



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:11 PM UTC

PDB ID : 9SKM / pdb_00009skm
Title : Biocatalytic Regioselective C-Formylation of Resorcinol Derivatives (CsATase C88S)
Authors : Gal, L.; Rohan, S.; Tittmann, K.; Kroutil, W.
Deposited on : 2025-09-02
Resolution : 1.87 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:

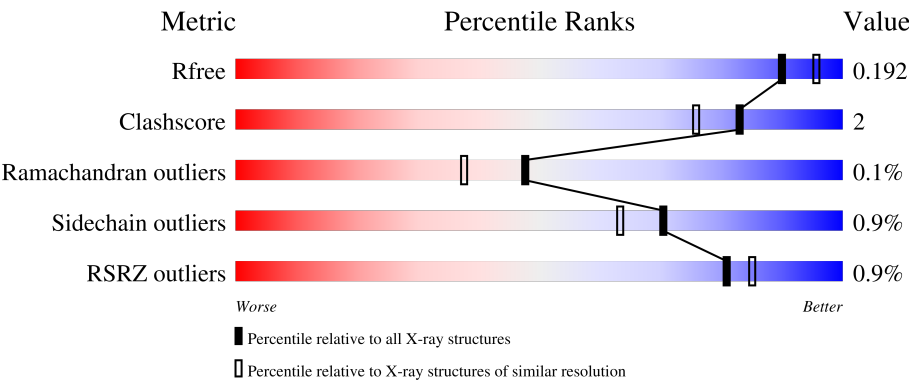
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.87 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	1220 (1.88-1.88)
Clashscore	190562	1234 (1.88-1.88)
Ramachandran outliers	187476	1222 (1.88-1.88)
Sidechain outliers	187428	1222 (1.88-1.88)
RSRZ outliers	180081	1220 (1.88-1.88)

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	360	<div><div></div><div>94%5%</div></div>
1	B	360	<div><div></div><div>92%8%</div></div>
1	C	360	<div><div></div><div>94%6%</div></div>
1	D	360	<div><div></div><div>96%..</div></div>
2	E	145	<div><div></div><div>94%...</div></div>

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Mol	Chain	Length	Quality of chain
2	F	145	
2	G	145	
2	H	145	
3	I	398	
3	J	398	
3	K	398	
3	L	398	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	B	403	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 56670 atoms, of which 26747 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 2,4-diacetylphloroglucinol biosynthesis protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	358	Total	C	H	N	O	S	0	1	0
			5305	1666	2640	457	531	11			
1	B	358	Total	C	H	N	O	S	0	0	0
			5296	1663	2636	456	530	11			
1	C	359	Total	C	H	N	O	S	0	1	0
			5337	1674	2660	461	531	11			
1	D	358	Total	C	H	N	O	S	0	1	0
			5302	1665	2639	456	531	11			

- Molecule 2 is a protein called 2,4-diacetylphloroglucinol biosynthesis protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	E	144	Total	C	H	N	O	S	0	0	0
			2299	722	1154	213	199	11			
2	F	144	Total	C	H	N	O	S	0	0	0
			2298	722	1153	213	199	11			
2	G	144	Total	C	H	N	O	S	0	1	0
			2316	727	1163	216	199	11			
2	H	144	Total	C	H	N	O	S	0	1	0
			2317	727	1164	216	199	11			

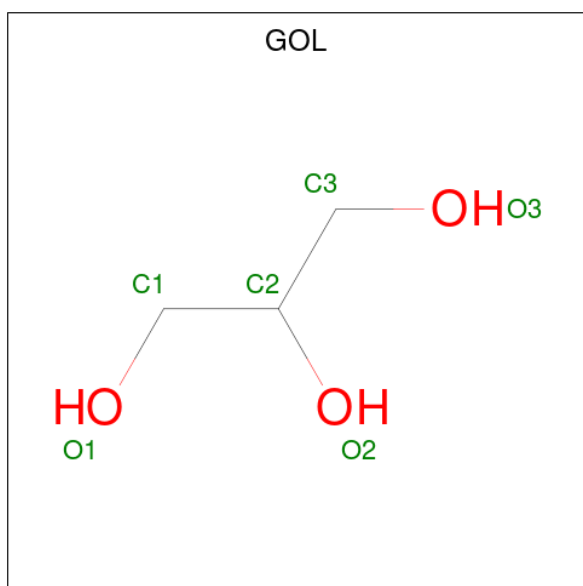
- Molecule 3 is a protein called 2,4-diacetylphloroglucinol biosynthesis protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	I	396	Total	C	H	N	O	S	0	0	0
			5837	1872	2853	517	576	19			
3	J	396	Total	C	H	N	O	S	0	0	0
			5837	1872	2853	517	576	19			
3	K	396	Total	C	H	N	O	S	0	0	0
			5837	1872	2853	517	576	19			
3	L	396	Total	C	H	N	O	S	0	1	0
			5856	1877	2864	520	576	19			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	88	SER	CYS	engineered mutation	UNP A0A1S1X4K0
I	168	VAL	ALA	conflict	UNP A0A1S1X4K0
J	88	SER	CYS	engineered mutation	UNP A0A1S1X4K0
J	168	VAL	ALA	conflict	UNP A0A1S1X4K0
K	88	SER	CYS	engineered mutation	UNP A0A1S1X4K0
K	168	VAL	ALA	conflict	UNP A0A1S1X4K0
L	88	SER	CYS	engineered mutation	UNP A0A1S1X4K0
L	168	VAL	ALA	conflict	UNP A0A1S1X4K0

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



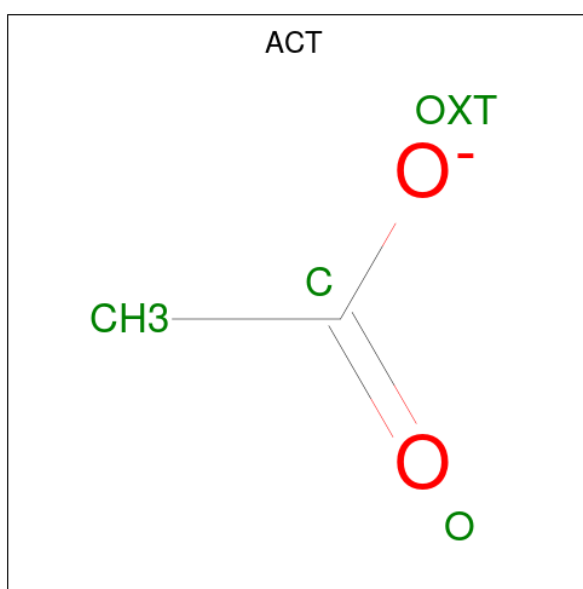
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			14	3	8	3		
4	B	1	Total	C	H	O	0	0
			14	3	8	3		
4	C	1	Total	C	H	O	0	0
			14	3	8	3		
4	D	1	Total	C	H	O	0	0
			14	3	8	3		
4	I	1	Total	C	H	O	0	0
			14	3	8	3		
4	J	1	Total	C	H	O	0	0
			14	3	8	3		
4	J	1	Total	C	H	O	0	0
			14	3	8	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	K	1	Total	C	H	O	0	0
			14	3	8	3		
4	L	1	Total	C	H	O	0	0
			14	3	8	3		
4	L	1	Total	C	H	O	0	0
			14	3	8	3		
4	L	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			7	2	3	2		
5	B	1	Total	C	H	O	0	0
			7	2	3	2		
5	B	1	Total	C	H	O	0	0
			7	2	3	2		
5	D	1	Total	C	H	O	0	0
			7	2	3	2		
5	D	1	Total	C	H	O	0	0
			7	2	3	2		
5	G	1	Total	C	H	O	0	0
			7	2	3	2		
5	H	1	Total	C	H	O	0	0
			7	2	3	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	1	Total	C	H	O	0	0
			7	2	3	2		
5	L	1	Total	C	H	O	0	0
			7	2	3	2		

- Molecule 6 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	E	1	Total	Zn	0	0
			1	1		
6	F	1	Total	Zn	0	0
			1	1		
6	G	1	Total	Zn	0	0
			1	1		
6	H	1	Total	Zn	0	0
			1	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	259	Total	O	0	0
			259	259		
7	B	250	Total	O	0	0
			250	250		
7	C	278	Total	O	0	0
			278	278		
7	D	254	Total	O	0	0
			254	254		
7	E	137	Total	O	0	0
			137	137		
7	F	134	Total	O	0	0
			134	134		
7	G	137	Total	O	0	0
			137	137		
7	H	139	Total	O	0	0
			139	139		
7	I	235	Total	O	0	0
			235	235		
7	J	272	Total	O	0	0
			272	272		
7	K	267	Total	O	0	0
			267	267		

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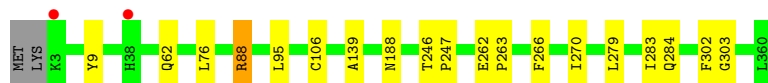
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	L	250	Total 250	O 250	0	0

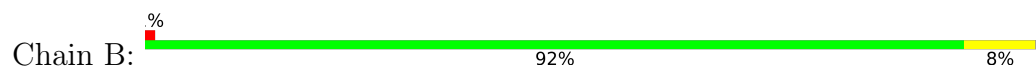
3 Residue-property plots [i](#)

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: 2,4-diacetylphloroglucinol biosynthesis protein



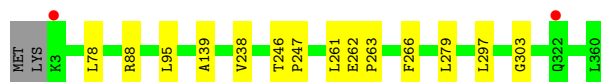
- Molecule 1: 2,4-diacetylphloroglucinol biosynthesis protein



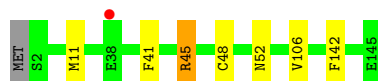
- Molecule 1: 2,4-diacetylphloroglucinol biosynthesis protein



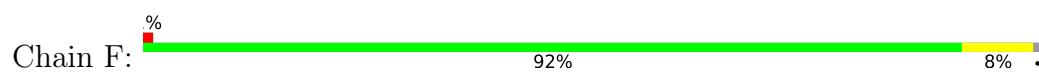
- Molecule 1: 2,4-diacetylphloroglucinol biosynthesis protein



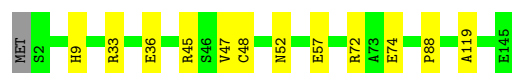
- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein



- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein



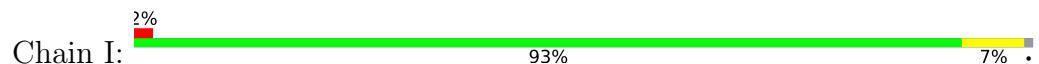
- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein



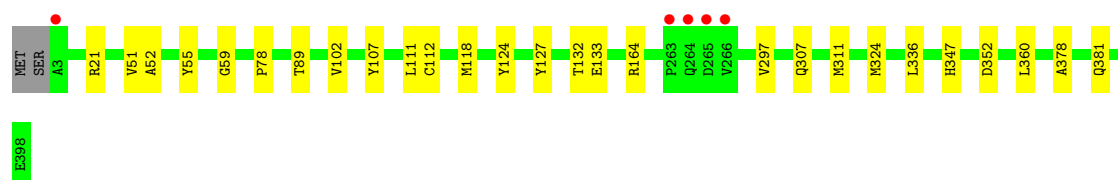
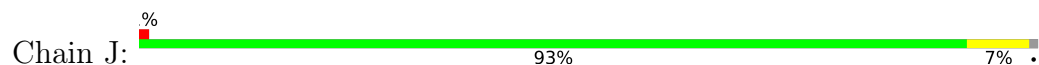
- Molecule 2: 2,4-diacetylphloroglucinol biosynthesis protein



- Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein



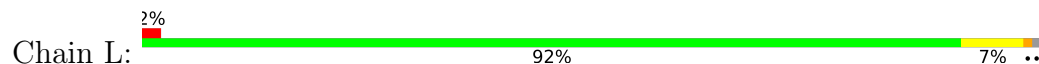
- Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein

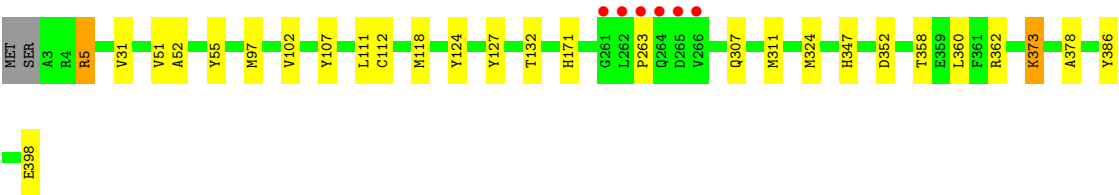


- Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein



- Molecule 3: 2,4-diacetylphloroglucinol biosynthesis protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.73Å 184.36Å 120.78Å 90.00° 103.66° 90.00°	Depositor
Resolution (Å)	64.92 – 1.87 64.92 – 1.87	Depositor EDS
% Data completeness (in resolution range)	97.4 (64.92-1.87) 97.9 (64.92-1.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.30 (at 1.87Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.165 , 0.193 0.165 , 0.192	Depositor DCC
R_{free} test set	16005 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	17.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	56670	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.09% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACT, GOL, ZN

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	0.36	0/2708	0.57	2/3673 (0.1%)
1	B	0.38	1/2700 (0.0%)	0.59	2/3662 (0.1%)
1	C	0.36	0/2720	0.57	2/3687 (0.1%)
1	D	0.36	1/2706 (0.0%)	0.58	2/3670 (0.1%)
2	E	0.36	0/1169	0.52	0/1570
2	F	0.35	0/1169	0.54	0/1570
2	G	0.38	0/1180	0.55	0/1584
2	H	0.34	0/1180	0.52	0/1584
3	I	0.33	0/3051	0.54	0/4128
3	J	0.34	0/3051	0.54	0/4128
3	K	0.33	0/3051	0.55	0/4128
3	L	0.34	0/3062	0.57	1/4142 (0.0%)
All	All	0.35	2/27747 (0.0%)	0.56	9/37526 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	I	0	1
3	J	0	1
3	K	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	70	SER	C-O	-6.26	1.21	1.23
1	D	78	LEU	C-N	5.13	1.36	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	303	GLY	CA-C-N	9.32	138.47	121.70
1	B	303	GLY	C-N-CA	9.32	138.47	121.70
1	C	303	GLY	CA-C-N	7.69	135.54	121.70
1	C	303	GLY	C-N-CA	7.69	135.54	121.70
1	D	303	GLY	CA-C-N	7.50	135.21	121.70
1	D	303	GLY	C-N-CA	7.50	135.21	121.70
1	A	303	GLY	CA-C-N	6.63	133.64	121.70
1	A	303	GLY	C-N-CA	6.63	133.64	121.70
3	L	386	TYR	CA-CB-CG	-5.29	104.38	113.90

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	133	GLU	Peptide
3	J	133	GLU	Peptide
3	K	133	GLU	Peptide

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	2665	2640	2647	10	0
1	B	2660	2636	2641	18	0
1	C	2677	2660	2667	13	0
1	D	2663	2639	2646	7	0
2	E	1145	1154	1156	4	0
2	F	1145	1153	1156	7	0
2	G	1153	1163	1169	8	0
2	H	1153	1164	1169	5	0
3	I	2984	2853	2871	16	0
3	J	2984	2853	2871	12	0
3	K	2984	2853	2871	15	0
3	L	2992	2864	2884	16	0
4	A	6	8	8	0	0
4	B	6	8	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	C	6	8	8	3	0
4	D	6	8	8	0	0
4	I	6	8	8	0	0
4	J	12	16	16	1	0
4	K	6	8	8	2	0
4	L	18	24	24	1	0
5	B	12	9	9	3	0
5	D	8	6	6	1	0
5	G	4	3	3	1	0
5	H	4	3	3	1	0
5	I	4	3	3	0	0
5	L	4	3	3	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	259	0	0	0	0
7	B	250	0	0	4	0
7	C	278	0	0	2	0
7	D	254	0	0	1	0
7	E	137	0	0	1	0
7	F	134	0	0	0	0
7	G	137	0	0	0	0
7	H	139	0	0	2	0
7	I	235	0	0	3	0
7	J	272	0	0	1	0
7	K	267	0	0	2	0
7	L	250	0	0	1	0
All	All	29923	26747	26863	128	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 (128) 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)
3:I:263:PRO:O	7:I:501:HOH:O	1.92	0.85
3:K:164:ARG:NH2	3:K:324:MET:HE1	2.00	0.77
2:G:33:ARG:NH2	2:G:57:GLU:OE2	2.19	0.76
1:B:178:THR:N	5:B:402:ACT:OXT	2.19	0.75
3:K:263:PRO:O	7:K:501:HOH:O	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:347:HIS:ND1	3:I:352:ASP:OD2	2.32	0.60
3:I:280:MET:HE1	3:J:78:PRO:HG2	1.84	0.58
3:L:5:ARG:NH2	3:L:398:GLU:O	2.35	0.58
1:C:248[A]:ARG:NH1	7:C:502:HOH:O	2.37	0.57
2:F:108:ASP:OD2	2:F:126:ARG:NH2	2.36	0.55
2:F:72:ARG:NH1	2:F:74:GLU:OE1	2.39	0.55
1:B:245:SER:HB2	5:B:403:ACT:H1	1.90	0.53
3:J:164:ARG:NH2	3:J:324:MET:HE1	2.24	0.53
1:C:111:PHE:CD2	1:C:114:LYS:HE3	2.44	0.53
2:E:11:MET:HE2	7:E:351:HOH:O	2.09	0.52
2:G:45:ARG:NE	2:G:47:VAL:O	2.39	0.52
1:A:95:LEU:C	1:A:95:LEU:HD23	2.37	0.50
3:K:333:GLN:HG3	7:K:676:HOH:O	2.10	0.50
1:A:88:ARG:HD2	1:B:189:ILE:HG22	1.94	0.49
3:J:118:MET:HB2	3:J:124:TYR:CG	2.47	0.49
2:E:41:PHE:CG	2:E:45:ARG:HD3	2.47	0.49
2:H:48:CYS:O	2:H:52:ASN:HA	2.12	0.49
3:L:307:GLN:O	3:L:311:MET:HG3	2.13	0.49
3:L:52:ALA:O	3:L:112:CYS:HA	2.12	0.49
3:K:263:PRO:HG2	3:K:270:LEU:HD21	1.95	0.49
1:D:246:THR:HB	1:D:247:PRO:HD3	1.95	0.48
1:B:111:PHE:CD2	1:B:114:LYS:HE3	2.48	0.48
1:C:99:GLY:HA2	4:C:401:GOL:C1	2.43	0.48
2:G:9:HIS:ND1	5:H:901:ACT:H1	2.29	0.48
2:F:48:CYS:O	2:F:52:ASN:HA	2.14	0.48
2:F:74:GLU:HB3	2:F:88:PRO:HB3	1.96	0.48
1:D:238:VAL:CG1	1:D:297:LEU:HD13	2.43	0.48
1:C:262:GLU:N	1:C:263:PRO:CD	2.77	0.47
2:G:47:VAL:HG23	3:L:31:VAL:HG11	1.95	0.47
1:A:266:PHE:CE1	1:A:270:ILE:HD11	2.49	0.47
1:C:99:GLY:C	4:C:401:GOL:H11	2.39	0.47
3:K:118:MET:HB2	3:K:124:TYR:CG	2.50	0.47
3:K:360:LEU:HD22	3:K:378:ALA:HB1	1.98	0.46
3:K:119:THR:HG22	4:K:401:GOL:H31	1.96	0.46
1:C:99:GLY:HA2	4:C:401:GOL:H11	1.98	0.46
3:J:52:ALA:O	3:J:112:CYS:HA	2.16	0.46
1:D:262:GLU:N	1:D:263:PRO:CD	2.78	0.45
2:F:11:MET:HE1	3:J:59:GLY:HA2	1.98	0.45
3:I:288:THR:OG1	3:I:290:LYS:HG2	2.17	0.45
1:B:62:GLN:HG2	7:B:725:HOH:O	2.16	0.45
3:J:51:VAL:HA	3:J:111:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:164:ARG:HH22	3:K:324:MET:HE1	1.76	0.45
3:L:171:HIS:CE1	3:L:324:MET:HE3	2.51	0.45
1:D:95:LEU:HD23	1:D:95:LEU:C	2.43	0.44
2:H:41:PHE:CG	2:H:45:ARG:HD3	2.52	0.44
3:J:297:VAL:HG22	3:J:336:LEU:HD21	1.99	0.44
1:B:95:LEU:C	1:B:95:LEU:HD23	2.43	0.44
3:I:250:THR:O	3:I:254:ASN:HB2	2.18	0.44
5:D:402:ACT:H3	7:D:673:HOH:O	2.17	0.44
3:L:118:MET:HB2	3:L:124:TYR:CG	2.53	0.44
2:G:72:ARG:HD3	2:G:74:GLU:CD	2.43	0.44
1:A:188:ASN:HB2	1:A:302:PHE:CG	2.53	0.43
1:B:343:ILE:HG23	1:B:348:LYS:HB2	2.00	0.43
3:L:358:THR:O	3:L:362:ARG:HG3	2.18	0.43
2:G:48:CYS:O	2:G:52:ASN:HA	2.18	0.43
3:I:259:TYR:CE1	3:I:280:MET:HE3	2.53	0.43
4:J:402:GOL:H11	7:J:706:HOH:O	2.18	0.43
3:K:51:VAL:HA	3:K:111:LEU:O	2.18	0.43
3:K:58:GLU:OE2	3:L:127:TYR:OH	2.18	0.43
3:K:119:THR:HG22	4:K:401:GOL:C3	2.49	0.43
1:B:258:ALA:O	1:B:262:GLU:HG3	2.18	0.43
1:A:9:TYR:CE1	1:A:283:ILE:HG23	2.54	0.43
1:A:266:PHE:HE1	1:A:270:ILE:HD11	1.83	0.43
3:I:89:THR:HG23	3:I:383:LEU:C	2.43	0.43
3:J:307:GLN:O	3:J:311:MET:HG3	2.17	0.43
2:H:74:GLU:HB3	2:H:88:PRO:HB3	2.00	0.43
3:I:251:ARG:O	3:I:266:VAL:HG22	2.18	0.43
3:K:52:ALA:O	3:K:112:CYS:HA	2.18	0.43
3:I:259:TYR:CD1	3:I:280:MET:HE3	2.54	0.42
3:I:266:VAL:HG21	7:I:680:HOH:O	2.18	0.42
3:J:297:VAL:HA	3:J:381:GLN:O	2.18	0.42
1:B:28:LYS:NZ	7:B:509:HOH:O	2.45	0.42
1:C:290:LYS:HD3	7:C:528:HOH:O	2.19	0.42
3:L:51:VAL:HA	3:L:111:LEU:O	2.19	0.42
1:A:246:THR:HB	1:A:247:PRO:HD3	2.00	0.42
3:K:102:VAL:HA	3:K:107:TYR:O	2.18	0.42
3:L:102:VAL:HA	3:L:107:TYR:O	2.19	0.42
2:F:41:PHE:CG	2:F:45:ARG:HD3	2.54	0.42
2:H:125:ILE:HD11	7:H:1022:HOH:O	2.19	0.42
3:K:171:HIS:CD2	3:K:324:MET:HE3	2.54	0.42
3:I:186:ALA:HB1	3:I:345:ARG:HA	2.01	0.42
1:C:31:ASP:OD2	1:C:33:ASP:HB3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:213:GLU:OE1	7:B:501:HOH:O	2.22	0.42
1:C:38:HIS:O	1:C:245:SER:HB3	2.20	0.42
1:D:139:ALA:CB	1:D:279:LEU:HD12	2.50	0.42
3:I:44:HIS:HE1	3:I:46:ARG:HG3	1.84	0.42
3:I:52:ALA:O	3:I:112:CYS:HA	2.20	0.41
3:I:209:LEU:C	3:I:209:LEU:HD12	2.45	0.41
1:A:139:ALA:CB	1:A:279:LEU:HD12	2.49	0.41
1:A:262:GLU:N	1:A:263:PRO:CD	2.83	0.41
3:L:373:LYS:NZ	7:L:507:HOH:O	2.48	0.41
1:B:139:ALA:CB	1:B:279:LEU:HD12	2.50	0.41
2:G:74:GLU:HB3	2:G:88:PRO:HB3	2.02	0.41
3:L:347:HIS:ND1	3:L:352:ASP:OD2	2.48	0.41
1:B:262:GLU:N	1:B:263:PRO:CD	2.84	0.41
2:H:86:ALA:HB3	7:H:1111:HOH:O	2.20	0.41
3:I:339:ASP:OD2	3:I:345:ARG:HD3	2.21	0.41
3:L:360:LEU:HD22	3:L:378:ALA:HB1	2.02	0.41
3:I:262:LEU:HB3	7:I:501:HOH:O	2.21	0.41
1:C:188:ASN:HB2	1:C:302:PHE:CG	2.55	0.41
2:E:106:VAL:HA	2:E:142:PHE:O	2.20	0.41
3:J:360:LEU:HD22	3:J:378:ALA:HB1	2.01	0.41
1:B:266:PHE:CD1	1:B:266:PHE:C	2.99	0.41
3:J:347:HIS:ND1	3:J:352:ASP:OD2	2.48	0.41
1:B:175:ILE:HG12	1:B:311:LEU:CD1	2.51	0.41
1:B:188:ASN:HB2	1:B:302:PHE:CG	2.56	0.41
1:B:248:ARG:HH12	1:B:262:GLU:CD	2.29	0.41
1:C:297:LEU:C	1:C:297:LEU:HD23	2.45	0.41
2:E:48:CYS:O	2:E:52:ASN:HA	2.21	0.41
3:J:102:VAL:HA	3:J:107:TYR:O	2.21	0.41
3:K:97:MET:HE3	3:L:97:MET:HE3	2.02	0.41
5:B:403:ACT:H2	7:B:675:HOH:O	2.21	0.41
1:C:244:VAL:O	1:C:247:PRO:HD2	2.21	0.40
1:C:343:ILE:HG23	1:C:348:LYS:HB2	2.03	0.40
1:B:61:ALA:HB1	1:B:136:LEU:HD21	2.03	0.40
1:D:266:PHE:CD1	1:D:266:PHE:C	3.00	0.40
2:G:119:ALA:HA	5:G:201:ACT:H2	2.03	0.40
3:L:171:HIS:ND1	3:L:324:MET:HE3	2.37	0.40
1:A:76:LEU:O	1:A:106:CYS:HA	2.22	0.40
1:B:261:LEU:C	1:B:261:LEU:HD12	2.46	0.40
1:D:261:LEU:HD12	1:D:261:LEU:C	2.47	0.40
2:F:108:ASP:CG	2:F:126:ARG:HH22	2.27	0.40
3:L:124:TYR:HB3	4:L:402:GOL:H31	2.03	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	357/360 (99%)	346 (97%)	10 (3%)	1 (0%)	36	26
1	B	356/360 (99%)	346 (97%)	9 (2%)	1 (0%)	36	26
1	C	358/360 (99%)	347 (97%)	10 (3%)	1 (0%)	36	26
1	D	357/360 (99%)	346 (97%)	10 (3%)	1 (0%)	36	26
2	E	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
2	F	142/145 (98%)	138 (97%)	4 (3%)	0	100	100
2	G	143/145 (99%)	140 (98%)	3 (2%)	0	100	100
2	H	143/145 (99%)	139 (97%)	4 (3%)	0	100	100
3	I	394/398 (99%)	381 (97%)	13 (3%)	0	100	100
3	J	394/398 (99%)	377 (96%)	17 (4%)	0	100	100
3	K	394/398 (99%)	382 (97%)	12 (3%)	0	100	100
3	L	395/398 (99%)	379 (96%)	15 (4%)	1 (0%)	36	26
All	All	3575/3612 (99%)	3459 (97%)	111 (3%)	5 (0%)	48	37

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	88	ARG
1	B	88	ARG
1	D	88	ARG
1	C	88	ARG
3	L	263	PRO

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	278/279 (100%)	276 (99%)	2 (1%)	76	69
1	B	277/279 (99%)	277 (100%)	0	100	100
1	C	279/279 (100%)	277 (99%)	2 (1%)	76	69
1	D	278/279 (100%)	278 (100%)	0	100	100
2	E	120/121 (99%)	119 (99%)	1 (1%)	73	68
2	F	120/121 (99%)	119 (99%)	1 (1%)	73	68
2	G	121/121 (100%)	120 (99%)	1 (1%)	73	68
2	H	121/121 (100%)	121 (100%)	0	100	100
3	I	304/306 (99%)	300 (99%)	4 (1%)	61	50
3	J	304/306 (99%)	299 (98%)	5 (2%)	55	43
3	K	304/306 (99%)	299 (98%)	5 (2%)	55	43
3	L	305/306 (100%)	301 (99%)	4 (1%)	61	50
All	All	2811/2824 (100%)	2786 (99%)	25 (1%)	70	63

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	284	GLN
1	C	284	GLN
1	C	311	LEU
2	E	45	ARG
2	F	120	ARG
2	G	36	GLU
3	I	21	ARG
3	I	55	TYR
3	I	127	TYR
3	I	132	THR
3	J	21	ARG
3	J	55	TYR
3	J	89	THR

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Mol	Chain	Res	Type
3	J	127	TYR
3	J	132	THR
3	K	55	TYR
3	K	127	TYR
3	K	132	THR
3	K	187	THR
3	K	196	LEU
3	L	5	ARG
3	L	55	TYR
3	L	132	THR
3	L	373	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN
1	A	215	GLN
1	A	322	GLN
1	B	215	GLN
1	B	288	GLN
1	C	121	GLN
1	C	134	HIS
1	C	288	GLN
1	C	330	GLN
3	I	157	HIS
3	I	318	GLN
3	J	318	GLN
3	J	333	GLN
3	K	318	GLN
3	L	100	GLN
3	L	227	HIS
3	L	318	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 4 are monoatomic - leaving 20 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	$\# Z > 2$
5	ACT	I	402	-	3,3,3	1.36	0	3,3,3	1.39	0
5	ACT	L	403	-	3,3,3	1.34	0	3,3,3	1.47	0
4	GOL	J	402	-	5,5,5	0.84	0	5,5,5	0.93	0
4	GOL	L	401	-	5,5,5	1.31	1 (20%)	5,5,5	0.82	0
4	GOL	B	401	-	5,5,5	0.60	0	5,5,5	1.23	1 (20%)
4	GOL	J	401	-	5,5,5	0.97	0	5,5,5	1.11	0
4	GOL	D	401	-	5,5,5	0.81	0	5,5,5	1.23	1 (20%)
5	ACT	B	402	-	3,3,3	1.31	0	3,3,3	1.17	0
5	ACT	B	404	-	3,3,3	1.36	1 (33%)	3,3,3	1.35	0
4	GOL	C	401	-	5,5,5	0.86	0	5,5,5	0.83	0
4	GOL	L	402	-	5,5,5	1.26	1 (20%)	5,5,5	1.15	0
4	GOL	A	401	-	5,5,5	0.90	0	5,5,5	0.85	0
4	GOL	K	401	-	5,5,5	1.05	1 (20%)	5,5,5	1.49	1 (20%)
5	ACT	H	901	-	3,3,3	1.51	1 (33%)	3,3,3	1.33	0
5	ACT	D	402	-	3,3,3	1.60	0	3,3,3	1.34	0
5	ACT	G	201	-	3,3,3	1.60	1 (33%)	3,3,3	1.23	0
5	ACT	B	403	-	3,3,3	1.79	1 (33%)	3,3,3	1.22	0
4	GOL	L	404	-	5,5,5	0.79	0	5,5,5	0.90	0
5	ACT	D	403	-	3,3,3	1.60	1 (33%)	3,3,3	1.19	0
4	GOL	I	401	-	5,5,5	1.01	0	5,5,5	0.84	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
4	GOL	D	401	-	-	0/4/4/4	-
4	GOL	L	402	-	-	2/4/4/4	-
4	GOL	A	401	-	-	3/4/4/4	-
4	GOL	K	401	-	-	2/4/4/4	-
4	GOL	J	402	-	-	2/4/4/4	-
4	GOL	L	401	-	-	0/4/4/4	-
4	GOL	B	401	-	-	2/4/4/4	-
4	GOL	L	404	-	-	0/4/4/4	-
4	GOL	J	401	-	-	2/4/4/4	-
4	GOL	I	401	-	-	0/4/4/4	-
4	GOL	C	401	-	-	2/4/4/4	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	403	ACT	CH3-C	2.77	1.60	1.49
4	L	402	GOL	C3-C2	2.62	1.61	1.51
5	G	201	ACT	CH3-C	2.38	1.58	1.49
5	H	901	ACT	CH3-C	2.33	1.58	1.49
5	D	403	ACT	CH3-C	2.32	1.58	1.49
4	L	401	GOL	O2-C2	-2.21	1.37	1.43
5	B	404	ACT	CH3-C	2.09	1.57	1.49
4	K	401	GOL	C1-C2	2.01	1.59	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	401	GOL	C3-C2-C1	-2.65	102.07	111.80
4	B	401	GOL	C3-C2-C1	-2.34	103.22	111.80
4	D	401	GOL	C3-C2-C1	-2.18	103.82	111.80

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	401	GOL	O1-C1-C2-O2
4	C	401	GOL	O1-C1-C2-C3
4	J	402	GOL	C1-C2-C3-O3
4	K	401	GOL	O1-C1-C2-C3
4	A	401	GOL	O1-C1-C2-C3
4	A	401	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	B	401	GOL	C1-C2-C3-O3
4	J	401	GOL	C1-C2-C3-O3
4	L	402	GOL	C1-C2-C3-O3
4	B	401	GOL	O2-C2-C3-O3
4	J	401	GOL	O2-C2-C3-O3
4	J	402	GOL	O2-C2-C3-O3
4	K	401	GOL	O1-C1-C2-O2
4	A	401	GOL	O2-C2-C3-O3
4	L	402	GOL	O2-C2-C3-O3

There are no ring outliers.

9 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	J	402	GOL	1	0
5	B	402	ACT	1	0
4	C	401	GOL	3	0
4	L	402	GOL	1	0
4	K	401	GOL	2	0
5	H	901	ACT	1	0
5	D	402	ACT	1	0
5	G	201	ACT	1	0
5	B	403	ACT	2	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	358/360 (99%)	-0.30	2 (0%) 85 89	14, 22, 37, 64	1 (0%)
1	B	358/360 (99%)	-0.35	2 (0%) 85 89	12, 21, 36, 57	0
1	C	359/360 (99%)	-0.29	1 (0%) 90 93	13, 22, 37, 66	1 (0%)
1	D	358/360 (99%)	-0.30	2 (0%) 85 89	14, 23, 38, 60	1 (0%)
2	E	144/145 (99%)	-0.21	1 (0%) 84 88	14, 24, 44, 58	0
2	F	144/145 (99%)	-0.22	1 (0%) 84 88	15, 23, 43, 55	0
2	G	144/145 (99%)	-0.22	0 100 100	14, 22, 42, 56	1 (0%)
2	H	144/145 (99%)	-0.21	0 100 100	14, 22, 44, 63	1 (0%)
3	I	396/398 (99%)	-0.11	7 (1%) 67 73	16, 26, 44, 89	0
3	J	396/398 (99%)	-0.24	5 (1%) 75 80	16, 24, 41, 75	0
3	K	396/398 (99%)	-0.20	5 (1%) 75 80	15, 24, 43, 80	0
3	L	396/398 (99%)	-0.18	6 (1%) 72 77	12, 24, 43, 84	1 (0%)
All	All	3593/3612 (99%)	-0.24	32 (0%) 81 85	12, 23, 41, 89	6 (0%)

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	265	ASP	4.7
3	L	263	PRO	3.8
3	J	265	ASP	3.8
3	L	264	GLN	3.6
3	I	263	PRO	3.6
3	K	265	ASP	3.6
3	J	263	PRO	3.5
3	K	263	PRO	3.4
3	I	266	VAL	3.2
3	K	162	ALA	3.1
3	K	266	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
3	K	264	GLN	3.0
3	L	266	VAL	3.0
1	C	322	GLN	2.9
3	I	162	ALA	2.9
3	I	265	ASP	2.9
3	L	261	GLY	2.9
3	J	264	GLN	2.8
3	I	264	GLN	2.7
3	J	3	ALA	2.7
1	D	3	LYS	2.7
3	L	262	LEU	2.6
3	I	44	HIS	2.5
1	D	322	GLN	2.5
3	J	266	VAL	2.5
1	A	3	LYS	2.3
1	A	38	HIS	2.3
2	E	38	GLU	2.1
1	B	38	HIS	2.1
2	F	2	SER	2.1
1	B	3	LYS	2.0
3	I	262	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no 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(\AA^2)	Q<0.9
5	ACT	B	404	4/4	0.63	0.21	35,42,46,49	0
5	ACT	D	403	4/4	0.71	0.20	38,46,56,57	0

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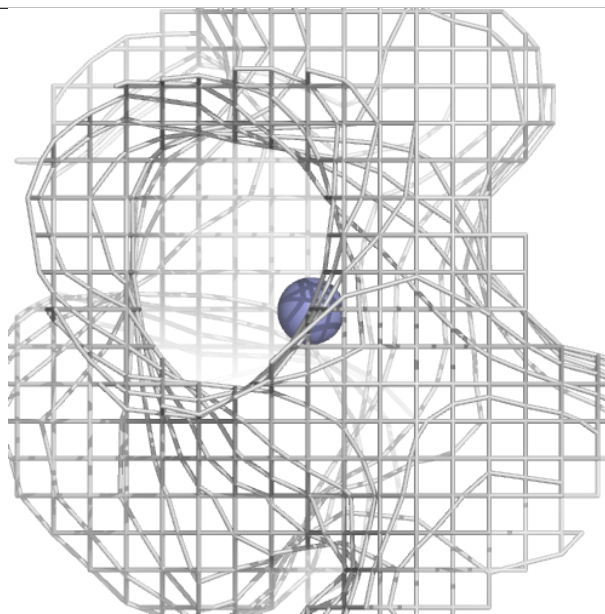
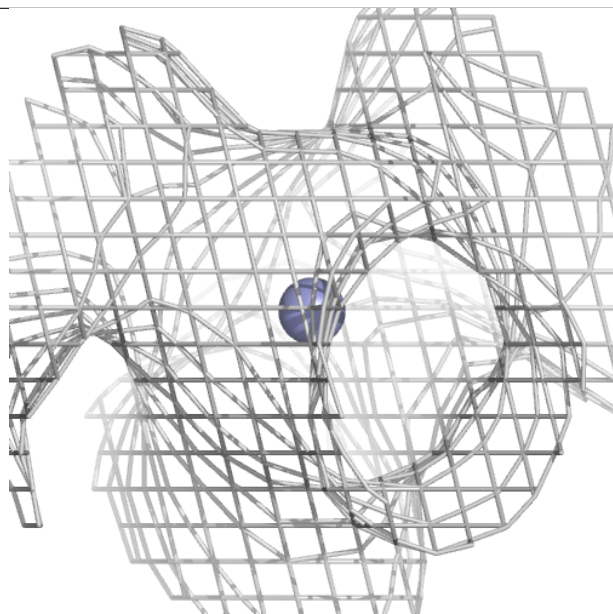
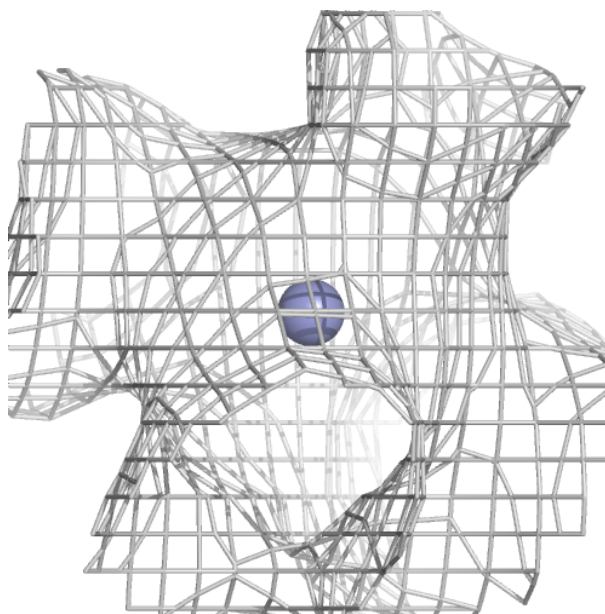
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	GOL	J	401	6/6	0.78	0.13	31,38,46,54	0
5	ACT	B	403	4/4	0.78	0.19	30,37,44,57	0
5	ACT	B	402	4/4	0.79	0.17	31,37,39,44	0
5	ACT	G	201	4/4	0.79	0.16	39,46,49,57	0
5	ACT	I	402	4/4	0.81	0.13	38,46,46,47	0
4	GOL	L	404	6/6	0.84	0.12	41,50,57,60	0
4	GOL	C	401	6/6	0.86	0.13	26,35,46,48	0
5	ACT	L	403	4/4	0.86	0.14	29,35,37,40	0
4	GOL	D	401	6/6	0.87	0.13	25,33,40,41	0
5	ACT	H	901	4/4	0.87	0.13	25,30,31,32	0
4	GOL	B	401	6/6	0.88	0.14	20,32,42,42	0
4	GOL	A	401	6/6	0.89	0.12	22,32,41,41	0
5	ACT	D	402	4/4	0.90	0.10	30,36,43,43	0
4	GOL	K	401	6/6	0.90	0.13	18,27,36,36	0
4	GOL	L	401	6/6	0.91	0.13	27,34,43,43	0
4	GOL	L	402	6/6	0.92	0.10	15,28,34,39	0
4	GOL	J	402	6/6	0.95	0.10	15,30,43,43	0
4	GOL	I	401	6/6	0.95	0.10	15,24,28,28	0
6	ZN	E	201	1/1	0.99	0.03	31,31,31,31	1
6	ZN	F	201	1/1	0.99	0.02	26,26,26,26	1
6	ZN	G	202	1/1	0.99	0.02	25,25,25,25	1
6	ZN	H	902	1/1	0.99	0.03	30,30,30,30	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.

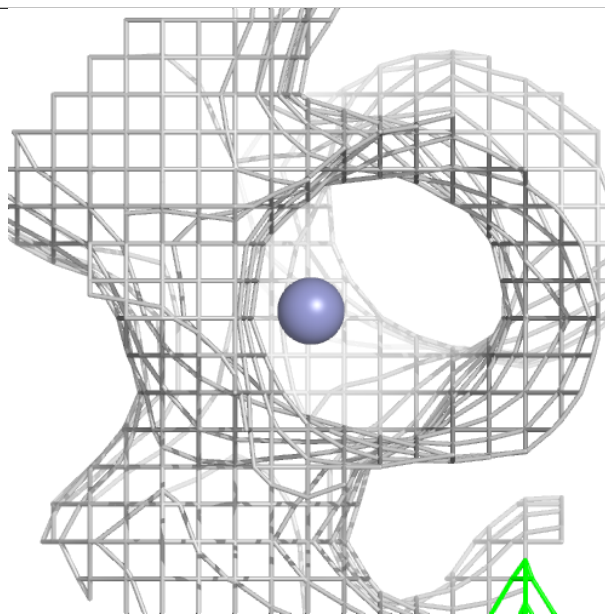
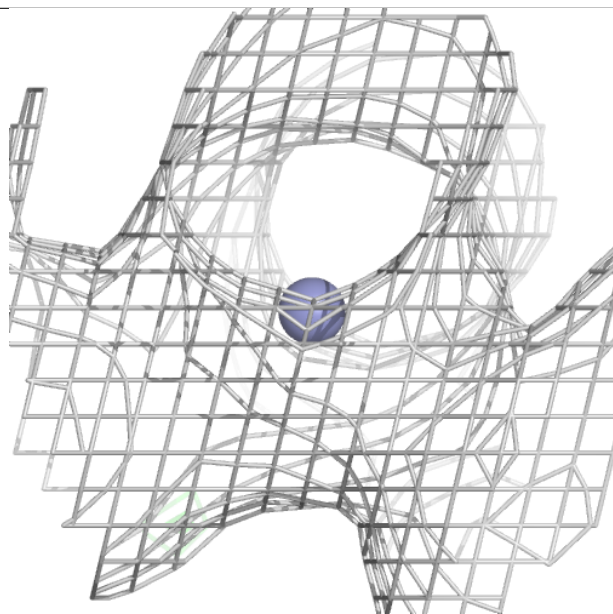
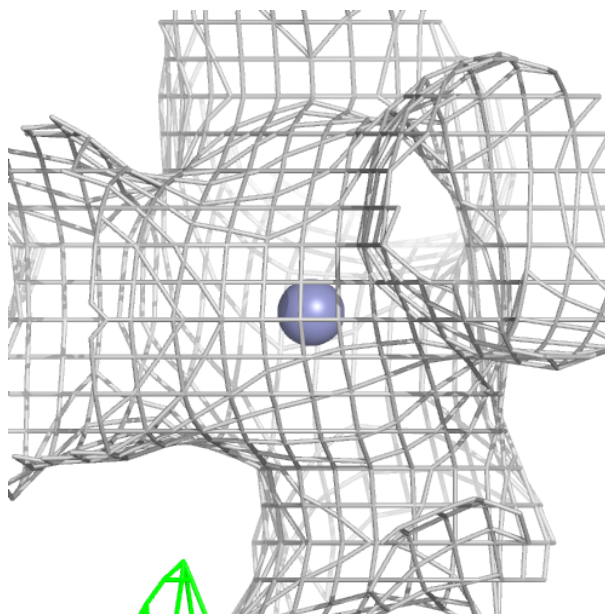
Electron density around ZN E 201:

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



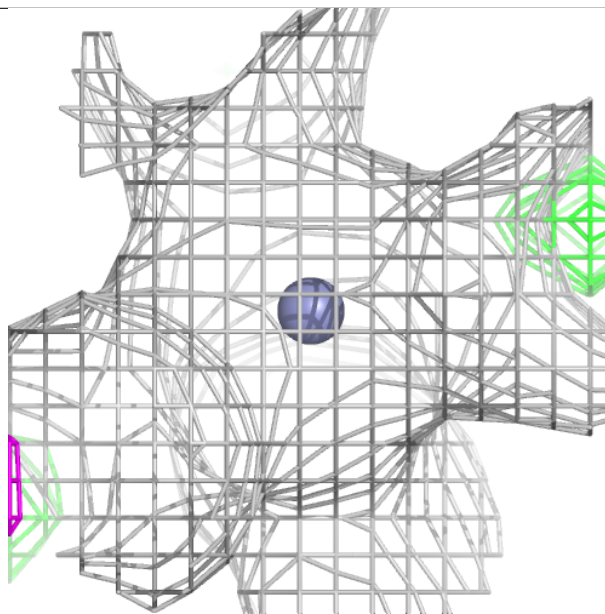
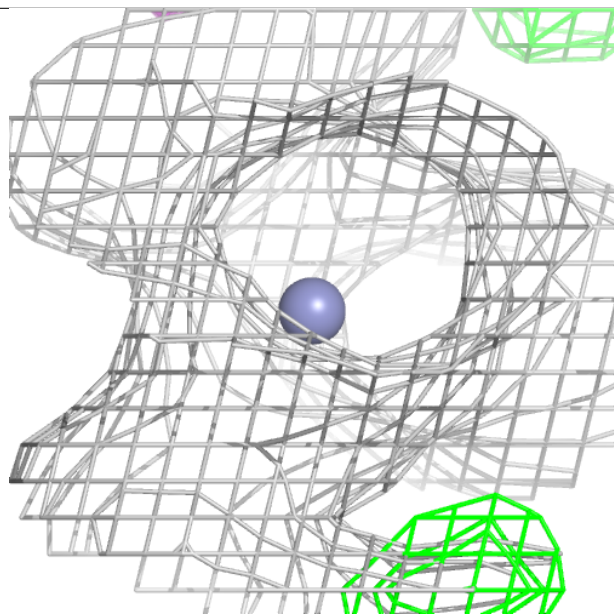
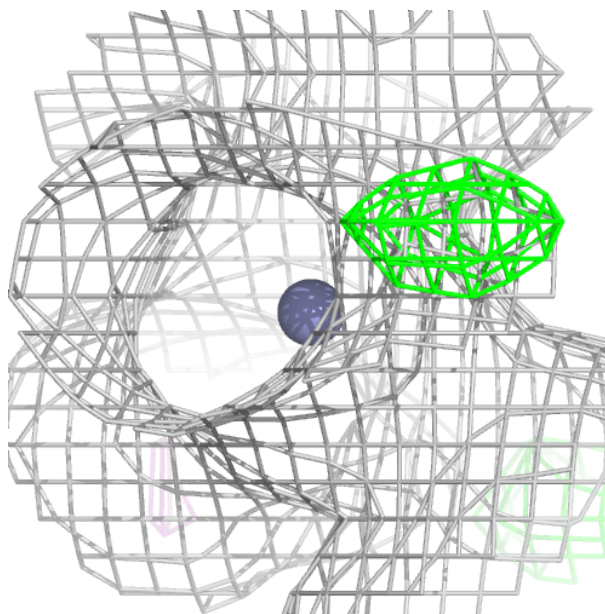
Electron density around ZN F 201:

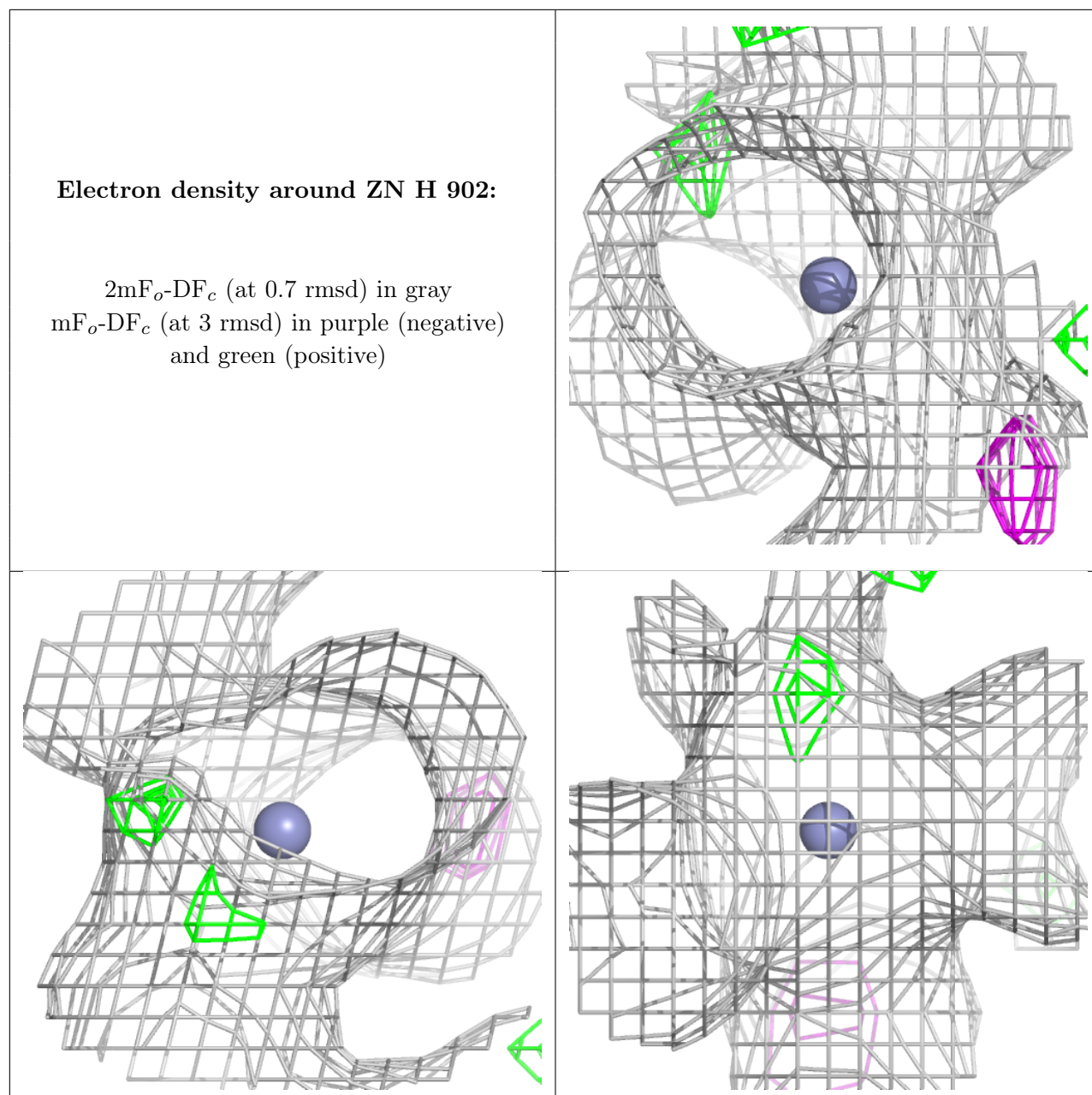
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN G 202:

$2mF_o-DF_c$ (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.