



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 12:35 AM UTC

PDB ID : 9JP7 / pdb_00009jp7
Title : 4,5-dihydroxyphthalate decarboxylase from Comamonas testosteroni (strain DSM 14576 / KF-1)
Authors : Kumar, K.A.; Kumar, P.
Deposited on : 2024-09-25
Resolution : 3.05 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
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

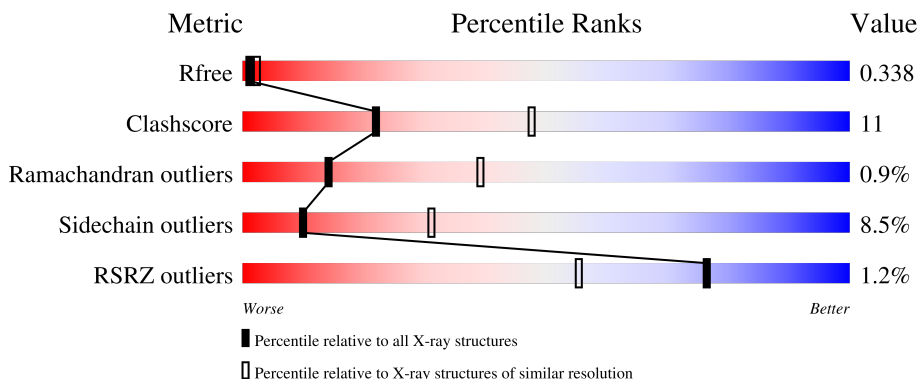
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.05 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	2469 (3.10-3.02)
Clashscore	190562	2569 (3.10-3.02)
Ramachandran outliers	187476	2424 (3.10-3.02)
Sidechain outliers	187428	2423 (3.10-3.02)
RSRZ outliers	180081	2469 (3.10-3.02)

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	349	% 63% 28% 6%
1	B	349	68% 22% 6%
1	C	349	% 69% 21% 7%
1	D	349	3% 66% 17% 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10450 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 4,5-dihydroxyphthalate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	329	Total	C	N	O	S	0	0	0
			2626	1672	466	479	9			
1	B	328	Total	C	N	O	S	0	0	0
			2618	1667	465	478	8			
1	C	325	Total	C	N	O	S	0	0	0
			2592	1650	462	471	9			
1	D	307	Total	C	N	O	S	0	0	0
			2447	1557	436	447	7			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP B7WQU9
A	-18	GLY	-	expression tag	UNP B7WQU9
A	-17	SER	-	expression tag	UNP B7WQU9
A	-16	SER	-	expression tag	UNP B7WQU9
A	-15	HIS	-	expression tag	UNP B7WQU9
A	-14	HIS	-	expression tag	UNP B7WQU9
A	-13	HIS	-	expression tag	UNP B7WQU9
A	-12	HIS	-	expression tag	UNP B7WQU9
A	-11	HIS	-	expression tag	UNP B7WQU9
A	-10	HIS	-	expression tag	UNP B7WQU9
A	-9	SER	-	expression tag	UNP B7WQU9
A	-8	SER	-	expression tag	UNP B7WQU9
A	-7	GLY	-	expression tag	UNP B7WQU9
A	-6	LEU	-	expression tag	UNP B7WQU9
A	-5	VAL	-	expression tag	UNP B7WQU9
A	-4	PRO	-	expression tag	UNP B7WQU9
A	-3	ARG	-	expression tag	UNP B7WQU9
A	-2	GLY	-	expression tag	UNP B7WQU9
A	-1	SER	-	expression tag	UNP B7WQU9
A	0	HIS	-	expression tag	UNP B7WQU9
B	-19	MET	-	initiating methionine	UNP B7WQU9

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP B7WQU9
B	-17	SER	-	expression tag	UNP B7WQU9
B	-16	SER	-	expression tag	UNP B7WQU9
B	-15	HIS	-	expression tag	UNP B7WQU9
B	-14	HIS	-	expression tag	UNP B7WQU9
B	-13	HIS	-	expression tag	UNP B7WQU9
B	-12	HIS	-	expression tag	UNP B7WQU9
B	-11	HIS	-	expression tag	UNP B7WQU9
B	-10	HIS	-	expression tag	UNP B7WQU9
B	-9	SER	-	expression tag	UNP B7WQU9
B	-8	SER	-	expression tag	UNP B7WQU9
B	-7	GLY	-	expression tag	UNP B7WQU9
B	-6	LEU	-	expression tag	UNP B7WQU9
B	-5	VAL	-	expression tag	UNP B7WQU9
B	-4	PRO	-	expression tag	UNP B7WQU9
B	-3	ARG	-	expression tag	UNP B7WQU9
B	-2	GLY	-	expression tag	UNP B7WQU9
B	-1	SER	-	expression tag	UNP B7WQU9
B	0	HIS	-	expression tag	UNP B7WQU9
C	-19	MET	-	initiating methionine	UNP B7WQU9
C	-18	GLY	-	expression tag	UNP B7WQU9
C	-17	SER	-	expression tag	UNP B7WQU9
C	-16	SER	-	expression tag	UNP B7WQU9
C	-15	HIS	-	expression tag	UNP B7WQU9
C	-14	HIS	-	expression tag	UNP B7WQU9
C	-13	HIS	-	expression tag	UNP B7WQU9
C	-12	HIS	-	expression tag	UNP B7WQU9
C	-11	HIS	-	expression tag	UNP B7WQU9
C	-10	HIS	-	expression tag	UNP B7WQU9
C	-9	SER	-	expression tag	UNP B7WQU9
C	-8	SER	-	expression tag	UNP B7WQU9
C	-7	GLY	-	expression tag	UNP B7WQU9
C	-6	LEU	-	expression tag	UNP B7WQU9
C	-5	VAL	-	expression tag	UNP B7WQU9
C	-4	PRO	-	expression tag	UNP B7WQU9
C	-3	ARG	-	expression tag	UNP B7WQU9
C	-2	GLY	-	expression tag	UNP B7WQU9
C	-1	SER	-	expression tag	UNP B7WQU9
C	0	HIS	-	expression tag	UNP B7WQU9
D	-19	MET	-	initiating methionine	UNP B7WQU9
D	-18	GLY	-	expression tag	UNP B7WQU9
D	-17	SER	-	expression tag	UNP B7WQU9

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP B7WQU9
D	-15	HIS	-	expression tag	UNP B7WQU9
D	-14	HIS	-	expression tag	UNP B7WQU9
D	-13	HIS	-	expression tag	UNP B7WQU9
D	-12	HIS	-	expression tag	UNP B7WQU9
D	-11	HIS	-	expression tag	UNP B7WQU9
D	-10	HIS	-	expression tag	UNP B7WQU9
D	-9	SER	-	expression tag	UNP B7WQU9
D	-8	SER	-	expression tag	UNP B7WQU9
D	-7	GLY	-	expression tag	UNP B7WQU9
D	-6	LEU	-	expression tag	UNP B7WQU9
D	-5	VAL	-	expression tag	UNP B7WQU9
D	-4	PRO	-	expression tag	UNP B7WQU9
D	-3	ARG	-	expression tag	UNP B7WQU9
D	-2	GLY	-	expression tag	UNP B7WQU9
D	-1	SER	-	expression tag	UNP B7WQU9
D	0	HIS	-	expression tag	UNP B7WQU9

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mg 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	47	Total O 47 47	0	0

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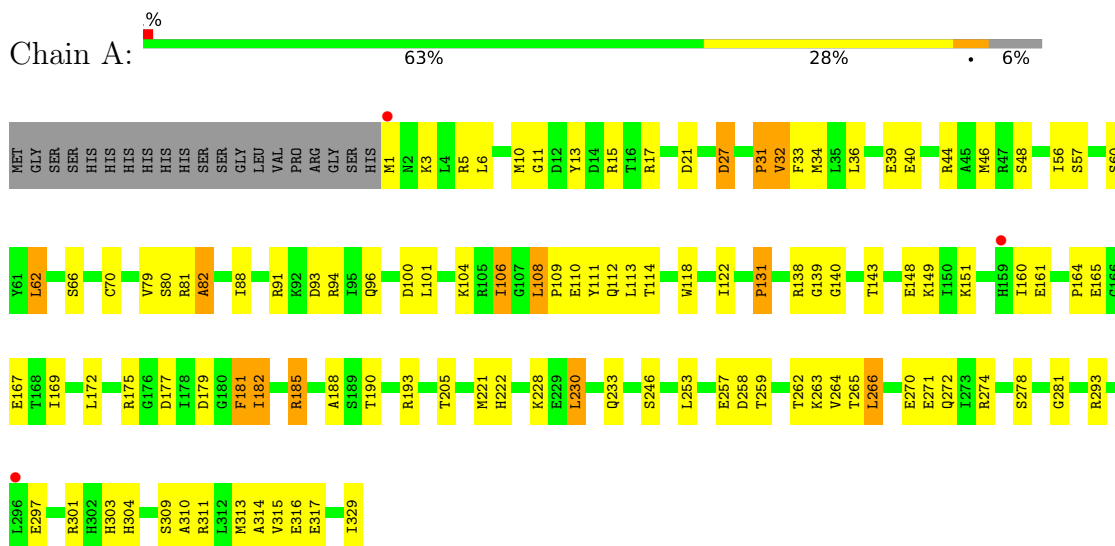
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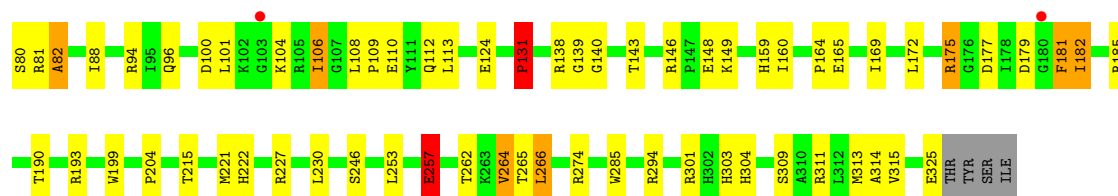
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	52	Total 52	O 52	0	0
4	C	36	Total 36	O 36	0	0
4	D	28	Total 28	O 28	0	0

3 Residue-property plots [i](#)

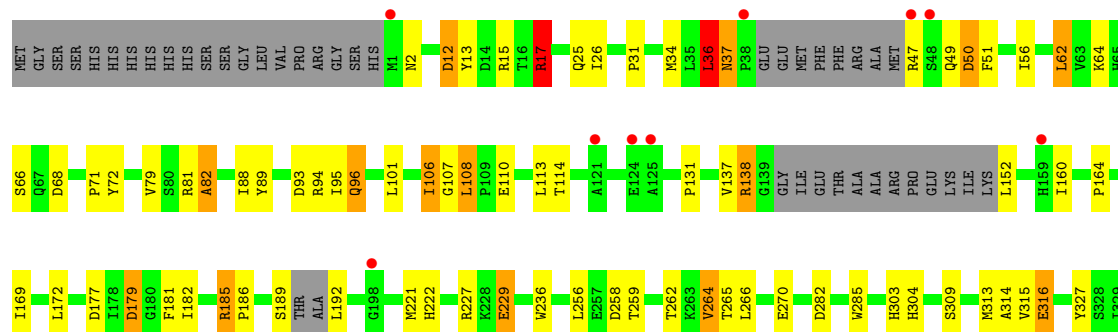
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 4,5-dihydroxyphthalate decarboxylase





• Molecule 1: 4,5-dihydroxyphthalate decarboxylase



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	128.04Å 270.20Å 113.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.22 – 3.05 25.22 – 3.05	Depositor EDS
% Data completeness (in resolution range)	98.1 (25.22-3.05) 98.0 (25.22-3.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.76 (at 3.05Å)	Xtriage
Refinement program	REFMAC 5.8.0415	Depositor
R, R_{free}	0.264 , 0.335 0.265 , 0.338	Depositor DCC
R_{free} test set	1829 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.403	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	10450	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% 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: MG, 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	0.61	0/2695	1.17	7/3659 (0.2%)
1	B	0.60	0/2687	1.12	3/3649 (0.1%)
1	C	0.54	0/2660	1.07	3/3612 (0.1%)
1	D	0.55	0/2510	1.13	8/3407 (0.2%)
All	All	0.58	0/10552	1.12	21/14327 (0.1%)

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
1	A	0	6
1	B	0	3
1	C	0	1
1	D	0	4
All	All	0	14

There are no bond length outliers.

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	PRO	N-CA-C	11.05	128.89	113.53
1	B	262	THR	CB-CA-C	7.48	122.03	109.84
1	A	161	GLU	CB-CG-CD	7.32	125.05	112.60
1	D	17	ARG	CB-CG-CD	7.25	127.98	111.30
1	D	12	ASP	CA-CB-CG	6.70	119.30	112.60
1	C	262	THR	CB-CA-C	6.65	120.68	109.84
1	A	21	ASP	CB-CA-C	-6.51	97.00	109.95
1	A	262	THR	CB-CA-C	6.19	119.94	109.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	262	THR	CB-CA-C	6.15	119.87	109.84
1	B	233	GLN	CB-CG-CD	-5.94	102.50	112.60
1	C	181	PHE	CA-CB-CG	5.90	119.70	113.80
1	D	179	ASP	CA-CB-CG	5.79	118.39	112.60
1	D	96	GLN	CB-CA-C	5.59	120.94	110.70
1	B	181	PHE	CA-CB-CG	5.54	119.33	113.80
1	D	51	PHE	CA-CB-CG	-5.51	108.29	113.80
1	C	257	GLU	CB-CG-CD	5.48	121.91	112.60
1	A	40	GLU	CB-CG-CD	5.36	121.71	112.60
1	D	36	LEU	N-CA-C	5.30	117.32	109.69
1	A	181	PHE	CA-CB-CG	5.29	119.09	113.80
1	D	2	ASN	CB-CA-C	5.26	118.82	110.19
1	A	281	GLY	CA-C-O	-5.12	118.89	122.22

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	ARG	Sidechain
1	A	185	ARG	Sidechain
1	A	193	ARG	Sidechain
1	A	293	ARG	Sidechain
1	A	5	ARG	Sidechain
1	A	91	ARG	Sidechain
1	B	15	ARG	Sidechain
1	B	213	ARG	Sidechain
1	B	84	ARG	Sidechain
1	C	15	ARG	Sidechain
1	D	138	ARG	Peptide
1	D	15	ARG	Sidechain
1	D	17	ARG	Sidechain
1	D	36	LEU	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	2626	0	2596	65	0
1	B	2618	0	2584	53	0
1	C	2592	0	2564	65	0
1	D	2447	0	2405	56	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	47	0	0	2	0
4	B	52	0	0	3	0
4	C	36	0	0	5	0
4	D	28	0	0	2	0
All	All	10450	0	10149	219	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 11.

All (219) 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:259:THR:HG21	1:A:270:GLU:HG3	1.45	0.95
1:C:164:PRO:HD3	4:C:530:HOH:O	1.73	0.88
1:B:110:GLU:HB2	1:B:113:LEU:HD13	1.56	0.87
1:D:47:ARG:HG2	1:D:64:LYS:NZ	1.97	0.79
1:A:66:SER:HB3	1:A:313:MET:HE3	1.66	0.78
1:D:50:ASP:HB3	1:D:227:ARG:HH12	1.50	0.77
1:A:6:LEU:O	1:A:31:PRO:O	2.02	0.76
1:C:66:SER:HB3	1:C:313:MET:HE3	1.67	0.75
1:A:259:THR:CG2	1:A:270:GLU:HG3	2.15	0.74
1:C:172:LEU:HD23	1:C:175:ARG:NH1	2.01	0.74
1:B:164:PRO:HD2	1:B:172:LEU:HD11	1.73	0.71
1:B:57:SER:HB3	1:B:60:SER:HB2	1.73	0.70
1:D:66:SER:HB3	1:D:313:MET:HE3	1.73	0.70
1:C:172:LEU:HD23	1:C:175:ARG:HH12	1.57	0.69
1:A:164:PRO:HD2	1:A:172:LEU:HD11	1.73	0.69
1:C:266:LEU:HD21	1:D:256:LEU:HD21	1.75	0.69
1:A:39:GLU:OE2	1:A:185:ARG:NH1	2.26	0.68
1:C:138:ARG:NH2	4:C:501:HOH:O	2.27	0.67
1:D:164:PRO:HD2	1:D:172:LEU:HD11	1.76	0.67
1:A:111:TYR:N	1:A:148:GLU:OE1	2.27	0.66
1:C:124:GLU:OE2	1:C:131:PRO:HD2	1.95	0.66
1:C:39:GLU:OE2	1:C:185:ARG:NH1	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:GLU:OE2	1:B:185:ARG:NH1	2.29	0.66
1:D:229:GLU:OE1	1:D:229:GLU:HA	1.94	0.66
1:A:272:GLN:HG3	1:B:272:GLN:OE1	1.96	0.65
1:C:164:PRO:HD2	1:C:172:LEU:HD11	1.78	0.65
1:C:66:SER:CB	1:C:313:MET:HE3	2.27	0.64
1:B:110:GLU:HB2	1:B:113:LEU:CD1	2.28	0.64
1:C:215:THR:O	1:C:294:ARG:HD3	1.98	0.64
1:C:64:LYS:HD2	4:C:502:HOH:O	1.98	0.64
1:C:266:LEU:CD2	1:D:256:LEU:HD21	2.29	0.63
1:B:88:ILE:HG12	1:B:182:ILE:CG2	2.29	0.62
1:A:88:ILE:HG12	1:A:182:ILE:CG2	2.29	0.62
1:C:46:MET:HE2	1:C:46:MET:HA	1.81	0.62
1:C:190:THR:HG22	1:C:193:ARG:HH22	1.65	0.62
1:D:229:GLU:OE1	1:D:229:GLU:CA	2.48	0.61
1:B:172:LEU:HD23	1:B:175:ARG:NH1	2.15	0.61
1:A:1:MET:HG2	1:A:1:MET:O	2.00	0.61
1:A:188:ALA:HB1	4:A:526:HOH:O	2.01	0.60
1:D:101:LEU:HD22	1:D:106:ILE:CD1	2.32	0.60
1:C:88:ILE:HG12	1:C:182:ILE:CG2	2.31	0.60
1:B:253:LEU:O	1:B:257:GLU:HG3	2.01	0.59
1:D:259:THR:CG2	1:D:270:GLU:HG3	2.32	0.59
1:A:253:LEU:O	1:A:257:GLU:HG3	2.02	0.59
1:B:50:ASP:HB3	1:D:236:TRP:HB3	1.85	0.59
1:C:109:PRO:HG2	1:C:113:LEU:HD12	1.84	0.58
1:D:95:ILE:HD11	1:D:179:ASP:HB3	1.85	0.58
1:D:189:SER:C	1:D:192:LEU:N	2.61	0.58
1:A:100:ASP:O	1:A:104:LYS:HE3	2.03	0.57
1:A:167:GLU:CD	1:A:175:ARG:HH12	2.13	0.56
1:C:66:SER:CB	1:C:313:MET:CE	2.84	0.56
1:D:47:ARG:HG2	1:D:64:LYS:HZ2	1.70	0.56
1:D:259:THR:HG22	1:D:270:GLU:HG3	1.88	0.56
1:B:42:PHE:HB2	1:B:149:LYS:HE2	1.88	0.55
1:C:101:LEU:HD22	1:C:106:ILE:CD1	2.36	0.55
1:A:17:ARG:HD2	1:B:17:ARG:HD2	1.88	0.55
1:A:172:LEU:HD23	1:A:175:ARG:NH2	2.22	0.55
1:A:66:SER:CB	1:A:313:MET:HE3	2.36	0.55
1:B:259:THR:CG2	1:B:270:GLU:HG3	2.36	0.55
1:A:271:GLU:HG2	1:B:205:THR:OG1	2.07	0.55
1:B:249:LYS:CE	4:B:533:HOH:O	2.55	0.54
1:B:42:PHE:CB	1:B:149:LYS:HE2	2.38	0.54
1:B:101:LEU:HD22	1:B:106:ILE:CD1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:VAL:HG11	1:D:264:VAL:HG11	1.90	0.54
1:B:259:THR:HG22	1:B:270:GLU:HG3	1.89	0.54
1:D:101:LEU:HD22	1:D:106:ILE:HD11	1.90	0.54
1:A:56:ILE:HG22	1:A:57:SER:N	2.23	0.54
1:A:66:SER:CB	1:A:313:MET:CE	2.86	0.54
1:A:109:PRO:HG2	1:A:113:LEU:HD12	1.90	0.53
1:B:112:GLN:HE22	1:B:150:ILE:HD12	1.73	0.53
1:A:140:GLY:HA3	1:A:143:THR:O	2.09	0.53
1:D:66:SER:CB	1:D:313:MET:CE	2.87	0.52
1:A:66:SER:HB2	1:A:313:MET:HE1	1.91	0.52
1:C:100:ASP:O	1:C:104:LYS:HE2	2.08	0.52
1:A:259:THR:HG21	1:A:270:GLU:CG	2.30	0.52
1:B:140:GLY:HA3	1:B:143:THR:O	2.10	0.51
1:C:17:ARG:HD2	1:D:17:ARG:HD3	1.91	0.51
1:D:88:ILE:HG12	1:D:182:ILE:CG2	2.40	0.51
1:D:47:ARG:HH21	1:D:71:PRO:HG3	1.76	0.51
1:C:190:THR:HG22	1:C:193:ARG:NH2	2.26	0.50
1:C:264:VAL:CG1	1:D:264:VAL:HG11	2.41	0.50
1:D:13:TYR:O	1:D:17:ARG:HG2	2.12	0.50
1:A:205:THR:OG1	1:B:271:GLU:HG2	2.12	0.50
1:C:265:THR:HG23	1:D:285:TRP:CD2	2.46	0.50
1:B:93:ASP:OD1	1:B:94:ARG:HG3	2.12	0.50
1:D:221:MET:HB3	1:D:222:HIS:HD2	1.77	0.50
1:A:70:CYS:O	1:A:228:LYS:HD3	2.12	0.49
1:D:66:SER:HB3	1:D:313:MET:CE	2.41	0.49
1:A:329:ILE:HD13	1:C:185:ARG:NH1	2.28	0.49
1:D:110:GLU:OE1	1:D:138:ARG:HD2	2.12	0.49
1:D:169:ILE:HG22	1:D:181:PHE:CD1	2.47	0.49
1:B:46:MET:HE2	1:B:46:MET:HA	1.95	0.49
1:C:101:LEU:HD22	1:C:106:ILE:HD11	1.94	0.49
1:C:110:GLU:OE2	1:C:149:LYS:HG3	2.12	0.49
1:D:108:LEU:O	1:D:138:ARG:HA	2.12	0.48
1:C:215:THR:O	1:C:294:ARG:CD	2.60	0.48
1:C:112:GLN:HG2	1:C:148:GLU:OE2	2.14	0.48
1:A:44:ARG:O	1:A:48:SER:HB3	2.13	0.48
1:D:66:SER:CB	1:D:313:MET:HE3	2.41	0.48
1:B:66:SER:HA	1:B:313:MET:CE	2.43	0.48
1:A:17:ARG:HH11	1:B:17:ARG:HH11	1.61	0.48
1:D:71:PRO:HG2	1:D:72:TYR:CD2	2.49	0.47
1:D:93:ASP:OD1	1:D:94:ARG:HG3	2.13	0.47
1:A:172:LEU:CD2	1:A:175:ARG:NH2	2.77	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:MET:HE2	1:A:46:MET:HA	1.96	0.47
1:A:93:ASP:OD1	1:A:94:ARG:HG3	2.14	0.47
1:C:94:ARG:HD2	1:C:179:ASP:OD1	2.14	0.47
1:C:164:PRO:HG2	1:C:172:LEU:HD21	1.97	0.47
1:D:26:ILE:HD12	1:D:31:PRO:HB3	1.96	0.47
1:D:185:ARG:NE	4:D:502:HOH:O	2.41	0.47
1:A:108:LEU:O	1:A:138:ARG:HA	2.14	0.47
1:A:297:GLU:HG3	1:A:301:ARG:NH1	2.31	0.47
1:C:227:ARG:HB2	1:C:230:LEU:HD22	1.96	0.46
1:A:139:GLY:O	1:A:169:ILE:HG12	2.15	0.46
1:C:140:GLY:HA3	1:C:143:THR:O	2.16	0.46
1:A:81:ARG:O	1:A:82:ALA:HB2	2.14	0.46
1:A:329:ILE:HA	1:C:146:ARG:NH1	2.30	0.46
1:C:108:LEU:O	1:C:138:ARG:HA	2.14	0.46
1:A:112:GLN:HG2	1:A:148:GLU:OE2	2.15	0.46
1:B:81:ARG:O	1:B:82:ALA:HB2	2.16	0.46
1:C:81:ARG:O	1:C:82:ALA:HB2	2.14	0.46
1:C:304:HIS:HA	1:C:309:SER:HB2	1.98	0.46
1:A:27:ASP:OD1	1:A:27:ASP:N	2.49	0.46
1:D:304:HIS:HA	1:D:309:SER:HB2	1.98	0.46
1:A:304:HIS:HA	1:A:309:SER:HB2	1.98	0.46
1:B:101:LEU:HD22	1:B:106:ILE:HD11	1.98	0.46
1:B:139:GLY:O	1:B:169:ILE:HG12	2.16	0.46
1:B:66:SER:HA	1:B:313:MET:HE1	1.97	0.45
1:C:165:GLU:HG3	4:C:534:HOH:O	2.16	0.45
1:C:253:LEU:O	1:C:257:GLU:CG	2.65	0.45
1:D:169:ILE:CG2	1:D:181:PHE:CD1	2.99	0.45
1:A:109:PRO:HA	1:A:139:GLY:O	2.17	0.45
1:B:80:SER:HB3	1:B:222:HIS:CG	2.52	0.45
1:B:314:ALA:O	1:B:315:VAL:C	2.60	0.45
1:D:314:ALA:O	1:D:315:VAL:C	2.58	0.45
1:C:253:LEU:O	1:C:257:GLU:HG3	2.17	0.45
1:D:169:ILE:CG2	1:D:181:PHE:HD1	2.30	0.45
1:A:66:SER:HB3	1:A:313:MET:CE	2.38	0.45
1:C:172:LEU:CD2	1:C:175:ARG:HH12	2.25	0.45
1:A:265:THR:OG1	1:B:15:ARG:HD3	2.16	0.45
1:B:109:PRO:HA	1:B:139:GLY:O	2.17	0.45
1:C:109:PRO:HG2	1:C:113:LEU:CD1	2.44	0.45
1:C:109:PRO:HA	1:C:139:GLY:O	2.17	0.44
1:C:264:VAL:CG1	1:D:264:VAL:CG1	2.95	0.44
1:B:56:ILE:HD12	1:B:223:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ALA:O	1:C:315:VAL:C	2.59	0.44
1:D:229:GLU:OE1	1:D:229:GLU:N	2.50	0.44
1:C:139:GLY:O	1:C:169:ILE:HG12	2.17	0.44
1:B:169:ILE:HG22	1:B:181:PHE:CD2	2.52	0.44
1:D:81:ARG:O	1:D:82:ALA:HB2	2.18	0.44
1:D:169:ILE:HG22	1:D:181:PHE:HD1	1.81	0.44
1:A:36:LEU:HA	4:A:514:HOH:O	2.18	0.44
1:A:101:LEU:HD22	1:A:106:ILE:CD1	2.48	0.44
1:A:314:ALA:O	1:A:317:GLU:HG2	2.17	0.44
1:B:10:MET:HE2	1:B:33:PHE:CD1	2.52	0.44
1:B:34:MET:HB2	1:B:34:MET:HE3	1.87	0.44
1:B:108:LEU:O	1:B:138:ARG:HA	2.17	0.43
1:D:25:GLN:NE2	4:D:503:HOH:O	2.50	0.43
1:C:80:SER:HB3	1:C:222:HIS:CG	2.54	0.43
1:B:68:ASP:OD1	1:B:311:ARG:NH2	2.52	0.43
1:C:169:ILE:HG22	1:C:181:PHE:CD2	2.53	0.43
1:A:80:SER:HB3	1:A:222:HIS:CG	2.54	0.43
1:C:199:TRP:CE3	1:C:204:PRO:HG3	2.53	0.43
1:D:110:GLU:HB3	1:D:113:LEU:HG	2.00	0.43
1:C:39:GLU:CD	1:C:185:ARG:NH1	2.76	0.43
1:C:54:THR:HG23	1:C:56:ILE:HG12	2.01	0.43
1:C:66:SER:HB2	1:C:313:MET:HE1	2.00	0.43
1:C:62:LEU:HB3	1:C:303:HIS:CE1	2.54	0.43
1:A:62:LEU:HB3	1:A:303:HIS:CE1	2.53	0.42
1:B:62:LEU:HB3	1:B:303:HIS:CE1	2.54	0.42
1:B:118:TRP:O	1:B:122:ILE:HG13	2.19	0.42
1:B:136:TRP:CZ3	1:B:182:ILE:HD11	2.54	0.42
1:D:221:MET:CB	1:D:222:HIS:HD2	2.32	0.42
1:A:314:ALA:O	1:A:315:VAL:C	2.59	0.42
1:B:249:LYS:HE3	4:B:533:HOH:O	2.16	0.42
1:A:110:GLU:HB2	1:A:113:LEU:HG	2.02	0.42
1:A:11:GLY:HA3	1:A:13:TYR:CZ	2.55	0.42
1:A:169:ILE:HG22	1:A:181:PHE:CD2	2.55	0.42
1:D:66:SER:CB	1:D:313:MET:HE1	2.49	0.42
1:B:95:ILE:HD11	1:B:179:ASP:HB3	2.00	0.42
1:C:110:GLU:HB2	1:C:113:LEU:HG	2.00	0.42
1:D:62:LEU:HB3	1:D:303:HIS:CE1	2.55	0.42
1:A:10:MET:HE2	1:A:33:PHE:CD1	2.54	0.42
1:A:94:ARG:HD2	1:A:179:ASP:OD1	2.20	0.42
1:A:57:SER:HB3	1:A:60:SER:HB2	2.02	0.42
1:D:114:THR:HG21	1:D:221:MET:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:TRP:O	1:A:122:ILE:HG13	2.20	0.42
1:B:96:GLN:H	1:B:96:GLN:HG2	1.72	0.42
1:C:11:GLY:HA3	1:C:13:TYR:CZ	2.55	0.42
1:C:34:MET:HE1	1:C:51:PHE:CD1	2.54	0.42
1:D:66:SER:HB2	1:D:313:MET:HE1	2.01	0.42
1:B:227:ARG:HB2	1:B:230:LEU:HD22	2.02	0.41
1:B:249:LYS:HE2	4:B:533:HOH:O	2.20	0.41
1:A:139:GLY:O	1:A:169:ILE:CG1	2.68	0.41
1:A:88:ILE:HG12	1:A:182:ILE:HG22	2.02	0.41
1:B:199:TRP:CE3	1:B:204:PRO:HG3	2.55	0.41
1:C:172:LEU:HD22	1:C:177:ASP:HB3	2.02	0.41
1:D:259:THR:HG21	1:D:270:GLU:HG3	2.02	0.41
1:A:109:PRO:HG2	1:A:113:LEU:CD1	2.50	0.41
1:A:114:THR:HG21	1:A:221:MET:O	2.21	0.41
1:A:110:GLU:OE2	1:A:149:LYS:HG2	2.21	0.41
1:A:230:LEU:HD12	1:A:230:LEU:HA	1.92	0.41
1:C:221:MET:HB3	1:C:222:HIS:CD2	2.56	0.41
1:B:40:GLU:HA	1:D:327:TYR:CG	2.56	0.41
1:A:314:ALA:C	1:A:316:GLU:N	2.78	0.41
1:B:167:GLU:OE1	1:B:175:ARG:NH1	2.53	0.41
1:C:28:GLY:HA3	4:C:531:HOH:O	2.21	0.41
1:C:57:SER:HB3	1:C:60:SER:HB2	2.02	0.41
1:C:285:TRP:CD2	1:D:265:THR:HG23	2.55	0.41
1:B:314:ALA:C	1:B:316:GLU:N	2.77	0.41
1:C:139:GLY:O	1:C:169:ILE:CG1	2.69	0.41
1:D:314:ALA:C	1:D:316:GLU:N	2.79	0.41
1:A:66:SER:CB	1:A:313:MET:HE1	2.51	0.40
1:C:264:VAL:HG11	1:D:264:VAL:CG1	2.50	0.40
1:D:107:GLY:HA2	1:D:137:VAL:O	2.21	0.40
1:A:266:LEU:HD21	1:B:256:LEU:HD21	2.03	0.40
1:B:304:HIS:HA	1:B:309:SER:HB2	2.03	0.40
1:C:10:MET:HE2	1:C:33:PHE:CD1	2.57	0.40
1:D:89:TYR:OH	1:D:186:PRO:HB3	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	327/349 (94%)	313 (96%)	10 (3%)	4 (1%)	10	32
1	B	326/349 (93%)	313 (96%)	11 (3%)	2 (1%)	21	48
1	C	323/349 (93%)	309 (96%)	12 (4%)	2 (1%)	21	48
1	D	299/349 (86%)	286 (96%)	9 (3%)	4 (1%)	9	31
All	All	1275/1396 (91%)	1221 (96%)	42 (3%)	12 (1%)	14	39

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	VAL
1	D	37	ASN
1	A	82	ALA
1	C	82	ALA
1	D	82	ALA
1	B	82	ALA
1	D	50	ASP
1	A	310	ALA
1	B	131	PRO
1	A	131	PRO
1	C	131	PRO
1	D	131	PRO

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	277/294 (94%)	251 (91%)	26 (9%)	8	27
1	B	276/294 (94%)	254 (92%)	22 (8%)	11	33
1	C	273/294 (93%)	252 (92%)	21 (8%)	12	35
1	D	259/294 (88%)	236 (91%)	23 (9%)	9	29
All	All	1085/1176 (92%)	993 (92%)	92 (8%)	10	31

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	27	ASP
1	A	32	VAL
1	A	34	MET
1	A	62	LEU
1	A	79	VAL
1	A	96	GLN
1	A	106	ILE
1	A	108	LEU
1	A	131	PRO
1	A	151	LYS
1	A	160	ILE
1	A	165	GLU
1	A	177	ASP
1	A	182	ILE
1	A	190	THR
1	A	230	LEU
1	A	233	GLN
1	A	246	SER
1	A	258	ASP
1	A	263	LYS
1	A	264	VAL
1	A	266	LEU
1	A	274	ARG
1	A	278	SER
1	A	311	ARG
1	B	3	LYS
1	B	5	ARG
1	B	56	ILE
1	B	62	LEU
1	B	79	VAL
1	B	96	GLN
1	B	106	ILE

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Mol	Chain	Res	Type
1	B	131	PRO
1	B	150	ILE
1	B	159	HIS
1	B	160	ILE
1	B	182	ILE
1	B	190	THR
1	B	230	LEU
1	B	246	SER
1	B	258	ASP
1	B	264	VAL
1	B	266	LEU
1	B	278	SER
1	B	282	ASP
1	B	297	GLU
1	B	313	MET
1	C	3	LYS
1	C	5	ARG
1	C	34	MET
1	C	56	ILE
1	C	62	LEU
1	C	79	VAL
1	C	96	GLN
1	C	106	ILE
1	C	131	PRO
1	C	159	HIS
1	C	160	ILE
1	C	175	ARG
1	C	182	ILE
1	C	246	SER
1	C	257	GLU
1	C	264	VAL
1	C	266	LEU
1	C	274	ARG
1	C	301	ARG
1	C	311	ARG
1	C	325	GLU
1	D	12	ASP
1	D	17	ARG
1	D	34	MET
1	D	36	LEU
1	D	37	ASN
1	D	49	GLN

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Mol	Chain	Res	Type
1	D	56	ILE
1	D	62	LEU
1	D	68	ASP
1	D	79	VAL
1	D	96	GLN
1	D	106	ILE
1	D	108	LEU
1	D	152	LEU
1	D	160	ILE
1	D	177	ASP
1	D	185	ARG
1	D	229	GLU
1	D	258	ASP
1	D	264	VAL
1	D	266	LEU
1	D	282	ASP
1	D	316	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	162	ASN
1	A	272	GLN
1	A	302	HIS
1	B	112	GLN
1	B	162	ASN
1	B	302	HIS
1	C	112	GLN
1	D	25	GLN
1	D	112	GLN
1	D	222	HIS

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 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

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 [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	329/349 (94%)	0.19	3 (0%) 81 61	6, 14, 37, 62	0
1	B	328/349 (93%)	0.09	1 (0%) 90 80	5, 15, 39, 66	0
1	C	325/349 (93%)	0.26	3 (0%) 81 61	20, 36, 55, 100	0
1	D	307/349 (87%)	0.45	9 (2%) 53 31	17, 47, 73, 100	0
All	All	1289/1396 (92%)	0.24	16 (1%) 76 55	5, 29, 62, 100	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	48	SER	3.1
1	C	1	MET	3.0
1	D	38	PRO	2.8
1	B	147	PRO	2.8
1	A	159	HIS	2.8
1	D	47	ARG	2.6
1	A	1	MET	2.6
1	D	159	HIS	2.4
1	C	180	GLY	2.3
1	D	198	GLY	2.3
1	A	296	LEU	2.2
1	D	124	GLU	2.2
1	D	125	ALA	2.1
1	C	103	GLY	2.1
1	D	121	ALA	2.0
1	D	1	MET	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](#)

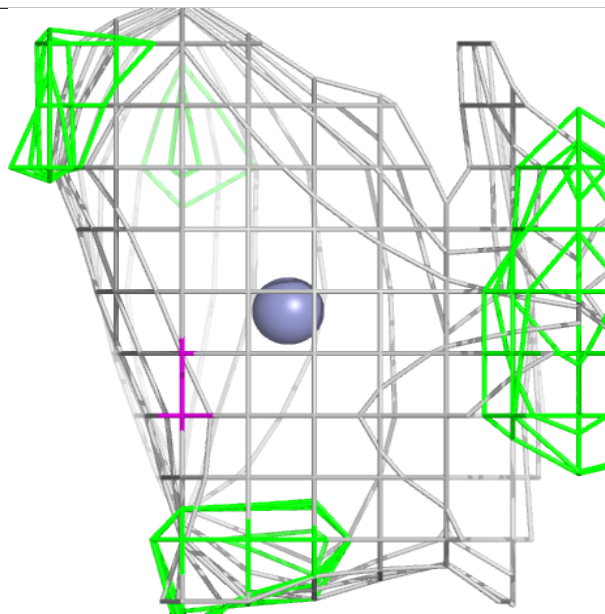
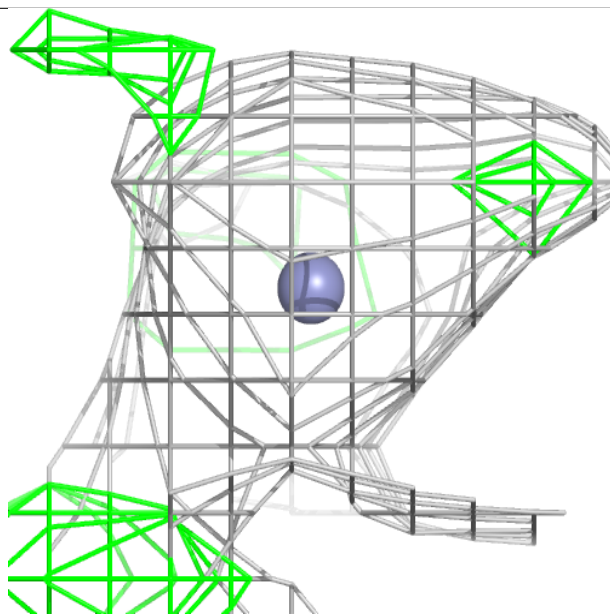
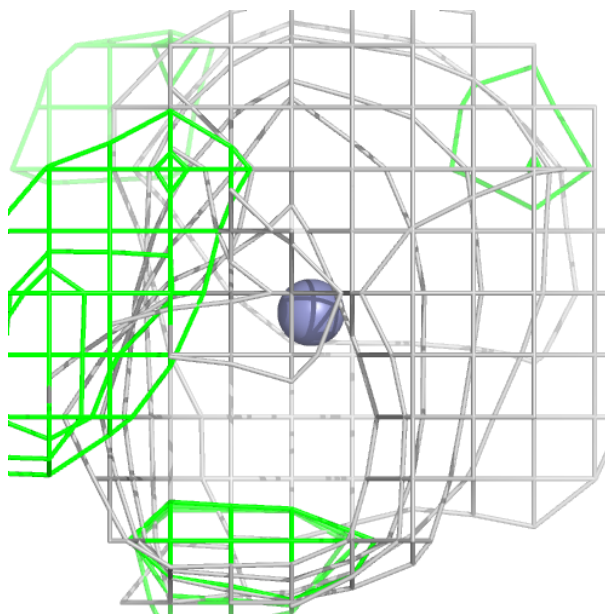
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	401	1/1	0.90	0.08	74,74,74,74	0
2	ZN	B	401	1/1	0.96	0.06	67,67,67,67	0
2	ZN	C	401	1/1	0.97	0.05	68,68,68,68	0
3	MG	D	401	1/1	0.97	0.15	34,34,34,34	0

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.

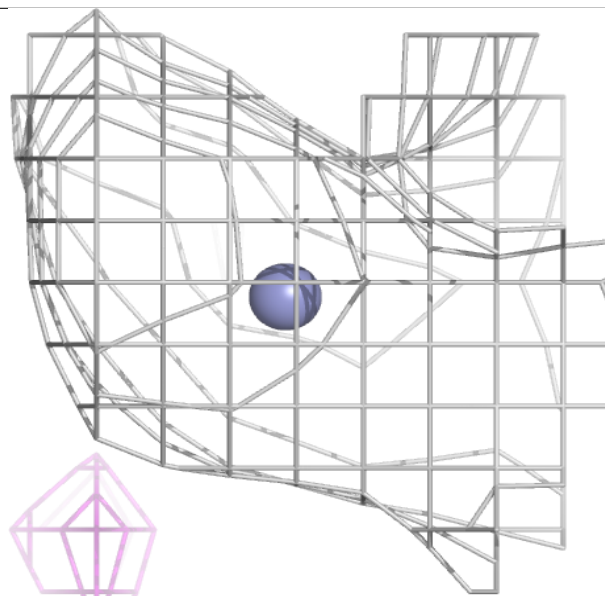
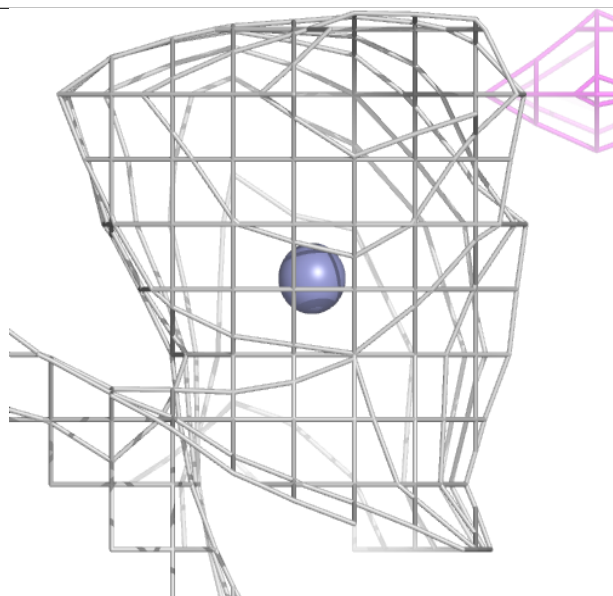
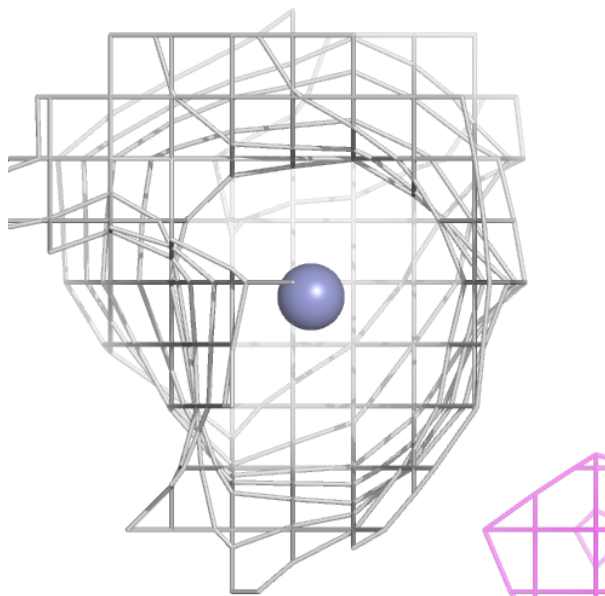
Electron density around ZN A 401:

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



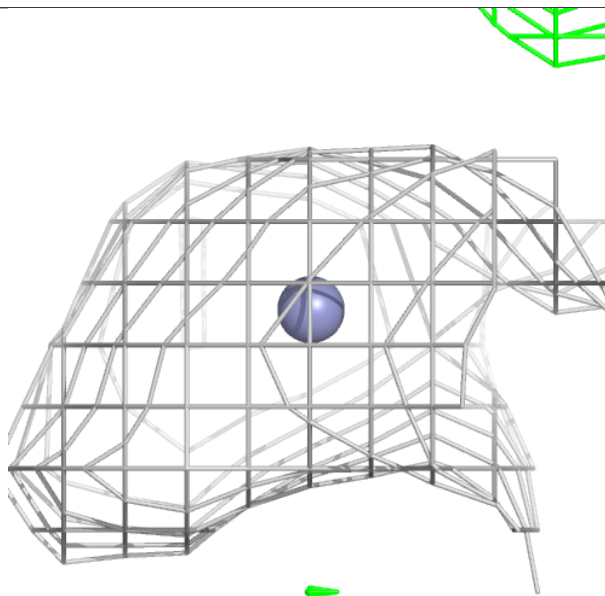
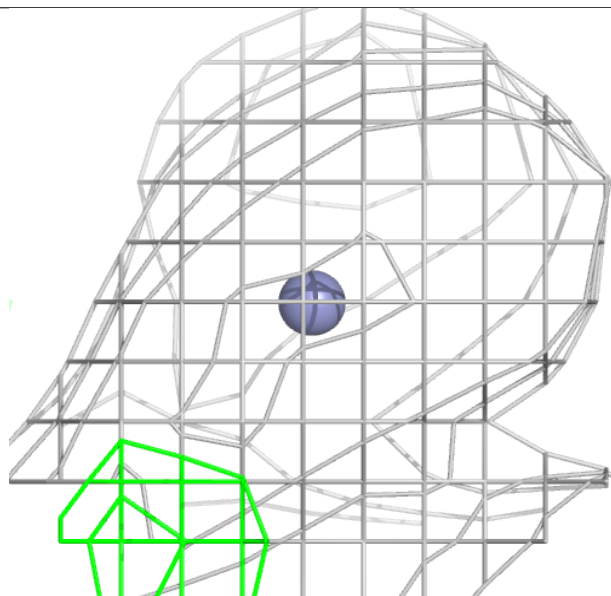
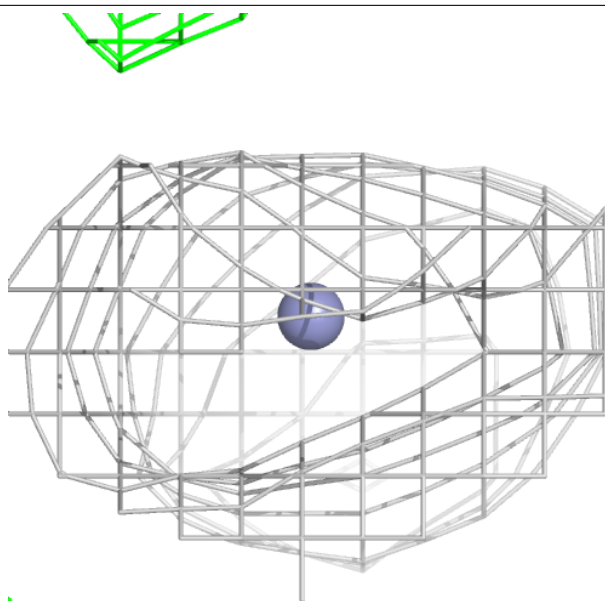
Electron density around ZN B 401:

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



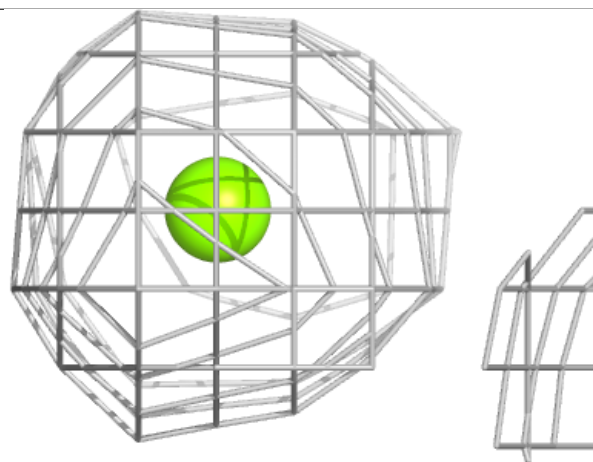
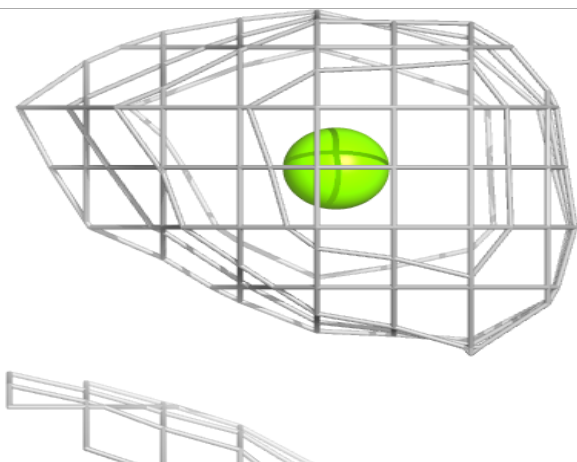
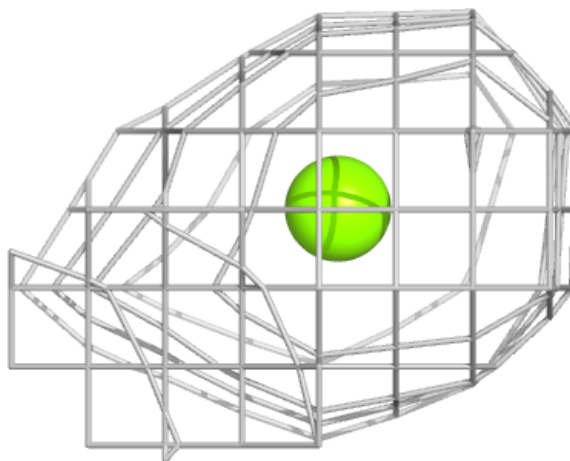
Electron density around ZN C 401:

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



Electron density around MG D 401:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.