



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:42 AM UTC

PDB ID : 9GL0 / pdb_00009gl0
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	:	4-5-2 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

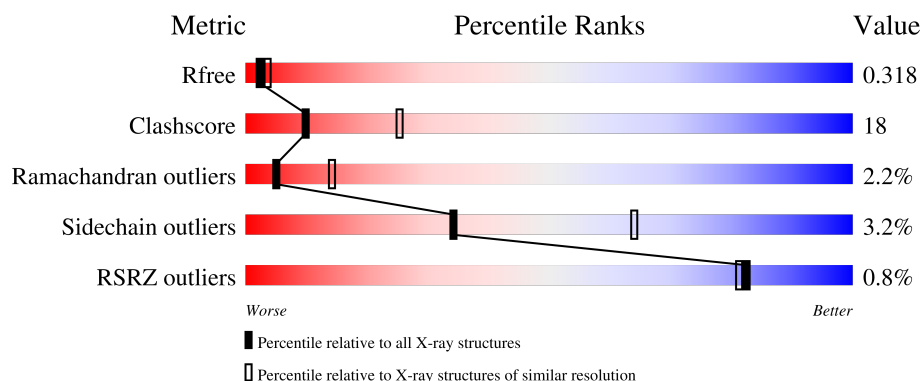
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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}	180053	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 $\leq 5\%$. 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	437	% 57% 32% • 10%
1	B	437	% 62% 27% • 10%
1	C	437	54% 34% • 10%
1	D	437	% 49% 38% • 11%

2 Entry composition

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 A0A2S6EWW0
A	-9	ALA	-	expression tag	UNP A0A2S6EWW0
A	-8	HIS	-	expression tag	UNP A0A2S6EWW0
A	-7	HIS	-	expression tag	UNP A0A2S6EWW0
A	-6	HIS	-	expression tag	UNP A0A2S6EWW0
A	-5	HIS	-	expression tag	UNP A0A2S6EWW0
A	-4	HIS	-	expression tag	UNP A0A2S6EWW0
A	-3	HIS	-	expression tag	UNP A0A2S6EWW0
A	-2	VAL	-	expression tag	UNP A0A2S6EWW0
A	-1	GLY	-	expression tag	UNP A0A2S6EWW0
A	0	THR	-	expression tag	UNP A0A2S6EWW0
B	-10	MET	-	initiating methionine	UNP A0A2S6EWW0
B	-9	ALA	-	expression tag	UNP A0A2S6EWW0
B	-8	HIS	-	expression tag	UNP A0A2S6EWW0
B	-7	HIS	-	expression tag	UNP A0A2S6EWW0
B	-6	HIS	-	expression tag	UNP A0A2S6EWW0
B	-5	HIS	-	expression tag	UNP A0A2S6EWW0
B	-4	HIS	-	expression tag	UNP A0A2S6EWW0
B	-3	HIS	-	expression tag	UNP A0A2S6EWW0
B	-2	VAL	-	expression tag	UNP A0A2S6EWW0
B	-1	GLY	-	expression tag	UNP A0A2S6EWW0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	0	THR	-	expression tag	UNP A0A2S6EWW0
C	-10	MET	-	initiating methionine	UNP A0A2S6EWW0
C	-9	ALA	-	expression tag	UNP A0A2S6EWW0
C	-8	HIS	-	expression tag	UNP A0A2S6EWW0
C	-7	HIS	-	expression tag	UNP A0A2S6EWW0
C	-6	HIS	-	expression tag	UNP A0A2S6EWW0
C	-5	HIS	-	expression tag	UNP A0A2S6EWW0
C	-4	HIS	-	expression tag	UNP A0A2S6EWW0
C	-3	HIS	-	expression tag	UNP A0A2S6EWW0
C	-2	VAL	-	expression tag	UNP A0A2S6EWW0
C	-1	GLY	-	expression tag	UNP A0A2S6EWW0
C	0	THR	-	expression tag	UNP A0A2S6EWW0
D	-10	MET	-	initiating methionine	UNP A0A2S6EWW0
D	-9	ALA	-	expression tag	UNP A0A2S6EWW0
D	-8	HIS	-	expression tag	UNP A0A2S6EWW0
D	-7	HIS	-	expression tag	UNP A0A2S6EWW0
D	-6	HIS	-	expression tag	UNP A0A2S6EWW0
D	-5	HIS	-	expression tag	UNP A0A2S6EWW0
D	-4	HIS	-	expression tag	UNP A0A2S6EWW0
D	-3	HIS	-	expression tag	UNP A0A2S6EWW0
D	-2	VAL	-	expression tag	UNP A0A2S6EWW0
D	-1	GLY	-	expression tag	UNP A0A2S6EWW0
D	0	THR	-	expression tag	UNP A0A2S6EWW0

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

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

- Molecule 3 is POTASSIUM ION (CCD ID: 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	0	0
			1	1		

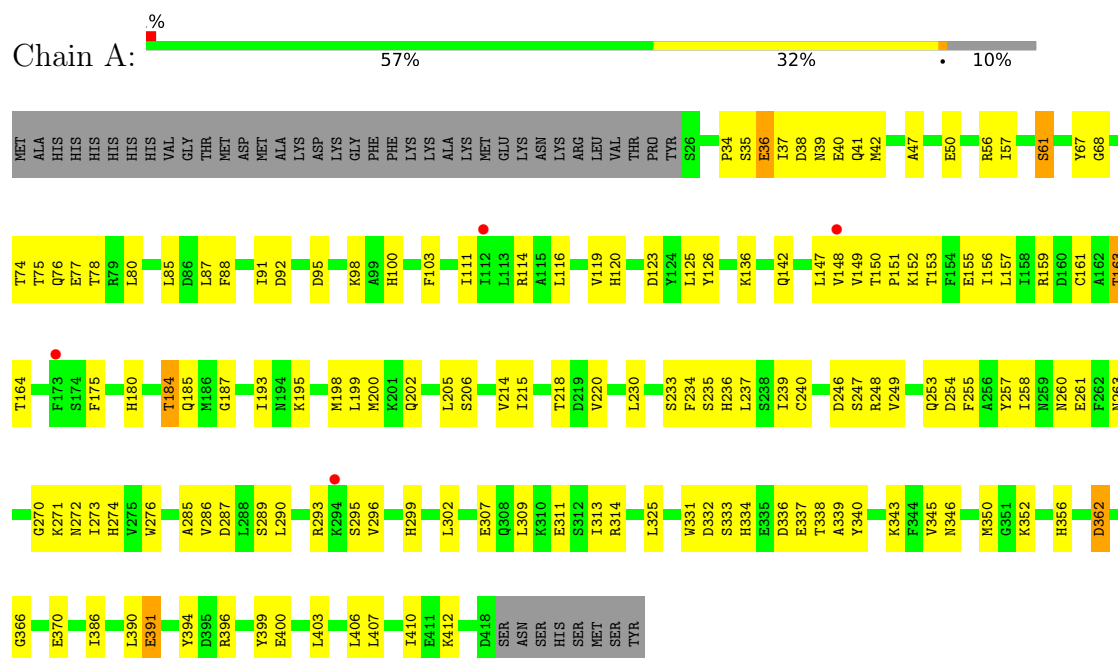
- Molecule 4 is water.

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

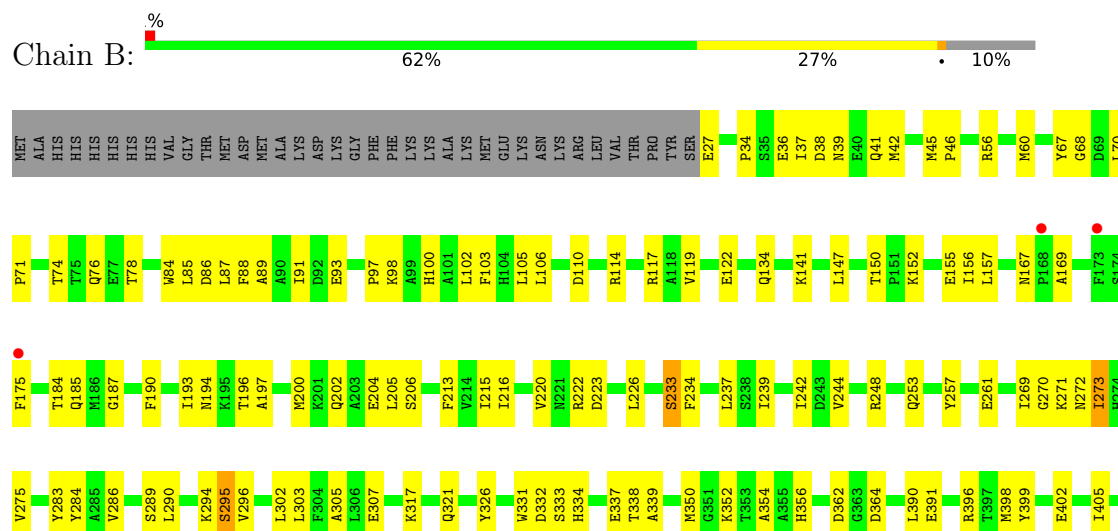
3 Residue-property plots [i](#)

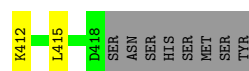
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



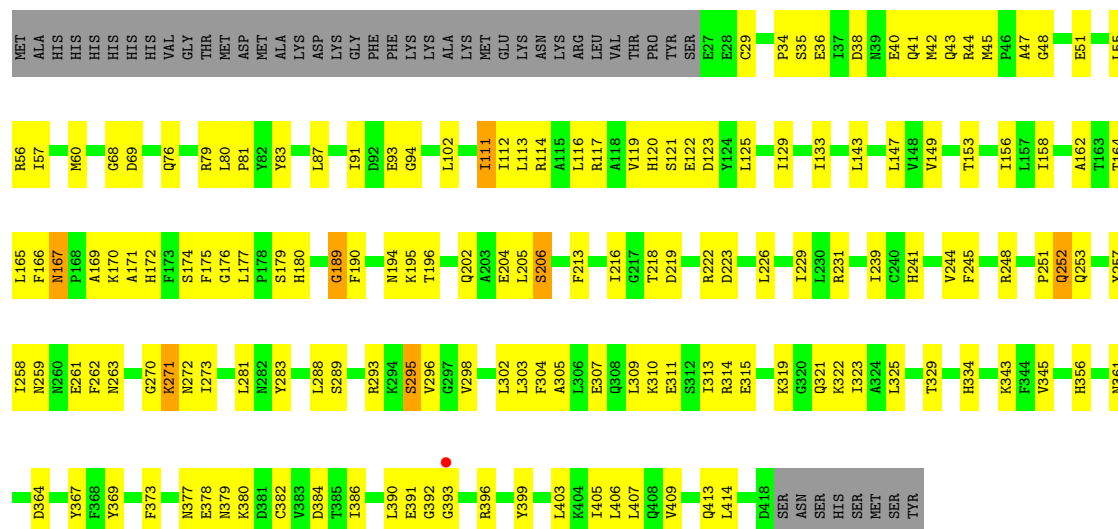
• Molecule 1: Acetypolyamine aminohydrolase





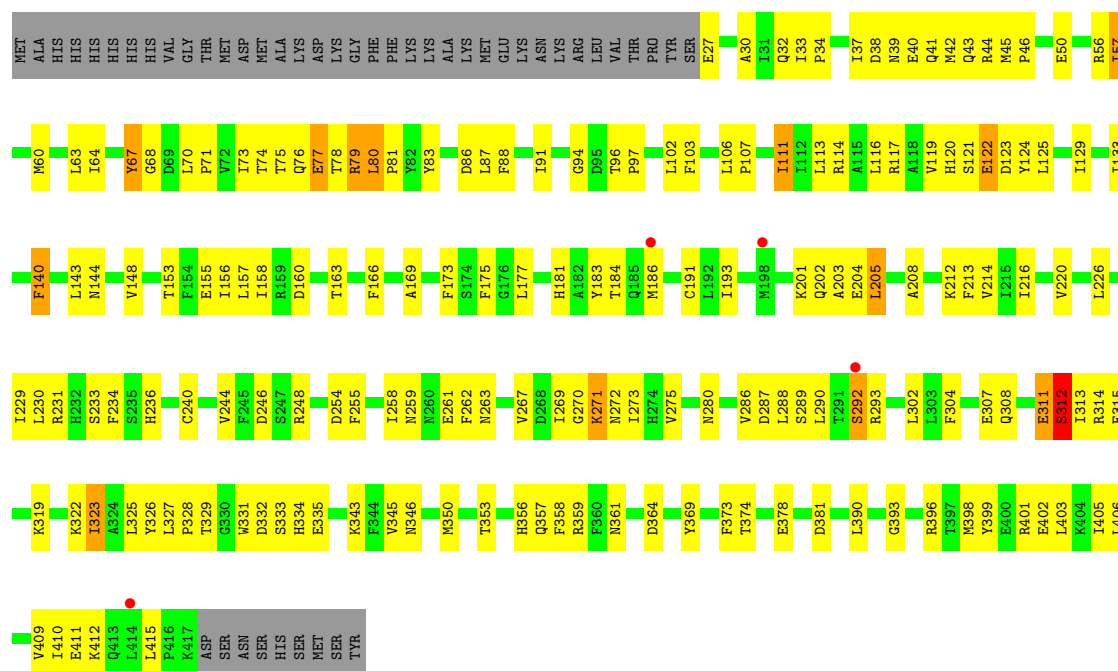
• Molecule 1: Acetylpolyamine aminohydrolase

Chain C: 54% 34% 10%



• Molecule 1: Acetylpolyamine aminohydrolase

Chain D: 49% 38% 11%



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ ¹	0.87 (at 2.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.240 , 0.316 0.243 , 0.318	Depositor DCC
R_{free} test set	3378 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	92.2	Xtrriage
Anisotropy	0.512	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 79.5	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	0.96	EDS
Total number of atoms	12712	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtrriage'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.*

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: K, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.41	1/3261 (0.0%)	0.59	0/4413
1	B	0.39	0/3254	0.59	0/4406
1	C	0.40	0/3243	0.61	0/4390
1	D	0.39	0/3246	0.60	0/4393
All	All	0.40	1/13004 (0.0%)	0.60	0/17602

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	391	GLU	CA-C	-5.37	1.49	1.52

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	3182	0	3107	108	0
1	B	3175	0	3096	81	0
1	C	3164	0	3088	120	0
1	D	3167	0	3094	143	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	440	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 18.

All (440) 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	1.35	1.05
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: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:B:60:MET:HE1	1:B:390:LEU:CD1	2.13	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
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:C:42:MET:HE1	1:C:57:ILE:HG13	1.72	0.72
1:D:56:ARG:NH1	1:D:393:GLY:O	2.23	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:CYS:SG	1:A:198:MET:HE1	2.29	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:B:60:MET:CE	1:B:390:LEU:HD11	2.21	0.67
1:D:356:HIS:O	1:D:356:HIS:ND1	2.27	0.67
1:A:202:GLN:O	1:A:206:SER:OG	2.08	0.66
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: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: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: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:A:39:ASN:HD22	1:A:42:MET:HE2	1.63	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:C:79:ARG:C	1:C:79:ARG:HD2	2.25	0.61
1:D:63:LEU:HD23	1:D:403:LEU:HD23	1.82	0.61
1:C:60:MET:HE1	1:C:390:LEU:HG	1.83	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
1:A:78:THR:OG1	1:A:163:THR:HG22	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:47:ALA:C	1:C:190:PHE:HE2	2.10	0.59
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:A:195:LYS:HA	1:A:198:MET:HE2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:157:LEU:HB3	1:D:193:ILE:HD11	1.86	0.57
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:165:LEU:HD22	1:C:202:GLN:HG3	1.87	0.56
1:D:287:ASP:OD1	1:D:289:SER:OG	2.20	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: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:A:220:VAL:HG12	1:A:332:ASP:CG	2.33	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:C:170:LYS:NZ	1:C:384:ASP:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:314:ARG:HD3	1:D:314:ARG:C	2.33	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:220:VAL:HG12	1:D:332:ASP:CG	2.34	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:A:345:VAL:HG21	1:A:350:MET:HE3	1.92	0.52
1:B:67:TYR:HD2	1:B:70:LEU:HD11	1.75	0.52
1:B:147:LEU:HD11	1:B:187:GLY:C	2.35	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:321:GLN:C	1:C:322:LYS:HD2	2.35	0.51
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:B:334:HIS:HB3	1:B:398:MET:HE2	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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:84:TRP:HE1	1:B:110:ASP:CG	2.20	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:356:HIS:HD1	1:D:356:HIS:C	2.19	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:43:GLN:C	1:C:45:MET:H	2.20	0.48
1:A:119:VAL:HG23	1:A:120:HIS:CD2	2.49	0.48
1:B:352:LYS:HZ3	1:B:356:HIS:HB2	1.78	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
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:A:39:ASN:ND2	1:A:42:MET:HE2	2.29	0.47
1:A:147:LEU:HD11	1:A:187:GLY:C	2.39	0.47
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: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:194:ASN:HD21	1:B:226:LEU:CD1	2.21	0.47
1:B:200:MET:HE3	1:B:213:PHE:CD2	2.50	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:304:PHE:C	1:C:304:PHE:CD2	2.93	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:C:245:PHE:C	1:C:288:LEU:HD12	2.40	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:356:HIS:ND1	1:D:356:HIS:C	2.74	0.46
1:B:45:MET:HB3	1:B:45:MET:HE2	1.58	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
1:B:331:TRP:HB3	1:B:398:MET:HE1	1.98	0.46
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:D:331:TRP:HB3	1:D:398:MET:HE1	1.98	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:42:MET:HE3	1:D:177:LEU:HD11	1.99	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: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:C:356:HIS:ND1	1:C:356:HIS:C	2.77	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:CE	3.05	0.43
1:C:47:ALA:C	1:C:190:PHE:CE2	2.95	0.43
1:D:326:TYR:O	1:D:327:LEU:HD23	2.19	0.43
1:D:345:VAL:HG11	1:D:350:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:ARG:HA	1:D:399:TYR:CE2	2.54	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:D:334:HIS:HE2	1:D:361:ASN:HA	1.83	0.43
1:A:180:HIS:N	1:A:391:GLU:OE1	2.41	0.42
1:C:194:ASN:HD21	1:C:226:LEU:HB2	1.83	0.42
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:C:189:GLY:C	1:C:190:PHE:HD1	2.28	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: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:A:331:TRP:HH2	1:A:403:LEU:HD13	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:TYR:C	1:A:340:TYR:CD2	2.98	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:C:167:ASN:ND2	1:C:167:ASN:C	2.77	0.41
1:C:165:LEU:CD2	1:C:202:GLN:HG3	2.49	0.41
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:C:356:HIS:C	1:C:356:HIS:HD1	2.29	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:D:45:MET:HE3	1:D:148:VAL:O	2.20	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:200:MET:HE2	1:B:200:MET:HB3	1.86	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:A:246:ASP:C	1:A:248:ARG:H	2.28	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:A:200:MET:HE1	1:A:230:LEU:HD11	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	6	18
1	D	390/437 (89%)	346 (89%)	30 (8%)	14 (4%)	2	6
All	All	1563/1748 (89%)	1375 (88%)	153 (10%)	35 (2%)	5	14

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

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Mol	Chain	Res	Type
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
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 ⓘ

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%)	331 (96%)	12 (4%)	32	61
1	B	342/381 (90%)	331 (97%)	11 (3%)	34	64
1	C	340/381 (89%)	329 (97%)	11 (3%)	34	64
1	D	341/381 (90%)	330 (97%)	11 (3%)	34	64
All	All	1366/1524 (90%)	1321 (97%)	45 (3%)	34	63

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	GLU
1	A	61	SER
1	A	111	ILE
1	A	123	ASP
1	A	150	THR
1	A	163	THR
1	A	184	THR
1	A	218	THR
1	A	235	SER
1	A	274	HIS
1	A	338	THR
1	A	362	ASP
1	B	78	THR
1	B	105	LEU
1	B	150	THR
1	B	167[A]	ASN
1	B	167[B]	ASN
1	B	184	THR
1	B	223	ASP
1	B	233	SER
1	B	261	GLU
1	B	321	GLN
1	B	338	THR
1	C	38	ASP
1	C	111	ILE
1	C	123	ASP
1	C	167	ASN
1	C	196	THR
1	C	206	SER
1	C	218	THR
1	C	271	LYS
1	C	281	LEU
1	C	295	SER
1	C	329	THR
1	D	38	ASP
1	D	57	ILE
1	D	80	LEU
1	D	111	ILE
1	D	140	PHE
1	D	205	LEU
1	D	233	SER
1	D	312	SER

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Mol	Chain	Res	Type
1	D	323	ILE
1	D	353	THR
1	D	406	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	GLN
1	A	202	GLN
1	A	260	ASN
1	A	272	ASN
1	B	59	HIS
1	B	100	HIS
1	B	127	GLN
1	B	194	ASN
1	B	202	GLN
1	B	277	HIS
1	C	100	HIS
1	C	104	HIS
1	C	167	ASN
1	C	232	HIS
1	C	282	ASN
1	C	308	GLN
1	C	346	ASN
1	C	379	ASN
1	C	413	GLN
1	D	43	GLN
1	D	108	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 [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	393/437 (89%)	-0.21	4 (1%) 79 78	57, 108, 131, 164	1 (0%)
1	B	392/437 (89%)	-0.23	3 (0%) 82 81	61, 111, 134, 159	1 (0%)
1	C	392/437 (89%)	-0.22	1 (0%) 90 89	90, 113, 138, 156	0
1	D	391/437 (89%)	-0.22	4 (1%) 79 78	59, 115, 143, 158	1 (0%)
All	All	1568/1748 (89%)	-0.22	12 (0%) 82 81	57, 112, 138, 164	3 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	186[A]	MET	5.9
1	A	294[A]	LYS	4.1
1	B	173	PHE	3.2
1	D	414	LEU	3.1
1	A	112	ILE	2.6
1	A	173	PHE	2.4
1	A	148	VAL	2.3
1	B	175	PHE	2.3
1	B	168	PRO	2.3
1	D	198	MET	2.2
1	D	292	SER	2.1
1	C	393	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

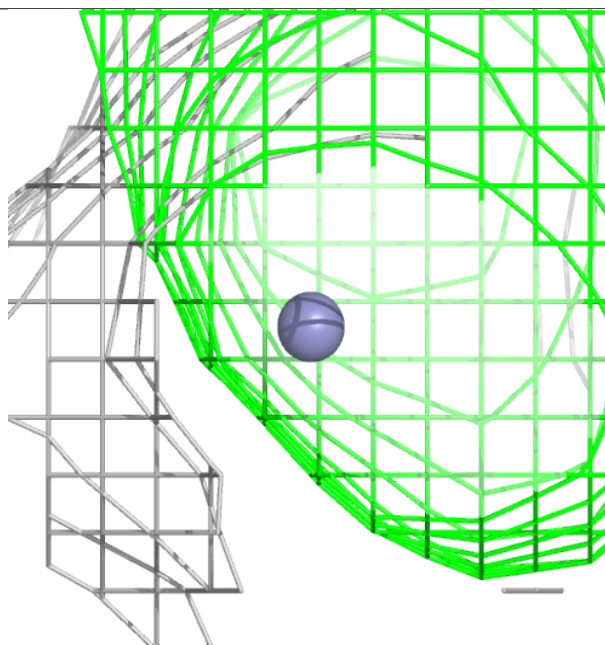
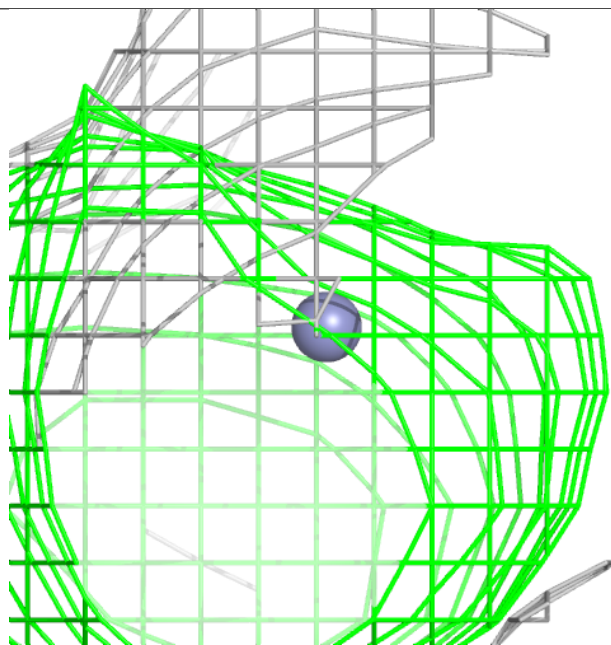
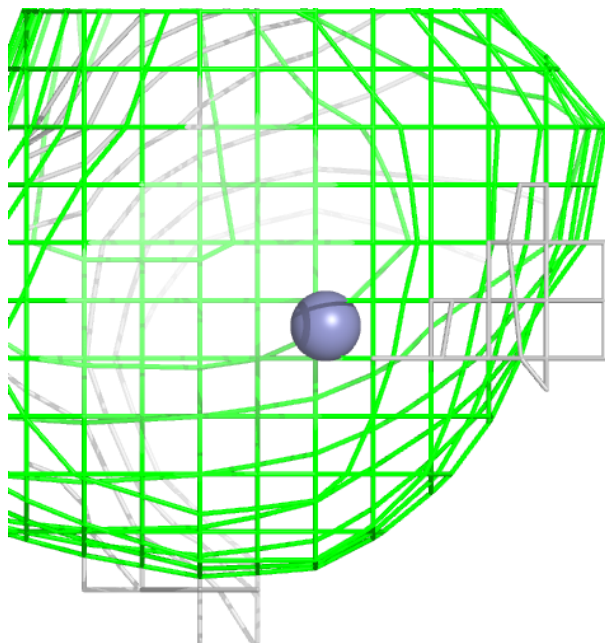
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	B	501	1/1	0.63	0.20	101,101,101,101	1
2	ZN	A	501	1/1	0.67	0.18	103,103,103,103	1
2	ZN	D	501	1/1	0.75	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	0.10	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.

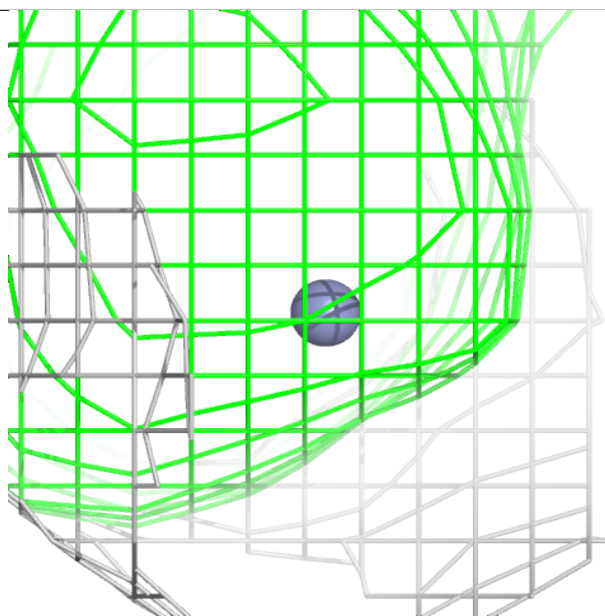
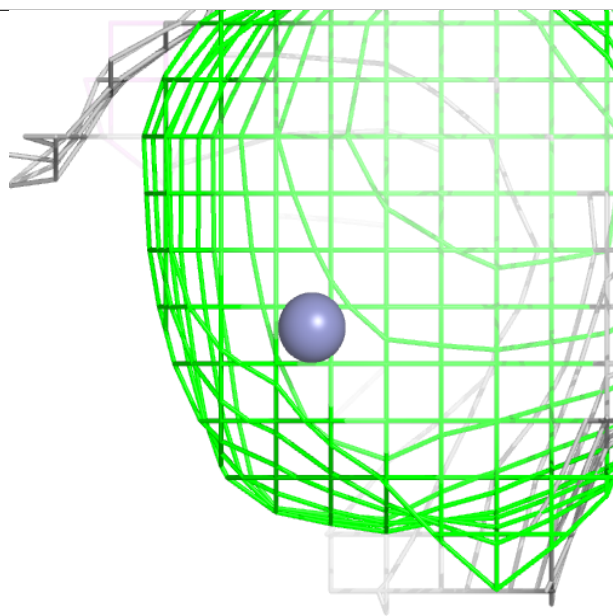
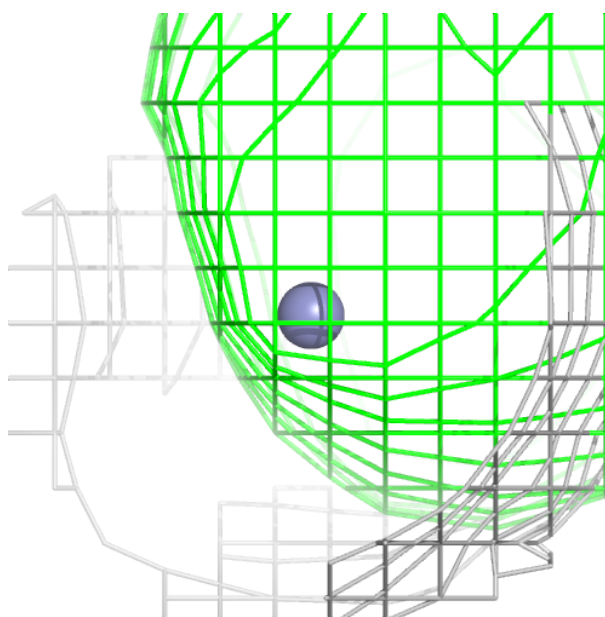
Electron density around ZN B 501:

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



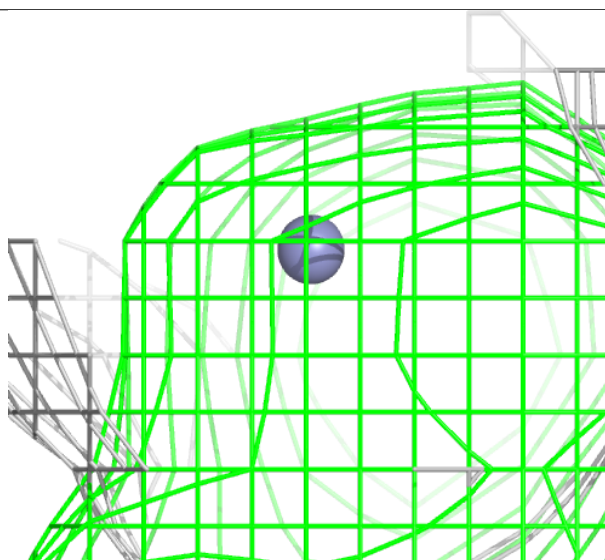
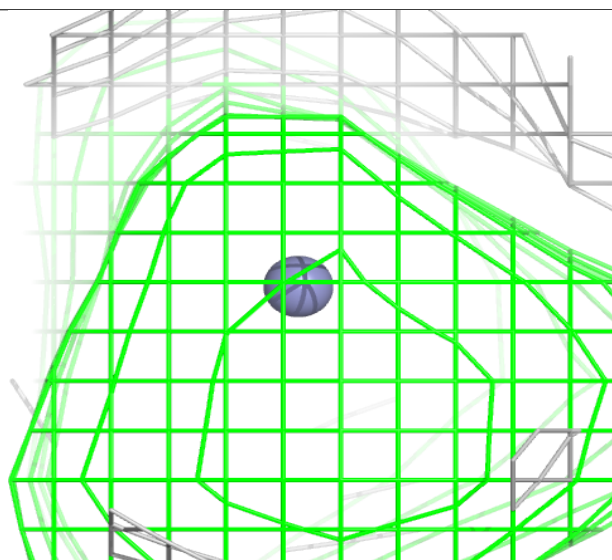
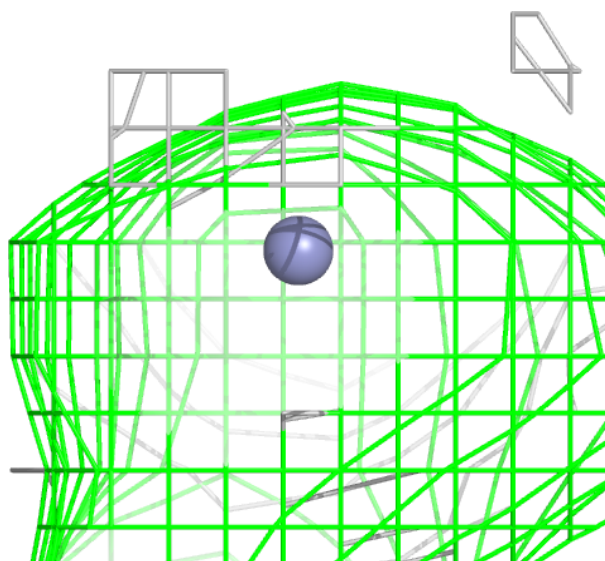
Electron density around ZN A 501:

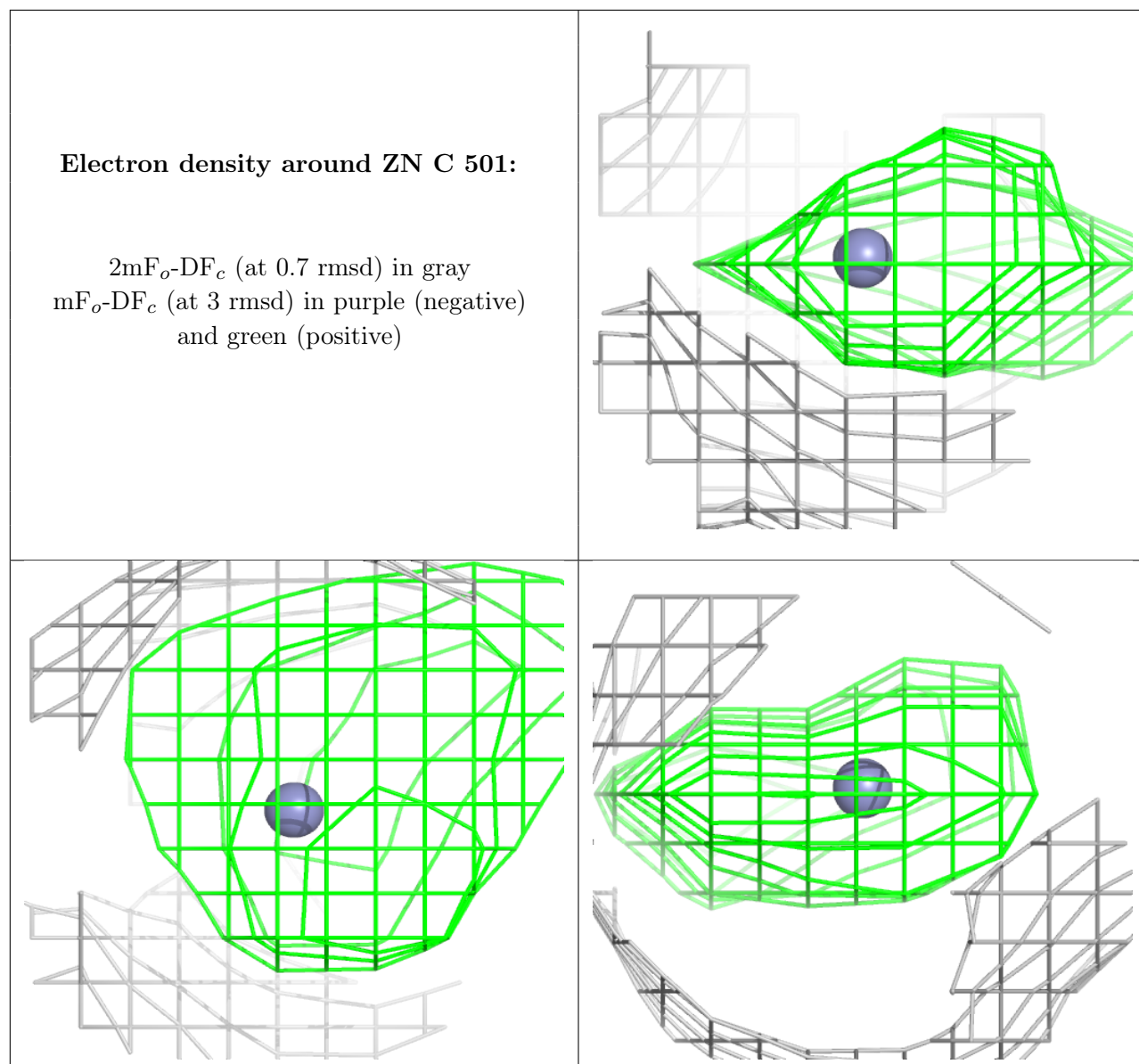
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers ⓘ

There are no such residues in this entry.