SO4	C	836	-	-	0/0/0/0	0/0/0/0
2	NAG	D	1081	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1191	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1434	1	-	0/6/23/26	0/1/1/1
6	SO4	D	840	-	-	0/0/0/0	0/0/0/0
6	SO4	D	841	-	-	0/0/0/0	0/0/0/0
6	SO4	D	842	-	-	0/0/0/0	0/0/0/0
6	SO4	D	843	-	-	0/0/0/0	0/0/0/0
6	SO4	D	844	-	-	0/0/0/0	0/0/0/0
6	SO4	D	845	-	-	0/0/0/0	0/0/0/0
6	SO4	D	846	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1434	NAG	C2-N2-C7	-2.61	119.69	123.04
2	C	1191	NAG	C6-C5-C4	-2.43	107.03	113.02
2	B	1434	NAG	C2-N2-C7	-2.24	120.16	123.04
2	D	1434	NAG	C2-N2-C7	-2.18	120.24	123.04
2	A	1081	NAG	C2-N2-C7	-2.15	120.28	123.04
2	B	1191	NAG	O5-C5-C6	2.17	112.04	107.35
2	C	1309	NAG	C1-O5-C5	2.41	115.31	112.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1081	NAG	C4-C3-C2	2.57	115.23	111.23
2	C	1081	NAG	C3-C4-C5	2.95	115.34	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	734/787 (93%)	-0.29	15 (2%) 68 71	9, 15, 30, 68	2 (0%)
1	B	734/787 (93%)	-0.33	21 (2%) 55 56	8, 13, 30, 63	2 (0%)
1	C	734/787 (93%)	-0.30	20 (2%) 58 59	8, 13, 31, 65	3 (0%)
1	D	734/787 (93%)	-0.28	16 (2%) 65 67	9, 15, 30, 71	2 (0%)
All	All	2936/3148 (93%)	-0.30	72 (2%) 61 61	8, 14, 30, 71	9 (0%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	41	ALA	9.6
1	D	41	ALA	9.0
1	C	41	ALA	8.6
1	B	41	ALA	8.5
1	A	739	ASP	7.7
1	D	740	GLU	6.8
1	D	739	ASP	6.7
1	A	740	GLU	5.5
1	C	740	GLU	4.9
1	A	741	THR	4.9
1	B	739	ASP	4.6
1	C	739	ASP	4.5
1	B	740	GLU	4.4
1	D	742	GLU	4.3
1	A	149	ASP	4.1
1	A	742	GLU	4.0
1	C	149	ASP	4.0
1	B	311	SER	3.7
1	C	774	THR	3.5
1	C	150	GLU	3.5
1	C	311	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	288	ASP	3.4
1	A	288	ASP	3.4
1	B	774	THR	3.4
1	B	149	ASP	3.3
1	A	456	ALA	3.3
1	A	770	TYR	3.3
1	D	115	ASP	3.3
1	C	743	GLU	3.2
1	D	741	THR	3.1
1	B	288	ASP	3.1
1	D	770	TYR	3.0
1	C	42	SER	3.0
1	B	771	GLY	3.0
1	C	770	TYR	3.0
1	D	149	ASP	3.0
1	D	288	ASP	3.0
1	C	742	GLU	2.9
1	A	150	GLU	2.9
1	C	310	ASP	2.9
1	A	42	SER	2.9
1	B	742	GLU	2.8
1	D	775	ARG	2.8
1	D	738	ASP	2.8
1	D	150	GLU	2.7
1	A	738	ASP	2.5
1	B	769	THR	2.5
1	B	775	ARG	2.5
1	C	456	ALA	2.5
1	B	115	ASP	2.4
1	C	289	ASP	2.4
1	D	42	SER	2.4
1	C	775	ARG	2.3
1	C	115	ASP	2.3
1	B	770	TYR	2.3
1	B	289	ASP	2.3
1	B	741	THR	2.3
1	B	772	ARG	2.3
1	A	115	ASP	2.3
1	A	743	GLU	2.2
1	D	737	TYR	2.2
1	B	310	ASP	2.2
1	B	150	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	42	SER	2.2
1	C	133	GLU	2.2
1	B	133	GLU	2.1
1	B	743	GLU	2.1
1	C	772	ARG	2.0
1	D	769	THR	2.0
1	A	133	GLU	2.0
1	D	289	ASP	2.0
1	C	737	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TPQ	A	478	14/15	0.94	0.12	-	12,26,46,52	0
1	TPQ	D	478	14/15	0.94	0.15	-	14,28,48,51	0
1	TPQ	B	478	14/15	0.94	0.13	-	12,23,45,52	0
1	TPQ	C	478	14/15	0.93	0.17	-	13,23,46,53	0

6.3 Carbohydrates [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	NAG	D	1104	14/15	0.91	0.14	1.93	16,30,38,39	0
3	NAG	B	1104	14/15	0.93	0.10	1.28	15,23,30,37	0
3	NAG	C	1104	14/15	0.94	0.10	1.05	16,24,36,37	0
3	NAG	A	1104	14/15	0.93	0.10	0.85	22,30,39,45	0
3	NAG	B	1105	14/15	0.59	0.30	-	30,44,53,56	0
3	NAG	D	1105	14/15	0.83	0.20	-	38,46,53,54	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	1105	14/15	0.87	0.20	-	36,44,52,54	0
3	NAG	C	1105	14/15	0.77	0.26	-	28,38,56,58	0

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(\AA^2)	Q<0.9
6	SO4	B	826	5/5	0.87	0.26	25.52	35,52,56,58	0
6	SO4	A	816	5/5	0.81	0.26	20.72	52,58,63,65	0
6	SO4	C	835	5/5	0.81	0.27	17.97	18,30,45,46	0
6	SO4	C	830	5/5	0.91	0.20	16.64	23,25,26,33	0
6	SO4	B	825	5/5	0.86	0.30	15.30	15,30,41,43	0
6	SO4	B	820	5/5	0.92	0.20	14.71	20,26,32,35	0
6	SO4	D	840	5/5	0.85	0.23	14.31	22,27,32,36	0
6	SO4	A	815	5/5	0.76	0.32	13.78	23,32,44,48	0
6	SO4	D	846	5/5	0.84	0.21	12.37	61,62,69,70	0
6	SO4	A	810	5/5	0.87	0.20	12.09	21,26,29,34	0
6	SO4	D	845	5/5	0.85	0.28	9.28	20,36,45,47	0
6	SO4	C	832	5/5	0.71	0.30	3.31	38,49,51,59	0
6	SO4	A	812	5/5	0.91	0.26	2.98	30,41,45,48	0
6	SO4	D	842	5/5	0.89	0.27	2.82	39,46,51,54	0
6	SO4	B	822	5/5	0.80	0.28	2.69	33,44,49,55	0
2	NAG	C	1081	14/15	0.47	0.33	1.31	55,66,74,77	0
2	NAG	B	1081	14/15	0.79	0.30	1.18	36,44,48,50	0
5	CA	C	3802	1/1	1.00	0.06	-0.97	10,10,10,10	0
5	CA	D	5802	1/1	0.99	0.05	-1.40	12,12,12,12	0
5	CA	B	1803	1/1	1.00	0.04	-1.62	10,10,10,10	0
5	CA	B	1802	1/1	1.00	0.04	-2.05	8,8,8,8	0
5	CA	C	3803	1/1	1.00	0.04	-2.15	10,10,10,10	0
5	CA	A	803	1/1	1.00	0.04	-2.57	13,13,13,13	0
5	CA	A	802	1/1	1.00	0.04	-2.72	11,11,11,11	0
5	CA	D	5803	1/1	0.99	0.04	-4.14	14,14,14,14	0
2	NAG	B	1434	14/15	0.65	0.34	-	48,61,66,67	0
2	NAG	D	1081	14/15	0.69	0.39	-	61,70,76,76	0
6	SO4	D	843	5/5	0.91	0.33	-	29,39,45,47	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	D	1434	14/15	0.64	0.37	-	50,63,75,77	0
6	SO4	D	844	5/5	0.92	0.30	-	34,34,43,46	0
4	CU	B	801	1/1	0.99	0.03	-	16,16,16,16	0
2	NAG	D	1309	14/15	0.81	0.22	-	30,37,45,46	0
6	SO4	A	813	5/5	0.91	0.26	-	22,31,42,42	0
6	SO4	C	836	5/5	0.74	0.29	-	44,51,59,61	0
6	SO4	B	823	5/5	0.93	0.18	-	19,30,33,35	0
2	NAG	C	1309	14/15	0.30	0.51	-	65,69,73,76	0
2	NAG	A	1081	14/15	0.77	0.34	-	45,51,68,71	0
6	SO4	B	824	5/5	0.94	0.27	-	26,29,36,38	0
2	NAG	A	1309	14/15	0.87	0.16	-	23,33,42,43	0
2	NAG	C	1434	14/15	0.68	0.33	-	51,64,68,71	0
2	NAG	B	1309	14/15	0.40	0.44	-	67,75,77,79	0
6	SO4	C	831	5/5	-	-	-	7,39,48,50	5
6	SO4	A	814	5/5	0.84	0.37	-	26,31,45,47	0
4	CU	D	801	1/1	0.99	0.03	-	17,17,17,17	0
6	SO4	A	811	5/5	-	-	-	10,36,47,52	5
6	SO4	B	821	5/5	-	-	-	7,34,44,51	5
6	SO4	D	841	5/5	-	-	-	14,37,52,58	5
2	NAG	D	1191	14/15	0.90	0.17	-	23,28,34,39	0
4	CU	C	801	1/1	0.99	0.02	-	16,16,16,16	0
2	NAG	C	1191	14/15	0.94	0.10	-	12,19,23,25	0
6	SO4	C	834	5/5	0.91	0.24	-	24,27,35,37	0
2	NAG	A	1191	14/15	0.89	0.15	-	23,27,37,37	0
4	CU	A	801	1/1	0.99	0.02	-	16,16,16,16	0
6	SO4	C	833	5/5	0.93	0.23	-	23,38,42,42	0
2	NAG	B	1191	14/15	0.92	0.12	-	15,25,30,41	0
2	NAG	A	1434	14/15	0.64	0.34	-	51,62,70,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.