



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:34 AM UTC

PDB ID : 8RUF / pdb_00008ruf
Title : Crystal structure of Rhizobium etli L-asparaginase ReAV D187A mutant
Authors : Pokrywka, K.; Grzechowiak, M.; Sliwiak, J.; Worsztynowicz, P.; Loch, J.I.;
Ruszkowski, M.; Gilski, M.; Jaskolski, M.
Deposited on : 2024-01-30
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

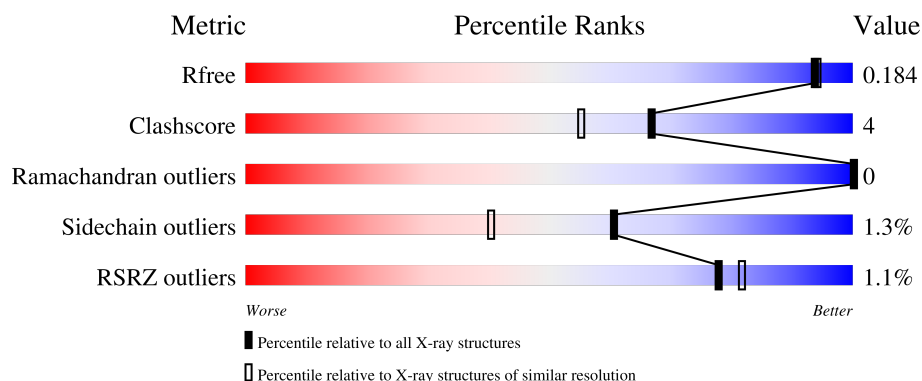
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	88% 5% 6%
1	B	373	86% 8% 6%
1	C	373	2% 89% • 6%
1	D	373	86% 7% • 6%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 12462 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 L-asparaginase II protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	19	0
			2683	1665	490	505	23			
1	B	349	Total	C	N	O	S	0	22	0
			2694	1678	489	504	23			
1	C	350	Total	C	N	O	S	0	20	0
			2687	1670	489	505	23			
1	D	350	Total	C	N	O	S	0	20	0
			2692	1675	488	506	23			

There are 28 discrepancies between the modelled and reference sequences:

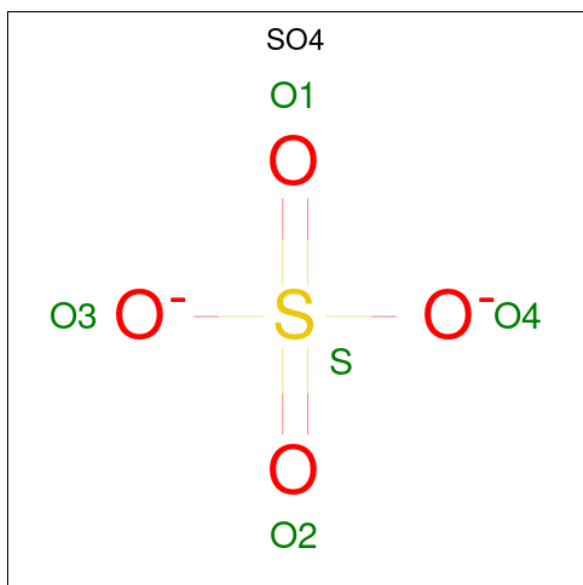
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q2K0Z2
A	-4	ILE	-	expression tag	UNP Q2K0Z2
A	-3	ASP	-	expression tag	UNP Q2K0Z2
A	-2	PRO	-	expression tag	UNP Q2K0Z2
A	-1	PHE	-	expression tag	UNP Q2K0Z2
A	0	THR	-	expression tag	UNP Q2K0Z2
A	187	ALA	ASP	engineered mutation	UNP Q2K0Z2
B	-5	GLY	-	expression tag	UNP Q2K0Z2
B	-4	ILE	-	expression tag	UNP Q2K0Z2
B	-3	ASP	-	expression tag	UNP Q2K0Z2
B	-2	PRO	-	expression tag	UNP Q2K0Z2
B	-1	PHE	-	expression tag	UNP Q2K0Z2
B	0	THR	-	expression tag	UNP Q2K0Z2
B	187	ALA	ASP	engineered mutation	UNP Q2K0Z2
C	-5	GLY	-	expression tag	UNP Q2K0Z2
C	-4	ILE	-	expression tag	UNP Q2K0Z2
C	-3	ASP	-	expression tag	UNP Q2K0Z2
C	-2	PRO	-	expression tag	UNP Q2K0Z2
C	-1	PHE	-	expression tag	UNP Q2K0Z2
C	0	THR	-	expression tag	UNP Q2K0Z2
C	187	ALA	ASP	engineered mutation	UNP Q2K0Z2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	GLY	-	expression tag	UNP Q2K0Z2
D	-4	ILE	-	expression tag	UNP Q2K0Z2
D	-3	ASP	-	expression tag	UNP Q2K0Z2
D	-2	PRO	-	expression tag	UNP Q2K0Z2
D	-1	PHE	-	expression tag	UNP Q2K0Z2
D	0	THR	-	expression tag	UNP Q2K0Z2
D	187	ALA	ASP	engineered mutation	UNP Q2K0Z2

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

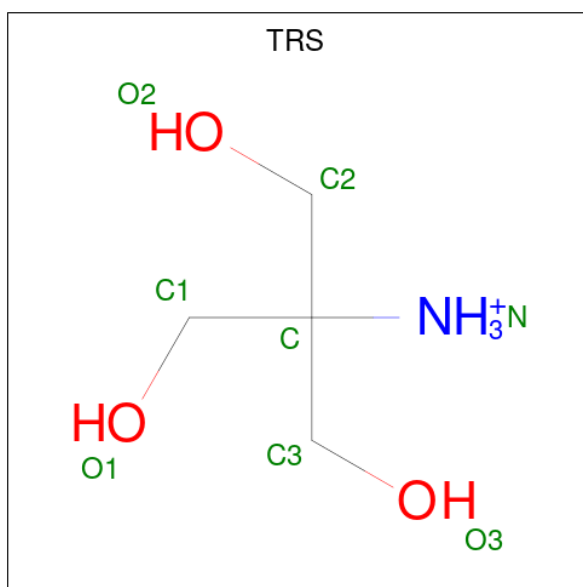
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Cl 1 1	0	0
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



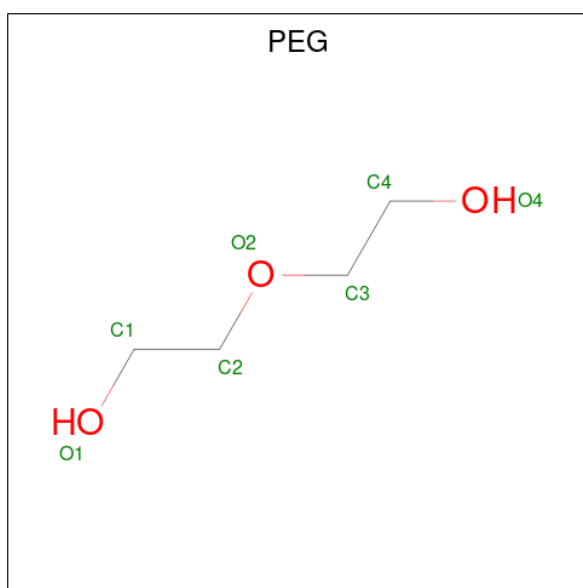
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			8	4	1	3		
7	D	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 8 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			7	4	3		
8	D	1	Total	C	O	0	0
			7	4	3		

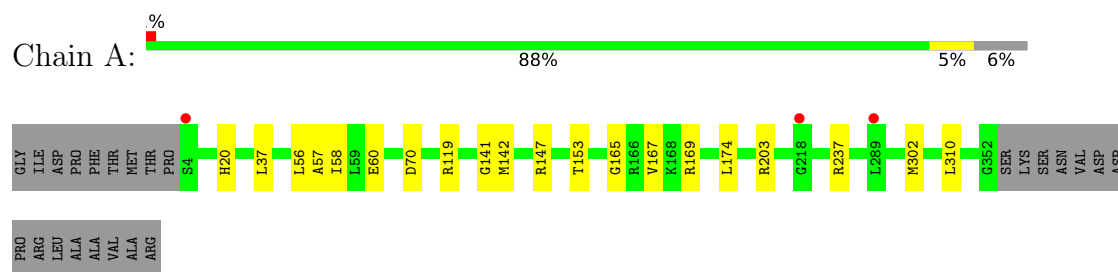
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	366	Total 366	O 366	0	0
9	B	390	Total 390	O 390	0	0
9	C	379	Total 379	O 379	0	0
9	D	399	Total 399	O 399	0	0

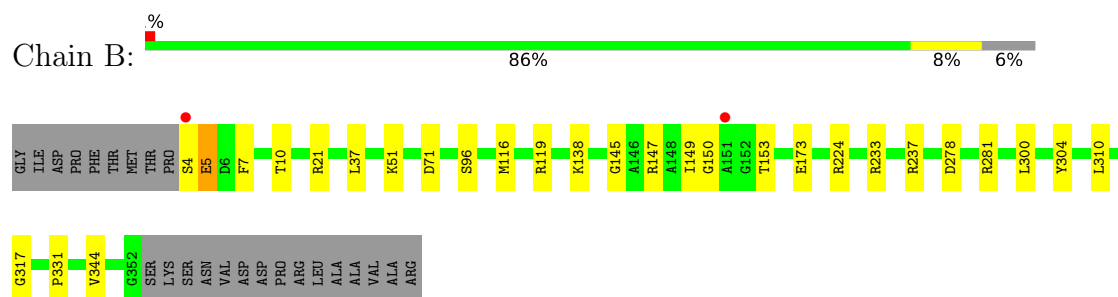
3 Residue-property plots [i](#)

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

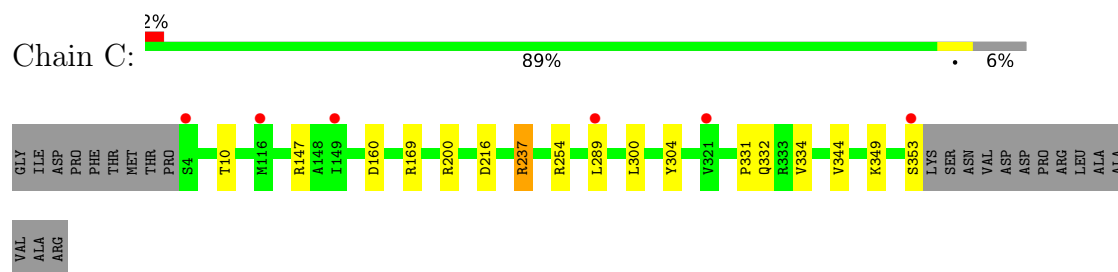
- Molecule 1: L-asparaginase II protein



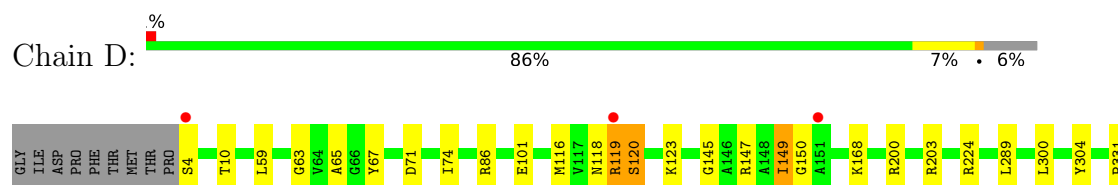
- Molecule 1: L-asparaginase II protein



- Molecule 1: L-asparaginase II protein



- Molecule 1: L-asparaginase II protein



V344	S353	LYS
		SER
		ASN
		VAL
		ASP
		ASP
		PRO
		ARG
		LEU
		ALA
		ALA
		VAL
		ALA
		ARG

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.72Å 91.26Å 114.20Å 90.00° 96.95° 90.00°	Depositor
Resolution (Å)	48.57 – 1.60 48.57 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.57-1.60) 100.0 (48.57-1.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.57 (at 1.60Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.158 , 0.184 0.158 , 0.184	Depositor DCC
R_{free} test set	2090 reflections (1.00%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtrriage
Anisotropy	0.468	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	12462	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.34 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.2218e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: TRS, GOL, SO4, EDO, CL, ZN, PEG

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	0.42	0/2785	0.59	0/3759
1	B	0.46	0/2804	0.61	0/3783
1	C	0.42	0/2792	0.60	0/3768
1	D	0.45	0/2796	0.64	0/3772
All	All	0.44	0/11177	0.61	0/15082

There are no bond length outliers.

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	2683	0	2699	18	0
1	B	2694	0	2737	21	0
1	C	2687	0	2715	12	0
1	D	2692	0	2725	28	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	20	0	30	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	20	0	30	4	0
3	C	16	0	24	3	0
3	D	28	0	42	6	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	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	6	0	8	3	0
6	B	12	0	16	2	0
6	C	6	0	8	1	0
6	D	6	0	8	2	0
7	B	8	0	12	2	0
7	D	8	0	12	3	0
8	D	14	0	20	5	0
9	A	366	0	0	2	0
9	B	390	0	0	3	0
9	C	379	0	0	4	0
9	D	399	0	0	1	0
All	All	12462	0	11086	81	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 4.

All (81) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:GLY:H	8:D:411:PEG:H31	1.19	1.02
1:D:71:ASP:HB2	7:D:409:TRS:H31	1.52	0.90
1:A:237:ARG:HH12	3:A:407:EDO:H22	1.37	0.88
1:D:200:ARG:HH12	8:D:406:PEG:H21	1.43	0.84
1:B:96[A]:SER:OG	1:D:101[A]:GLU:OE1	1.97	0.82
1:C:331:PRO:HD2	1:C:344[B]:VAL:HG21	1.66	0.78
1:B:173:GLU:HB3	7:B:409:TRS:H22	1.68	0.75
1:A:237:ARG:NH1	3:A:407:EDO:H22	2.02	0.73
1:B:71:ASP:HB2	6:B:406:GOL:H11	1.69	0.72
1:D:63:GLY:N	8:D:411:PEG:H31	2.01	0.72
1:B:5:GLU:HG3	1:B:7:PHE:HE1	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:ARG:HH22	3:D:413:EDO:H22	1.56	0.68
1:A:203:ARG:HH22	6:A:409:GOL:H2	1.59	0.67
1:D:71:ASP:H	7:D:409:TRS:H32	1.60	0.66
1:D:331:PRO:HD2	1:D:344[B]:VAL:HG21	1.77	0.66
1:B:153:THR:HG23	3:B:403:EDO:H12	1.80	0.62
1:C:147:ARG:HH21	3:C:402:EDO:H22	1.66	0.60
1:D:10:THR:HG22	1:D:344[B]:VAL:HG12	1.84	0.60
1:B:147:ARG:HE	3:B:403:EDO:H11	1.67	0.59
1:C:200:ARG:HH12	6:C:405:GOL:H11	1.67	0.59
1:D:10:THR:HG22	1:D:344[A]:VAL:HG22	1.85	0.59
1:A:174:LEU:HD23	3:A:403:EDO:H11	1.83	0.59
1:A:60[B]:GLU:HG3	9:A:524:HOH:O	2.02	0.58
1:D:145:GLY:O	1:D:149[B]:ILE:HG23	2.04	0.58
1:C:349:LYS:NZ	9:C:506:HOH:O	2.34	0.56
1:B:10:THR:HG22	1:B:344[B]:VAL:HG22	1.87	0.56
1:A:147:ARG:HH21	3:A:406:EDO:H11	1.71	0.55
1:B:278[A]:ASP:OD1	1:B:281:ARG:NH2	2.39	0.55
1:C:10:THR:HG22	1:C:344[B]:VAL:HG12	1.88	0.55
1:C:237:ARG:NH2	3:C:408:EDO:H12	2.21	0.55
1:A:203:ARG:HH22	6:A:409:GOL:C2	2.20	0.54
1:D:224:ARG:HH11	6:D:410:GOL:H32	1.75	0.52
1:D:147[B]:ARG:HH12	3:D:405:EDO:H11	1.74	0.52
3:D:404:EDO:H11	9:D:577:HOH:O	2.09	0.52
1:D:203:ARG:HH12	8:D:406:PEG:H31	1.75	0.51
1:B:317:GLY:HA2	3:B:407:EDO:H12	1.93	0.50
6:A:409:GOL:O3	6:A:409:GOL:O1	2.28	0.50
1:D:120:SER:HA	1:D:123[B]:LYS:HE2	1.93	0.50
1:D:147[B]:ARG:NH1	3:D:405:EDO:H11	2.27	0.50
1:C:169[A]:ARG:HD3	9:C:786:HOH:O	2.11	0.49
1:D:67:TYR:OH	1:D:147[B]:ARG:HG2	2.12	0.49
1:B:300[B]:LEU:HD11	1:B:304:TYR:CZ	2.48	0.48
1:D:149[B]:ILE:HG13	1:D:150:GLY:N	2.29	0.48
1:A:142[B]:MET:HE2	1:A:167:VAL:HG21	1.97	0.47
1:D:86:ARG:HH22	3:D:413:EDO:C2	2.23	0.47
1:D:147[A]:ARG:HE	3:D:405:EDO:H11	1.80	0.47
1:D:65:ALA:HB3	8:D:411:PEG:H32	1.97	0.47
1:D:116:MET:HA	1:D:116:MET:HE2	1.97	0.47
1:A:37:LEU:HD11	1:A:310[B]:LEU:HD21	1.97	0.46
6:B:406:GOL:H2	9:B:650:HOH:O	2.16	0.46
1:B:37:LEU:HD11	1:B:310[B]:LEU:HD21	1.99	0.45
1:D:224:ARG:HH11	6:D:410:GOL:C3	2.28	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ARG:HH11	7:B:409:TRS:C3	2.29	0.45
1:C:237:ARG:NH1	9:C:521:HOH:O	2.48	0.45
1:B:21:ARG:HD2	9:B:792:HOH:O	2.16	0.45
1:A:56:LEU:O	1:A:60[B]:GLU:HG2	2.17	0.45
1:A:119:ARG:NH1	9:A:520:HOH:O	2.50	0.44
1:D:59:LEU:HD21	1:D:74[B]:ILE:HD12	2.00	0.44
1:C:147:ARG:HH21	3:C:402:EDO:C2	2.29	0.44
1:A:70:ASP:HB2	3:A:407:EDO:H11	2.00	0.44
1:B:116:MET:HA	1:B:116:MET:HE2	2.00	0.43
1:C:254:ARG:HD2	9:C:553:HOH:O	2.19	0.43
1:D:300[B]:LEU:HD11	1:D:304:TYR:CZ	2.54	0.43
1:D:118:ASN:HD22	1:D:119:ARG:NH2	2.17	0.43
1:B:237:ARG:HG3	9:B:780:HOH:O	2.18	0.42
1:A:58:ILE:HD13	1:A:141:GLY:HA3	2.00	0.42
1:B:149[B]:ILE:HG13	1:B:150:GLY:N	2.34	0.42
1:C:332[B]:GLN:HG3	1:C:334:VAL:HG23	2.01	0.42
1:B:147:ARG:HH21	3:B:403:EDO:H11	1.83	0.42
1:B:145:GLY:O	1:B:149[B]:ILE:HG23	2.19	0.42
1:D:71:ASP:N	7:D:409:TRS:H32	2.32	0.42
1:A:20:HIS:CD2	1:A:302:MET:HG3	2.55	0.41
1:B:51:LYS:HE2	1:B:138:LYS:HE2	2.03	0.41
1:B:116:MET:HE1	1:B:119:ARG:HE	1.85	0.41
1:A:153:THR:H	3:A:406:EDO:H12	1.85	0.41
1:D:118:ASN:HD22	1:D:119:ARG:HH21	1.67	0.41
1:A:165:GLY:O	1:A:169[A]:ARG:HG3	2.20	0.41
1:B:331:PRO:HD2	1:B:344[A]:VAL:HG11	2.02	0.41
1:A:57:ALA:HA	1:A:60[B]:GLU:HG2	2.03	0.40
1:A:147:ARG:HE	3:A:406:EDO:H11	1.85	0.40
1:C:300[B]:LEU:HD11	1:C:304:TYR:CZ	2.57	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	366/373 (98%)	356 (97%)	10 (3%)	0	100	100
1	B	369/373 (99%)	360 (98%)	9 (2%)	0	100	100
1	C	368/373 (99%)	358 (97%)	10 (3%)	0	100	100
1	D	368/373 (99%)	359 (98%)	9 (2%)	0	100	100
All	All	1471/1492 (99%)	1433 (97%)	38 (3%)	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	281/282 (100%)	281 (100%)	0	100	100
1	B	284/282 (101%)	280 (99%)	4 (1%)	59	38
1	C	283/282 (100%)	278 (98%)	5 (2%)	51	28
1	D	283/282 (100%)	275 (97%)	8 (3%)	38	15
All	All	1131/1128 (100%)	1114 (98%)	17 (2%)	61	35

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	SER
1	B	5	GLU
1	B	233[A]	ARG
1	B	233[B]	ARG
1	C	160	ASP
1	C	216	ASP
1	C	237	ARG
1	C	289	LEU
1	C	353	SER
1	D	4	SER
1	D	119	ARG
1	D	120	SER
1	D	149[A]	ILE

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Mol	Chain	Res	Type
1	D	149[B]	ILE
1	D	168[A]	LYS
1	D	168[B]	LYS
1	D	289	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	ASN
1	B	124	GLN
1	B	221	GLN
1	B	324	GLN
1	C	134	ASN
1	D	118	ASN
1	D	124	GLN
1	D	324	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 8 are monoatomic - leaving 34 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	EDO	B	411	-	3,3,3	0.38	0	2,2,2	0.79	0
8	PEG	D	406	-	6,6,6	0.08	0	5,5,5	0.44	0
3	EDO	D	402	-	3,3,3	0.32	0	2,2,2	0.80	0
3	EDO	A	406	-	3,3,3	0.26	0	2,2,2	0.62	0
2	SO4	A	401	-	4,4,4	0.47	0	6,6,6	0.11	0
3	EDO	A	402	-	3,3,3	0.52	0	2,2,2	0.34	0
3	EDO	B	403	-	3,3,3	0.42	0	2,2,2	0.24	0
3	EDO	C	406	-	3,3,3	0.47	0	2,2,2	0.21	0
7	TRS	B	409	-	7,7,7	0.31	0	9,9,9	1.02	0
3	EDO	D	407	-	3,3,3	0.56	0	2,2,2	0.58	0
6	GOL	B	410	-	5,5,5	0.88	0	5,5,5	1.02	0
6	GOL	B	406	-	5,5,5	0.82	0	5,5,5	1.06	0
3	EDO	A	408	-	3,3,3	0.33	0	2,2,2	0.80	0
3	EDO	A	403	-	3,3,3	0.40	0	2,2,2	0.48	0
3	EDO	D	413	-	3,3,3	0.57	0	2,2,2	0.21	0
7	TRS	D	409	-	7,7,7	0.58	0	9,9,9	1.18	0
2	SO4	B	401	-	4,4,4	0.49	0	6,6,6	0.07	0
3	EDO	C	402	-	3,3,3	0.36	0	2,2,2	0.62	0
3	EDO	D	405	-	3,3,3	0.39	0	2,2,2	0.37	0
3	EDO	C	408	-	3,3,3	0.58	0	2,2,2	0.18	0
6	GOL	D	410	-	5,5,5	0.43	0	5,5,5	1.30	1 (20%)
3	EDO	B	402	-	3,3,3	0.54	0	2,2,2	0.12	0
6	GOL	A	409	-	5,5,5	0.80	0	5,5,5	1.34	0
3	EDO	D	404	-	3,3,3	0.48	0	2,2,2	0.23	0
3	EDO	A	407	-	3,3,3	0.62	0	2,2,2	0.36	0
3	EDO	B	408	-	3,3,3	0.56	0	2,2,2	0.43	0
3	EDO	C	407	-	3,3,3	0.42	0	2,2,2	0.61	0
8	PEG	D	411	-	6,6,6	0.10	0	5,5,5	0.19	0
6	GOL	C	405	-	5,5,5	1.18	1 (20%)	5,5,5	0.97	0
3	EDO	D	412	-	3,3,3	0.48	0	2,2,2	0.39	0
3	EDO	D	403	-	3,3,3	0.42	0	2,2,2	0.31	0
2	SO4	C	401	-	4,4,4	0.48	0	6,6,6	0.16	0
3	EDO	B	407	-	3,3,3	0.56	0	2,2,2	0.18	0
2	SO4	D	401	-	4,4,4	0.49	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
3	EDO	B	411	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	PEG	D	406	-	-	2/4/4/4	-
3	EDO	D	402	-	-	1/1/1/1	-
3	EDO	A	406	-	-	1/1/1/1	-
3	EDO	A	402	-	-	1/1/1/1	-
3	EDO	B	403	-	-	0/1/1/1	-
3	EDO	C	406	-	-	0/1/1/1	-
7	TRS	B	409	-	-	9/9/9/9	-
3	EDO	D	407	-	-	1/1/1/1	-
6	GOL	B	410	-	-	0/4/4/4	-
6	GOL	B	406	-	-	2/4/4/4	-
3	EDO	A	408	-	-	1/1/1/1	-
3	EDO	A	403	-	-	1/1/1/1	-
3	EDO	D	413	-	-	1/1/1/1	-
7	TRS	D	409	-	-	6/9/9/9	-
3	EDO	C	402	-	-	0/1/1/1	-
3	EDO	D	405	-	-	1/1/1/1	-
3	EDO	C	408	-	-	0/1/1/1	-
6	GOL	D	410	-	-	3/4/4/4	-
3	EDO	B	402	-	-	0/1/1/1	-
6	GOL	A	409	-	-	1/4/4/4	-
3	EDO	D	404	-	-	1/1/1/1	-
3	EDO	A	407	-	-	0/1/1/1	-
3	EDO	B	408	-	-	1/1/1/1	-
3	EDO	C	407	-	-	1/1/1/1	-
8	PEG	D	411	-	-	1/4/4/4	-
6	GOL	C	405	-	-	3/4/4/4	-
3	EDO	D	412	-	-	0/1/1/1	-
3	EDO	D	403	-	-	0/1/1/1	-
3	EDO	B	407	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	405	GOL	C1-C2	2.16	1.60	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	410	GOL	C3-C2-C1	-2.20	103.74	111.80

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	406	GOL	O1-C1-C2-C3
6	C	405	GOL	C1-C2-C3-O3
6	D	410	GOL	C1-C2-C3-O3
7	B	409	TRS	C2-C-C1-O1
7	B	409	TRS	N-C-C3-O3
7	D	409	TRS	C2-C-C1-O1
7	D	409	TRS	C3-C-C1-O1
7	D	409	TRS	N-C-C1-O1
6	D	410	GOL	O2-C2-C3-O3
8	D	406	PEG	O1-C1-C2-O2
6	B	406	GOL	O1-C1-C2-O2
7	B	409	TRS	C1-C-C3-O3
3	A	402	EDO	O1-C1-C2-O2
3	C	407	EDO	O1-C1-C2-O2
3	D	413	EDO	O1-C1-C2-O2
6	C	405	GOL	O2-C2-C3-O3
3	A	406	EDO	O1-C1-C2-O2
7	B	409	TRS	C3-C-C1-O1
7	B	409	TRS	N-C-C1-O1
7	B	409	TRS	C2-C-C3-O3
7	D	409	TRS	C1-C-C3-O3
7	D	409	TRS	N-C-C3-O3
3	A	403	EDO	O1-C1-C2-O2
8	D	411	PEG	C1-C2-O2-C3
8	D	406	PEG	O2-C3-C4-O4
7	D	409	TRS	C2-C-C3-O3
6	C	405	GOL	O1-C1-C2-C3
3	D	405	EDO	O1-C1-C2-O2
6	A	409	GOL	O2-C2-C3-O3
3	B	408	EDO	O1-C1-C2-O2
3	D	402	EDO	O1-C1-C2-O2
3	D	407	EDO	O1-C1-C2-O2
7	B	409	TRS	C1-C-C2-O2
7	B	409	TRS	C3-C-C2-O2
3	D	404	EDO	O1-C1-C2-O2
3	A	408	EDO	O1-C1-C2-O2
7	B	409	TRS	N-C-C2-O2
6	D	410	GOL	O1-C1-C2-O2

There are no ring outliers.

18 monomers are involved in 38 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	406	PEG	2	0
3	A	406	EDO	3	0
3	B	403	EDO	3	0
7	B	409	TRS	2	0
6	B	406	GOL	2	0
3	A	403	EDO	1	0
3	D	413	EDO	2	0
7	D	409	TRS	3	0
3	C	402	EDO	2	0
3	D	405	EDO	3	0
3	C	408	EDO	1	0
6	D	410	GOL	2	0
6	A	409	GOL	3	0
3	D	404	EDO	1	0
3	A	407	EDO	3	0
8	D	411	PEG	3	0
6	C	405	GOL	1	0
3	B	407	EDO	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	349/373 (93%)	-0.27	3 (0%) 81 84	11, 22, 43, 60	19 (5%)
1	B	349/373 (93%)	-0.47	2 (0%) 85 88	9, 18, 35, 54	22 (6%)
1	C	350/373 (93%)	-0.31	6 (1%) 69 72	11, 21, 40, 68	20 (5%)
1	D	350/373 (93%)	-0.46	4 (1%) 78 82	10, 18, 33, 60	20 (5%)
All	All	1398/1492 (93%)	-0.38	15 (1%) 78 82	9, 20, 38, 68	81 (5%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	353	SER	4.4
1	C	4	SER	3.2
1	B	151	ALA	2.8
1	D	119	ARG	2.8
1	A	4	SER	2.8
1	C	289	LEU	2.6
1	D	353	SER	2.6
1	C	116[A]	MET	2.5
1	D	151	ALA	2.5
1	C	149	ILE	2.3
1	A	218	GLY	2.3
1	B	4	SER	2.3
1	D	4	SER	2.2
1	A	289	LEU	2.1
1	C	321	VAL	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	A	406	4/4	0.73	0.20	35,37,40,53	0
6	GOL	A	409	6/6	0.73	0.16	36,43,46,51	6
3	EDO	B	403	4/4	0.76	0.14	42,49,50,55	0
3	EDO	C	407	4/4	0.77	0.18	42,42,53,54	0
3	EDO	D	412	4/4	0.78	0.14	44,48,50,54	0
6	GOL	C	405	6/6	0.78	0.13	43,47,48,49	0
8	PEG	D	406	7/7	0.80	0.15	27,35,42,48	7
8	PEG	D	411	7/7	0.83	0.17	20,28,31,39	7
3	EDO	C	402	4/4	0.84	0.15	39,45,47,51	0
3	EDO	A	408	4/4	0.84	0.16	41,42,45,50	0
6	GOL	B	410	6/6	0.84	0.12	35,44,49,50	0
3	EDO	B	407	4/4	0.85	0.13	35,35,37,40	0
3	EDO	B	411	4/4	0.85	0.12	33,37,40,42	0
3	EDO	D	407	4/4	0.85	0.24	26,31,34,35	0
3	EDO	C	408	4/4	0.86	0.15	29,34,40,47	0
7	TRS	B	409	8/8	0.86	0.16	27,31,38,40	8
6	GOL	D	410	6/6	0.87	0.12	33,37,43,51	0
3	EDO	D	413	4/4	0.87	0.14	18,32,39,49	0
7	TRS	D	409	8/8	0.88	0.14	21,35,44,45	8
3	EDO	A	407	4/4	0.88	0.13	26,34,37,39	0
3	EDO	A	403	4/4	0.88	0.11	35,37,41,48	0
3	EDO	B	408	4/4	0.89	0.19	29,31,32,36	0
6	GOL	B	406	6/6	0.89	0.12	22,36,43,57	0
3	EDO	A	402	4/4	0.89	0.13	41,44,46,51	0
2	SO4	A	401	5/5	0.90	0.13	27,35,39,42	0
3	EDO	D	404	4/4	0.90	0.10	26,36,37,41	0
3	EDO	D	405	4/4	0.90	0.11	39,41,41,42	0
2	SO4	C	401	5/5	0.91	0.11	28,35,36,40	0
3	EDO	C	406	4/4	0.91	0.10	39,43,44,47	0
3	EDO	D	402	4/4	0.92	0.11	26,33,33,39	0
3	EDO	D	403	4/4	0.94	0.09	30,31,37,41	0
3	EDO	B	402	4/4	0.94	0.10	26,29,29,38	0

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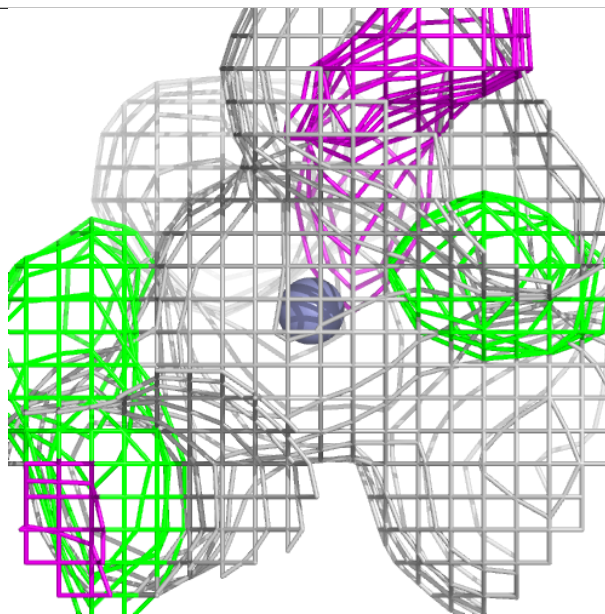
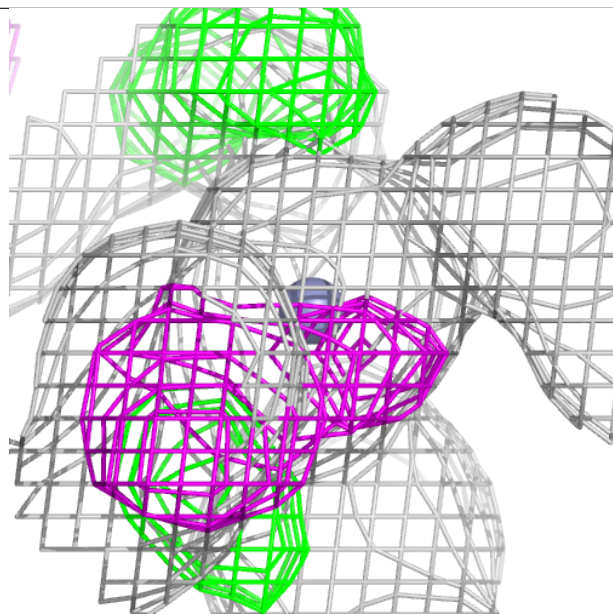
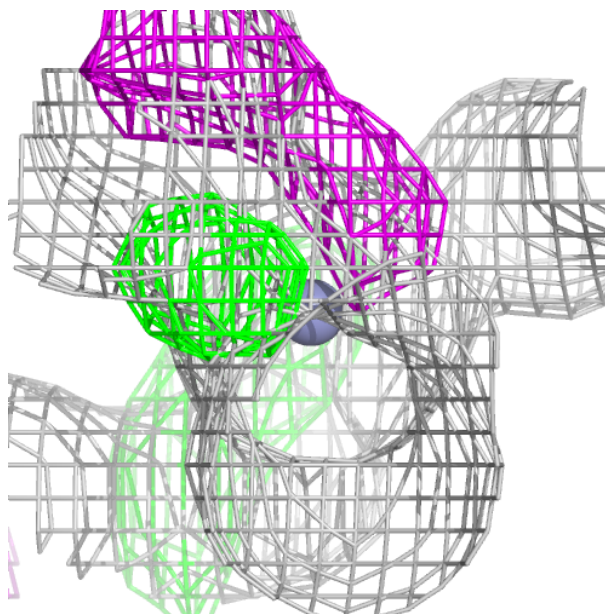
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	SO4	D	401	5/5	0.94	0.09	28,29,36,37	0
2	SO4	B	401	5/5	0.96	0.08	27,29,32,34	0
5	CL	C	404	1/1	0.97	0.06	35,35,35,35	0
5	CL	B	405	1/1	0.97	0.07	39,39,39,39	0
4	ZN	B	404	1/1	0.98	0.04	20,20,20,20	1
5	CL	A	405	1/1	0.98	0.06	36,36,36,36	0
5	CL	D	414	1/1	0.98	0.08	34,34,34,34	0
4	ZN	D	408	1/1	0.99	0.04	20,20,20,20	1
4	ZN	A	404	1/1	0.99	0.03	21,21,21,21	1
4	ZN	C	403	1/1	1.00	0.02	19,19,19,19	1

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

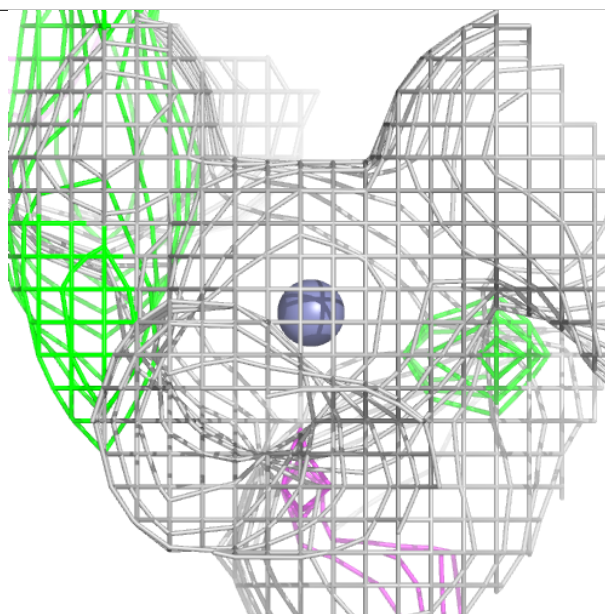
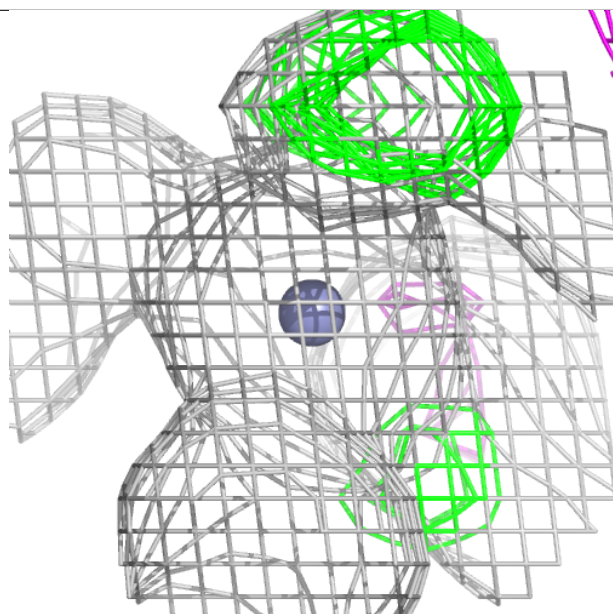
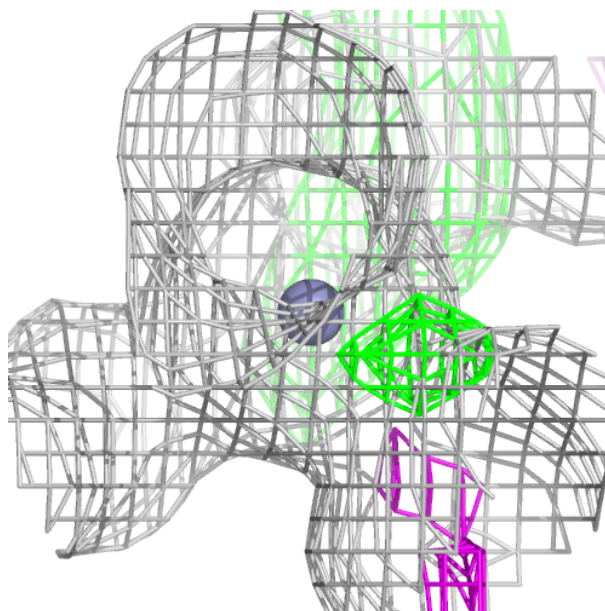
Electron density around ZN B 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



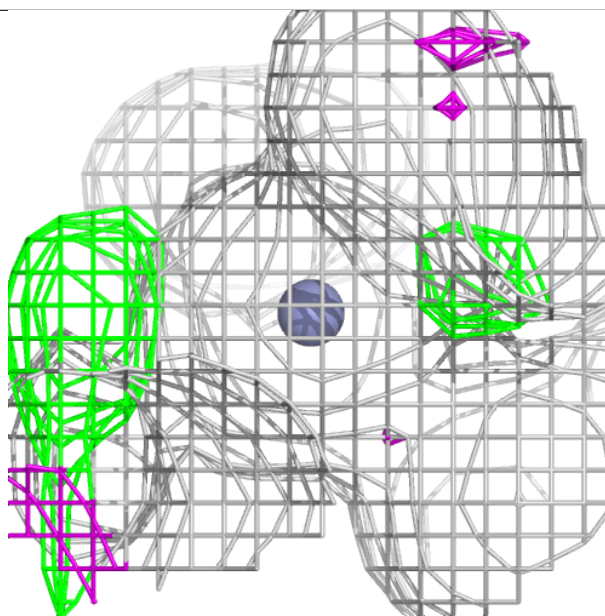
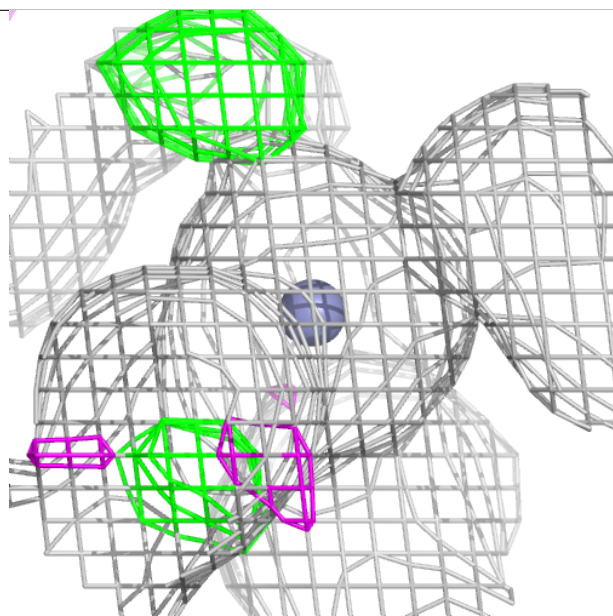
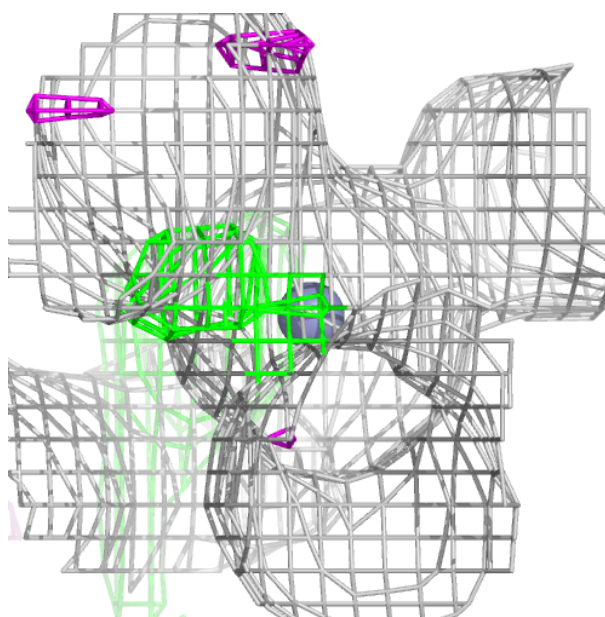
Electron density around ZN D 408:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



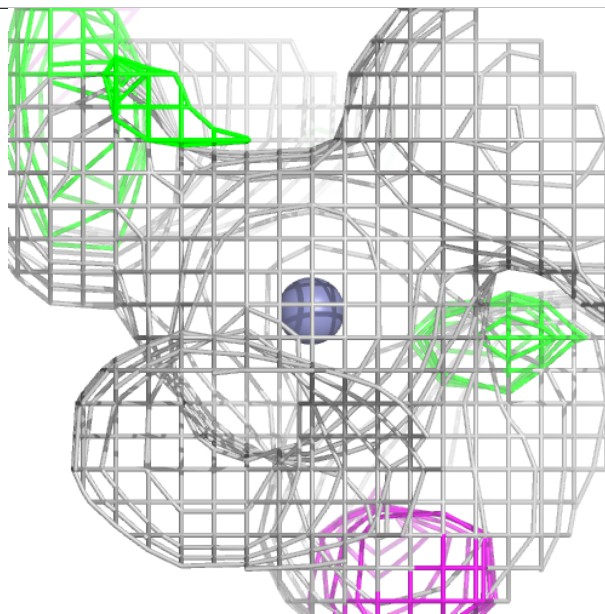
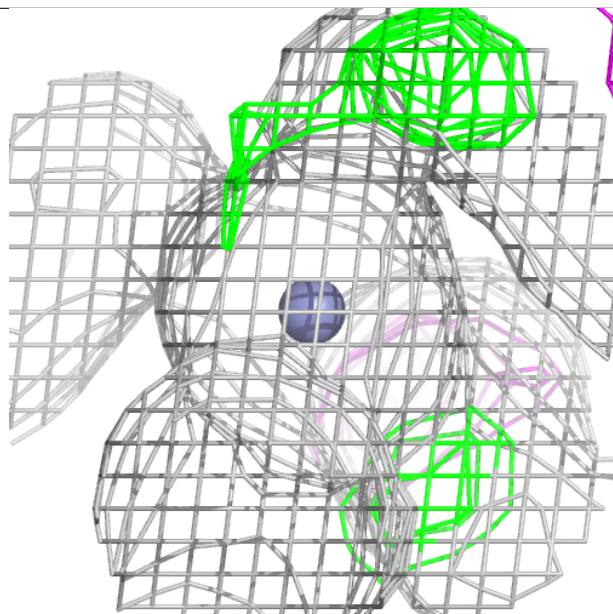
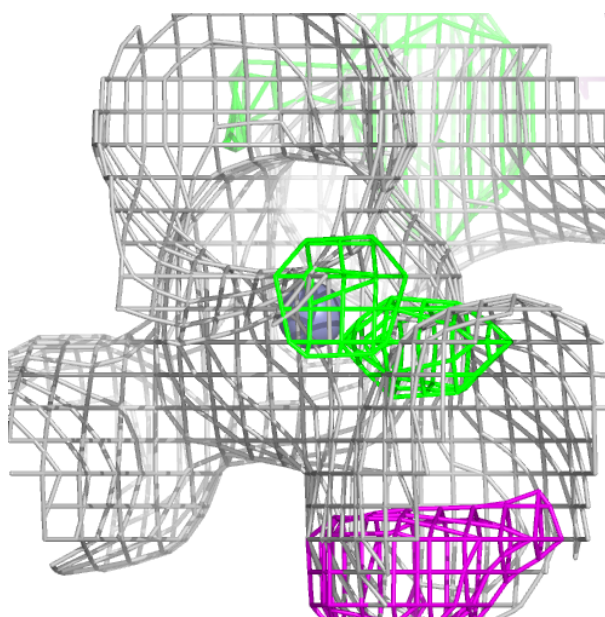
Electron density around ZN A 404:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN C 403:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.