



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 03:06 PM UTC

PDB ID : 6LTD / pdb_00006ltd
Title : Crystal Structure of Nonribosomal peptide synthetases (NRPS), FmoA3 (S10 46A)-alpha-methyl-L-serine-AMP bound form
Authors : Senda, T.; Harada, A.
Deposited on : 2020-01-22
Resolution : 4.10 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

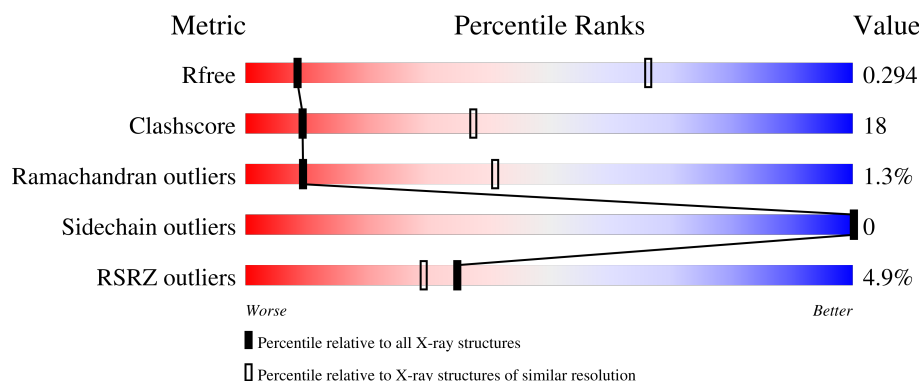
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.10 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	1243 (4.40-3.80)
Clashscore	190562	1293 (4.40-3.80)
Ramachandran outliers	187476	1206 (4.40-3.80)
Sidechain outliers	187428	1193 (4.40-3.80)
RSRZ outliers	180081	1240 (4.40-3.80)

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	1153	3% 52% 25% 23%
1	B	1153	4% 52% 24% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	AMP	B	1201	-	X	-	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12031 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 Nonribosomal peptide synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	883	Total	C	N	O	S	0	1	0
			5996	3805	1032	1149	10			
1	B	882	Total	C	N	O	S	0	0	0
			5975	3786	1035	1142	12			

There are 54 discrepancies between the modelled and reference sequences:

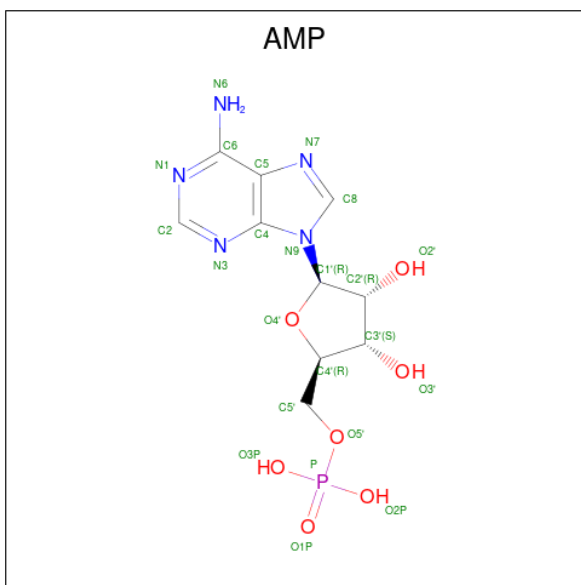
Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP A0A077JG85
A	-14	ASN	-	expression tag	UNP A0A077JG85
A	-13	HIS	-	expression tag	UNP A0A077JG85
A	-12	LYS	-	expression tag	UNP A0A077JG85
A	-11	VAL	-	expression tag	UNP A0A077JG85
A	-10	HIS	-	expression tag	UNP A0A077JG85
A	-9	HIS	-	expression tag	UNP A0A077JG85
A	-8	HIS	-	expression tag	UNP A0A077JG85
A	-7	HIS	-	expression tag	UNP A0A077JG85
A	-6	HIS	-	expression tag	UNP A0A077JG85
A	-5	HIS	-	expression tag	UNP A0A077JG85
A	-4	ILE	-	expression tag	UNP A0A077JG85
A	-3	GLU	-	expression tag	UNP A0A077JG85
A	-2	GLY	-	expression tag	UNP A0A077JG85
A	-1	ARG	-	expression tag	UNP A0A077JG85
A	0	HIS	-	expression tag	UNP A0A077JG85
A	1046	ALA	SER	engineered mutation	UNP A0A077JG85
A	1128	SER	-	expression tag	UNP A0A077JG85
A	1129	ALA	-	expression tag	UNP A0A077JG85
A	1130	TRP	-	expression tag	UNP A0A077JG85
A	1131	SER	-	expression tag	UNP A0A077JG85
A	1132	HIS	-	expression tag	UNP A0A077JG85
A	1133	PRO	-	expression tag	UNP A0A077JG85
A	1134	GLN	-	expression tag	UNP A0A077JG85
A	1135	PHE	-	expression tag	UNP A0A077JG85

Continued on next page...

Continued from previous page...

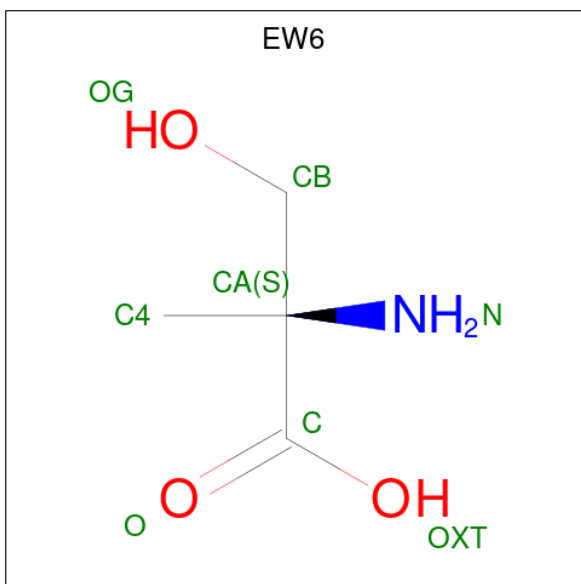
Chain	Residue	Modelled	Actual	Comment	Reference
A	1136	GLU	-	expression tag	UNP A0A077JG85
A	1137	LYS	-	expression tag	UNP A0A077JG85
B	-15	MET	-	expression tag	UNP A0A077JG85
B	-14	ASN	-	expression tag	UNP A0A077JG85
B	-13	HIS	-	expression tag	UNP A0A077JG85
B	-12	LYS	-	expression tag	UNP A0A077JG85
B	-11	VAL	-	expression tag	UNP A0A077JG85
B	-10	HIS	-	expression tag	UNP A0A077JG85
B	-9	HIS	-	expression tag	UNP A0A077JG85
B	-8	HIS	-	expression tag	UNP A0A077JG85
B	-7	HIS	-	expression tag	UNP A0A077JG85
B	-6	HIS	-	expression tag	UNP A0A077JG85
B	-5	HIS	-	expression tag	UNP A0A077JG85
B	-4	ILE	-	expression tag	UNP A0A077JG85
B	-3	GLU	-	expression tag	UNP A0A077JG85
B	-2	GLY	-	expression tag	UNP A0A077JG85
B	-1	ARG	-	expression tag	UNP A0A077JG85
B	0	HIS	-	expression tag	UNP A0A077JG85
B	1046	ALA	SER	engineered mutation	UNP A0A077JG85
B	1128	SER	-	expression tag	UNP A0A077JG85
B	1129	ALA	-	expression tag	UNP A0A077JG85
B	1130	TRP	-	expression tag	UNP A0A077JG85
B	1131	SER	-	expression tag	UNP A0A077JG85
B	1132	HIS	-	expression tag	UNP A0A077JG85
B	1133	PRO	-	expression tag	UNP A0A077JG85
B	1134	GLN	-	expression tag	UNP A0A077JG85
B	1135	PHE	-	expression tag	UNP A0A077JG85
B	1136	GLU	-	expression tag	UNP A0A077JG85
B	1137	LYS	-	expression tag	UNP A0A077JG85

- Molecule 2 is ADENOSINE MONOPHOSPHATE (CCD ID: AMP) (formula: $C_{10}H_{14}N_5O_7P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			23	10	5	7	1		
2	B	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 3 is alpha-methyl-L-serine (CCD ID: EW6) (formula: $C_4H_9NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			7	4	1	2		

Continued on next page...

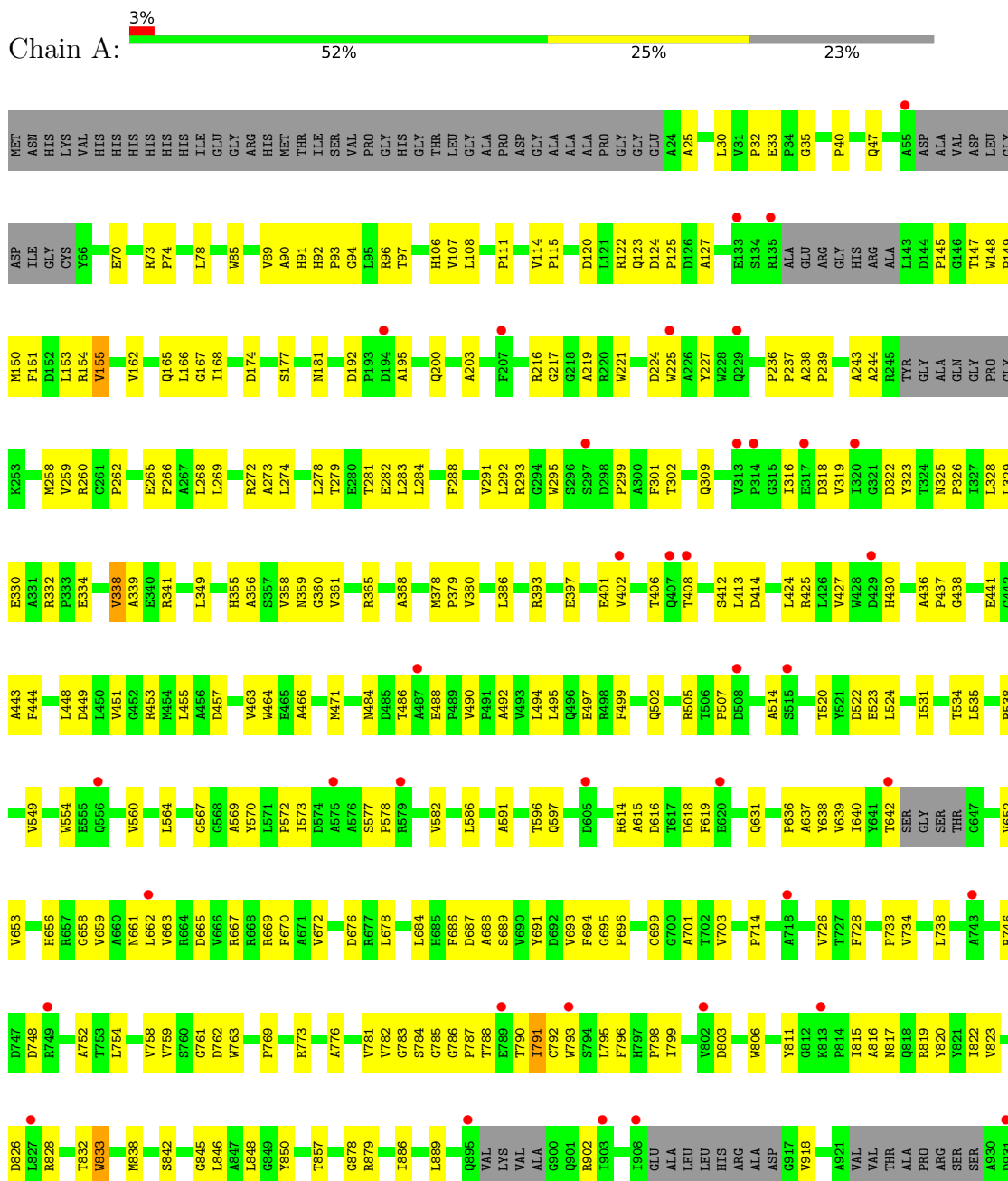
Continued from previous page...

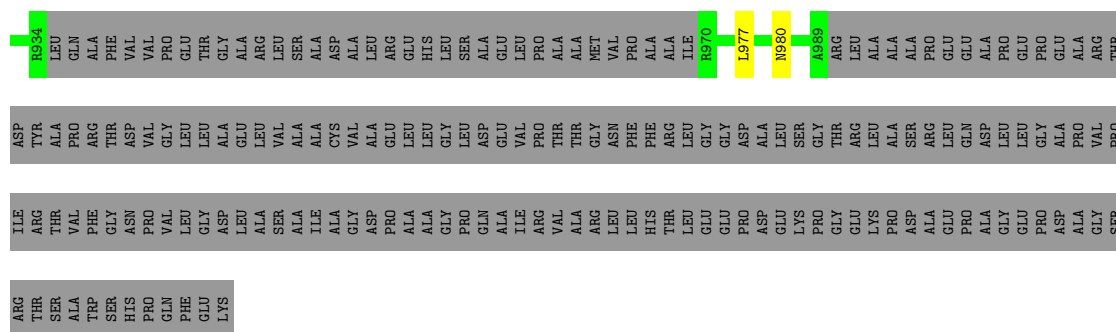
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			7	4	1	2		

3 Residue-property plots

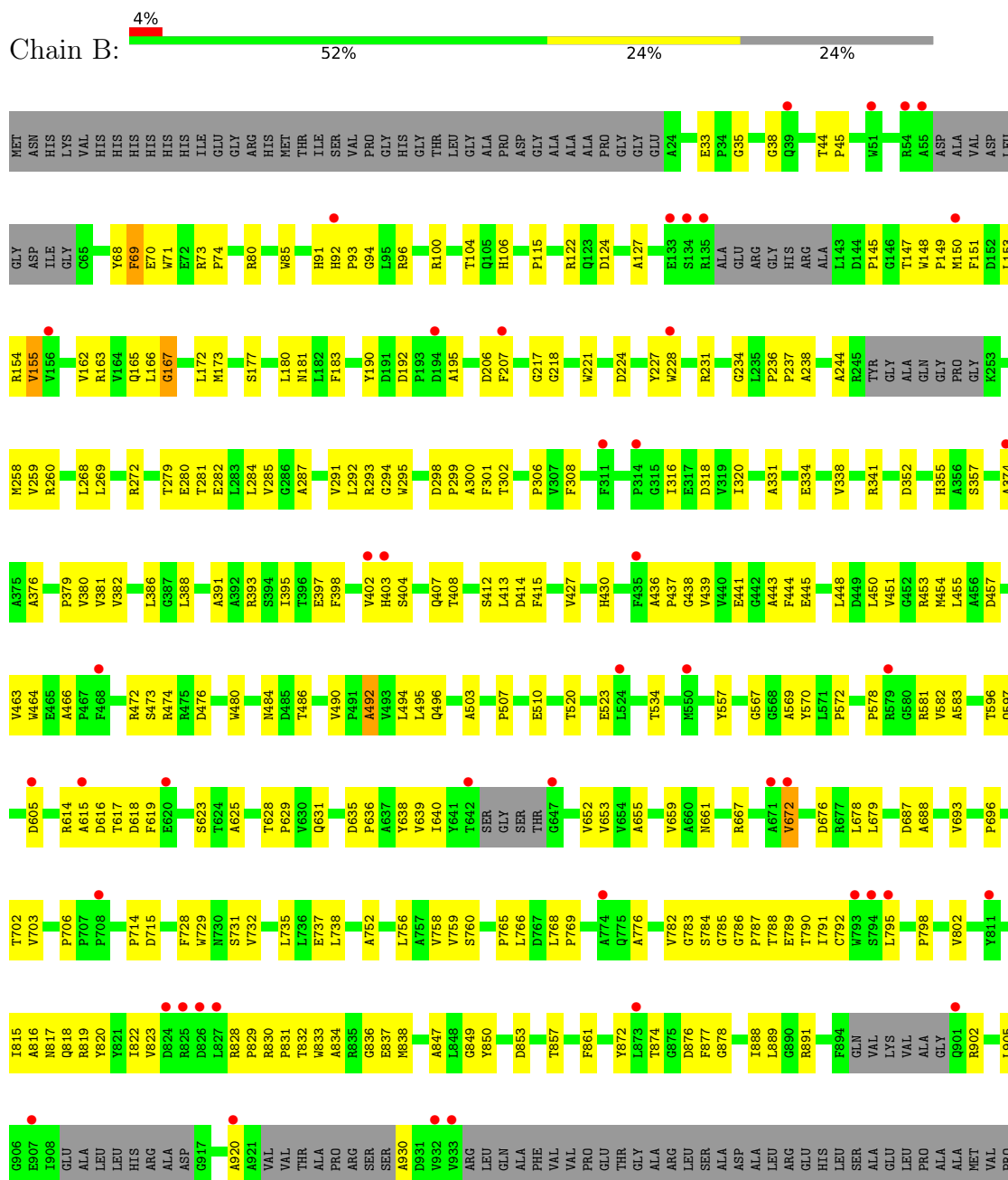
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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





• Molecule 1: Nonribosomal peptide synthetase



[illegible]

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	96.62Å 97.05Å 107.82Å 69.71° 74.91° 63.96°	Depositor
Resolution (Å)	48.15 – 4.10 48.15 – 4.10	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.15-4.10) 98.8 (48.15-4.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 4.14Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.237 , 0.297 0.236 , 0.294	Depositor DCC
R_{free} test set	1204 reflections (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	133.6	Xtriage
Anisotropy	0.615	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 175.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	12031	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EW6, AMP

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	0.50	0/6145	0.76	0/8493
1	B	0.52	0/6128	0.79	0/8471
All	All	0.51	0/12273	0.77	0/16964

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5996	0	5204	212	0
1	B	5975	0	5103	190	0
2	A	23	0	12	5	0
2	B	23	0	11	5	0
3	A	7	0	0	2	0
3	B	7	0	0	2	0
All	All	12031	0	10330	403	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (403) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:787:PRO:O	1:B:790:THR:HG22	1.52	1.09
1:A:787:PRO:O	1:A:790:THR:HG22	1.53	1.09
1:B:258:MET:HB2	1:B:427:VAL:HG22	1.47	0.96
1:A:329:LEU:HD22	1:A:349:LEU:HD13	1.53	0.89
1:B:787:PRO:HB3	2:B:1201:AMP:H5'2	1.54	0.87
1:B:520:THR:HG23	1:B:523:GLU:H	1.37	0.87
1:A:549:VAL:HG22	1:A:573:ILE:HB	1.58	0.85
1:B:667:ARG:HA	1:B:672:VAL:HG21	1.60	0.83
1:B:920:ALA:HA	1:B:930:ALA:HA	1.62	0.81
1:B:484:ASN:HB3	1:B:819:ARG:HG2	1.61	0.81
1:B:147:THR:HG22	1:B:149:PRO:HD2	1.64	0.78
1:A:334:GLU:O	1:A:341:ARG:HA	1.85	0.75
1:A:379:PRO:HB2	1:A:412:SER:OG	1.86	0.75
1:A:260:ARG:NH2	1:A:425:ARG:HE	1.86	0.74
1:A:484:ASN:HB3	1:A:819:ARG:HG2	1.70	0.73
1:A:279:THR:H	1:A:282:GLU:HB2	1.54	0.72
1:B:334:GLU:O	1:B:341:ARG:HA	1.89	0.71
1:B:413:LEU:HD13	1:B:430:HIS:HB3	1.72	0.71
1:B:490:VAL:HG21	1:B:661:ASN:HB2	1.71	0.71
1:B:822:ILE:O	1:B:830:ARG:HG2	1.90	0.71
1:A:639:VAL:HA	1:A:652:VAL:O	1.91	0.71
1:B:678:LEU:HD12	1:B:728:PHE:CD2	2.26	0.70
1:A:273:ALA:HB2	1:A:283:LEU:HD23	1.72	0.70
1:A:878:GLY:HA2	1:A:889:LEU:HG	1.74	0.69
1:B:295:TRP:CH2	1:B:443:ALA:HA	2.27	0.69
1:B:878:GLY:HA2	1:B:889:LEU:HG	1.75	0.69
1:B:244:ALA:HB2	1:B:436:ALA:HA	1.75	0.68
1:A:279:THR:HG23	1:A:282:GLU:HG3	1.75	0.68
1:B:850:TYR:HB2	1:B:857:THR:OG1	1.93	0.68
1:A:258:MET:HB2	1:A:427:VAL:HG22	1.76	0.68
1:B:227:TYR:CE1	1:B:231:ARG:HD2	2.29	0.68
1:B:679:LEU:HD23	1:B:729:TRP:HZ3	1.58	0.67
1:A:787:PRO:HB3	2:A:1201:AMP:H5'2	1.77	0.67
1:B:639:VAL:HA	1:B:652:VAL:O	1.94	0.67
1:A:413:LEU:HD13	1:A:430:HIS:HB3	1.77	0.67
1:A:96:ARG:HA	1:A:148:TRP:HE1	1.60	0.66
1:A:326:PRO:HG2	1:A:360:GLY:HA3	1.77	0.66
1:A:787:PRO:HB3	2:A:1201:AMP:H3'	1.77	0.66
1:A:850:TYR:HB2	1:A:857:THR:OG1	1.96	0.66
1:B:752:ALA:HA	1:B:776:ALA:HB2	1.78	0.66
1:A:678:LEU:HD12	1:A:728:PHE:CD2	2.31	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:842:SER:HB3	1:A:846:LEU:HG	1.77	0.65
1:B:572:PRO:HD2	1:B:639:VAL:O	1.97	0.65
1:B:891:ARG:HD2	2:B:1201:AMP:O2'	1.97	0.65
1:A:90:ALA:O	1:A:92:HIS:N	2.30	0.64
1:A:237:PRO:O	1:A:301:PHE:HA	1.97	0.64
1:A:815:ILE:HG12	1:A:816:ALA:H	1.61	0.64
1:A:520:THR:HG23	1:A:523:GLU:H	1.62	0.64
1:B:69:PHE:HA	1:B:404:SER:HB2	1.80	0.64
1:B:495:LEU:HD11	1:B:659:VAL:HB	1.81	0.63
1:A:260:ARG:HH22	1:A:425:ARG:HE	1.46	0.63
1:B:760:SER:HB3	1:B:784:SER:H	1.63	0.63
1:B:438:GLY:O	1:B:441:GLU:N	2.32	0.62
1:A:272:ARG:HD2	1:A:464:TRP:CZ2	2.35	0.62
1:B:281:THR:O	1:B:285:VAL:HG23	1.99	0.62
1:A:272:ARG:HD2	1:A:464:TRP:HZ2	1.64	0.61
1:B:687:ASP:HB2	1:B:788:THR:OG1	2.00	0.61
1:A:166:LEU:HG	1:A:167:GLY:O	2.00	0.61
1:A:502:GLN:OE1	1:A:505:ARG:NH2	2.31	0.61
1:B:80:ARG:NH1	1:B:190:TYR:O	2.32	0.61
1:A:217:GLY:H	1:A:221:TRP:CG	2.18	0.61
1:A:782:VAL:HG22	1:A:798:PRO:HA	1.83	0.61
1:B:714:PRO:HG3	1:B:738:LEU:HB3	1.81	0.61
1:B:823:VAL:HG12	1:B:829:PRO:HA	1.83	0.61
1:A:822:ILE:HD11	1:A:838:MET:HG2	1.82	0.61
1:B:667:ARG:HA	1:B:672:VAL:CG2	2.29	0.61
1:B:70:GLU:HG3	1:B:165:GLN:HG2	1.82	0.60
1:A:490:VAL:HG21	1:A:661:ASN:HB2	1.82	0.60
1:B:306:PRO:HD2	1:B:382:VAL:O	2.01	0.60
1:B:679:LEU:HD23	1:B:729:TRP:CZ3	2.35	0.60
1:A:269:LEU:HD11	1:A:283:LEU:HD11	1.83	0.60
1:A:258:MET:HE3	1:A:260:ARG:HG3	1.83	0.60
1:A:572:PRO:HD2	1:A:639:VAL:O	2.01	0.60
1:B:166:LEU:HG	1:B:167:GLY:O	2.01	0.59
1:B:379:PRO:HB2	1:B:412:SER:OG	2.02	0.59
1:A:642:THR:HG21	1:A:788:THR:HG21	1.84	0.59
1:B:293:ARG:HG2	1:B:299:PRO:HA	1.83	0.59
1:A:787:PRO:HD2	1:A:790:THR:HG21	1.85	0.59
1:A:746:ARG:NH2	1:A:748:ASP:OD2	2.34	0.58
1:B:688:ALA:HA	1:B:792:CYS:SG	2.42	0.58
1:A:823:VAL:HA	1:A:828:ARG:O	2.02	0.58
1:B:338:VAL:O	1:B:341:ARG:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ARG:O	1:B:162:VAL:HG12	2.03	0.58
1:A:89:VAL:HG21	1:A:114:VAL:HG22	1.86	0.58
1:B:33:GLU:O	1:B:35:GLY:N	2.36	0.57
1:A:244:ALA:HB2	1:A:436:ALA:HA	1.86	0.57
1:B:486:THR:O	1:B:817:ASN:N	2.34	0.57
1:A:295:TRP:CH2	1:A:443:ALA:HA	2.40	0.57
1:B:259:VAL:HG11	1:B:448:LEU:HD21	1.86	0.57
1:B:486:THR:HB	1:B:816:ALA:HA	1.86	0.57
1:A:444:PHE:CE2	1:A:448:LEU:HD11	2.40	0.57
1:A:691:TYR:O	1:A:696:PRO:HD3	2.05	0.56
1:A:258:MET:HG3	1:A:259:VAL:N	2.21	0.56
1:A:70:GLU:HG3	1:A:165:GLN:HG2	1.87	0.56
1:B:457:ASP:OD2	1:B:463:VAL:HG12	2.05	0.56
1:A:273:ALA:CB	1:A:283:LEU:HD23	2.35	0.56
1:B:782:VAL:HG22	1:B:798:PRO:HA	1.88	0.56
1:B:192:ASP:HB3	1:B:195:ALA:HB2	1.88	0.56
1:B:279:THR:O	1:B:282:GLU:N	2.33	0.56
1:A:781:VAL:HG12	1:A:799:ILE:HD12	1.86	0.55
1:A:495:LEU:HD11	1:A:659:VAL:HB	1.88	0.55
1:B:154:ARG:O	1:B:155:VAL:HG23	2.07	0.55
1:A:437:PRO:HD2	1:A:833:TRP:CZ2	2.42	0.55
1:B:236:PRO:O	1:B:302:THR:OG1	2.19	0.55
1:B:450:LEU:HD11	1:B:454:MET:HE3	1.89	0.55
1:A:667:ARG:HA	1:A:672:VAL:HB	1.88	0.55
1:B:795:LEU:HD13	1:B:820:TYR:CE2	2.41	0.55
1:A:586:LEU:HD23	1:A:591:ALA:HB3	1.89	0.54
1:A:492:ALA:O	1:B:268:LEU:HD22	2.07	0.54
1:A:616:ASP:OD1	1:A:616:ASP:N	2.39	0.54
1:B:572:PRO:CG	1:B:640:ILE:HG12	2.38	0.54
1:B:224:ASP:OD2	1:B:357:SER:OG	2.24	0.54
1:B:163:ARG:CZ	1:B:402:VAL:HG11	2.37	0.54
1:A:784:SER:HB2	1:A:796:PHE:CE1	2.42	0.54
1:B:616:ASP:OD1	1:B:616:ASP:N	2.35	0.54
1:B:653:VAL:O	1:B:847:ALA:HB1	2.07	0.54
1:A:451:VAL:O	1:A:455:LEU:HG	2.08	0.54
1:B:758:VAL:HA	1:B:782:VAL:O	2.07	0.54
1:A:769:PRO:O	1:A:773:ARG:HB2	2.08	0.54
1:A:686:PHE:HB2	1:A:980:ASN:OD1	2.08	0.53
1:B:731:SER:O	1:B:759:VAL:HA	2.08	0.53
1:B:557:TYR:HE2	1:B:693:VAL:HA	1.72	0.53
1:B:765:PRO:HB2	1:B:768:LEU:HB2	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:787:PRO:CD	1:A:790:THR:HG21	2.38	0.53
1:B:269:LEU:HD21	1:B:284:LEU:HD11	1.88	0.53
1:B:788:THR:HB	2:B:1201:AMP:P	2.48	0.53
1:A:258:MET:HE1	1:A:260:ARG:HH21	1.74	0.53
1:A:614:ARG:O	1:A:618:ASP:HB2	2.09	0.53
1:A:678:LEU:HD12	1:A:728:PHE:CG	2.43	0.53
1:B:614:ARG:O	1:B:618:ASP:HB2	2.08	0.53
1:A:85:TRP:CH2	1:A:153:LEU:HD11	2.44	0.53
1:B:784:SER:OG	1:B:785:GLY:N	2.41	0.53
1:A:147:THR:HG22	1:A:149:PRO:HD2	1.91	0.52
1:A:653:VAL:HG12	1:A:848:LEU:HB2	1.91	0.52
1:A:149:PRO:C	1:A:151:PHE:H	2.16	0.52
1:A:328:LEU:HD13	1:A:378:MET:HE3	1.92	0.52
1:A:567:GLY:HA2	1:A:631:GLN:NE2	2.25	0.52
1:A:393:ARG:NH2	1:A:397:GLU:OE1	2.40	0.52
1:A:784:SER:HB2	1:A:796:PHE:CD1	2.44	0.52
1:A:457:ASP:OD2	1:A:463:VAL:HG12	2.10	0.52
1:A:499:PHE:CZ	1:A:524:LEU:HD23	2.45	0.51
1:A:30:LEU:O	1:A:32:PRO:HD3	2.10	0.51
1:B:413:LEU:HD12	1:B:414:ASP:H	1.75	0.51
1:B:623:SER:C	1:B:625:ALA:H	2.19	0.51
1:B:115:PRO:HD3	1:B:148:TRP:HZ3	1.74	0.51
1:B:227:TYR:HB2	1:B:355:HIS:CD2	2.45	0.51
1:A:758:VAL:HG11	1:A:793:TRP:CE2	2.46	0.51
1:B:44:THR:HB	1:B:45:PRO:HD2	1.92	0.51
1:B:567:GLY:HA2	1:B:631:GLN:NE2	2.24	0.51
1:B:849:GLY:HA3	1:B:857:THR:HG23	1.92	0.51
1:B:473:SER:O	1:B:476:ASP:HB2	2.10	0.51
1:B:687:ASP:OD2	1:B:792:CYS:HA	2.11	0.51
1:A:192:ASP:HB3	1:A:195:ALA:HB2	1.92	0.51
1:A:762:ASP:CG	1:A:763:TRP:H	2.19	0.51
1:A:826:ASP:HB2	1:A:828:ARG:HG3	1.93	0.51
1:B:217:GLY:H	1:B:221:TRP:CG	2.28	0.51
1:B:815:ILE:HG22	1:B:818:GLN:HG3	1.92	0.51
1:A:319:VAL:O	1:A:323:TYR:OH	2.22	0.51
1:B:787:PRO:O	1:B:790:THR:N	2.43	0.51
1:B:836:GLY:O	1:B:877:PHE:HA	2.11	0.51
1:A:200:GLN:NE2	1:A:318:ASP:O	2.43	0.51
1:A:687:ASP:HB2	1:A:788:THR:OG1	2.10	0.51
1:B:503:ALA:O	1:B:507:PRO:HB3	2.10	0.50
1:B:177:SER:HA	1:B:181:ASN:OD1	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:766:LEU:O	1:B:802:VAL:HG21	2.10	0.50
1:A:25:ALA:HB1	1:A:219:ALA:HB1	1.94	0.50
1:B:124:ASP:O	1:B:127:ALA:HB2	2.12	0.50
1:A:560:VAL:HG22	1:A:570:TYR:CD2	2.47	0.50
1:B:393:ARG:HE	1:B:397:GLU:CD	2.19	0.50
1:B:765:PRO:O	1:B:769:PRO:HD3	2.11	0.50
1:B:737:GLU:HB2	1:B:768:LEU:HD22	1.94	0.50
1:A:393:ARG:HE	1:A:397:GLU:CD	2.19	0.49
1:A:406:THR:HG22	1:A:408:THR:H	1.77	0.49
1:A:124:ASP:O	1:A:127:ALA:HB2	2.12	0.49
1:B:830:ARG:HH12	1:B:834:ALA:C	2.21	0.49
1:A:40:PRO:HG3	1:A:106:HIS:HB3	1.93	0.49
1:A:167:GLY:O	1:A:168:ILE:HB	2.11	0.49
1:B:437:PRO:HD2	1:B:833:TRP:CZ2	2.47	0.49
1:B:636:PRO:HA	1:B:655:ALA:HA	1.94	0.49
1:A:359:ASN:OD1	1:A:361:VAL:HG23	2.12	0.49
1:B:85:TRP:CE2	1:B:153:LEU:HD21	2.48	0.49
1:B:279:THR:O	1:B:280:GLU:C	2.55	0.49
1:B:823:VAL:O	1:B:837:GLU:N	2.45	0.49
1:A:291:VAL:HA	1:A:471:MET:HE3	1.95	0.49
1:A:438:GLY:HA2	1:A:441:GLU:OE1	2.13	0.48
1:B:293:ARG:NH1	1:B:299:PRO:O	2.42	0.48
1:A:330:GLU:HG2	1:A:332:ARG:HG3	1.95	0.48
1:A:752:ALA:HA	1:A:776:ALA:HB2	1.94	0.48
1:A:833:TRP:O	1:A:879:ARG:HD2	2.14	0.48
1:A:73:ARG:O	1:A:162:VAL:HG12	2.13	0.48
1:A:615:ALA:HA	1:A:619:PHE:HD2	1.78	0.48
1:B:759:VAL:O	1:B:783:GLY:HA2	2.13	0.48
1:A:878:GLY:HA2	1:A:889:LEU:CG	2.41	0.48
1:A:260:ARG:CZ	1:A:425:ARG:HE	2.27	0.48
1:A:488:GLU:H	1:A:817:ASN:HD21	1.60	0.48
1:A:534:THR:HB	1:A:619:PHE:HE1	1.78	0.48
1:B:231:ARG:O	1:B:234:GLY:N	2.41	0.48
1:B:849:GLY:CA	1:B:857:THR:HG23	2.44	0.48
1:A:578:PRO:O	1:A:582:VAL:HG23	2.14	0.48
1:A:811:TYR:N	1:A:886:ILE:O	2.43	0.47
1:B:258:MET:HE1	1:B:260:ARG:NH2	2.29	0.47
1:A:258:MET:HE1	1:A:260:ARG:NH2	2.28	0.47
1:A:534:THR:O	1:A:538:ARG:HG3	2.14	0.47
1:A:795:LEU:HD13	1:A:820:TYR:CE2	2.49	0.47
1:B:382:VAL:HG22	1:B:415:PHE:HB3	1.96	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PHE:O	1:A:269:LEU:N	2.47	0.47
1:B:237:PRO:O	1:B:301:PHE:HA	2.15	0.47
1:A:637:ALA:HB2	1:A:656:HIS:CD2	2.50	0.47
1:A:758:VAL:HA	1:A:782:VAL:O	2.14	0.47
1:A:784:SER:OG	1:A:785:GLY:N	2.48	0.47
1:B:473:SER:O	1:B:476:ASP:N	2.47	0.47
1:B:815:ILE:HG12	1:B:816:ALA:H	1.79	0.47
1:A:115:PRO:HD3	1:A:148:TRP:HZ3	1.79	0.47
1:A:177:SER:HA	1:A:181:ASN:OD1	2.15	0.47
1:A:236:PRO:O	1:A:302:THR:OG1	2.23	0.47
1:A:570:TYR:CE1	1:A:638:TYR:HB3	2.50	0.47
1:B:38:GLY:O	1:B:106:HIS:HB2	2.14	0.47
1:B:85:TRP:CZ2	1:B:153:LEU:HD11	2.50	0.47
1:A:569:ALA:HB2	1:A:636:PRO:O	2.14	0.47
1:B:295:TRP:CH2	1:B:443:ALA:CA	2.97	0.47
1:B:381:VAL:HG22	1:B:414:ASP:HA	1.97	0.47
1:A:689:SER:O	1:A:693:VAL:HG23	2.15	0.47
1:B:578:PRO:HG2	1:B:581:ARG:CB	2.44	0.47
1:A:449:ASP:O	1:A:453:ARG:HG3	2.16	0.46
1:A:787:PRO:HD2	1:A:790:THR:CG2	2.45	0.46
1:A:832:THR:O	1:A:833:TRP:HB2	2.15	0.46
1:A:848:LEU:HD23	1:A:848:LEU:HA	1.78	0.46
1:B:857:THR:O	1:B:861:PHE:HB2	2.15	0.46
1:A:33:GLU:O	1:A:35:GLY:N	2.47	0.46
1:B:453:ARG:HB2	1:B:463:VAL:HG11	1.97	0.46
1:A:243:ALA:O	1:A:436:ALA:HB2	2.15	0.46
1:A:107:VAL:HG12	1:A:108:LEU:O	2.16	0.46
1:A:148:TRP:HB3	1:A:149:PRO:HD3	1.97	0.46
1:A:279:THR:N	1:A:282:GLU:HB2	2.28	0.46
1:A:413:LEU:HD12	1:A:414:ASP:H	1.81	0.46
1:B:578:PRO:O	1:B:582:VAL:HG23	2.16	0.46
1:A:669:ARG:HG2	1:A:670:PHE:CE1	2.51	0.45
1:A:684:LEU:HA	1:A:689:SER:CB	2.46	0.45
1:B:679:LEU:HD11	1:B:706:PRO:HB3	1.98	0.45
1:A:216:ARG:HA	1:A:221:TRP:CD1	2.51	0.45
1:A:273:ALA:CA	1:A:283:LEU:HD23	2.47	0.45
1:B:569:ALA:HB2	1:B:636:PRO:O	2.16	0.45
1:B:888:ILE:O	1:B:888:ILE:HG23	2.15	0.45
1:A:47:GLN:HE21	1:A:322:ASP:HB2	1.82	0.45
1:A:293:ARG:HG3	1:A:301:PHE:HE2	1.81	0.45
1:A:652:VAL:HG21	1:A:788:THR:CG2	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:564:LEU:HD23	1:A:564:LEU:HA	1.76	0.45
1:A:693:VAL:HB	1:A:694:PHE:CD1	2.51	0.45
1:A:274:LEU:HD23	1:A:278:LEU:O	2.16	0.45
1:B:33:GLU:HG2	1:B:206:ASP:OD1	2.16	0.45
1:B:308:PHE:HB2	1:B:388:LEU:HD11	1.98	0.45
1:B:472:ARG:HA	1:B:831:PRO:HB3	1.98	0.45
1:B:832:THR:O	1:B:833:TRP:HB2	2.17	0.45
1:B:977:LEU:HD22	1:B:982:LYS:O	2.17	0.45
1:A:309:GLN:O	1:A:323:TYR:HB3	2.16	0.45
1:A:338:VAL:O	1:A:339:ALA:C	2.59	0.45
1:B:172:LEU:O	1:B:173:MET:HG2	2.17	0.45
1:B:386:LEU:HA	1:B:386:LEU:HD23	1.72	0.45
1:B:678:LEU:HD12	1:B:728:PHE:CG	2.52	0.45
1:A:93:PRO:HG2	1:A:203:ALA:HB1	1.98	0.45
1:A:658:GLY:O	1:A:661:ASN:HB3	2.17	0.44
1:B:73:ARG:NH1	1:B:398:PHE:O	2.50	0.44
1:B:207:PHE:CE2	1:B:316:ILE:HG12	2.52	0.44
1:B:570:TYR:CE1	1:B:638:TYR:HB3	2.53	0.44
1:B:728:PHE:CE1	1:B:756:LEU:HG	2.53	0.44
1:A:325:ASN:ND2	1:A:356:ALA:O	2.50	0.44
1:A:514:ALA:HB3	1:A:554:TRP:HB3	1.98	0.44
1:B:238:ALA:CB	1:B:379:PRO:HD2	2.47	0.44
1:B:445:GLU:OE2	1:B:474:ARG:HG3	2.18	0.44
1:B:494:LEU:CD1	1:B:631:GLN:HG2	2.47	0.44
1:A:47:GLN:NE2	1:A:322:ASP:HB2	2.33	0.44
1:A:676:ASP:O	1:A:701:ALA:HB1	2.17	0.44
1:B:68:TYR:O	1:B:69:PHE:CG	2.71	0.44
1:B:69:PHE:HB3	1:B:71:TRP:CZ2	2.53	0.44
1:B:100:ARG:N	1:B:104:THR:O	2.50	0.44
1:B:183:PHE:HB3	1:B:395:ILE:HD13	2.00	0.44
1:B:272:ARG:HD2	1:B:464:TRP:CZ2	2.53	0.44
1:B:395:ILE:HD12	1:B:395:ILE:HA	1.84	0.44
1:B:838:MET:N	1:B:876:ASP:O	2.49	0.44
1:A:78:LEU:HD12	1:A:78:LEU:H	1.82	0.44
1:A:714:PRO:HG3	1:A:738:LEU:HB3	1.99	0.44
1:A:759:VAL:O	1:A:783:GLY:HA2	2.17	0.44
1:B:615:ALA:HA	1:B:619:PHE:HD2	1.83	0.44
1:B:787:PRO:N	1:B:790:THR:HG22	2.33	0.44
1:A:266:PHE:O	1:A:269:LEU:HB3	2.17	0.44
1:B:145:PRO:HA	1:B:150:MET:SD	2.58	0.44
1:A:438:GLY:HA2	1:A:441:GLU:CD	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:MET:HB2	1:B:320:ILE:HG23	2.00	0.44
1:B:295:TRP:CZ3	1:B:443:ALA:HA	2.53	0.44
1:A:486:THR:HB	1:A:816:ALA:HA	1.99	0.43
1:A:822:ILE:CD1	1:A:838:MET:HG2	2.46	0.43
1:A:293:ARG:HG2	1:A:299:PRO:HA	1.99	0.43
1:A:507:PRO:HB2	1:A:522:ASP:HB2	1.99	0.43
1:A:652:VAL:HG21	1:A:788:THR:HG23	2.01	0.43
1:A:734:VAL:HG21	1:A:977:LEU:HD21	2.00	0.43
1:B:520:THR:CG2	1:B:523:GLU:H	2.21	0.43
1:B:876:ASP:OD2	2:B:1201:AMP:H2'	2.18	0.43
1:A:365:ARG:O	1:A:368:ALA:N	2.51	0.43
1:A:761:GLY:HA2	2:A:1201:AMP:N7	2.33	0.43
1:A:663:VAL:HG22	1:A:695:GLY:HA2	2.01	0.43
1:A:748:ASP:OD1	1:A:748:ASP:N	2.49	0.43
1:B:878:GLY:HA2	1:B:889:LEU:CG	2.45	0.43
1:B:316:ILE:C	1:B:318:ASP:H	2.25	0.43
1:A:262:PRO:HD2	1:A:265:GLU:HB2	2.01	0.43
1:A:733:PRO:CD	1:A:762:ASP:HB3	2.49	0.43
1:B:451:VAL:O	1:B:455:LEU:HG	2.19	0.43
1:A:284:LEU:HD23	1:A:284:LEU:HA	1.61	0.43
1:A:401:GLU:HG2	1:A:402:VAL:H	1.83	0.43
1:A:672:VAL:HG12	1:A:699:CYS:SG	2.58	0.43
1:A:696:PRO:HG2	1:A:703:VAL:HG22	2.01	0.43
1:B:494:LEU:HD12	1:B:629:PRO:HB3	2.00	0.43
1:A:266:PHE:CZ	1:A:424:LEU:HD13	2.54	0.43
1:A:281:THR:HG22	1:A:281:THR:O	2.18	0.43
1:A:338:VAL:HG23	1:A:466:ALA:O	2.18	0.43
1:A:569:ALA:HB1	1:A:637:ALA:C	2.44	0.43
1:A:572:PRO:CG	1:A:640:ILE:HG12	2.48	0.43
1:B:407:GLN:O	1:B:408:THR:C	2.62	0.43
1:B:292:LEU:C	1:B:294:GLY:N	2.76	0.42
1:B:628:THR:OG1	1:B:629:PRO:HD2	2.20	0.42
1:B:287:ALA:O	1:B:291:VAL:HG23	2.19	0.42
1:A:224:ASP:HB2	1:A:358:VAL:HG23	2.01	0.42
1:A:279:THR:OG1	1:A:282:GLU:HG2	2.19	0.42
1:A:596:THR:HG22	1:A:597:GLN:O	2.18	0.42
1:B:96:ARG:HA	1:B:148:TRP:HE1	1.84	0.42
2:B:1201:AMP:O1P	3:B:1202:EW6:O	2.37	0.42
1:A:225:TRP:HE3	1:A:358:VAL:HG11	1.84	0.42
1:A:803:ASP:HB3	1:A:806:TRP:CD2	2.54	0.42
1:A:73:ARG:HG3	1:A:162:VAL:CG1	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:PRO:HG2	1:B:703:VAL:HG22	2.01	0.42
1:A:239:PRO:HG2	1:A:380:VAL:HG21	2.02	0.42
1:B:71:TRP:O	1:B:163:ARG:HD2	2.20	0.42
1:B:510:GLU:O	1:B:702:THR:OG1	2.32	0.42
1:B:672:VAL:HG23	1:B:672:VAL:O	2.19	0.42
1:B:786:GLY:O	3:B:1202:EW6:C4	2.67	0.42
1:B:902:ARG:O	1:B:905:LEU:N	2.53	0.42
1:A:174:ASP:HB3	1:A:322:ASP:HA	2.02	0.42
1:A:288:PHE:CE2	1:A:292:LEU:HD11	2.55	0.42
1:B:92:HIS:HA	1:B:93:PRO:HD3	1.85	0.42
1:B:438:GLY:O	1:B:439:VAL:C	2.62	0.42
1:B:557:TYR:CE2	1:B:693:VAL:HA	2.53	0.42
1:B:672:VAL:HA	1:B:676:ASP:OD2	2.20	0.42
1:A:577:SER:HB2	1:A:582:VAL:HG22	2.02	0.42
1:A:688:ALA:HA	1:A:792:CYS:SG	2.60	0.42
1:A:758:VAL:HG11	1:A:793:TRP:CZ2	2.55	0.42
1:A:790:THR:O	1:A:791:ILE:HB	2.19	0.42
1:B:122:ARG:H	1:B:122:ARG:HG3	1.65	0.42
1:B:180:LEU:HD23	1:B:391:ALA:HB2	2.01	0.42
1:B:616:ASP:C	1:B:617:THR:HG23	2.44	0.42
1:A:386:LEU:HD23	1:A:386:LEU:HA	1.67	0.41
1:A:85:TRP:O	1:A:89:VAL:HG23	2.19	0.41
1:A:123:GLN:O	1:A:125:PRO:HD3	2.21	0.41
1:A:174:ASP:OD1	1:A:174:ASP:C	2.63	0.41
1:A:726:VAL:O	1:A:754:LEU:HD23	2.20	0.41
1:A:120:ASP:OD1	1:A:122:ARG:NE	2.43	0.41
1:A:145:PRO:HA	1:A:150:MET:SD	2.60	0.41
1:A:795:LEU:H	1:A:795:LEU:HD23	1.84	0.41
1:B:534:THR:HB	1:B:619:PHE:HE1	1.85	0.41
1:A:268:LEU:HD22	1:B:492:ALA:O	2.21	0.41
2:A:1201:AMP:C8	3:A:1202:EW6:N	2.88	0.41
1:B:635:ASP:HA	1:B:636:PRO:HD3	1.89	0.41
1:A:316:ILE:C	1:A:318:ASP:H	2.27	0.41
1:B:94:GLY:C	1:B:96:ARG:H	2.29	0.41
1:A:238:ALA:CB	1:A:379:PRO:HD2	2.51	0.41
1:A:494:LEU:HB2	1:A:497:GLU:HB2	2.02	0.41
1:B:596:THR:HG22	1:B:597:GLN:N	2.36	0.41
1:B:715:ASP:OD1	1:B:715:ASP:N	2.53	0.41
1:A:786:GLY:O	3:A:1202:EW6:C4	2.69	0.41
1:A:791:ILE:HD12	1:A:845:GLY:HA2	2.02	0.41
1:B:496:GLN:H	1:B:496:GLN:CD	2.28	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:GLN:OE1	1:B:496:GLN:N	2.41	0.41
1:B:732:VAL:HG22	1:B:735:LEU:HG	2.03	0.41
1:B:787:PRO:N	1:B:790:THR:CG2	2.83	0.41
1:A:94:GLY:O	1:A:97:THR:N	2.53	0.41
1:A:227:TYR:HB2	1:A:355:HIS:CD2	2.56	0.41
1:A:266:PHE:CE1	1:A:424:LEU:HD22	2.56	0.41
1:A:316:ILE:HD12	1:A:316:ILE:HA	1.92	0.41
1:A:338:VAL:O	1:A:341:ARG:N	2.53	0.41
1:A:815:ILE:HD13	1:A:815:ILE:HG21	1.85	0.41
1:B:292:LEU:HD11	1:B:380:VAL:HG11	2.02	0.41
1:B:484:ASN:O	1:B:819:ARG:NH1	2.51	0.41
1:B:976:PRO:HG3	1:B:988:LEU:HD21	2.02	0.41
1:B:977:LEU:O	1:B:984:ASP:HB2	2.21	0.41
1:A:531:ILE:O	1:A:535:LEU:HG	2.20	0.41
2:A:1201:AMP:N3	2:A:1201:AMP:O2'	2.54	0.41
1:B:259:VAL:HG12	1:B:444:PHE:HZ	1.86	0.41
1:B:300:ALA:HA	1:B:331:ALA:O	2.21	0.41
1:A:733:PRO:HG2	1:A:762:ASP:HB3	2.02	0.40
1:B:151:PHE:CD2	1:B:151:PHE:N	2.90	0.40
1:B:583:ALA:HB2	1:B:605:ASP:O	2.20	0.40
1:A:154:ARG:O	1:A:155:VAL:HG23	2.21	0.40
1:A:665:ASP:OD1	1:A:815:ILE:HD11	2.21	0.40
1:A:684:LEU:HA	1:A:689:SER:OG	2.20	0.40
1:B:374:ALA:C	1:B:376:ALA:H	2.29	0.40
1:B:872:TYR:CE2	1:B:874:THR:HA	2.56	0.40
1:B:830:ARG:HH12	1:B:834:ALA:HB1	1.85	0.40
1:A:659:VAL:O	1:A:662:LEU:HB3	2.21	0.40
1:A:669:ARG:HD3	1:A:796:PHE:CD2	2.56	0.40
1:B:228:TRP:HH2	1:B:352:ASP:HB3	1.85	0.40
1:B:480:TRP:CD1	1:B:484:ASN:ND2	2.90	0.40
1:A:816:ALA:O	1:A:817:ASN:HB2	2.21	0.40
1:A:846:LEU:HA	1:A:846:LEU:HD23	1.84	0.40
1:B:298:ASP:HA	1:B:299:PRO:HD3	1.93	0.40
1:B:463:VAL:HA	1:B:466:ALA:HB2	2.04	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	866/1153 (75%)	752 (87%)	105 (12%)	9 (1%)	12	46
1	B	864/1153 (75%)	736 (85%)	114 (13%)	14 (2%)	7	37
All	All	1730/2306 (75%)	1488 (86%)	219 (13%)	23 (1%)	9	41

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	91	HIS
1	A	918	VAL
1	B	69	PHE
1	B	492	ALA
1	A	791	ILE
1	B	789	GLU
1	A	902	ARG
1	B	403	HIS
1	A	111	PRO
1	B	74	PRO
1	B	91	HIS
1	B	973	PRO
1	A	833	TRP
1	B	155	VAL
1	B	828	ARG
1	B	791	ILE
1	B	218	GLY
1	A	74	PRO
1	A	155	VAL
1	B	167	GLY
1	A	338	VAL
1	B	672	VAL
1	B	853	ASP

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	501/902 (56%)	501 (100%)	0	100	100
1	B	491/902 (54%)	491 (100%)	0	100	100
All	All	992/1804 (55%)	992 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	200	GLN
1	A	481	ASN
1	A	631	GLN
1	A	817	ASN
1	B	123	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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	$\# Z > 2$
3	EW6	B	1202	2	2,6,7	0.63	0	2,8,10	1.98	1 (50%)
3	EW6	A	1202	2	2,6,7	0.70	0	2,8,10	0.92	0
2	AMP	A	1201	3	25,25,25	1.68	7 (28%)	37,38,38	3.07	24 (64%)
2	AMP	B	1201	3	25,25,25	2.20	11 (44%)	37,38,38	3.36	24 (64%)

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
3	EW6	B	1202	2	-	1/4/6/9	-
3	EW6	A	1202	2	-	3/4/6/9	-
2	AMP	A	1201	3	-	5/10/26/26	0/3/3/3
2	AMP	B	1201	3	-	5/10/26/26	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1201	AMP	P-O1P	3.74	1.62	1.50
2	B	1201	AMP	C2'-C3'	3.67	1.63	1.53
2	B	1201	AMP	C2-N1	3.59	1.40	1.33
2	B	1201	AMP	C5-N7	-3.44	1.32	1.39
2	A	1201	AMP	C2'-C3'	3.33	1.62	1.53
2	B	1201	AMP	C8-N9	-3.08	1.32	1.37
2	A	1201	AMP	P-O1P	3.03	1.59	1.50
2	B	1201	AMP	P-O5'	2.92	1.69	1.60
2	A	1201	AMP	C8-N7	2.85	1.37	1.31
2	B	1201	AMP	C2-N3	2.80	1.38	1.33
2	B	1201	AMP	C5-C4	2.53	1.43	1.39
2	B	1201	AMP	O3'-C3'	2.42	1.49	1.43
2	A	1201	AMP	C5-C4	2.26	1.43	1.39
2	B	1201	AMP	P-O3P	2.24	1.63	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	AMP	O4'-C1'	-2.23	1.36	1.42
2	B	1201	AMP	O4'-C1'	-2.03	1.37	1.42
2	A	1201	AMP	P-O5'	2.03	1.66	1.60
2	A	1201	AMP	P-O3P	2.02	1.62	1.54

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1201	AMP	C6-C5-C4	8.44	128.71	117.18
2	B	1201	AMP	C5-C4-N3	-6.88	117.24	126.72
2	B	1201	AMP	C4-C5-N7	-5.54	104.25	110.58
2	B	1201	AMP	O3'-C3'-C2'	5.41	129.17	111.82
2	A	1201	AMP	C4-C5-N7	-5.38	104.43	110.58
2	A	1201	AMP	O2'-C2'-C3'	5.32	128.85	111.82
2	A	1201	AMP	C5-N7-C8	4.91	111.17	103.45
2	B	1201	AMP	O2'-C2'-C3'	4.87	127.44	111.82
2	A	1201	AMP	O4'-C4'-C3'	-4.83	95.57	105.15
2	A	1201	AMP	C6-C5-C4	4.81	123.74	117.18
2	A	1201	AMP	O3'-C3'-C2'	4.75	127.05	111.82
2	B	1201	AMP	C5-N7-C8	4.73	110.89	103.45
2	A	1201	AMP	O3P-P-O5'	4.60	118.67	106.67
2	A	1201	AMP	N9-C8-N7	-4.56	107.46	113.94
2	B	1201	AMP	O4'-C4'-C3'	-4.47	96.28	105.15
2	B	1201	AMP	O5'-P-O1P	4.43	118.40	106.44
2	A	1201	AMP	C5-C4-N3	-4.36	120.71	126.72
2	B	1201	AMP	N3-C4-N9	4.36	134.58	127.17
2	A	1201	AMP	C4'-O4'-C1'	-4.15	100.31	109.47
2	A	1201	AMP	C3'-C2'-C1'	-3.91	94.07	101.46
2	B	1201	AMP	O4'-C1'-N9	3.48	114.78	108.09
2	B	1201	AMP	C3'-C2'-C1'	-3.47	94.89	101.46
2	A	1201	AMP	C4-N9-C8	3.39	109.29	105.74
2	B	1201	AMP	O4'-C4'-C5'	3.15	119.43	109.33
2	B	1201	AMP	O2'-C2'-C1'	-3.15	99.26	110.10
2	B	1201	AMP	O3'-C3'-C4'	3.13	120.07	111.08
2	A	1201	AMP	O3'-C3'-C4'	3.13	120.06	111.08
2	A	1201	AMP	C1'-N9-C8	-3.06	120.30	127.09
2	B	1201	AMP	C1'-N9-C8	-2.97	120.51	127.09
2	A	1201	AMP	O4'-C4'-C5'	2.96	118.80	109.33
2	B	1201	AMP	O3P-P-O5'	2.83	114.05	106.67
3	B	1202	EW6	C4-CA-C	-2.79	98.55	109.75
2	B	1201	AMP	C4-N9-C1'	2.72	133.00	126.63
2	B	1201	AMP	N9-C8-N7	-2.65	110.17	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1201	AMP	N3-C4-N9	2.64	131.66	127.17
2	A	1201	AMP	C5-C6-N1	-2.62	110.86	117.51
2	B	1201	AMP	C6-C5-N7	-2.62	127.04	132.09
2	A	1201	AMP	O2'-C2'-C1'	-2.54	101.37	110.10
2	A	1201	AMP	C5-C6-N6	2.41	129.25	123.29
2	B	1201	AMP	C5-C6-N1	-2.37	111.49	117.51
2	B	1201	AMP	C4'-O4'-C1'	-2.34	104.30	109.47
2	A	1201	AMP	C2-N1-C6	2.27	122.45	118.73
2	A	1201	AMP	C5'-C4'-C3'	-2.24	107.14	115.21
2	A	1201	AMP	O4'-C1'-N9	2.18	112.28	108.09
2	B	1201	AMP	C5-C4-N9	2.17	108.18	105.81
2	A	1201	AMP	O2P-P-O5'	-2.16	101.03	106.67
2	A	1201	AMP	C2'-C1'-N9	-2.16	107.94	113.30
2	B	1201	AMP	N6-C6-N1	2.10	123.06	118.38
2	B	1201	AMP	O2P-P-O5'	-2.09	101.23	106.67

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	AMP	C5'-O5'-P-O1P
2	A	1201	AMP	C5'-O5'-P-O2P
2	A	1201	AMP	C5'-O5'-P-O3P
2	A	1201	AMP	C4'-C5'-O5'-P
2	B	1201	AMP	C5'-O5'-P-O1P
2	B	1201	AMP	C5'-O5'-P-O2P
2	B	1201	AMP	C5'-O5'-P-O3P
2	B	1201	AMP	C4'-C5'-O5'-P
3	A	1202	EW6	N-CA-CB-OG
2	A	1201	AMP	C3'-C4'-C5'-O5'
3	A	1202	EW6	C4-CA-CB-OG
2	B	1201	AMP	C3'-C4'-C5'-O5'
3	A	1202	EW6	O-C-CA-C4
3	B	1202	EW6	O-C-CA-C4

There are no ring outliers.

4 monomers are involved in 12 short contacts:

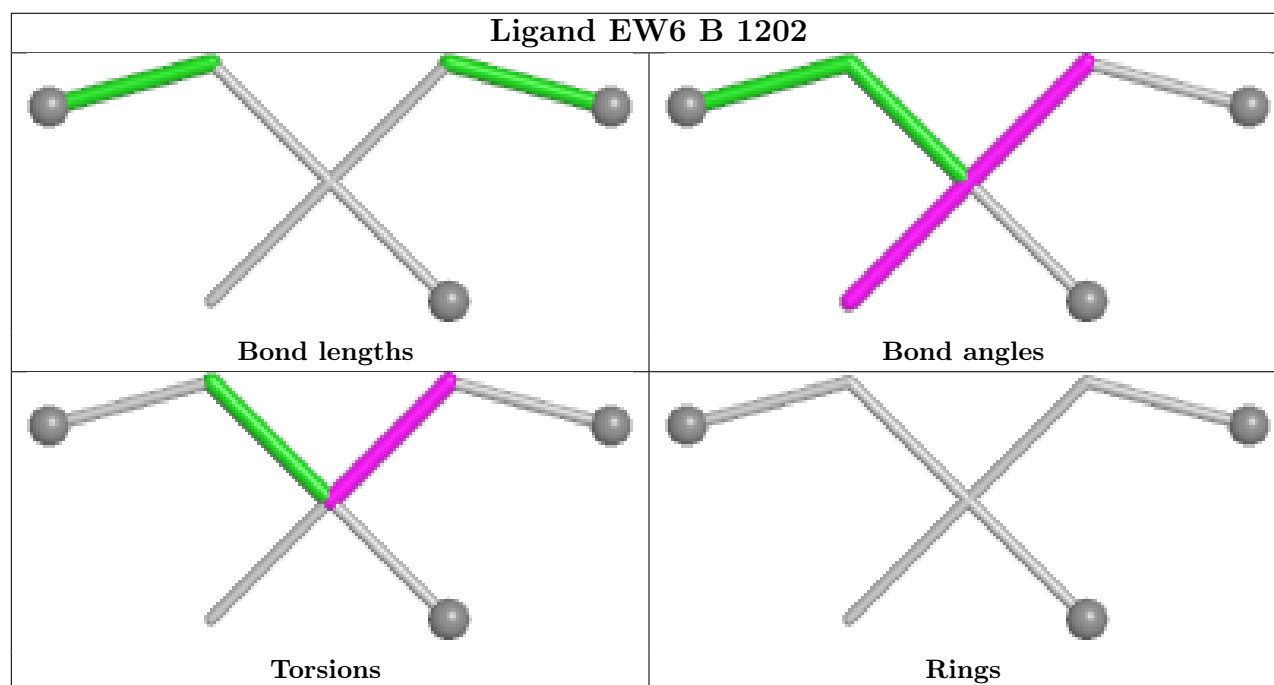
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1202	EW6	2	0
3	A	1202	EW6	2	0

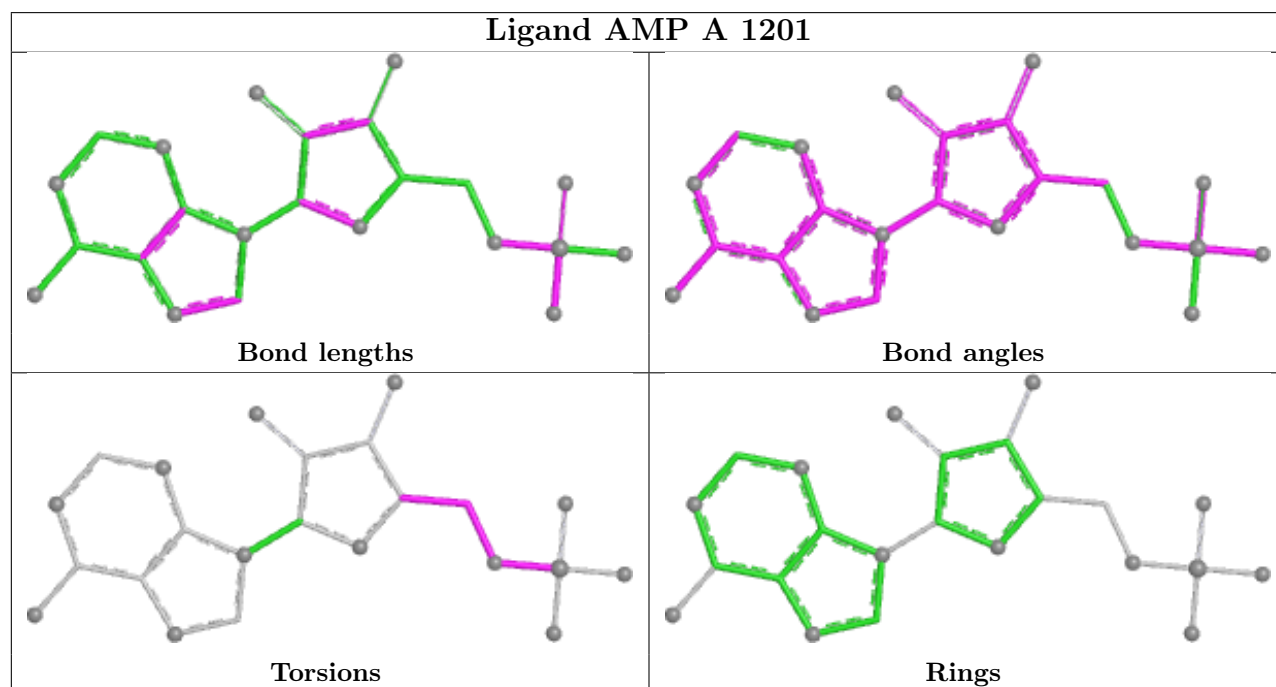
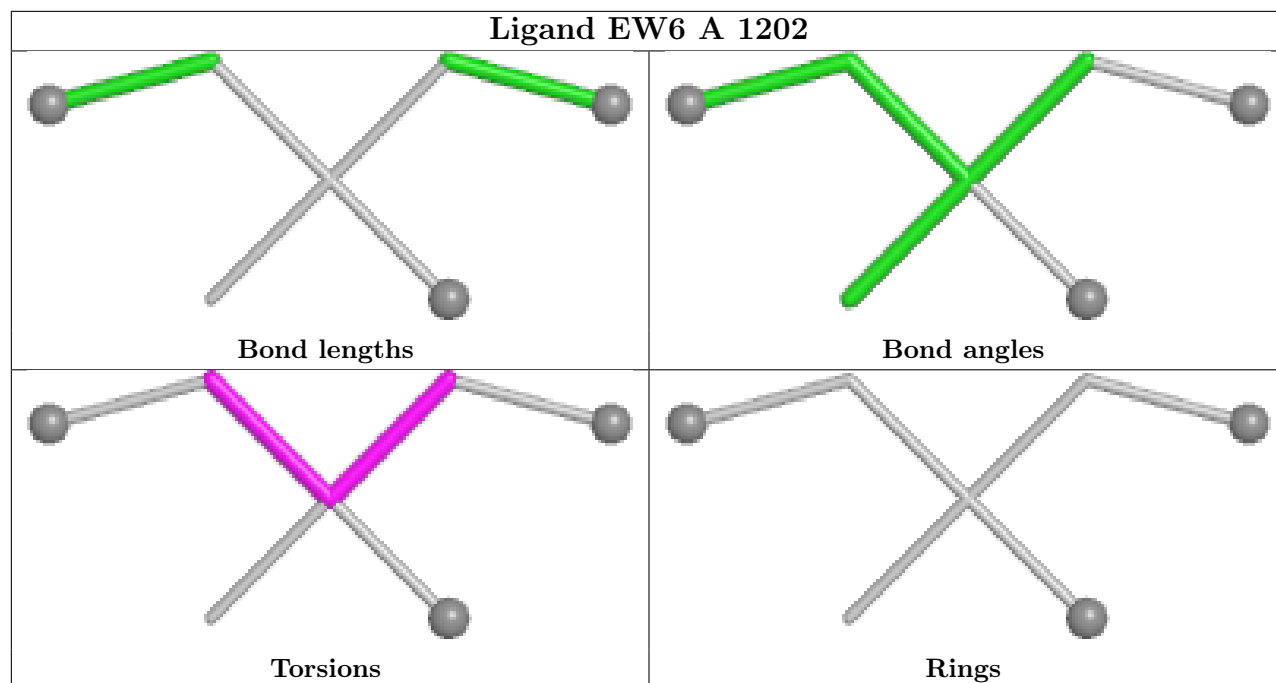
Continued on next page...

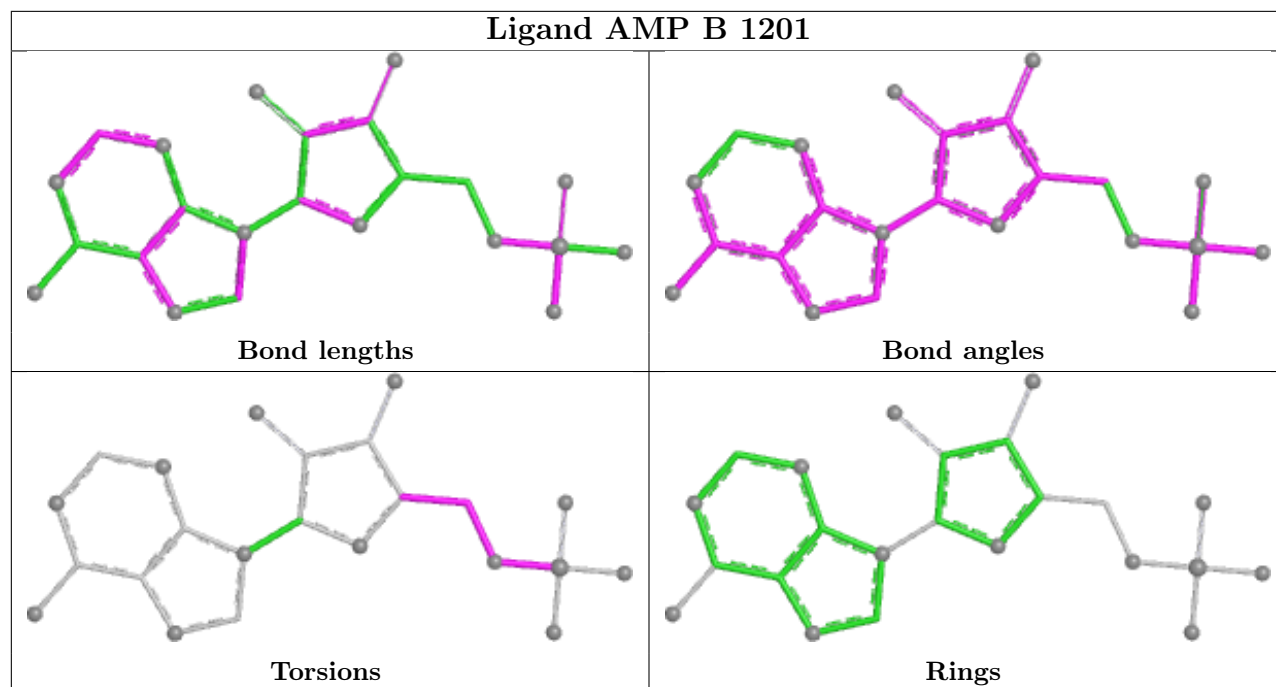
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	AMP	5	0
2	B	1201	AMP	5	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.







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	883/1153 (76%)	0.52	38 (4%) 40 32	97, 145, 185, 217	1 (0%)
1	B	882/1153 (76%)	0.50	48 (5%) 31 27	93, 142, 185, 211	0
All	All	1765/2306 (76%)	0.51	86 (4%) 35 29	93, 144, 185, 217	1 (0%)

All (86) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	793	TRP	4.6
1	B	933	VAL	4.0
1	B	55	ALA	4.0
1	A	605	ASP	3.8
1	B	194	ASP	3.6
1	A	579	ARG	3.4
1	A	718	ALA	3.4
1	A	407	GLN	3.2
1	B	794	SER	3.2
1	A	194	ASP	3.2
1	B	824	ASP	3.1
1	B	156	VAL	2.9
1	B	524	LEU	2.9
1	A	297	SER	2.9
1	B	468	PHE	2.9
1	A	895	GLN	2.8
1	B	901	GLN	2.8
1	B	402	VAL	2.8
1	A	133	GLU	2.8
1	A	402	VAL	2.7
1	A	908	ILE	2.7
1	A	642	THR	2.7
1	A	313	VAL	2.7
1	B	207	PHE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	920	ALA	2.6
1	B	620	GLU	2.6
1	B	671	ALA	2.6
1	A	903	ILE	2.6
1	B	134	SER	2.6
1	A	789	GLU	2.5
1	B	647	GLY	2.5
1	B	969	ILE	2.5
1	A	802	VAL	2.5
1	A	793	TRP	2.5
1	A	575	ALA	2.5
1	A	620	GLU	2.5
1	B	550	MET	2.5
1	A	320	ILE	2.5
1	A	487	ALA	2.5
1	B	774	ALA	2.4
1	A	207	PHE	2.4
1	A	55	ALA	2.4
1	B	435	PHE	2.3
1	A	225	TRP	2.3
1	B	826	ASP	2.3
1	B	92	HIS	2.3
1	B	827	LEU	2.3
1	A	931	ASP	2.3
1	B	708	PRO	2.3
1	A	508	ASP	2.3
1	B	228	TRP	2.3
1	A	827	LEU	2.3
1	B	54	ARG	2.3
1	B	873	LEU	2.3
1	A	317	GLU	2.2
1	B	314	PRO	2.2
1	B	795	LEU	2.2
1	B	811	TYR	2.2
1	B	989	ALA	2.2
1	A	429	ASP	2.2
1	A	556	GLN	2.2
1	A	813	LYS	2.2
1	B	135	ARG	2.2
1	A	515	SER	2.2
1	B	605	ASP	2.2
1	A	743	ALA	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	39	GLN	2.2
1	B	642	THR	2.1
1	B	51	TRP	2.1
1	B	374	ALA	2.1
1	B	403	HIS	2.1
1	B	133	GLU	2.1
1	A	135	ARG	2.1
1	B	150	MET	2.1
1	B	932	VAL	2.1
1	A	408	THR	2.1
1	A	229	GLN	2.1
1	A	662	LEU	2.1
1	B	615	ALA	2.1
1	B	311	PHE	2.1
1	B	579	ARG	2.0
1	B	825	ARG	2.0
1	B	672	VAL	2.0
1	A	749	ARG	2.0
1	A	314	PRO	2.0
1	B	907	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [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.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	AMP	A	1201	23/23	0.68	0.18	134,161,175,186	0
3	EW6	B	1202	7/8	0.76	0.22	104,130,140,141	0
2	AMP	B	1201	23/23	0.79	0.14	121,160,174,184	0

Continued on next page...

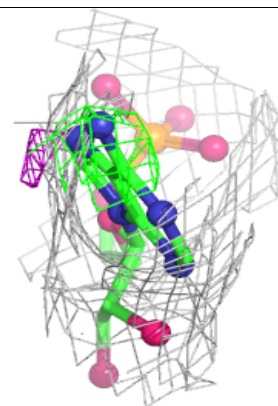
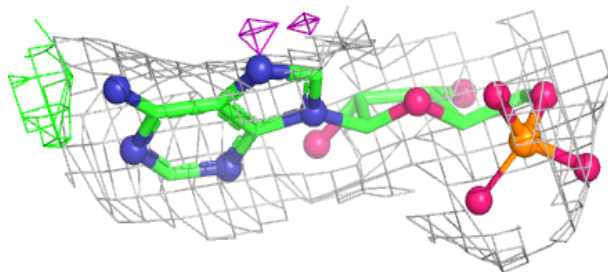
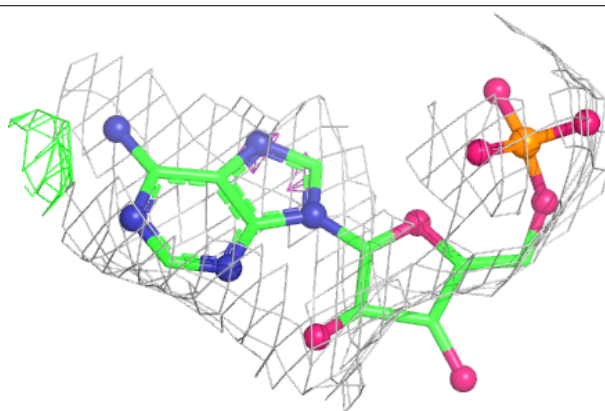
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EW6	A	1202	7/8	0.89	0.16	137,143,148,150	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.

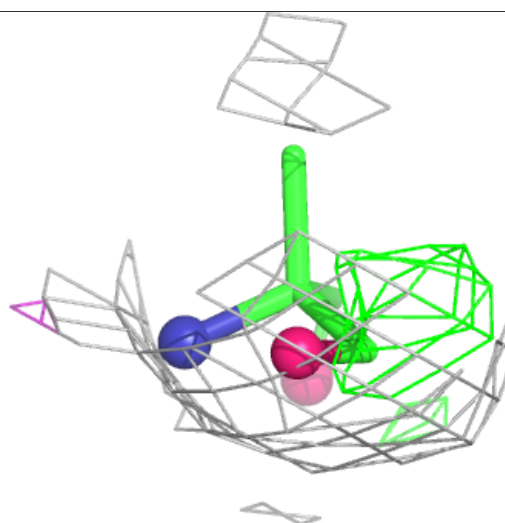
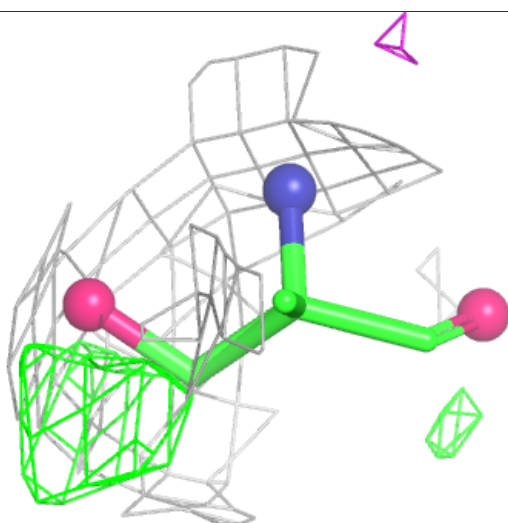
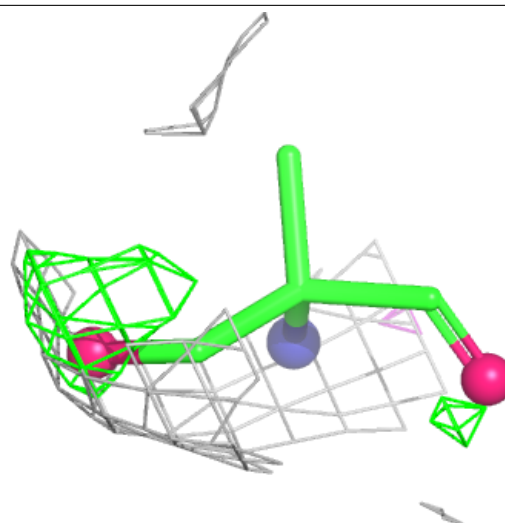
Electron density around AMP A 1201:

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



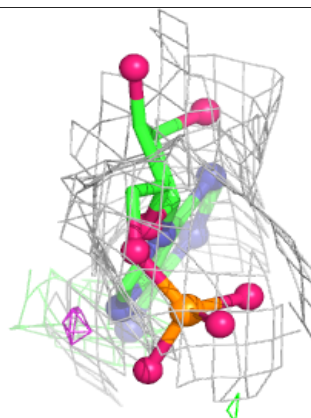
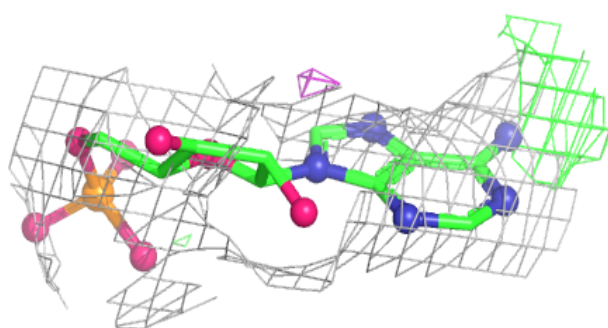
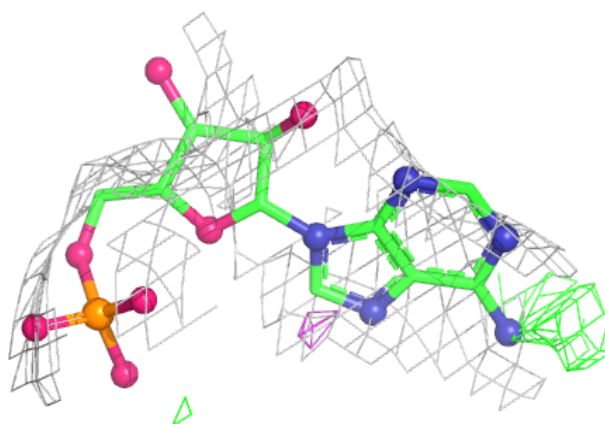
Electron density around EW6 B 1202:

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

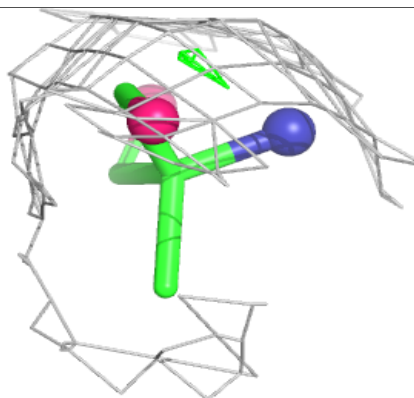
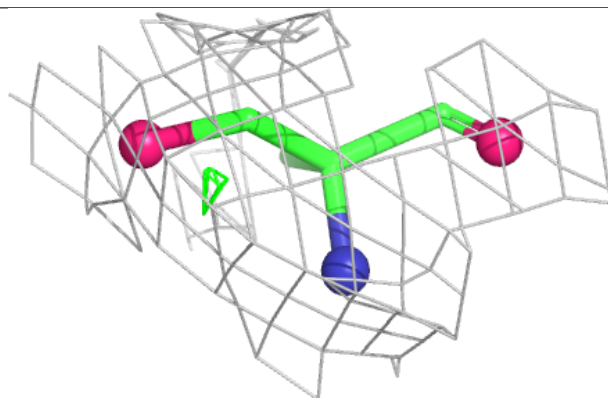
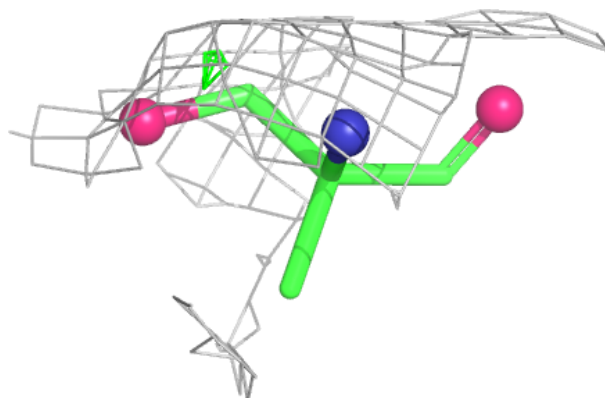


Electron density around AMP B 1201:

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

**Electron density around EW6 A 1202:**

$2mF_o-DF_c$ (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.