



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:38 PM UTC

PDB ID : 9KOV / pdb_00009kov
Title : Crystal structure of an amidohydrolase mutant from Thermonema
Authors : Xu, N.N.; Jian, G.; Wei, H.L.; Chen, Y.Y.; Wu, P.; Han, X.; Liu, W.
Deposited on : 2024-11-21
Resolution : 2.56 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
Xtrriage (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

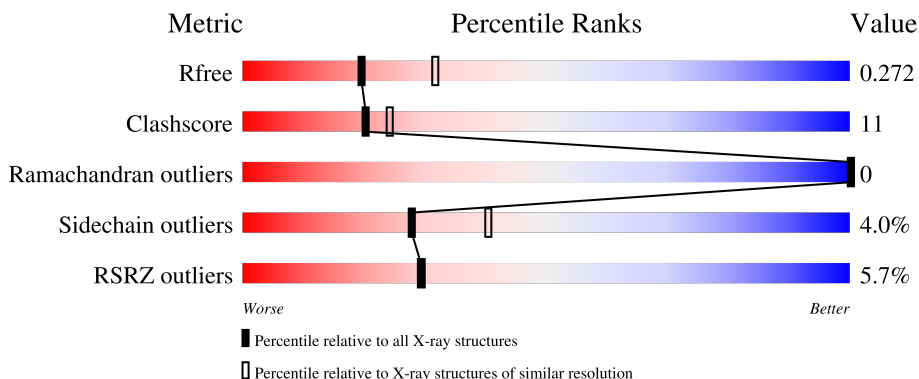
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.56 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.



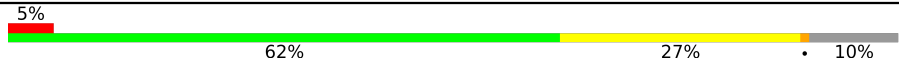

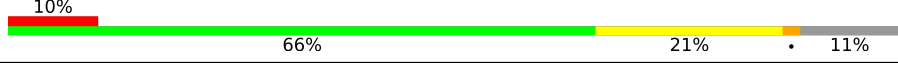
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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	422	 4% 68% 24% • 8%
1	B	422	 5% 63% 24% • 11%
1	C	422	 4% 64% 23% • 12%
1	D	422	 4% 69% 19% 12%
1	E	422	 7% 68% 23% • 8%

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Mol	Chain	Length	Quality of chain
1	F	422	 5% 62% 27% • 10%
1	G	422	 3% 69% 20% • 10%
1	H	422	 10% 66% 21% • 11%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 22609 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 trum-mut.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	390	2903	1832	512	546	13	0	0	0
1	B	375	2811	1769	496	533	13	0	0	0
1	C	373	2777	1749	492	523	13	0	0	0
1	D	372	2748	1731	483	521	13	0	0	0
1	E	389	2838	1796	495	534	13	0	0	0
1	F	378	2768	1746	485	524	13	0	0	0
1	G	379	2796	1758	488	537	13	0	0	0
1	H	376	2745	1729	480	523	13	0	0	0

- 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	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

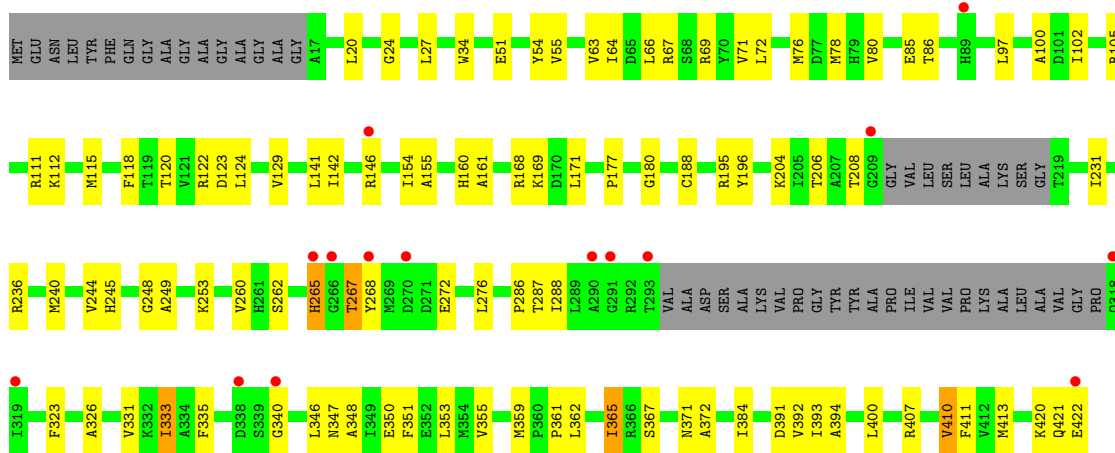
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	35	Total	O	0	0
			35	35		

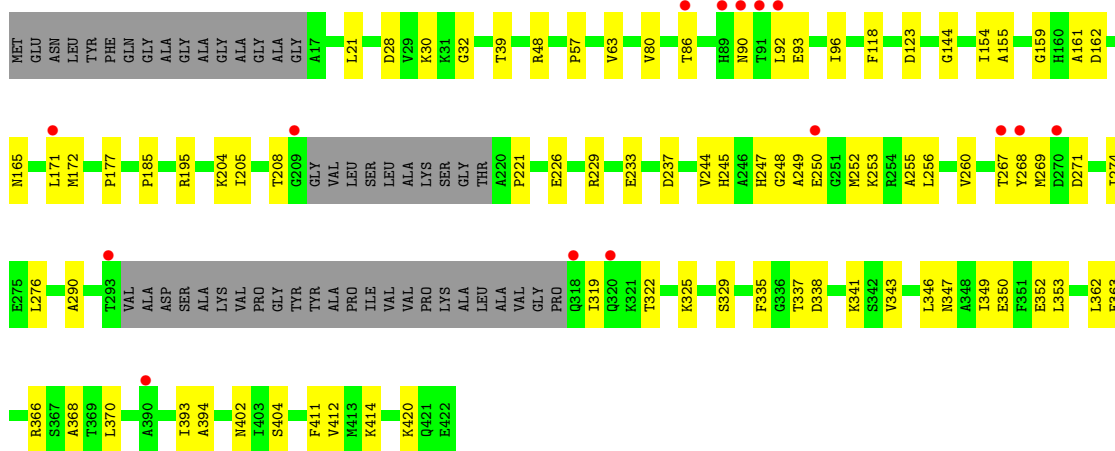
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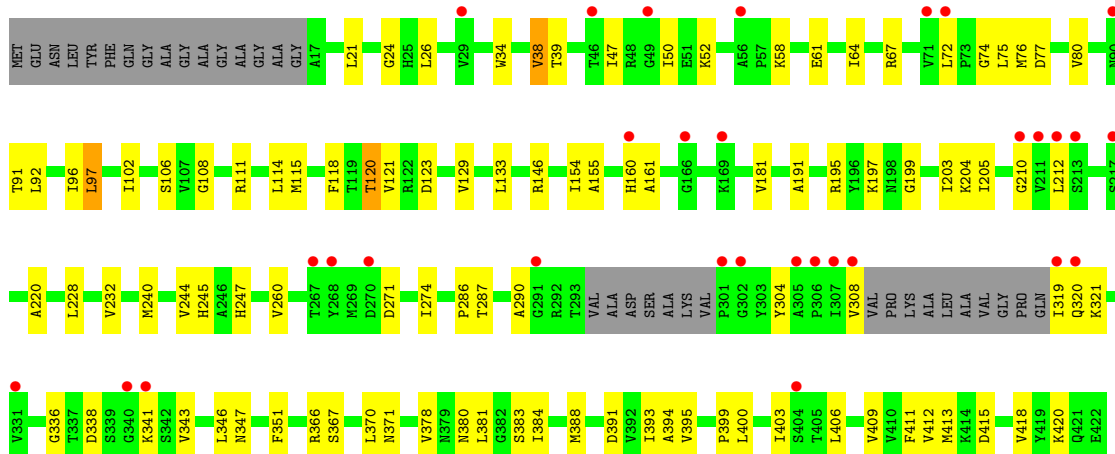
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	28	Total 28	O 28	0	0
3	D	28	Total 28	O 28	0	0
3	E	22	Total 22	O 22	0	0
3	F	23	Total 23	O 23	0	0
3	G	35	Total 35	O 35	0	0
3	H	20	Total 20	O 20	0	0



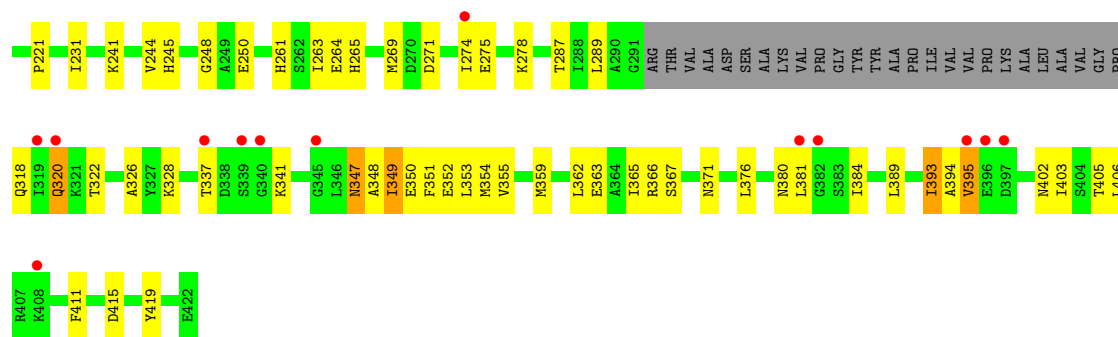
• Molecule 1: trum-mut



• Molecule 1: trum-mut



• Molecule 1: trum-mut



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	84.64Å 205.75Å 105.27Å 90.00° 103.08° 90.00°	Depositor
Resolution (Å)	49.92 – 2.56 49.92 – 2.56	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.92-2.56) 99.5 (49.92-2.56)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.82 (at 2.54Å)	Xtrriage
Refinement program	PHENIX (1.21_5207: ???)	Depositor
R, R_{free}	0.222 , 0.264 0.242 , 0.272	Depositor DCC
R_{free} test set	5000 reflections (4.43%)	wwPDB-VP
Wilson B-factor (Å ²)	33.1	Xtrriage
Anisotropy	0.230	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22609	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% 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:
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	0.28	0/2953	0.59	2/3998 (0.1%)
1	B	0.37	0/2858	0.70	5/3865 (0.1%)
1	C	0.36	0/2823	0.65	0/3820
1	D	0.31	0/2793	0.67	2/3784 (0.1%)
1	E	0.23	0/2888	0.52	0/3920
1	F	0.34	0/2815	0.65	2/3814 (0.1%)
1	G	0.30	0/2842	0.60	2/3852 (0.1%)
1	H	0.32	0/2791	0.61	1/3786 (0.0%)
All	All	0.32	0/22763	0.63	14/30839 (0.0%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	LYS	N-CA-C	-10.20	100.24	111.36
1	A	340	GLY	N-CA-C	-9.33	103.59	114.69
1	B	341	LYS	N-CA-C	-8.07	102.48	111.28
1	B	292	ARG	N-CA-C	-8.00	102.64	111.36
1	H	341	LYS	N-CA-C	-7.26	103.37	111.28
1	F	95	PHE	CA-C-N	-5.78	114.98	121.85
1	F	95	PHE	C-N-CA	-5.78	114.98	121.85
1	D	48	ARG	CA-C-N	-5.67	113.55	120.92
1	D	48	ARG	C-N-CA	-5.67	113.55	120.92
1	B	267	THR	CA-C-N	-5.37	115.54	123.05
1	B	267	THR	C-N-CA	-5.37	115.54	123.05
1	B	291	GLY	N-CA-C	-5.26	108.81	115.08
1	G	272	GLU	CB-CA-C	-5.26	101.74	110.68
1	G	272	GLU	N-CA-C	5.21	117.63	111.33

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	2903	0	2902	60	0
1	B	2811	0	2813	72	0
1	C	2777	0	2770	63	0
1	D	2748	0	2716	48	0
1	E	2838	0	2797	67	0
1	F	2768	0	2734	81	0
1	G	2796	0	2752	54	0
1	H	2745	0	2686	73	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	30	0	0	0	0
3	B	35	0	0	1	0
3	C	28	0	0	2	0
3	D	28	0	0	0	0
3	E	22	0	0	0	0
3	F	23	0	0	2	0
3	G	35	0	0	0	0
3	H	20	0	0	2	0
All	All	22609	0	22170	505	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (505) 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:E:38:VAL:HB	1:E:50:ILE:HD11	1.50	0.92
1:H:289:LEU:HD23	1:H:337:THR:HG23	1.52	0.92
1:F:76:MET:HG2	1:F:120:THR:HB	1.48	0.92
1:D:86:THR:HA	1:D:90:ASN:HD21	1.40	0.87
1:A:394:ALA:HB3	1:A:411:PHE:HB3	1.58	0.84
1:F:394:ALA:HB3	1:F:411:PHE:HB3	1.57	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:78:MET:HE3	1:F:372:ALA:HB1	1.59	0.84
1:H:76:MET:HE1	1:H:381:LEU:HB3	1.59	0.84
1:H:394:ALA:HB3	1:H:411:PHE:HB3	1.61	0.82
1:H:25:HIS:HD2	1:H:70:TYR:CE2	2.00	0.80
1:E:74:GLY:HA2	1:E:393:ILE:HD13	1.63	0.80
1:G:394:ALA:HB3	1:G:411:PHE:HB3	1.64	0.79
1:A:94:ARG:HH21	1:A:167:TYR:HE1	1.33	0.77
1:G:76:MET:HG2	1:G:120:THR:HB	1.66	0.77
1:E:394:ALA:HB3	1:E:411:PHE:HB3	1.66	0.77
1:D:271:ASP:HA	1:D:274:ILE:HD12	1.65	0.76
1:C:78:MET:HE3	1:C:372:ALA:HB1	1.67	0.76
1:F:74:GLY:HA2	1:F:393:ILE:HG12	1.66	0.75
1:F:206:THR:HG22	1:F:245:HIS:CE1	2.22	0.75
1:H:120:THR:HG23	1:H:146:ARG:HB2	1.67	0.74
1:B:93:GLU:HA	1:B:96:ILE:HG12	1.70	0.73
1:C:410:VAL:HG23	1:C:422:GLU:HG2	1.69	0.73
1:F:30:LYS:HG2	1:F:370:LEU:HD11	1.71	0.73
1:B:87:ASN:HD22	1:B:88:PRO:HD2	1.52	0.72
1:D:394:ALA:HB3	1:D:411:PHE:HB3	1.71	0.72
1:F:271:ASP:HA	1:F:274:ILE:HD12	1.72	0.72
1:G:320:GLN:NE2	1:G:356:GLU:OE1	2.21	0.72
1:H:289:LEU:HD23	1:H:337:THR:CG2	2.21	0.71
1:A:346:LEU:O	1:A:349:ILE:HG12	1.91	0.70
1:G:244:VAL:HG21	1:G:260:VAL:HG11	1.72	0.70
1:D:144:GLY:O	1:D:414:LYS:NZ	2.22	0.70
1:E:399:PRO:HB3	1:E:406:LEU:HD21	1.73	0.69
1:B:394:ALA:HB3	1:B:411:PHE:HB3	1.75	0.69
1:B:144:GLY:O	1:B:414:LYS:NZ	2.25	0.69
1:C:394:ALA:HB3	1:C:411:PHE:HB3	1.74	0.69
1:E:80:VAL:HG21	1:E:121:VAL:HB	1.73	0.68
1:H:21:LEU:HB2	1:H:40:VAL:HB	1.75	0.68
1:E:58:LYS:N	1:E:61:GLU:OE2	2.26	0.68
1:F:21:LEU:HD23	1:F:64:ILE:HB	1.76	0.68
1:H:269:MET:HE1	1:H:326:ALA:HB2	1.76	0.67
1:A:244:VAL:HG21	1:A:260:VAL:HG11	1.76	0.67
1:F:76:MET:HE3	1:F:369:THR:HA	1.76	0.67
1:B:87:ASN:ND2	1:B:88:PRO:HD2	2.10	0.66
1:G:155:ALA:HB2	1:G:161:ALA:HB3	1.76	0.66
1:H:365:ILE:HD11	1:H:403:ILE:HD11	1.77	0.66
1:E:154:ILE:HB	1:E:205:ILE:HG22	1.77	0.66
1:C:188:CYS:HB3	1:C:231:ILE:HG13	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:177:PRO:O	1:D:195:ARG:NH2	2.29	0.65
1:H:155:ALA:HB2	1:H:161:ALA:HB3	1.76	0.65
1:C:69:ARG:NH1	3:C:501:HOH:O	2.29	0.65
1:H:245:HIS:HD1	1:H:265:HIS:HE1	1.43	0.65
1:C:72:LEU:HG	1:C:393:ILE:HG13	1.79	0.65
1:C:20:LEU:HB2	1:C:63:VAL:HG22	1.78	0.64
1:C:420:LYS:HE2	1:C:422:GLU:OE1	1.98	0.64
1:B:20:LEU:HB2	1:B:63:VAL:HG22	1.80	0.63
1:A:267:THR:HG22	1:A:319:ILE:HD12	1.79	0.63
1:H:241:LYS:HE3	1:H:261:HIS:CD2	2.34	0.63
1:A:76:MET:HG2	1:A:120:THR:HB	1.80	0.63
1:E:197:LYS:HE2	1:F:172:MET:HE2	1.81	0.62
1:D:118:PHE:CE2	1:D:347:ASN:HB2	2.34	0.62
1:G:27:LEU:HB2	1:G:34:TRP:CZ3	2.34	0.62
1:F:262:SER:HB2	1:F:375:LEU:HD11	1.80	0.62
1:F:417:LYS:HE2	1:F:419:TYR:CZ	2.34	0.62
1:F:83:GLU:OE1	1:F:127:THR:HG22	2.00	0.62
1:G:154:ILE:HB	1:G:205:ILE:HG22	1.80	0.62
1:B:410:VAL:HG13	1:B:422:GLU:HB2	1.80	0.62
1:D:92:LEU:HA	1:E:92:LEU:HD13	1.80	0.62
1:F:87:ASN:HB2	1:F:88:PRO:HD2	1.82	0.62
1:G:351:PHE:HB3	1:G:403:ILE:HG12	1.82	0.62
1:D:159:GLY:O	1:D:165:ASN:ND2	2.32	0.62
1:B:87:ASN:HB3	1:B:90:ASN:OD1	1.99	0.61
1:F:249:ALA:O	1:F:253:LYS:HG3	2.00	0.61
1:G:188:CYS:HB3	1:G:231:ILE:HG13	1.82	0.61
1:C:66:LEU:HD23	1:C:71:VAL:HG22	1.81	0.61
1:A:270:ASP:OD2	1:A:271:ASP:N	2.33	0.61
1:D:229:ARG:O	1:D:233:GLU:HG3	2.01	0.61
1:E:39:THR:O	1:E:50:ILE:HD12	2.00	0.61
1:F:80:VAL:HG21	1:F:121:VAL:HB	1.82	0.61
1:A:46:THR:HB	1:A:48:ARG:HH21	1.66	0.60
1:F:154:ILE:HB	1:F:205:ILE:HD13	1.83	0.60
1:H:194:GLN:HG3	1:H:195:ARG:HH12	1.65	0.60
1:H:245:HIS:ND1	1:H:265:HIS:HE1	1.99	0.60
1:C:286:PRO:HB2	1:C:288:ILE:HG13	1.81	0.60
1:G:383:SER:HB3	1:G:388:MET:HE2	1.82	0.60
1:D:343:VAL:HB	1:D:346:LEU:HD12	1.81	0.60
1:F:206:THR:HG22	1:F:245:HIS:ND1	2.16	0.60
1:F:250:GLU:HA	1:F:253:LYS:HZ2	1.67	0.59
1:B:245:HIS:HD1	1:B:265:HIS:CE1	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:155:ALA:HB2	1:B:161:ALA:HB3	1.83	0.59
1:H:350:GLU:O	1:H:354:MET:HG3	2.02	0.59
1:E:320:GLN:CD	1:E:320:GLN:H	2.09	0.59
1:F:352:GLU:O	1:F:355:VAL:HG12	2.03	0.59
1:F:209:GLY:HA3	1:F:218:GLY:HA2	1.83	0.59
1:D:350:GLU:HA	1:D:353:LEU:HD23	1.84	0.59
1:F:34:TRP:NE1	1:F:400:LEU:HD12	2.18	0.59
1:B:57:PRO:HB3	1:B:61:GLU:HB2	1.85	0.58
1:C:204:LYS:HE2	1:C:245:HIS:HB2	1.85	0.58
1:C:177:PRO:O	1:C:195:ARG:NH2	2.36	0.58
1:A:352:GLU:OE2	1:A:407:ARG:HD2	2.04	0.58
1:C:287:THR:O	1:C:287:THR:HG22	2.04	0.57
1:B:92:LEU:HG	1:B:96:ILE:HD13	1.86	0.57
1:G:264:GLU:HG3	1:G:285:VAL:HB	1.87	0.57
1:D:86:THR:HA	1:D:90:ASN:ND2	2.16	0.57
1:F:346:LEU:O	1:F:349:ILE:HG13	2.05	0.57
1:H:122:ARG:NH2	1:H:264:GLU:OE2	2.38	0.57
1:F:221:PRO:HG3	1:F:250:GLU:HG2	1.87	0.57
1:H:274:ILE:O	1:H:278:LYS:HG2	2.05	0.57
1:F:244:VAL:HB	1:F:263:ILE:HD13	1.86	0.57
1:D:30:LYS:HG3	1:D:370:LEU:HD11	1.87	0.56
1:B:171:LEU:HD13	1:C:171:LEU:HD13	1.86	0.56
1:B:204:LYS:HE2	1:B:245:HIS:HB2	1.88	0.56
1:G:270:ASP:O	1:G:274:ILE:HG13	2.04	0.56
1:H:352:GLU:O	1:H:355:VAL:HG22	2.05	0.56
1:F:189:ARG:HG3	1:F:234:THR:OG1	2.06	0.56
1:A:189:ARG:HG3	1:A:234:THR:OG1	2.06	0.56
1:D:319:ILE:HA	1:D:322:THR:HG22	1.86	0.56
1:E:108:GLY:HA2	1:E:111:ARG:NH1	2.21	0.56
1:E:212:LEU:HD12	1:E:341:LYS:HD2	1.87	0.56
1:E:212:LEU:HD21	1:E:304:TYR:CE1	2.41	0.56
1:A:94:ARG:NH1	1:A:214:LEU:HD23	2.21	0.55
1:C:206:THR:HG22	1:C:245:HIS:HB3	1.89	0.55
1:C:118:PHE:CE1	1:C:347:ASN:HB2	2.41	0.55
1:F:118:PHE:CE1	1:F:347:ASN:HB2	2.41	0.55
1:H:118:PHE:CE1	1:H:347:ASN:HB2	2.41	0.55
1:D:221:PRO:HB3	1:D:250:GLU:HG2	1.89	0.55
1:G:69:ARG:HD2	1:G:410:VAL:HG21	1.89	0.55
1:A:245:HIS:ND1	1:A:265:HIS:HD2	2.05	0.55
1:H:170:ASP:OD1	1:H:170:ASP:N	2.39	0.55
1:E:120:THR:HG23	1:E:146:ARG:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:VAL:HG21	1:D:260:VAL:HG11	1.90	0.54
1:B:171:LEU:HD22	1:C:171:LEU:HD22	1.87	0.54
1:D:57:PRO:HG3	1:D:63:VAL:HG21	1.89	0.54
1:E:343:VAL:HB	1:E:346:LEU:HD12	1.89	0.54
1:A:118:PHE:CE1	1:A:347:ASN:HB2	2.43	0.54
1:D:402:ASN:OD1	1:D:404:SER:OG	2.24	0.54
1:G:288:ILE:HD11	1:G:323:PHE:CD2	2.43	0.54
1:A:160:HIS:CD2	1:A:213:SER:HB3	2.43	0.54
1:F:393:ILE:HD12	1:F:412:VAL:HG22	1.90	0.54
1:G:115:MET:HE1	1:G:419:TYR:HB3	1.88	0.54
1:C:160:HIS:ND1	1:C:206:THR:HG21	2.23	0.54
1:D:335:PHE:HB3	1:D:368:ALA:HA	1.89	0.54
1:D:154:ILE:HB	1:D:205:ILE:HG22	1.90	0.54
1:H:78:MET:HE1	1:H:376:LEU:HG	1.88	0.54
1:A:205:ILE:HG21	1:A:231:ILE:HD13	1.90	0.54
1:E:38:VAL:HG12	1:E:52:LYS:HA	1.89	0.53
1:H:245:HIS:ND1	1:H:265:HIS:CE1	2.76	0.53
1:B:191:ALA:O	1:B:195:ARG:HG2	2.08	0.53
1:F:168:ARG:HB2	1:H:95:PHE:O	2.08	0.53
1:H:204:LYS:HE2	1:H:245:HIS:HB2	1.89	0.53
1:E:111:ARG:CZ	1:E:111:ARG:HB3	2.37	0.53
1:F:160:HIS:H	1:F:222:GLN:HE22	1.55	0.53
1:F:250:GLU:HA	1:F:253:LYS:NZ	2.24	0.53
1:F:287:THR:HG22	1:F:287:THR:O	2.07	0.53
1:A:154:ILE:HB	1:A:205:ILE:HG22	1.90	0.53
1:B:335:PHE:CE1	1:B:350:GLU:HG2	2.44	0.53
1:G:33:LYS:HD3	1:G:35:LEU:CD2	2.39	0.53
1:A:220:ALA:HB1	1:D:237:ASP:O	2.08	0.53
1:H:359:MET:HE2	1:H:363:GLU:C	2.34	0.53
1:D:346:LEU:HB3	1:D:349:ILE:HD12	1.90	0.53
1:H:180:GLY:HA2	1:H:195:ARG:HH21	1.74	0.53
1:H:35:LEU:HB3	1:H:38:VAL:HG11	1.89	0.53
1:H:244:VAL:HB	1:H:263:ILE:HD13	1.91	0.53
1:B:45:ASN:HB2	1:B:415:ASP:OD1	2.08	0.52
1:E:146:ARG:NH2	1:E:391:ASP:OD1	2.37	0.52
1:E:244:VAL:HG21	1:E:260:VAL:HG11	1.90	0.52
1:G:74:GLY:HA2	1:G:393:ILE:HG23	1.91	0.52
1:A:270:ASP:OD2	1:A:272:GLU:N	2.41	0.52
1:G:34:TRP:CZ2	1:G:399:PRO:HD2	2.44	0.52
1:H:89:HIS:O	1:H:93:GLU:HG3	2.09	0.52
1:E:47:ILE:HD12	1:E:388:MET:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ALA:HB2	1:A:202:LEU:HD11	1.92	0.52
1:B:76:MET:HG2	1:B:120:THR:HB	1.91	0.52
1:C:78:MET:HA	1:C:122:ARG:HB3	1.92	0.52
1:D:247:HIS:O	1:D:268:TYR:HD1	1.93	0.51
1:D:249:ALA:O	1:D:253:LYS:HG3	2.10	0.51
1:E:413:MET:HE3	1:E:418:VAL:HG22	1.92	0.51
1:A:155:ALA:HB2	1:A:161:ALA:HB3	1.92	0.51
1:A:255:ALA:HB1	1:A:260:VAL:HG11	1.92	0.51
1:B:31:LYS:HB3	1:B:33:LYS:HD2	1.92	0.51
1:D:325:LYS:O	1:D:329:SER:OG	2.20	0.51
1:F:73:PRO:HG3	1:F:384:ILE:HG12	1.92	0.51
1:F:159:GLY:O	1:F:165:ASN:ND2	2.44	0.51
1:A:79:HIS:NE2	1:A:338:ASP:OD2	2.44	0.51
1:E:220:ALA:HB1	1:G:237:ASP:O	2.11	0.51
1:B:118:PHE:CE2	1:B:347:ASN:HB2	2.45	0.51
1:C:27:LEU:HB2	1:C:34:TRP:CZ3	2.45	0.51
1:D:93:GLU:HA	1:D:96:ILE:HG12	1.91	0.51
1:F:76:MET:HE1	1:F:382:GLY:HA2	1.93	0.51
1:A:351:PHE:HB3	1:A:403:ILE:HG12	1.91	0.51
1:C:54:TYR:CE2	1:C:67:ARG:HD2	2.46	0.51
1:C:76:MET:HA	1:C:120:THR:O	2.11	0.51
1:H:275:GLU:OE1	1:H:278:LYS:HE2	2.10	0.51
1:C:236:ARG:NH2	3:C:505:HOH:O	2.44	0.51
1:F:130:ASN:OD1	1:F:130:ASN:N	2.44	0.51
1:H:271:ASP:HA	1:H:274:ILE:HD12	1.93	0.51
1:H:349:ILE:O	1:H:353:LEU:HD12	2.11	0.51
1:A:27:LEU:HD23	1:A:29:VAL:HG12	1.94	0.50
1:B:244:VAL:HG21	1:B:260:VAL:HG11	1.93	0.50
1:C:362:LEU:HD13	1:C:400:LEU:HD21	1.92	0.50
1:G:346:LEU:HB3	1:G:349:ILE:HD12	1.92	0.50
1:B:66:LEU:HD21	1:B:411:PHE:CG	2.46	0.50
1:A:188:CYS:HB3	1:A:231:ILE:HG13	1.93	0.50
1:D:28:ASP:O	1:D:32:GLY:N	2.44	0.50
1:B:115:MET:HE2	1:B:419:TYR:HB3	1.93	0.50
1:F:120:THR:HG23	1:F:146:ARG:HB2	1.94	0.50
1:B:271:ASP:HA	1:B:274:ILE:HD12	1.93	0.50
1:A:352:GLU:O	1:A:356:GLU:HG3	2.11	0.50
1:G:118:PHE:CE1	1:G:347:ASN:HB2	2.47	0.50
1:B:318:GLN:OE1	1:B:321:LYS:NZ	2.36	0.49
1:C:326:ALA:HB1	1:C:331:VAL:HG11	1.93	0.49
1:C:391:ASP:HA	1:C:413:MET:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:PRO:HG3	1:D:226:GLU:HG3	1.94	0.49
1:E:290:ALA:HB2	1:E:338:ASP:HB3	1.93	0.49
1:A:226:GLU:O	1:A:229:ARG:HB3	2.11	0.49
1:B:99:PRO:HD2	1:C:169:LYS:HE2	1.94	0.49
1:A:74:GLY:HA2	1:A:393:ILE:HG12	1.93	0.49
1:D:290:ALA:HB2	1:D:338:ASP:HB3	1.93	0.49
1:E:26:LEU:HD11	1:E:384:ILE:HD13	1.95	0.49
1:F:167:TYR:HB2	1:F:172:MET:HB2	1.93	0.49
1:B:244:VAL:HB	1:B:263:ILE:HD13	1.94	0.49
1:B:226:GLU:OE2	3:B:601:HOH:O	2.20	0.49
1:D:204:LYS:NZ	1:D:245:HIS:HB2	2.27	0.49
1:E:114:LEU:O	1:E:412:VAL:HG11	2.13	0.49
1:B:93:GLU:HB3	1:B:97:LEU:HD22	1.94	0.49
1:E:228:LEU:O	1:E:232:VAL:HG23	2.13	0.49
1:D:337:THR:HG21	1:D:347:ASN:HB3	1.95	0.49
1:A:367:SER:HA	1:A:371:ASN:HB2	1.93	0.49
1:D:80:VAL:O	1:D:123:ASP:HA	2.13	0.49
1:F:244:VAL:HG21	1:F:260:VAL:HG11	1.94	0.49
1:C:168:ARG:HE	1:C:171:LEU:HG	1.77	0.48
1:E:108:GLY:HA2	1:E:111:ARG:HH12	1.79	0.48
1:E:393:ILE:HG23	1:E:409:VAL:HG13	1.94	0.48
1:F:154:ILE:HB	1:F:205:ILE:CD1	2.44	0.48
1:H:217:SER:OG	1:H:218:GLY:N	2.46	0.48
1:H:347:ASN:H	1:H:347:ASN:ND2	2.12	0.48
1:E:160:HIS:CE1	1:E:210:GLY:HA3	2.48	0.48
1:F:413:MET:HE2	1:F:416:GLY:O	2.14	0.48
1:B:27:LEU:HB2	1:B:34:TRP:CZ3	2.47	0.48
1:B:87:ASN:HD22	1:B:88:PRO:CD	2.21	0.48
1:B:376:LEU:HB3	1:B:378:VAL:HG23	1.96	0.48
1:B:337:THR:HG21	1:B:347:ASN:HB3	1.94	0.48
1:F:164:THR:HB	1:F:172:MET:HA	1.96	0.48
1:B:89:HIS:O	1:B:93:GLU:HB2	2.14	0.48
1:B:410:VAL:CG1	1:B:422:GLU:HB2	2.44	0.48
1:C:323:PHE:CE1	1:C:333:ILE:HD13	2.49	0.48
1:A:241:LYS:HD3	1:A:261:HIS:CD2	2.49	0.48
1:B:245:HIS:ND1	1:B:265:HIS:CE1	2.82	0.48
1:A:93:GLU:HA	1:A:96:ILE:HG12	1.96	0.47
1:C:97:LEU:HD21	1:C:105:ARG:NH1	2.29	0.47
1:D:155:ALA:HB2	1:D:161:ALA:HB3	1.94	0.47
1:D:256:LEU:HB2	1:D:276:LEU:HD13	1.96	0.47
1:H:318:GLN:N	3:H:501:HOH:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ARG:HH21	1:A:389:LEU:HD13	1.78	0.47
1:B:28:ASP:O	1:B:32:GLY:N	2.40	0.47
1:E:155:ALA:HB2	1:E:161:ALA:HB3	1.95	0.47
1:A:18:THR:CG2	1:A:61:GLU:HG2	2.44	0.47
1:A:45:ASN:HB2	1:A:415:ASP:OD2	2.14	0.47
1:A:155:ALA:O	1:A:181:VAL:HA	2.15	0.47
1:G:78:MET:O	1:G:122:ARG:NH2	2.37	0.47
1:A:77:ASP:HB3	1:A:121:VAL:HG12	1.97	0.47
1:B:190:LYS:HD2	1:G:183:ASN:ND2	2.28	0.47
1:A:94:ARG:HH12	1:A:214:LEU:HD23	1.77	0.47
1:E:380:ASN:HA	1:E:388:MET:SD	2.55	0.47
1:G:124:LEU:HB3	1:G:204:LYS:HD3	1.95	0.47
1:H:76:MET:HA	1:H:120:THR:O	2.15	0.47
1:H:83:GLU:CD	1:H:129:VAL:HB	2.40	0.47
1:G:177:PRO:HB2	1:G:190:LYS:HD3	1.95	0.47
1:H:29:VAL:HG12	3:H:507:HOH:O	2.15	0.47
1:A:130:ASN:OD1	1:A:130:ASN:N	2.48	0.47
1:C:76:MET:HG2	1:C:120:THR:HB	1.96	0.47
1:C:265:HIS:CE1	1:C:287:THR:HG21	2.50	0.47
1:E:118:PHE:CZ	1:E:347:ASN:HB2	2.50	0.47
1:H:353:LEU:HD12	1:H:353:LEU:H	1.80	0.47
1:A:21:LEU:HD23	1:A:64:ILE:HB	1.96	0.46
1:A:21:LEU:O	1:A:39:THR:HA	2.16	0.46
1:B:155:ALA:O	1:B:181:VAL:HA	2.15	0.46
1:E:347:ASN:OD1	1:E:347:ASN:N	2.47	0.46
1:F:146:ARG:NH2	1:F:415:ASP:OD1	2.47	0.46
1:F:352:GLU:HA	1:F:403:ILE:HG21	1.97	0.46
1:G:152:LYS:NZ	1:G:153:SER:O	2.47	0.46
1:C:348:ALA:O	1:C:351:PHE:HB2	2.15	0.46
1:F:34:TRP:HE1	1:F:400:LEU:HD12	1.79	0.46
1:A:255:ALA:O	1:A:260:VAL:HG13	2.15	0.46
1:B:154:ILE:HB	1:B:205:ILE:HG22	1.97	0.46
1:E:76:MET:HA	1:E:120:THR:O	2.16	0.46
1:D:93:GLU:HA	1:D:96:ILE:CG1	2.45	0.46
1:E:72:LEU:C	1:E:384:ILE:HD11	2.40	0.46
1:F:33:LYS:NZ	3:F:502:HOH:O	2.47	0.46
1:H:320:GLN:HE21	1:H:320:GLN:HB3	1.58	0.46
1:H:347:ASN:H	1:H:347:ASN:HD22	1.63	0.46
1:A:209:GLY:HA3	1:A:218:GLY:HA2	1.97	0.46
1:D:248:GLY:O	1:D:252:MET:HG3	2.15	0.46
1:E:191:ALA:O	1:E:195:ARG:HG2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:367:SER:HA	1:F:371:ASN:HB2	1.98	0.46
1:E:74:GLY:HA2	1:E:393:ILE:CD1	2.42	0.46
1:H:269:MET:HE2	1:H:322:THR:HG22	1.98	0.46
1:A:252:MET:HG3	1:A:263:ILE:HG21	1.98	0.46
1:E:106:SER:OG	1:E:133:LEU:HD22	2.16	0.46
1:H:115:MET:HE1	1:H:419:TYR:O	2.16	0.46
1:H:188:CYS:HB3	1:H:231:ILE:HG13	1.98	0.46
1:A:183:ASN:N	1:A:187:GLU:OE1	2.41	0.46
1:E:96:ILE:HG22	1:E:97:LEU:HD23	1.97	0.46
1:G:21:LEU:HD23	1:G:64:ILE:HB	1.98	0.46
1:H:362:LEU:HD11	1:H:366:ARG:CZ	2.45	0.46
1:B:188:CYS:HB3	1:B:231:ILE:HG13	1.98	0.46
1:C:288:ILE:HD11	1:C:323:PHE:CG	2.51	0.46
1:G:255:ALA:HB1	1:G:260:VAL:HG11	1.98	0.46
1:A:264:GLU:OE1	1:A:285:VAL:HB	2.16	0.46
1:G:72:LEU:HD11	1:G:395:VAL:HG22	1.98	0.46
1:E:395:VAL:HG11	1:E:406:LEU:HA	1.98	0.45
1:F:37:GLY:HA2	1:F:54:TYR:CE1	2.51	0.45
1:G:294:VAL:CG2	1:G:341:LYS:HE3	2.47	0.45
1:H:380:ASN:HB3	1:H:389:LEU:HD12	1.97	0.45
1:D:162:ASP:HB3	1:D:165:ASN:CG	2.41	0.45
1:E:366:ARG:HG2	1:E:370:LEU:HD12	1.98	0.45
1:A:18:THR:HG22	1:A:61:GLU:HG2	1.98	0.45
1:D:269:MET:HE2	1:D:269:MET:HB2	1.60	0.45
1:H:395:VAL:HG11	1:H:406:LEU:HA	1.98	0.45
1:A:27:LEU:HD11	1:A:400:LEU:HD11	1.98	0.45
1:A:212:LEU:HD23	1:A:212:LEU:HA	1.71	0.45
1:C:72:LEU:HD11	1:C:393:ILE:HD11	1.97	0.45
1:C:154:ILE:HA	1:C:180:GLY:O	2.17	0.45
1:C:361:PRO:O	1:C:365:ILE:HD12	2.15	0.45
1:E:102:ILE:HG22	1:E:129:VAL:HG11	1.99	0.45
1:G:335:PHE:CE1	1:G:350:GLU:HG2	2.52	0.45
1:G:385:GLU:HG2	1:G:388:MET:HG3	1.98	0.45
1:B:59:ALA:O	1:B:60:GLY:C	2.59	0.45
1:B:367:SER:HA	1:B:371:ASN:HB2	1.97	0.45
1:D:271:ASP:HA	1:D:274:ILE:CD1	2.42	0.45
1:F:156:THR:HG22	1:F:182:ALA:O	2.16	0.45
1:B:385:GLU:HG2	1:B:388:MET:HG3	1.99	0.45
1:A:69:ARG:NH2	1:A:422:GLU:O	2.50	0.45
1:B:287:THR:HG23	1:B:338:ASP:HB2	1.99	0.45
1:B:290:ALA:HB1	1:B:341:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:407:ARG:HE	1:C:407:ARG:HB3	1.59	0.45
1:H:25:HIS:CD2	1:H:70:TYR:CE2	2.91	0.45
1:H:367:SER:HA	1:H:371:ASN:HB2	1.98	0.45
1:A:27:LEU:HD23	1:A:29:VAL:CG1	2.46	0.45
1:A:380:ASN:C	1:A:388:MET:HE3	2.42	0.45
1:D:362:LEU:HG	1:D:366:ARG:HD2	1.99	0.45
1:E:160:HIS:ND1	1:E:210:GLY:HA3	2.31	0.45
1:G:79:HIS:ND1	1:G:264:GLU:HG2	2.32	0.44
1:E:351:PHE:HB3	1:E:403:ILE:HD13	1.99	0.44
1:G:350:GLU:O	1:G:354:MET:HG3	2.16	0.44
1:F:150:ALA:HA	1:F:202:LEU:O	2.18	0.44
1:H:348:ALA:O	1:H:351:PHE:HB2	2.18	0.44
1:B:93:GLU:HG2	1:B:97:LEU:CD1	2.48	0.44
1:B:290:ALA:CB	1:B:338:ASP:HB3	2.47	0.44
1:C:384:ILE:HD11	1:C:392:VAL:HG13	2.00	0.44
1:D:255:ALA:HB1	1:D:260:VAL:HG11	1.99	0.44
1:F:153:SER:OG	1:F:204:LYS:HD2	2.17	0.44
1:H:194:GLN:CG	1:H:195:ARG:HH12	2.30	0.44
1:H:221:PRO:HG3	1:H:250:GLU:HG3	1.99	0.44
1:H:393:ILE:HD13	1:H:393:ILE:HA	1.80	0.44
1:A:27:LEU:HB2	1:A:34:TRP:CZ3	2.53	0.44
1:G:287:THR:HG22	1:G:290:ALA:HB3	1.98	0.44
1:B:58:LYS:HB3	1:B:58:LYS:HE2	1.64	0.44
1:C:64:ILE:HG23	1:C:421:GLN:NE2	2.32	0.44
1:C:100:ALA:HB2	1:F:129:VAL:HG22	1.99	0.44
1:E:21:LEU:CD1	1:E:64:ILE:HB	2.47	0.44
1:G:33:LYS:HD3	1:G:35:LEU:HD23	1.98	0.44
1:G:54:TYR:CE2	1:G:67:ARG:HG2	2.53	0.44
1:B:284:TYR:HD2	1:B:333:ILE:CD1	2.30	0.44
1:C:111:ARG:O	1:C:115:MET:HG2	2.18	0.44
1:F:380:ASN:HA	1:F:388:MET:HG2	1.99	0.44
1:F:417:LYS:HG2	1:F:419:TYR:CE1	2.52	0.44
1:A:157:THR:OG1	1:A:183:ASN:ND2	2.47	0.44
1:C:112:LYS:HB3	1:C:112:LYS:HE2	1.86	0.44
1:F:76:MET:HB2	1:F:368:ALA:O	2.18	0.44
1:A:196:TYR:HB2	1:A:240:MET:HE1	2.00	0.43
1:G:290:ALA:HA	1:G:293:THR:OG1	2.18	0.43
1:B:126:GLY:HA3	1:B:130:ASN:ND2	2.32	0.43
1:E:24:GLY:HA3	1:E:67:ARG:O	2.18	0.43
1:F:85:GLU:HB2	1:F:109:TYR:CZ	2.53	0.43
1:H:25:HIS:HA	1:H:35:LEU:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ILE:HG23	1:A:409:VAL:HG13	2.00	0.43
3:F:522:HOH:O	1:H:168:ARG:HD3	2.17	0.43
1:H:275:GLU:CD	1:H:278:LYS:HE2	2.42	0.43
1:B:28:ASP:CG	1:B:31:LYS:HB2	2.43	0.43
1:B:341:LYS:HB3	1:B:341:LYS:HE3	1.69	0.43
1:D:255:ALA:O	1:D:260:VAL:HG13	2.18	0.43
1:D:393:ILE:HA	1:D:411:PHE:O	2.19	0.43
1:F:74:GLY:HA3	1:F:119:THR:OG1	2.18	0.43
1:C:102:ILE:HG22	1:C:129:VAL:HG11	1.99	0.43
1:E:210:GLY:HA2	1:E:247:HIS:CD2	2.54	0.43
1:F:245:HIS:HB2	1:F:264:GLU:HB2	2.00	0.43
1:G:118:PHE:CZ	1:G:347:ASN:HB2	2.53	0.43
1:H:85:GLU:HB2	1:H:109:TYR:CZ	2.54	0.43
1:B:362:LEU:O	1:B:362:LEU:HD12	2.18	0.43
1:C:288:ILE:HG22	1:C:353:LEU:HD13	1.99	0.43
1:H:287:THR:HG22	1:H:287:THR:O	2.18	0.43
1:A:164:THR:HB	1:A:172:MET:HA	2.01	0.43
1:E:212:LEU:HD23	1:E:212:LEU:HA	1.76	0.43
1:B:237:ASP:CG	1:G:254:ARG:HH22	2.26	0.43
1:C:155:ALA:HB2	1:C:161:ALA:HB3	2.00	0.43
1:H:150:ALA:HA	1:H:202:LEU:O	2.19	0.43
1:C:335:PHE:CE1	1:C:350:GLU:HG2	2.53	0.43
1:E:21:LEU:HD12	1:E:64:ILE:HB	2.00	0.43
1:E:77:ASP:OD1	1:E:336:GLY:HA2	2.18	0.43
1:F:82:LEU:HD23	1:F:82:LEU:HA	1.85	0.43
1:F:262:SER:OG	1:F:264:GLU:OE2	2.32	0.43
1:C:51:GLU:OE1	1:C:55:VAL:HG21	2.19	0.43
1:E:118:PHE:CE1	1:E:347:ASN:HB2	2.54	0.43
1:F:403:ILE:HD12	1:F:403:ILE:HA	1.89	0.43
1:H:21:LEU:O	1:H:39:THR:HA	2.19	0.43
1:H:39:THR:HG22	1:H:51:GLU:HB2	2.00	0.43
1:C:141:LEU:C	1:C:142:ILE:HD12	2.44	0.42
1:C:267:THR:O	1:C:268:TYR:C	2.62	0.42
1:F:25:HIS:HA	1:F:35:LEU:O	2.19	0.42
1:F:80:VAL:O	1:F:123:ASP:HA	2.19	0.42
1:F:204:LYS:NZ	1:F:245:HIS:HB3	2.33	0.42
1:G:323:PHE:CE2	1:G:354:MET:HB3	2.54	0.42
1:B:223:PHE:HB3	1:B:228:LEU:HG	2.00	0.42
1:E:75:LEU:HD13	1:E:351:PHE:CE2	2.54	0.42
1:F:146:ARG:NH1	1:F:391:ASP:OD2	2.52	0.42
1:G:191:ALA:O	1:G:195:ARG:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:ILE:HD11	1:B:244:VAL:HG22	2.01	0.42
1:C:85:GLU:HA	1:C:340:GLY:O	2.19	0.42
1:C:208:THR:HG21	1:C:248:GLY:H	1.84	0.42
1:D:402:ASN:HD22	1:D:402:ASN:HA	1.68	0.42
1:G:45:ASN:HB2	1:G:415:ASP:OD1	2.19	0.42
1:E:378:VAL:HG11	1:E:381:LEU:HD12	2.01	0.42
1:G:271:ASP:HA	1:G:274:ILE:HG13	2.01	0.42
1:G:362:LEU:HD13	1:G:400:LEU:HD11	2.01	0.42
1:B:93:GLU:HG2	1:B:97:LEU:HD13	2.02	0.42
1:D:412:VAL:HB	1:D:420:LYS:HB3	2.00	0.42
1:F:73:PRO:HA	1:F:384:ILE:HD11	2.02	0.42
1:G:76:MET:HA	1:G:120:THR:O	2.20	0.42
1:G:136:ALA:HB3	1:G:142:ILE:HD11	2.00	0.42
1:A:146:ARG:HG3	1:A:414:LYS:HE3	2.01	0.42
1:E:199:GLY:HA2	1:F:216:LYS:HE2	2.02	0.42
1:H:39:THR:CG2	1:H:51:GLU:HB2	2.50	0.42
1:H:82:LEU:HD23	1:H:82:LEU:HA	1.88	0.42
1:H:337:THR:O	1:H:337:THR:HG22	2.19	0.42
1:B:76:MET:HA	1:B:120:THR:O	2.20	0.42
1:B:398:ASN:ND2	1:B:401:GLU:HG3	2.35	0.42
1:B:420:LYS:HE2	1:B:422:GLU:CD	2.44	0.42
1:E:80:VAL:O	1:E:123:ASP:HA	2.20	0.42
1:F:250:GLU:O	1:F:254:ARG:HG3	2.20	0.42
1:G:50:ILE:HD11	1:G:384:ILE:HG22	2.02	0.42
1:G:54:TYR:CZ	1:G:67:ARG:HG2	2.55	0.42
1:C:249:ALA:O	1:C:253:LYS:HE2	2.19	0.42
1:D:21:LEU:O	1:D:39:THR:HA	2.20	0.42
1:E:34:TRP:HE1	1:E:400:LEU:HD12	1.84	0.41
1:G:97:LEU:HD22	1:G:101:ASP:HB2	2.02	0.41
1:B:287:THR:CG2	1:B:338:ASP:HB2	2.50	0.41
1:E:271:ASP:HA	1:E:274:ILE:HD12	2.02	0.41
1:F:170:ASP:OD1	1:F:170:ASP:N	2.50	0.41
1:E:203:ILE:HG12	1:E:240:MET:HE2	2.01	0.41
1:E:338:ASP:OD1	1:E:341:LYS:HG2	2.19	0.41
1:F:245:HIS:CB	1:F:264:GLU:HB2	2.50	0.41
1:B:183:ASN:ND2	1:F:190:LYS:HD2	2.35	0.41
1:C:244:VAL:HG21	1:C:260:VAL:HG11	2.03	0.41
1:F:155:ALA:O	1:F:181:VAL:HA	2.20	0.41
1:H:70:TYR:O	1:H:394:ALA:HA	2.19	0.41
1:B:269:MET:HE3	1:B:269:MET:HB2	1.80	0.41
1:C:24:GLY:HA2	1:C:54:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:LEU:HD23	1:C:124:LEU:HA	1.83	0.41
1:E:155:ALA:O	1:E:181:VAL:HA	2.20	0.41
1:E:204:LYS:HE2	1:E:245:HIS:CB	2.51	0.41
1:G:347:ASN:OD1	1:G:347:ASN:N	2.53	0.41
1:H:73:PRO:HG3	1:H:384:ILE:CD1	2.50	0.41
1:C:118:PHE:CZ	1:C:347:ASN:HB2	2.56	0.41
1:C:367:SER:HA	1:C:371:ASN:HB2	2.03	0.41
1:F:66:LEU:HB3	1:F:69:ARG:HB2	2.02	0.41
1:H:27:LEU:HD23	1:H:29:VAL:HB	2.01	0.41
1:D:352:GLU:OE2	1:D:404:SER:HB3	2.21	0.41
1:E:286:PRO:O	1:E:287:THR:OG1	2.32	0.41
1:H:208:THR:HG21	1:H:248:GLY:H	1.86	0.41
1:A:392:VAL:O	1:A:393:ILE:HD13	2.21	0.41
1:B:75:LEU:HD13	1:B:351:PHE:CE2	2.55	0.41
1:C:80:VAL:O	1:C:123:ASP:HA	2.21	0.41
1:C:196:TYR:HB2	1:C:240:MET:HE1	2.03	0.41
1:C:355:VAL:HA	1:C:359:MET:O	2.21	0.41
1:D:208:THR:HG1	1:D:247:HIS:H	1.67	0.41
1:E:304:TYR:HB3	1:E:308:VAL:HB	2.03	0.41
1:F:79:HIS:CG	1:F:124:LEU:HD12	2.55	0.41
1:G:255:ALA:O	1:G:260:VAL:HG13	2.21	0.41
1:H:402:ASN:O	1:H:405:THR:HG22	2.20	0.41
1:A:122:ARG:HH12	1:A:243:ALA:HB2	1.86	0.41
1:A:146:ARG:NH2	1:A:389:LEU:HD13	2.36	0.41
1:B:103:ALA:O	1:B:107:VAL:HG23	2.21	0.41
1:E:383:SER:HB3	1:E:388:MET:HE2	2.03	0.41
1:F:107:VAL:HG22	1:F:142:ILE:HD12	2.03	0.41
1:H:73:PRO:HG3	1:H:384:ILE:HD11	2.02	0.41
1:B:290:ALA:HB3	1:B:338:ASP:HB3	2.03	0.40
1:C:362:LEU:HD12	1:C:362:LEU:HA	1.82	0.40
1:F:27:LEU:HB2	1:F:34:TRP:CZ3	2.56	0.40
1:F:76:MET:HE1	1:F:382:GLY:CA	2.49	0.40
1:F:206:THR:CG2	1:F:245:HIS:CE1	2.99	0.40
1:F:207:ALA:HB3	1:F:246:ALA:HB2	2.03	0.40
1:B:93:GLU:HA	1:B:96:ILE:CG1	2.47	0.40
1:C:393:ILE:HA	1:C:411:PHE:O	2.21	0.40
1:E:115:MET:CE	1:E:420:LYS:HB2	2.51	0.40
1:E:367:SER:HA	1:E:371:ASN:HB2	2.04	0.40
1:F:204:LYS:HZ1	1:F:245:HIS:HB3	1.86	0.40
1:H:278:LYS:HG2	1:H:278:LYS:H	1.74	0.40
1:H:328:LYS:HB2	1:H:328:LYS:HE3	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:THR:O	1:B:238:TYR:HD1	2.05	0.40
1:F:33:LYS:HE3	1:F:33:LYS:HB3	1.62	0.40
1:H:47:ILE:HD13	1:H:384:ILE:HG23	2.02	0.40
1:B:335:PHE:HD1	1:B:354:MET:HE1	1.86	0.40
1:G:290:ALA:O	1:G:294:VAL:HG23	2.21	0.40
1:G:367:SER:HA	1:G:371:ASN:HB2	2.02	0.40
1:B:249:ALA:O	1:B:253:LYS:HG3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/422 (91%)	372 (97%)	12 (3%)	0	100	100
1	B	369/422 (87%)	357 (97%)	12 (3%)	0	100	100
1	C	367/422 (87%)	361 (98%)	6 (2%)	0	100	100
1	D	366/422 (87%)	360 (98%)	6 (2%)	0	100	100
1	E	383/422 (91%)	368 (96%)	15 (4%)	0	100	100
1	F	372/422 (88%)	361 (97%)	11 (3%)	0	100	100
1	G	373/422 (88%)	363 (97%)	10 (3%)	0	100	100
1	H	370/422 (88%)	360 (97%)	10 (3%)	0	100	100
All	All	2984/3376 (88%)	2902 (97%)	82 (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	294/323 (91%)	281 (96%)	13 (4%)	25	37
1	B	288/323 (89%)	266 (92%)	22 (8%)	12	17
1	C	281/323 (87%)	270 (96%)	11 (4%)	28	41
1	D	275/323 (85%)	270 (98%)	5 (2%)	51	67
1	E	281/323 (87%)	274 (98%)	7 (2%)	42	58
1	F	276/323 (85%)	264 (96%)	12 (4%)	26	38
1	G	281/323 (87%)	271 (96%)	10 (4%)	31	44
1	H	272/323 (84%)	261 (96%)	11 (4%)	28	40
All	All	2248/2584 (87%)	2157 (96%)	91 (4%)	28	40

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	18	THR
1	A	39	THR
1	A	51	GLU
1	A	58	LYS
1	A	86	THR
1	A	89	HIS
1	A	106	SER
1	A	170	ASP
1	A	202	LEU
1	A	211	VAL
1	A	279	LYS
1	A	331	VAL
1	A	339	SER
1	B	29	VAL
1	B	30	LYS
1	B	31	LYS
1	B	52	LYS
1	B	58	LYS
1	B	62	LYS
1	B	67	ARG
1	B	86	THR
1	B	170	ASP
1	B	204	LYS

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Mol	Chain	Res	Type
1	B	231	ILE
1	B	250	GLU
1	B	267	THR
1	B	271	ASP
1	B	278	LYS
1	B	293	THR
1	B	319	ILE
1	B	331	VAL
1	B	339	SER
1	B	341	LYS
1	B	342	SER
1	B	347	ASN
1	C	86	THR
1	C	146	ARG
1	C	262	SER
1	C	265	HIS
1	C	267	THR
1	C	272	GLU
1	C	276	LEU
1	C	333	ILE
1	C	346	LEU
1	C	365	ILE
1	C	410	VAL
1	D	171	LEU
1	D	172	MET
1	D	267	THR
1	D	341	LYS
1	D	363	GLU
1	E	38	VAL
1	E	91	THR
1	E	97	LEU
1	E	120	THR
1	E	319	ILE
1	E	321	LYS
1	E	415	ASP
1	F	19	THR
1	F	62	LYS
1	F	63	VAL
1	F	86	THR
1	F	97	LEU
1	F	129	VAL
1	F	202	LEU

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Mol	Chain	Res	Type
1	F	288	ILE
1	F	293	THR
1	F	355	VAL
1	F	385	GLU
1	F	397	ASP
1	G	27	LEU
1	G	36	GLU
1	G	38	VAL
1	G	39	THR
1	G	58	LYS
1	G	62	LYS
1	G	63	VAL
1	G	142	ILE
1	G	204	LYS
1	G	346	LEU
1	H	21	LEU
1	H	76	MET
1	H	89	HIS
1	H	91	THR
1	H	170	ASP
1	H	320	GLN
1	H	347	ASN
1	H	349	ILE
1	H	393	ILE
1	H	395	VAL
1	H	415	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	194	GLN
1	A	198	ASN
1	A	402	ASN
1	B	81	HIS
1	B	87	ASN
1	B	89	HIS
1	B	160	HIS
1	B	402	ASN
1	B	421	GLN
1	C	81	HIS
1	C	245	HIS

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Mol	Chain	Res	Type
1	C	421	GLN
1	D	87	ASN
1	D	90	ASN
1	D	160	HIS
1	D	245	HIS
1	D	421	GLN
1	E	344	HIS
1	E	421	GLN
1	F	79	HIS
1	F	81	HIS
1	F	194	GLN
1	F	222	GLN
1	F	245	HIS
1	F	261	HIS
1	F	421	GLN
1	G	160	HIS
1	G	344	HIS
1	H	25	HIS
1	H	265	HIS
1	H	320	GLN
1	H	347	ASN
1	H	421	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

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, 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	390/422 (92%)	0.51	18 (4%) 37 38	13, 33, 68, 109	0
1	B	375/422 (88%)	0.52	19 (5%) 33 34	17, 33, 61, 86	0
1	C	373/422 (88%)	0.50	15 (4%) 42 43	21, 35, 59, 89	0
1	D	372/422 (88%)	0.48	15 (4%) 42 43	14, 31, 62, 116	0
1	E	389/422 (92%)	0.76	31 (7%) 18 18	21, 42, 66, 114	0
1	F	378/422 (89%)	0.74	22 (5%) 29 29	19, 44, 65, 87	0
1	G	379/422 (89%)	0.41	11 (2%) 53 55	15, 30, 61, 101	0
1	H	376/422 (89%)	0.90	41 (10%) 10 10	21, 47, 82, 102	0
All	All	3032/3376 (89%)	0.60	172 (5%) 29 29	13, 36, 69, 116	0

All (172) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	VAL	5.5
1	H	397	ASP	5.3
1	A	215	ALA	4.9
1	B	340	GLY	4.7
1	E	267	THR	4.7
1	C	265	HIS	4.2
1	A	213	SER	4.2
1	F	334	ALA	4.1
1	H	319	ILE	4.1
1	C	319	ILE	4.1
1	E	212	LEU	4.0
1	E	307	ILE	3.9
1	D	91	THR	3.9
1	A	307	ILE	3.8
1	E	319	ILE	3.8
1	A	214	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	295	ALA	3.7
1	H	211	VAL	3.7
1	H	17	ALA	3.7
1	B	319	ILE	3.7
1	F	217	SER	3.6
1	C	290	ALA	3.6
1	E	211	VAL	3.5
1	B	293	THR	3.5
1	E	301	PRO	3.5
1	A	212	LEU	3.5
1	D	250	GLU	3.4
1	B	59	ALA	3.4
1	E	302	GLY	3.4
1	A	210	GLY	3.3
1	H	37	GLY	3.3
1	H	95	PHE	3.3
1	H	216	LYS	3.3
1	G	317	PRO	3.3
1	E	306	PRO	3.2
1	E	49	GLY	3.2
1	H	59	ALA	3.2
1	E	217	SER	3.2
1	E	308	VAL	3.2
1	A	218	GLY	3.1
1	H	337	THR	3.1
1	A	170	ASP	3.1
1	C	340	GLY	3.0
1	F	216	LYS	3.0
1	D	267	THR	3.0
1	C	338	ASP	3.0
1	E	270	ASP	3.0
1	G	273	ALA	3.0
1	C	270	ASP	3.0
1	H	218	GLY	3.0
1	F	319	ILE	2.9
1	E	268	TYR	2.9
1	F	416	GLY	2.9
1	D	320	GLN	2.9
1	H	320	GLN	2.9
1	H	53	GLY	2.9
1	D	90	ASN	2.8
1	G	293	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	210	GLY	2.8
1	A	294	VAL	2.8
1	B	294	VAL	2.8
1	A	317	PRO	2.8
1	C	293	THR	2.8
1	F	292	ARG	2.8
1	E	305	ALA	2.8
1	C	266	GLY	2.8
1	H	24	GLY	2.7
1	G	142	ILE	2.7
1	B	317	PRO	2.7
1	A	268	TYR	2.7
1	D	171	LEU	2.7
1	B	339	SER	2.7
1	F	90	ASN	2.7
1	G	294	VAL	2.6
1	E	320	GLN	2.6
1	D	89	HIS	2.6
1	B	290	ALA	2.6
1	G	295	ALA	2.6
1	C	268	TYR	2.6
1	H	58	LYS	2.6
1	C	422	GLU	2.6
1	H	36	GLU	2.6
1	E	340	GLY	2.6
1	H	29	VAL	2.6
1	E	213	SER	2.6
1	C	318	GLN	2.5
1	D	293	THR	2.5
1	B	60	GLY	2.5
1	H	60	GLY	2.5
1	D	86	THR	2.5
1	H	217	SER	2.5
1	G	94	ARG	2.5
1	H	69	ARG	2.5
1	D	92	LEU	2.5
1	F	48	ARG	2.5
1	F	404	SER	2.5
1	A	216	LYS	2.5
1	B	58	LYS	2.5
1	F	289	LEU	2.4
1	H	26	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	217	SER	2.4
1	F	251	GLY	2.4
1	C	146	ARG	2.4
1	E	71	VAL	2.4
1	H	34	TRP	2.4
1	B	51	GLU	2.4
1	H	396	GLU	2.4
1	H	382	GLY	2.4
1	H	50	ILE	2.4
1	B	92	LEU	2.3
1	B	338	ASP	2.3
1	E	169	LYS	2.3
1	E	341	LYS	2.3
1	A	267	THR	2.3
1	D	209	GLY	2.3
1	C	89	HIS	2.3
1	F	23	CYS	2.3
1	E	331	VAL	2.3
1	H	38	VAL	2.3
1	D	318	GLN	2.3
1	E	29	VAL	2.3
1	D	268	TYR	2.3
1	E	160	HIS	2.2
1	E	166	GLY	2.2
1	F	358	GLY	2.2
1	B	403	ILE	2.2
1	E	404	SER	2.2
1	H	42	ILE	2.2
1	F	407	ARG	2.2
1	G	297	SER	2.2
1	A	305	ALA	2.2
1	F	348	ALA	2.2
1	G	341	LYS	2.2
1	G	267	THR	2.2
1	C	209	GLY	2.2
1	E	72	LEU	2.2
1	G	292	ARG	2.2
1	H	408	LYS	2.2
1	E	90	ASN	2.2
1	H	44	GLY	2.2
1	H	55	VAL	2.1
1	H	395	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	17	ALA	2.1
1	H	274	ILE	2.1
1	B	270	ASP	2.1
1	D	270	ASP	2.1
1	E	46	THR	2.1
1	B	61	GLU	2.1
1	F	89	HIS	2.1
1	D	390	ALA	2.1
1	C	291	GLY	2.1
1	H	340	GLY	2.1
1	F	50	ILE	2.1
1	A	341	LYS	2.1
1	B	170	ASP	2.1
1	B	341	LYS	2.1
1	H	25	HIS	2.1
1	E	56	ALA	2.1
1	F	56	ALA	2.1
1	H	161	ALA	2.1
1	F	316	GLY	2.1
1	F	62	LYS	2.1
1	B	88	PRO	2.1
1	H	381	LEU	2.0
1	E	291	GLY	2.0
1	H	70	TYR	2.0
1	H	27	LEU	2.0
1	H	56	ALA	2.0
1	H	180	GLY	2.0
1	H	345	GLY	2.0
1	F	174	ASP	2.0
1	H	339	SER	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

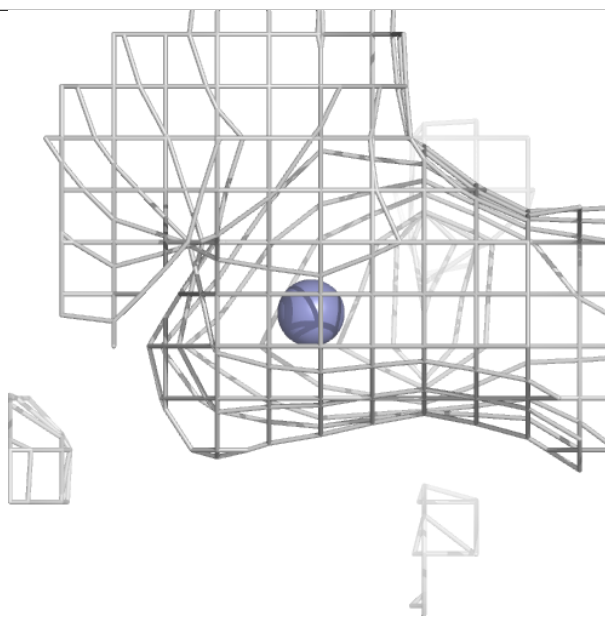
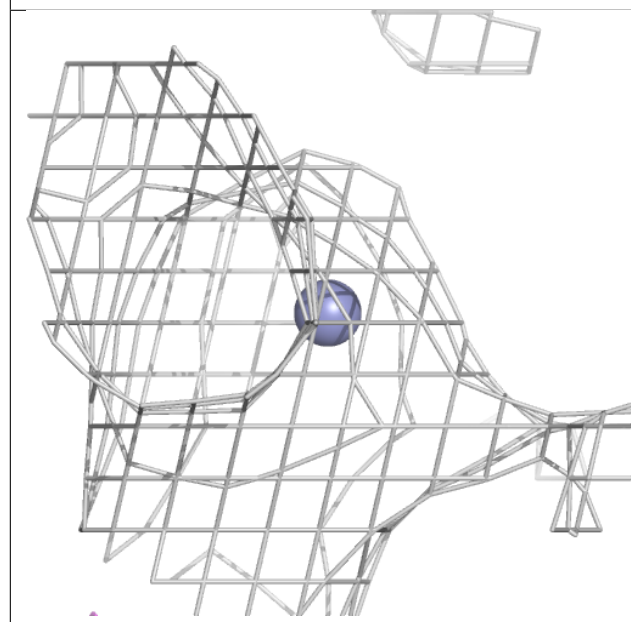
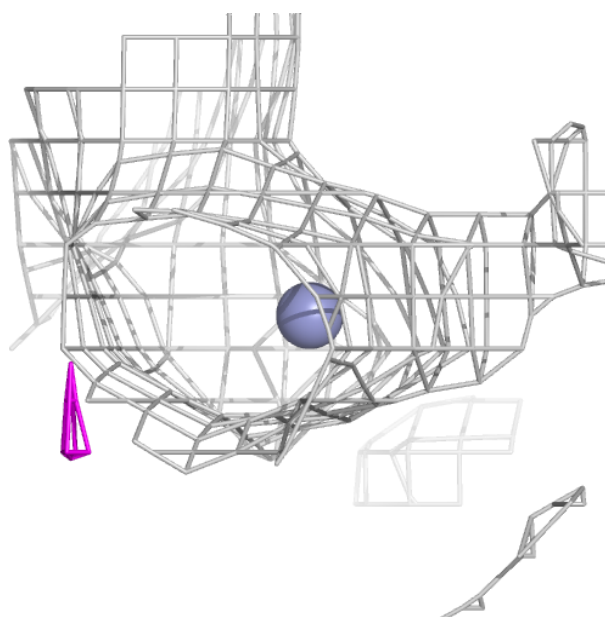
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists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

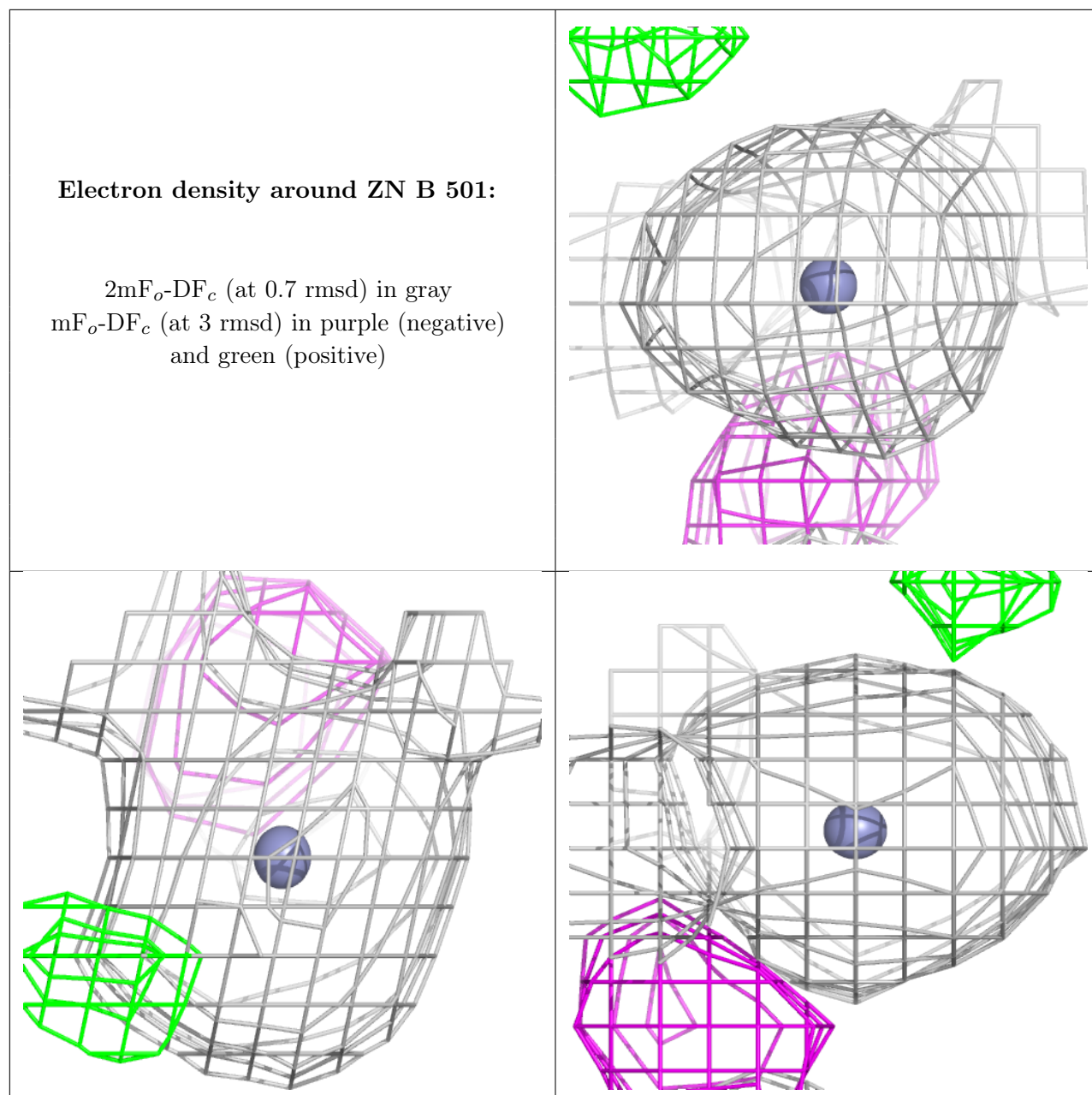
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ZN	A	501	1/1	0.85	0.22	172,172,172,172	0
2	ZN	B	501	1/1	0.88	0.11	102,102,102,102	0

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

Electron density around ZN A 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.