Full wwPDB X-ray Structure Validation Report ⓘ

Oct 31, 2024 – 12:30 pm GMT

PDB ID	:	9GL0
Title	:	Crystal Structure of Acetylpolyamine aminohydrolase (ApaH) from Legionella pneumophila
Authors	:	Graf, L.G.; Schulze, S.; Palm, G.J.; Lammers, M.
Deposited on	:	2024-08-26
Resolution	:	2.70 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:

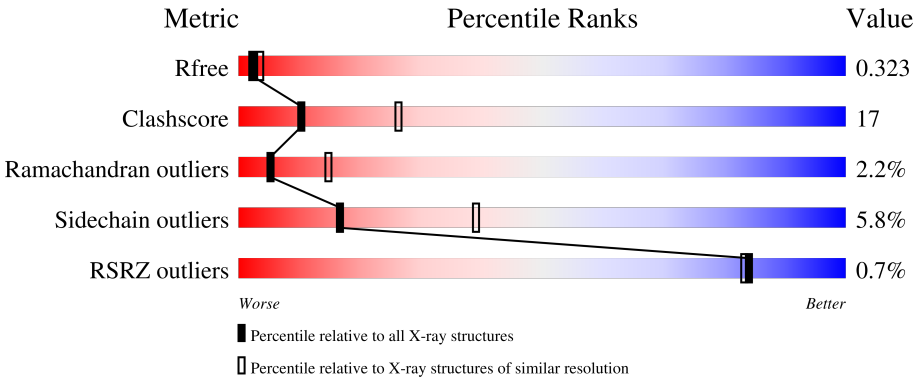
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

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 2.70 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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (2.70-2.70)

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 <=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	437	57% 31% 10%
1	B	437	60% 28% 10%
1	C	437	54% 32% 10%
1	D	437	49% 37% 11%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12712 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 Acetylpolyamine aminohydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	1	0
			3182	2037	538	590	17			
1	B	392	Total	C	N	O	S	0	1	0
			3175	2032	537	589	17			
1	C	392	Total	C	N	O	S	0	0	0
			3164	2027	535	585	17			
1	D	391	Total	C	N	O	S	0	1	0
			3167	2029	535	585	18			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	MET	-	initiating methionine	UNP A0A2S6EWV0
A	-9	ALA	-	expression tag	UNP A0A2S6EWV0
A	-8	HIS	-	expression tag	UNP A0A2S6EWV0
A	-7	HIS	-	expression tag	UNP A0A2S6EWV0
A	-6	HIS	-	expression tag	UNP A0A2S6EWV0
A	-5	HIS	-	expression tag	UNP A0A2S6EWV0
A	-4	HIS	-	expression tag	UNP A0A2S6EWV0
A	-3	HIS	-	expression tag	UNP A0A2S6EWV0
A	-2	VAL	-	expression tag	UNP A0A2S6EWV0
A	-1	GLY	-	expression tag	UNP A0A2S6EWV0
A	0	THR	-	expression tag	UNP A0A2S6EWV0
B	-10	MET	-	initiating methionine	UNP A0A2S6EWV0
B	-9	ALA	-	expression tag	UNP A0A2S6EWV0
B	-8	HIS	-	expression tag	UNP A0A2S6EWV0
B	-7	HIS	-	expression tag	UNP A0A2S6EWV0
B	-6	HIS	-	expression tag	UNP A0A2S6EWV0
B	-5	HIS	-	expression tag	UNP A0A2S6EWV0
B	-4	HIS	-	expression tag	UNP A0A2S6EWV0
B	-3	HIS	-	expression tag	UNP A0A2S6EWV0
B	-2	VAL	-	expression tag	UNP A0A2S6EWV0
B	-1	GLY	-	expression tag	UNP A0A2S6EWV0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	THR	-	expression tag	UNP A0A2S6EWV0
C	-10	MET	-	initiating methionine	UNP A0A2S6EWV0
C	-9	ALA	-	expression tag	UNP A0A2S6EWV0
C	-8	HIS	-	expression tag	UNP A0A2S6EWV0
C	-7	HIS	-	expression tag	UNP A0A2S6EWV0
C	-6	HIS	-	expression tag	UNP A0A2S6EWV0
C	-5	HIS	-	expression tag	UNP A0A2S6EWV0
C	-4	HIS	-	expression tag	UNP A0A2S6EWV0
C	-3	HIS	-	expression tag	UNP A0A2S6EWV0
C	-2	VAL	-	expression tag	UNP A0A2S6EWV0
C	-1	GLY	-	expression tag	UNP A0A2S6EWV0
C	0	THR	-	expression tag	UNP A0A2S6EWV0
D	-10	MET	-	initiating methionine	UNP A0A2S6EWV0
D	-9	ALA	-	expression tag	UNP A0A2S6EWV0
D	-8	HIS	-	expression tag	UNP A0A2S6EWV0
D	-7	HIS	-	expression tag	UNP A0A2S6EWV0
D	-6	HIS	-	expression tag	UNP A0A2S6EWV0
D	-5	HIS	-	expression tag	UNP A0A2S6EWV0
D	-4	HIS	-	expression tag	UNP A0A2S6EWV0
D	-3	HIS	-	expression tag	UNP A0A2S6EWV0
D	-2	VAL	-	expression tag	UNP A0A2S6EWV0
D	-1	GLY	-	expression tag	UNP A0A2S6EWV0
D	0	THR	-	expression tag	UNP A0A2S6EWV0

- Molecule 2 is ZINC ION (three-letter code: 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
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total K 1 1	0	0

- Molecule 4 is water.

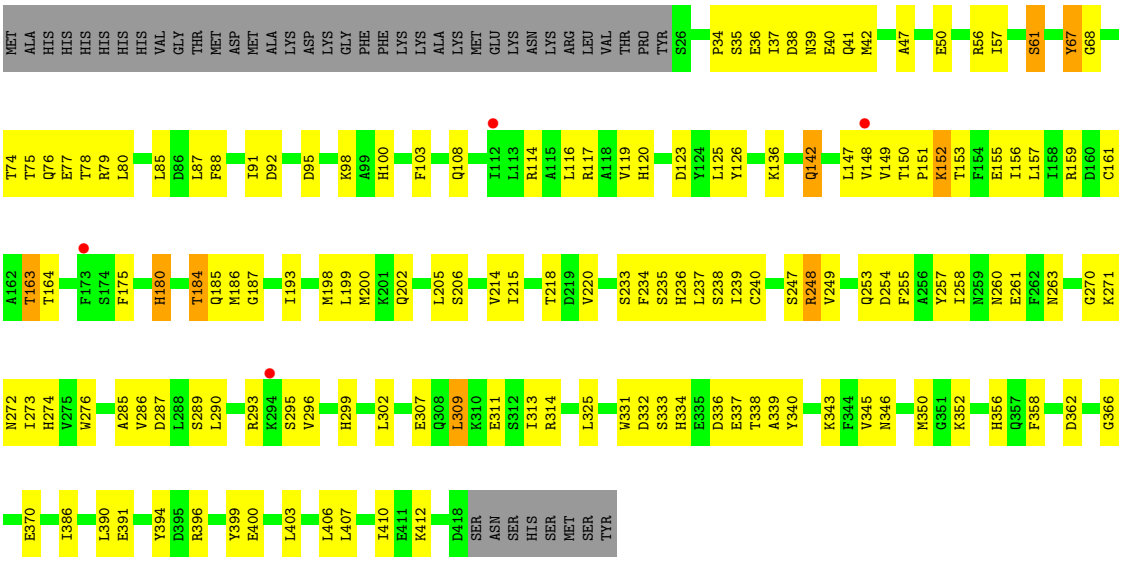
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total O 4 4	0	0
4	B	4	Total O 4 4	0	0
4	C	4	Total O 4 4	0	0
4	D	6	Total O 6 6	0	0

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.

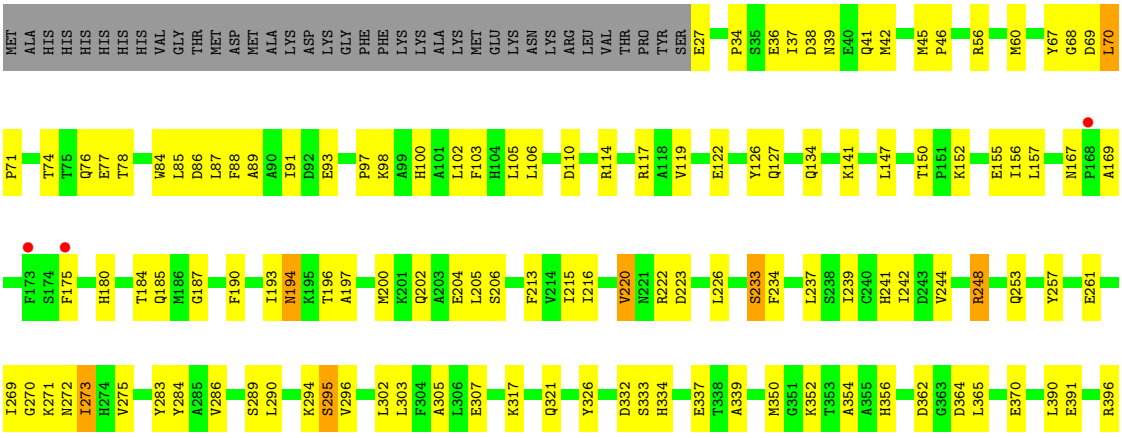
• Molecule 1: Acetylpolyamine aminohydrolase

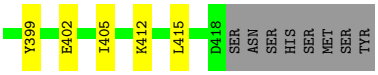
Chain A:



• Molecule 1: Acetylpolyamine aminohydrolase

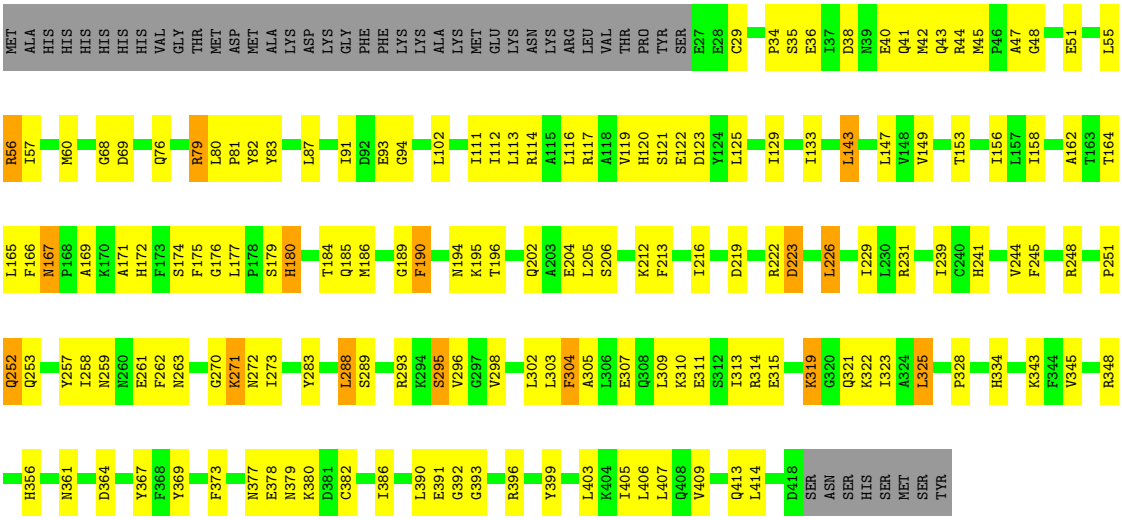
Chain B:





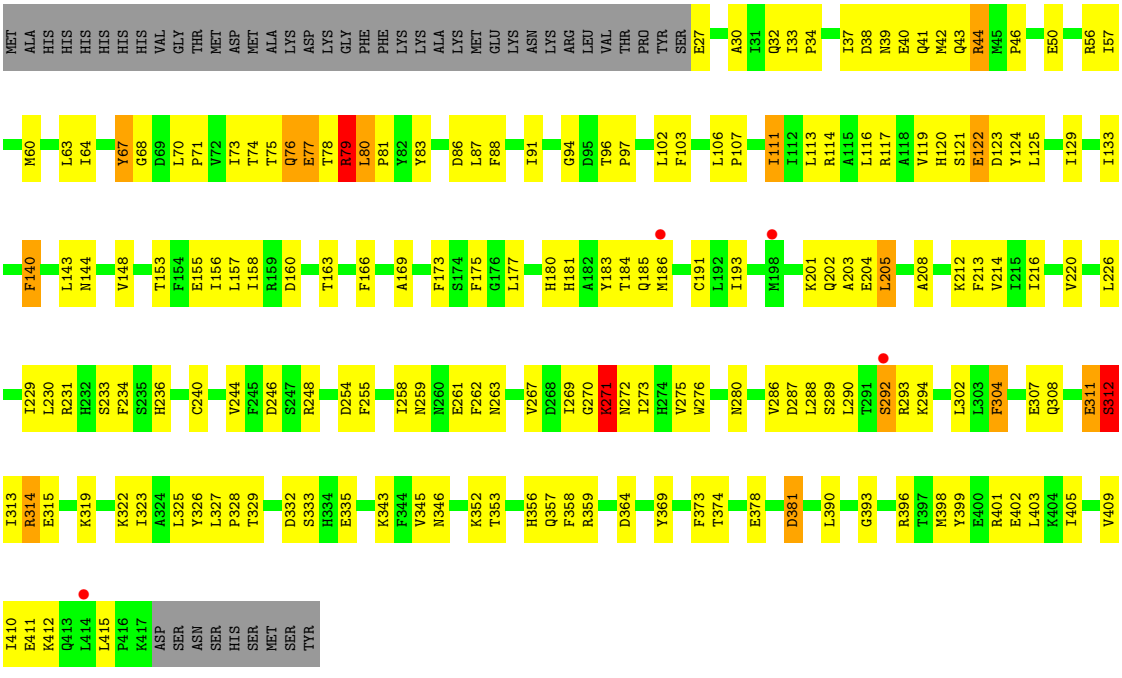
• Molecule 1: Acetylpolyamine aminohydrolase

Chain C:



• Molecule 1: Acetylpolyamine aminohydrolase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	109.12Å 109.12Å 400.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.96 – 2.70 45.96 – 2.70	Depositor EDS
% Data completeness (in resolution range)	94.6 (45.96-2.70) 94.5 (45.96-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.16	Depositor
$< I/\sigma(I) >$ [1]	0.87 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.240 , 0.316 0.251 , 0.323	Depositor DCC
R_{free} test set	3452 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	92.2	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 79.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	12712	wwPDB-VP
Average B, all atoms (Å^2)	113.0	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 45.67 % 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 1.2778e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: ZN, K

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	0.45	0/3261	0.65	1/4413 (0.0%)
1	B	0.47	1/3254 (0.0%)	0.65	1/4406 (0.0%)
1	C	0.47	0/3243	0.67	1/4390 (0.0%)
1	D	0.45	0/3246	0.63	0/4393
All	All	0.46	1/13004 (0.0%)	0.65	3/17602 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	69	ASP	CA-CB	6.89	1.69	1.53

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	220	VAL	CG1-CB-CG2	5.77	120.14	110.90
1	C	325	LEU	CA-CB-CG	5.69	128.39	115.30
1	A	309	LEU	CA-CB-CG	5.68	128.37	115.30

There are no chirality outliers.

There are no planarity outliers.

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	3182	0	3107	104	0
1	B	3175	0	3096	78	0
1	C	3164	0	3088	114	0
1	D	3167	0	3094	138	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	C	1	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	6	0	0	0	0
All	All	12712	0	12385	422	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 17.

All (422) 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:60:MET:HE1	1:B:390:LEU:HD11	1.28	1.12
1:A:41:GLN:OE1	1:A:152:LYS:HE3	1.57	1.02
1:C:213:PHE:HB2	1:C:239:ILE:HG12	1.53	0.90
1:C:114:ARG:HH11	1:C:205:LEU:HD23	1.34	0.90
1:A:41:GLN:HB2	1:A:156:ILE:HD11	1.54	0.89
1:B:194:ASN:HD21	1:B:226:LEU:HD12	1.41	0.86
1:D:231:ARG:HH21	1:D:262:PHE:HA	1.40	0.85
1:D:41:GLN:HB2	1:D:156:ILE:HD11	1.58	0.83
1:C:41:GLN:HB2	1:C:156:ILE:HD11	1.62	0.82
1:B:60:MET:HE1	1:B:390:LEU:CD1	2.11	0.81
1:C:216:ILE:HD13	1:C:305:ALA:HB1	1.63	0.80
1:D:293:ARG:NH1	1:D:356:HIS:O	2.14	0.80
1:A:37:ILE:HD12	1:A:38:ASP:N	1.97	0.79
1:D:292:SER:HB2	1:D:357:GLN:HG2	1.64	0.77
1:A:260:ASN:HD21	1:D:40:GLU:HB3	1.49	0.77
1:C:311:GLU:OE1	1:C:314:ARG:NH1	2.17	0.76
1:A:95:ASP:HB3	1:A:98:LYS:HB3	1.68	0.76
1:A:370:GLU:OE2	1:A:412:LYS:NZ	2.18	0.76
1:D:248:ARG:HH11	1:D:289:SER:HB3	1.52	0.75
1:D:124:TYR:HE2	1:D:186[B]:MET:HA	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:ILE:HD12	1:A:286:VAL:HG22	1.69	0.74
1:B:36:GLU:OE2	1:B:36:GLU:N	2.21	0.74
1:C:114:ARG:NH1	1:C:205:LEU:HD23	2.02	0.73
1:D:56:ARG:NH1	1:D:393:GLY:O	2.23	0.72
1:A:151:PRO:HB2	1:A:152:LYS:HD3	1.72	0.71
1:D:181:HIS:HB2	1:D:191:CYS:SG	2.29	0.71
1:A:50:GLU:OE2	1:A:50:GLU:N	2.14	0.69
1:C:273:ILE:HG21	1:C:304:PHE:HE1	1.55	0.69
1:D:32:GLN:NE2	1:D:160:ASP:OD1	2.27	0.67
1:D:83:TYR:CE2	1:D:107:PRO:HD2	2.30	0.67
1:A:116:LEU:CD1	1:A:125:LEU:HD21	2.24	0.67
1:C:378:GLU:OE2	1:C:379:ASN:ND2	2.28	0.67
1:D:269:ILE:HG23	1:D:273:ILE:HD11	1.76	0.67
1:D:356:HIS:O	1:D:356:HIS:ND1	2.27	0.67
1:B:117:ARG:CZ	1:B:122:GLU:HG2	2.25	0.66
1:D:77:GLU:N	1:D:77:GLU:OE2	2.28	0.66
1:D:288:LEU:HD23	1:D:358:PHE:O	1.96	0.65
1:C:319:LYS:HE3	1:C:321:GLN:NE2	2.11	0.65
1:B:93:GLU:N	1:B:93:GLU:OE1	2.29	0.64
1:D:60:MET:HE1	1:D:390:LEU:HG	1.79	0.64
1:C:325:LEU:HD12	1:C:386:ILE:HG12	1.80	0.64
1:A:92:ASP:O	1:A:136:LYS:NZ	2.26	0.64
1:B:152:LYS:HB3	1:B:156:ILE:HD13	1.79	0.64
1:A:202:GLN:O	1:A:206:SER:OG	2.08	0.63
1:B:294:LYS:O	1:B:296:VAL:N	2.30	0.63
1:D:255:PHE:O	1:D:259:ASN:ND2	2.31	0.63
1:C:42:MET:HE1	1:C:57:ILE:HG13	1.80	0.63
1:D:411:GLU:HA	1:D:415:LEU:HD13	1.80	0.63
1:D:153:THR:O	1:D:157:LEU:HD12	1.98	0.63
1:B:114:ARG:HE	1:B:205:LEU:HD12	1.64	0.63
1:A:248:ARG:HB3	1:A:345:VAL:HG13	1.80	0.63
1:C:60:MET:HE1	1:C:390:LEU:HG	1.81	0.62
1:D:311:GLU:O	1:D:313:ILE:N	2.32	0.62
1:B:34:PRO:HD3	1:B:175:PHE:O	1.98	0.62
1:C:309:LEU:HD22	1:C:313:ILE:HD11	1.82	0.62
1:A:260:ASN:ND2	1:D:40:GLU:OE1	2.33	0.62
1:C:111:ILE:HG22	1:C:114:ARG:HH21	1.64	0.62
1:A:103:PHE:CZ	1:A:125:LEU:HD23	2.35	0.61
1:D:63:LEU:HD23	1:D:403:LEU:HD23	1.82	0.61
1:A:136:LYS:HA	1:A:151:PRO:HG3	1.82	0.61
1:C:93:GLU:OE1	1:C:93:GLU:N	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:THR:OG1	1:A:163:THR:HG22	2.01	0.60
1:B:194:ASN:ND2	1:B:197:ALA:H	1.98	0.60
1:B:396:ARG:HA	1:B:399:TYR:CE2	2.37	0.60
1:D:37:ILE:HA	1:D:40:GLU:HG3	1.83	0.60
1:A:37:ILE:HD12	1:A:38:ASP:H	1.63	0.60
1:A:184:THR:HG23	1:A:185:GLN:HG2	1.82	0.60
1:D:46:PRO:HD3	1:D:148:VAL:HB	1.83	0.59
1:B:117:ARG:HD2	1:B:122:GLU:OE2	2.02	0.59
1:C:111:ILE:HG22	1:C:114:ARG:NH2	2.16	0.59
1:D:64:ILE:HG13	1:D:403:LEU:HD21	1.84	0.59
1:C:319:LYS:HE3	1:C:321:GLN:HE22	1.67	0.59
1:A:396:ARG:HA	1:A:399:TYR:CE2	2.38	0.59
1:D:335:GLU:O	1:D:343:LYS:NZ	2.28	0.59
1:B:237:LEU:HB2	1:B:239:ILE:HD11	1.85	0.59
1:C:334:HIS:CE1	1:C:361:ASN:HA	2.38	0.59
1:C:309:LEU:O	1:C:313:ILE:HG13	2.02	0.59
1:A:214:VAL:HG22	1:A:240:CYS:HB3	1.85	0.58
1:D:216:ILE:O	1:D:328:PRO:HD2	2.03	0.58
1:C:94:GLY:HA2	1:C:133:ILE:HG23	1.84	0.58
1:D:153:THR:HG22	1:D:157:LEU:HD11	1.85	0.58
1:B:27:GLU:O	1:B:169:ALA:HA	2.03	0.58
1:B:71:PRO:HD3	1:B:415:LEU:HD11	1.84	0.58
1:C:35:SER:HB3	1:C:76:GLN:HB2	1.85	0.58
1:D:41:GLN:HB2	1:D:156:ILE:CD1	2.31	0.58
1:A:403:LEU:HG	1:A:407:LEU:HD13	1.85	0.58
1:D:76:GLN:N	1:D:77:GLU:OE2	2.36	0.58
1:A:272:ASN:HB2	1:A:290:LEU:HB3	1.85	0.57
1:B:202:GLN:NE2	1:B:206:SER:OG	2.37	0.57
1:B:67:TYR:CD2	1:B:70:LEU:HD11	2.39	0.57
1:C:373:PHE:HB3	1:C:413:GLN:HG2	1.87	0.57
1:D:244:VAL:HG12	1:D:288:LEU:HD11	1.85	0.57
1:B:37:ILE:HG13	1:B:38:ASP:H	1.70	0.57
1:C:112:ILE:H	1:C:112:ILE:HD12	1.69	0.57
1:A:159:ARG:O	1:A:163:THR:HG23	2.05	0.57
1:B:37:ILE:O	1:B:41:GLN:HG2	2.05	0.57
1:B:242:ILE:HA	1:B:284:TYR:HB2	1.87	0.57
1:C:149:VAL:HG23	1:C:153:THR:HB	1.87	0.57
1:A:34:PRO:HD3	1:A:175:PHE:O	2.04	0.57
1:A:57:ILE:O	1:A:61:SER:OG	2.22	0.57
1:C:177:LEU:HD12	1:C:177:LEU:H	1.69	0.57
1:D:157:LEU:HB3	1:D:193:ILE:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:SER:HB3	1:A:76:GLN:HB3	1.87	0.56
1:C:202:GLN:OE1	1:C:206:SER:OG	2.22	0.56
1:C:79:ARG:C	1:C:79:ARG:HD2	2.25	0.56
1:C:165:LEU:HD22	1:C:202:GLN:HG3	1.87	0.56
1:A:273:ILE:HD12	1:A:286:VAL:CG2	2.34	0.56
1:B:87:LEU:O	1:B:91:ILE:HG13	2.05	0.56
1:B:194:ASN:ND2	1:B:226:LEU:HD12	2.16	0.56
1:C:112:ILE:HD11	1:C:166:PHE:CE1	2.41	0.56
1:D:157:LEU:HD22	1:D:193:ILE:HG12	1.88	0.56
1:A:116:LEU:HD11	1:A:125:LEU:HD21	1.87	0.56
1:D:246:ASP:OD2	1:D:359:ARG:NH2	2.39	0.56
1:D:106:LEU:HD12	1:D:113:LEU:HD22	1.86	0.55
1:C:112:ILE:O	1:C:116:LEU:HB2	2.07	0.55
1:D:81:PRO:HB2	1:D:83:TYR:CE1	2.41	0.55
1:D:398:MET:O	1:D:402:GLU:HG2	2.07	0.55
1:A:153:THR:HG22	1:A:157:LEU:HD23	1.89	0.55
1:B:194:ASN:HD22	1:B:197:ALA:H	1.54	0.55
1:C:47:ALA:C	1:C:190:PHE:HE2	2.10	0.55
1:D:302:LEU:HD12	1:D:364:ASP:HB3	1.88	0.55
1:A:337:GLU:O	1:A:343:LYS:HG3	2.07	0.55
1:C:257:TYR:CE1	1:C:261:GLU:HG3	2.42	0.55
1:A:88:PHE:CG	1:A:155:GLU:HG3	2.42	0.55
1:A:406:LEU:O	1:A:410:ILE:HG13	2.07	0.55
1:C:396:ARG:HA	1:C:399:TYR:CE2	2.42	0.55
1:A:260:ASN:HB3	1:D:43:GLN:OE1	2.06	0.54
1:D:44:ARG:HD2	1:D:44:ARG:N	2.22	0.54
1:C:41:GLN:HB2	1:C:156:ILE:CD1	2.36	0.54
1:D:117:ARG:NH1	1:D:121:SER:HA	2.22	0.54
1:C:356:HIS:O	1:C:356:HIS:ND1	2.40	0.54
1:B:244:VAL:HA	1:B:286:VAL:HB	1.89	0.54
1:C:231:ARG:HD3	1:C:262:PHE:CE1	2.42	0.54
1:B:216:ILE:HD13	1:B:305:ALA:HB1	1.89	0.54
1:D:410:ILE:HG22	1:D:415:LEU:HD11	1.90	0.54
1:A:100:HIS:CD2	1:A:126:TYR:HD1	2.24	0.54
1:C:117:ARG:NH1	1:C:121:SER:HA	2.23	0.54
1:D:201:LYS:O	1:D:204:GLU:HG3	2.08	0.54
1:C:180:HIS:CD2	1:C:391:GLU:HG3	2.43	0.54
1:A:149:VAL:HG12	1:A:153:THR:HG21	1.90	0.53
1:C:35:SER:CB	1:C:76:GLN:HB2	2.38	0.53
1:B:303:LEU:O	1:B:307:GLU:HG3	2.08	0.53
1:C:273:ILE:HG21	1:C:304:PHE:CE1	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:LEU:O	1:C:91:ILE:HG13	2.08	0.53
1:C:248:ARG:NE	1:C:345:VAL:HG11	2.24	0.53
1:C:48:GLY:N	1:C:190:PHE:HE2	2.07	0.53
1:A:35:SER:CB	1:A:76:GLN:HB3	2.39	0.53
1:A:164:THR:HG21	1:A:199:LEU:HD11	1.89	0.53
1:D:272:ASN:HB3	1:D:290:LEU:HD23	1.90	0.53
1:B:220:VAL:HB	1:B:333:SER:HA	1.90	0.53
1:C:270:GLY:O	1:C:272:ASN:N	2.42	0.53
1:D:43:GLN:O	1:D:44:ARG:HB2	2.09	0.53
1:D:67:TYR:HB3	1:D:70:LEU:HD11	1.91	0.53
1:C:119:VAL:O	1:C:184:THR:OG1	2.19	0.53
1:A:41:GLN:HB3	1:A:152:LYS:HE2	1.90	0.52
1:C:204:GLU:HG2	1:C:205:LEU:HD12	1.92	0.52
1:D:79:ARG:O	1:D:79:ARG:HG3	2.09	0.52
1:D:230:LEU:HA	1:D:234:PHE:HB2	1.91	0.52
1:D:322:LYS:NZ	1:D:381:ASP:O	2.39	0.52
1:A:37:ILE:O	1:A:41:GLN:HG2	2.10	0.52
1:D:270:GLY:O	1:D:273:ILE:HG13	2.09	0.52
1:C:259:ASN:O	1:C:263:ASN:N	2.42	0.52
1:A:261:GLU:OE2	1:D:44:ARG:NH2	2.42	0.52
1:B:222:ARG:NH1	1:B:253:GLN:OE1	2.42	0.52
1:D:34:PRO:HD3	1:D:175:PHE:O	2.10	0.52
1:D:56:ARG:HH21	1:D:390:LEU:HD11	1.74	0.52
1:D:236:HIS:O	1:D:280:ASN:ND2	2.35	0.52
1:B:67:TYR:HD2	1:B:70:LEU:HD11	1.75	0.52
1:C:405:ILE:O	1:C:409:VAL:HG23	2.10	0.52
1:D:114:ARG:NH2	1:D:205:LEU:HG	2.25	0.52
1:C:167:ASN:ND2	1:C:167:ASN:O	2.43	0.51
1:D:125:LEU:HD12	1:D:125:LEU:H	1.75	0.51
1:C:112:ILE:HD11	1:C:166:PHE:CZ	2.46	0.51
1:C:34:PRO:HD3	1:C:175:PHE:O	2.11	0.51
1:D:374:THR:O	1:D:378:GLU:HG2	2.11	0.51
1:D:231:ARG:NE	1:D:261:GLU:O	2.43	0.51
1:D:410:ILE:HG22	1:D:415:LEU:CD1	2.41	0.51
1:A:270:GLY:O	1:A:272:ASN:N	2.43	0.50
1:A:309:LEU:HD22	1:A:313:ILE:HD13	1.93	0.50
1:C:248:ARG:HE	1:C:345:VAL:HG11	1.77	0.50
1:D:183:TYR:HB2	1:D:186[A]:MET:O	2.11	0.50
1:A:74:THR:O	1:A:77:GLU:HG3	2.12	0.50
1:B:352:LYS:NZ	1:B:356:HIS:HB2	2.26	0.50
1:D:405:ILE:O	1:D:409:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:TYR:CE2	1:D:186[B]:MET:HA	2.41	0.50
1:B:412:LYS:HD3	1:D:405:ILE:HD11	1.94	0.50
1:C:295:SER:OG	1:C:296:VAL:N	2.42	0.50
1:B:98:LYS:O	1:B:102:LEU:HG	2.11	0.50
1:B:253:GLN:HB3	1:B:257:TYR:CD1	2.46	0.50
1:D:120:HIS:HD1	1:D:184:THR:HA	1.77	0.50
1:D:254:ASP:O	1:D:258:ILE:HG13	2.11	0.50
1:A:220:VAL:HG12	1:A:332:ASP:CG	2.33	0.49
1:B:270:GLY:O	1:B:272:ASN:N	2.42	0.49
1:D:111:ILE:HD11	1:D:202:GLN:OE1	2.12	0.49
1:D:314:ARG:HD3	1:D:315:GLU:N	2.27	0.49
1:D:94:GLY:HA2	1:D:133:ILE:HG23	1.93	0.49
1:D:231:ARG:NH2	1:D:262:PHE:HA	2.19	0.49
1:A:75:THR:HA	1:A:163:THR:HG21	1.93	0.49
1:A:80:LEU:HB2	1:A:85:LEU:CD1	2.42	0.49
1:A:255:PHE:HD1	1:A:276:TRP:HH2	1.59	0.49
1:C:369:TYR:CD2	1:C:406:LEU:HD23	2.48	0.49
1:D:177:LEU:HD12	1:D:177:LEU:H	1.77	0.49
1:A:80:LEU:HD21	1:A:159:ARG:HG2	1.94	0.49
1:A:248:ARG:NE	1:A:289:SER:HB3	2.28	0.49
1:A:350:MET:HE1	1:A:358:PHE:HD2	1.76	0.49
1:A:100:HIS:CD2	1:A:126:TYR:CD1	3.01	0.49
1:C:343:LYS:O	1:C:345:VAL:HG23	2.13	0.49
1:D:214:VAL:HG12	1:D:325:LEU:HD13	1.94	0.49
1:A:36:GLU:O	1:A:40:GLU:HG3	2.13	0.49
1:A:234:PHE:HB3	1:A:237:LEU:HD13	1.94	0.49
1:B:86:ASP:HA	1:B:89:ALA:HB3	1.93	0.48
1:B:296:VAL:HG11	1:D:307:GLU:HG3	1.95	0.48
1:A:56:ARG:NH1	1:A:390:LEU:HD21	2.28	0.48
1:C:298:VAL:HG21	1:C:367:TYR:CD2	2.47	0.48
1:D:80:LEU:HD12	1:D:81:PRO:HD2	1.94	0.48
1:D:214:VAL:HG22	1:D:240:CYS:HB3	1.95	0.48
1:B:46:PRO:HG2	1:B:190:PHE:HD1	1.79	0.48
1:D:119:VAL:HG13	1:D:229:ILE:HD13	1.95	0.48
1:D:314:ARG:HD3	1:D:314:ARG:C	2.33	0.48
1:D:246:ASP:OD1	1:D:248:ARG:HG3	2.13	0.48
1:A:103:PHE:HZ	1:A:125:LEU:HD23	1.77	0.48
1:A:362:ASP:N	1:A:362:ASP:OD1	2.45	0.48
1:A:119:VAL:HG23	1:A:120:HIS:CD2	2.49	0.48
1:D:27:GLU:O	1:D:169:ALA:HA	2.14	0.48
1:D:248:ARG:NH1	1:D:289:SER:HB3	2.26	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:34:PRO:HG2	1:C:57:ILE:HG21	1.95	0.48
1:C:248:ARG:NH1	1:C:289:SER:OG	2.41	0.48
1:D:231:ARG:HH21	1:D:262:PHE:CA	2.20	0.48
1:B:337:GLU:HG3	1:B:339:ALA:H	1.79	0.47
1:C:119:VAL:HG23	1:C:120:HIS:CD2	2.48	0.47
1:C:311:GLU:O	1:C:315:GLU:HG3	2.14	0.47
1:D:201:LYS:HB2	1:D:234:PHE:CZ	2.49	0.47
1:A:153:THR:O	1:A:157:LEU:HD23	2.15	0.47
1:C:36:GLU:O	1:C:40:GLU:HG3	2.14	0.47
1:C:125:LEU:O	1:C:129:ILE:HD12	2.15	0.47
1:D:30:ALA:HA	1:D:71:PRO:HB2	1.95	0.47
1:A:56:ARG:HH12	1:A:390:LEU:HD21	1.79	0.47
1:C:258:ILE:O	1:C:262:PHE:HB2	2.14	0.47
1:D:220:VAL:HG12	1:D:332:ASP:CG	2.34	0.47
1:D:226:LEU:O	1:D:230:LEU:HG	2.15	0.47
1:A:302:LEU:HD12	1:A:302:LEU:H	1.80	0.47
1:D:121:SER:O	1:D:124:TYR:N	2.47	0.47
1:B:405:ILE:HG12	1:D:412:LYS:HE2	1.95	0.47
1:C:251:PRO:O	1:C:253:GLN:N	2.48	0.47
1:A:352:LYS:NZ	1:A:356:HIS:HB2	2.29	0.47
1:B:147:LEU:HD11	1:B:187:GLY:C	2.35	0.47
1:B:194:ASN:HD21	1:B:226:LEU:CD1	2.21	0.47
1:C:51:GLU:HB3	1:C:55:LEU:HB2	1.97	0.47
1:D:56:ARG:O	1:D:60:MET:HG3	2.15	0.47
1:B:56:ARG:HH12	1:B:390:LEU:HD22	1.78	0.47
1:B:196:THR:O	1:B:200:MET:HG3	2.15	0.47
1:C:321:GLN:C	1:C:322:LYS:HD2	2.35	0.47
1:D:87:LEU:O	1:D:91:ILE:HG13	2.15	0.47
1:B:37:ILE:HG13	1:B:38:ASP:N	2.28	0.47
1:B:233:SER:HB2	1:B:234:PHE:CD2	2.50	0.47
1:C:47:ALA:HB3	1:C:51:GLU:O	2.15	0.47
1:D:103:PHE:O	1:D:106:LEU:HG	2.14	0.47
1:B:39:ASN:HA	1:B:42:MET:SD	2.55	0.47
1:B:157:LEU:HD13	1:B:193:ILE:HG12	1.96	0.47
1:B:175:PHE:HB3	1:B:390:LEU:HD12	1.97	0.46
1:D:271:LYS:H	1:D:271:LYS:HD3	1.79	0.46
1:C:253:GLN:HG2	1:C:257:TYR:CD1	2.51	0.46
1:B:134:GLN:OE1	1:B:141:LYS:NZ	2.35	0.46
1:B:302:LEU:HD12	1:B:364:ASP:HB3	1.97	0.46
1:C:117:ARG:HD3	1:C:122:GLU:HB3	1.96	0.46
1:D:122:GLU:HA	1:D:125:LEU:HD13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ARG:NH1	1:D:120:HIS:O	2.43	0.46
1:C:113:LEU:HD23	1:C:113:LEU:O	2.16	0.46
1:C:302:LEU:HD12	1:C:364:ASP:HB3	1.97	0.46
1:B:119:VAL:HG12	1:B:234:PHE:CZ	2.51	0.46
1:A:220:VAL:HB	1:A:333:SER:CA	2.46	0.46
1:B:269:ILE:HG13	1:B:273:ILE:O	2.15	0.46
1:A:220:VAL:HB	1:A:333:SER:HB3	1.98	0.45
1:B:295:SER:OG	1:B:296:VAL:N	2.49	0.45
1:C:122:GLU:OE2	1:C:122:GLU:N	2.49	0.45
1:D:173:PHE:HZ	1:D:373:PHE:CZ	2.35	0.45
1:B:317:LYS:HB3	1:B:317:LYS:HE2	1.73	0.45
1:C:111:ILE:CG2	1:C:114:ARG:HH21	2.28	0.45
1:A:214:VAL:HA	1:A:240:CYS:O	2.17	0.45
1:C:158:ILE:HD13	1:C:158:ILE:HA	1.77	0.45
1:D:287:ASP:OD1	1:D:289:SER:OG	2.20	0.45
1:B:248:ARG:NE	1:B:289:SER:HB3	2.32	0.45
1:C:29:CYS:HA	1:C:171:ALA:O	2.17	0.45
1:C:222:ARG:HG3	1:C:223:ASP:N	2.30	0.45
1:B:215:ILE:HG12	1:B:326:TYR:HB2	1.98	0.45
1:A:273:ILE:HG13	1:A:285:ALA:O	2.17	0.45
1:B:334:HIS:NE2	1:B:402:GLU:OE1	2.50	0.45
1:D:125:LEU:O	1:D:129:ILE:HG13	2.16	0.45
1:B:185:GLN:OE1	1:B:185:GLN:N	2.50	0.45
1:B:204:GLU:OE2	1:B:237:LEU:HD21	2.16	0.45
1:C:56:ARG:NH1	1:C:393:GLY:O	2.49	0.45
1:C:325:LEU:HD12	1:C:386:ILE:CG1	2.45	0.45
1:C:413:GLN:HB3	1:C:414:LEU:HD13	1.98	0.45
1:D:312:SER:O	1:D:323:ILE:HD11	2.17	0.45
1:C:403:LEU:O	1:C:407:LEU:HG	2.17	0.45
1:D:304:PHE:CE1	1:D:308:GLN:HG2	2.51	0.45
1:D:124:TYR:HE2	1:D:186[A]:MET:HA	1.81	0.45
1:A:311:GLU:OE2	1:A:314:ARG:HB3	2.17	0.45
1:C:176:GLY:O	1:C:390:LEU:HD12	2.16	0.45
1:A:39:ASN:O	1:A:42:MET:HG3	2.18	0.44
1:A:307:GLU:HG3	1:C:296:VAL:HG11	1.99	0.44
1:A:237:LEU:HB2	1:A:239:ILE:HD11	1.99	0.44
1:C:80:LEU:HD21	1:C:162:ALA:CB	2.46	0.44
1:A:114:ARG:HD2	1:A:205:LEU:CD1	2.47	0.44
1:C:179:SER:HB2	1:C:195:LYS:H	1.83	0.44
1:D:116:LEU:HG	1:D:125:LEU:HD21	2.00	0.44
1:A:198:MET:HB2	1:A:198:MET:HE3	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:84:TRP:HE1	1:B:110:ASP:CG	2.20	0.44
1:D:78:THR:OG1	1:D:163:THR:OG1	2.26	0.44
1:D:244:VAL:HG22	1:D:286:VAL:HB	2.00	0.44
1:D:329:THR:HG21	1:D:369:TYR:OH	2.18	0.44
1:A:161:CYS:SG	1:A:198:MET:CE	3.05	0.44
1:D:220:VAL:HB	1:D:333:SER:HA	1.99	0.44
1:D:270:GLY:O	1:D:272:ASN:N	2.51	0.44
1:D:33:ILE:O	1:D:74:THR:HA	2.18	0.44
1:D:88:PHE:O	1:D:91:ILE:N	2.51	0.44
1:D:248:ARG:HH21	1:D:345:VAL:HG21	1.81	0.44
1:B:45:MET:HE2	1:B:45:MET:HB3	1.90	0.44
1:D:75:THR:HG22	1:D:163:THR:OG1	2.18	0.44
1:A:220:VAL:HB	1:A:333:SER:HA	1.98	0.43
1:A:233:SER:O	1:A:236:HIS:HE1	2.01	0.43
1:C:43:GLN:C	1:C:45:MET:H	2.20	0.43
1:C:174:SER:OG	1:C:195:LYS:NZ	2.51	0.43
1:D:319:LYS:HA	1:D:319:LYS:HD3	1.85	0.43
1:D:356:HIS:HD1	1:D:356:HIS:C	2.19	0.43
1:B:370:GLU:OE2	1:B:412:LYS:NZ	2.50	0.43
1:A:396:ARG:O	1:A:400:GLU:HG3	2.19	0.43
1:A:47:ALA:HB1	1:A:394:TYR:CE2	2.53	0.43
1:A:325:LEU:HD12	1:A:386:ILE:HG12	2.01	0.43
1:B:275:VAL:HA	1:B:283:TYR:O	2.18	0.43
1:C:304:PHE:HD2	1:C:304:PHE:O	2.01	0.43
1:A:87:LEU:O	1:A:91:ILE:HG13	2.19	0.43
1:A:152:LYS:HE2	1:A:152:LYS:HB2	1.84	0.43
1:A:287:ASP:HB3	1:A:290:LEU:HD23	2.01	0.43
1:C:143:LEU:HB2	1:C:147:LEU:HB3	2.00	0.43
1:D:73:ILE:O	1:D:73:ILE:HG13	2.18	0.43
1:A:161:CYS:SG	1:A:198:MET:HE2	2.58	0.43
1:D:326:TYR:O	1:D:327:LEU:HD23	2.19	0.43
1:D:396:ARG:HA	1:D:399:TYR:CE2	2.54	0.43
1:A:147:LEU:HD11	1:A:187:GLY:C	2.39	0.43
1:C:179:SER:HB2	1:C:194:ASN:HA	2.00	0.43
1:C:202:GLN:O	1:C:206:SER:OG	2.36	0.43
1:D:83:TYR:CD2	1:D:107:PRO:HD2	2.54	0.43
1:C:253:GLN:HG2	1:C:257:TYR:CG	2.54	0.43
1:D:86:ASP:HB3	1:D:102:LEU:HD22	2.01	0.43
1:A:180:HIS:N	1:A:391:GLU:OE1	2.41	0.42
1:B:200:MET:HE3	1:B:213:PHE:CD2	2.53	0.42
1:C:194:ASN:HD21	1:C:226:LEU:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:LEU:HD22	1:A:80:LEU:H	1.84	0.42
1:C:244:VAL:HG12	1:C:288:LEU:HD11	2.01	0.42
1:B:38:ASP:O	1:B:42:MET:HG3	2.20	0.42
1:B:175:PHE:CB	1:B:390:LEU:HD12	2.49	0.42
1:D:158:ILE:HD13	1:D:158:ILE:HA	1.86	0.42
1:A:254:ASP:O	1:A:258:ILE:HG12	2.19	0.42
1:D:34:PRO:HG2	1:D:57:ILE:HG21	2.01	0.42
1:A:47:ALA:HB1	1:A:394:TYR:CD2	2.55	0.42
1:A:157:LEU:HB3	1:A:193:ILE:HD11	2.01	0.42
1:A:296:VAL:HG13	1:C:310:LYS:HE2	2.01	0.42
1:A:334:HIS:ND1	1:A:336:ASP:HB2	2.35	0.42
1:A:366:GLY:O	1:A:370:GLU:HB2	2.20	0.42
1:C:378:GLU:O	1:C:380:LYS:N	2.51	0.42
1:A:339:ALA:HB2	1:A:394:TYR:HB2	2.01	0.42
1:B:134:GLN:HB3	1:B:141:LYS:HZ3	1.84	0.42
1:B:362:ASP:OD1	1:B:362:ASP:N	2.51	0.42
1:C:69:ASP:OD1	1:C:69:ASP:N	2.52	0.42
1:C:403:LEU:HA	1:C:403:LEU:HD12	1.75	0.42
1:D:121:SER:O	1:D:123:ASP:N	2.52	0.42
1:A:299:HIS:HB3	1:A:302:LEU:HD12	2.02	0.42
1:C:245:PHE:C	1:C:288:LEU:HD12	2.40	0.42
1:C:149:VAL:HG23	1:C:153:THR:CB	2.49	0.42
1:D:203:ALA:HB3	1:D:213:PHE:HZ	1.85	0.42
1:D:267:VAL:HG12	1:D:275:VAL:HG12	2.01	0.42
1:A:200:MET:SD	1:A:215:ILE:HD11	2.60	0.42
1:C:81:PRO:HB2	1:C:83:TYR:CE1	2.55	0.42
1:C:377:ASN:HD22	1:C:413:GLN:HG3	1.85	0.42
1:D:111:ILE:HD13	1:D:114:ARG:NH2	2.35	0.42
1:A:260:ASN:HD21	1:D:40:GLU:CB	2.27	0.41
1:B:157:LEU:HD23	1:B:157:LEU:HA	1.78	0.41
1:C:167:ASN:HD21	1:C:169:ALA:CB	2.33	0.41
1:D:356:HIS:ND1	1:D:356:HIS:C	2.74	0.41
1:A:331:TRP:HH2	1:A:403:LEU:HD13	1.86	0.41
1:B:352:LYS:HZ1	1:B:356:HIS:HB2	1.85	0.41
1:C:241:HIS:CD2	1:C:283:TYR:HD1	2.37	0.41
1:D:212:LYS:HB2	1:D:212:LYS:HE2	1.65	0.41
1:A:253:GLN:HG2	1:A:257:TYR:CD2	2.54	0.41
1:B:272:ASN:HB2	1:B:290:LEU:HB3	2.03	0.41
1:C:164:THR:HG23	1:C:172:HIS:CD2	2.55	0.41
1:A:350:MET:HE1	1:A:358:PHE:CD2	2.54	0.41
1:C:165:LEU:CD2	1:C:202:GLN:HG3	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:GLN:N	1:C:252:GLN:OE1	2.53	0.41
1:D:88:PHE:CE1	1:D:155:GLU:HA	2.55	0.41
1:D:111:ILE:HD12	1:D:111:ILE:HA	1.82	0.41
1:B:74:THR:HG23	1:B:76:GLN:H	1.85	0.41
1:A:293:ARG:NH1	1:A:356:HIS:O	2.53	0.41
1:A:340:TYR:HE2	1:D:50:GLU:OE2	2.03	0.41
1:C:377:ASN:ND2	1:C:413:GLN:HG3	2.35	0.41
1:C:391:GLU:HB3	1:C:392:GLY:H	1.72	0.41
1:A:257:TYR:CZ	1:D:43:GLN:HG2	2.55	0.41
1:C:323:ILE:HG13	1:C:382:CYS:SG	2.61	0.41
1:D:96:THR:HB	1:D:97:PRO:HD3	2.03	0.41
1:D:401:ARG:O	1:D:405:ILE:HD13	2.21	0.41
1:A:116:LEU:HA	1:A:198:MET:SD	2.61	0.41
1:D:43:GLN:HE21	1:D:43:GLN:HB2	1.55	0.41
1:B:350:MET:HG3	1:B:354:ALA:HB3	2.02	0.41
1:C:293:ARG:NH1	1:C:356:HIS:O	2.54	0.41
1:D:119:VAL:HG12	1:D:120:HIS:CD2	2.56	0.41
1:D:166:PHE:CD1	1:D:166:PHE:N	2.89	0.41
1:D:244:VAL:CG1	1:D:288:LEU:HD11	2.50	0.41
1:B:85:LEU:O	1:B:89:ALA:N	2.39	0.41
1:C:373:PHE:CB	1:C:413:GLN:HG2	2.49	0.41
1:A:114:ARG:NH2	1:A:202:GLN:HE22	2.20	0.40
1:B:88:PHE:CE1	1:B:155:GLU:HA	2.56	0.40
1:C:167:ASN:HD21	1:C:169:ALA:HB2	1.86	0.40
1:D:114:ARG:CZ	1:D:205:LEU:HG	2.52	0.40
1:D:153:THR:CG2	1:D:157:LEU:HD11	2.51	0.40
1:B:103:PHE:HA	1:B:106:LEU:HG	2.04	0.40
1:C:303:LEU:O	1:C:307:GLU:OE1	2.40	0.40
1:D:44:ARG:HG2	1:D:140:PHE:CE1	2.57	0.40
1:B:97:PRO:HA	1:B:100:HIS:HB2	2.04	0.40
1:C:229:ILE:H	1:C:229:ILE:HG13	1.76	0.40
1:A:142:GLN:HG2	1:A:148:VAL:HG22	2.04	0.40
1:D:39:ASN:HA	1:D:42:MET:SD	2.61	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	392/437 (90%)	341 (87%)	43 (11%)	8 (2%)	6 16
1	B	391/437 (90%)	347 (89%)	38 (10%)	6 (2%)	8 22
1	C	390/437 (89%)	341 (87%)	42 (11%)	7 (2%)	7 18
1	D	390/437 (89%)	346 (89%)	30 (8%)	14 (4%)	3 6
All	All	1563/1748 (89%)	1375 (88%)	153 (10%)	35 (2%)	5 15

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	GLY
1	B	295	SER
1	C	252	GLN
1	C	271	LYS
1	D	122	GLU
1	D	143	LEU
1	D	208	ALA
1	D	263	ASN
1	D	271	LYS
1	D	346	ASN
1	A	247	SER
1	A	263	ASN
1	B	332	ASP
1	C	189	GLY
1	D	67	TYR
1	D	292	SER
1	D	312	SER
1	A	67	TYR
1	A	271	LYS
1	A	295	SER
1	B	271	LYS
1	D	79	ARG

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Mol	Chain	Res	Type
1	A	346	ASN
1	B	391	GLU
1	C	102	LEU
1	C	219	ASP
1	D	311	GLU
1	D	144	ASN
1	C	44	ARG
1	C	68	GLY
1	D	77	GLU
1	A	68	GLY
1	B	273	ILE
1	D	68	GLY
1	A	249	VAL

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	343/381 (90%)	324 (94%)	19 (6%)	18	41
1	B	342/381 (90%)	323 (94%)	19 (6%)	17	41
1	C	340/381 (89%)	318 (94%)	22 (6%)	14	34
1	D	341/381 (90%)	321 (94%)	20 (6%)	16	38
All	All	1366/1524 (90%)	1286 (94%)	80 (6%)	17	38

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	SER
1	A	67	TYR
1	A	79	ARG
1	A	108	GLN
1	A	117	ARG
1	A	123	ASP
1	A	142	GLN
1	A	150	THR

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Mol	Chain	Res	Type
1	A	152	LYS
1	A	163	THR
1	A	180	HIS
1	A	184	THR
1	A	186	MET
1	A	218	THR
1	A	235	SER
1	A	238	SER
1	A	248	ARG
1	A	274	HIS
1	A	338	THR
1	B	70	LEU
1	B	77	GLU
1	B	78	THR
1	B	105	LEU
1	B	126	TYR
1	B	127	GLN
1	B	150	THR
1	B	167[A]	ASN
1	B	167[B]	ASN
1	B	180	HIS
1	B	184	THR
1	B	194	ASN
1	B	223	ASP
1	B	233	SER
1	B	241	HIS
1	B	248	ARG
1	B	261	GLU
1	B	321	GLN
1	B	365	LEU
1	C	38	ASP
1	C	56	ARG
1	C	79	ARG
1	C	82	TYR
1	C	123	ASP
1	C	143	LEU
1	C	167	ASN
1	C	180	HIS
1	C	185	GLN
1	C	186	MET
1	C	190	PHE
1	C	196	THR

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Mol	Chain	Res	Type
1	C	212	LYS
1	C	223	ASP
1	C	226	LEU
1	C	271	LYS
1	C	288	LEU
1	C	295	SER
1	C	304	PHE
1	C	319	LYS
1	C	328	PRO
1	C	348	ARG
1	D	38	ASP
1	D	44	ARG
1	D	76	GLN
1	D	79	ARG
1	D	80	LEU
1	D	111	ILE
1	D	140	PHE
1	D	180	HIS
1	D	185	GLN
1	D	205	LEU
1	D	233	SER
1	D	271	LYS
1	D	276	TRP
1	D	294	LYS
1	D	304	PHE
1	D	312	SER
1	D	314	ARG
1	D	352	LYS
1	D	353	THR
1	D	381	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	202	GLN
1	A	260	ASN
1	B	59	HIS
1	B	100	HIS
1	B	194	ASN
1	B	277	HIS
1	C	167	ASN

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Mol	Chain	Res	Type
1	C	180	HIS
1	C	232	HIS
1	C	308	GLN
1	C	379	ASN
1	C	413	GLN
1	D	43	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 6 ligands modelled in this entry, 6 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	393/437 (89%)	-0.35	4 (1%) 79 79	57, 108, 131, 164	1 (0%)
1	B	392/437 (89%)	-0.37	3 (0%) 82 82	61, 111, 134, 159	1 (0%)
1	C	392/437 (89%)	-0.35	0 100 100	90, 113, 138, 156	0
1	D	391/437 (89%)	-0.36	4 (1%) 79 79	59, 115, 143, 158	1 (0%)
All	All	1568/1748 (89%)	-0.36	11 (0%) 84 83	57, 112, 138, 164	3 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	186[A]	MET	5.8
1	A	294[A]	LYS	4.0
1	B	173	PHE	3.1
1	D	414	LEU	3.0
1	A	112	ILE	2.5
1	A	173	PHE	2.3
1	A	148	VAL	2.2
1	B	175	PHE	2.2
1	B	168	PRO	2.2
1	D	198	MET	2.1
1	D	292	SER	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 monosaccharides in this entry.

6.4 Ligands (i)

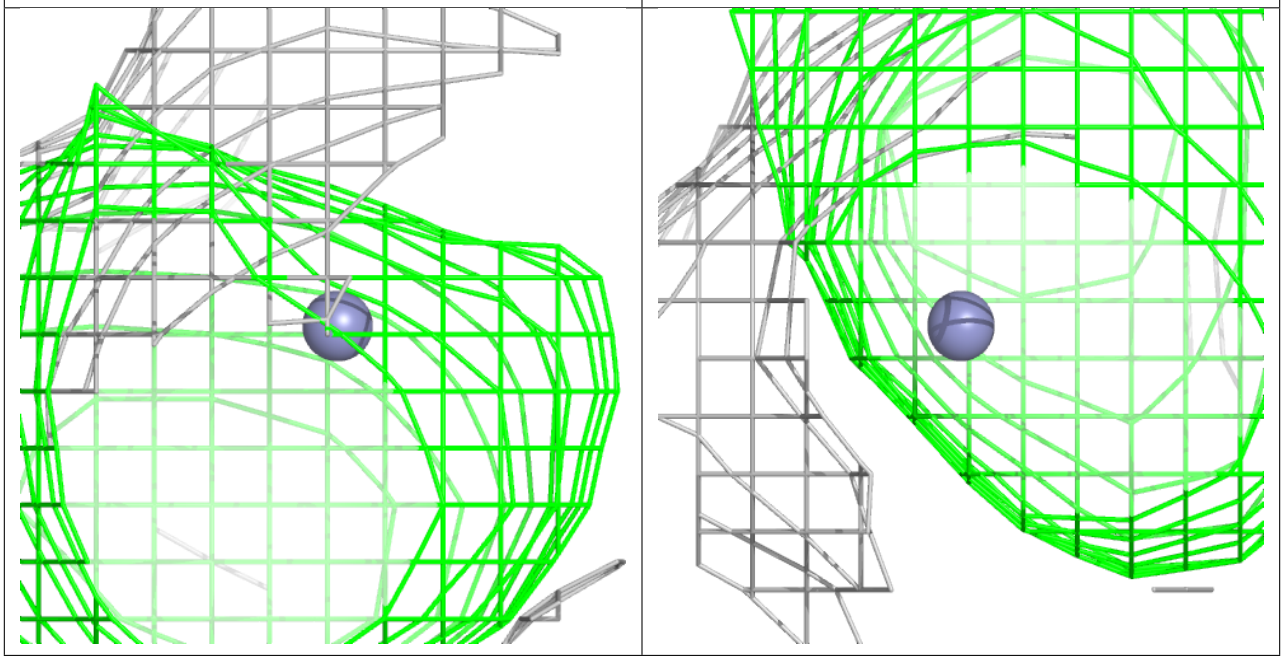
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	ZN	B	501	1/1	0.64	0.20	101,101,101,101	1
2	ZN	A	501	1/1	0.66	0.18	103,103,103,103	1
2	ZN	D	501	1/1	0.76	0.20	111,111,111,111	1
3	K	C	502	1/1	0.90	0.06	113,113,113,113	0
3	K	A	502	1/1	0.96	0.04	100,100,100,100	0
2	ZN	C	501	1/1	0.99	0.09	113,113,113,113	1

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

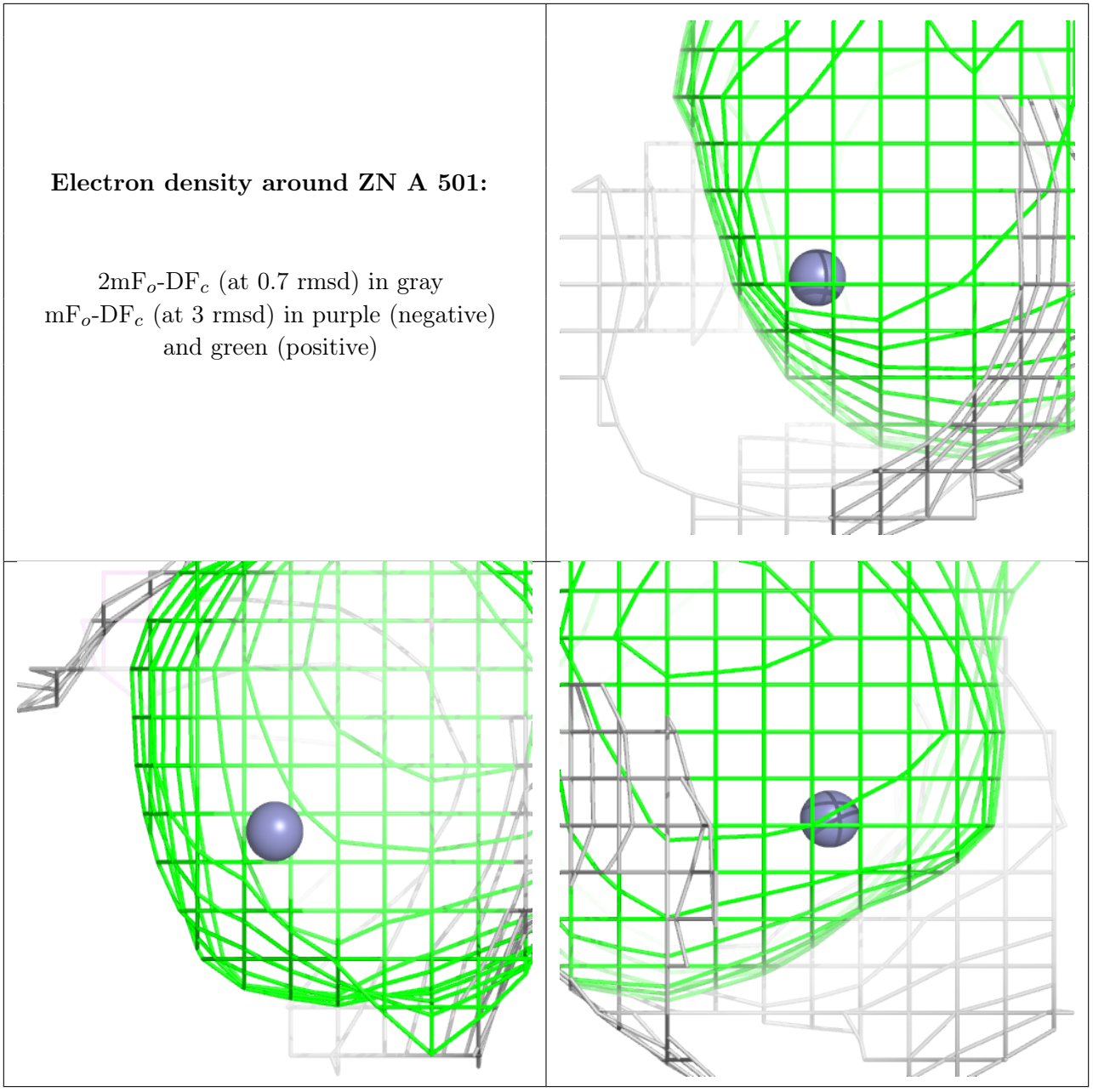
Electron density around ZN B 501:

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



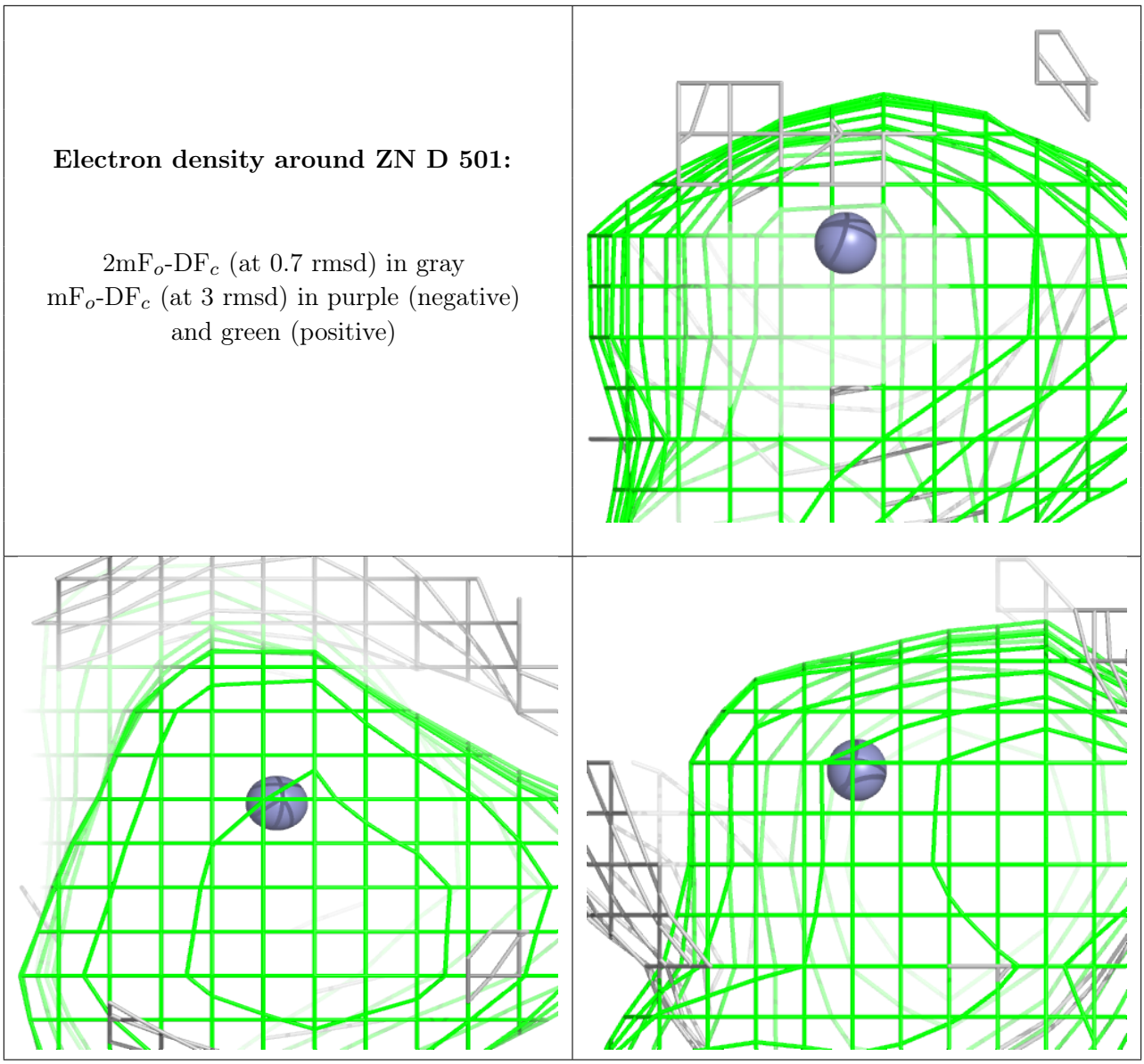
Electron density around ZN A 501:

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



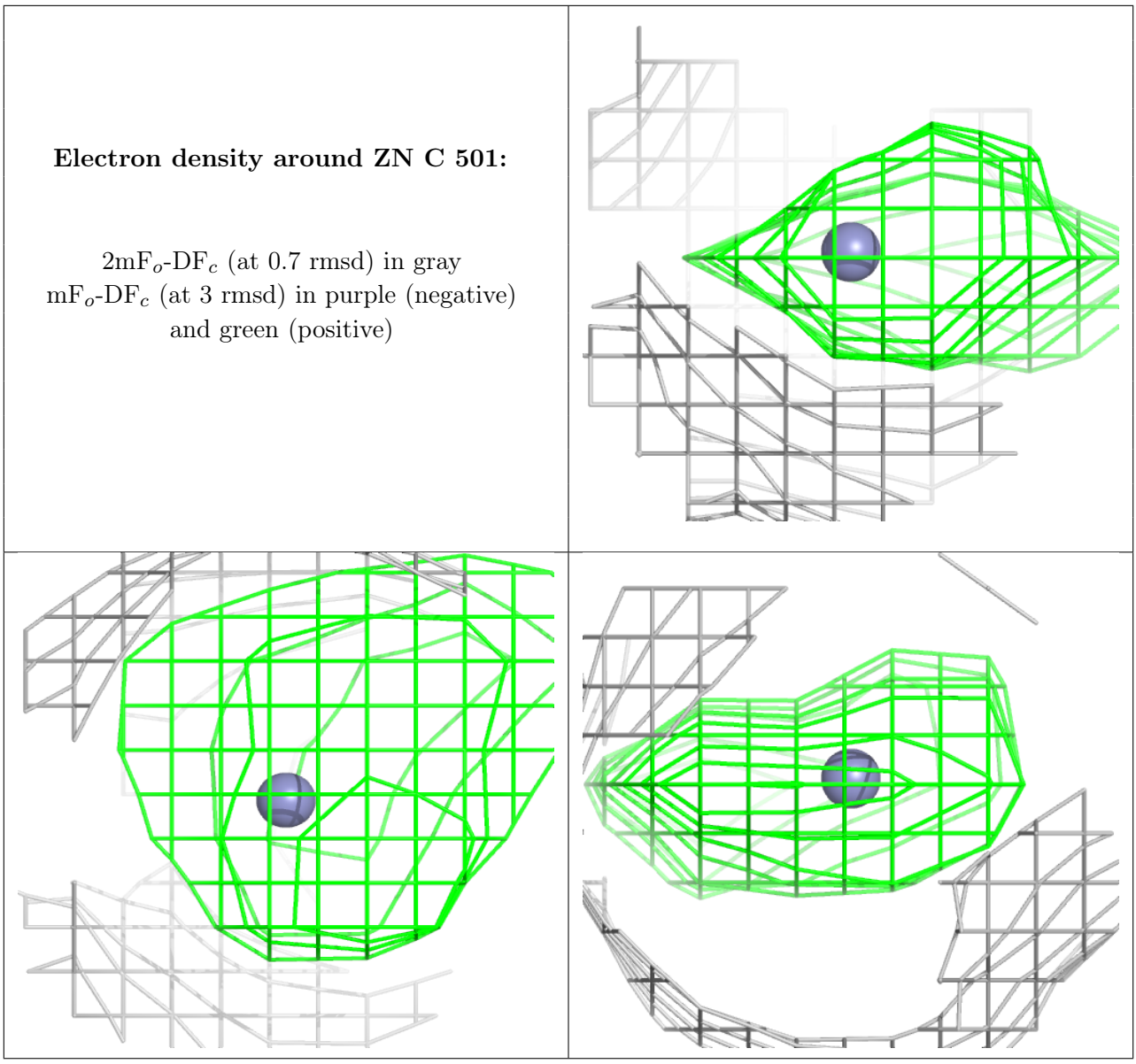
Electron density around ZN D 501:

$2mF_o$-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 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.