



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 04:30 PM EDT

PDB ID : 3FCT / pdb_00003fct
Title : MATURE METAL CHELATASE CATALYTIC ANTIBODY WITH HAP-
TEN
Authors : Romesberg, F.E.; Santarsiero, B.D.; Barnes, D.; Yin, J.; Spiller, B.; Schultz,
P.G.; Stevens, R.C.
Deposited on : 1999-06-13
Resolution : 2.40 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
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

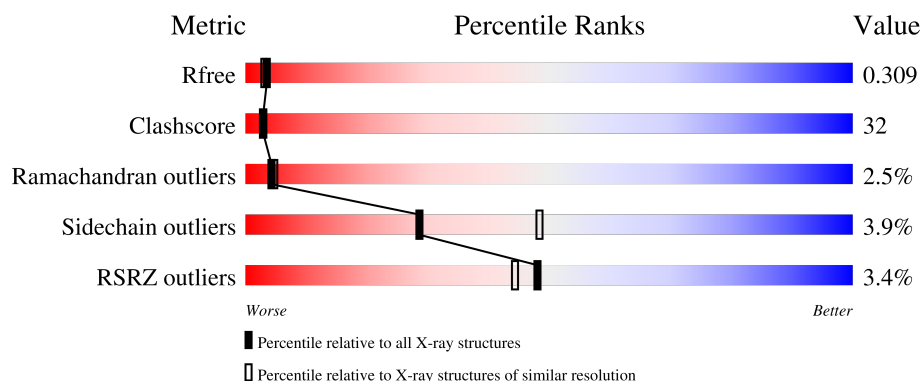
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	213	2% 57% 38% 5%
1	C	213	6% 52% 43% .
2	B	216	5% 56% 40% .
2	D	216	2% 46% 49% 5%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 7178 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 PROTEIN (METAL CHELATASE CATALYTIC ANTI-BODY).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	213	Total	C	N	O	S	0	0	0
			1646	1029	274	336	7			
1	C	213	Total	C	N	O	S	0	0	0
			1646	1029	274	336	7			

- Molecule 2 is a protein called PROTEIN (METAL CHELATASE CATALYTIC ANTI-BODY).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	0	0	0
			1622	1025	269	320	8			
2	D	216	Total	C	N	O	S	0	0	0
			1622	1025	269	320	8			

- Molecule 3 is CADMIUM ION (CCD ID: CD) (formula: Cd).

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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		

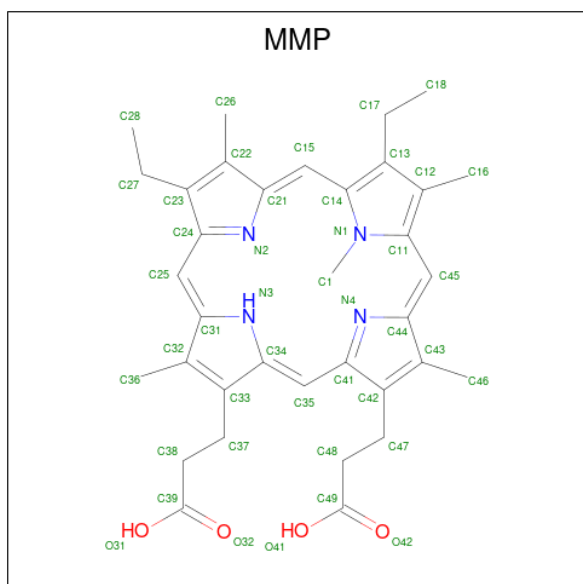
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		
6	B	2	Total	Na	0	0
			2	2		
6	C	4	Total	Na	0	0
			4	4		

- Molecule 7 is N-METHYLMESOPORPHYRIN (CCD ID: MMP) (formula: $C_{35}H_{40}N_4O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	B	1	Total	C	N	O	0	0
			43	35	4	4		
7	D	1	Total	C	N	O	0	0
			43	35	4	4		

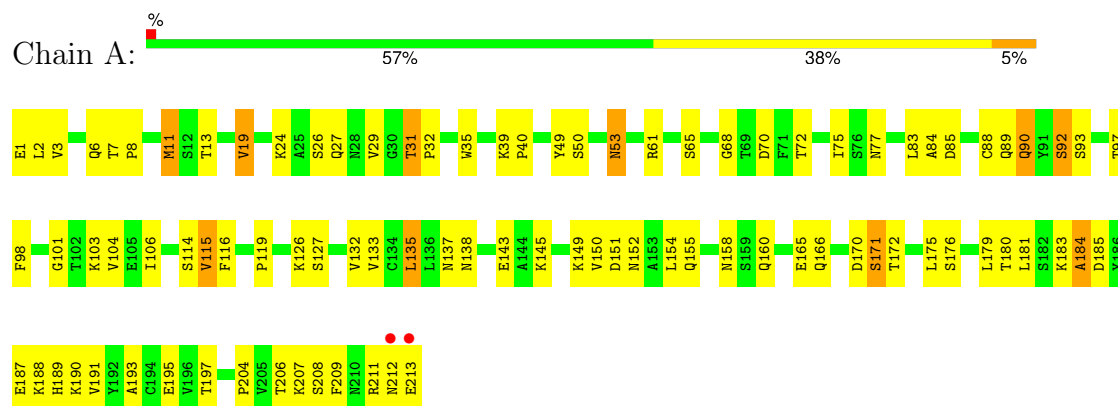
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	135	Total	O	0	0
			135	135		
8	B	167	Total	O	0	0
			167	167		
8	C	129	Total	O	0	0
			129	129		
8	D	115	Total	O	0	0
			115	115		

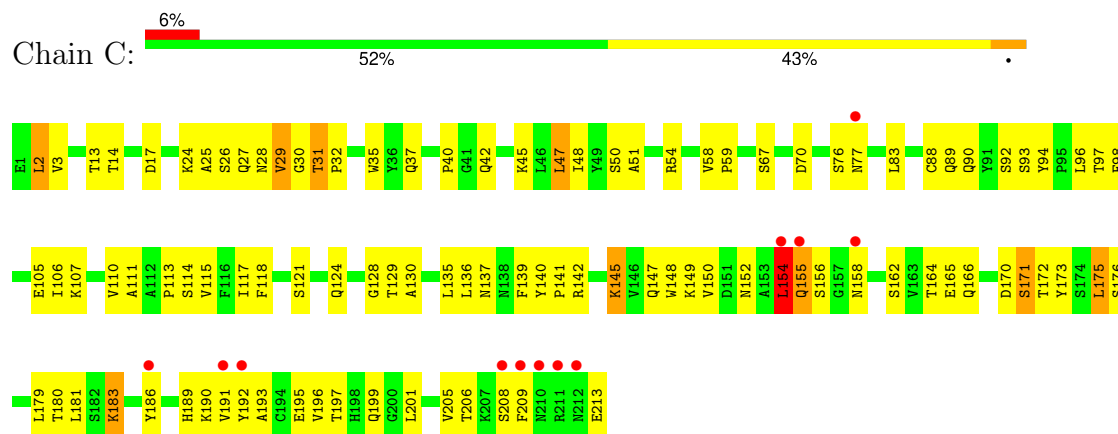
3 Residue-property plots

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.

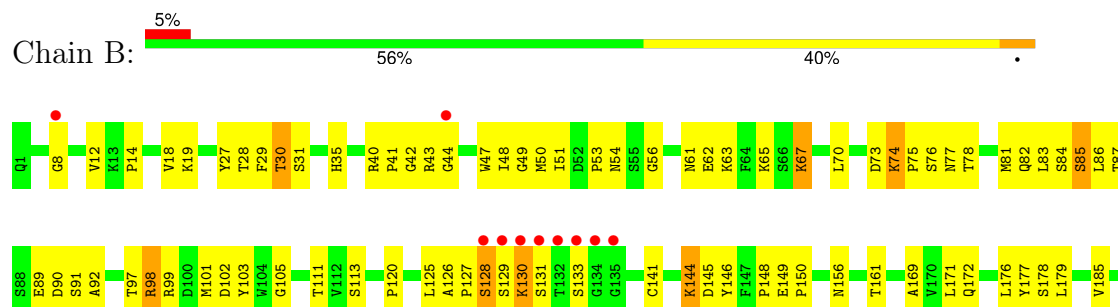
• Molecule 1: PROTEIN (METAL CHELATASE CATALYTIC ANTIBODY)

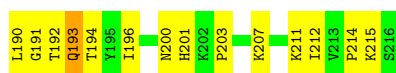


• Molecule 1: PROTEIN (METAL CHELATASE CATALYTIC ANTIBODY)

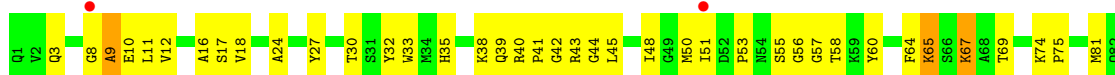


• Molecule 2: PROTEIN (METAL CHELATASE CATALYTIC ANTIBODY)





● Molecule 2: PROTEIN (METAL CHELATASE CATALYTIC ANTIBODY)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.29Å 100.69Å 73.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.40 50.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	69.9 (50.00-2.40) 85.2 (50.00-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.41Å)	Xtriage
Refinement program	CNS 0.4	Depositor
R, R_{free}	0.206 , 0.293 0.227 , 0.309	Depositor DCC
R_{free} test set	1680 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 60.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7178	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.41% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MMP, CD, NA, MG

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	0.43	0/1681	0.99	8/2281 (0.4%)
1	C	0.43	0/1681	1.00	8/2281 (0.4%)
2	B	0.44	0/1662	0.97	4/2261 (0.2%)
2	D	0.42	0/1662	1.01	9/2261 (0.4%)
All	All	0.43	0/6686	1.00	29/9084 (0.3%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	118	PHE	CA-C-N	8.69	125.92	119.66
1	C	118	PHE	C-N-CA	8.69	125.92	119.66
2	B	144	LYS	N-CA-C	8.31	121.79	109.24
1	C	171	SER	N-CA-C	-7.57	102.27	113.40
1	C	114	SER	N-CA-C	-7.12	97.12	108.73
1	A	115	VAL	N-CA-C	6.45	117.20	108.17
2	D	144	LYS	N-CA-C	6.23	119.69	109.85
2	B	56	GLY	N-CA-C	-6.22	106.83	114.92
2	D	67	LYS	N-CA-C	5.86	118.45	111.71
1	A	133	VAL	N-CA-C	5.83	116.33	108.17
2	D	119	GLY	CA-C-N	5.70	125.89	120.31
2	D	119	GLY	C-N-CA	5.70	125.89	120.31
2	B	149	GLU	N-CA-C	-5.65	101.92	110.39
1	A	165	GLU	N-CA-C	-5.64	103.08	110.53
1	A	171	SER	N-CA-C	-5.61	106.38	113.23
2	D	96	CYS	N-CA-C	-5.50	100.43	109.40
1	C	137	ASN	N-CA-C	5.49	117.90	109.07
1	C	196	VAL	N-CA-C	5.44	116.82	108.71
2	D	99	ARG	N-CA-C	5.44	117.91	111.33
1	A	92	SER	N-CA-C	-5.35	106.89	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	125	LEU	N-CA-C	-5.35	101.60	109.62
2	B	105	GLY	N-CA-C	-5.32	104.29	112.85
1	A	114	SER	N-CA-C	-5.32	100.58	109.24
1	C	29	VAL	N-CA-C	-5.17	107.72	111.90
2	D	123	PHE	CA-C-N	5.12	125.28	119.90
2	D	123	PHE	C-N-CA	5.12	125.28	119.90
1	A	127	SER	N-CA-C	-5.12	106.89	113.23
1	C	209	PHE	N-CA-C	5.05	116.66	109.14
1	A	135	LEU	N-CA-C	5.01	117.07	108.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1646	0	1595	94	0
1	C	1646	0	1596	115	0
2	B	1622	0	1609	99	0
2	D	1622	0	1609	118	0
3	A	1	0	0	0	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	4	0	0	0	0
7	B	43	0	40	1	0
7	D	43	0	40	1	0
8	A	135	0	0	17	0
8	B	167	0	0	11	0
8	C	129	0	0	12	0
8	D	115	0	0	9	0
All	All	7178	0	6489	424	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 32.

All (424) 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)
2:B:200:ASN:HD21	2:B:207:LYS:HE2	1.01	1.09
2:B:200:ASN:ND2	2:B:207:LYS:HE2	1.69	1.06
2:B:130:LYS:HG3	2:B:131:SER:H	1.26	0.98
1:C:90:GLN:HE21	1:C:92:SER:H	1.08	0.98
2:D:200:ASN:HD21	2:D:207:LYS:HE2	1.26	0.98
1:A:11:MET:HA	1:A:11:MET:HE2	1.44	0.96
1:A:83:LEU:HD13	1:A:106:ILE:HG13	1.47	0.94
1:C:90:GLN:NE2	1:C:93:SER:H	1.65	0.93
2:B:194:THR:HB	2:B:211:LYS:HE2	1.50	0.91
1:A:197:THR:HG22	1:A:204:PRO:HB3	1.52	0.91
1:A:150:VAL:HG22	1:A:155:GLN:NE2	1.86	0.91
1:A:185:ASP:HA	1:A:188:LYS:HE2	1.52	0.90
1:C:170:ASP:HB3	1:C:172:THR:HG23	1.53	0.89
1:C:31:THR:HG22	8:C:934:HOH:O	1.71	0.89
1:C:201:LEU:HD13	1:C:205:VAL:HG23	1.53	0.88
2:D:127:PRO:HB3	2:D:139:LEU:HB3	1.55	0.87
1:C:90:GLN:HE21	1:C:92:SER:N	1.71	0.87
2:D:141:CYS:SG	2:D:212:ILE:HD11	2.15	0.87
1:C:195:GLU:HA	1:C:206:THR:HG22	1.56	0.86
1:C:13:THR:HG23	1:C:17:ASP:OD2	1.76	0.86
1:C:31:THR:H	1:C:32:PRO:HD3	1.43	0.83
2:D:189:SER:HB2	2:D:193:GLN:NE2	1.94	0.83
1:A:31:THR:H	1:A:32:PRO:HD3	1.43	0.83
2:D:157:SER:H	2:D:198:ASN:HD21	1.23	0.82
2:D:156:ASN:ND2	2:D:196:ILE:H	1.78	0.82
2:B:98:ARG:HH11	2:B:98:ARG:HB3	1.43	0.82
2:B:200:ASN:HD21	2:B:207:LYS:CE	1.89	0.82
2:B:111:THR:HB	8:B:1006:HOH:O	1.79	0.81
1:C:149:LYS:HE2	1:C:191:VAL:HG11	1.63	0.80
1:C:175:LEU:C	1:C:175:LEU:HD23	2.07	0.79
1:A:195:GLU:HG2	1:A:206:THR:OG1	1.83	0.78
2:D:30:THR:HA	2:D:53:PRO:HB2	1.65	0.78
1:A:83:LEU:HD21	1:A:166:GLN:HG2	1.65	0.78
2:D:154:SER:HB2	2:D:198:ASN:HD22	1.48	0.77
1:C:90:GLN:HE22	1:C:93:SER:H	1.30	0.77
2:D:97:THR:CG2	2:D:101:MET:HA	2.15	0.77
1:A:180:THR:HG23	8:A:965:HOH:O	1.82	0.77
2:D:97:THR:HG22	2:D:101:MET:HA	1.66	0.76
2:B:19:LYS:HD2	2:B:82:GLN:HB2	1.67	0.76
2:D:156:ASN:HD21	2:D:196:ILE:H	1.34	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:154:LEU:HD23	1:C:154:LEU:H	1.52	0.75
1:A:211:ARG:NH1	1:A:211:ARG:HB3	2.00	0.75
2:D:174:SER:HB2	8:D:254:HOH:O	1.86	0.74
2:B:194:THR:CB	2:B:211:LYS:HE2	2.18	0.74
2:B:8:GLY:HA2	8:B:940:HOH:O	1.86	0.74
2:D:12:VAL:HG11	2:D:18:VAL:HB	1.70	0.73
1:A:158:ASN:ND2	1:A:179:LEU:HD11	2.03	0.73
2:D:43:ARG:HE	2:D:43:ARG:HA	1.53	0.73
2:D:16:ALA:O	2:D:86:LEU:HD23	1.88	0.73
2:B:98:ARG:HH11	2:B:98:ARG:CB	2.02	0.73
2:D:38:LYS:HE2	2:D:40:ARG:HD2	1.71	0.72
2:B:156:ASN:ND2	2:B:196:ILE:H	1.87	0.72
1:A:103:LYS:HE2	8:A:924:HOH:O	1.90	0.70
2:B:127:PRO:HD2	2:B:214:PRO:HA	1.73	0.70
1:A:2:LEU:HD13	8:A:941:HOH:O	1.90	0.70
2:B:97:THR:HG22	2:B:101:MET:HA	1.73	0.70
1:C:128:GLY:O	1:C:183:LYS:HB2	1.91	0.69
2:B:156:ASN:HD21	2:B:196:ILE:H	1.37	0.69
1:C:2:LEU:CD2	1:C:27:GLN:HB2	2.22	0.69
1:C:128:GLY:C	1:C:183:LYS:HB2	2.16	0.69
1:A:11:MET:HA	1:A:11:MET:CE	2.20	0.68
2:D:84:SER:O	2:D:86:LEU:HD22	1.93	0.68
1:C:110:VAL:HG21	1:C:199:GLN:HE21	1.57	0.68
8:A:1029:HOH:O	2:B:44:GLY:HA2	1.93	0.68
1:A:211:ARG:HB3	1:A:211:ARG:HH11	1.58	0.68
2:B:111:THR:HG23	8:B:923:HOH:O	1.94	0.68
2:D:65:LYS:HA	2:D:65:LYS:HE2	1.75	0.67
1:A:145:LYS:HB3	1:A:197:THR:OG1	1.93	0.67
1:C:149:LYS:HD2	1:C:193:ALA:HB3	1.75	0.67
2:D:74:LYS:HB2	2:D:75:PRO:CD	2.24	0.67
1:A:2:LEU:HD23	1:A:27:GLN:OE1	1.95	0.67
1:A:2:LEU:CD1	1:A:93:SER:HB3	2.24	0.67
1:C:31:THR:H	1:C:32:PRO:CD	2.07	0.66
2:D:43:ARG:HA	2:D:43:ARG:NE	2.10	0.66
2:B:41:PRO:HD3	8:B:1011:HOH:O	1.94	0.66
2:B:12:VAL:HG11	2:B:86:LEU:HD12	1.75	0.66
2:B:129:SER:HA	2:B:215:LYS:HB3	1.77	0.66
1:C:110:VAL:HG21	1:C:199:GLN:NE2	2.09	0.66
1:C:162:SER:OG	2:D:168:PRO:HD2	1.95	0.66
1:C:2:LEU:HD22	1:C:27:GLN:HB2	1.77	0.66
1:C:149:LYS:HE3	1:C:152:ASN:N	2.11	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:130:LYS:HG3	2:B:131:SER:N	2.07	0.66
2:D:120:PRO:HB3	2:D:146:TYR:HB3	1.77	0.65
1:C:115:VAL:HA	1:C:135:LEU:O	1.95	0.65
1:A:149:LYS:HG3	1:A:195:GLU:OE2	1.95	0.65
2:B:169:ALA:HB2	2:B:179:LEU:HD23	1.78	0.65
2:B:99:ARG:NH1	7:B:910:MMP:H481	2.12	0.65
1:A:29:VAL:HG23	1:A:92:SER:OG	1.96	0.64
1:C:90:GLN:NE2	1:C:92:SER:H	1.89	0.64
2:B:126:ALA:HB1	2:B:215:LYS:HB2	1.78	0.64
2:D:175:GLY:C	2:D:176:LEU:HD12	2.23	0.64
1:A:31:THR:N	1:A:32:PRO:HD3	2.12	0.63
1:C:149:LYS:HE2	1:C:191:VAL:CG1	2.29	0.63
1:C:201:LEU:HD13	1:C:205:VAL:CG2	2.27	0.63
2:D:38:LYS:HE2	2:D:40:ARG:CD	2.27	0.63
2:D:111:THR:HG22	8:D:261:HOH:O	1.96	0.63
2:B:35:HIS:CE1	2:B:50:MET:HE2	2.33	0.63
1:A:103:LYS:HE3	8:A:920:HOH:O	1.97	0.63
1:C:40:PRO:HG3	1:C:165:GLU:HG2	1.80	0.63
1:C:90:GLN:NE2	1:C:92:SER:N	2.45	0.63
2:D:81:MET:HE2	2:D:83:LEU:HD21	1.81	0.63
2:B:144:LYS:HE2	2:B:145:ASP:OD2	1.99	0.62
1:C:77:ASN:HB2	8:C:1006:HOH:O	1.98	0.62
1:C:105:GLU:HG3	1:C:166:GLN:OE1	1.99	0.62
2:B:97:THR:CG2	2:B:101:MET:HA	2.30	0.62
1:C:205:VAL:HA	8:C:941:HOH:O	2.00	0.62
2:D:33:TRP:HB2	2:D:99:ARG:HB3	1.81	0.62
2:B:193:GLN:HE21	2:B:194:THR:N	1.96	0.61
1:C:136:LEU:HD13	1:C:175:LEU:HD22	1.82	0.61
1:C:170:ASP:O	1:C:171:SER:HB2	2.01	0.61
1:A:211:ARG:HH11	1:A:211:ARG:CB	2.14	0.61
1:C:149:LYS:HE3	1:C:152:ASN:H	1.65	0.61
2:D:127:PRO:O	2:D:128:SER:HB3	2.01	0.60
1:A:180:THR:HG22	8:A:919:HOH:O	2.00	0.60
2:B:67:LYS:HB2	2:B:67:LYS:NZ	2.16	0.60
1:C:37:GLN:NE2	8:C:937:HOH:O	2.33	0.60
1:A:27:GLN:HG3	8:A:1000:HOH:O	2.01	0.60
1:C:180:THR:HG22	8:C:944:HOH:O	2.00	0.60
2:B:29:PHE:C	2:B:31:SER:H	2.09	0.60
1:C:189:HIS:HA	8:C:980:HOH:O	2.00	0.60
2:B:127:PRO:O	2:B:128:SER:C	2.45	0.60
2:B:193:GLN:NE2	2:B:194:THR:N	2.49	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:48:ILE:HD13	2:D:81:MET:HE1	1.82	0.59
1:C:195:GLU:CA	1:C:206:THR:HG22	2.32	0.59
2:D:200:ASN:HD21	2:D:207:LYS:CE	2.08	0.59
2:D:87:THR:HG22	2:D:90:ASP:OD2	2.03	0.59
2:D:139:LEU:C	2:D:139:LEU:HD12	2.28	0.58
1:C:76:SER:O	1:C:77:ASN:ND2	2.37	0.58
2:D:40:ARG:HG3	2:D:92:ALA:HB2	1.85	0.58
1:C:190:LYS:HD2	1:C:213:GLU:HB3	1.86	0.58
2:D:99:ARG:NH1	2:D:100:ASP:OD1	2.36	0.58
1:A:188:LYS:HG3	1:A:189:HIS:CD2	2.39	0.58
1:A:24:LYS:HZ1	1:A:70:ASP:CG	2.12	0.57
1:A:170:ASP:HB3	1:A:172:THR:HG23	1.87	0.57
1:C:192:TYR:HB2	8:C:999:HOH:O	2.05	0.57
1:A:143:GLU:H	1:A:143:GLU:CD	2.12	0.57
2:D:157:SER:N	2:D:198:ASN:HD21	2.00	0.57
1:A:197:THR:CG2	1:A:204:PRO:HB3	2.29	0.56
2:B:97:THR:HG23	2:B:103:TYR:O	2.04	0.56
2:D:137:ALA:HB2	2:D:187:SER:HB3	1.87	0.56
2:B:141:CYS:SG	2:B:212:ILE:HD11	2.45	0.56
1:C:107:LYS:HD2	1:C:140:TYR:OH	2.06	0.56
2:B:35:HIS:HE1	2:B:50:MET:HE2	1.70	0.56
1:C:31:THR:N	1:C:32:PRO:CD	2.67	0.56
2:B:194:THR:HG22	8:B:1075:HOH:O	2.05	0.56
2:D:125:LEU:HD23	2:D:141:CYS:CA	2.36	0.56
1:A:31:THR:N	1:A:32:PRO:CD	2.69	0.56
2:B:179:LEU:HD12	2:B:179:LEU:C	2.31	0.55
2:D:39:GLN:HB2	2:D:45:LEU:HD23	1.88	0.55
1:C:47:LEU:C	1:C:48:ILE:HD12	2.31	0.55
1:C:28:ASN:HD22	1:C:29:VAL:N	2.05	0.55
1:A:19:VAL:HG23	1:A:75:ILE:HB	1.87	0.55
2:B:190:LEU:O	2:B:192:THR:N	2.35	0.55
2:B:145:ASP:HB3	2:B:176:LEU:HD13	1.89	0.55
2:D:97:THR:HG21	2:D:101:MET:HA	1.89	0.55
2:D:84:SER:O	2:D:85:SER:C	2.51	0.54
1:A:190:LYS:HG3	1:A:191:VAL:HG23	1.90	0.54
1:A:212:ASN:O	1:A:213:GLU:HB2	2.07	0.54
1:C:35:TRP:CZ3	1:C:88:CYS:HB3	2.43	0.54
1:C:37:GLN:HE21	1:C:45:LYS:NZ	2.05	0.54
1:A:24:LYS:HE2	1:A:24:LYS:HA	1.89	0.54
2:D:154:SER:CB	2:D:198:ASN:HD22	2.19	0.54
2:D:69:THR:HG23	8:D:295:HOH:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:170:VAL:HG23	8:D:314:HOH:O	2.06	0.54
2:D:51:ILE:HG13	2:D:58:THR:HG22	1.90	0.54
2:D:65:LYS:HE2	2:D:65:LYS:CA	2.38	0.54
1:C:149:LYS:O	1:C:149:LYS:HD3	2.08	0.54
1:C:175:LEU:C	1:C:175:LEU:CD2	2.80	0.53
1:A:149:LYS:HD3	1:A:154:LEU:HA	1.89	0.53
1:C:180:THR:HG23	8:C:913:HOH:O	2.08	0.53
1:C:142:ARG:HB2	1:C:173:TYR:CE2	2.43	0.53
2:B:125:LEU:HD13	2:B:141:CYS:CA	2.38	0.53
1:C:155:GLN:CD	1:C:179:LEU:HD11	2.33	0.53
2:D:122:VAL:HG21	2:D:199:VAL:HG21	1.89	0.53
2:D:74:LYS:HB2	2:D:75:PRO:HD3	1.90	0.53
1:A:183:LYS:O	1:A:187:GLU:HG3	2.09	0.53
1:C:147:GLN:NE2	1:C:154:LEU:HB2	2.24	0.53
2:B:30:THR:HB	2:B:54:ASN:HD22	1.73	0.53
1:C:28:ASN:ND2	1:C:29:VAL:N	2.57	0.53
1:C:96:LEU:HD12	1:C:96:LEU:N	2.23	0.52
1:C:170:ASP:HB3	1:C:172:THR:CG2	2.35	0.52
2:B:193:GLN:HE21	2:B:193:GLN:C	2.18	0.52
1:A:24:LYS:NZ	1:A:70:ASP:OD2	2.39	0.52
1:A:175:LEU:HD23	1:A:176:SER:N	2.24	0.52
2:D:55:SER:O	2:D:57:GLY:N	2.42	0.52
2:D:192:THR:C	2:D:193:GLN:HG3	2.33	0.52
1:A:65:SER:HB2	1:A:72:THR:CG2	2.40	0.52
1:C:190:LYS:HD2	1:C:213:GLU:CD	2.35	0.52
1:C:24:LYS:HE3	1:C:70:ASP:OD1	2.10	0.52
1:C:183:LYS:HD2	1:C:183:LYS:O	2.09	0.52
2:D:35:HIS:NE2	2:D:99:ARG:HA	2.25	0.51
1:A:2:LEU:HD22	8:A:941:HOH:O	2.09	0.51
1:C:121:SER:HA	8:C:981:HOH:O	2.09	0.51
2:D:202:LYS:HE2	2:D:202:LYS:HA	1.93	0.51
2:D:17:SER:HA	2:D:86:LEU:CD2	2.41	0.51
2:B:29:PHE:CD2	2:B:77:ASN:HA	2.45	0.51
2:B:18:VAL:HG12	2:B:86:LEU:HD11	1.93	0.51
2:B:185:VAL:HG12	8:B:995:HOH:O	2.10	0.51
1:C:136:LEU:HD13	1:C:175:LEU:CD2	2.40	0.51
1:C:149:LYS:HE3	1:C:152:ASN:CA	2.40	0.51
1:C:158:ASN:C	1:C:158:ASN:HD22	2.18	0.51
1:C:181:LEU:CD1	1:C:186:TYR:HB2	2.41	0.51
2:D:94:TYR:O	2:D:107:GLY:HA2	2.09	0.51
2:D:214:PRO:C	2:D:215:LYS:HD2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:GLN:HG2	1:A:90:GLN:N	2.26	0.51
2:D:17:SER:HA	2:D:86:LEU:HD23	1.93	0.51
2:D:33:TRP:CB	2:D:99:ARG:HB3	2.41	0.50
1:C:175:LEU:HD23	1:C:176:SER:N	2.25	0.50
2:D:132:THR:O	2:D:132:THR:HG23	2.12	0.50
2:D:125:LEU:HD23	2:D:141:CYS:N	2.27	0.50
1:A:40:PRO:HG2	8:A:944:HOH:O	2.11	0.50
2:B:28:THR:O	2:B:31:SER:HB3	2.11	0.50
1:C:47:LEU:O	1:C:48:ILE:HD12	2.12	0.50
1:C:28:ASN:HD22	1:C:29:VAL:H	1.60	0.50
2:B:28:THR:HA	8:B:1057:HOH:O	2.12	0.50
1:C:83:LEU:C	1:C:83:LEU:HD12	2.37	0.50
1:A:1:GLU:O	1:A:2:LEU:HB2	2.11	0.50
1:A:65:SER:HB2	1:A:72:THR:HG23	1.93	0.50
2:B:48:ILE:CD1	2:B:81:MET:HE1	2.41	0.50
2:B:129:SER:HA	2:B:215:LYS:CB	2.42	0.50
1:C:2:LEU:HD21	1:C:27:GLN:O	2.12	0.50
1:C:164:THR:HG23	2:D:167:PHE:CE1	2.46	0.50
2:D:87:THR:CG2	2:D:89:GLU:HB2	2.42	0.50
1:C:83:LEU:HD12	1:C:83:LEU:O	2.12	0.49
1:C:130:ALA:HB3	1:C:181:LEU:HD12	1.94	0.49
2:D:8:GLY:O	2:D:9:ALA:C	2.54	0.49
2:D:43:ARG:HG3	2:D:44:GLY:N	2.27	0.49
2:B:53:PRO:O	2:B:74:LYS:HD2	2.12	0.49
2:B:70:LEU:HD21	2:B:81:MET:HE3	1.93	0.49
2:D:199:VAL:HG22	2:D:208:VAL:HB	1.93	0.49
1:A:39:LYS:HG2	1:A:84:ALA:HB2	1.94	0.49
2:B:73:ASP:OD1	2:B:75:PRO:HD2	2.13	0.49
2:B:125:LEU:HD13	2:B:141:CYS:HA	1.95	0.49
2:B:48:ILE:HG21	2:B:81:MET:HE1	1.94	0.49
2:D:12:VAL:HG21	2:D:86:LEU:HG	1.94	0.49
2:D:184:THR:HB	8:D:296:HOH:O	2.11	0.49
2:B:67:LYS:HE2	2:B:90:ASP:OD2	2.13	0.48
2:D:152:THR:HA	8:D:253:HOH:O	2.12	0.48
2:D:213:VAL:HG13	2:D:214:PRO:HD2	1.95	0.48
1:A:2:LEU:CD2	1:A:27:GLN:HB2	2.43	0.48
2:B:67:LYS:HB2	2:B:67:LYS:HZ2	1.77	0.48
2:B:12:VAL:HG11	2:B:86:LEU:CD1	2.42	0.48
2:D:48:ILE:HG21	2:D:81:MET:CE	2.44	0.48
1:A:183:LYS:HD2	8:A:1001:HOH:O	2.14	0.48
1:A:50:SER:HB2	1:A:53:ASN:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:43:ARG:HG3	2:D:44:GLY:H	1.79	0.48
2:D:163:GLY:O	2:D:183:VAL:HA	2.14	0.48
1:A:35:TRP:CZ3	1:A:88:CYS:HB3	2.49	0.48
1:A:135:LEU:HD12	1:A:175:LEU:O	2.13	0.48
2:D:11:LEU:HD22	2:D:148:PRO:HD3	1.95	0.48
2:D:166:THR:HG21	8:D:331:HOH:O	2.13	0.48
1:A:150:VAL:HA	1:A:191:VAL:O	2.13	0.48
2:B:29:PHE:HB2	8:B:932:HOH:O	2.13	0.47
1:C:149:LYS:HD3	1:C:149:LYS:C	2.39	0.47
2:B:144:LYS:HB3	2:B:178:SER:OG	2.14	0.47
2:D:87:THR:HG23	2:D:89:GLU:HB2	1.97	0.47
1:A:61:ARG:HD2	1:A:77:ASN:O	2.15	0.47
2:B:65:LYS:HE3	8:B:970:HOH:O	2.13	0.47
1:A:83:LEU:HD21	1:A:166:GLN:CG	2.40	0.47
1:A:104:VAL:HG13	8:A:1043:HOH:O	2.13	0.47
2:B:84:SER:O	2:B:85:SER:C	2.57	0.47
2:D:111:THR:HG21	2:D:148:PRO:HG3	1.95	0.47
1:A:3:VAL:CG1	1:A:26:SER:HB3	2.45	0.47
2:D:35:HIS:CD2	2:D:99:ARG:HA	2.50	0.47
2:D:149:GLU:HG3	2:D:177:TYR:CE2	2.49	0.47
1:A:132:VAL:HB	1:A:179:LEU:HB3	1.97	0.47
1:A:170:ASP:O	1:A:171:SER:HB2	2.15	0.47
1:C:89:GLN:HG2	1:C:90:GLN:N	2.30	0.47
1:A:126:LYS:HD2	8:A:1017:HOH:O	2.15	0.47
2:B:40:ARG:O	2:B:43:ARG:HB3	2.15	0.46
1:C:113:PRO:HB3	1:C:139:PHE:CD2	2.50	0.46
2:D:215:LYS:HD2	2:D:215:LYS:N	2.30	0.46
2:B:91:SER:O	2:B:92:ALA:HB2	2.15	0.46
2:D:201:HIS:CD2	2:D:203:PRO:HD2	2.51	0.46
2:B:128:SER:O	2:B:129:SER:C	2.59	0.46
2:D:99:ARG:NH1	2:D:100:ASP:CG	2.73	0.46
1:A:119:PRO:HG3	1:A:209:PHE:CE2	2.50	0.46
1:A:193:ALA:CB	1:A:208:SER:HB3	2.45	0.46
1:C:124:GLN:HG2	1:C:129:THR:O	2.15	0.46
1:A:49:TYR:O	1:A:53:ASN:HB2	2.14	0.46
1:C:13:THR:O	1:C:106:ILE:HA	2.16	0.46
1:C:42:GLN:HG2	8:C:939:HOH:O	2.15	0.46
2:B:47:TRP:CZ2	2:B:49:GLY:HA2	2.51	0.46
2:D:97:THR:HG21	2:D:101:MET:HG2	1.96	0.46
2:D:129:SER:O	2:D:130:LYS:HB2	2.15	0.46
2:D:140:GLY:HA2	2:D:155:TRP:CH2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:LEU:HD23	1:A:155:GLN:O	2.16	0.46
1:A:175:LEU:HD23	1:A:175:LEU:C	2.41	0.46
2:B:161:THR:HG23	8:B:1035:HOH:O	2.15	0.46
1:C:50:SER:O	1:C:51:ALA:HB3	2.15	0.46
2:D:51:ILE:CG1	2:D:58:THR:HG22	2.45	0.46
2:D:125:LEU:HD23	2:D:140:GLY:C	2.41	0.46
1:A:212:ASN:O	1:A:213:GLU:CB	2.64	0.46
2:B:127:PRO:O	2:B:129:SER:N	2.49	0.46
2:B:145:ASP:HA	2:B:176:LEU:HB3	1.98	0.46
2:B:193:GLN:NE2	2:B:194:THR:H	2.14	0.46
1:C:13:THR:HG22	1:C:17:ASP:HB3	1.97	0.46
2:D:179:LEU:HD12	2:D:179:LEU:C	2.41	0.46
2:D:3:GLN:HB3	8:D:248:HOH:O	2.16	0.45
2:D:24:ALA:HB1	2:D:27:TYR:CE1	2.52	0.45
2:D:99:ARG:NH1	2:D:100:ASP:OD2	2.50	0.45
2:B:29:PHE:C	2:B:31:SER:N	2.75	0.45
1:C:97:THR:HG22	1:C:98:PHE:N	2.32	0.45
1:A:151:ASP:O	1:A:152:ASN:HB2	2.17	0.45
2:D:51:ILE:CB	2:D:58:THR:HG22	2.47	0.45
1:A:29:VAL:HG12	1:A:68:GLY:O	2.17	0.45
1:C:58:VAL:HG12	1:C:59:PRO:O	2.16	0.45
2:B:41:PRO:O	2:B:42:GLY:C	2.60	0.45
1:C:165:GLU:HG3	8:C:912:HOH:O	2.17	0.45
1:C:37:GLN:HG2	1:C:45:LYS:HZ2	1.82	0.45
2:D:55:SER:C	2:D:57:GLY:N	2.75	0.45
2:B:35:HIS:HE1	2:B:50:MET:CE	2.28	0.45
2:B:201:HIS:CD2	2:B:203:PRO:HD2	2.52	0.45
1:C:181:LEU:HD12	1:C:181:LEU:O	2.17	0.45
1:C:13:THR:HG22	1:C:14:THR:N	2.32	0.44
1:C:142:ARG:HB2	1:C:173:TYR:CD2	2.53	0.44
2:D:55:SER:C	2:D:57:GLY:H	2.24	0.44
2:D:147:PHE:C	2:D:147:PHE:CD1	2.94	0.44
2:D:200:ASN:ND2	2:D:207:LYS:HG2	2.31	0.44
1:A:1:GLU:HB3	8:A:1032:HOH:O	2.17	0.44
1:C:140:TYR:CG	1:C:141:PRO:HA	2.53	0.44
2:D:111:THR:HG21	2:D:148:PRO:CG	2.47	0.44
1:C:37:GLN:HE21	1:C:45:LYS:HZ2	1.65	0.44
2:B:83:LEU:CB	2:B:86:LEU:HD21	2.47	0.44
1:C:170:ASP:O	1:C:171:SER:CB	2.65	0.44
2:D:128:SER:O	2:D:215:LYS:NZ	2.47	0.44
2:D:189:SER:HB2	2:D:193:GLN:CD	2.42	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:214:PRO:O	2:D:215:LYS:C	2.61	0.44
1:A:97:THR:HG21	8:A:943:HOH:O	2.17	0.44
1:A:150:VAL:O	1:A:150:VAL:HG23	2.16	0.44
2:B:29:PHE:CE2	2:B:53:PRO:HB3	2.53	0.44
2:B:27:TYR:CE2	2:B:98:ARG:HD3	2.52	0.44
2:B:172:GLN:NE2	2:B:178:SER:HB2	2.33	0.44
2:B:63:LYS:HD2	8:B:1000:HOH:O	2.18	0.44
7:D:217:MMP:H35	7:D:217:MMP:H381	1.99	0.44
1:A:184:ALA:O	1:A:185:ASP:C	2.61	0.44
1:A:29:VAL:HG23	1:A:92:SER:CB	2.48	0.44
2:B:83:LEU:HB3	2:B:86:LEU:HD21	2.00	0.43
1:C:2:LEU:HD11	1:C:25:ALA:HB1	2.00	0.43
1:C:29:VAL:HG23	1:C:30:GLY:N	2.33	0.43
2:B:51:ILE:O	2:B:53:PRO:HD3	2.18	0.43
1:C:155:GLN:NE2	1:C:179:LEU:HD11	2.33	0.43
1:A:193:ALA:HA	1:A:208:SER:HB3	2.01	0.43
1:C:193:ALA:HA	1:C:208:SER:OG	2.17	0.43
2:D:32:TYR:HB3	2:D:98:ARG:HG2	2.00	0.43
2:D:120:PRO:CB	2:D:146:TYR:HB3	2.46	0.43
1:A:150:VAL:CG2	1:A:155:GLN:NE2	2.72	0.43
1:C:156:SER:C	1:C:158:ASN:H	2.27	0.43
2:B:102:ASP:OD1	2:B:102:ASP:N	2.49	0.43
2:B:130:LYS:CG	2:B:131:SER:H	2.09	0.43
1:A:6:GLN:NE2	1:A:101:GLY:C	2.77	0.43
2:B:120:PRO:HB3	2:B:146:TYR:HB3	2.00	0.43
2:D:10:GLU:HA	8:D:255:HOH:O	2.17	0.43
2:B:97:THR:HG21	2:B:101:MET:HG2	2.00	0.43
1:C:154:LEU:H	1:C:154:LEU:CD2	2.27	0.43
2:D:38:LYS:HB2	2:D:48:ILE:HD11	2.00	0.43
2:D:120:PRO:HB3	2:D:146:TYR:CB	2.48	0.43
2:D:199:VAL:CG2	2:D:208:VAL:HB	2.48	0.43
1:A:2:LEU:HD11	1:A:93:SER:HB3	2.00	0.43
1:C:3:VAL:HG22	1:C:26:SER:HB3	2.00	0.43
1:A:115:VAL:HG12	1:A:207:LYS:HG3	2.00	0.43
2:B:61:ASN:O	2:B:63:LYS:N	2.52	0.43
2:B:126:ALA:HA	2:B:127:PRO:HD3	1.85	0.43
1:C:13:THR:CG2	1:C:17:ASP:HB3	2.49	0.43
1:C:54:ARG:NH1	1:C:54:ARG:HB2	2.34	0.43
2:D:156:ASN:HD21	2:D:196:ILE:N	2.09	0.43
1:A:2:LEU:HD23	1:A:27:GLN:HB2	2.00	0.42
2:B:48:ILE:HG21	2:B:81:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LYS:CD	2:B:90:ASP:OD1	2.67	0.42
1:C:142:ARG:HG2	8:C:1023:HOH:O	2.19	0.42
1:C:145:LYS:HB3	1:C:197:THR:HB	2.02	0.42
1:C:150:VAL:HG23	1:C:150:VAL:O	2.19	0.42
2:D:143:VAL:HG11	2:D:151:VAL:HG11	2.01	0.42
1:A:7:THR:OG1	1:A:8:PRO:HA	2.20	0.42
2:B:144:LYS:HE3	2:B:144:LYS:HB2	1.93	0.42
1:A:116:PHE:CD1	1:A:116:PHE:N	2.88	0.42
2:B:97:THR:CG2	2:B:101:MET:HG2	2.50	0.42
2:D:43:ARG:HE	2:D:43:ARG:CA	2.28	0.42
2:D:202:LYS:N	2:D:203:PRO:CD	2.82	0.42
1:C:110:VAL:CG1	1:C:111:ALA:N	2.82	0.42
1:A:83:LEU:HD11	1:A:166:GLN:OE1	2.20	0.42
1:A:209:PHE:CD1	1:A:209:PHE:C	2.97	0.42
2:D:41:PRO:O	2:D:42:GLY:C	2.63	0.42
2:B:76:SER:C	2:B:78:THR:N	2.78	0.42
1:C:94:TYR:OH	2:D:50:MET:HE1	2.20	0.42
1:C:96:LEU:N	1:C:96:LEU:CD1	2.82	0.42
1:A:119:PRO:HG3	1:A:209:PHE:CD2	2.55	0.42
2:B:67:LYS:HD3	2:B:90:ASP:CG	2.44	0.42
2:D:60:TYR:CD1	2:D:60:TYR:N	2.88	0.42
2:B:129:SER:O	2:B:131:SER:N	2.53	0.41
1:C:156:SER:C	1:C:158:ASN:N	2.78	0.41
1:C:155:GLN:OE1	1:C:155:GLN:O	2.37	0.41
2:B:14:PRO:HD3	2:B:113:SER:O	2.20	0.41
1:A:97:THR:HG22	1:A:98:PHE:N	2.35	0.41
2:B:86:LEU:HA	2:B:90:ASP:OD2	2.20	0.41
1:C:96:LEU:CD1	1:C:96:LEU:H	2.33	0.41
2:D:40:ARG:HH11	2:D:40:ARG:HG2	1.86	0.41
1:A:3:VAL:HG13	1:A:26:SER:HB3	2.03	0.41
1:A:115:VAL:O	1:A:207:LYS:HE3	2.20	0.41
1:C:40:PRO:CG	1:C:165:GLU:HG2	2.50	0.41
2:D:127:PRO:O	2:D:128:SER:CB	2.68	0.41
1:A:158:ASN:ND2	1:A:179:LEU:CD1	2.81	0.41
1:A:195:GLU:HB3	8:A:1015:HOH:O	2.20	0.41
1:C:110:VAL:HG12	1:C:111:ALA:N	2.34	0.41
2:D:175:GLY:O	2:D:176:LEU:HD12	2.20	0.41
2:B:14:PRO:HD3	2:B:113:SER:C	2.45	0.41
2:B:171:LEU:HD13	2:B:177:TYR:CZ	2.55	0.41
1:C:117:ILE:HD11	1:C:148:TRP:CH2	2.55	0.41
1:C:154:LEU:HD23	1:C:154:LEU:N	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:51:ILE:HB	2:D:58:THR:HG22	2.02	0.41
2:B:87:THR:C	2:B:89:GLU:N	2.78	0.41
1:C:145:LYS:C	1:C:145:LYS:HD3	2.46	0.41
2:D:127:PRO:O	2:D:215:LYS:NZ	2.40	0.41
2:D:64:PHE:O	2:D:65:LYS:C	2.64	0.40
2:D:65:LYS:HE2	2:D:65:LYS:O	2.20	0.40
1:A:90:GLN:O	1:A:90:GLN:NE2	2.54	0.40
1:A:189:HIS:CE1	8:A:950:HOH:O	2.75	0.40
1:A:189:HIS:O	1:A:211:ARG:NH1	2.54	0.40
1:A:193:ALA:HB2	1:A:208:SER:HB3	2.04	0.40
1:C:35:TRP:CE3	1:C:88:CYS:HB3	2.57	0.40
1:A:181:LEU:C	8:A:964:HOH:O	2.64	0.40
2:B:48:ILE:HD13	2:B:81:MET:HE1	2.03	0.40
2:D:126:ALA:HA	2:D:127:PRO:HD2	1.89	0.40
1:A:90:GLN:HE21	1:A:90:GLN:HB3	1.67	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	211/213 (99%)	192 (91%)	16 (8%)	3 (1%)	9	13
1	C	211/213 (99%)	191 (90%)	17 (8%)	3 (1%)	9	13
2	B	214/216 (99%)	189 (88%)	18 (8%)	7 (3%)	3	2
2	D	214/216 (99%)	190 (89%)	16 (8%)	8 (4%)	2	2
All	All	850/858 (99%)	762 (90%)	67 (8%)	21 (2%)	4	5

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	133	SER
2	D	85	SER
2	D	130	LYS
2	B	62	GLU
2	B	128	SER
2	B	130	LYS
1	C	154	LEU
2	D	9	ALA
2	D	56	GLY
2	D	215	LYS
1	A	138	ASN
2	B	30	THR
1	C	67	SER
1	A	184	ALA
2	D	115	ALA
2	D	133	SER
2	B	85	SER
1	C	31	THR
1	A	31	THR
2	D	134	GLY
2	B	191	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	189/189 (100%)	181 (96%)	8 (4%)	26	45
1	C	189/189 (100%)	182 (96%)	7 (4%)	30	51
2	B	185/185 (100%)	179 (97%)	6 (3%)	34	56
2	D	185/185 (100%)	177 (96%)	8 (4%)	26	44
All	All	748/748 (100%)	719 (96%)	29 (4%)	28	48

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	MET

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Mol	Chain	Res	Type
1	A	13	THR
1	A	19	VAL
1	A	53	ASN
1	A	85	ASP
1	A	90	GLN
1	A	137	ASN
1	A	160	GLN
2	B	67	LYS
2	B	74	LYS
2	B	98	ARG
2	B	148	PRO
2	B	150	PRO
2	B	193	GLN
1	C	2	LEU
1	C	47	LEU
1	C	145	LYS
1	C	154	LEU
1	C	155	GLN
1	C	175	LEU
1	C	183	LYS
2	D	65	LYS
2	D	67	LYS
2	D	148	PRO
2	D	150	PRO
2	D	151	VAL
2	D	202	LYS
2	D	211	LYS
2	D	215	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	6	GLN
1	A	28	ASN
1	A	77	ASN
1	A	79	GLN
1	A	90	GLN
1	A	160	GLN
1	A	189	HIS
2	B	54	ASN
2	B	77	ASN
2	B	156	ASN

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Mol	Chain	Res	Type
2	B	165	HIS
2	B	193	GLN
2	B	200	ASN
2	B	205	ASN
1	C	6	GLN
1	C	28	ASN
1	C	37	GLN
1	C	38	GLN
1	C	77	ASN
1	C	79	GLN
1	C	90	GLN
1	C	138	ASN
1	C	147	GLN
1	C	155	GLN
1	C	158	ASN
1	C	160	GLN
1	C	199	GLN
1	C	210	ASN
2	D	39	GLN
2	D	54	ASN
2	D	82	GLN
2	D	156	ASN
2	D	165	HIS
2	D	172	GLN
2	D	193	GLN
2	D	198	ASN
2	D	200	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MMP	D	217	-	36,47,47	2.67	17 (47%)	29,70,70	2.01	5 (17%)
7	MMP	B	910	-	36,47,47	2.64	17 (47%)	29,70,70	1.97	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MMP	D	217	-	-	7/14/62/62	0/4/5/5
7	MMP	B	910	-	-	5/14/62/62	0/4/5/5

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	217	MMP	C34-C33	6.54	1.46	1.39
7	B	910	MMP	C34-C33	6.20	1.46	1.39
7	D	217	MMP	C31-C32	5.79	1.45	1.39
7	B	910	MMP	C31-C32	5.52	1.45	1.39
7	D	217	MMP	C11-C12	5.32	1.45	1.39
7	B	910	MMP	C11-C12	4.98	1.45	1.39
7	D	217	MMP	O42-C49	4.76	1.37	1.22
7	B	910	MMP	O42-C49	4.74	1.37	1.22
7	D	217	MMP	O32-C39	4.66	1.37	1.22
7	B	910	MMP	O32-C39	4.64	1.37	1.22
7	B	910	MMP	C47-C42	4.49	1.58	1.51
7	D	217	MMP	C47-C42	4.35	1.57	1.51
7	D	217	MMP	C28-C27	-3.99	1.34	1.51
7	B	910	MMP	C28-C27	-3.88	1.35	1.51
7	B	910	MMP	C46-C43	3.14	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	217	MMP	C26-C22	2.98	1.55	1.50
7	D	217	MMP	C1-N1	2.84	1.52	1.46
7	B	910	MMP	C1-N1	2.81	1.52	1.46
7	B	910	MMP	C26-C22	2.79	1.54	1.50
7	D	217	MMP	C11-N1	2.74	1.42	1.38
7	D	217	MMP	C46-C43	2.74	1.54	1.50
7	D	217	MMP	C18-C17	-2.62	1.33	1.50
7	B	910	MMP	C18-C17	-2.60	1.33	1.50
7	B	910	MMP	C16-C12	2.54	1.56	1.51
7	B	910	MMP	C11-N1	2.52	1.42	1.38
7	D	217	MMP	C14-N1	2.38	1.42	1.38
7	D	217	MMP	C37-C33	2.37	1.57	1.52
7	D	217	MMP	C16-C12	2.30	1.56	1.51
7	B	910	MMP	C14-N1	2.23	1.42	1.38
7	B	910	MMP	O41-C49	2.19	1.38	1.30
7	B	910	MMP	C37-C33	2.13	1.57	1.52
7	D	217	MMP	O31-C39	2.07	1.37	1.30
7	B	910	MMP	O31-C39	2.04	1.37	1.30
7	D	217	MMP	O41-C49	2.00	1.37	1.30

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	217	MMP	C28-C27-C23	5.75	121.10	112.87
7	B	910	MMP	C28-C27-C23	5.48	120.71	112.87
7	D	217	MMP	C14-N1-C11	-4.74	105.36	108.59
7	B	910	MMP	C14-N1-C11	-4.62	105.44	108.59
7	D	217	MMP	C18-C17-C13	4.13	122.21	112.32
7	B	910	MMP	C1-N1-C14	-3.75	117.31	124.58
7	B	910	MMP	C18-C17-C13	3.73	121.26	112.32
7	D	217	MMP	C1-N1-C14	-3.58	117.63	124.58
7	B	910	MMP	C1-N1-C11	-3.00	118.76	124.58
7	D	217	MMP	C1-N1-C11	-2.90	118.96	124.58

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	D	217	MMP	C32-C33-C37-C38
7	D	217	MMP	C34-C33-C37-C38
7	D	217	MMP	C42-C47-C48-C49
7	B	910	MMP	C42-C47-C48-C49

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Mol	Chain	Res	Type	Atoms
7	B	910	MMP	C37-C38-C39-O32
7	B	910	MMP	C37-C38-C39-O31
7	B	910	MMP	C47-C48-C49-O41
7	D	217	MMP	C37-C38-C39-O31
7	D	217	MMP	C37-C38-C39-O32
7	B	910	MMP	C47-C48-C49-O42
7	D	217	MMP	C47-C48-C49-O41
7	D	217	MMP	C47-C48-C49-O42

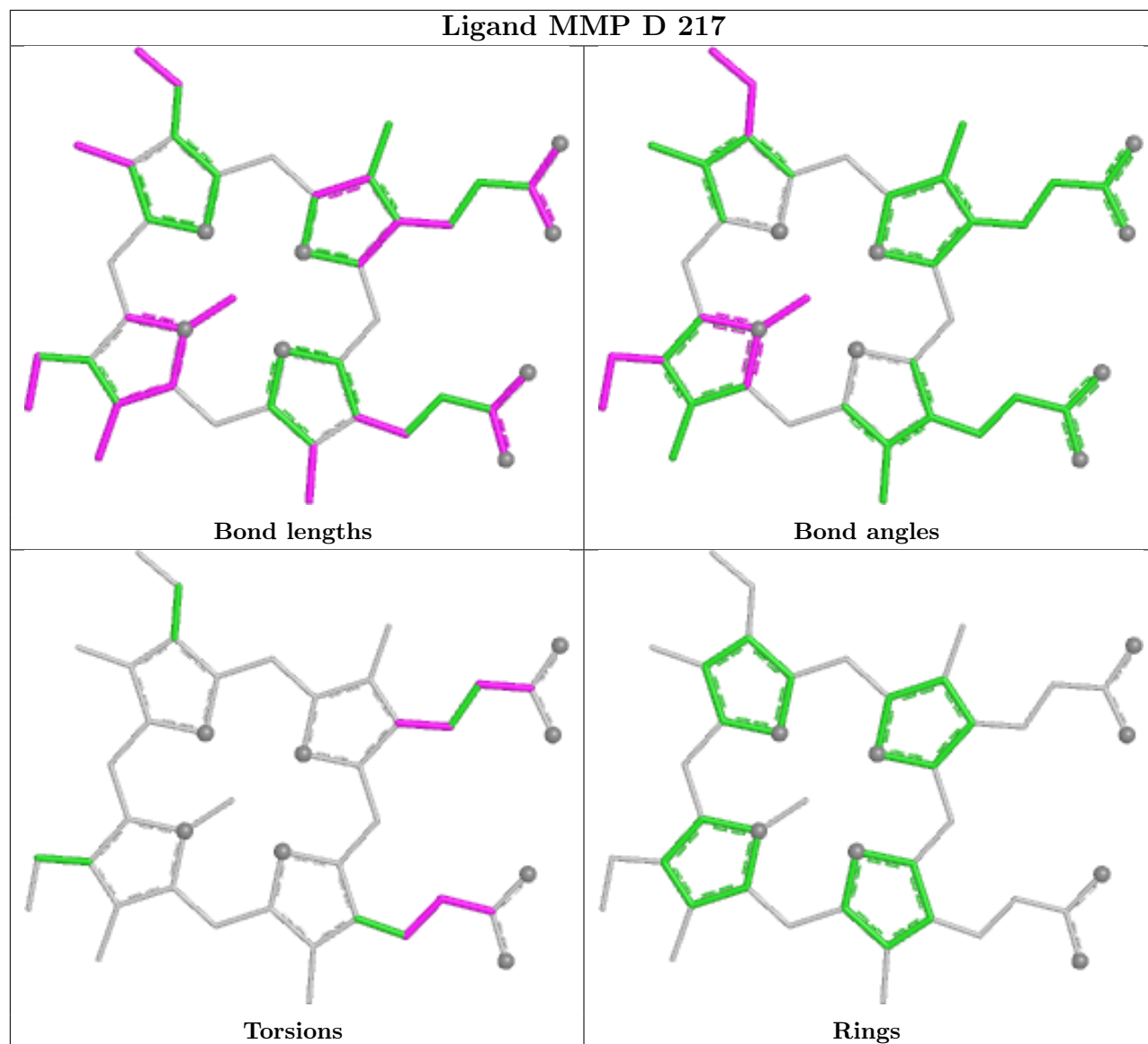
There are no ring outliers.

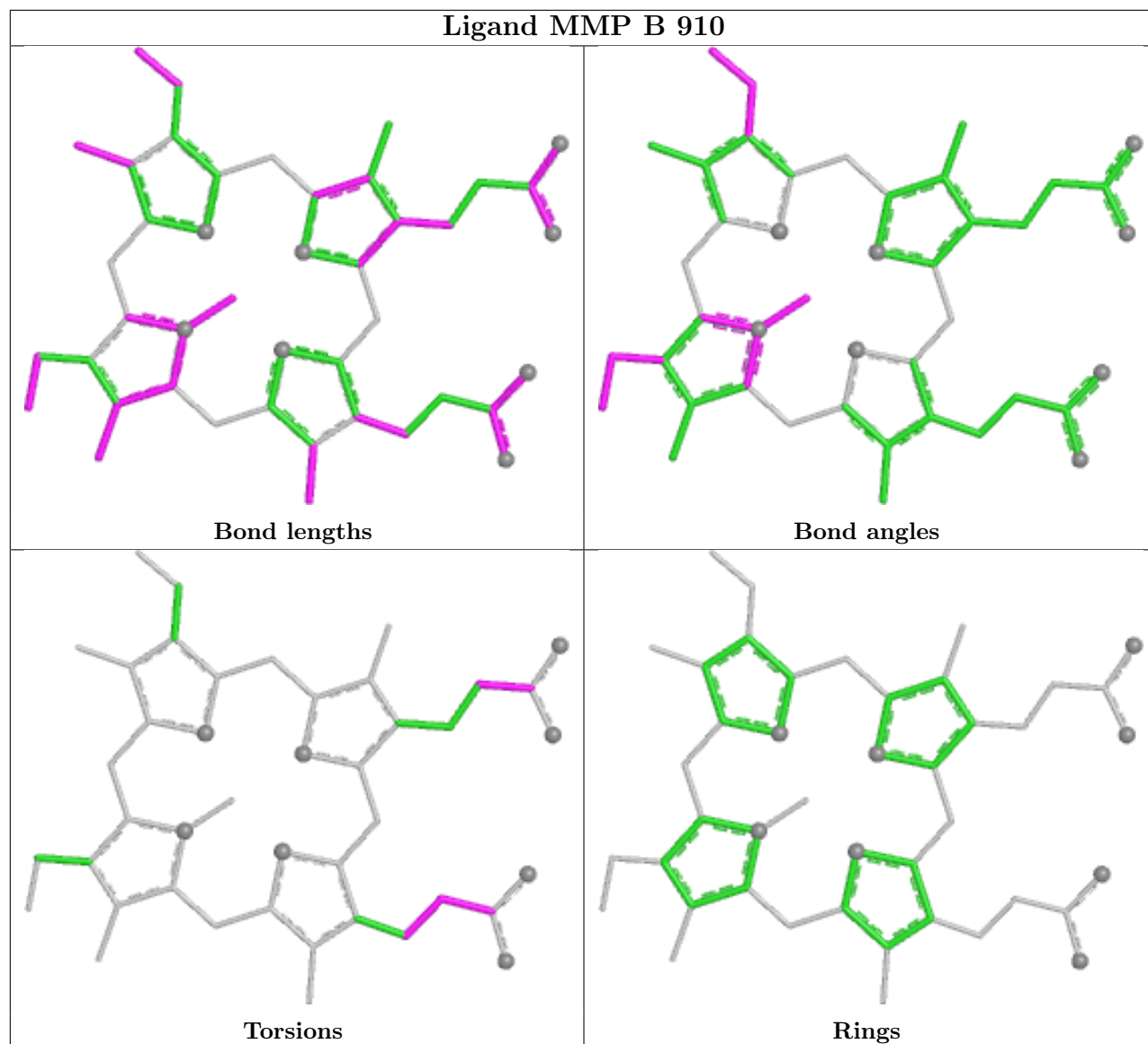
2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	D	217	MMP	1	0
7	B	910	MMP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand MMP D 217





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	213/213 (100%)	-0.02	2 (0%) 81 78	12, 28, 43, 70	0
1	C	213/213 (100%)	0.36	12 (5%) 30 26	14, 31, 67, 99	0
2	B	216/216 (100%)	0.04	10 (4%) 37 33	8, 26, 54, 78	0
2	D	216/216 (100%)	0.33	5 (2%) 61 57	17, 37, 59, 90	0
All	All	858/858 (100%)	0.18	29 (3%) 48 44	8, 30, 60, 99	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	158	ASN	4.8
2	B	132	THR	4.1
1	A	212	ASN	3.7
2	B	133	SER	3.6
1	C	192	TYR	3.4
2	B	129	SER	3.4
2	B	130	LYS	3.2
2	D	132	THR	3.1
1	A	213	GLU	3.0
1	C	209	PHE	2.9
1	C	155	GLN	2.8
1	C	212	ASN	2.8
1	C	210	ASN	2.8
2	D	129	SER	2.8
1	C	191	VAL	2.7
2	B	8	GLY	2.6
2	D	8	GLY	2.4
1	C	77	ASN	2.4
2	D	92	ALA	2.4
1	C	154	LEU	2.2
1	C	211	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	186	TYR	2.2
2	B	128	SER	2.2
2	B	134	GLY	2.1
2	B	131	SER	2.1
2	B	135	GLY	2.1
1	C	208	SER	2.1
2	B	44	GLY	2.1
2	D	51	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

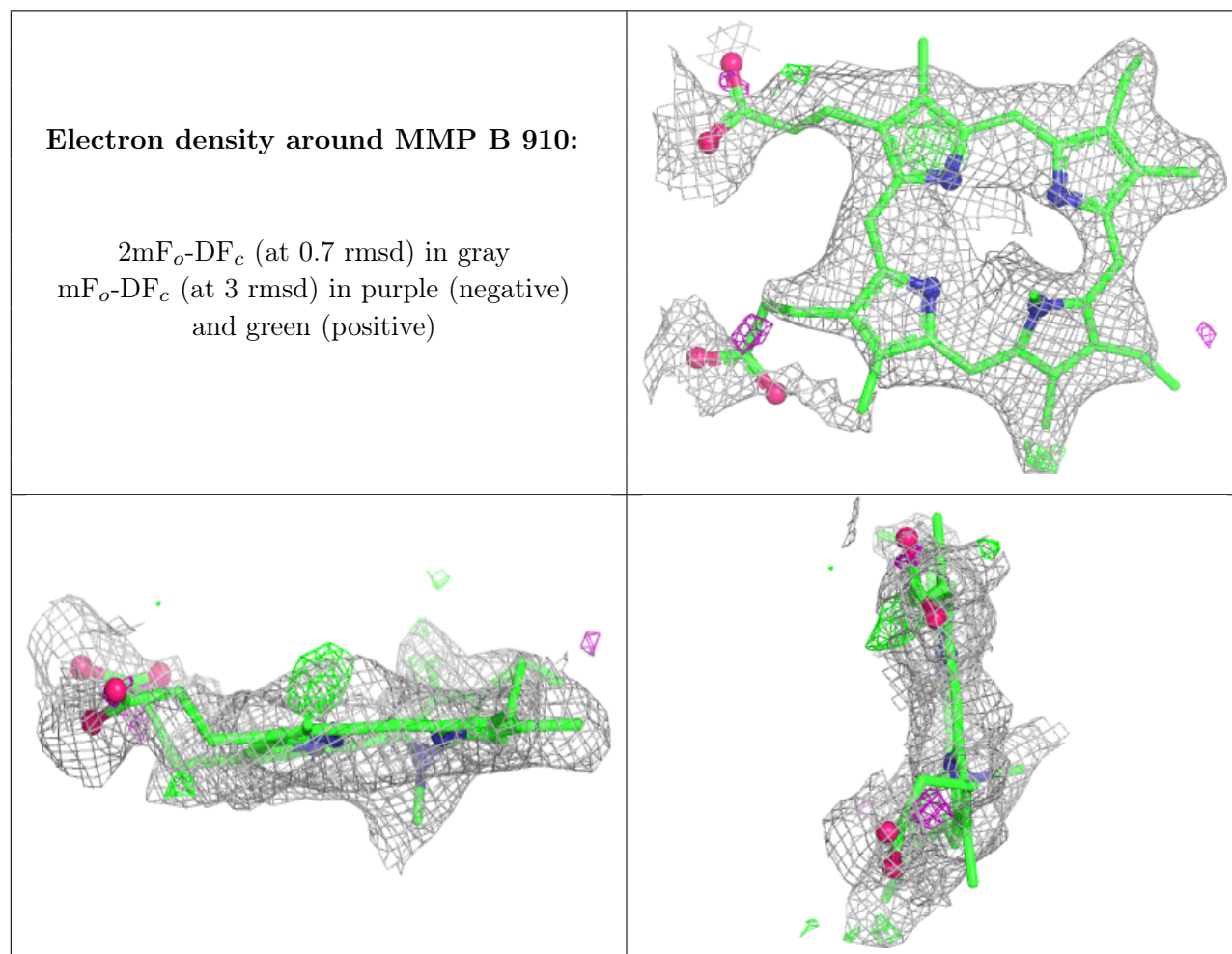
6.4 Ligands ⓘ

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
7	MMP	B	910	43/43	0.78	0.15	47,55,63,66	0
6	NA	C	904	1/1	0.82	0.14	50,50,50,50	0
7	MMP	D	217	43/43	0.83	0.14	39,49,58,62	0
6	NA	C	907	1/1	0.91	0.11	14,14,14,14	0
6	NA	A	908	1/1	0.94	0.09	14,14,14,14	0
6	NA	B	905	1/1	0.95	0.08	16,16,16,16	0
6	NA	C	906	1/1	0.96	0.05	19,19,19,19	0
6	NA	C	910	1/1	0.96	0.07	20,20,20,20	0
5	MG	A	903	1/1	0.97	0.06	20,20,20,20	0
6	NA	B	909	1/1	0.97	0.11	16,16,16,16	0
4	CA	A	902	1/1	0.98	0.06	35,35,35,35	0
3	CD	A	901	1/1	0.99	0.02	27,27,27,27	0

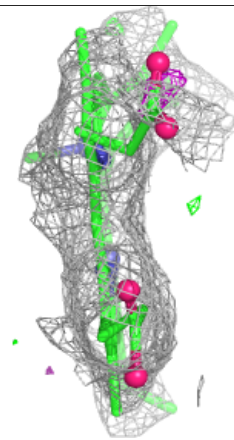
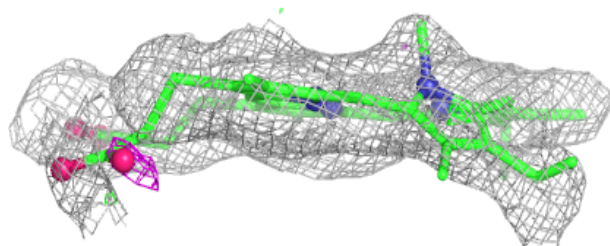
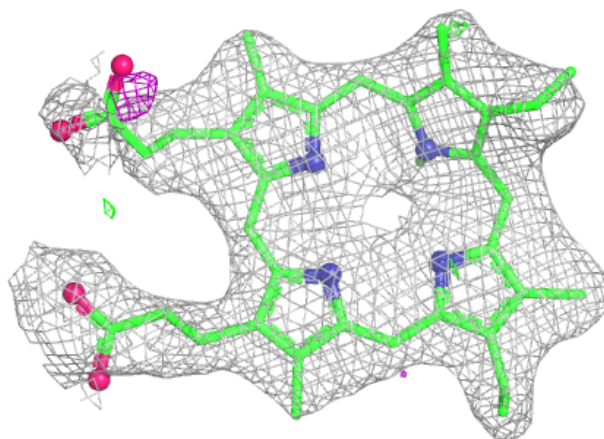
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

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 MMP D 217:

$2mF_o - DF_c$ (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.