



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 02:14 PM EDT

PDB ID : 8D1X
Title : Crystal Structure of aminopeptidase A from Neisseria gonorrhoeae
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2022-05-27
Resolution : 2.80 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35.1

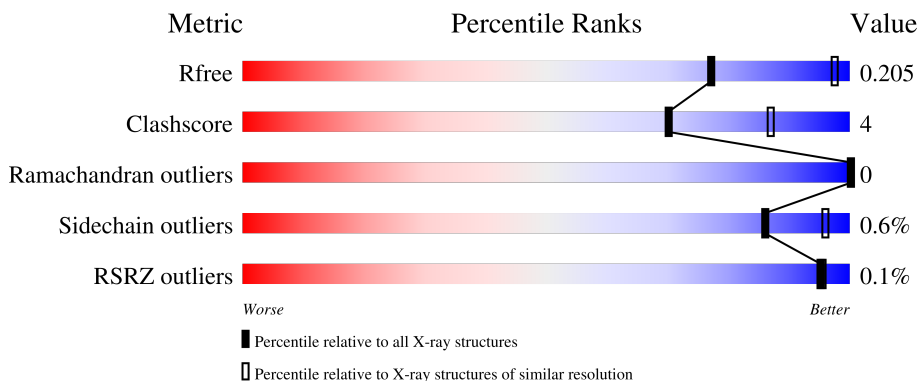
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	476	89% (0% poor fit, 9% outliers)
1	B	476	89% (0% poor fit, 9% outliers)
1	C	476	91% (0% poor fit, 8% outliers)
1	D	476	88% (10% poor fit, 10% outliers)
1	E	476	90% (0% poor fit, 8% outliers)

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Mol	Chain	Length	Quality of chain
1	F	476	 89% 9%

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
4	TAR	B	502	-	X	-	-
4	TAR	F	502	-	X	-	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 21162 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 Probable cytosol aminopeptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	468	3472	2198	583	675	16	0	0	0
1	B	468	3458	2194	582	666	16	0	0	0
1	C	467	3380	2144	567	653	16	0	0	0
1	D	469	3456	2188	578	674	16	0	0	0
1	E	468	3426	2173	574	663	16	0	0	0
1	F	469	3474	2202	583	673	16	0	0	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP B4RJ22
A	-6	ALA	-	expression tag	UNP B4RJ22
A	-5	HIS	-	expression tag	UNP B4RJ22
A	-4	HIS	-	expression tag	UNP B4RJ22
A	-3	HIS	-	expression tag	UNP B4RJ22
A	-2	HIS	-	expression tag	UNP B4RJ22
A	-1	HIS	-	expression tag	UNP B4RJ22
A	0	HIS	-	expression tag	UNP B4RJ22
B	-7	MET	-	initiating methionine	UNP B4RJ22
B	-6	ALA	-	expression tag	UNP B4RJ22
B	-5	HIS	-	expression tag	UNP B4RJ22
B	-4	HIS	-	expression tag	UNP B4RJ22
B	-3	HIS	-	expression tag	UNP B4RJ22
B	-2	HIS	-	expression tag	UNP B4RJ22
B	-1	HIS	-	expression tag	UNP B4RJ22
B	0	HIS	-	expression tag	UNP B4RJ22
C	-7	MET	-	initiating methionine	UNP B4RJ22

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-6	ALA	-	expression tag	UNP B4RJ22
C	-5	HIS	-	expression tag	UNP B4RJ22
C	-4	HIS	-	expression tag	UNP B4RJ22
C	-3	HIS	-	expression tag	UNP B4RJ22
C	-2	HIS	-	expression tag	UNP B4RJ22
C	-1	HIS	-	expression tag	UNP B4RJ22
C	0	HIS	-	expression tag	UNP B4RJ22
D	-7	MET	-	initiating methionine	UNP B4RJ22
D	-6	ALA	-	expression tag	UNP B4RJ22
D	-5	HIS	-	expression tag	UNP B4RJ22
D	-4	HIS	-	expression tag	UNP B4RJ22
D	-3	HIS	-	expression tag	UNP B4RJ22
D	-2	HIS	-	expression tag	UNP B4RJ22
D	-1	HIS	-	expression tag	UNP B4RJ22
D	0	HIS	-	expression tag	UNP B4RJ22
E	-7	MET	-	initiating methionine	UNP B4RJ22
E	-6	ALA	-	expression tag	UNP B4RJ22
E	-5	HIS	-	expression tag	UNP B4RJ22
E	-4	HIS	-	expression tag	UNP B4RJ22
E	-3	HIS	-	expression tag	UNP B4RJ22
E	-2	HIS	-	expression tag	UNP B4RJ22
E	-1	HIS	-	expression tag	UNP B4RJ22
E	0	HIS	-	expression tag	UNP B4RJ22
F	-7	MET	-	initiating methionine	UNP B4RJ22
F	-6	ALA	-	expression tag	UNP B4RJ22
F	-5	HIS	-	expression tag	UNP B4RJ22
F	-4	HIS	-	expression tag	UNP B4RJ22
F	-3	HIS	-	expression tag	UNP B4RJ22
F	-2	HIS	-	expression tag	UNP B4RJ22
F	-1	HIS	-	expression tag	UNP B4RJ22
F	0	HIS	-	expression tag	UNP B4RJ22

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn) (labeled as "Ligand of Interest" by depositor).

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

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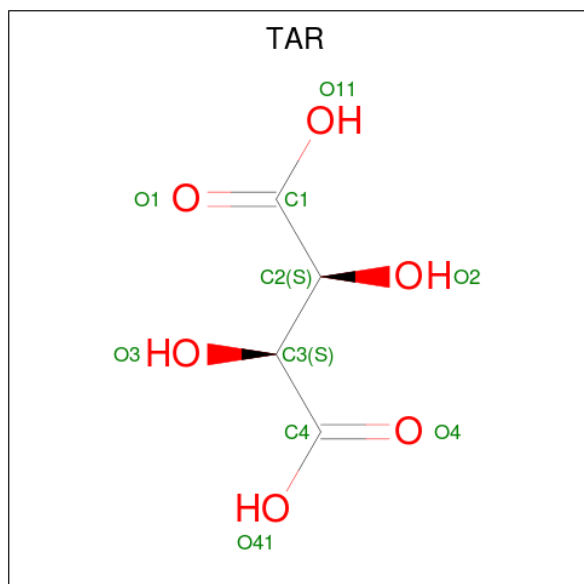
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

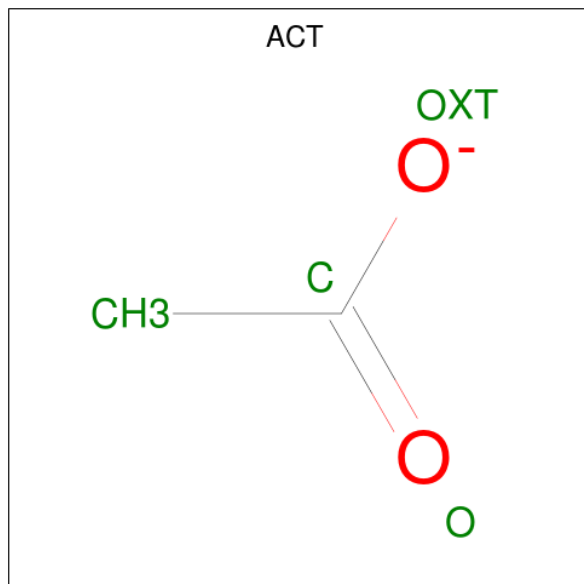
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 10 4 6	0	0
4	B	1	Total C O 10 4 6	0	0
4	C	1	Total C O 10 4 6	0	0
4	D	1	Total C O 10 4 6	0	0
4	E	1	Total C O 10 4 6	0	0
4	F	1	Total C O 10 4 6	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: $C_2H_3O_2$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	86	Total O 86 86	0	0
6	B	77	Total O 77 77	0	0
6	C	31	Total O 31 31	0	0
6	D	62	Total O 62 62	0	0
6	E	77	Total O 77 77	0	0
6	F	75	Total O 75 75	0	0



- Molecule 1: Probable cytosol aminopeptidase

Chain E: 90% 8% ..



- Molecule 1: Probable cytosol aminopeptidase

Chain F: 89% 9% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.61Å 93.25Å 179.47Å 90.00° 101.32° 90.00°	Depositor
Resolution (Å)	48.17 – 2.80 48.17 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.9 (48.17-2.80) 99.9 (48.17-2.80)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.62 (at 2.81Å)	Xtrriage
Refinement program	PHENIX 1.20.1	Depositor
R, R_{free}	0.170 , 0.203 0.173 , 0.205	Depositor DCC
R_{free} test set	2016 reflections (2.61%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtrriage
Anisotropy	0.343	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 29.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	21162	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.01% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TAR, CL, ACT, MN

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	0.31	0/3540	0.49	0/4817
1	B	0.30	0/3526	0.49	0/4797
1	C	0.29	0/3447	0.48	0/4702
1	D	0.30	0/3523	0.49	0/4798
1	E	0.29	0/3493	0.49	0/4760
1	F	0.31	0/3542	0.49	0/4818
All	All	0.30	0/21071	0.49	0/28692

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	3472	0	3376	27	0
1	B	3458	0	3372	27	0
1	C	3380	0	3221	23	0
1	D	3456	0	3339	30	0
1	E	3426	0	3304	25	0
1	F	3474	0	3384	28	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	1	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	10	0	4	1	0
4	B	10	0	4	0	0
4	C	10	0	4	3	0
4	D	10	0	4	0	0
4	E	10	0	4	0	0
4	F	10	0	4	1	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	E	4	0	3	0	0
5	F	4	0	3	0	0
6	A	86	0	0	0	0
6	B	77	0	0	2	0
6	C	31	0	0	1	0
6	D	62	0	0	1	0
6	E	77	0	0	2	0
6	F	75	0	0	2	0
All	All	21162	0	20032	146	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (146) 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:265:ASP:OD2	6:B:601:HOH:O	2.06	0.71
1:D:210:SER:HA	1:D:213:LYS:HE3	1.74	0.69
1:E:265:ASP:OD2	6:E:601:HOH:O	2.10	0.68
1:C:388:LYS:HE3	1:D:397:THR:HG21	1.77	0.65
1:C:19:LEU:HD11	1:C:63:VAL:HG23	1.78	0.64
1:E:44:GLN:O	1:E:64:ARG:NH2	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:305:LYS:HE3	1:F:170:PRO:HB2	1.80	0.63
1:B:65:LEU:HD21	1:B:73:LEU:HD13	1.80	0.62
1:A:210:SER:HA	1:A:213:LYS:HE3	1.81	0.62
1:B:275:THR:HG21	1:B:461:LEU:HB3	1.81	0.62
1:F:275:THR:HG21	1:F:461:LEU:HB3	1.82	0.61
1:F:210:SER:HA	1:F:213:LYS:HE3	1.81	0.61
1:E:97:PHE:HB3	1:E:101:GLN:HB3	1.83	0.60
1:F:139:SER:HB3	6:F:662:HOH:O	2.02	0.59
1:D:99:GLU:HG3	1:D:141:HIS:HB3	1.85	0.59
1:A:224:LEU:HB2	1:A:290:ALA:HB3	1.84	0.59
1:D:305:LYS:HE3	1:E:170:PRO:HB2	1.83	0.58
1:C:275:THR:HG21	1:C:461:LEU:HB3	1.86	0.58
1:D:198:LYS:HB3	1:D:219:PRO:HD2	1.85	0.57
1:E:210:SER:HA	1:E:213:LYS:HE3	1.85	0.57
1:E:275:THR:HG21	1:E:461:LEU:HB3	1.86	0.57
1:D:328:ARG:NH1	3:D:501:CL:CL	2.74	0.57
1:D:275:THR:HG21	1:D:461:LEU:HB3	1.87	0.57
1:C:170:PRO:HB2	1:F:305:LYS:HE3	1.87	0.56
1:E:198:LYS:HB3	1:E:219:PRO:HD2	1.86	0.56
1:E:196:ILE:HB	1:E:221:LEU:HB3	1.86	0.56
1:A:388:LYS:HE3	1:B:397:THR:HG21	1.88	0.56
1:C:196:ILE:HB	1:C:221:LEU:HB3	1.87	0.56
1:D:19:LEU:HD11	1:D:63:VAL:HG23	1.86	0.56
1:F:224:LEU:HB2	1:F:290:ALA:HB3	1.88	0.56
1:F:368:MET:O	1:F:437:HIS:N	2.38	0.55
1:C:397:THR:HG21	1:D:388:LYS:HE3	1.88	0.55
1:A:170:PRO:HB2	1:E:305:LYS:HE3	1.88	0.55
1:A:275:THR:HG21	1:A:461:LEU:HB3	1.89	0.55
1:C:198:LYS:HB3	1:C:219:PRO:HD2	1.89	0.55
1:B:242:LYS:NZ	6:B:601:HOH:O	2.28	0.54
1:A:328:ARG:NH1	3:A:501:CL:CL	2.77	0.54
1:B:99:GLU:HG3	1:B:141:HIS:HB3	1.89	0.54
1:B:210:SER:HA	1:B:213:LYS:HE3	1.90	0.54
1:C:122:ARG:HB2	4:C:502:TAR:H2	1.89	0.53
1:F:242:LYS:NZ	6:F:603:HOH:O	2.42	0.53
1:C:224:LEU:HB2	1:C:290:ALA:HB3	1.90	0.53
1:C:22:CYS:SG	1:C:27:PRO:HD3	2.50	0.52
1:B:198:LYS:HB3	1:B:219:PRO:HD2	1.91	0.51
1:A:445:TRP:HA	1:A:454:THR:HG23	1.94	0.50
1:B:196:ILE:HB	1:B:221:LEU:HB3	1.93	0.50
1:B:46:PHE:HD1	1:B:63:VAL:HG22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:LEU:HD11	1:A:63:VAL:HG23	1.93	0.49
1:A:198:LYS:HB3	1:A:219:PRO:HD2	1.94	0.49
1:E:19:LEU:HD11	1:E:63:VAL:HG23	1.94	0.49
1:D:440:ILE:HG21	1:D:457:PRO:HD3	1.93	0.49
1:A:22:CYS:SG	1:A:27:PRO:HD3	2.53	0.49
1:F:99:GLU:HG3	1:F:141:HIS:HB3	1.95	0.48
1:A:3:PHE:HD1	1:A:135:ALA:HB3	1.78	0.48
1:C:325:ALA:HB1	1:C:328:ARG:HD2	1.94	0.48
1:F:242:LYS:HG3	1:F:330:ILE:HD11	1.94	0.48
1:A:242:LYS:HD2	1:A:327:GLY:HA3	1.95	0.48
1:F:440:ILE:HG21	1:F:457:PRO:HD3	1.94	0.48
1:B:22:CYS:SG	1:B:27:PRO:HD3	2.54	0.47
1:A:36:LEU:HD11	1:A:49:THR:HG22	1.96	0.47
1:A:461:LEU:HD23	1:A:461:LEU:HA	1.74	0.47
1:B:242:LYS:HD2	1:B:327:GLY:HA3	1.97	0.47
1:D:3:PHE:HD1	1:D:135:ALA:HB3	1.79	0.47
1:D:242:LYS:HD2	1:D:327:GLY:HA3	1.97	0.47
1:B:381:ALA:HB1	1:B:463:ASN:HB3	1.96	0.47
1:D:94:VAL:HG23	1:D:139:SER:HB2	1.97	0.47
1:F:198:LYS:HB3	1:F:219:PRO:HD2	1.97	0.47
1:C:440:ILE:HG21	1:C:457:PRO:HD3	1.96	0.47
1:A:44:GLN:O	1:A:64:ARG:NH2	2.46	0.46
1:B:44:GLN:O	1:B:64:ARG:NH2	2.46	0.46
1:C:46:PHE:HD1	1:C:63:VAL:HG22	1.80	0.46
1:D:238:VAL:HB	1:D:346:VAL:HG22	1.98	0.46
1:C:122:ARG:HE	4:C:502:TAR:C1	2.29	0.46
1:E:46:PHE:HD1	1:E:63:VAL:HG22	1.80	0.46
1:A:328:ARG:NH2	1:A:422:ALA:HB2	2.30	0.46
1:B:224:LEU:HB2	1:B:290:ALA:HB3	1.98	0.46
1:E:242:LYS:NZ	6:E:601:HOH:O	2.42	0.46
1:D:224:LEU:HB2	1:D:290:ALA:HB3	1.96	0.45
1:D:65:LEU:HD21	1:D:73:LEU:HD13	1.98	0.45
1:A:173:CYS:HA	1:A:177:PHE:CD1	2.52	0.45
1:D:19:LEU:HD23	1:D:92:VAL:HG13	1.98	0.45
1:E:22:CYS:SG	1:E:27:PRO:HD3	2.57	0.45
1:F:9:ILE:HD13	1:F:95:HIS:CG	2.51	0.45
1:F:336:THR:O	1:F:339:GLU:HG2	2.17	0.45
1:C:238:VAL:HB	1:C:346:VAL:HG22	1.99	0.45
1:E:224:LEU:HB2	1:E:290:ALA:HB3	1.97	0.45
1:B:238:VAL:HG22	1:B:289:ILE:HB	1.99	0.45
1:C:121:ASP:N	4:C:502:TAR:O41	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:VAL:O	1:E:348:ASP:HA	2.18	0.44
1:F:30:ASN:HB3	1:F:33:ALA:HB3	1.99	0.44
1:A:182:ALA:HB2	1:A:273:ILE:HD13	1.99	0.44
1:C:336:THR:O	1:C:339:GLU:HG2	2.17	0.44
1:D:242:LYS:NZ	1:D:265:ASP:OD2	2.42	0.44
1:E:397:THR:HG21	1:F:388:LYS:HE3	1.99	0.44
1:D:326:GLU:OE2	6:D:601:HOH:O	2.20	0.44
1:B:240:VAL:O	1:B:348:ASP:HA	2.18	0.44
1:C:242:LYS:NZ	6:C:602:HOH:O	2.45	0.43
1:F:22:CYS:SG	1:F:27:PRO:HD3	2.58	0.43
1:A:65:LEU:HD21	1:A:73:LEU:HD13	2.01	0.43
1:F:85:GLN:HA	1:F:132:PHE:HB2	2.01	0.43
1:F:107:GLU:HB2	1:F:148:ALA:HB1	2.01	0.43
1:A:240:VAL:O	1:A:348:ASP:HA	2.19	0.43
1:C:242:LYS:HG3	1:C:330:ILE:HD11	2.01	0.43
1:D:196:ILE:HB	1:D:221:LEU:HB3	2.01	0.43
1:B:440:ILE:HG21	1:B:457:PRO:HD3	2.01	0.43
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.79	0.43
1:D:44:GLN:O	1:D:64:ARG:NH2	2.45	0.43
1:F:461:LEU:HD23	1:F:461:LEU:HA	1.76	0.43
1:D:87:GLN:O	1:D:132:PHE:HA	2.19	0.42
1:C:210:SER:HA	1:C:213:LYS:HE3	2.00	0.42
1:E:461:LEU:HD23	1:E:461:LEU:HA	1.82	0.42
1:F:248:THR:OG1	1:F:299:PRO:HD3	2.19	0.42
1:B:445:TRP:HA	1:B:454:THR:HG23	2.01	0.42
1:E:94:VAL:HG23	1:E:139:SER:HB2	2.02	0.42
1:B:226:TYR:CG	1:B:280:VAL:HG22	2.54	0.42
1:D:244:ILE:HG21	1:D:247:ASP:HB2	2.01	0.42
1:F:3:PHE:HD1	1:F:135:ALA:HB3	1.84	0.42
1:E:332:CYS:HB2	1:E:429:PHE:CD1	2.54	0.42
1:F:240:VAL:O	1:F:348:ASP:HA	2.20	0.42
1:D:7:THR:HA	1:D:139:SER:O	2.20	0.42
1:A:122:ARG:HB2	4:A:502:TAR:H2	2.02	0.42
1:A:446:LYS:HE2	1:A:446:LYS:HB3	1.80	0.41
1:E:336:THR:O	1:E:339:GLU:HG2	2.20	0.41
1:A:302:ALA:HB2	1:D:216:VAL:HG11	2.01	0.41
1:B:328:ARG:NH2	1:B:422:ALA:HB2	2.34	0.41
1:B:170:PRO:HB2	1:C:305:LYS:HE3	2.02	0.41
1:D:291:ILE:HD13	1:D:337:TYR:HD1	1.84	0.41
1:E:179:ALA:HA	1:E:222:VAL:HG21	2.02	0.41
1:F:122:ARG:HB2	4:F:502:TAR:H2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:GLU:O	1:F:146:LYS:HB2	2.20	0.41
1:B:85:GLN:HA	1:B:132:PHE:HB2	2.02	0.41
1:C:242:LYS:HD2	1:C:327:GLY:HA3	2.02	0.41
1:D:240:VAL:O	1:D:348:ASP:HA	2.21	0.41
1:F:44:GLN:O	1:F:64:ARG:NH2	2.49	0.41
1:D:336:THR:O	1:D:339:GLU:HG2	2.21	0.41
1:A:397:THR:HG21	1:B:388:LYS:HE3	2.02	0.41
1:C:182:ALA:HB2	1:C:273:ILE:HD13	2.03	0.41
1:E:388:LYS:HE3	1:F:397:THR:HG21	2.02	0.41
1:E:238:VAL:HG22	1:E:289:ILE:HB	2.03	0.40
1:A:305:LYS:HE3	1:D:170:PRO:HB2	2.02	0.40
1:E:65:LEU:HD23	1:E:65:LEU:HA	1.98	0.40
1:E:242:LYS:HD2	1:E:327:GLY:HA3	2.03	0.40
1:A:325:ALA:HB1	1:A:328:ARG:HD2	2.03	0.40
1:A:406:PHE:O	1:D:123:TYR:HB2	2.21	0.40
1:B:3:PHE:HD1	1:B:135:ALA:HB3	1.86	0.40
1:F:7:THR:HA	1:F:139:SER:O	2.21	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	466/476 (98%)	452 (97%)	14 (3%)	0	100	100
1	B	466/476 (98%)	452 (97%)	14 (3%)	0	100	100
1	C	465/476 (98%)	450 (97%)	15 (3%)	0	100	100
1	D	467/476 (98%)	452 (97%)	15 (3%)	0	100	100
1	E	466/476 (98%)	452 (97%)	14 (3%)	0	100	100
1	F	467/476 (98%)	453 (97%)	14 (3%)	0	100	100
All	All	2797/2856 (98%)	2711 (97%)	86 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	346/365 (95%)	345 (100%)	1 (0%)	92	98
1	B	342/365 (94%)	340 (99%)	2 (1%)	86	96
1	C	323/365 (88%)	321 (99%)	2 (1%)	86	96
1	D	341/365 (93%)	339 (99%)	2 (1%)	86	96
1	E	334/365 (92%)	331 (99%)	3 (1%)	78	94
1	F	345/365 (94%)	343 (99%)	2 (1%)	86	96
All	All	2031/2190 (93%)	2019 (99%)	12 (1%)	86	96

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	265	ASP
1	B	265	ASP
1	B	348	ASP
1	C	265	ASP
1	C	348	ASP
1	D	265	ASP
1	D	348	ASP
1	E	101	GLN
1	E	265	ASP
1	E	348	ASP
1	F	265	ASP
1	F	348	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	401	GLN
1	C	258	ASN

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Mol	Chain	Res	Type
1	C	401	GLN
1	D	258	ASN
1	D	401	GLN
1	E	258	ASN
1	E	401	GLN
1	F	138	HIS
1	F	401	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 12 are monoatomic - leaving 10 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	B	503	-	3,3,3	1.36	0	3,3,3	1.46	0
5	ACT	E	503	-	3,3,3	1.39	1 (33%)	3,3,3	1.43	0
5	ACT	F	503	-	3,3,3	1.58	1 (33%)	3,3,3	1.70	1 (33%)
5	ACT	A	503	-	3,3,3	1.46	1 (33%)	3,3,3	1.51	0
4	TAR	E	502	-	9,9,9	1.37	2 (22%)	12,12,12	1.29	2 (16%)
4	TAR	A	502	-	9,9,9	1.97	4 (44%)	12,12,12	1.90	4 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	TAR	B	502	-	9,9,9	1.44	2 (22%)	12,12,12	1.27	2 (16%)
4	TAR	D	502	-	9,9,9	1.35	2 (22%)	12,12,12	1.36	2 (16%)
4	TAR	F	502	-	9,9,9	1.95	4 (44%)	12,12,12	1.87	4 (33%)
4	TAR	C	502	-	9,9,9	1.40	2 (22%)	12,12,12	1.33	2 (16%)

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	TAR	E	502	-	-	8/12/12/12	-
4	TAR	A	502	-	-	4/12/12/12	-
4	TAR	B	502	-	-	10/12/12/12	-
4	TAR	D	502	-	-	4/12/12/12	-
4	TAR	F	502	-	-	8/12/12/12	-
4	TAR	C	502	-	-	4/12/12/12	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	502	TAR	O1-C1	3.24	1.32	1.22
4	B	502	TAR	O1-C1	3.19	1.31	1.22
4	F	502	TAR	O4-C4	3.16	1.31	1.22
4	E	502	TAR	O1-C1	3.13	1.31	1.22
4	A	502	TAR	O4-C4	3.07	1.31	1.22
4	C	502	TAR	O4-C4	3.07	1.31	1.22
4	A	502	TAR	O1-C1	3.03	1.31	1.22
4	D	502	TAR	O4-C4	2.98	1.31	1.22
4	C	502	TAR	O41-C4	-2.67	1.21	1.30
4	D	502	TAR	O41-C4	-2.67	1.21	1.30
4	F	502	TAR	O41-C4	-2.65	1.21	1.30
4	A	502	TAR	O41-C4	-2.65	1.21	1.30
4	E	502	TAR	O11-C1	-2.62	1.22	1.30
4	A	502	TAR	O11-C1	-2.60	1.22	1.30
4	B	502	TAR	O11-C1	-2.54	1.22	1.30
4	F	502	TAR	O11-C1	-2.49	1.22	1.30
5	F	503	ACT	CH3-C	2.36	1.59	1.49
5	A	503	ACT	CH3-C	2.11	1.57	1.49
5	E	503	ACT	CH3-C	2.11	1.57	1.49

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	502	TAR	O41-C4-C3	3.47	122.66	113.27
4	D	502	TAR	O41-C4-C3	3.37	122.39	113.27
4	C	502	TAR	O41-C4-C3	3.33	122.26	113.27
4	F	502	TAR	O41-C4-C3	3.32	122.25	113.27
4	A	502	TAR	O4-C4-C3	-3.30	112.96	121.63
4	A	502	TAR	O11-C1-C2	3.30	122.19	113.27
4	D	502	TAR	O4-C4-C3	-3.27	113.04	121.63
4	F	502	TAR	O11-C1-C2	3.26	122.08	113.27
4	E	502	TAR	O11-C1-C2	3.23	121.99	113.27
4	F	502	TAR	O1-C1-C2	-3.20	113.21	121.63
4	B	502	TAR	O11-C1-C2	3.19	121.89	113.27
4	C	502	TAR	O4-C4-C3	-3.14	113.36	121.63
4	F	502	TAR	O4-C4-C3	-3.12	113.43	121.63
4	E	502	TAR	O1-C1-C2	-3.06	113.58	121.63
4	A	502	TAR	O1-C1-C2	-2.98	113.81	121.63
4	B	502	TAR	O1-C1-C2	-2.94	113.91	121.63
5	F	503	ACT	O-C-CH3	-2.14	113.99	122.33

There are no chirality outliers.

All (38) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	502	TAR	O3-C3-C4-O4
4	A	502	TAR	O3-C3-C4-O41
4	B	502	TAR	O3-C3-C4-O4
4	B	502	TAR	O3-C3-C4-O41
4	C	502	TAR	O3-C3-C4-O4
4	C	502	TAR	O3-C3-C4-O41
4	E	502	TAR	O3-C3-C4-O4
4	E	502	TAR	O3-C3-C4-O41
4	F	502	TAR	O3-C3-C4-O4
4	F	502	TAR	O3-C3-C4-O41
4	F	502	TAR	C2-C3-C4-O41
4	A	502	TAR	O1-C1-C2-O2
4	A	502	TAR	O11-C1-C2-O2
4	D	502	TAR	O1-C1-C2-O2
4	D	502	TAR	O11-C1-C2-O2
4	D	502	TAR	O3-C3-C4-O4
4	D	502	TAR	O3-C3-C4-O41
4	E	502	TAR	O1-C1-C2-O2
4	F	502	TAR	C2-C3-C4-O4

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Mol	Chain	Res	Type	Atoms
4	E	502	TAR	O11-C1-C2-O2
4	B	502	TAR	C1-C2-C3-O3
4	B	502	TAR	O2-C2-C3-C4
4	B	502	TAR	O2-C2-C3-O3
4	F	502	TAR	O11-C1-C2-O2
4	C	502	TAR	C2-C3-C4-O41
4	B	502	TAR	C1-C2-C3-C4
4	C	502	TAR	C2-C3-C4-O4
4	F	502	TAR	O1-C1-C2-O2
4	F	502	TAR	O1-C1-C2-C3
4	F	502	TAR	O11-C1-C2-C3
4	B	502	TAR	O1-C1-C2-C3
4	B	502	TAR	O11-C1-C2-O2
4	B	502	TAR	O11-C1-C2-C3
4	E	502	TAR	C2-C3-C4-O4
4	E	502	TAR	O1-C1-C2-C3
4	B	502	TAR	O1-C1-C2-O2
4	E	502	TAR	C2-C3-C4-O41
4	E	502	TAR	O11-C1-C2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	TAR	1	0
4	F	502	TAR	1	0
4	C	502	TAR	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	468/476 (98%)	-0.52	0 100 100	29, 40, 60, 92	0
1	B	468/476 (98%)	-0.34	1 (0%) 95 94	30, 42, 70, 92	0
1	C	467/476 (98%)	-0.35	0 100 100	36, 57, 95, 110	0
1	D	469/476 (98%)	-0.48	1 (0%) 95 94	35, 48, 75, 100	0
1	E	468/476 (98%)	-0.41	1 (0%) 95 94	30, 45, 87, 106	0
1	F	469/476 (98%)	-0.46	0 100 100	28, 40, 57, 81	0
All	All	2809/2856 (98%)	-0.42	3 (0%) 95 95	28, 45, 81, 110	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	16	GLY	3.6
1	B	5	THR	2.2
1	D	94	VAL	2.2

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 monosaccharides 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,

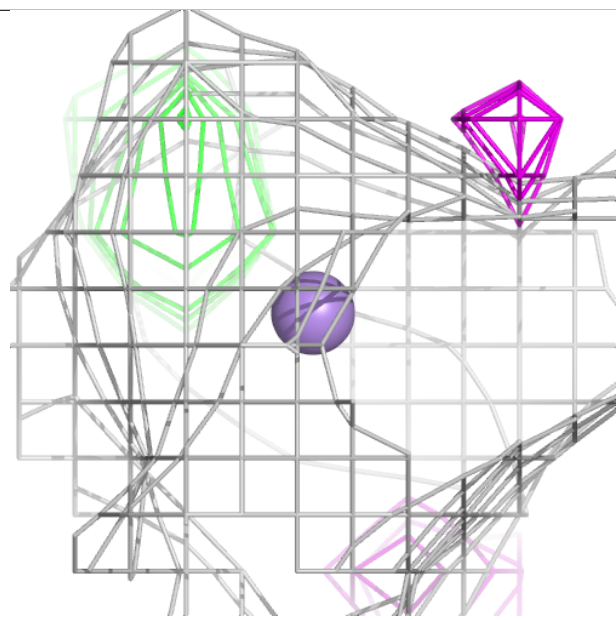
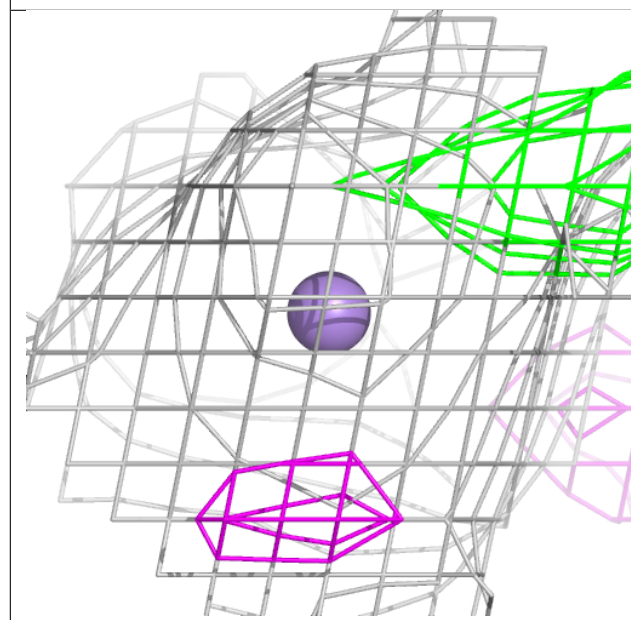
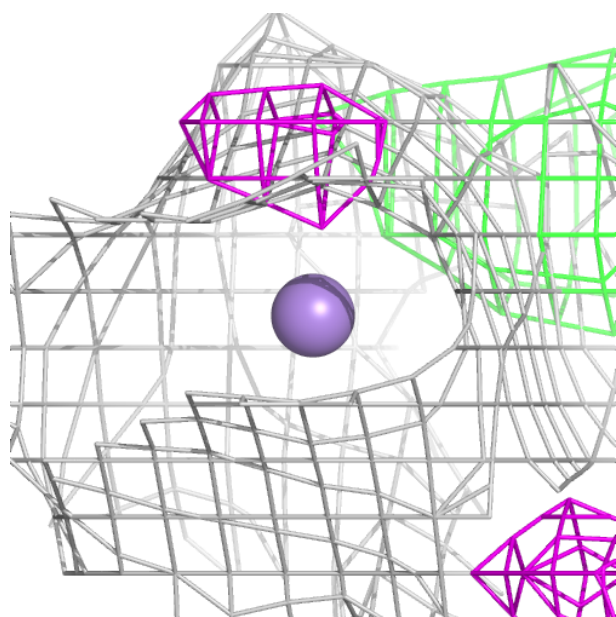
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	TAR	B	502	10/10	0.81	0.31	54,58,63,70	0
5	ACT	F	503	4/4	0.82	0.36	42,43,52,54	0
4	TAR	D	502	10/10	0.83	0.29	45,50,55,55	10
3	CL	C	501	1/1	0.86	0.19	61,61,61,61	0
4	TAR	E	502	10/10	0.88	0.29	51,60,62,64	0
5	ACT	E	503	4/4	0.88	0.36	53,59,60,62	0
4	TAR	C	502	10/10	0.88	0.32	61,64,69,74	0
4	TAR	A	502	10/10	0.90	0.34	47,52,56,58	0
4	TAR	F	502	10/10	0.90	0.31	42,48,52,57	0
5	ACT	B	503	4/4	0.91	0.39	46,54,54,56	0
2	MN	A	500	1/1	0.92	0.12	59,59,59,59	0
3	CL	E	501	1/1	0.93	0.16	57,57,57,57	0
2	MN	C	500	1/1	0.93	0.10	68,68,68,68	0
3	CL	B	501	1/1	0.93	0.26	57,57,57,57	0
2	MN	B	500	1/1	0.93	0.12	61,61,61,61	0
3	CL	D	501	1/1	0.93	0.12	57,57,57,57	0
5	ACT	A	503	4/4	0.94	0.22	47,49,52,52	0
3	CL	F	501	1/1	0.95	0.13	52,52,52,52	0
3	CL	A	501	1/1	0.96	0.19	50,50,50,50	0
2	MN	D	500	1/1	0.97	0.10	62,62,62,62	0
2	MN	E	500	1/1	0.98	0.10	62,62,62,62	0
2	MN	F	500	1/1	0.98	0.06	64,64,64,64	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.

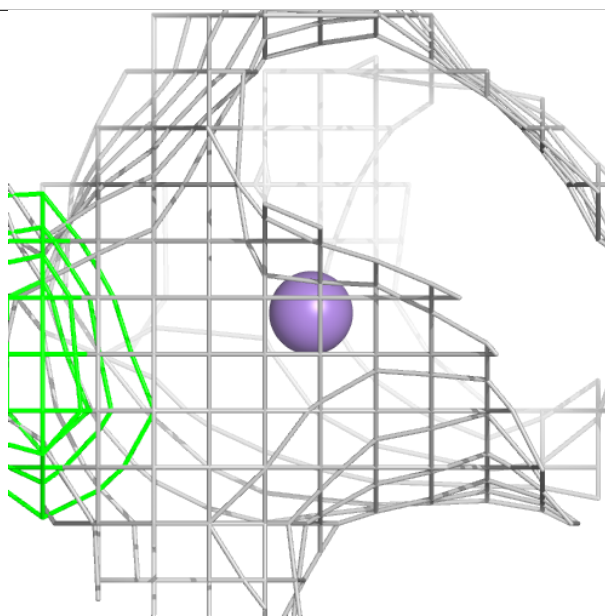
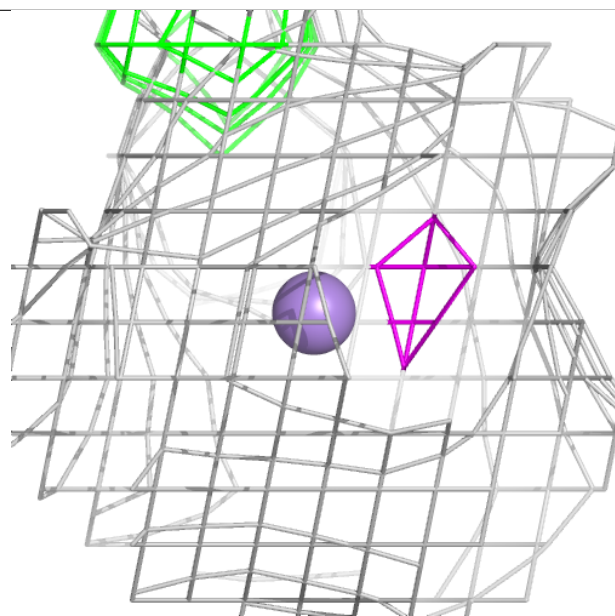
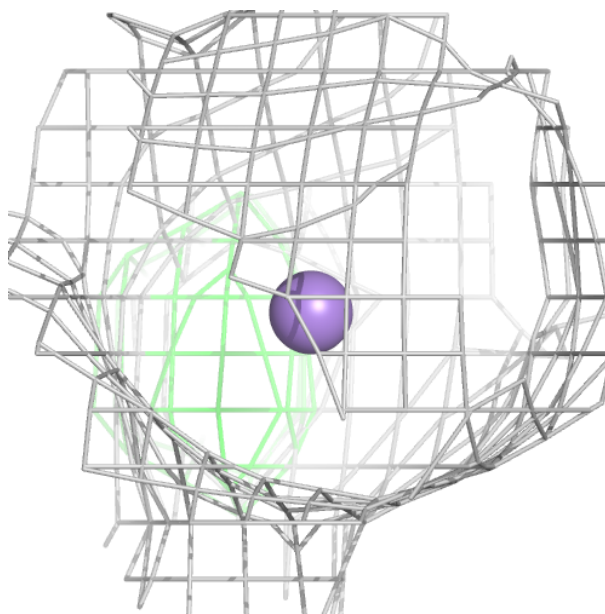
Electron density around MN A 500:

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



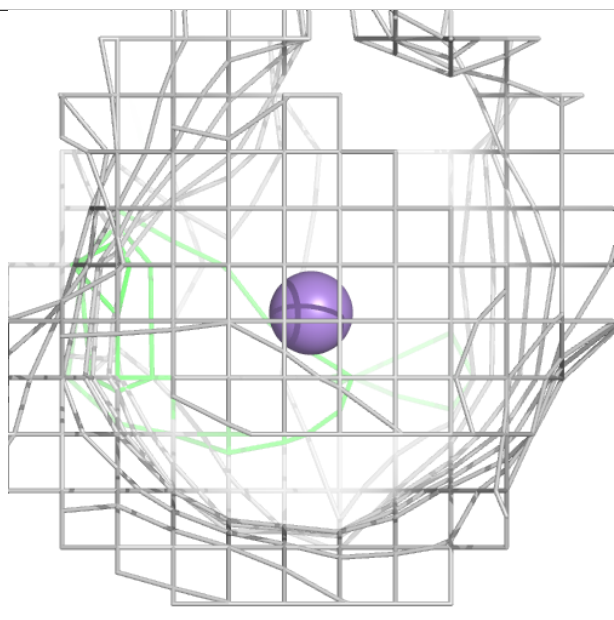
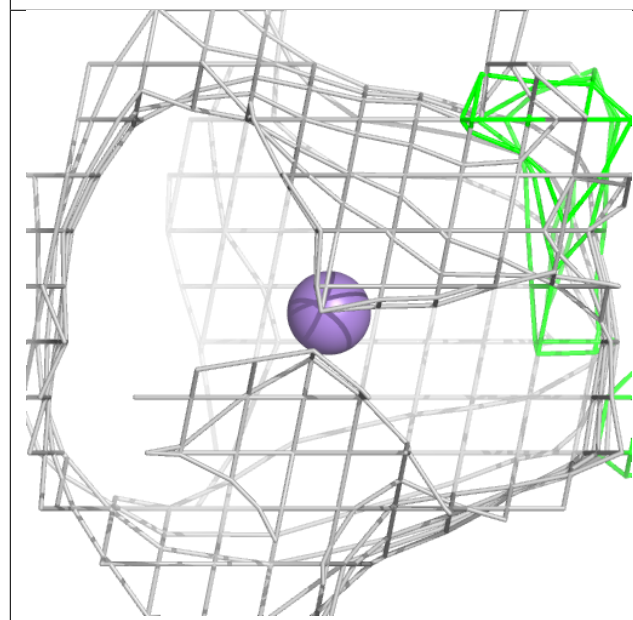
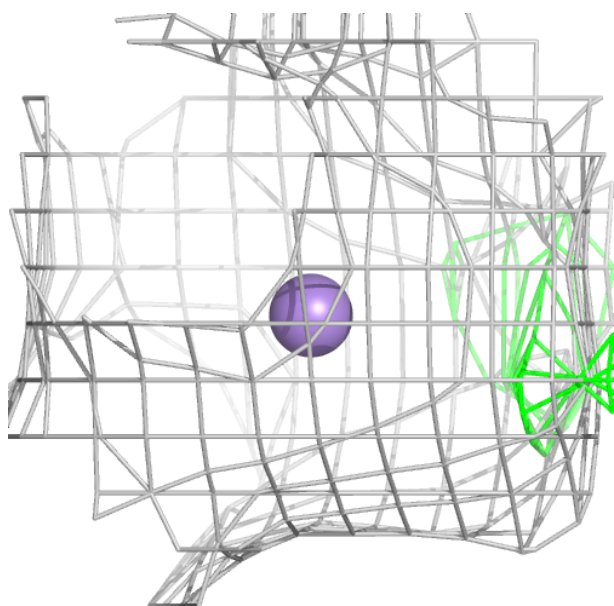
Electron density around MN C 500:

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



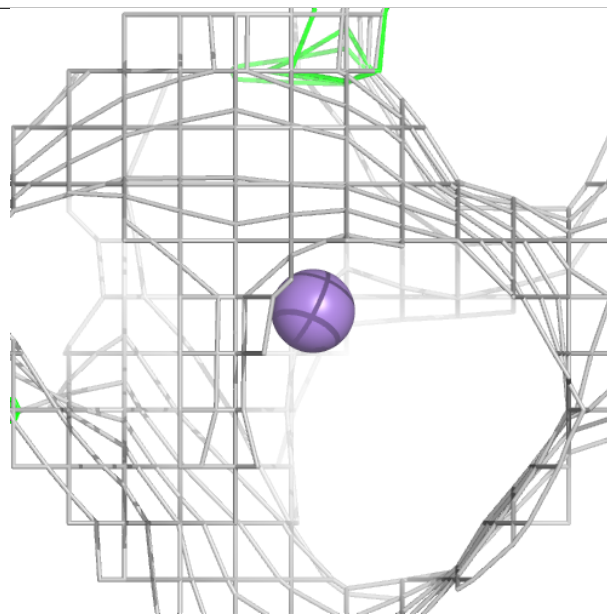
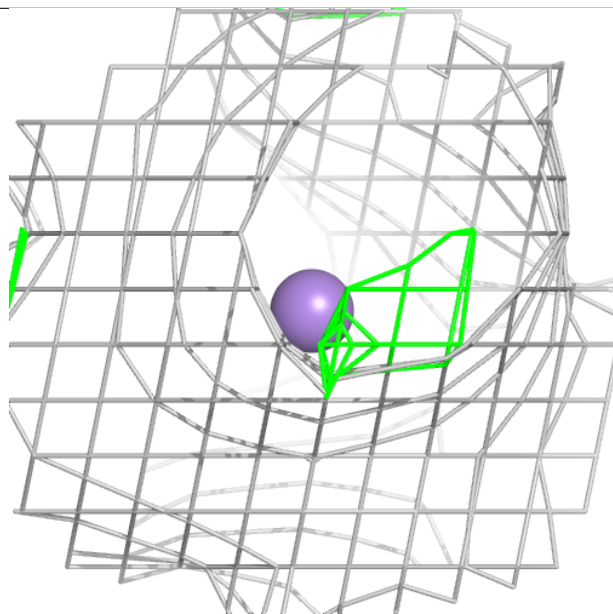
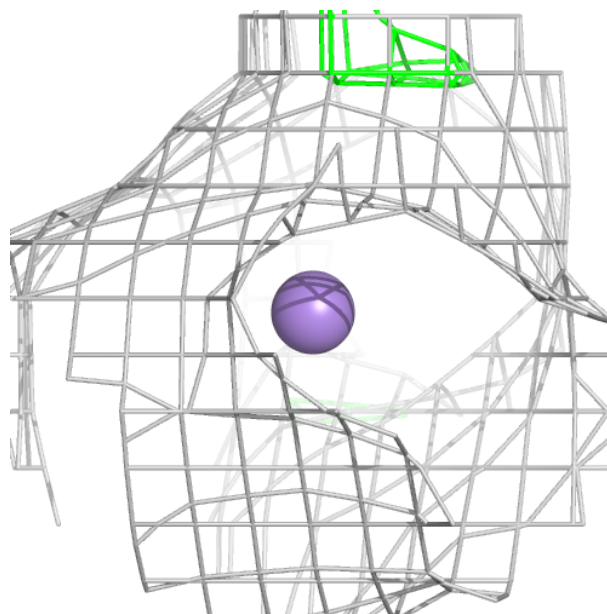
Electron density around MN B 500:

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



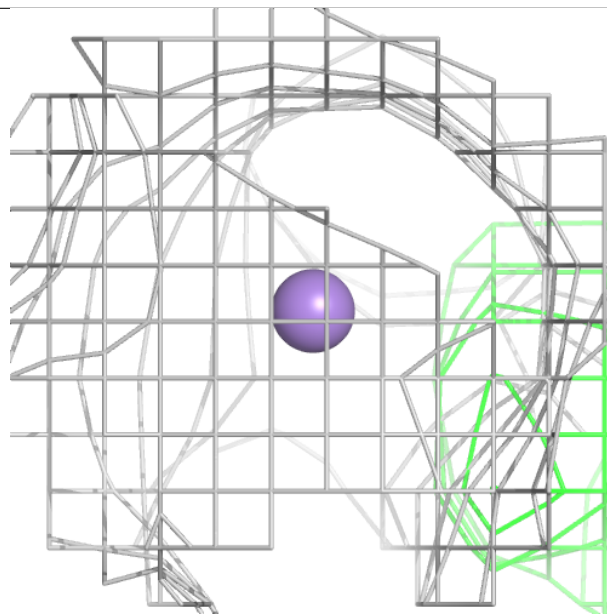
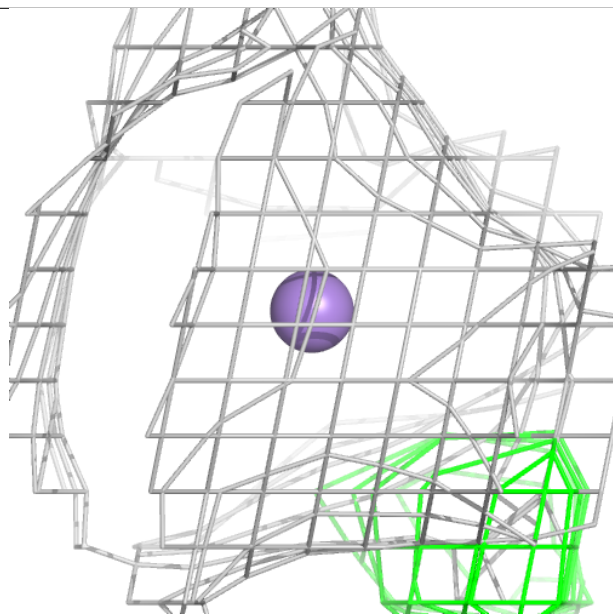
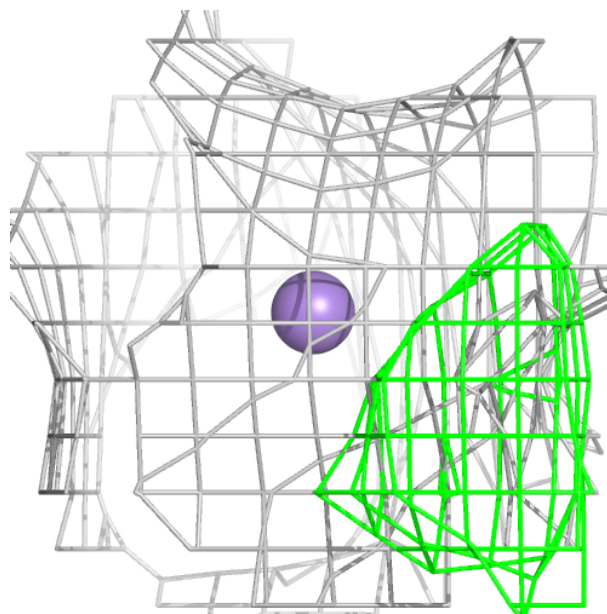
Electron density around MN D 500:

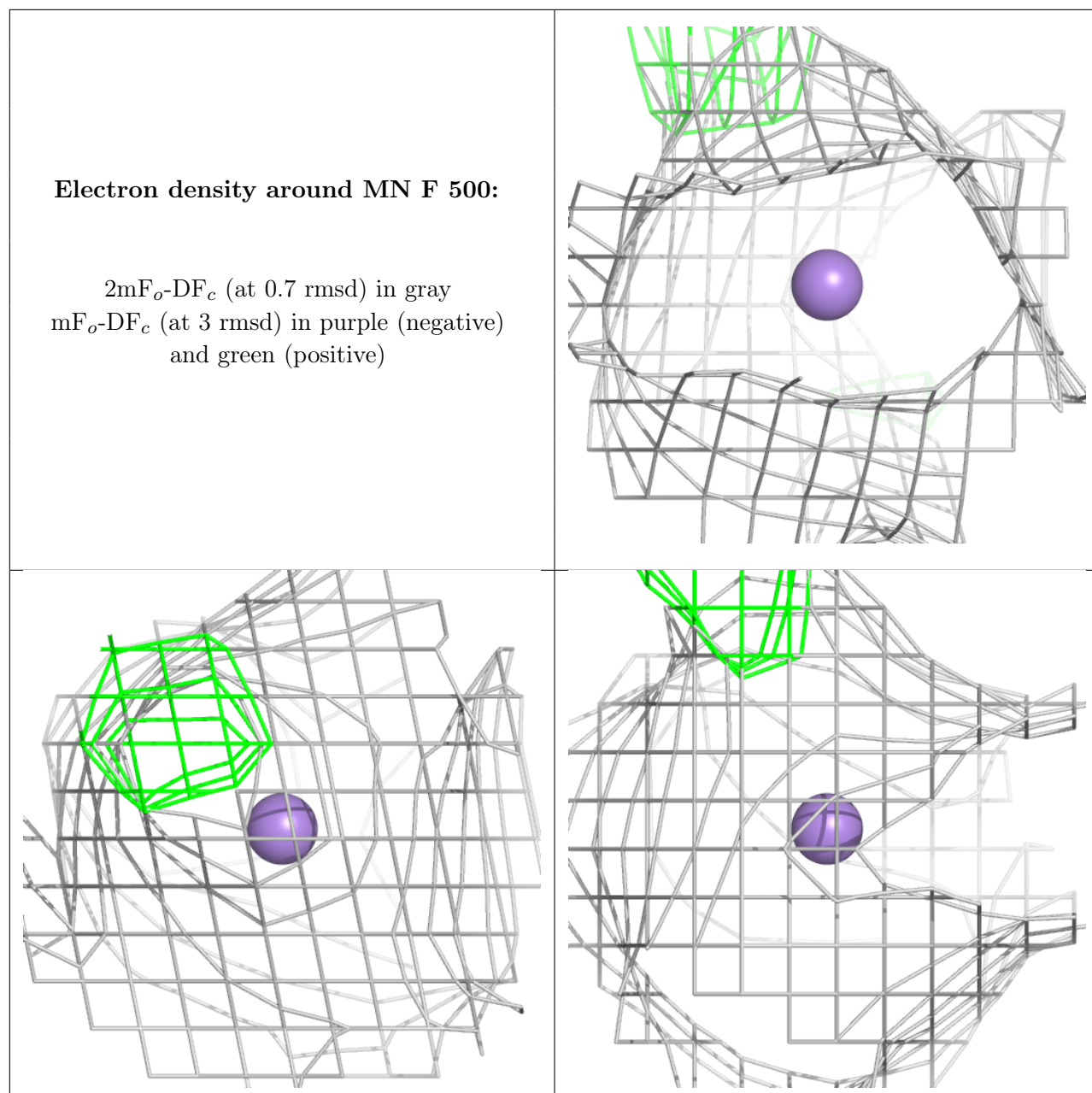
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MN E 500:

$2mF_o-DF_c$ (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.