



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:36 PM UTC

PDB ID : 8E8U / pdb_00008e8u
Title : Structure of the LOR domain of human AASS
Authors : Khamrui, S.; Lazarus, M.B.
Deposited on : 2022-08-25
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

<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

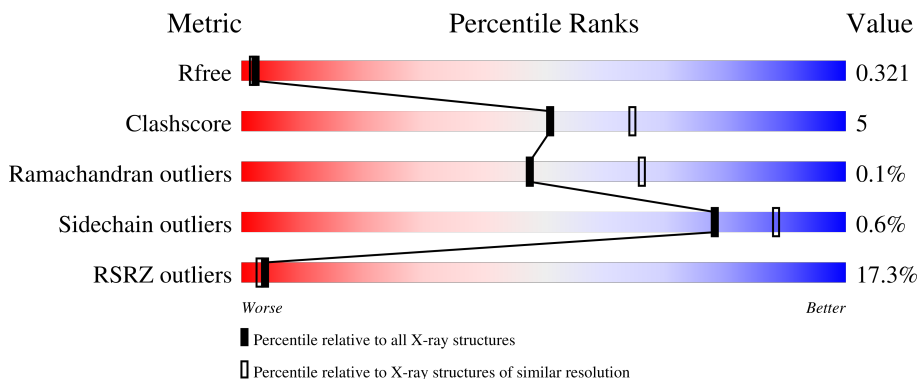
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1110 (2.66-2.66)
Clashscore	190562	1141 (2.66-2.66)
Ramachandran outliers	187476	1126 (2.66-2.66)
Sidechain outliers	187428	1126 (2.66-2.66)
RSRZ outliers	180081	1110 (2.66-2.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	452	24% 80% 15% 5%
1	B	452	10% 83% 12% 5%
1	C	452	24% 83% 12% •
1	D	452	8% 82% 13% 5%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13531 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 Alpha-aminoadipic semialdehyde synthase, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	430	Total	C	N	O	S	0	0	0
			3367	2135	588	622	22			
1	B	431	Total	C	N	O	S	0	0	0
			3371	2137	589	623	22			
1	C	432	Total	C	N	O	S	0	0	0
			3380	2142	590	626	22			
1	D	431	Total	C	N	O	S	0	0	0
			3371	2137	589	623	22			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP Q9UDR5
A	20	SER	-	expression tag	UNP Q9UDR5
A	97	ALA	GLU	conflict	UNP Q9UDR5
A	98	ALA	GLU	conflict	UNP Q9UDR5
A	99	ALA	LYS	conflict	UNP Q9UDR5
A	313	ALA	GLU	conflict	UNP Q9UDR5
A	314	ALA	GLN	conflict	UNP Q9UDR5
B	19	GLY	-	expression tag	UNP Q9UDR5
B	20	SER	-	expression tag	UNP Q9UDR5
B	97	ALA	GLU	conflict	UNP Q9UDR5
B	98	ALA	GLU	conflict	UNP Q9UDR5
B	99	ALA	LYS	conflict	UNP Q9UDR5
B	313	ALA	GLU	conflict	UNP Q9UDR5
B	314	ALA	GLN	conflict	UNP Q9UDR5
C	19	GLY	-	expression tag	UNP Q9UDR5
C	20	SER	-	expression tag	UNP Q9UDR5
C	97	ALA	GLU	conflict	UNP Q9UDR5
C	98	ALA	GLU	conflict	UNP Q9UDR5
C	99	ALA	LYS	conflict	UNP Q9UDR5
C	313	ALA	GLU	conflict	UNP Q9UDR5
C	314	ALA	GLN	conflict	UNP Q9UDR5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	19	GLY	-	expression tag	UNP Q9UDR5
D	20	SER	-	expression tag	UNP Q9UDR5
D	97	ALA	GLU	conflict	UNP Q9UDR5
D	98	ALA	GLU	conflict	UNP Q9UDR5
D	99	ALA	LYS	conflict	UNP Q9UDR5
D	313	ALA	GLU	conflict	UNP Q9UDR5
D	314	ALA	GLN	conflict	UNP Q9UDR5

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

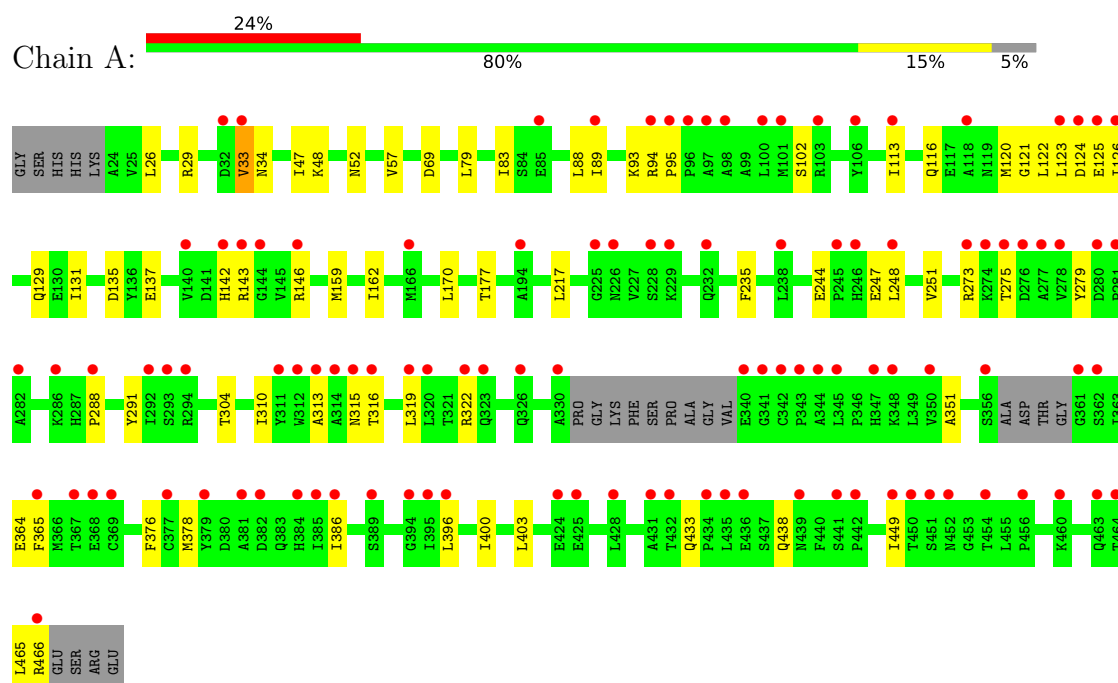
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	10	Total O 10 10	0	0
3	B	8	Total O 8 8	0	0
3	C	11	Total O 11 11	0	0
3	D	11	Total O 11 11	0	0

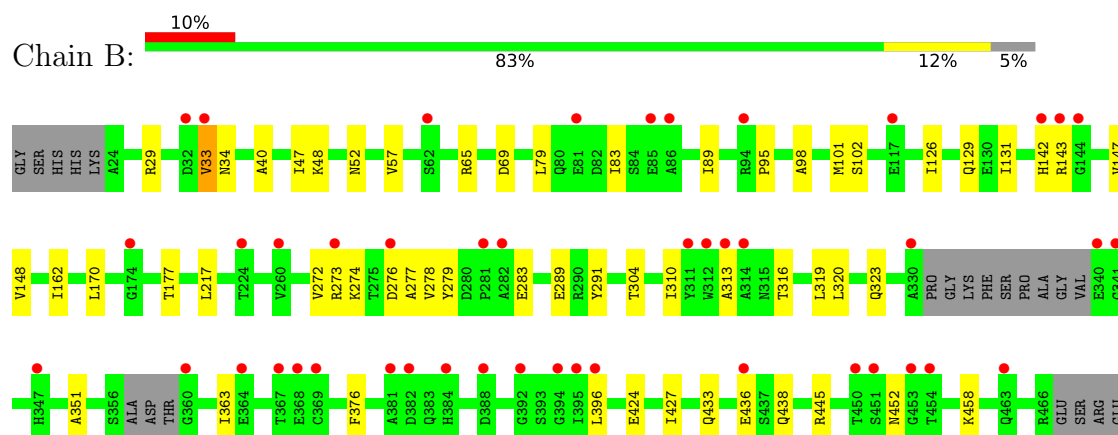
3 Residue-property plots [i](#)

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.

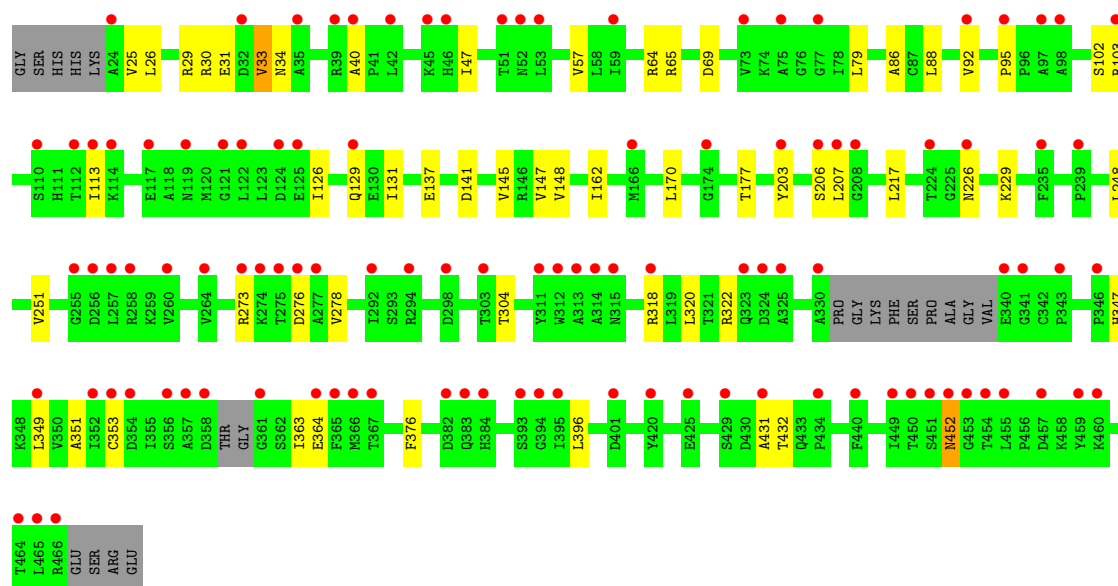
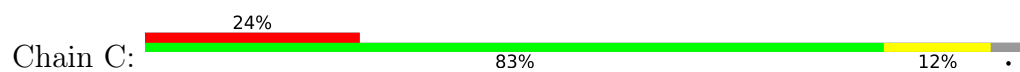
- Molecule 1: Alpha-aminoadipic semialdehyde synthase, mitochondrial



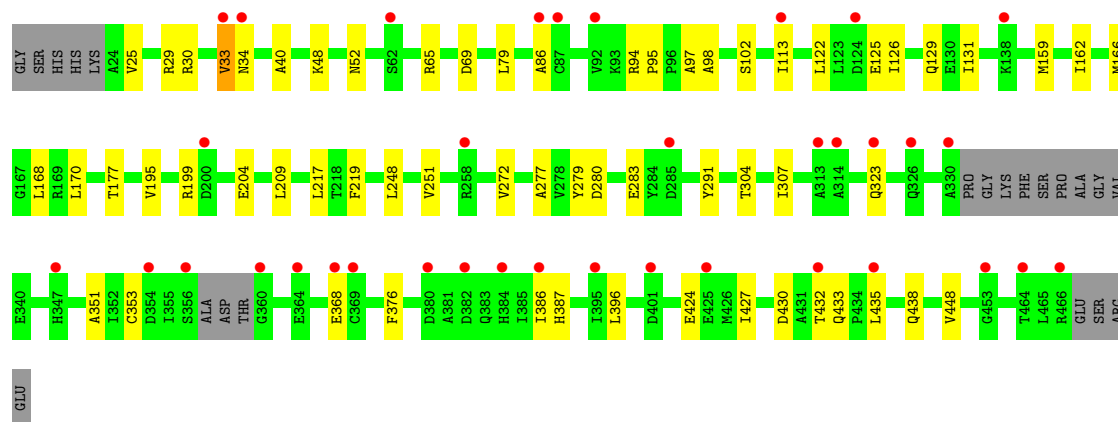
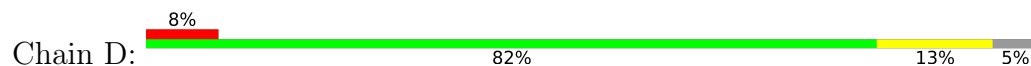
- Molecule 1: Alpha-aminoadipic semialdehyde synthase, mitochondrial



- Molecule 1: Alpha-aminoadipic semialdehyde synthase, mitochondrial



- Molecule 1: Alpha-aminoadipic semialdehyde synthase, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	73.00Å 131.94Å 96.49Å 90.00° 100.72° 90.00°	Depositor
Resolution (Å)	47.41 – 2.65 47.41 – 2.65	Depositor EDS
% Data completeness (in resolution range)	96.0 (47.41-2.65) 96.2 (47.41-2.65)	Depositor EDS
R_{merge}	0.41	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.51 (at 2.65Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.278 , 0.319 0.278 , 0.321	Depositor DCC
R_{free} test set	2497 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	34.3	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.57$, $\langle L^2 \rangle = 0.41$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	13531	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 59.02 % 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 1.8778e-05. 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: MG

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	0.11	0/3441	0.32	0/4667
1	B	0.10	0/3445	0.30	0/4672
1	C	0.12	0/3454	0.33	0/4685
1	D	0.10	0/3445	0.31	0/4672
All	All	0.11	0/13785	0.32	0/18696

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	3367	0	3352	42	0
1	B	3371	0	3355	32	0
1	C	3380	0	3361	36	0
1	D	3371	0	3355	32	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	10	0	0	1	0
3	B	8	0	0	0	0
3	C	11	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	11	0	0	0	0
All	All	13531	0	13423	140	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 5.

All (140) 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:B:436:GLU:OE1	1:B:445:ARG:NH2	2.24	0.70
1:C:273:ARG:HD2	1:C:276:ASP:HB2	1.75	0.69
1:B:69:ASP:HB3	1:B:79:LEU:HD11	1.76	0.67
1:C:273:ARG:HG3	1:C:276:ASP:H	1.60	0.66
1:A:135:ASP:HB2	1:A:449:ILE:HD11	1.78	0.65
1:C:40:ALA:HB2	1:C:65:ARG:HD3	1.79	0.65
1:C:69:ASP:HB3	1:C:79:LEU:HD11	1.79	0.64
1:D:69:ASP:HB3	1:D:79:LEU:HD11	1.79	0.64
1:D:40:ALA:HB2	1:D:65:ARG:HD3	1.80	0.64
1:A:288:PRO:HG2	1:A:315:ASN:HB2	1.81	0.63
1:B:273:ARG:NH2	1:B:283:GLU:OE2	2.31	0.63
1:D:113:ILE:HD12	1:D:113:ILE:H	1.63	0.62
1:D:48:LYS:NZ	1:D:52:ASN:OD1	2.33	0.61
1:B:126:ILE:HG23	1:B:131:ILE:HB	1.81	0.61
1:C:203:TYR:O	1:C:207:LEU:N	2.33	0.61
1:B:273:ARG:HG2	1:B:278:VAL:H	1.66	0.60
1:A:120:MET:SD	1:A:466:ARG:NE	2.75	0.60
1:A:137:GLU:HA	1:A:146:ARG:HD2	1.83	0.60
1:C:126:ILE:HG23	1:C:131:ILE:HB	1.84	0.59
1:D:126:ILE:HG23	1:D:131:ILE:HB	1.83	0.59
1:D:166:MET:HE1	1:D:219:PHE:HE2	1.66	0.59
1:A:378:MET:HB2	1:A:386:ILE:HG13	1.85	0.57
1:B:48:LYS:NZ	1:B:52:ASN:OD1	2.38	0.57
1:D:97:ALA:HB1	1:D:125:GLU:HG3	1.85	0.57
1:A:159:MET:HE2	1:A:235:PHE:HB2	1.87	0.56
1:A:170:LEU:HD13	1:A:177:THR:HG21	1.86	0.56
1:B:40:ALA:HB2	1:B:65:ARG:HD3	1.87	0.56
1:C:320:LEU:HB2	1:C:363:ILE:HD12	1.88	0.56
1:A:126:ILE:HG23	1:A:131:ILE:HB	1.87	0.55
1:A:310:ILE:HD12	1:A:319:LEU:HD11	1.88	0.55
1:A:273:ARG:HG2	1:A:275:THR:H	1.72	0.55
1:D:159:MET:HE1	1:D:307:ILE:HG13	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:ARG:NH2	1:C:364:GLU:OE1	2.40	0.54
1:D:217:LEU:HD22	1:D:304:THR:HG21	1.90	0.54
1:A:162:ILE:HD11	1:A:351:ALA:HB1	1.90	0.53
1:B:433:GLN:HB2	1:B:438:GLN:NE2	2.24	0.53
1:C:47:ILE:HD12	1:C:57:VAL:HG11	1.91	0.53
1:D:102:SER:HA	1:D:129:GLN:HB3	1.91	0.53
1:D:376:PHE:HB3	1:D:396:LEU:HD11	1.90	0.52
1:A:69:ASP:HB3	1:A:79:LEU:HD11	1.91	0.52
1:B:436:GLU:HA	1:B:445:ARG:NH2	2.25	0.52
1:A:33:VAL:HG11	1:A:93:LYS:HD3	1.91	0.52
1:A:248:LEU:HA	1:A:251:VAL:HG22	1.92	0.51
1:A:217:LEU:HD22	1:A:304:THR:HG21	1.92	0.51
1:A:433:GLN:HB2	1:A:438:GLN:NE2	2.26	0.51
1:B:83:ILE:HD12	1:B:89:ILE:HD12	1.93	0.51
1:D:435:LEU:HD21	1:D:448:VAL:HG11	1.92	0.51
1:B:33:VAL:HG13	1:B:34:ASN:H	1.75	0.51
1:A:322:ARG:HG3	1:A:364:GLU:HG3	1.93	0.50
1:C:103:ARG:HD3	1:C:432:THR:HG22	1.93	0.50
1:B:102:SER:HA	1:B:129:GLN:HB3	1.94	0.50
1:A:322:ARG:HG2	1:A:365:PHE:HB3	1.93	0.50
1:D:272:VAL:HB	1:D:277:ALA:HA	1.91	0.50
1:A:123:LEU:HD23	1:A:466:ARG:HH21	1.77	0.50
1:A:433:GLN:HB2	1:A:438:GLN:HE21	1.77	0.50
1:B:217:LEU:HD22	1:B:304:THR:HG21	1.93	0.50
1:B:310:ILE:HD12	1:B:319:LEU:HD11	1.94	0.50
1:D:433:GLN:HB2	1:D:438:GLN:NE2	2.26	0.50
1:B:272:VAL:HB	1:B:277:ALA:HA	1.94	0.49
1:B:274:LYS:NZ	1:B:289:GLU:O	2.45	0.49
1:C:322:ARG:N	1:C:364:GLU:OE2	2.33	0.49
1:C:162:ILE:HD11	1:C:351:ALA:HB1	1.93	0.49
1:B:162:ILE:HD11	1:B:351:ALA:HB1	1.94	0.49
1:A:48:LYS:NZ	1:A:52:ASN:OD1	2.46	0.49
1:B:98:ALA:HB2	1:D:323:GLN:NE2	2.27	0.49
1:A:29:ARG:CZ	1:A:95:PRO:HB3	2.43	0.49
1:A:94:ARG:HG3	1:A:122:LEU:HD22	1.94	0.49
1:D:33:VAL:HG13	1:D:34:ASN:H	1.77	0.49
1:B:83:ILE:HG13	1:B:101:MET:HE1	1.95	0.49
1:C:376:PHE:HB3	1:C:396:LEU:HD11	1.95	0.49
1:D:424:GLU:O	1:D:427:ILE:HG22	2.12	0.48
1:A:102:SER:HA	1:A:129:GLN:HB3	1.95	0.48
1:A:33:VAL:HG13	1:A:34:ASN:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:GLN:O	1:A:120:MET:HG2	2.12	0.48
1:D:162:ILE:HD11	1:D:351:ALA:HB1	1.95	0.48
1:B:424:GLU:O	1:B:427:ILE:HG22	2.13	0.48
1:B:376:PHE:HB3	1:B:396:LEU:HD11	1.96	0.48
1:C:217:LEU:HD22	1:C:304:THR:HG21	1.94	0.48
1:C:170:LEU:HD13	1:C:177:THR:HG21	1.94	0.48
1:B:170:LEU:HD13	1:B:177:THR:HG21	1.95	0.48
1:D:368:GLU:OE1	1:D:387:HIS:NE2	2.44	0.48
1:C:248:LEU:HA	1:C:251:VAL:HG22	1.96	0.47
1:D:170:LEU:HD13	1:D:177:THR:HG21	1.96	0.47
1:B:273:ARG:HG3	1:B:276:ASP:H	1.78	0.47
1:D:162:ILE:HD13	1:D:353:CYS:HB2	1.97	0.47
1:D:248:LEU:HA	1:D:251:VAL:HG22	1.96	0.47
1:C:273:ARG:HD2	1:C:276:ASP:CB	2.41	0.47
1:A:83:ILE:HD12	1:A:89:ILE:HD12	1.97	0.47
1:C:33:VAL:HG13	1:C:34:ASN:H	1.79	0.46
1:D:94:ARG:HG3	1:D:122:LEU:HD22	1.96	0.46
1:A:26:LEU:HD13	1:A:88:LEU:HD23	1.98	0.46
1:C:102:SER:HA	1:C:129:GLN:HB3	1.98	0.46
1:C:226:ASN:HA	1:C:229:LYS:HE2	1.97	0.46
1:B:320:LEU:HB2	1:B:363:ILE:HD12	1.96	0.46
1:D:166:MET:HE1	1:D:219:PHE:CE2	2.49	0.46
1:B:47:ILE:HG23	1:B:57:VAL:HG11	1.98	0.46
1:C:203:TYR:HA	1:C:206:SER:OG	2.16	0.46
1:D:280:ASP:HB3	1:D:283:GLU:HB3	1.97	0.46
1:C:162:ILE:HD13	1:C:353:CYS:HB2	1.99	0.45
1:A:376:PHE:HB3	1:A:396:LEU:HD11	1.98	0.45
1:A:135:ASP:OD1	1:A:137:GLU:HG2	2.17	0.45
1:C:273:ARG:HG2	1:C:278:VAL:H	1.81	0.45
1:A:279:TYR:HA	1:A:291:TYR:HE2	1.80	0.45
1:C:25:VAL:HB	1:C:86:ALA:HA	1.98	0.45
1:C:31:GLU:CD	1:C:92:VAL:HG22	2.42	0.45
1:C:113:ILE:HD13	1:C:137:GLU:OE2	2.17	0.44
1:A:47:ILE:HD12	1:A:57:VAL:HG11	1.99	0.44
1:C:141:ASP:OD1	1:C:145:VAL:N	2.50	0.44
1:A:244:GLU:HB2	1:A:247:GLU:HG3	2.00	0.44
1:C:113:ILE:H	1:C:113:ILE:HD12	1.82	0.44
1:A:33:VAL:HG22	1:A:34:ASN:HD22	1.83	0.44
1:B:142:HIS:CD2	1:B:143:ARG:HG3	2.52	0.44
1:B:147:VAL:HG23	1:B:148:VAL:HG23	2.00	0.44
1:B:313:ALA:HB3	1:B:316:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ILE:HB	1:A:403:LEU:HG	2.00	0.44
1:C:431:ALA:O	1:C:452:ASN:ND2	2.51	0.44
1:C:29:ARG:CZ	1:C:95:PRO:HB3	2.49	0.43
1:A:113:ILE:HG12	3:A:601:HOH:O	2.18	0.43
1:B:323:GLN:NE2	1:D:98:ALA:HB2	2.34	0.43
1:D:430:ASP:OD1	1:D:432:THR:HG22	2.18	0.43
1:A:142:HIS:CD2	1:A:143:ARG:HG3	2.54	0.43
1:B:29:ARG:CZ	1:B:95:PRO:HB3	2.49	0.43
1:D:29:ARG:CZ	1:D:95:PRO:HB3	2.49	0.42
1:D:25:VAL:HB	1:D:86:ALA:HA	2.00	0.42
1:B:458:LYS:H	1:B:458:LYS:HG2	1.59	0.42
1:C:33:VAL:HG22	1:C:34:ASN:HD22	1.84	0.42
1:C:347:HIS:ND1	1:C:349:LEU:O	2.54	0.41
1:A:93:LYS:HB3	1:A:93:LYS:HE2	1.85	0.41
1:B:279:TYR:HA	1:B:291:TYR:HE2	1.86	0.41
1:C:26:LEU:HD13	1:C:88:LEU:HD23	2.02	0.41
1:D:195:VAL:O	1:D:199:ARG:HG3	2.20	0.41
1:C:273:ARG:CG	1:C:276:ASP:H	2.31	0.41
1:A:273:ARG:HA	1:A:291:TYR:HA	2.02	0.40
1:C:147:VAL:HG23	1:C:148:VAL:HG23	2.03	0.40
1:C:31:GLU:O	1:C:64:ARG:NH1	2.48	0.40
1:D:204:GLU:HB3	1:D:209:LEU:HD12	2.04	0.40
1:D:279:TYR:HA	1:D:291:TYR:HE2	1.86	0.40
1:A:121:GLY:O	1:A:125:GLU:HG2	2.21	0.40
1:A:124:ASP:OD1	1:A:125:GLU:N	2.55	0.40
1:A:313:ALA:HB3	1:A:316:THR:HG23	2.03	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	424/452 (94%)	418 (99%)	6 (1%)	0	100	100
1	B	425/452 (94%)	418 (98%)	6 (1%)	1 (0%)	43	60
1	C	426/452 (94%)	419 (98%)	6 (1%)	1 (0%)	43	60
1	D	425/452 (94%)	422 (99%)	3 (1%)	0	100	100
All	All	1700/1808 (94%)	1677 (99%)	21 (1%)	2 (0%)	48	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	452	ASN
1	B	452	ASN

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	363/379 (96%)	361 (99%)	2 (1%)	78	88
1	B	363/379 (96%)	362 (100%)	1 (0%)	86	94
1	C	364/379 (96%)	362 (100%)	2 (0%)	81	91
1	D	363/379 (96%)	359 (99%)	4 (1%)	65	80
All	All	1453/1516 (96%)	1444 (99%)	9 (1%)	78	88

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	465	LEU
1	B	33	VAL
1	C	30	ARG
1	C	33	VAL
1	D	30	ARG
1	D	33	VAL
1	D	168	LEU
1	D	386	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	175	HIS
1	A	226	ASN
1	A	287	HIS
1	B	111	HIS
1	B	246	HIS
1	B	287	HIS
1	B	452	ASN
1	C	119	ASN
1	C	152	GLN
1	C	246	HIS
1	C	268	HIS
1	C	326	GLN
1	C	384	HIS
1	C	387	HIS
1	C	433	GLN
1	C	452	ASN
1	D	63	ASN
1	D	161	ASN
1	D	308	ASN
1	D	326	GLN
1	D	406	GLN
1	D	452	ASN

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 2 ligands modelled in this entry, 2 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 ⓘ

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	430/452 (95%)	1.38	109 (25%) 1 1	26, 46, 82, 105	0
1	B	431/452 (95%)	0.82	45 (10%) 11 9	12, 39, 69, 105	0
1	C	432/452 (95%)	1.45	108 (25%) 2 1	18, 47, 78, 105	0
1	D	431/452 (95%)	0.81	36 (8%) 17 12	15, 40, 70, 93	0
All	All	1724/1808 (95%)	1.12	298 (17%) 4 3	12, 44, 77, 105	0

All (298) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	451	SER	7.2
1	A	314	ALA	6.7
1	C	364	GLU	6.2
1	C	206	SER	5.9
1	C	466	ARG	5.7
1	B	314	ALA	5.6
1	C	258	ARG	5.6
1	A	347	HIS	5.4
1	A	395	ILE	5.4
1	A	313	ALA	5.4
1	A	125	GLU	5.2
1	A	466	ARG	5.0
1	C	454	THR	4.9
1	A	451	SER	4.8
1	C	51	THR	4.8
1	C	357	ALA	4.7
1	C	275	THR	4.6
1	C	366	MET	4.6
1	C	274	LYS	4.5
1	C	315	ASN	4.5
1	A	382	ASP	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	382	ASP	4.4
1	C	358	ASP	4.4
1	C	356	SER	4.3
1	D	323	GLN	4.3
1	A	439	ASN	4.2
1	A	367	THR	4.1
1	C	457	ASP	4.0
1	D	369	CYS	4.0
1	A	362	SER	3.9
1	D	62	SER	3.9
1	A	288	PRO	3.9
1	C	330	ALA	3.9
1	A	312	TRP	3.9
1	D	382	ASP	3.8
1	C	449	ILE	3.8
1	D	360	GLY	3.8
1	A	246	HIS	3.8
1	B	330	ALA	3.8
1	B	360	GLY	3.8
1	A	311	TYR	3.7
1	A	340	GLU	3.7
1	D	356	SER	3.6
1	C	367	THR	3.6
1	C	273	ARG	3.6
1	C	276	ASP	3.6
1	A	389	SER	3.6
1	B	142	HIS	3.5
1	A	144	GLY	3.5
1	A	330	ALA	3.5
1	B	463	GLN	3.5
1	A	368	GLU	3.5
1	B	368	GLU	3.5
1	B	94	ARG	3.5
1	C	361	GLY	3.5
1	A	450	THR	3.4
1	C	453	GLY	3.4
1	A	463	GLN	3.4
1	A	377	CYS	3.4
1	A	95	PRO	3.4
1	A	103	ARG	3.4
1	B	347	HIS	3.4
1	C	292	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	85	GLU	3.3
1	C	122	LEU	3.3
1	C	52	ASN	3.3
1	A	386	ILE	3.3
1	C	294	ARG	3.3
1	C	341	GLY	3.3
1	C	313	ALA	3.3
1	B	33	VAL	3.3
1	C	117	GLU	3.2
1	D	432	THR	3.2
1	A	425	GLU	3.2
1	D	368	GLU	3.2
1	C	110	SER	3.2
1	A	278	VAL	3.2
1	C	314	ALA	3.2
1	D	330	ALA	3.2
1	A	292	ILE	3.1
1	D	34	ASN	3.1
1	A	396	LEU	3.1
1	D	453	GLY	3.1
1	C	455	LEU	3.1
1	A	142	HIS	3.1
1	C	343	PRO	3.1
1	C	312	TRP	3.1
1	A	348	LYS	3.0
1	A	89	ILE	3.0
1	B	273	ARG	3.0
1	C	98	ALA	3.0
1	D	425	GLU	3.0
1	C	124	ASP	3.0
1	A	294	ARG	3.0
1	C	24	ALA	3.0
1	D	87	CYS	3.0
1	B	384	HIS	3.0
1	D	258	ARG	3.0
1	A	275	THR	3.0
1	B	144	GLY	3.0
1	C	255	GLY	3.0
1	A	286	LYS	3.0
1	A	379	TYR	3.0
1	C	401	ASP	3.0
1	C	465	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	436	GLU	2.9
1	A	248	LEU	2.9
1	C	384	HIS	2.9
1	A	369	CYS	2.9
1	D	466	ARG	2.9
1	D	200	ASP	2.9
1	A	394	GLY	2.9
1	A	85	GLU	2.9
1	A	96	PRO	2.9
1	A	464	THR	2.9
1	C	431	ALA	2.9
1	A	126	ILE	2.8
1	B	174	GLY	2.8
1	B	388	ASP	2.8
1	A	100	LEU	2.8
1	A	345	LEU	2.8
1	A	434	PRO	2.8
1	C	324	ASP	2.8
1	A	435	LEU	2.8
1	A	33	VAL	2.8
1	A	385	ILE	2.8
1	B	81	GLU	2.8
1	C	95	PRO	2.8
1	C	318	ARG	2.8
1	C	298	ASP	2.8
1	D	313	ALA	2.8
1	A	460	LYS	2.7
1	A	361	GLY	2.7
1	A	277	ALA	2.7
1	D	33	VAL	2.7
1	A	273	ARG	2.7
1	C	40	ALA	2.7
1	B	62	SER	2.7
1	D	326	GLN	2.6
1	A	98	ALA	2.6
1	B	260	VAL	2.6
1	B	451	SER	2.6
1	C	365	PHE	2.6
1	C	429	SER	2.6
1	C	224	THR	2.6
1	B	276	ASP	2.6
1	D	354	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	449	ILE	2.6
1	D	113	ILE	2.6
1	A	320	LEU	2.6
1	A	342	CYS	2.6
1	A	350	VAL	2.6
1	C	383	GLN	2.6
1	C	450	THR	2.6
1	C	32	ASP	2.6
1	A	194	ALA	2.6
1	A	365	PHE	2.6
1	B	86	ALA	2.6
1	A	101	MET	2.5
1	C	46	HIS	2.5
1	A	341	GLY	2.5
1	A	456	PRO	2.5
1	A	118	ALA	2.5
1	A	226	ASN	2.5
1	A	454	THR	2.5
1	A	166	MET	2.5
1	A	276	ASP	2.5
1	C	349	LEU	2.5
1	B	394	GLY	2.5
1	C	303	THR	2.5
1	C	452	ASN	2.5
1	A	143	ARG	2.5
1	C	103	ARG	2.5
1	D	384	HIS	2.5
1	B	340	GLU	2.5
1	B	367	THR	2.5
1	D	395	ILE	2.5
1	D	285	ASP	2.5
1	D	347	HIS	2.5
1	C	460	LYS	2.4
1	C	354	ASP	2.4
1	D	92	VAL	2.4
1	A	432	THR	2.4
1	C	394	GLY	2.4
1	A	323	GLN	2.4
1	D	86	ALA	2.4
1	A	245	PRO	2.4
1	C	92	VAL	2.4
1	C	277	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	123	LEU	2.4
1	B	450	THR	2.4
1	A	315	ASN	2.4
1	A	441	SER	2.4
1	A	343	PRO	2.4
1	C	346	PRO	2.4
1	C	352	ILE	2.3
1	A	124	ASP	2.3
1	A	442	PRO	2.3
1	B	453	GLY	2.3
1	C	59	ILE	2.3
1	C	113	ILE	2.3
1	D	386	ILE	2.3
1	A	274	LYS	2.3
1	A	424	GLU	2.3
1	D	401	ASP	2.3
1	B	312	TRP	2.3
1	C	434	PRO	2.3
1	A	431	ALA	2.3
1	A	316	THR	2.3
1	B	311	TYR	2.3
1	C	420	TYR	2.3
1	C	45	LYS	2.3
1	C	382	ASP	2.3
1	A	97	ALA	2.3
1	B	395	ILE	2.3
1	C	75	ALA	2.3
1	C	112	THR	2.3
1	A	326	GLN	2.3
1	B	392	GLY	2.3
1	C	73	VAL	2.3
1	C	114	LYS	2.2
1	B	364	GLU	2.2
1	A	280	ASP	2.2
1	B	32	ASP	2.2
1	A	428	LEU	2.2
1	C	42	LEU	2.2
1	A	229	LYS	2.2
1	B	313	ALA	2.2
1	C	39	ARG	2.2
1	B	369	CYS	2.2
1	C	353	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	364	GLU	2.2
1	A	106	TYR	2.2
1	A	452	ASN	2.2
1	A	281	PRO	2.2
1	A	238	LEU	2.2
1	A	282	ALA	2.2
1	C	340	GLU	2.2
1	B	224	THR	2.2
1	C	174	GLY	2.2
1	A	32	ASP	2.2
1	D	124	ASP	2.2
1	A	113	ILE	2.2
1	C	264	VAL	2.2
1	C	440	PHE	2.2
1	A	381	ALA	2.1
1	B	117	GLU	2.1
1	A	232	GLN	2.1
1	C	207	LEU	2.1
1	B	341	GLY	2.1
1	A	384	HIS	2.1
1	C	256	ASP	2.1
1	B	381	ALA	2.1
1	C	97	ALA	2.1
1	A	146	ARG	2.1
1	B	143	ARG	2.1
1	A	319	LEU	2.1
1	C	166	MET	2.1
1	C	257	LEU	2.1
1	A	140	VAL	2.1
1	A	228	SER	2.1
1	C	235	PHE	2.1
1	A	344	ALA	2.1
1	B	282	ALA	2.1
1	C	35	ALA	2.1
1	C	325	ALA	2.1
1	B	454	THR	2.1
1	C	464	THR	2.1
1	D	464	THR	2.1
1	C	129	GLN	2.1
1	C	323	GLN	2.1
1	C	77	GLY	2.1
1	C	121	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	208	GLY	2.1
1	C	311	TYR	2.1
1	C	395	ILE	2.1
1	C	393	SER	2.1
1	A	94	ARG	2.1
1	B	436	GLU	2.1
1	C	425	GLU	2.1
1	D	314	ALA	2.1
1	D	138	LYS	2.1
1	C	239	PRO	2.1
1	C	119	ASN	2.1
1	A	225	GLY	2.1
1	A	322	ARG	2.0
1	D	380	ASP	2.0
1	C	125	GLU	2.0
1	B	281	PRO	2.0
1	C	203	TYR	2.0
1	C	260	VAL	2.0
1	A	293	SER	2.0
1	A	356	SER	2.0
1	B	396	LEU	2.0
1	C	53	LEU	2.0
1	D	435	LEU	2.0
1	C	226	ASN	2.0
1	C	459	TYR	2.0

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

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

6.3 Carbohydrates ⓘ

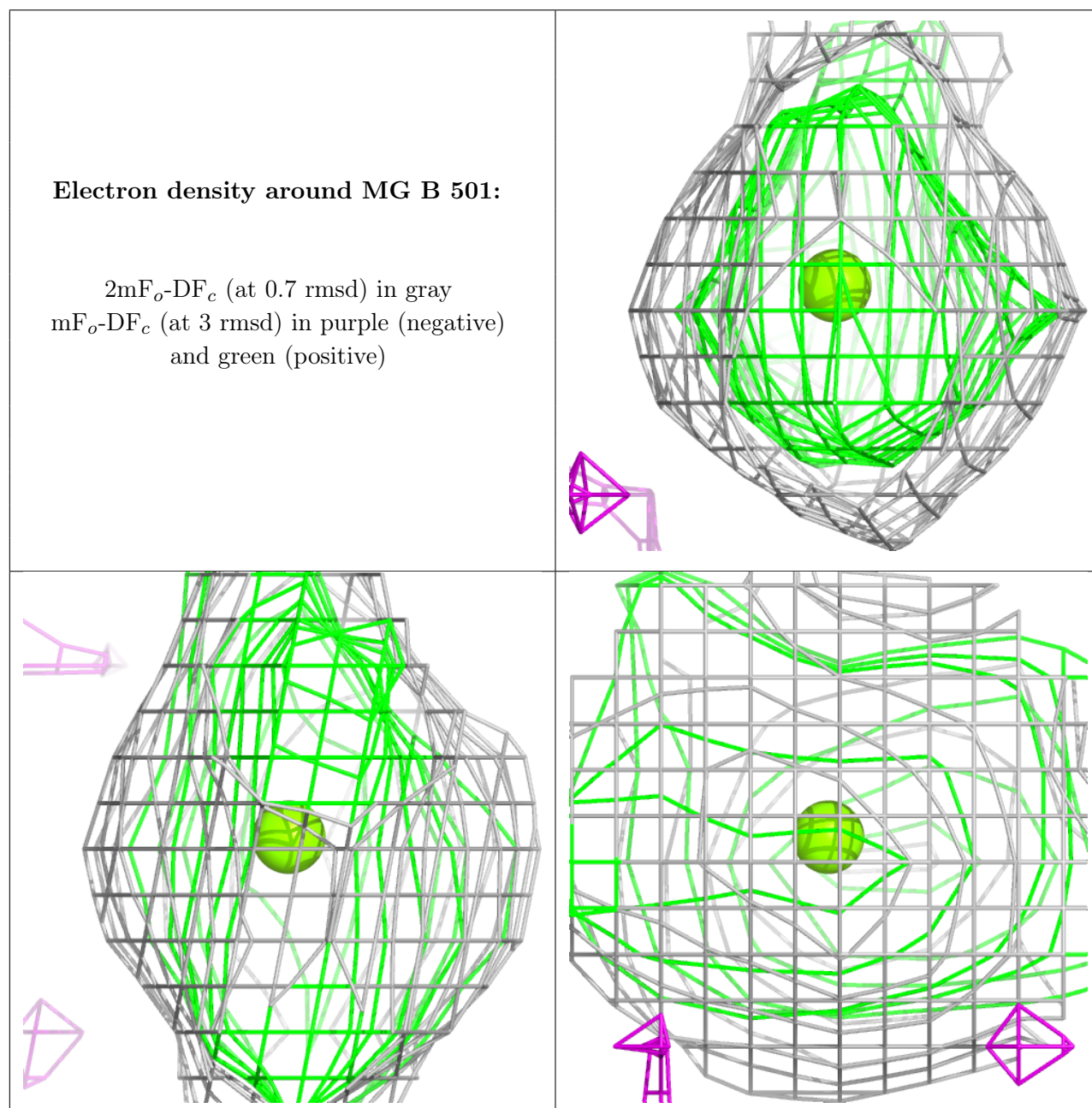
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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

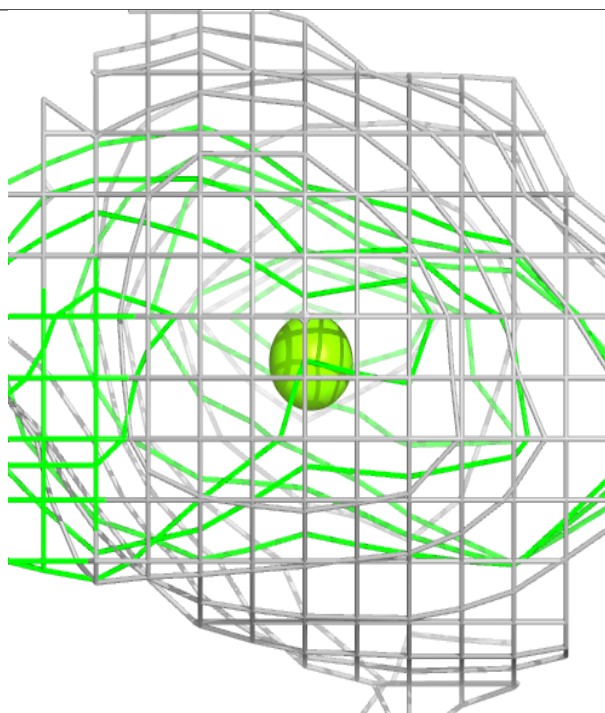
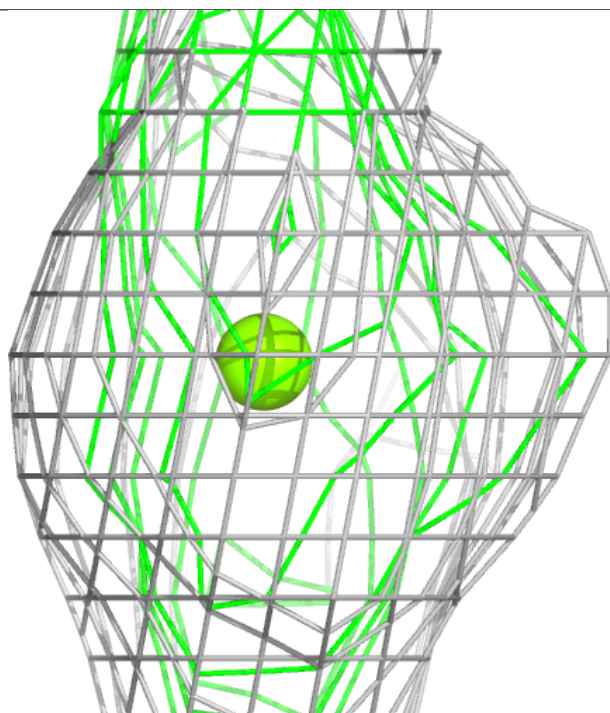
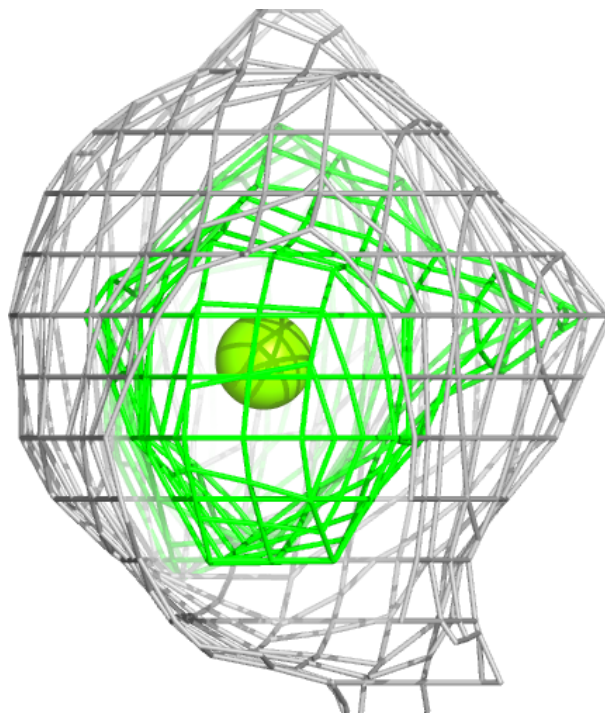
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	B	501	1/1	0.94	0.32	32,32,32,32	0
2	MG	A	501	1/1	0.97	0.25	25,25,25,25	0

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 MG A 501:

$2mF_o-DF_c$ (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.