



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 19, 2021 – 12:11 PM JST

PDB ID : 7BYQ
Title : The mutant variant of PNGM-1. H279A was substituted for alanine to study metal coordination.
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Deposited on : 2020-04-24
Resolution : 1.96 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 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 : 2.18
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

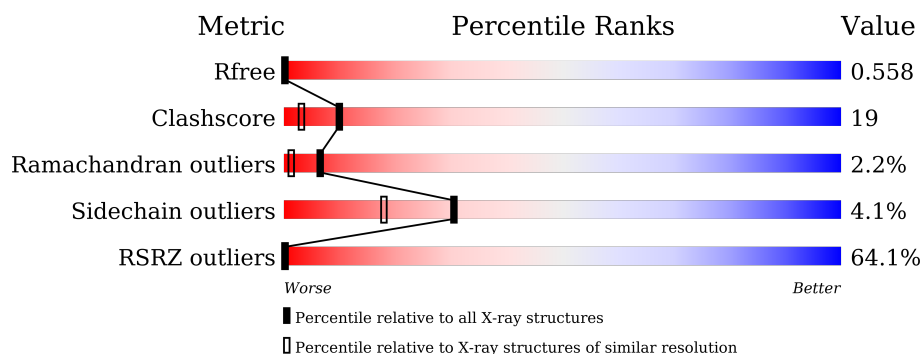
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	372	<div> <div>53%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>..</div> </div> </div>
1	B	372	<div> <div>61%</div> <div> <div></div> <div>67%</div> <div>28%</div> <div>..</div> </div> </div>
1	C	372	<div> <div>69%</div> <div> <div></div> <div>64%</div> <div>31%</div> <div>..</div> </div> </div>
1	D	372	<div> <div>66%</div> <div> <div></div> <div>69%</div> <div>24%</div> <div>..</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11914 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 Metallo-beta-lactamase PNGM-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	0	0
			2851	1805	490	536	20			
1	B	360	Total	C	N	O	S	0	0	0
			2823	1789	481	533	20			
1	C	360	Total	C	N	O	S	0	0	0
			2823	1789	481	533	20			
1	D	362	Total	C	N	O	S	0	0	0
			2847	1804	487	536	20			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
B	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
C	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6
D	279	ALA	HIS	engineered mutation	UNP A0A2U8UYM6

- 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	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

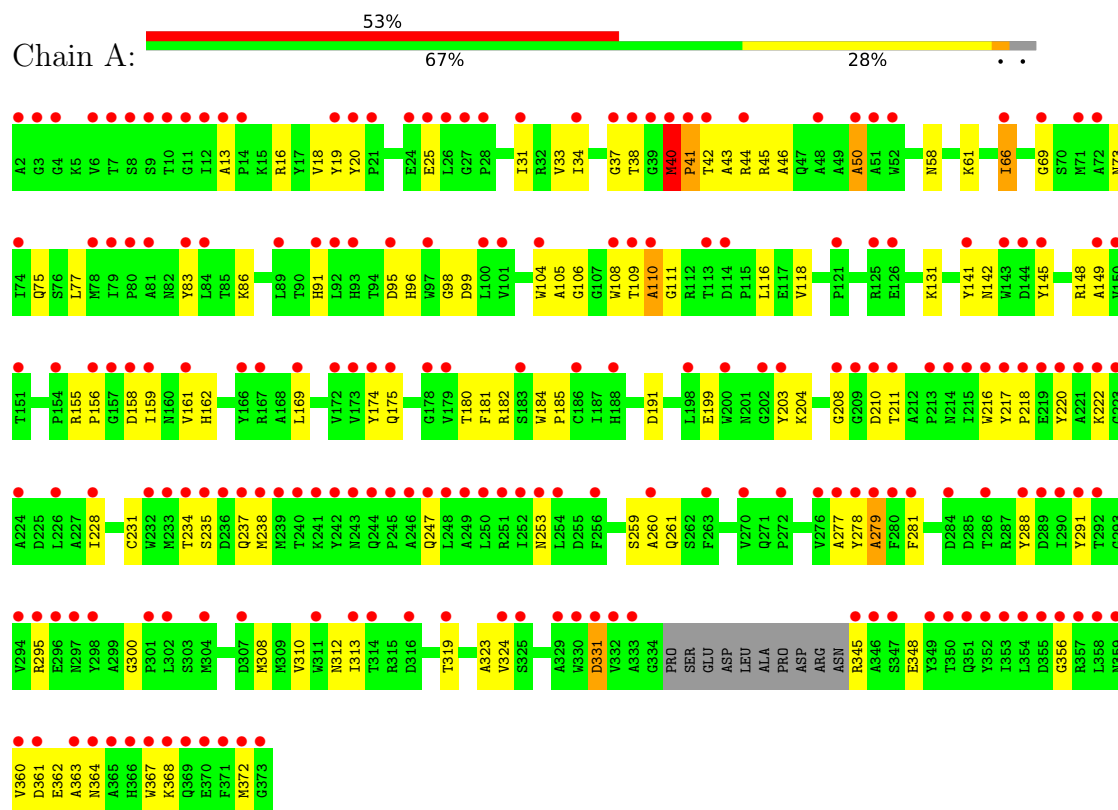
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	145	Total 145	O 145	0	0
3	B	144	Total 144	O 144	0	0
3	C	148	Total 148	O 148	0	0
3	D	129	Total 129	O 129	0	0

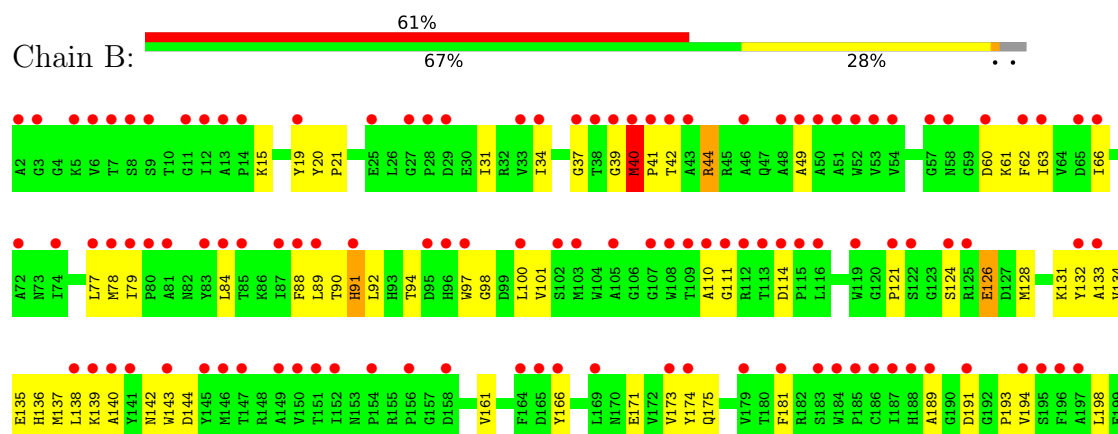
3 Residue-property plots

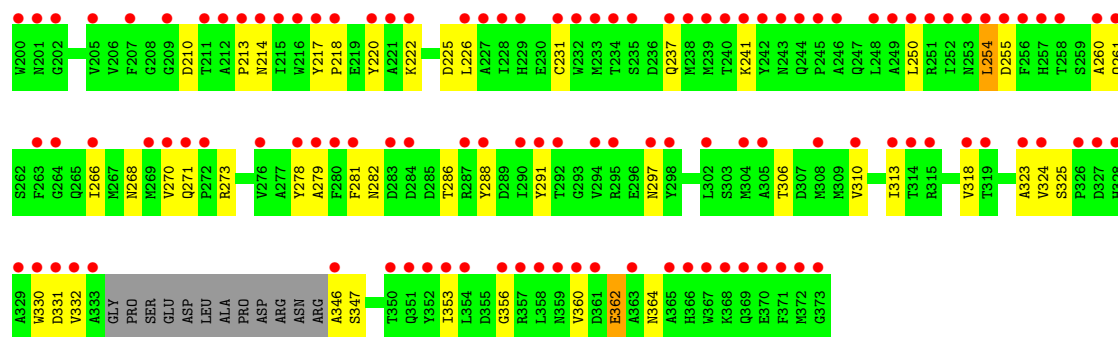
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Metallo-beta-lactamase PNGM-1

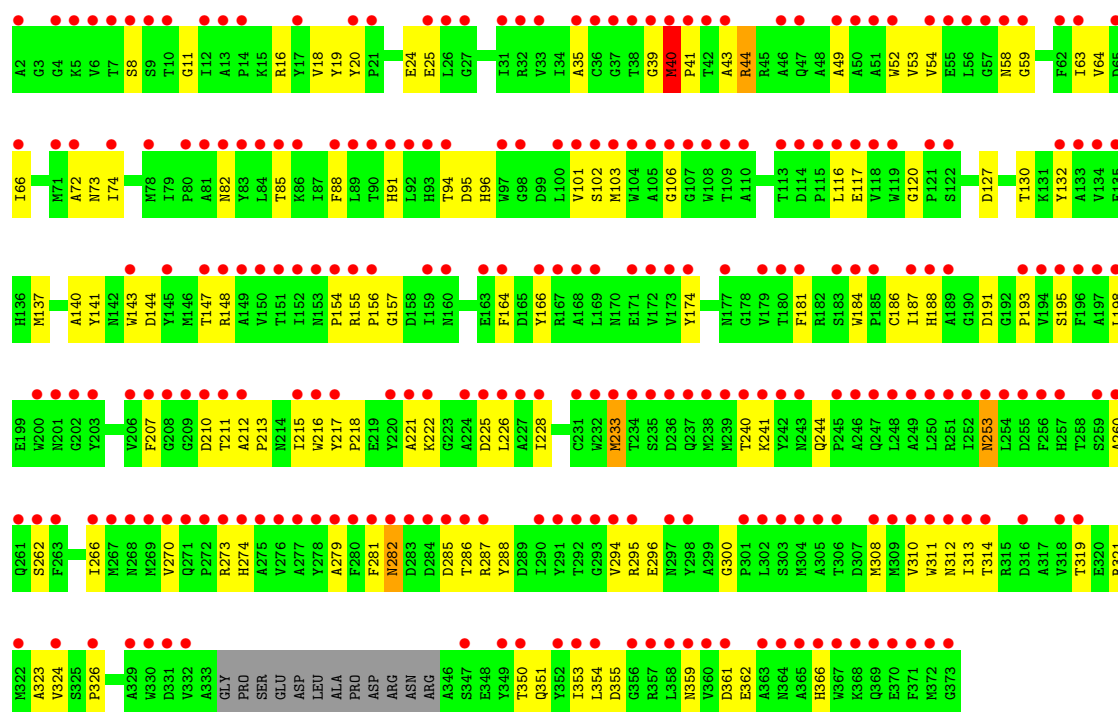


• Molecule 1: Metallo-beta-lactamase PNGM-1



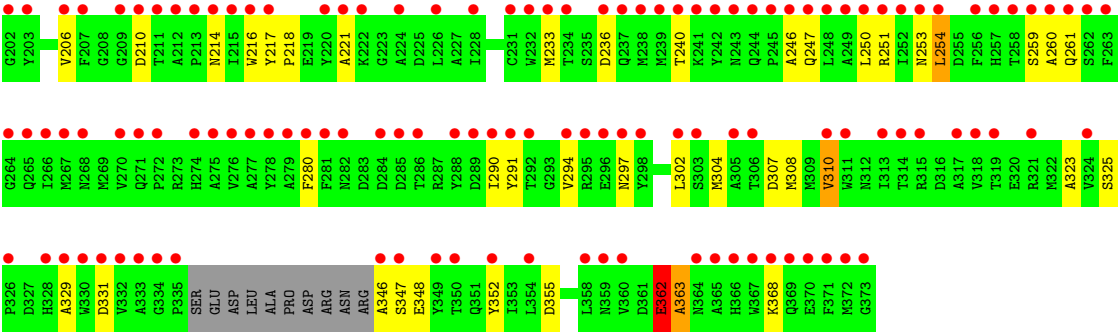


• Molecule 1: Metallo-beta-lactamase PNGM-1



• Molecule 1: Metallo-beta-lactamase PNGM-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	121.38Å 83.06Å 163.58Å 90.00° 110.69° 90.00°	Depositor
Resolution (Å)	49.04 – 1.96 49.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	95.1 (49.04-1.96) 95.2 (49.00-1.94)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 1.94Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.519 , 0.557 0.520 , 0.558	Depositor DCC
R_{free} test set	10778 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	21.3	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 65.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.024 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.51	EDS
Total number of atoms	11914	wwPDB-VP
Average B, all atoms (Å ²)	22.0	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 83.68 % 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 2.0365e-07. 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: 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	0.69	0/2933	0.81	0/3995
1	B	0.73	2/2905 (0.1%)	0.83	0/3960
1	C	0.68	0/2905	0.79	0/3960
1	D	0.69	0/2930	0.83	2/3993 (0.1%)
All	All	0.70	2/11673 (0.0%)	0.82	2/15908 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	126	GLU	CD-OE1	7.83	1.34	1.25
1	B	126	GLU	CD-OE2	6.50	1.32	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	83	TYR	CB-CG-CD1	5.94	124.56	121.00
1	D	346	ALA	O-C-N	5.64	131.73	122.70

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	2851	0	2683	102	0
1	B	2823	0	2641	117	0
1	C	2823	0	2641	128	0
1	D	2847	0	2677	96	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	145	0	0	46	0
3	B	144	0	0	62	0
3	C	148	0	0	70	0
3	D	129	0	0	53	0
All	All	11914	0	10642	420	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 19.

All (420) 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:C:187:ILE:HB	3:C:568:HOH:O	1.37	1.20
1:B:213:PRO:HA	3:B:574:HOH:O	1.39	1.18
1:D:210:ASP:OD2	3:D:501:HOH:O	1.62	1.15
1:B:310:VAL:HB	3:B:593:HOH:O	1.49	1.12
1:C:210:ASP:OD2	3:C:501:HOH:O	1.65	1.11
1:D:233:MET:SD	3:D:599:HOH:O	2.07	1.10
1:A:204:LYS:NZ	1:A:220:TYR:O	1.88	1.04
1:C:266:ILE:HG21	3:C:583:HOH:O	1.60	1.01
1:D:40:MET:HB3	1:D:41:PRO:HD2	1.44	0.98
1:C:188:HIS:CD2	3:C:600:HOH:O	2.15	0.98
1:A:260:ALA:HA	3:A:575:HOH:O	1.62	0.97
1:A:312:ASN:HB2	3:A:605:HOH:O	1.64	0.95
1:C:294:VAL:HG23	3:C:532:HOH:O	1.67	0.94
1:A:184:TRP:CZ2	3:A:608:HOH:O	2.20	0.94
1:B:124:SER:CB	3:B:506:HOH:O	2.16	0.94
1:D:214:ASN:HB3	3:D:588:HOH:O	1.69	0.91
1:B:132:TYR:CD2	3:B:559:HOH:O	2.23	0.91
1:A:105:ALA:HB1	3:D:554:HOH:O	1.71	0.90
1:B:40:MET:HB2	1:B:41:PRO:CD	2.02	0.90
1:B:166:TYR:CZ	3:B:573:HOH:O	2.24	0.89
1:D:40:MET:HB3	1:D:41:PRO:CD	2.04	0.88
1:A:108:TRP:HH2	3:A:504:HOH:O	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:GLY:HA3	1:B:49:ALA:O	1.74	0.88
1:B:126:GLU:O	3:B:501:HOH:O	1.92	0.87
1:A:25:GLU:OE2	3:A:501:HOH:O	1.91	0.87
1:A:217:TYR:CD2	3:A:608:HOH:O	2.27	0.86
1:C:311:TRP:CD1	3:C:587:HOH:O	2.29	0.85
1:A:149:ALA:HB2	3:A:504:HOH:O	1.75	0.85
1:B:286:THR:HG22	3:B:632:HOH:O	1.76	0.84
1:A:210:ASP:OD2	3:A:502:HOH:O	1.96	0.84
1:C:88:PHE:CZ	3:C:610:HOH:O	2.31	0.84
1:D:75:GLN:HB2	3:D:514:HOH:O	1.77	0.84
1:B:79:ILE:O	3:B:502:HOH:O	1.96	0.83
1:B:128:MET:CE	3:C:599:HOH:O	2.25	0.83
1:B:97:TRP:HB2	3:B:575:HOH:O	1.77	0.82
1:D:89:LEU:HD22	3:D:568:HOH:O	1.78	0.82
1:C:312:ASN:OD1	3:C:502:HOH:O	1.96	0.82
1:B:173:VAL:HG23	3:B:614:HOH:O	1.79	0.81
1:C:266:ILE:HD13	3:C:583:HOH:O	1.79	0.80
1:A:46:ALA:HB3	3:A:543:HOH:O	1.82	0.80
1:B:124:SER:HB3	3:B:506:HOH:O	1.78	0.80
1:B:286:THR:CG2	3:B:632:HOH:O	2.29	0.80
1:C:221:ALA:HB2	3:C:608:HOH:O	1.82	0.80
1:A:184:TRP:HZ2	3:A:608:HOH:O	1.60	0.79
1:A:313:ILE:HG22	3:A:552:HOH:O	1.83	0.79
1:C:191:ASP:O	3:C:503:HOH:O	2.01	0.79
1:C:143:TRP:CD1	3:C:599:HOH:O	2.35	0.77
1:B:134:VAL:HG23	3:B:533:HOH:O	1.85	0.77
1:B:40:MET:HB2	1:B:41:PRO:HD2	1.64	0.77
1:A:161:VAL:HG13	3:A:554:HOH:O	1.84	0.77
1:A:83:TYR:CD2	3:B:634:HOH:O	2.38	0.76
1:C:260:ALA:HB1	3:C:532:HOH:O	1.84	0.76
1:C:154:PRO:HB3	3:C:613:HOH:O	1.84	0.76
1:A:40:MET:HB3	1:A:41:PRO:HD2	1.65	0.76
1:A:203:TYR:CE1	3:A:552:HOH:O	2.39	0.76
1:A:319:THR:HB	3:A:605:HOH:O	1.85	0.76
1:A:217:TYR:CE2	3:A:608:HOH:O	2.39	0.75
1:B:171:GLU:OE1	3:B:503:HOH:O	2.04	0.75
1:A:203:TYR:CZ	3:A:552:HOH:O	2.40	0.75
1:C:74:ILE:O	3:C:504:HOH:O	2.04	0.74
1:D:260:ALA:HA	3:D:569:HOH:O	1.87	0.74
1:D:294:VAL:CG2	3:D:569:HOH:O	2.35	0.74
3:B:506:HOH:O	1:C:350:THR:HG23	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:294:VAL:HG22	3:D:569:HOH:O	1.88	0.73
1:A:261:GLN:OE1	1:A:261:GLN:N	2.21	0.73
1:B:94:THR:HG22	1:C:141:TYR:CD1	2.24	0.73
1:C:72:ALA:O	3:C:505:HOH:O	2.06	0.73
3:B:522:HOH:O	1:C:353:ILE:HG12	1.88	0.73
1:A:253:ASN:ND2	3:A:506:HOH:O	2.22	0.72
1:B:128:MET:HE2	3:C:599:HOH:O	1.86	0.72
1:A:364:ASN:ND2	3:A:505:HOH:O	2.22	0.72
1:A:118:VAL:HB	3:A:554:HOH:O	1.89	0.71
1:D:355:ASP:HB3	3:D:531:HOH:O	1.87	0.71
1:D:97:TRP:HB3	3:D:568:HOH:O	1.90	0.71
1:C:94:THR:HB	3:C:566:HOH:O	1.90	0.71
1:B:126:GLU:HG2	3:B:559:HOH:O	1.89	0.71
1:B:60:ASP:CB	3:B:540:HOH:O	2.37	0.71
1:B:268:ASN:O	1:B:271:GLN:HG2	1.92	0.70
1:B:346:ALA:O	3:B:504:HOH:O	2.10	0.69
1:C:212:ALA:HB3	3:C:568:HOH:O	1.93	0.69
1:D:290:ILE:HD13	3:D:544:HOH:O	1.93	0.69
1:C:174:TYR:CD1	3:C:610:HOH:O	2.46	0.68
1:B:194:VAL:HG13	3:B:513:HOH:O	1.92	0.68
1:A:98:GLY:O	3:A:503:HOH:O	2.12	0.68
1:B:193:PRO:HD2	3:B:511:HOH:O	1.93	0.68
1:A:61:LYS:O	1:A:86:LYS:NZ	2.27	0.68
1:B:191:ASP:HB3	3:B:573:HOH:O	1.93	0.68
1:B:144:ASP:OD2	1:C:94:THR:HG23	1.94	0.67
1:C:143:TRP:HD1	3:C:599:HOH:O	1.74	0.67
1:D:71:MET:HG3	3:D:514:HOH:O	1.94	0.67
1:B:210:ASP:OD2	3:B:505:HOH:O	2.11	0.67
1:D:186:CYS:SG	1:D:195:SER:OG	2.52	0.67
1:A:40:MET:HB3	1:A:41:PRO:CD	2.24	0.67
1:C:43:ALA:HA	3:C:545:HOH:O	1.96	0.66
1:B:132:TYR:HD2	3:B:559:HOH:O	1.71	0.66
1:C:294:VAL:CG2	3:C:532:HOH:O	2.35	0.66
1:A:20:TYR:CD2	1:B:20:TYR:HB3	2.30	0.66
1:B:261:GLN:N	1:B:261:GLN:OE1	2.29	0.65
1:C:52:TRP:O	3:C:506:HOH:O	2.14	0.65
1:D:187:ILE:HD12	3:D:588:HOH:O	1.96	0.65
1:C:53:VAL:HG22	3:C:506:HOH:O	1.97	0.65
1:A:96:HIS:NE2	3:A:502:HOH:O	2.29	0.65
1:B:225:ASP:O	1:B:273:ARG:HB2	1.97	0.64
1:B:19:TYR:CB	1:B:310:VAL:HG11	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:ASP:OD2	3:B:506:HOH:O	2.14	0.64
1:C:66:ILE:N	1:C:96:HIS:O	2.29	0.64
1:C:103:MET:SD	3:C:558:HOH:O	2.55	0.64
1:C:188:HIS:HD2	3:C:600:HOH:O	1.64	0.63
1:A:182:ARG:HD2	3:A:629:HOH:O	1.99	0.63
1:B:282:ASN:HD22	1:B:306:THR:HB	1.63	0.63
1:A:238:MET:HG3	3:A:506:HOH:O	1.98	0.63
1:C:40:MET:SD	1:C:279:ALA:HA	2.39	0.63
1:D:260:ALA:CA	3:D:569:HOH:O	2.43	0.62
1:D:260:ALA:HB1	3:D:569:HOH:O	1.99	0.62
3:B:519:HOH:O	1:C:215:ILE:HG21	1.98	0.62
1:C:49:ALA:HB1	1:C:95:ASP:HB2	1.82	0.61
1:A:58:ASN:HA	3:A:621:HOH:O	2.00	0.61
1:C:262:SER:HB3	3:C:627:HOH:O	1.98	0.61
1:D:261:GLN:N	1:D:261:GLN:OE1	2.33	0.61
1:B:92:LEU:HA	1:B:97:TRP:CD1	2.34	0.61
1:B:40:MET:CB	1:B:41:PRO:CD	2.79	0.61
1:D:290:ILE:CD1	3:D:544:HOH:O	2.48	0.61
1:D:260:ALA:CB	3:D:569:HOH:O	2.47	0.61
1:A:363:ALA:HB3	3:A:505:HOH:O	2.00	0.61
1:C:24:GLU:OE1	3:C:507:HOH:O	2.16	0.60
1:A:18:VAL:HG23	3:A:596:HOH:O	2.02	0.60
1:C:295:ARG:HG2	3:C:531:HOH:O	2.01	0.60
1:D:105:ALA:O	1:D:148:ARG:NH1	2.29	0.60
1:C:130:THR:HB	3:C:509:HOH:O	2.00	0.60
1:C:63:ILE:HG12	3:C:506:HOH:O	1.99	0.60
1:A:40:MET:CB	1:A:41:PRO:CD	2.80	0.60
1:B:44:ARG:HA	3:C:505:HOH:O	2.00	0.60
1:C:73:ASN:HB3	1:C:308:MET:SD	2.43	0.59
1:B:166:TYR:CE2	3:B:573:HOH:O	2.49	0.59
1:B:60:ASP:HB3	3:B:540:HOH:O	2.00	0.59
1:C:226:LEU:HD13	3:C:587:HOH:O	2.02	0.59
1:C:154:PRO:O	1:C:157:GLY:N	2.34	0.59
1:A:324:VAL:HG12	1:B:324:VAL:HG12	1.83	0.59
1:B:100:LEU:HB2	3:B:575:HOH:O	2.03	0.59
1:B:166:TYR:CE1	3:B:573:HOH:O	2.54	0.58
1:C:351:GLN:HG3	1:C:355:ASP:OD2	2.03	0.58
1:A:363:ALA:HB1	1:D:297:ASN:ND2	2.18	0.58
1:C:186:CYS:O	3:C:508:HOH:O	2.16	0.58
1:D:348:GLU:OE1	1:D:348:GLU:HA	2.04	0.57
1:C:120:GLY:C	3:C:509:HOH:O	2.41	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:254:LEU:CD2	3:D:524:HOH:O	2.52	0.57
1:A:38:THR:HA	3:A:528:HOH:O	2.03	0.57
1:A:131:LYS:HB3	3:A:579:HOH:O	2.04	0.57
1:C:44:ARG:HD3	1:C:281:PHE:CE1	2.39	0.57
1:C:354:LEU:HD23	3:C:596:HOH:O	2.05	0.57
1:B:19:TYR:O	1:B:323:ALA:HA	2.05	0.57
1:C:40:MET:CB	1:C:41:PRO:CD	2.83	0.57
1:C:314:THR:HG23	3:C:550:HOH:O	2.05	0.57
1:D:291:TYR:CE1	1:D:302:LEU:HD23	2.40	0.57
1:C:226:LEU:CD1	3:C:587:HOH:O	2.53	0.56
1:A:98:GLY:C	3:A:503:HOH:O	2.43	0.56
1:D:294:VAL:HG23	3:D:569:HOH:O	2.03	0.56
1:A:162:HIS:HA	3:A:630:HOH:O	2.05	0.56
1:B:94:THR:HB	3:B:536:HOH:O	2.05	0.56
1:B:250:LEU:HD12	3:B:554:HOH:O	2.05	0.56
1:B:217:TYR:HB3	1:B:218:PRO:HD3	1.88	0.56
1:C:39:GLY:C	1:C:40:MET:SD	2.84	0.56
1:B:353:ILE:HG21	3:C:508:HOH:O	2.05	0.56
1:B:94:THR:HG21	1:C:101:VAL:HG22	1.87	0.55
1:A:19:TYR:O	1:A:323:ALA:HA	2.07	0.55
1:D:131:LYS:HD2	3:D:622:HOH:O	2.06	0.55
1:A:75:GLN:NE2	3:A:516:HOH:O	2.37	0.55
1:C:226:LEU:HB2	1:C:313:ILE:HD11	1.87	0.54
1:B:135:GLU:OE1	3:B:508:HOH:O	2.18	0.54
1:C:260:ALA:CB	3:C:532:HOH:O	2.49	0.54
3:B:519:HOH:O	1:C:215:ILE:CG2	2.55	0.54
1:C:82:ASN:O	1:C:85:THR:HG23	2.07	0.54
1:C:166:TYR:OH	1:C:191:ASP:OD2	2.14	0.54
1:D:160:ASN:HA	3:D:577:HOH:O	2.07	0.54
1:D:91:HIS:CD2	1:D:93:HIS:HD1	2.26	0.54
1:C:324:VAL:HG21	3:D:523:HOH:O	2.08	0.54
1:A:16:ARG:NH2	3:A:523:HOH:O	2.39	0.54
1:A:110:ALA:HB1	1:A:331:ASP:OD2	2.07	0.53
1:A:259:SER:HA	3:A:532:HOH:O	2.07	0.53
1:C:274:HIS:CD2	3:C:587:HOH:O	2.61	0.53
1:C:288:TYR:N	3:C:514:HOH:O	2.31	0.53
1:C:282:ASN:OD1	1:C:287:ARG:NE	2.39	0.53
1:B:220:TYR:O	3:B:509:HOH:O	2.19	0.53
1:D:132:TYR:O	1:D:135:GLU:HB3	2.08	0.53
1:D:108:TRP:CD2	3:D:535:HOH:O	2.53	0.53
1:D:40:MET:CB	1:D:41:PRO:HD2	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:279:ALA:HB3	3:C:529:HOH:O	2.09	0.53
1:A:360:VAL:O	1:A:364:ASN:ND2	2.41	0.53
1:D:34:ILE:HG23	3:D:526:HOH:O	2.09	0.53
1:B:189:ALA:HB1	1:C:147:THR:HB	1.91	0.52
1:C:213:PRO:HG3	3:C:627:HOH:O	2.08	0.52
1:A:13:ALA:O	1:A:16:ARG:NH1	2.43	0.52
1:C:217:TYR:HB3	1:C:218:PRO:HD3	1.92	0.52
1:B:88:PHE:HE2	3:B:614:HOH:O	1.92	0.52
1:C:213:PRO:HA	3:C:602:HOH:O	2.10	0.52
1:C:270:VAL:HA	3:C:518:HOH:O	2.09	0.52
1:A:161:VAL:HG23	3:A:547:HOH:O	2.09	0.52
1:B:40:MET:HB2	1:B:41:PRO:HD3	1.86	0.52
1:B:136:HIS:CE1	3:B:531:HOH:O	2.63	0.52
1:D:233:MET:HG3	3:D:599:HOH:O	2.09	0.51
1:B:174:TYR:HB3	1:B:181:PHE:HB2	1.93	0.51
1:D:107:GLY:HA2	1:D:110:ALA:HB3	1.92	0.51
1:B:19:TYR:HB3	1:B:310:VAL:HG11	1.91	0.51
1:B:98:GLY:HA3	3:B:536:HOH:O	2.11	0.51
1:C:184:TRP:HZ2	3:C:608:HOH:O	1.93	0.51
1:D:304:MET:CE	3:D:615:HOH:O	2.58	0.51
1:B:40:MET:CB	1:B:41:PRO:HD2	2.35	0.51
1:C:64:VAL:HG21	1:C:207:PHE:CE2	2.45	0.51
1:C:279:ALA:CB	3:C:529:HOH:O	2.57	0.51
1:B:63:ILE:HD11	1:B:84:LEU:HB3	1.92	0.51
1:C:164:PHE:HA	3:C:575:HOH:O	2.09	0.51
1:C:351:GLN:O	1:C:355:ASP:OD2	2.28	0.51
1:D:156:PRO:C	3:D:535:HOH:O	2.48	0.51
1:C:20:TYR:CD1	1:D:20:TYR:CD1	2.99	0.51
1:A:20:TYR:CD1	1:B:20:TYR:CD1	2.99	0.51
1:D:67:GLY:O	1:D:70:SER:OG	2.17	0.51
1:B:21:PRO:HG2	1:B:325:SER:HB3	1.92	0.51
1:B:254:LEU:CD2	3:B:554:HOH:O	2.59	0.51
1:C:359:ASN:OD1	1:C:361:ASP:OD2	2.28	0.51
1:B:332:VAL:HB	3:B:628:HOH:O	2.11	0.50
1:A:142:ASN:CB	3:D:513:HOH:O	2.60	0.50
1:D:214:ASN:CB	3:D:588:HOH:O	2.41	0.50
1:A:34:ILE:HD13	1:A:77:LEU:HD22	1.94	0.50
1:D:127:ASP:HB2	3:D:513:HOH:O	2.12	0.50
1:B:31:ILE:HG22	1:B:313:ILE:HD12	1.94	0.50
1:D:280:PHE:O	3:D:502:HOH:O	2.19	0.50
1:A:174:TYR:HB3	1:A:181:PHE:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:GLU:OE1	1:D:162:HIS:NE2	2.45	0.49
1:C:39:GLY:O	1:C:40:MET:SD	2.70	0.49
1:D:141:TYR:O	1:D:144:ASP:HB3	2.11	0.49
1:B:128:MET:HE3	3:C:599:HOH:O	2.02	0.49
1:B:266:ILE:O	1:B:270:VAL:HG23	2.12	0.49
1:A:142:ASN:HB3	3:D:513:HOH:O	2.12	0.49
1:B:31:ILE:CG2	1:B:313:ILE:HD12	2.42	0.49
1:B:101:VAL:HG11	3:B:551:HOH:O	2.11	0.49
1:C:154:PRO:CB	3:C:613:HOH:O	2.50	0.49
1:A:104:TRP:CD1	1:A:159:ILE:HD11	2.48	0.49
1:D:131:LYS:HE3	1:D:161:VAL:HB	1.93	0.49
1:C:116:LEU:HD21	3:C:558:HOH:O	2.12	0.48
1:C:244:GLN:HA	1:C:244:GLN:HE21	1.78	0.48
1:A:208:GLY:N	1:A:228:ILE:O	2.46	0.48
1:D:156:PRO:HB2	3:D:535:HOH:O	2.12	0.48
1:D:187:ILE:CD1	3:D:588:HOH:O	2.57	0.48
1:A:41:PRO:HA	1:A:95:ASP:OD2	2.13	0.48
1:B:110:ALA:HA	3:B:539:HOH:O	2.13	0.48
1:D:290:ILE:HB	3:D:615:HOH:O	2.14	0.48
1:B:66:ILE:HG23	1:B:66:ILE:O	2.14	0.48
1:B:194:VAL:N	3:B:513:HOH:O	2.47	0.48
1:C:240:THR:HA	3:C:554:HOH:O	2.13	0.48
1:A:45:ARG:NH2	1:D:325:SER:OG	2.42	0.48
1:B:143:TRP:HB2	3:B:546:HOH:O	2.13	0.48
1:B:356:GLY:HA3	1:C:216:TRP:CH2	2.49	0.48
1:C:16:ARG:HA	3:C:626:HOH:O	2.13	0.48
1:C:285:ASP:OD1	1:C:286:THR:HG23	2.13	0.47
1:D:246:ALA:HB3	3:D:603:HOH:O	2.14	0.47
1:D:34:ILE:HG12	3:D:629:HOH:O	2.14	0.47
1:C:52:TRP:CZ2	1:C:228:ILE:HG21	2.49	0.47
1:C:155:ARG:HB3	1:C:156:PRO:HD3	1.95	0.47
1:D:150:VAL:HG12	1:D:151:THR:HG23	1.95	0.47
1:A:40:MET:CG	1:A:41:PRO:HD3	2.45	0.47
1:A:367:TRP:CH2	3:D:524:HOH:O	2.56	0.47
1:B:323:ALA:HB2	3:B:593:HOH:O	2.14	0.47
1:C:18:VAL:HG22	1:D:78:MET:HE1	1.95	0.47
1:B:62:PHE:CE2	3:B:540:HOH:O	2.67	0.47
1:B:362:GLU:H	1:B:362:GLU:CD	2.17	0.47
1:C:156:PRO:HB2	3:C:525:HOH:O	2.14	0.47
1:D:24:GLU:OE2	3:D:503:HOH:O	2.21	0.47
1:A:73:ASN:HB3	1:A:308:MET:SD	2.54	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:181:PHE:CZ	1:B:198:LEU:HD12	2.49	0.47
1:A:44:ARG:HD2	1:A:281:PHE:CE1	2.50	0.47
1:D:233:MET:CG	3:D:599:HOH:O	2.48	0.47
1:B:313:ILE:HD13	3:B:537:HOH:O	2.14	0.47
1:C:310:VAL:CG1	1:C:321:ARG:HB2	2.44	0.47
1:D:174:TYR:HB3	1:D:181:PHE:HB2	1.95	0.47
1:A:217:TYR:HB3	1:A:218:PRO:HD3	1.95	0.46
1:D:250:LEU:HG	3:D:524:HOH:O	2.14	0.46
1:C:359:ASN:ND2	1:C:362:GLU:OE1	2.48	0.46
1:D:217:TYR:HB3	1:D:218:PRO:HD3	1.97	0.46
1:D:323:ALA:HB2	3:D:526:HOH:O	2.14	0.46
1:A:43:ALA:HB3	3:D:514:HOH:O	2.15	0.46
1:C:295:ARG:NH2	1:C:300:GLY:O	2.49	0.46
1:C:193:PRO:CG	3:C:600:HOH:O	2.63	0.46
1:B:132:TYR:HB2	3:B:559:HOH:O	2.15	0.46
1:B:137:MET:O	1:B:140:ALA:HB3	2.16	0.46
1:C:96:HIS:NE2	3:C:501:HOH:O	2.36	0.46
1:C:262:SER:CB	3:C:627:HOH:O	2.61	0.46
1:D:155:ARG:HB3	1:D:156:PRO:HD3	1.98	0.46
1:A:231:CYS:CB	1:A:277:ALA:HB1	2.46	0.46
1:C:20:TYR:HB3	1:D:20:TYR:CD2	2.51	0.46
1:C:225:ASP:O	1:C:273:ARG:HB2	2.16	0.46
1:A:141:TYR:HA	3:D:560:HOH:O	2.16	0.45
3:A:582:HOH:O	1:D:141:TYR:HA	2.16	0.45
1:B:39:GLY:O	1:B:40:MET:O	2.34	0.45
1:C:310:VAL:HG13	1:C:321:ARG:HB2	1.98	0.45
1:B:134:VAL:HG11	1:B:161:VAL:HG22	1.97	0.45
1:D:27:GLY:O	1:D:57:GLY:HA2	2.16	0.45
1:B:121:PRO:HB3	3:B:513:HOH:O	2.16	0.45
1:C:19:TYR:O	1:C:323:ALA:HA	2.17	0.45
1:A:345:ARG:NH1	3:A:537:HOH:O	2.48	0.45
1:B:288:TYR:HB3	1:D:291:TYR:CZ	2.51	0.45
1:A:295:ARG:NH2	1:A:300:GLY:O	2.39	0.45
1:B:360:VAL:O	1:B:364:ASN:ND2	2.49	0.45
1:C:91:HIS:HB3	1:C:193:PRO:HA	1.98	0.45
1:C:225:ASP:HA	1:C:273:ARG:HB2	1.99	0.45
1:D:253:ASN:O	1:D:259:SER:HB3	2.16	0.45
1:B:89:LEU:HD22	1:B:97:TRP:HB3	1.98	0.45
1:C:186:CYS:HB2	1:C:193:PRO:HB2	1.97	0.45
1:D:40:MET:CB	1:D:41:PRO:CD	2.82	0.45
1:C:274:HIS:CG	3:C:587:HOH:O	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:91:HIS:CD2	1:D:93:HIS:ND1	2.85	0.45
1:A:44:ARG:HB3	1:D:329:ALA:HB3	1.99	0.45
1:B:142:ASN:ND2	1:C:127:ASP:O	2.50	0.44
1:D:48:ALA:N	1:D:307:ASP:OD2	2.43	0.44
1:C:156:PRO:CB	3:C:525:HOH:O	2.66	0.44
1:A:145:TYR:O	3:A:504:HOH:O	2.21	0.44
1:B:231:CYS:SG	1:B:260:ALA:HA	2.57	0.44
1:A:16:ARG:CZ	3:A:523:HOH:O	2.65	0.44
1:A:231:CYS:HB3	1:A:277:ALA:HB1	2.00	0.44
1:C:102:SER:O	1:C:106:GLY:N	2.39	0.44
1:C:366:HIS:CD2	3:C:619:HOH:O	2.71	0.44
1:D:187:ILE:CG1	3:D:588:HOH:O	2.65	0.44
1:A:235:SER:O	1:A:238:MET:HB2	2.17	0.44
1:C:181:PHE:CZ	1:C:198:LEU:HD12	2.53	0.44
1:D:217:TYR:CE1	1:D:221:ALA:CB	2.99	0.44
1:B:19:TYR:HB2	1:B:310:VAL:HG11	1.99	0.44
1:C:144:ASP:OD1	1:C:148:ARG:NH1	2.50	0.44
1:D:120:GLY:HA3	1:D:130:THR:HG21	1.99	0.44
1:B:61:LYS:HE3	3:B:604:HOH:O	2.17	0.44
1:B:78:MET:HA	3:B:628:HOH:O	2.17	0.44
1:B:198:LEU:HD23	1:B:198:LEU:C	2.38	0.44
1:C:120:GLY:O	3:C:509:HOH:O	2.20	0.44
1:B:214:ASN:ND2	3:B:535:HOH:O	2.50	0.43
1:D:105:ALA:O	1:D:109:THR:HG23	2.18	0.43
1:A:278:TYR:O	1:A:279:ALA:HB3	2.18	0.43
1:B:42:THR:CG2	3:C:519:HOH:O	2.65	0.43
1:D:206:VAL:HG11	1:D:217:TYR:CZ	2.53	0.43
1:B:21:PRO:HB3	1:B:77:LEU:HA	2.01	0.43
1:C:66:ILE:HG23	1:C:66:ILE:O	2.19	0.43
1:C:137:MET:O	1:C:140:ALA:HB3	2.18	0.43
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.91	0.43
1:B:237:GLN:HB3	3:B:608:HOH:O	2.17	0.43
1:C:253:ASN:HA	3:C:573:HOH:O	2.19	0.43
1:D:83:TYR:C	3:D:512:HOH:O	2.56	0.43
1:C:186:CYS:SG	1:C:211:THR:HB	2.59	0.43
3:A:508:HOH:O	1:D:42:THR:HG22	2.17	0.43
1:B:226:LEU:N	3:B:537:HOH:O	2.52	0.43
1:D:304:MET:HE3	3:D:615:HOH:O	2.18	0.43
1:B:94:THR:HG22	1:C:141:TYR:CE1	2.52	0.43
1:D:34:ILE:HD13	1:D:77:LEU:HD13	2.00	0.43
1:A:40:MET:CG	1:A:41:PRO:CD	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:ILE:CG1	1:A:66:ILE:O	2.65	0.42
1:B:313:ILE:HG23	1:B:318:VAL:HG22	2.00	0.42
1:C:226:LEU:CB	1:C:313:ILE:HD11	2.49	0.42
1:D:33:VAL:O	1:D:310:VAL:HA	2.19	0.42
1:D:97:TRP:O	1:D:100:LEU:N	2.52	0.42
1:A:108:TRP:CE3	1:A:148:ARG:HD2	2.54	0.42
1:B:273:ARG:HB3	3:B:578:HOH:O	2.19	0.42
1:D:106:GLY:O	1:D:109:THR:N	2.52	0.42
1:D:290:ILE:O	1:D:294:VAL:HG23	2.19	0.42
1:A:20:TYR:CE2	3:A:596:HOH:O	2.71	0.42
1:A:348:GLU:N	3:A:526:HOH:O	2.42	0.42
1:A:356:GLY:HA3	1:D:216:TRP:CH2	2.54	0.42
1:B:181:PHE:CE1	1:B:198:LEU:HG	2.54	0.42
1:C:40:MET:HB2	1:C:41:PRO:CD	2.50	0.42
1:D:352:TYR:O	1:D:352:TYR:CD1	2.72	0.42
1:A:69:GLY:N	1:A:99:ASP:OD2	2.53	0.42
1:A:33:VAL:O	1:A:310:VAL:HA	2.19	0.42
1:A:313:ILE:C	3:A:552:HOH:O	2.58	0.42
1:B:291:TYR:HD2	3:B:514:HOH:O	2.01	0.42
1:D:66:ILE:HG23	1:D:66:ILE:O	2.19	0.42
1:A:118:VAL:CG1	3:A:554:HOH:O	2.67	0.42
1:A:185:PRO:HB2	1:A:216:TRP:CZ3	2.55	0.42
1:A:204:LYS:NZ	3:A:527:HOH:O	2.43	0.42
1:B:34:ILE:HD13	1:B:77:LEU:HD22	2.02	0.42
1:B:128:MET:HB3	3:C:599:HOH:O	2.19	0.42
1:C:54:VAL:HG21	1:C:207:PHE:HZ	1.84	0.42
1:B:330:TRP:CZ3	1:C:241:LYS:HG3	2.54	0.42
1:D:101:VAL:HG21	1:D:141:TYR:CE2	2.55	0.42
1:D:254:LEU:HD23	3:D:524:HOH:O	2.18	0.42
1:A:234:THR:O	1:A:237:GLN:N	2.51	0.42
1:A:367:TRP:O	1:A:367:TRP:CE3	2.72	0.42
1:C:18:VAL:HG21	3:D:523:HOH:O	2.19	0.41
1:D:149:ALA:O	1:D:150:VAL:C	2.58	0.41
1:A:31:ILE:CG2	1:A:313:ILE:HD12	2.50	0.41
1:A:66:ILE:O	1:A:66:ILE:HG12	2.19	0.41
1:B:90:THR:O	1:B:91:HIS:HB3	2.20	0.41
1:C:354:LEU:CD2	3:C:596:HOH:O	2.67	0.41
1:A:37:GLY:O	1:A:50:ALA:HA	2.20	0.41
1:A:104:TRP:HA	1:A:116:LEU:HD11	2.02	0.41
1:A:109:THR:O	1:A:111:GLY:N	2.53	0.41
1:B:261:GLN:O	1:B:297:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:LYS:HE3	3:B:632:HOH:O	2.20	0.41
1:D:108:TRP:CG	3:D:535:HOH:O	2.73	0.41
1:C:221:ALA:HB3	1:C:270:VAL:HG22	2.02	0.41
1:C:286:THR:C	3:C:514:HOH:O	2.59	0.41
1:A:175:GLN:NE2	3:A:549:HOH:O	2.54	0.41
1:A:20:TYR:HB3	1:B:20:TYR:CG	2.56	0.41
1:A:288:TYR:O	1:A:291:TYR:HB3	2.21	0.41
1:C:295:ARG:O	1:C:296:GLU:C	2.59	0.41
1:D:247:GLN:HA	3:D:585:HOH:O	2.20	0.41
1:A:20:TYR:HE2	1:B:21:PRO:O	2.04	0.41
1:A:105:ALA:HB1	1:A:148:ARG:HH12	1.84	0.41
1:B:139:LYS:HD3	1:C:132:TYR:OH	2.20	0.41
3:B:506:HOH:O	1:C:350:THR:CG2	2.58	0.41
1:A:91:HIS:HE1	1:A:96:HIS:CE1	2.39	0.41
1:C:8:SER:OG	1:C:11:GLY:HA3	2.21	0.41
1:C:58:ASN:OD1	1:C:59:GLY:N	2.54	0.41
1:D:178:GLY:O	1:D:200:TRP:HD1	2.04	0.41
1:A:175:GLN:NE2	1:A:180:THR:HG23	2.36	0.40
1:B:226:LEU:CB	3:B:537:HOH:O	2.69	0.40
1:B:271:GLN:CB	3:B:589:HOH:O	2.69	0.40
1:C:326:PRO:HG3	1:D:18:VAL:HG21	2.03	0.40
1:B:133:ALA:HB3	3:B:533:HOH:O	2.21	0.40
1:A:312:ASN:ND2	3:A:541:HOH:O	2.49	0.40
1:D:362:GLU:OE1	1:D:363:ALA:N	2.36	0.40
1:A:155:ARG:HB3	1:A:156:PRO:HD3	2.04	0.40
1:C:88:PHE:HZ	3:C:610:HOH:O	1.87	0.40
1:C:359:ASN:OD1	1:C:361:ASP:CG	2.59	0.40
1:D:93:HIS:CE1	1:D:188:HIS:NE2	2.90	0.40
1:D:187:ILE:HG13	3:D:588:HOH:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	358/372 (96%)	319 (89%)	30 (8%)	9 (2%)	5	1
1	B	356/372 (96%)	315 (88%)	37 (10%)	4 (1%)	14	5
1	C	356/372 (96%)	310 (87%)	40 (11%)	6 (2%)	9	2
1	D	358/372 (96%)	316 (88%)	30 (8%)	12 (3%)	3	0
All	All	1428/1488 (96%)	1260 (88%)	137 (10%)	31 (2%)	6	1

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	40	MET
1	B	40	MET
1	C	40	MET
1	D	65	ASP
1	D	150	VAL
1	A	110	ALA
1	A	222	LYS
1	A	279	ALA
1	C	35	ALA
1	C	222	LYS
1	D	98	GLY
1	D	188	HIS
1	D	362	GLU
1	A	50	ALA
1	A	211	THR
1	B	91	HIS
1	C	44	ARG
1	D	66	ILE
1	D	200	TRP
1	C	282	ASN
1	D	240	THR
1	B	279	ALA
1	D	40	MET
1	D	363	ALA
1	C	233	MET
1	D	308	MET
1	A	41	PRO
1	B	111	GLY
1	A	66	ILE
1	A	106	GLY
1	D	106	GLY

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	292/301 (97%)	280 (96%)	12 (4%)	30	18
1	B	288/301 (96%)	274 (95%)	14 (5%)	25	12
1	C	288/301 (96%)	281 (98%)	7 (2%)	49	40
1	D	292/301 (97%)	278 (95%)	14 (5%)	25	12
All	All	1160/1204 (96%)	1113 (96%)	47 (4%)	30	18

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	MET
1	A	42	THR
1	A	158	ASP
1	A	169	LEU
1	A	191	ASP
1	A	199	GLU
1	A	247	GLN
1	A	331	ASP
1	A	361	ASP
1	A	362	GLU
1	A	368	LYS
1	A	372	MET
1	B	15	LYS
1	B	40	MET
1	B	44	ARG
1	B	114	ASP
1	B	131	LYS
1	B	175	GLN
1	B	222	LYS
1	B	254	LEU
1	B	255	ASP
1	B	278	TYR
1	B	281	PHE
1	B	331	ASP

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Mol	Chain	Res	Type
1	B	347	SER
1	B	362	GLU
1	C	25	GLU
1	C	40	MET
1	C	117	GLU
1	C	195	SER
1	C	233	MET
1	C	253	ASN
1	C	319	THR
1	D	76	SER
1	D	109	THR
1	D	126	GLU
1	D	131	LYS
1	D	191	ASP
1	D	199	GLU
1	D	236	ASP
1	D	251	ARG
1	D	254	LEU
1	D	310	VAL
1	D	331	ASP
1	D	347	SER
1	D	362	GLU
1	D	368	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	175	GLN
1	B	142	ASN
1	B	162	HIS
1	B	175	GLN
1	B	243	ASN
1	C	75	GLN
1	C	175	GLN
1	C	177	ASN
1	C	244	GLN
1	C	351	GLN
1	C	366	HIS
1	D	175	GLN
1	D	244	GLN
1	D	297	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	362/372 (97%)	2.62	197 (54%) 0 0	6, 17, 41, 51	0
1	B	360/372 (96%)	2.84	227 (63%) 0 0	5, 20, 46, 58	0
1	C	360/372 (96%)	3.21	258 (71%) 0 0	13, 25, 41, 58	0
1	D	362/372 (97%)	2.97	244 (67%) 0 0	2, 21, 38, 60	0
All	All	1444/1488 (97%)	2.91	926 (64%) 0 0	2, 21, 41, 60	0

All (926) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	8	SER	20.1
1	C	254	LEU	16.6
1	C	368	LYS	15.9
1	A	360	VAL	15.0
1	D	254	LEU	14.3
1	C	8	SER	13.4
1	D	248	LEU	13.3
1	B	250	LEU	12.7
1	D	243	ASN	11.6
1	A	249	ALA	11.0
1	C	108	TRP	10.5
1	A	251	ARG	10.3
1	D	369	GLN	10.0
1	A	358	LEU	9.9
1	B	251	ARG	9.9
1	D	250	LEU	9.7
1	B	243	ASN	9.5
1	B	8	SER	9.5
1	B	371	PHE	9.3
1	B	9	SER	9.3
1	D	244	GLN	8.9

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Mol	Chain	Res	Type	RSRZ
1	B	248	LEU	8.9
1	A	252	ILE	8.8
1	B	369	GLN	8.8
1	C	5	LYS	8.8
1	D	314	THR	8.8
1	C	216	TRP	8.5
1	D	251	ARG	8.3
1	B	221	ALA	8.2
1	B	372	MET	8.2
1	B	353	ILE	8.2
1	C	240	THR	8.1
1	C	246	ALA	8.1
1	A	238	MET	8.0
1	A	241	LYS	8.0
1	D	365	ALA	8.0
1	C	110	ALA	7.9
1	B	152	ILE	7.9
1	B	365	ALA	7.7
1	D	12	ILE	7.6
1	D	9	SER	7.6
1	D	246	ALA	7.5
1	C	151	THR	7.5
1	D	13	ALA	7.5
1	A	365	ALA	7.4
1	C	7	THR	7.4
1	C	367	TRP	7.4
1	B	2	ALA	7.4
1	B	361	ASP	7.4
1	C	159	ILE	7.3
1	C	248	LEU	7.3
1	C	360	VAL	7.3
1	D	187	ILE	7.2
1	D	239	MET	7.2
1	B	367	TRP	7.1
1	D	329	ALA	7.1
1	D	10	THR	7.1
1	A	371	PHE	7.1
1	D	150	VAL	7.0
1	D	252	ILE	7.0
1	D	151	THR	7.0
1	B	6	VAL	7.0
1	C	366	HIS	7.0

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Mol	Chain	Res	Type	RSRZ
1	D	366	HIS	7.0
1	B	360	VAL	7.0
1	C	369	GLN	6.9
1	D	294	VAL	6.9
1	C	365	ALA	6.9
1	A	367	TRP	6.8
1	D	368	LYS	6.7
1	C	263	PHE	6.7
1	D	108	TRP	6.7
1	C	113	THR	6.6
1	C	150	VAL	6.6
1	A	368	LYS	6.6
1	A	12	ILE	6.6
1	C	114	ASP	6.6
1	A	361	ASP	6.5
1	C	116	LEU	6.5
1	C	203	TYR	6.5
1	C	13	ALA	6.5
1	C	200	TRP	6.5
1	B	330	TRP	6.4
1	C	83	TYR	6.4
1	C	290	ILE	6.4
1	A	250	LEU	6.4
1	D	372	MET	6.4
1	C	371	PHE	6.4
1	B	232	TRP	6.4
1	D	121	PRO	6.4
1	A	209	GLY	6.3
1	D	249	ALA	6.3
1	A	291	TYR	6.2
1	B	249	ALA	6.2
1	A	373	GLY	6.2
1	D	7	THR	6.2
1	B	254	LEU	6.2
1	A	372	MET	6.2
1	C	298	TYR	6.1
1	D	367	TRP	6.1
1	C	266	ILE	6.1
1	C	284	ASP	6.0
1	A	248	LEU	6.0
1	B	187	ILE	6.0
1	C	224	ALA	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	154	PRO	6.0
1	B	14	PRO	5.9
1	C	243	ASN	5.9
1	B	28	PRO	5.9
1	B	62	PHE	5.9
1	B	263	PHE	5.9
1	C	12	ILE	5.9
1	C	9	SER	5.9
1	D	313	ILE	5.9
1	C	292	THR	5.8
1	A	239	MET	5.8
1	A	363	ALA	5.8
1	C	353	ILE	5.8
1	C	14	PRO	5.8
1	B	116	LEU	5.8
1	A	232	TRP	5.7
1	D	247	GLN	5.7
1	D	213	PRO	5.7
1	D	215	ILE	5.7
1	D	242	TYR	5.7
1	B	215	ILE	5.7
1	C	237	GLN	5.7
1	A	256	PHE	5.6
1	B	244	GLN	5.6
1	B	209	GLY	5.6
1	C	250	LEU	5.6
1	D	25	GLU	5.6
1	D	335	PRO	5.6
1	B	240	THR	5.6
1	D	253	ASN	5.6
1	D	152	ILE	5.5
1	D	240	THR	5.5
1	C	233	MET	5.5
1	A	11	GLY	5.5
1	B	111	GLY	5.5
1	C	329	ALA	5.5
1	A	7	THR	5.5
1	A	235	SER	5.4
1	B	245	PRO	5.4
1	B	189	ALA	5.4
1	B	373	GLY	5.4
1	A	4	GLY	5.4

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Mol	Chain	Res	Type	RSRZ
1	C	40	MET	5.3
1	A	359	ASN	5.3
1	C	225	ASP	5.3
1	A	26	LEU	5.3
1	C	187	ILE	5.3
1	C	249	ALA	5.3
1	B	233	MET	5.3
1	A	245	PRO	5.2
1	D	221	ALA	5.2
1	B	288	TYR	5.2
1	D	110	ALA	5.2
1	A	158	ASP	5.2
1	D	371	PHE	5.2
1	C	242	TYR	5.2
1	A	150	VAL	5.2
1	B	290	ILE	5.1
1	A	279	ALA	5.1
1	A	221	ALA	5.1
1	B	13	ALA	5.1
1	C	236	ASP	5.1
1	D	256	PHE	5.1
1	D	245	PRO	5.1
1	C	115	PRO	5.0
1	C	104	TRP	5.0
1	D	101	VAL	5.0
1	C	255	ASP	5.0
1	A	253	ASN	5.0
1	A	10	THR	5.0
1	A	294	VAL	5.0
1	B	154	PRO	4.9
1	C	154	PRO	4.9
1	C	66	ILE	4.9
1	D	116	LEU	4.9
1	D	178	GLY	4.9
1	D	232	TRP	4.9
1	A	28	PRO	4.9
1	C	155	ARG	4.8
1	A	52	TRP	4.8
1	B	318	VAL	4.8
1	D	8	SER	4.8
1	A	288	TYR	4.8
1	D	266	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
1	C	274	HIS	4.8
1	C	280	PHE	4.8
1	B	313	ILE	4.8
1	B	29	ASP	4.8
1	C	109	THR	4.7
1	C	147	THR	4.7
1	C	160	ASN	4.7
1	C	220	TYR	4.7
1	C	31	ILE	4.7
1	B	242	TYR	4.7
1	D	149	ALA	4.7
1	B	241	LYS	4.7
1	D	263	PHE	4.7
1	B	280	PHE	4.7
1	C	59	GLY	4.7
1	B	235	SER	4.7
1	B	7	THR	4.6
1	D	100	LEU	4.6
1	B	278	TYR	4.6
1	C	222	LYS	4.6
1	D	212	ALA	4.6
1	C	373	GLY	4.6
1	B	197	ALA	4.6
1	B	246	ALA	4.6
1	A	354	LEU	4.6
1	D	6	VAL	4.6
1	A	41	PRO	4.5
1	C	238	MET	4.5
1	D	297	ASN	4.5
1	D	189	ALA	4.5
1	B	164	PHE	4.5
1	D	167	ARG	4.5
1	B	5	LYS	4.5
1	C	372	MET	4.5
1	B	108	TRP	4.5
1	C	52	TRP	4.5
1	C	247	GLN	4.5
1	A	242	TYR	4.5
1	D	147	THR	4.5
1	D	216	TRP	4.4
1	A	366	HIS	4.4
1	B	328	HIS	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	254	LEU	4.4
1	C	235	SER	4.4
1	C	330	TRP	4.4
1	A	25	GLU	4.4
1	A	211	THR	4.4
1	B	356	GLY	4.4
1	A	2	ALA	4.4
1	A	215	ILE	4.4
1	A	3	GLY	4.4
1	A	126	GLU	4.4
1	B	100	LEU	4.4
1	C	149	ALA	4.4
1	A	234	THR	4.3
1	A	244	GLN	4.3
1	B	216	TRP	4.3
1	D	207	PHE	4.3
1	A	6	VAL	4.3
1	B	110	ALA	4.3
1	C	215	ILE	4.3
1	A	356	GLY	4.2
1	D	43	ALA	4.2
1	A	69	GLY	4.2
1	A	243	ASN	4.2
1	C	183	SER	4.2
1	C	92	LEU	4.2
1	C	241	LYS	4.2
1	D	104	TRP	4.2
1	B	366	HIS	4.2
1	D	281	PHE	4.2
1	C	318	VAL	4.2
1	B	121	PRO	4.2
1	B	156	PRO	4.2
1	C	239	MET	4.2
1	D	233	MET	4.2
1	B	252	ILE	4.2
1	D	87	ILE	4.2
1	C	43	ALA	4.2
1	C	167	ARG	4.2
1	B	97	TRP	4.2
1	C	232	TRP	4.2
1	A	186	CYS	4.2
1	B	298	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
1	D	11	GLY	4.1
1	C	294	VAL	4.1
1	D	346	ALA	4.1
1	A	14	PRO	4.1
1	A	332	VAL	4.1
1	C	194	VAL	4.1
1	B	149	ALA	4.1
1	B	255	ASP	4.1
1	D	330	TRP	4.1
1	A	79	ILE	4.1
1	A	161	VAL	4.1
1	A	278	TYR	4.1
1	B	12	ILE	4.0
1	C	319	THR	4.0
1	D	290	ILE	4.0
1	D	332	VAL	4.0
1	C	256	PHE	4.0
1	D	234	THR	4.0
1	A	217	TYR	4.0
1	B	351	GLN	4.0
1	C	78	MET	4.0
1	D	373	GLY	4.0
1	C	152	ILE	4.0
1	C	221	ALA	4.0
1	C	185	PRO	4.0
1	B	169	LEU	4.0
1	C	282	ASN	4.0
1	C	198	LEU	4.0
1	A	240	THR	3.9
1	D	164	PHE	3.9
1	B	11	GLY	3.9
1	B	109	THR	3.9
1	B	234	THR	3.9
1	C	10	THR	3.9
1	C	46	ALA	3.9
1	C	81	ALA	3.9
1	C	262	SER	3.9
1	D	188	HIS	3.8
1	B	354	LEU	3.8
1	A	154	PRO	3.8
1	B	256	PHE	3.8
1	B	185	PRO	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	282	ASN	3.8
1	B	186	CYS	3.8
1	A	298	TYR	3.8
1	D	291	TYR	3.8
1	B	239	MET	3.8
1	A	350	THR	3.8
1	D	310	VAL	3.8
1	A	290	ILE	3.8
1	C	260	ALA	3.8
1	B	357	ARG	3.8
1	C	122	SER	3.8
1	B	266	ILE	3.8
1	C	38	THR	3.8
1	B	39	GLY	3.8
1	C	145	TYR	3.8
1	D	217	TYR	3.8
1	A	370	GLU	3.8
1	C	184	TRP	3.7
1	C	352	TYR	3.7
1	D	141	TYR	3.7
1	B	88	PHE	3.7
1	C	26	LEU	3.7
1	B	314	THR	3.7
1	C	6	VAL	3.7
1	D	319	THR	3.7
1	C	65	ASP	3.7
1	C	291	TYR	3.7
1	D	278	TYR	3.7
1	A	330	TRP	3.7
1	C	358	LEU	3.7
1	D	169	LEU	3.7
1	D	272	PRO	3.7
1	C	364	ASN	3.7
1	D	132	TYR	3.7
1	C	253	ASN	3.7
1	A	34	ILE	3.7
1	C	349	TYR	3.7
1	B	211	THR	3.7
1	C	350	THR	3.7
1	D	370	GLU	3.7
1	A	220	TYR	3.6
1	D	153	ASN	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	13	ALA	3.6
1	D	260	ALA	3.6
1	A	226	LEU	3.6
1	B	358	LEU	3.6
1	C	311	TRP	3.6
1	C	252	ILE	3.6
1	D	211	THR	3.6
1	A	173	VAL	3.6
1	D	206	VAL	3.6
1	C	297	ASN	3.6
1	A	219	GLU	3.6
1	A	352	TYR	3.6
1	D	203	TYR	3.6
1	D	92	LEU	3.6
1	A	270	VAL	3.6
1	C	97	TRP	3.6
1	C	106	GLY	3.6
1	B	34	ILE	3.6
1	C	188	HIS	3.6
1	D	126	GLU	3.6
1	D	358	LEU	3.6
1	D	173	VAL	3.6
1	A	222	LYS	3.6
1	C	133	ALA	3.6
1	D	120	GLY	3.6
1	B	200	TRP	3.5
1	A	91	HIS	3.5
1	D	306	THR	3.5
1	B	54	VAL	3.5
1	D	262	SER	3.5
1	A	110	ALA	3.5
1	B	218	PRO	3.5
1	D	94	THR	3.5
1	A	141	TYR	3.5
1	C	174	TYR	3.5
1	C	278	TYR	3.5
1	C	357	ARG	3.5
1	D	41	PRO	3.5
1	B	124	SER	3.5
1	C	74	ILE	3.5
1	A	179	VAL	3.5
1	B	279	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	363	ALA	3.5
1	C	121	PRO	3.5
1	A	151	THR	3.5
1	C	370	GLU	3.5
1	B	43	ALA	3.5
1	A	272	PRO	3.5
1	D	288	TYR	3.4
1	A	9	SER	3.4
1	B	324	VAL	3.4
1	A	319	THR	3.4
1	D	315	ARG	3.4
1	A	159	ILE	3.4
1	D	139	LYS	3.4
1	D	318	VAL	3.4
1	B	52	TRP	3.4
1	A	304	MET	3.4
1	C	62	PHE	3.4
1	B	258	THR	3.4
1	B	350	THR	3.4
1	C	172	VAL	3.4
1	D	292	THR	3.4
1	B	143	TRP	3.4
1	A	280	PHE	3.4
1	A	351	GLN	3.4
1	A	369	GLN	3.4
1	D	109	THR	3.4
1	D	39	GLY	3.4
1	C	42	THR	3.4
1	B	146	MET	3.4
1	A	145	TYR	3.4
1	D	226	LEU	3.4
1	C	359	ASN	3.3
1	C	41	PRO	3.3
1	B	166	TYR	3.3
1	A	143	TRP	3.3
1	B	297	ASN	3.3
1	C	231	CYS	3.3
1	D	231	CYS	3.3
1	B	173	VAL	3.3
1	A	331	ASP	3.3
1	D	222	LYS	3.3
1	D	317	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	331	ASP	3.3
1	A	346	ALA	3.3
1	B	113	THR	3.3
1	B	133	ALA	3.3
1	D	36	CYS	3.3
1	D	67	GLY	3.2
1	D	31	ILE	3.2
1	D	68	SER	3.2
1	C	134	VAL	3.2
1	C	302	LEU	3.2
1	B	46	ALA	3.2
1	B	105	ALA	3.2
1	C	50	ALA	3.2
1	D	259	SER	3.2
1	A	109	THR	3.2
1	C	234	THR	3.2
1	D	97	TRP	3.2
1	B	174	TYR	3.2
1	C	217	TYR	3.2
1	C	36	CYS	3.2
1	A	218	PRO	3.2
1	B	294	VAL	3.2
1	C	89	LEU	3.2
1	C	118	VAL	3.2
1	D	53	VAL	3.2
1	D	210	ASP	3.2
1	A	19	TYR	3.2
1	B	83	TYR	3.2
1	B	231	CYS	3.2
1	C	177	ASN	3.2
1	D	74	ILE	3.2
1	C	268	ASN	3.2
1	B	271	GLN	3.2
1	A	40	MET	3.2
1	B	212	ALA	3.1
1	C	35	ALA	3.1
1	C	276	VAL	3.1
1	C	169	LEU	3.1
1	A	48	ALA	3.1
1	C	279	ALA	3.1
1	B	269	MET	3.1
1	B	33	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	310	VAL	3.1
1	C	119	TRP	3.1
1	A	80	PRO	3.1
1	A	276	VAL	3.1
1	A	353	ILE	3.1
1	C	283	ASP	3.1
1	C	331	ASP	3.1
1	B	217	TYR	3.1
1	C	304	MET	3.1
1	D	220	TYR	3.1
1	D	280	PHE	3.1
1	A	329	ALA	3.1
1	D	2	ALA	3.1
1	B	19	TYR	3.1
1	D	19	TYR	3.1
1	A	247	GLN	3.1
1	C	195	SER	3.0
1	C	143	TRP	3.0
1	B	40	MET	3.0
1	C	72	ALA	3.0
1	A	349	TYR	3.0
1	B	352	TYR	3.0
1	C	132	TYR	3.0
1	A	213	PRO	3.0
1	D	296	GLU	3.0
1	A	104	TRP	3.0
1	C	281	PHE	3.0
1	D	122	SER	3.0
1	A	113	THR	3.0
1	A	314	THR	3.0
1	B	207	PHE	3.0
1	D	119	TRP	3.0
1	D	5	LYS	3.0
1	B	238	MET	3.0
1	A	333	ALA	3.0
1	D	194	VAL	3.0
1	D	224	ALA	3.0
1	B	115	PRO	3.0
1	C	226	LEU	3.0
1	D	258	THR	3.0
1	D	103	MET	3.0
1	D	333	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	158	ASP	3.0
1	C	153	ASN	3.0
1	A	97	TRP	2.9
1	A	108	TRP	2.9
1	B	141	TYR	2.9
1	C	51	ALA	2.9
1	B	85	THR	2.9
1	C	228	ILE	2.9
1	B	95	ASP	2.9
1	B	122	SER	2.9
1	B	253	ASN	2.9
1	B	91	HIS	2.9
1	C	295	ARG	2.9
1	C	322	MET	2.9
1	B	132	TYR	2.9
1	D	200	TRP	2.9
1	D	298	TYR	2.9
1	C	189	ALA	2.9
1	D	111	GLY	2.9
1	B	205	VAL	2.9
1	C	270	VAL	2.9
1	D	42	THR	2.9
1	D	324	VAL	2.9
1	B	89	LEU	2.9
1	A	246	ALA	2.9
1	A	324	VAL	2.9
1	C	54	VAL	2.9
1	D	18	VAL	2.9
1	C	272	PRO	2.9
1	A	313	ILE	2.9
1	A	355	ASP	2.9
1	D	261	GLN	2.9
1	C	33	VAL	2.9
1	B	315	ARG	2.9
1	D	334	GLY	2.9
1	B	49	ALA	2.9
1	D	145	TYR	2.8
1	A	289	ASP	2.8
1	B	41	PRO	2.8
1	D	179	VAL	2.8
1	C	107	GLY	2.8
1	C	212	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	363	ALA	2.8
1	A	284	ASP	2.8
1	B	65	ASP	2.8
1	D	114	ASP	2.8
1	D	241	LYS	2.8
1	A	216	TRP	2.8
1	A	224	ALA	2.8
1	B	3	GLY	2.8
1	C	57	GLY	2.8
1	D	349	TYR	2.8
1	C	347	SER	2.8
1	D	347	SER	2.8
1	D	284	ASP	2.8
1	C	197	ALA	2.8
1	A	297	ASN	2.8
1	A	27	GLY	2.8
1	C	245	PRO	2.8
1	D	3	GLY	2.8
1	A	345	ARG	2.8
1	D	91	HIS	2.8
1	B	179	VAL	2.8
1	D	302	LEU	2.8
1	B	283	ASP	2.8
1	D	161	VAL	2.8
1	D	49	ALA	2.7
1	A	223	GLY	2.7
1	D	98	GLY	2.7
1	B	191	ASP	2.7
1	C	32	ARG	2.7
1	B	194	VAL	2.7
1	B	227	ALA	2.7
1	D	35	ALA	2.7
1	D	279	ALA	2.7
1	B	188	HIS	2.7
1	C	93	HIS	2.7
1	B	359	ASN	2.7
1	B	66	ILE	2.7
1	C	63	ILE	2.7
1	D	79	ILE	2.7
1	A	167	ARG	2.7
1	B	114	ASP	2.7
1	C	39	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	62	PHE	2.7
1	C	2	ALA	2.7
1	D	274	HIS	2.7
1	B	48	ALA	2.7
1	B	333	ALA	2.7
1	C	164	PHE	2.7
1	D	168	ALA	2.7
1	D	311	TRP	2.7
1	B	332	VAL	2.7
1	C	332	VAL	2.7
1	C	103	MET	2.7
1	B	80	PRO	2.7
1	C	193	PRO	2.7
1	C	313	ILE	2.7
1	C	251	ARG	2.7
1	D	52	TRP	2.7
1	D	237	GLN	2.7
1	D	40	MET	2.7
1	D	359	ASN	2.7
1	A	286	THR	2.7
1	B	37	GLY	2.6
1	B	276	VAL	2.6
1	C	171	GLU	2.6
1	D	34	ILE	2.6
1	B	27	GLY	2.6
1	A	233	MET	2.6
1	C	196	PHE	2.6
1	B	145	TYR	2.6
1	C	179	VAL	2.6
1	C	210	ASP	2.6
1	D	20	TYR	2.6
1	D	354	LEU	2.6
1	C	168	ALA	2.6
1	C	275	ALA	2.6
1	D	63	ILE	2.6
1	D	228	ILE	2.6
1	B	284	ASP	2.6
1	D	78	MET	2.6
1	C	326	PRO	2.6
1	D	303	SER	2.6
1	A	149	ALA	2.6
1	C	4	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	95	ASP	2.6
1	A	78	MET	2.6
1	A	263	PHE	2.6
1	A	20	TYR	2.6
1	D	268	ASN	2.6
1	A	157	GLY	2.6
1	D	175	GLN	2.6
1	B	84	LEU	2.6
1	D	184	TRP	2.6
1	A	21	PRO	2.6
1	B	125	ARG	2.6
1	C	269	MET	2.6
1	C	293	GLY	2.6
1	B	281	PHE	2.5
1	A	203	TYR	2.5
1	D	257	HIS	2.5
1	A	84	LEU	2.5
1	C	21	PRO	2.5
1	B	331	ASP	2.5
1	A	292	THR	2.5
1	C	209	GLY	2.5
1	A	125	ARG	2.5
1	D	118	VAL	2.5
1	D	155	ARG	2.5
1	A	210	ASP	2.5
1	B	201	ASN	2.5
1	B	214	ASN	2.5
1	C	309	MET	2.5
1	A	37	GLY	2.5
1	A	202	GLY	2.5
1	B	53	VAL	2.5
1	B	81	ALA	2.5
1	D	275	ALA	2.5
1	B	213	PRO	2.5
1	D	146	MET	2.5
1	C	27	GLY	2.5
1	A	296	GLU	2.5
1	D	38	THR	2.5
1	B	165	ASP	2.5
1	C	361	ASP	2.5
1	A	72	ALA	2.5
1	A	156	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	156	PRO	2.5
1	C	277	ALA	2.5
1	A	178	GLY	2.5
1	B	220	TYR	2.5
1	A	237	GLN	2.5
1	C	211	THR	2.5
1	C	86	LYS	2.5
1	D	236	ASP	2.5
1	C	58	ASN	2.5
1	A	24	GLU	2.5
1	C	80	PRO	2.5
1	B	50	ALA	2.5
1	B	72	ALA	2.5
1	A	101	VAL	2.5
1	B	257	HIS	2.5
1	C	101	VAL	2.5
1	D	360	VAL	2.5
1	D	265	GLN	2.5
1	A	281	PHE	2.5
1	D	321	ARG	2.5
1	D	14	PRO	2.4
1	B	51	ALA	2.4
1	C	91	HIS	2.4
1	D	209	GLY	2.4
1	A	236	ASP	2.4
1	B	151	THR	2.4
1	A	83	TYR	2.4
1	D	84	LEU	2.4
1	C	37	GLY	2.4
1	B	25	GLU	2.4
1	D	197	ALA	2.4
1	B	58	ASN	2.4
1	D	160	ASN	2.4
1	A	357	ARG	2.4
1	B	74	ILE	2.4
1	B	183	SER	2.4
1	C	47	GLN	2.4
1	B	184	TRP	2.4
1	B	226	LEU	2.4
1	A	121	PRO	2.4
1	C	88	PHE	2.4
1	C	301	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	202	GLY	2.4
1	A	260	ALA	2.4
1	B	140	ALA	2.4
1	C	173	VAL	2.4
1	D	285	ASP	2.4
1	D	143	TRP	2.4
1	B	329	ALA	2.4
1	C	271	GLN	2.4
1	D	277	ALA	2.4
1	B	195	SER	2.4
1	C	286	THR	2.4
1	D	350	THR	2.4
1	A	228	ILE	2.4
1	B	87	ILE	2.4
1	B	295	ARG	2.4
1	C	287	ARG	2.4
1	D	96	HIS	2.4
1	A	198	LEU	2.4
1	A	200	TRP	2.4
1	C	267	MET	2.4
1	D	295	ARG	2.4
1	B	319	THR	2.4
1	C	180	THR	2.4
1	C	82	ASN	2.4
1	D	28	PRO	2.4
1	B	237	GLN	2.4
1	D	64	VAL	2.4
1	D	276	VAL	2.4
1	B	60	ASP	2.3
1	A	92	LEU	2.3
1	A	71	MET	2.3
1	B	305	ALA	2.3
1	C	20	TYR	2.3
1	B	38	THR	2.3
1	D	90	THR	2.3
1	C	202	GLY	2.3
1	B	272	PRO	2.3
1	B	79	ILE	2.3
1	B	270	VAL	2.3
1	D	270	VAL	2.3
1	C	25	GLU	2.3
1	B	103	MET	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	302	LEU	2.3
1	D	214	ASN	2.3
1	C	227	ALA	2.3
1	C	207	PHE	2.3
1	C	163	GLU	2.3
1	B	228	ILE	2.3
1	D	364	ASN	2.3
1	A	39	GLY	2.3
1	B	107	GLY	2.3
1	C	49	ALA	2.3
1	C	208	GLY	2.3
1	A	42	THR	2.3
1	A	89	LEU	2.3
1	C	56	LEU	2.3
1	D	26	LEU	2.3
1	A	316	ASP	2.3
1	D	166	TYR	2.3
1	A	325	SER	2.3
1	C	259	SER	2.3
1	D	238	MET	2.3
1	C	105	ALA	2.3
1	A	301	PRO	2.3
1	C	306	THR	2.3
1	D	198	LEU	2.3
1	D	17	TYR	2.3
1	D	177	ASN	2.3
1	B	96	HIS	2.3
1	C	285	ASP	2.3
1	B	150	VAL	2.3
1	C	310	VAL	2.3
1	B	323	ALA	2.3
1	D	50	ALA	2.3
1	D	138	LEU	2.3
1	A	114	ASP	2.3
1	A	166	TYR	2.2
1	B	291	TYR	2.2
1	D	93	HIS	2.3
1	D	352	TYR	2.2
1	D	37	GLY	2.2
1	C	305	ALA	2.2
1	D	305	ALA	2.2
1	C	257	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	271	GLN	2.2
1	D	196	PHE	2.2
1	A	51	ALA	2.2
1	A	277	ALA	2.2
1	D	51	ALA	2.2
1	D	72	ALA	2.2
1	A	172	VAL	2.2
1	B	327	ASP	2.2
1	C	324	VAL	2.2
1	A	93	HIS	2.2
1	B	119	TRP	2.2
1	B	77	LEU	2.2
1	B	222	LYS	2.2
1	A	174	TYR	2.2
1	B	326	PRO	2.2
1	C	85	THR	2.2
1	C	102	SER	2.2
1	A	50	ALA	2.2
1	D	66	ILE	2.2
1	A	44	ARG	2.2
1	B	138	LEU	2.2
1	D	326	PRO	2.2
1	C	308	MET	2.2
1	A	175	GLN	2.2
1	B	292	THR	2.2
1	C	314	THR	2.2
1	A	208	GLY	2.2
1	D	264	GLY	2.2
1	C	312	ASN	2.2
1	D	33	VAL	2.2
1	D	134	VAL	2.2
1	B	63	ILE	2.2
1	D	267	MET	2.2
1	B	147	THR	2.2
1	D	113	THR	2.2
1	D	201	ASN	2.2
1	A	144	ASP	2.2
1	A	100	LEU	2.1
1	A	169	LEU	2.1
1	C	94	THR	2.1
1	C	201	ASN	2.1
1	A	81	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	261	GLN	2.1
1	D	83	TYR	2.1
1	C	148	ARG	2.1
1	B	42	THR	2.1
1	D	165	ASP	2.1
1	A	302	LEU	2.1
1	D	89	LEU	2.1
1	B	260	ALA	2.1
1	C	135	GLU	2.1
1	A	311	TRP	2.1
1	B	368	LYS	2.1
1	B	57	GLY	2.1
1	C	90	THR	2.1
1	A	74	ILE	2.1
1	A	295	ARG	2.1
1	C	273	ARG	2.1
1	B	139	LYS	2.1
1	D	15	LYS	2.1
1	C	17	TYR	2.1
1	C	55	GLU	2.1
1	D	117	GLU	2.1
1	D	48	ALA	2.1
1	D	289	ASP	2.1
1	B	261	GLN	2.1
1	C	117	GLU	2.1
1	B	202	GLY	2.1
1	B	304	MET	2.1
1	D	286	THR	2.1
1	A	307	ASP	2.1
1	A	188	HIS	2.1
1	A	214	ASN	2.1
1	B	346	ALA	2.1
1	D	81	ALA	2.1
1	D	328	HIS	2.1
1	A	31	ILE	2.1
1	A	66	ILE	2.1
1	C	84	LEU	2.1
1	B	264	GLY	2.1
1	D	45	ARG	2.0
1	B	308	MET	2.0
1	C	166	TYR	2.0
1	A	183	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	347	SER	2.0
1	C	303	SER	2.0
1	B	196	PHE	2.0
1	C	181	PHE	2.0
1	C	100	LEU	2.0
1	D	163	GLU	2.0
1	C	316	ASP	2.0
1	B	112	ARG	2.0
1	C	206	VAL	2.0
1	B	181	PHE	2.0
1	C	98	GLY	2.0
1	C	356	GLY	2.0
1	D	69	GLY	2.0
1	D	115	PRO	2.0
1	B	370	GLU	2.0
1	A	364	ASN	2.0
1	C	354	LEU	2.0
1	A	38	THR	2.0
1	B	78	MET	2.0
1	B	102	SER	2.0
1	B	229	HIS	2.0
1	C	71	MET	2.0
1	B	287	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

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

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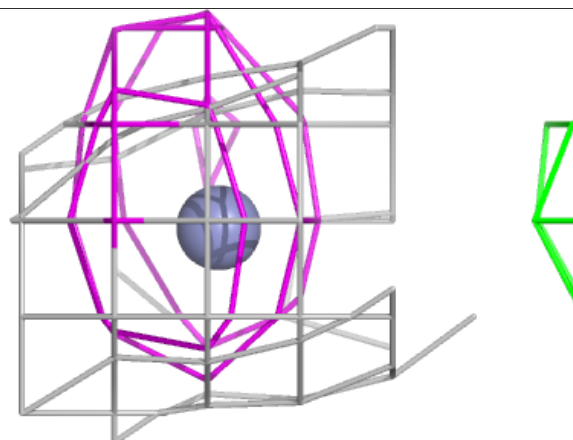
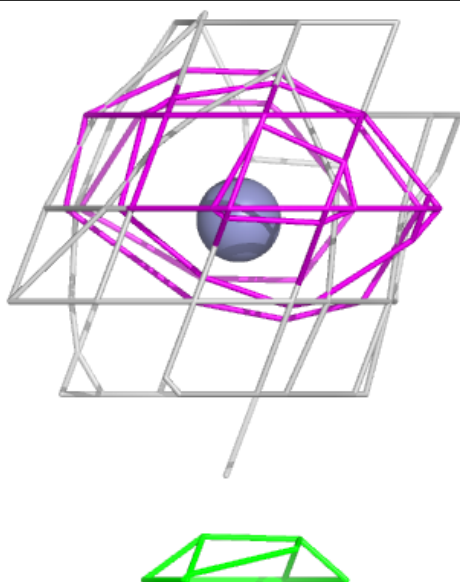
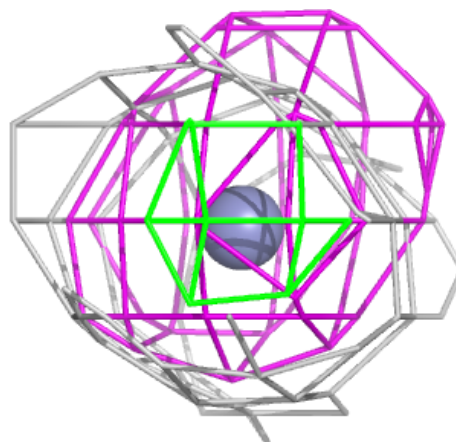
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	401	1/1	0.85	0.25	33,33,33,33	0
2	ZN	C	401	1/1	0.88	0.25	45,45,45,45	0
2	ZN	D	401	1/1	0.88	0.06	43,43,43,43	0
2	ZN	A	401	1/1	0.96	0.33	29,29,29,29	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.

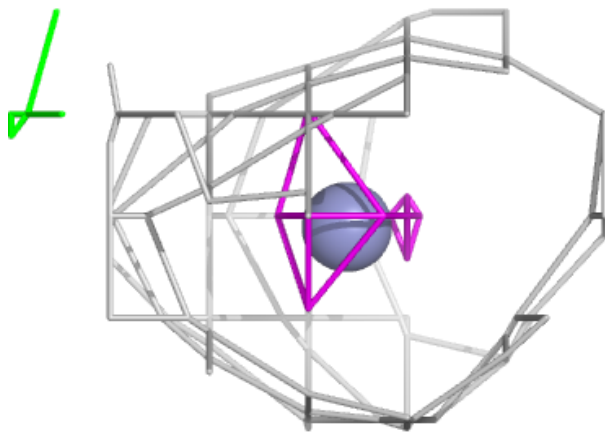
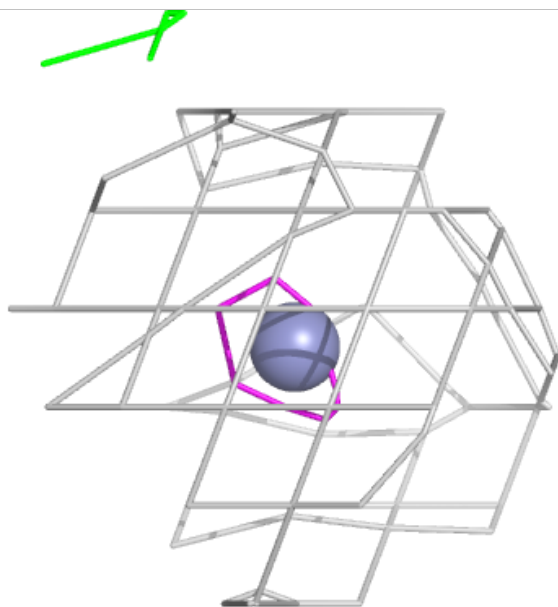
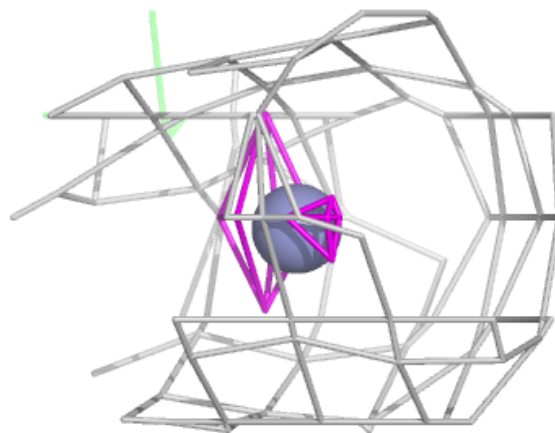
Electron density around ZN B 401:

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



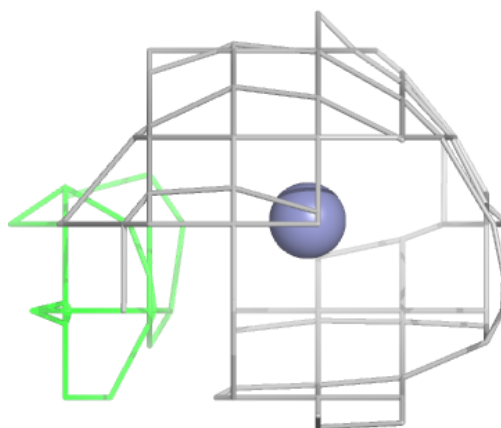
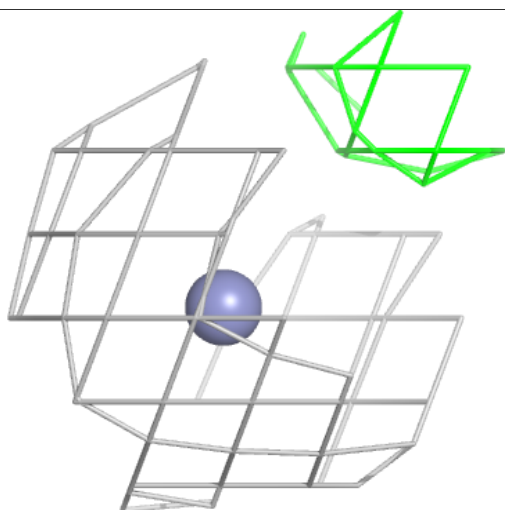
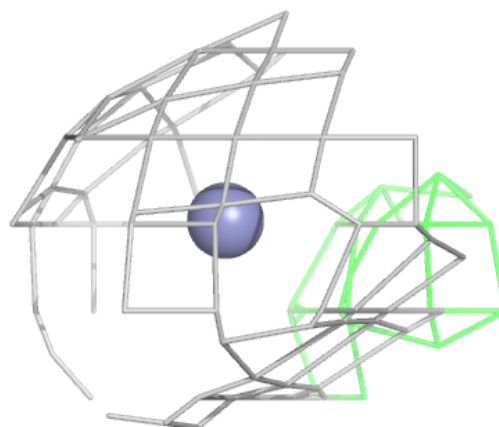
Electron density around ZN C 401:

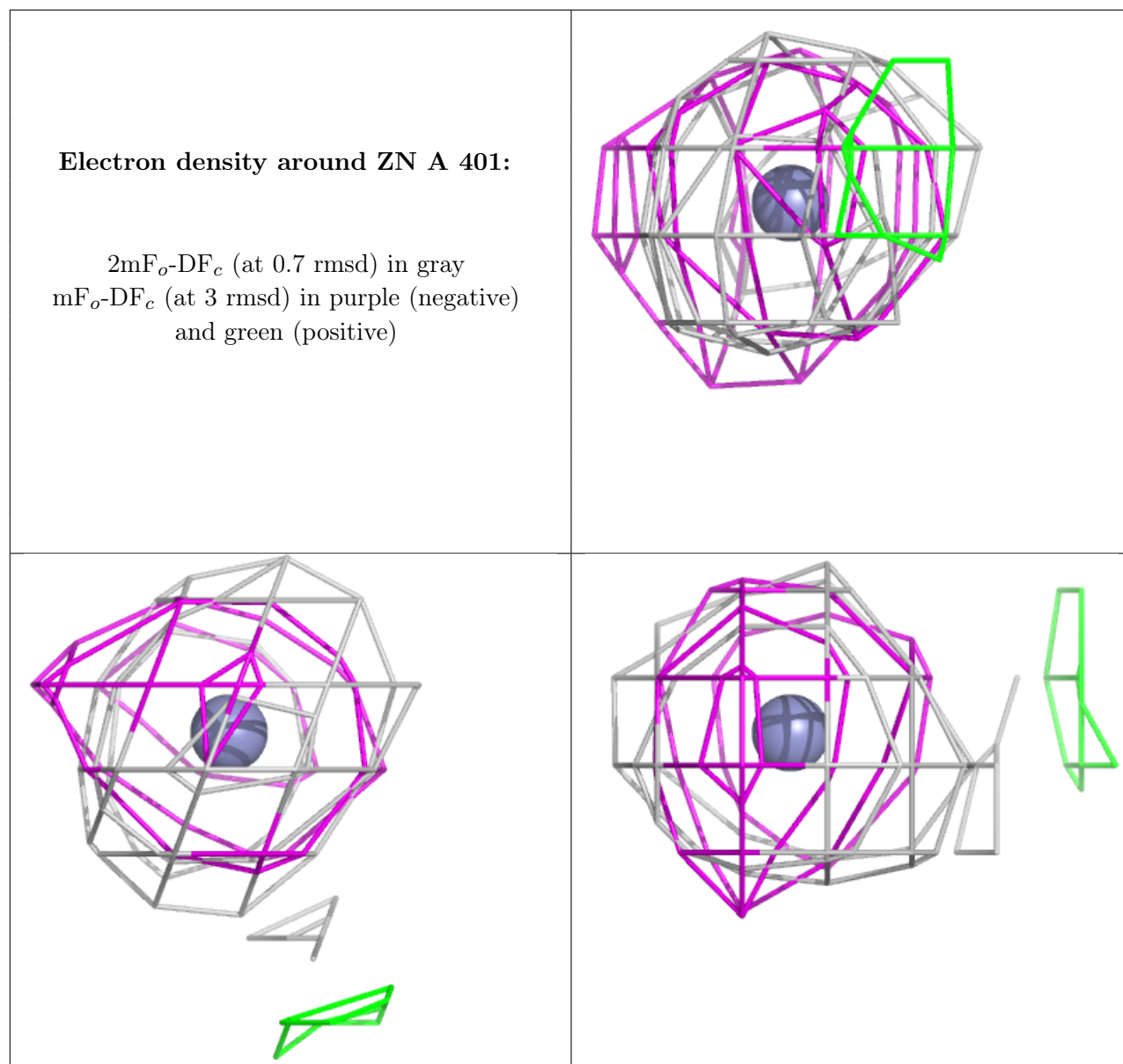
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around ZN D 401:

$2mF_o-DF_c$ (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.