Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2024 – 05:57 PM EDT

PDB ID	:	1XRS
Title	:	Crystal structure of Lysine 5,6-Aminomutase in complex with PLP, cobalamin, and 5'-deoxyadenosine
Authors	:	Berkovitch, F.; Behshad, E.; Tang, K.H.; Enns, E.A.; Frey, P.A.; Drennan, C.L.
Deposited on	:	2004-10-15
Resolution	:	2.80 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:

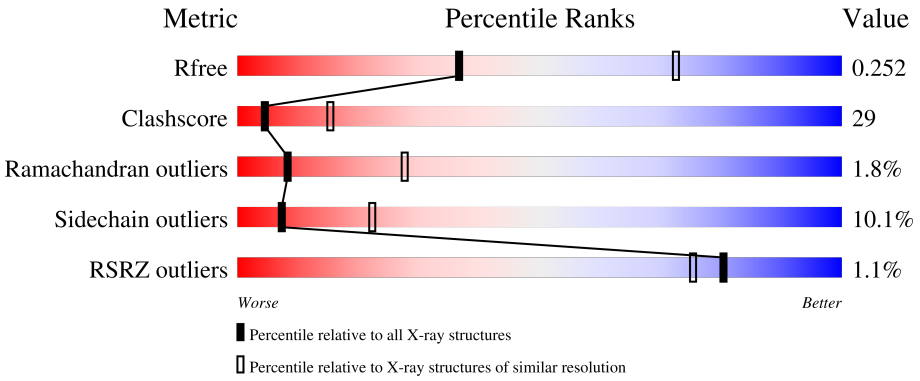
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

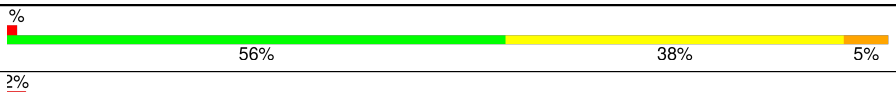
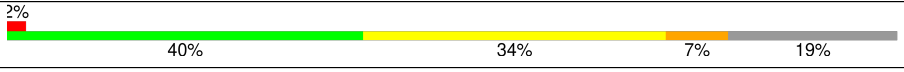
The reported resolution of this entry is 2.80 Å.

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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	516	
2	B	262	

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 5797 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.

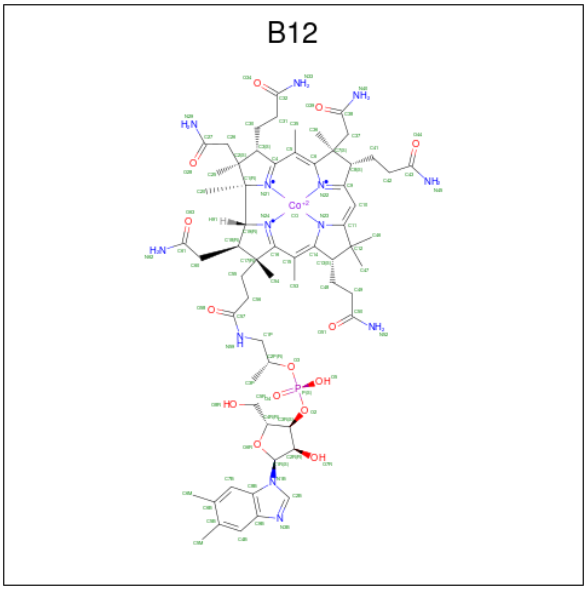
- Molecule 1 is a protein called D-lysine 5,6-aminomutase alpha subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	516	4022	2551	671	775	25	0	0	0

- Molecule 2 is a protein called D-lysine 5,6-aminomutase beta subunit.

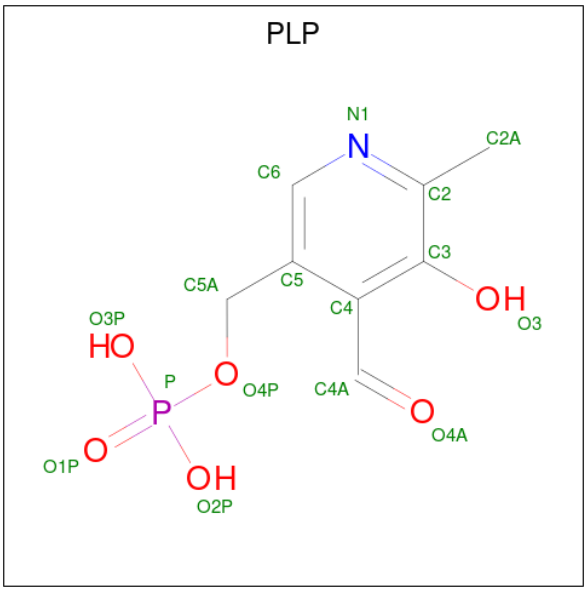
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	212	1651	1040	277	325	9	0	0	0

- Molecule 3 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



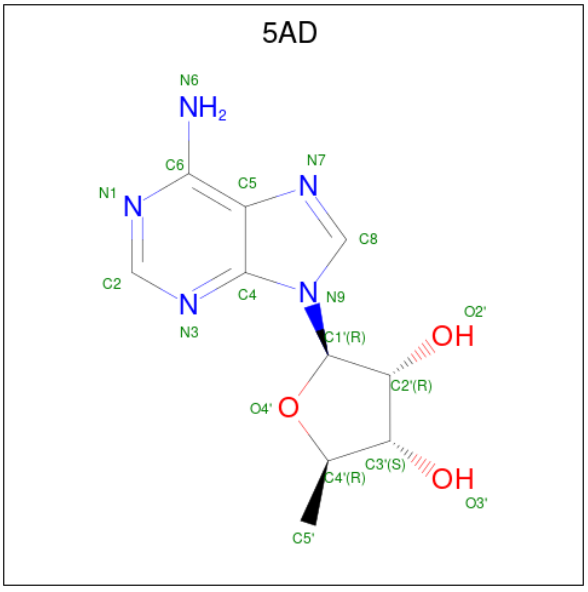
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	Co	N	O	P		
3	B	1	91	62	1	13	14	1	0	0

- Molecule 4 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 5 is 5'-DEOXYADENOSINE (three-letter code: 5AD) (formula: $C_{10}H_{13}N_5O_3$).

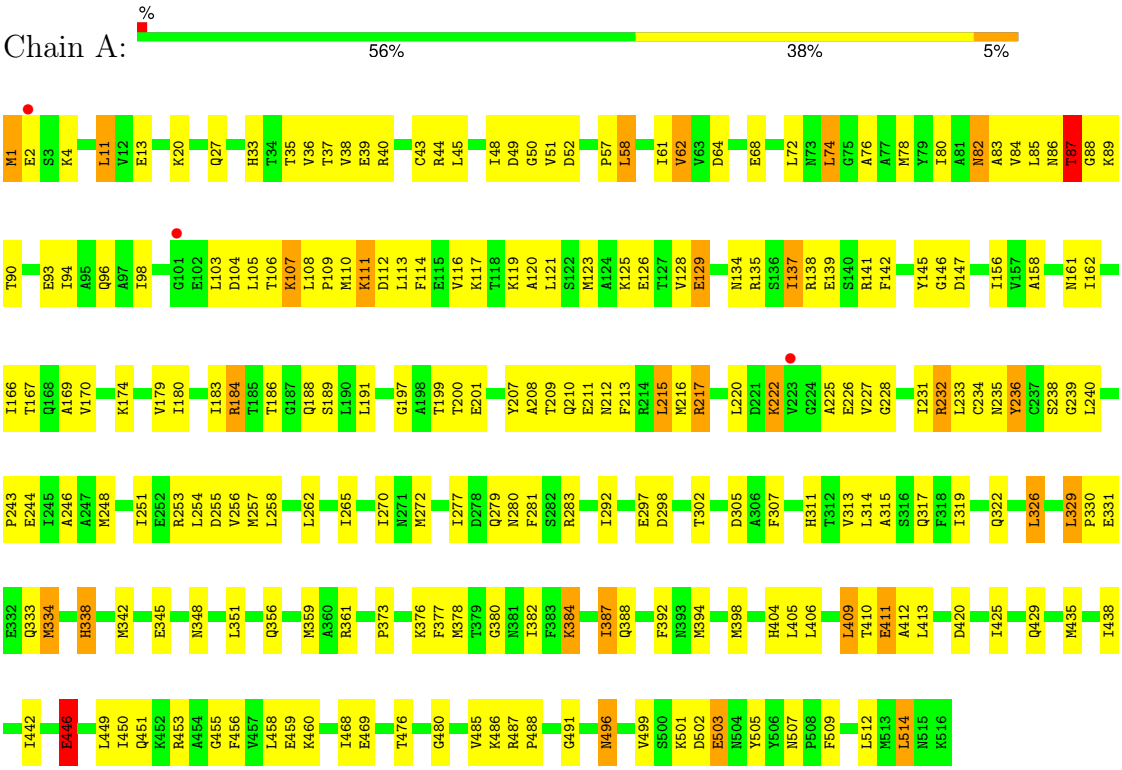


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	0
			18	10	5	3		

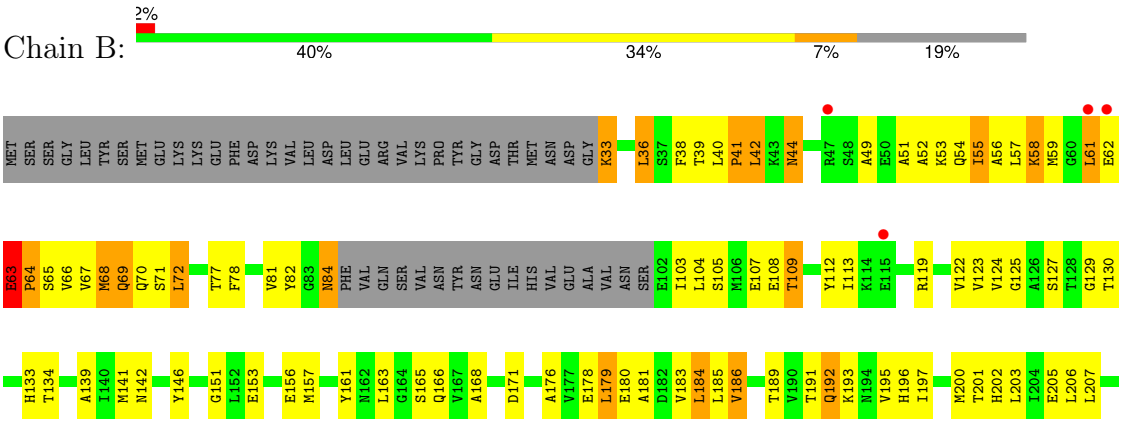
3 Residue-property plots (i)

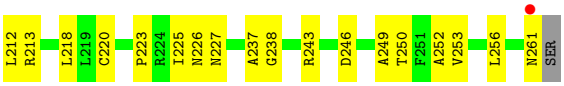
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: D-lysine 5,6-aminomutase alpha subunit



• Molecule 2: D-lysine 5,6-aminomutase beta subunit




L212
R213
L218
L219
C220
P223
R224
I225
N226
N227
A237
G238
R243
D246
A249
T250
F251
A252
V253
L256
N261
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	99.70Å 99.70Å 168.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.85 – 2.80 49.85 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.5 (49.85-2.80) 98.6 (49.85-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	8.49 (at 2.81Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.199 , 0.262 0.191 , 0.252	Depositor DCC
R_{free} test set	2403 reflections (9.88%)	wwPDB-VP
Wilson B-factor (Å^2)	38.0	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 55.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.027 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	5797	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 3.20% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 5AD, B12, PLP

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	0.65	0/4085	0.83	1/5510 (0.0%)
2	B	0.67	0/1673	0.84	1/2255 (0.0%)
All	All	0.66	0/5758	0.83	2/7765 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	449	LEU	CA-CB-CG	5.85	128.75	115.30
2	B	36	LEU	CA-CB-CG	5.46	127.85	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	207	TYR	Sidechain
1	A	505	TYR	Sidechain

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	4022	0	4034	223	0
2	B	1651	0	1631	107	0
3	B	91	0	82	9	0
4	B	15	0	6	0	0
5	B	18	0	13	0	0
All	All	5797	0	5766	330	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 29.

All (330) 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)
3:B:800:B12:C3R	3:B:800:B12:O2	1.64	1.44
2:B:192:GLN:HG3	2:B:193:LYS:H	1.03	1.10
1:A:184:ARG:HG2	1:A:184:ARG:HH11	1.18	1.08
1:A:217:ARG:HG3	1:A:217:ARG:HH11	1.23	1.03
2:B:192:GLN:HG3	2:B:193:LYS:N	1.79	0.98
2:B:189:THR:HG23	2:B:223:PRO:HG3	1.46	0.95
1:A:103:LEU:HD23	1:A:104:ASP:H	1.31	0.95
2:B:122:VAL:HG22	2:B:181:ALA:HA	1.47	0.94
2:B:66:VAL:HA	2:B:81:VAL:HG12	1.52	0.92
1:A:86:ASN:ND2	1:A:109:PRO:HG2	1.85	0.89
1:A:40:ARG:O	1:A:44:ARG:HG3	1.73	0.88
1:A:27:GLN:HE22	1:A:280:ASN:HD21	1.18	0.87
2:B:249:ALA:O	2:B:253:VAL:HG23	1.76	0.85
1:A:94:ILE:O	1:A:98:ILE:HG13	1.77	0.84
2:B:72:LEU:HD21	2:B:78:PHE:HB2	1.58	0.84
1:A:210:GLN:HB2	1:A:248:MET:HG2	1.61	0.82
1:A:27:GLN:HE22	1:A:280:ASN:ND2	1.77	0.82
1:A:87:THR:HG23	1:A:89:LYS:HG2	1.59	0.81
1:A:197:GLY:O	1:A:209:THR:HG21	1.79	0.81
1:A:44:ARG:HD2	1:A:244:GLU:HG2	1.62	0.80
2:B:192:GLN:CG	2:B:193:LYS:H	1.83	0.80
1:A:180:ILE:HD12	1:A:231:ILE:HG21	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:800:B12:H552	3:B:800:B12:H531	1.66	0.78
1:A:217:ARG:HG3	1:A:217:ARG:NH1	1.95	0.77
2:B:189:THR:HG23	2:B:223:PRO:CG	2.16	0.76
1:A:199:THR:HB	1:A:212:ASN:HD21	1.51	0.76
1:A:87:THR:CG2	1:A:89:LYS:HG2	2.16	0.76
2:B:51:ALA:O	2:B:55:ILE:HG22	1.86	0.74
1:A:134:ASN:O	1:A:137:ILE:HG22	1.86	0.74
1:A:58:LEU:O	1:A:62:VAL:HG12	1.87	0.74
2:B:57:LEU:HA	2:B:62:GLU:HB3	1.68	0.74
1:A:80:ILE:O	1:A:84:VAL:HG23	1.87	0.73
2:B:141:MET:O	2:B:153:GLU:HG2	1.87	0.73
1:A:158:ALA:HB2	1:A:183:ILE:HB	1.69	0.72
1:A:222:LYS:NZ	1:A:222:LYS:HB3	2.03	0.72
2:B:68:MET:CE	2:B:70:GLN:HG2	2.19	0.72
2:B:33:LYS:N	2:B:33:LYS:HE2	2.04	0.72
1:A:129:GLU:OE1	1:A:129:GLU:HA	1.90	0.71
2:B:69:GLN:O	2:B:69:GLN:HG3	1.89	0.71
1:A:74:LEU:HD22	1:A:78:MET:HG3	1.72	0.71
1:A:413:LEU:HD11	2:B:67:VAL:HG11	1.71	0.71
1:A:61:ILE:HD12	1:A:62:VAL:N	2.06	0.71
1:A:446:GLU:O	1:A:451:GLN:OE1	2.09	0.70
1:A:87:THR:HG23	1:A:89:LYS:H	1.57	0.70
1:A:253:ARG:O	1:A:253:ARG:HG3	1.91	0.69
2:B:122:VAL:CG2	2:B:181:ALA:HA	2.21	0.69
1:A:216:MET:HE2	1:A:220:LEU:HD21	1.72	0.69
2:B:66:VAL:HG22	2:B:81:VAL:CG1	2.21	0.69
1:A:162:ILE:HG22	1:A:199:THR:O	1.91	0.69
1:A:210:GLN:HB2	1:A:248:MET:CG	2.23	0.69
3:B:800:B12:C3R	3:B:800:B12:P	2.81	0.69
1:A:184:ARG:HG2	1:A:184:ARG:NH1	1.98	0.68
2:B:189:THR:CG2	2:B:223:PRO:HG3	2.22	0.67
1:A:83:ALA:O	1:A:87:THR:HB	1.94	0.67
1:A:222:LYS:HB3	1:A:222:LYS:HZ2	1.57	0.67
1:A:74:LEU:CD2	1:A:78:MET:HG3	2.25	0.67
1:A:103:LEU:HD23	1:A:104:ASP:N	2.07	0.66
1:A:378:MET:HG2	1:A:411:GLU:HB3	1.77	0.66
2:B:246:ASP:O	2:B:250:THR:HG22	1.96	0.66
1:A:378:MET:HE2	1:A:378:MET:HA	1.75	0.66
1:A:103:LEU:HD21	1:A:108:LEU:HD11	1.77	0.66
1:A:331:GLU:HA	1:A:334:MET:HG3	1.79	0.65
2:B:113:ILE:HG21	2:B:157:MET:HB3	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LEU:CD2	1:A:333:GLN:HB3	2.26	0.65
2:B:49:ALA:O	2:B:52:ALA:HB3	1.97	0.65
2:B:62:GLU:HB2	2:B:64:PRO:HD3	1.78	0.65
1:A:413:LEU:CD1	2:B:67:VAL:HG11	2.27	0.65
2:B:220:CYS:O	2:B:238:GLY:HA2	1.98	0.64
1:A:189:SER:HB2	1:A:239:GLY:CA	2.28	0.64
1:A:376:LYS:HG3	1:A:377:PHE:CD1	2.33	0.63
1:A:103:LEU:CD2	1:A:104:ASP:H	2.09	0.63
1:A:234:CYS:HA	1:A:256:VAL:O	1.99	0.63
1:A:35:THR:OG1	1:A:37:THR:HG22	1.98	0.63
2:B:107:GLU:HG3	2:B:108:GLU:N	2.12	0.63
1:A:387:ILE:HD12	1:A:387:ILE:O	1.99	0.62
1:A:209:THR:HG22	1:A:211:GLU:H	1.63	0.62
1:A:39:GLU:HG3	1:A:72:LEU:HD22	1.81	0.62
3:B:800:B12:H362	3:B:800:B12:H351	1.82	0.62
1:A:231:ILE:HD12	1:A:231:ILE:N	2.15	0.62
2:B:196:HIS:O	2:B:200:MET:HG3	2.00	0.62
1:A:87:THR:HG21	1:A:94:ILE:HD11	1.82	0.61
1:A:233:LEU:HD23	1:A:254:LEU:HD22	1.80	0.61
2:B:107:GLU:HG3	2:B:108:GLU:HG3	1.81	0.61
2:B:176:ALA:HB1	2:B:184:LEU:HD11	1.82	0.61
2:B:213:ARG:CZ	2:B:218:LEU:HD13	2.30	0.61
1:A:246:ALA:HA	1:A:257:MET:HE1	1.82	0.61
2:B:142:ASN:O	2:B:151:GLY:HA3	2.01	0.61
1:A:409:LEU:HD23	1:A:409:LEU:H	1.65	0.61
2:B:44:ASN:HB2	2:B:71:SER:HB3	1.82	0.61
1:A:279:GLN:O	1:A:283:ARG:HG2	2.00	0.60
1:A:394:MET:O	1:A:398:MET:HG3	2.01	0.60
1:A:87:THR:HG23	1:A:89:LYS:CG	2.32	0.60
1:A:184:ARG:NH2	1:A:238:SER:O	2.34	0.60
1:A:188:GLN:HE22	1:A:208:ALA:HB3	1.65	0.59
1:A:82:ASN:OD1	1:A:110:MET:HA	2.01	0.59
1:A:35:THR:HG23	1:A:277:ILE:HG21	1.84	0.59
1:A:82:ASN:HD22	1:A:82:ASN:C	2.06	0.59
2:B:68:MET:HE3	2:B:70:GLN:HG2	1.83	0.59
1:A:104:ASP:HB3	1:A:107:LYS:HG3	1.83	0.59
1:A:234:CYS:HB2	1:A:256:VAL:HG22	1.85	0.59
1:A:86:ASN:HD22	1:A:109:PRO:HG2	1.63	0.59
1:A:297:GLU:N	1:A:297:GLU:OE1	2.35	0.59
2:B:107:GLU:HG3	2:B:108:GLU:H	1.68	0.59
2:B:105:SER:O	2:B:109:THR:HG22	2.02	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ILE:O	1:A:429:GLN:HG2	2.04	0.58
1:A:33:HIS:O	1:A:501:LYS:HE3	2.04	0.58
2:B:66:VAL:HG22	2:B:81:VAL:HG11	1.83	0.58
1:A:235:ASN:ND2	1:A:236:TYR:H	2.01	0.58
2:B:66:VAL:HG22	2:B:81:VAL:HG12	1.85	0.58
2:B:178:GLU:C	2:B:180:GLU:H	2.06	0.58
1:A:37:THR:HG23	1:A:243:PRO:HG2	1.85	0.57
1:A:11:LEU:HD13	1:A:458:LEU:HG	1.84	0.57
1:A:188:GLN:NE2	1:A:208:ALA:HB3	2.19	0.57
1:A:83:ALA:HB1	1:A:94:ILE:HD12	1.86	0.57
1:A:119:LYS:O	1:A:123:MET:HG3	2.04	0.57
2:B:68:MET:HE1	2:B:70:GLN:HG2	1.85	0.57
2:B:192:GLN:CG	2:B:193:LYS:N	2.53	0.57
1:A:128:VAL:HG21	1:A:512:LEU:HD12	1.87	0.56
1:A:456:PHE:CE2	1:A:460:LYS:HD2	2.40	0.56
1:A:103:LEU:CD2	1:A:104:ASP:N	2.67	0.56
1:A:121:LEU:HD11	1:A:512:LEU:HD21	1.87	0.56
1:A:145:TYR:CE2	1:A:228:GLY:HA2	2.40	0.56
1:A:410:THR:HG21	1:A:420:ASP:OD1	2.06	0.56
2:B:201:THR:O	2:B:205:GLU:HG3	2.06	0.56
1:A:216:MET:CE	1:A:220:LEU:HD21	2.36	0.56
1:A:305:ASP:OD1	1:A:305:ASP:C	2.44	0.56
1:A:378:MET:O	1:A:412:ALA:HB2	2.06	0.55
1:A:488:PRO:HG2	1:A:491:GLY:HA3	1.88	0.55
1:A:496:ASN:ND2	1:A:496:ASN:H	2.02	0.55
2:B:112:TYR:CD2	2:B:253:VAL:HG12	2.42	0.55
1:A:413:LEU:CD2	2:B:67:VAL:HG13	2.37	0.55
1:A:209:THR:HG22	1:A:211:GLU:N	2.22	0.55
1:A:210:GLN:HE22	1:A:251:ILE:CD1	2.20	0.55
1:A:103:LEU:HD22	1:A:105:LEU:HD23	1.89	0.54
1:A:116:VAL:CG2	1:A:117:LYS:N	2.70	0.54
1:A:231:ILE:HD12	1:A:231:ILE:H	1.72	0.54
1:A:49:ASP:CG	1:A:50:GLY:H	2.10	0.54
1:A:158:ALA:CB	1:A:183:ILE:HB	2.38	0.54
1:A:162:ILE:O	1:A:166:ILE:HG13	2.08	0.54
1:A:183:ILE:HD13	1:A:236:TYR:OH	2.07	0.54
1:A:169:ALA:HB3	1:A:216:MET:HE1	1.90	0.54
2:B:185:LEU:HB3	3:B:800:B12:HM52	1.89	0.54
2:B:192:GLN:HG2	2:B:195:VAL:HG12	1.89	0.54
1:A:378:MET:HE2	1:A:378:MET:CA	2.37	0.54
1:A:404:HIS:CD2	1:A:406:LEU:HD23	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:THR:CG2	1:A:89:LYS:H	2.20	0.53
2:B:139:ALA:HB1	2:B:146:TYR:HB2	1.90	0.53
2:B:38:PHE:CE1	2:B:55:ILE:HD12	2.44	0.53
2:B:252:ALA:O	2:B:256:LEU:HG	2.09	0.53
2:B:176:ALA:CB	2:B:184:LEU:HD11	2.38	0.53
2:B:66:VAL:HG12	2:B:66:VAL:O	2.08	0.52
1:A:298:ASP:O	1:A:302:THR:HG23	2.09	0.52
2:B:225:ILE:HG22	2:B:226:ASN:N	2.25	0.52
1:A:110:MET:CE	1:A:116:VAL:HG11	2.40	0.52
2:B:57:LEU:HB2	2:B:62:GLU:OE2	2.09	0.52
1:A:227:VAL:HG12	1:A:227:VAL:O	2.09	0.52
1:A:373:PRO:HD3	1:A:405:LEU:O	2.10	0.52
1:A:179:VAL:HG22	1:A:232:ARG:HB2	1.91	0.52
1:A:382:ILE:HD11	1:A:409:LEU:CD1	2.40	0.52
1:A:258:LEU:N	1:A:258:LEU:HD12	2.25	0.52
1:A:480:GLY:HA2	1:A:485:VAL:O	2.09	0.52
1:A:126:GLU:O	1:A:129:GLU:HB2	2.10	0.52
2:B:55:ILE:HD13	2:B:55:ILE:C	2.30	0.51
1:A:507:ASN:OD1	1:A:509:PHE:HB2	2.10	0.51
1:A:52:ASP:OD2	1:A:52:ASP:C	2.47	0.51
1:A:382:ILE:HD11	1:A:409:LEU:HD12	1.91	0.51
1:A:199:THR:CB	1:A:212:ASN:HD21	2.21	0.51
1:A:258:LEU:HD12	1:A:258:LEU:H	1.75	0.51
1:A:236:TYR:N	1:A:236:TYR:CD2	2.79	0.51
2:B:161:TYR:CG	2:B:179:LEU:HD13	2.46	0.51
2:B:63:GLU:N	2:B:64:PRO:CD	2.73	0.50
2:B:191:THR:O	2:B:192:GLN:C	2.50	0.50
2:B:196:HIS:CE1	2:B:197:ILE:HG13	2.46	0.50
1:A:72:LEU:HB3	1:A:499:VAL:HG11	1.94	0.50
1:A:45:LEU:HB3	1:A:509:PHE:CZ	2.47	0.50
1:A:378:MET:CA	1:A:378:MET:CE	2.90	0.50
1:A:413:LEU:HD22	2:B:67:VAL:HG13	1.92	0.50
3:B:800:B12:O2	3:B:800:B12:C4R	2.52	0.50
1:A:378:MET:HG2	1:A:411:GLU:CB	2.42	0.49
1:A:61:ILE:HD12	1:A:61:ILE:C	2.31	0.49
2:B:105:SER:O	2:B:109:THR:CG2	2.59	0.49
1:A:409:LEU:HD23	1:A:409:LEU:N	2.28	0.49
1:A:488:PRO:CG	1:A:491:GLY:HA3	2.42	0.49
2:B:125:GLY:HA2	2:B:185:LEU:O	2.12	0.49
1:A:236:TYR:CD2	1:A:258:LEU:HD13	2.47	0.49
1:A:83:ALA:O	1:A:87:THR:CG2	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:186:VAL:O	2:B:220:CYS:HA	2.13	0.49
1:A:311:HIS:H	1:A:311:HIS:CD2	2.31	0.49
1:A:35:THR:HG23	1:A:277:ILE:CG2	2.43	0.48
1:A:351:LEU:HD22	1:A:450:ILE:HD11	1.96	0.48
1:A:486:LYS:C	1:A:487:ARG:HG2	2.34	0.48
1:A:184:ARG:HH22	1:A:189:SER:HB3	1.78	0.48
2:B:103:ILE:HG22	2:B:104:LEU:O	2.14	0.48
1:A:236:TYR:N	1:A:236:TYR:HD2	2.10	0.48
1:A:378:MET:HA	1:A:378:MET:CE	2.44	0.48
1:A:409:LEU:H	1:A:409:LEU:CD2	2.25	0.48
1:A:170:VAL:O	1:A:174:LYS:HG2	2.13	0.48
2:B:156:GLU:HG2	2:B:157:MET:CE	2.44	0.48
2:B:192:GLN:HG2	2:B:195:VAL:CG1	2.43	0.48
2:B:72:LEU:HD23	2:B:72:LEU:N	2.29	0.48
1:A:384:LYS:HG3	1:A:388:GLN:NE2	2.29	0.48
2:B:71:SER:HA	2:B:77:THR:HA	1.95	0.48
2:B:213:ARG:NH2	2:B:218:LEU:HD13	2.29	0.47
1:A:138:ARG:HD3	1:A:255:ASP:OD1	2.15	0.47
1:A:189:SER:HB2	1:A:239:GLY:HA2	1.96	0.47
1:A:456:PHE:CZ	1:A:460:LYS:HD2	2.49	0.47
1:A:51:VAL:CA	1:A:58:LEU:HD22	2.44	0.47
1:A:315:ALA:O	1:A:319:ILE:HG13	2.13	0.47
1:A:313:VAL:O	1:A:317:GLN:HG3	2.14	0.47
2:B:129:GLY:O	2:B:166:GLN:HA	2.15	0.47
1:A:51:VAL:HG12	1:A:57:PRO:HA	1.96	0.47
1:A:116:VAL:HG23	1:A:117:LYS:N	2.28	0.47
1:A:233:LEU:CD2	1:A:254:LEU:HD22	2.45	0.47
1:A:338:HIS:N	1:A:338:HIS:CD2	2.82	0.47
2:B:62:GLU:O	2:B:84:ASN:OD1	2.33	0.47
2:B:189:THR:HG23	2:B:223:PRO:CD	2.45	0.47
1:A:64:ASP:O	1:A:68:GLU:HG2	2.15	0.47
1:A:200:THR:C	1:A:201:GLU:HG3	2.36	0.46
2:B:55:ILE:HD13	2:B:55:ILE:O	2.16	0.46
1:A:36:VAL:HG13	1:A:40:ARG:NH2	2.30	0.46
1:A:244:GLU:O	1:A:248:MET:HB2	2.15	0.46
2:B:105:SER:OG	2:B:107:GLU:HG2	2.16	0.46
1:A:87:THR:HG22	1:A:88:GLY:N	2.31	0.46
1:A:112:ASP:OD2	1:A:113:LEU:N	2.49	0.46
1:A:329:LEU:HD23	1:A:330:PRO:HD2	1.97	0.46
1:A:348:ASN:OD1	1:A:351:LEU:HD12	2.16	0.46
1:A:455:GLY:O	1:A:459:GLU:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ASN:O	1:A:87:THR:HB	2.15	0.45
1:A:200:THR:HG22	1:A:201:GLU:HG3	1.97	0.45
1:A:405:LEU:C	1:A:405:LEU:HD23	2.37	0.45
2:B:122:VAL:HG21	2:B:179:LEU:O	2.15	0.45
1:A:83:ALA:O	1:A:87:THR:CB	2.63	0.45
3:B:800:B12:H531	3:B:800:B12:C55	2.43	0.45
1:A:184:ARG:CD	1:A:208:ALA:HB2	2.46	0.45
2:B:61:LEU:HB3	2:B:84:ASN:C	2.37	0.45
1:A:36:VAL:CG1	1:A:40:ARG:NH2	2.80	0.45
1:A:145:TYR:OH	1:A:225:ALA:HA	2.17	0.45
2:B:64:PRO:HA	2:B:82:TYR:O	2.17	0.45
1:A:38:VAL:HG13	1:A:281:PHE:CD2	2.51	0.45
1:A:58:LEU:HD13	1:A:58:LEU:HA	1.74	0.45
1:A:256:VAL:HA	1:A:292:ILE:O	2.16	0.45
2:B:124:VAL:HG23	2:B:181:ALA:HB2	1.98	0.45
1:A:305:ASP:OD1	1:A:307:PHE:N	2.48	0.44
2:B:127:SER:HB2	2:B:165:SER:HA	1.99	0.44
1:A:87:THR:CG2	1:A:88:GLY:N	2.80	0.44
2:B:62:GLU:N	2:B:62:GLU:OE1	2.51	0.44
2:B:178:GLU:C	2:B:180:GLU:N	2.71	0.44
1:A:104:ASP:OD1	1:A:106:THR:HB	2.17	0.44
1:A:380:GLY:C	2:B:68:MET:HB2	2.37	0.44
1:A:410:THR:HG21	1:A:420:ASP:CG	2.38	0.44
1:A:125:LYS:HE3	1:A:125:LYS:HB2	1.89	0.44
1:A:378:MET:CG	1:A:411:GLU:HB3	2.47	0.44
2:B:133:HIS:NE2	3:B:800:B12:H202	2.33	0.44
1:A:314:LEU:HD22	1:A:359:MET:HE1	2.00	0.44
1:A:373:PRO:HB3	1:A:392:PHE:CE2	2.53	0.44
1:A:446:GLU:HA	1:A:446:GLU:OE1	2.17	0.44
2:B:161:TYR:CD1	2:B:179:LEU:HD13	2.52	0.44
1:A:11:LEU:HD11	1:A:459:GLU:HG2	1.99	0.44
1:A:141:ARG:HH11	1:A:141:ARG:HG2	1.83	0.44
1:A:186:THR:HG23	2:B:146:TYR:CE1	2.53	0.43
2:B:38:PHE:C	2:B:38:PHE:CD2	2.91	0.43
1:A:35:THR:OG1	1:A:38:VAL:HG23	2.18	0.43
1:A:36:VAL:CG1	1:A:40:ARG:HH22	2.31	0.43
3:B:800:B12:H262	3:B:800:B12:H601	2.00	0.43
1:A:44:ARG:NH2	1:A:244:GLU:OE2	2.51	0.43
1:A:213:PHE:CE1	1:A:254:LEU:HD11	2.53	0.43
2:B:53:LYS:HZ3	2:B:65:SER:HA	1.84	0.43
2:B:62:GLU:HB2	2:B:63:GLU:H	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LEU:O	1:A:61:ILE:HG13	2.19	0.43
1:A:43:CYS:HB3	1:A:48:ILE:HD12	2.01	0.43
1:A:58:LEU:HD12	1:A:61:ILE:HG12	2.01	0.43
2:B:41:PRO:C	2:B:42:LEU:HD23	2.39	0.43
1:A:86:ASN:HD21	1:A:109:PRO:HG2	1.73	0.42
2:B:63:GLU:H	2:B:64:PRO:HD3	1.85	0.42
2:B:36:LEU:HD12	2:B:81:VAL:HG22	2.02	0.42
2:B:123:VAL:HB	2:B:183:VAL:HB	2.01	0.42
2:B:130:THR:O	2:B:130:THR:CG2	2.66	0.42
1:A:184:ARG:HD3	1:A:208:ALA:HB2	2.01	0.42
1:A:234:CYS:CB	1:A:256:VAL:HG22	2.48	0.42
1:A:326:LEU:HD12	1:A:326:LEU:HA	1.68	0.42
2:B:41:PRO:O	2:B:42:LEU:HD23	2.20	0.42
2:B:227:ASN:OD1	2:B:237:ALA:HA	2.19	0.42
1:A:1:MET:HG2	1:A:361:ARG:HG3	2.02	0.42
1:A:2:GLU:HG3	1:A:4:LYS:HG3	2.01	0.42
1:A:117:LYS:O	1:A:120:ALA:HB3	2.19	0.42
1:A:356:GLN:HE21	1:A:453:ARG:HE	1.68	0.42
1:A:156:ILE:CG2	1:A:183:ILE:HG12	2.49	0.42
2:B:104:LEU:HD12	2:B:109:THR:HA	2.01	0.42
2:B:156:GLU:HG2	2:B:157:MET:HE2	2.00	0.42
1:A:104:ASP:HB3	1:A:107:LYS:CG	2.49	0.42
1:A:183:ILE:CD1	1:A:236:TYR:OH	2.68	0.42
2:B:52:ALA:O	2:B:55:ILE:HG23	2.20	0.42
2:B:54:GLN:O	2:B:58:LYS:HB2	2.19	0.42
1:A:135:ARG:O	1:A:139:GLU:OE2	2.38	0.42
1:A:137:ILE:CG2	1:A:138:ARG:N	2.83	0.42
1:A:435:MET:HE3	1:A:438:ILE:HG21	2.02	0.42
1:A:20:LYS:N	1:A:322:GLN:HG3	2.34	0.42
1:A:110:MET:O	1:A:111:LYS:O	2.38	0.42
1:A:128:VAL:HG21	1:A:512:LEU:CD1	2.50	0.41
1:A:265:ILE:HG12	1:A:272:MET:HA	2.01	0.41
1:A:468:ILE:HG12	1:A:476:THR:HG21	2.02	0.41
1:A:82:ASN:OD1	1:A:110:MET:CE	2.68	0.41
1:A:236:TYR:CG	1:A:258:LEU:HD13	2.56	0.41
2:B:53:LYS:O	2:B:56:ALA:HB3	2.20	0.41
2:B:69:GLN:O	2:B:69:GLN:CG	2.64	0.41
1:A:413:LEU:HD13	2:B:67:VAL:HG21	2.01	0.41
2:B:57:LEU:O	2:B:59:MET:N	2.53	0.41
1:A:89:LYS:HB2	1:A:93:GLU:OE1	2.21	0.41
1:A:51:VAL:C	1:A:58:LEU:HD22	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:PHE:O	1:A:146:GLY:N	2.33	0.41
1:A:68:GLU:HG2	1:A:68:GLU:H	1.67	0.41
1:A:382:ILE:CD1	1:A:409:LEU:HD12	2.51	0.41
1:A:147:ASP:OD1	1:A:232:ARG:NH1	2.53	0.41
1:A:189:SER:HB2	1:A:239:GLY:HA3	2.02	0.41
1:A:240:LEU:HG	1:A:270:ILE:HD13	2.02	0.41
1:A:342:MET:CE	1:A:356:GLN:HE22	2.34	0.41
1:A:514:LEU:HD23	1:A:514:LEU:HA	1.94	0.41
1:A:254:LEU:HD12	1:A:257:MET:SD	2.61	0.40
1:A:114:PHE:CD1	1:A:114:PHE:O	2.74	0.40
1:A:329:LEU:CD2	1:A:333:GLN:CB	2.98	0.40
2:B:53:LYS:NZ	2:B:65:SER:HA	2.37	0.40
2:B:225:ILE:CG2	2:B:226:ASN:N	2.84	0.40
1:A:234:CYS:SG	1:A:256:VAL:HG22	2.61	0.40
1:A:378:MET:HB2	1:A:378:MET:HE3	1.85	0.40
2:B:57:LEU:C	2:B:59:MET:N	2.74	0.40
1:A:90:THR:OG1	1:A:93:GLU:HG3	2.21	0.40
1:A:211:GLU:HG3	1:A:215:LEU:HD22	2.03	0.40
2:B:38:PHE:CZ	2:B:55:ILE:HD12	2.57	0.40
2:B:168:ALA:HB3	2:B:171:ASP:OD1	2.20	0.40
2:B:202:HIS:CE1	2:B:206:LEU:HD11	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	514/516 (100%)	471 (92%)	36 (7%)	7 (1%)	11 34
2	B	208/262 (79%)	184 (88%)	18 (9%)	6 (3%)	4 15
All	All	722/778 (93%)	655 (91%)	54 (8%)	13 (2%)	8 28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	87	THR
1	A	111	LYS
1	A	446	GLU
2	B	192	GLN
2	B	44	ASN
1	A	503	GLU
1	A	76	ALA
2	B	58	LYS
1	A	85	LEU
1	A	411	GLU
2	B	179	LEU
2	B	41	PRO
2	B	63	GLU

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	429/429 (100%)	391 (91%)	38 (9%)	9 28
2	B	177/223 (79%)	154 (87%)	23 (13%)	4 13
All	All	606/652 (93%)	545 (90%)	61 (10%)	7 22

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	11	LEU
1	A	13	GLU
1	A	58	LEU
1	A	62	VAL
1	A	74	LEU
1	A	82	ASN
1	A	87	THR
1	A	96	GLN
1	A	107	LYS

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Mol	Chain	Res	Type
1	A	129	GLU
1	A	137	ILE
1	A	161	ASN
1	A	167	THR
1	A	184	ARG
1	A	191	LEU
1	A	215	LEU
1	A	217	ARG
1	A	222	LYS
1	A	226	GLU
1	A	232	ARG
1	A	236	TYR
1	A	262	LEU
1	A	326	LEU
1	A	329	LEU
1	A	334	MET
1	A	338	HIS
1	A	345	GLU
1	A	384	LYS
1	A	387	ILE
1	A	409	LEU
1	A	442	ILE
1	A	446	GLU
1	A	469	GLU
1	A	496	ASN
1	A	502	ASP
1	A	503	GLU
1	A	514	LEU
2	B	33	LYS
2	B	39	THR
2	B	40	LEU
2	B	42	LEU
2	B	55	ILE
2	B	61	LEU
2	B	63	GLU
2	B	64	PRO
2	B	68	MET
2	B	69	GLN
2	B	72	LEU
2	B	84	ASN
2	B	109	THR
2	B	119	ARG

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Mol	Chain	Res	Type
2	B	134	THR
2	B	163	LEU
2	B	184	LEU
2	B	186	VAL
2	B	203	LEU
2	B	207	LEU
2	B	212	LEU
2	B	243	ARG
2	B	261	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	33	HIS
1	A	69	ASN
1	A	133	ASN
1	A	161	ASN
1	A	168	GLN
1	A	210	GLN
1	A	235	ASN
1	A	280	ASN
1	A	294	ASN
1	A	311	HIS
1	A	356	GLN
1	A	388	GLN
1	A	393	ASN
1	A	434	ASN
1	A	443	GLN
1	A	496	ASN
2	B	35	GLN
2	B	54	GLN
2	B	84	ASN
2	B	166	GLN
2	B	169	ASN
2	B	192	GLN
2	B	194	ASN
2	B	202	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

3 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	$\#\|Z\| > 2$
5	5AD	B	500	3	16,20,20	1.54	3 (18%)	14,30,30	1.88	4 (28%)
3	B12	B	800	2,5	91,101,101	3.14	43 (47%)	140,166,166	2.57	40 (28%)
4	PLP	B	801	2	15,15,16	5.52	8 (53%)	21,22,23	2.37	7 (33%)

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
5	5AD	B	500	3	-	0/0/20/20	0/3/3/3
3	B12	B	800	2,5	-	6/52/223/223	0/3/11/11
4	PLP	B	801	2	-	1/6/6/8	0/1/1/1

All (54) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	B12	O6R-C1R	16.99	1.63	1.40
4	B	801	PLP	C5-C4	15.45	1.58	1.40
4	B	801	PLP	C6-C5	7.54	1.52	1.37
4	B	801	PLP	C6-N1	7.04	1.48	1.34
4	B	801	PLP	C2-N1	6.97	1.46	1.33
3	B	800	B12	C20-C1	6.70	1.66	1.53
3	B	800	B12	C4B-C9B	6.25	1.51	1.41
3	B	800	B12	O2-C3R	6.01	1.64	1.44
3	B	800	B12	C1-C19	-5.80	1.42	1.55
3	B	800	B12	C12-C11	5.38	1.61	1.52
3	B	800	B12	C4B-C5B	5.05	1.49	1.37
4	B	801	PLP	C3-C2	4.93	1.46	1.41
3	B	800	B12	C25-C2	4.59	1.62	1.54
3	B	800	B12	C7B-C6B	4.52	1.48	1.37
3	B	800	B12	C5M-C5B	-4.01	1.43	1.51
3	B	800	B12	C35-C5	4.00	1.59	1.50
3	B	800	B12	C56-C57	3.99	1.59	1.51
3	B	800	B12	C50-N52	-3.91	1.20	1.32
3	B	800	B12	C47-C12	3.85	1.61	1.54
3	B	800	B12	C49-C50	-3.80	1.36	1.51
3	B	800	B12	C6B-C5B	3.79	1.50	1.40
3	B	800	B12	O8R-C5R	-3.75	1.26	1.42
4	B	801	PLP	P-O4P	-3.72	1.48	1.60
3	B	800	B12	C8B-C9B	3.51	1.47	1.40
5	B	500	5AD	O4'-C1'	3.45	1.45	1.40
3	B	800	B12	C7B-C8B	3.40	1.47	1.40
4	B	801	PLP	O4P-C5A	-3.18	1.33	1.44
3	B	800	B12	C13-C14	3.12	1.58	1.52
3	B	800	B12	C2R-C3R	3.00	1.59	1.53
3	B	800	B12	O6R-C4R	-2.87	1.38	1.45
3	B	800	B12	C10-C9	-2.82	1.31	1.39
3	B	800	B12	C2-C3	-2.78	1.49	1.57
3	B	800	B12	C60-C18	-2.75	1.48	1.54
3	B	800	B12	C41-C42	-2.71	1.44	1.52
3	B	800	B12	C3-C4	2.71	1.58	1.51
3	B	800	B12	C61-N62	-2.70	1.24	1.32
3	B	800	B12	C17-C16	2.70	1.60	1.54
3	B	800	B12	C6M-C6B	2.64	1.55	1.51
3	B	800	B12	C43-N45	-2.58	1.24	1.32
3	B	800	B12	C54-C17	2.57	1.58	1.54
3	B	800	B12	C26-C27	-2.57	1.43	1.51
4	B	801	PLP	P-O3P	-2.56	1.45	1.54
3	B	800	B12	O34-C32	2.45	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	800	B12	C32-N33	-2.41	1.25	1.32
3	B	800	B12	C12-C13	-2.41	1.48	1.55
3	B	800	B12	C53-C15	-2.35	1.46	1.50
3	B	800	B12	C36-C7	2.29	1.58	1.54
5	B	500	5AD	C2-N1	2.28	1.38	1.33
3	B	800	B12	C27-N29	-2.27	1.25	1.32
3	B	800	B12	C14-N23	2.25	1.38	1.35
3	B	800	B12	C41-C8	-2.24	1.49	1.54
3	B	800	B12	C5R-C4R	-2.20	1.44	1.51
3	B	800	B12	C31-C32	2.20	1.60	1.51
5	B	500	5AD	C8-N7	-2.05	1.31	1.34

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	800	B12	C19-N24-C16	14.65	123.31	107.29
3	B	800	B12	C9-N22-C6	10.28	117.65	105.28
3	B	800	B12	C1-C19-N24	7.60	114.70	106.25
4	B	801	PLP	O4P-P-O1P	-6.64	88.49	106.44
3	B	800	B12	O58-C57-C56	-5.92	111.29	122.02
3	B	800	B12	C17-C16-N24	-5.44	102.87	111.17
3	B	800	B12	C2-C1-C19	5.34	126.91	118.61
3	B	800	B12	C4R-O6R-C1R	5.21	114.70	109.92
3	B	800	B12	C54-C17-C55	-5.10	100.80	109.27
3	B	800	B12	C17-C18-C19	4.51	109.20	102.36
3	B	800	B12	O39-C38-C37	-4.43	108.27	121.98
3	B	800	B12	O7R-C2R-C3R	-4.28	99.21	111.19
3	B	800	B12	C10-C9-N22	4.07	130.38	125.74
3	B	800	B12	C56-C57-N59	3.95	123.54	116.34
3	B	800	B12	C18-C19-N24	-3.74	96.71	102.33
5	B	500	5AD	C5'-C4'-C3'	-3.64	111.88	115.70
4	B	801	PLP	C2A-C2-C3	3.59	124.99	120.80
3	B	800	B12	C15-C16-N24	3.43	127.31	122.42
3	B	800	B12	C54-C17-C18	3.43	117.92	112.99
4	B	801	PLP	O4P-C5A-C5	-3.36	103.06	109.36
5	B	500	5AD	C4-C5-N7	3.33	112.85	109.34
3	B	800	B12	C5-C6-N22	3.28	128.84	123.88
3	B	800	B12	C20-C1-C2	-3.23	107.96	113.28
3	B	800	B12	O3-C2P-C1P	-3.22	100.56	106.94
3	B	800	B12	C7-C6-N22	-3.15	102.20	107.94
4	B	801	PLP	C4-C3-C2	3.07	124.47	119.89
3	B	800	B12	C35-C5-C4	-3.04	110.63	116.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	500	5AD	C5-C6-N6	3.01	124.89	120.31
3	B	800	B12	C2R-C3R-C4R	2.94	108.39	103.24
4	B	801	PLP	C6-C5-C4	-2.90	115.72	118.10
3	B	800	B12	C1-C2-C3	2.82	105.15	101.60
3	B	800	B12	C35-C5-C6	2.81	126.94	122.41
3	B	800	B12	C2-C26-C27	2.78	122.92	115.19
3	B	800	B12	O63-C61-C60	-2.73	115.16	120.87
3	B	800	B12	C37-C38-N40	2.63	124.64	116.49
3	B	800	B12	C26-C2-C3	-2.62	102.84	107.42
3	B	800	B12	C47-C12-C46	-2.59	105.12	109.41
4	B	801	PLP	C5A-C5-C4	2.52	127.61	122.64
3	B	800	B12	C1-C19-C18	2.41	125.81	121.90
4	B	801	PLP	O3P-P-O2P	2.36	116.65	107.80
3	B	800	B12	C8-C9-N22	-2.26	106.31	110.77
3	B	800	B12	C17-C16-C15	2.25	129.81	126.26
3	B	800	B12	C25-C2-C3	2.25	118.62	112.91
3	B	800	B12	C5B-C4B-C9B	-2.23	118.25	121.30
3	B	800	B12	C47-C12-C13	2.19	121.61	112.74
5	B	500	5AD	C2'-C3'-C4'	2.18	105.58	102.36
3	B	800	B12	O28-C27-N29	2.15	128.29	122.53
3	B	800	B12	C2P-C1P-N59	2.10	116.01	112.92
3	B	800	B12	C25-C2-C26	-2.08	105.61	109.74
3	B	800	B12	C10-C11-N23	2.04	127.87	124.42
3	B	800	B12	C1P-N59-C57	-2.01	118.38	122.69

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	800	B12	C14-C13-C48-C49
3	B	800	B12	C12-C13-C48-C49
3	B	800	B12	C42-C41-C8-C9
3	B	800	B12	C1P-C2P-O3-P
3	B	800	B12	C3R-O2-P-O4
3	B	800	B12	C3R-O2-P-O5
4	B	801	PLP	C4-C5-C5A-O4P

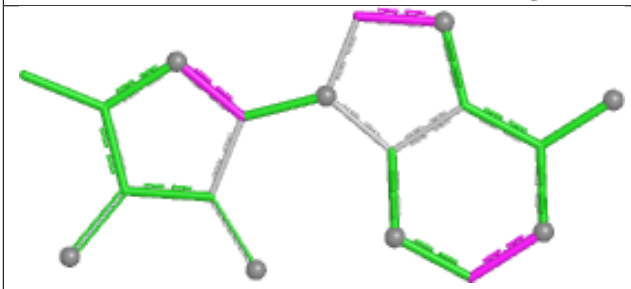
There are no ring outliers.

1 monomer is involved in 9 short contacts:

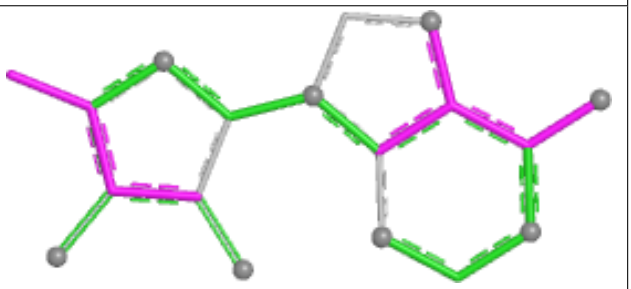
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	800	B12	9	0

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 then 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.

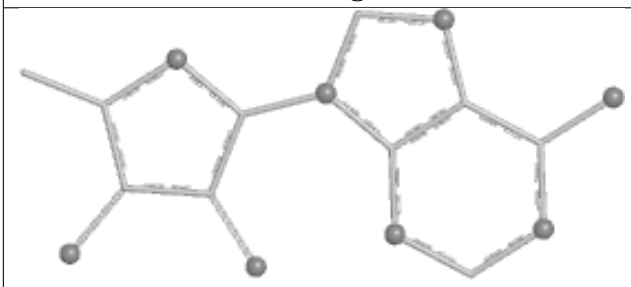
Ligand 5AD B 500



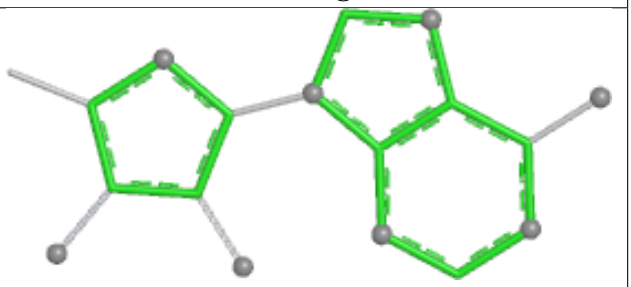
Bond lengths



Bond angles

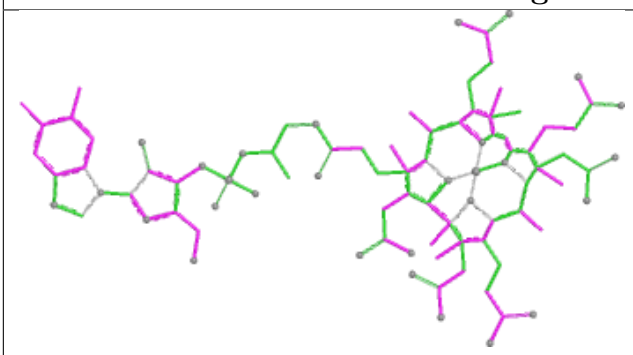


Torsions

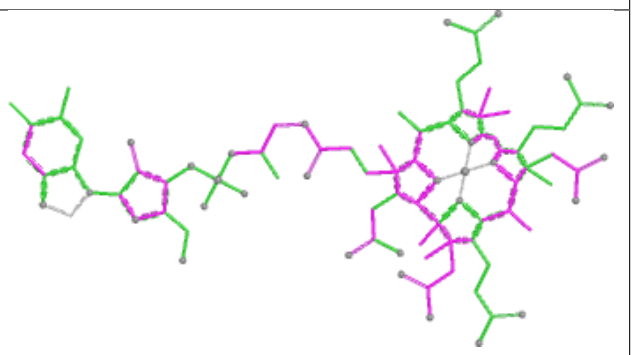


Rings

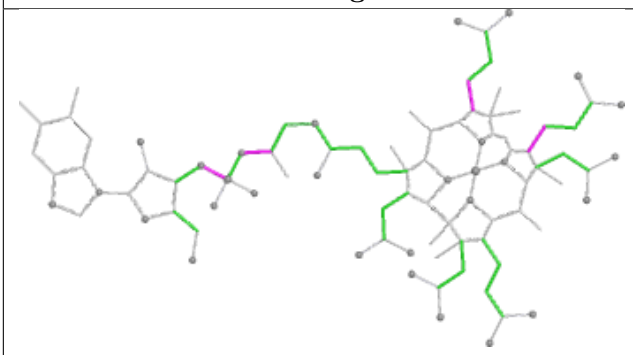
Ligand B12 B 800



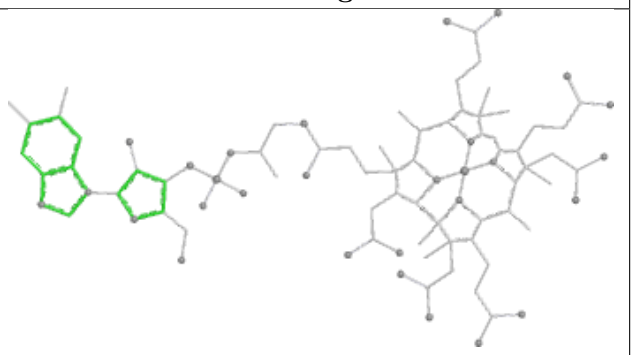
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	516/516 (100%)	-0.42	3 (0%)	89	86	9, 28, 54, 86	0
2	B	212/262 (80%)	-0.05	5 (2%)	59	49	12, 32, 74, 102	0
All	All	728/778 (93%)	-0.31	8 (1%)	80	75	9, 29, 61, 102	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	61	LEU	4.5
2	B	62	GLU	3.8
2	B	261	ASN	2.5
1	A	223	VAL	2.5
2	B	115	GLU	2.3
1	A	101	GLY	2.1
2	B	47	ARG	2.0
1	A	2	GLU	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 monosaccharides 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,

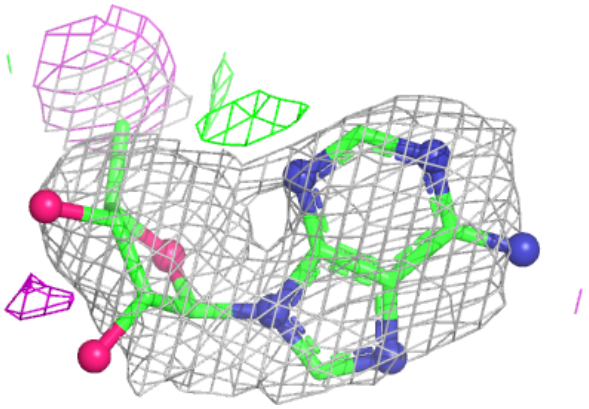
median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

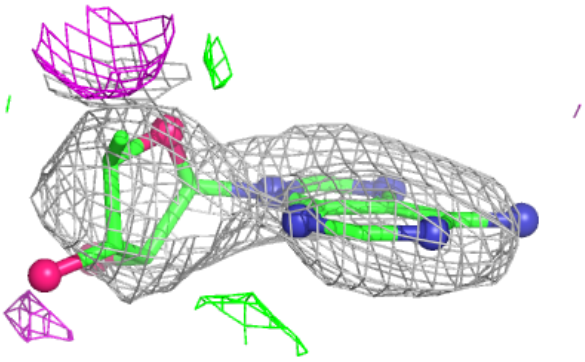
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	5AD	B	500	18/18	0.89	0.28	72,79,83,85	0
3	B12	B	800	91/91	0.93	0.16	0,30,48,55	0
4	PLP	B	801	15/16	0.98	0.17	22,25,30,33	0

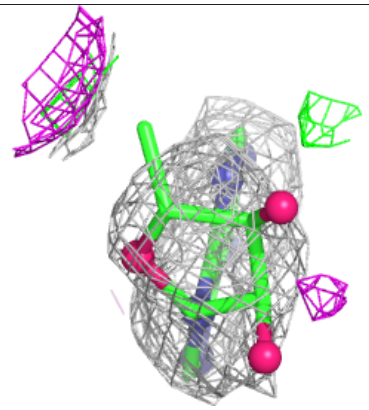
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 5AD B 500:

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

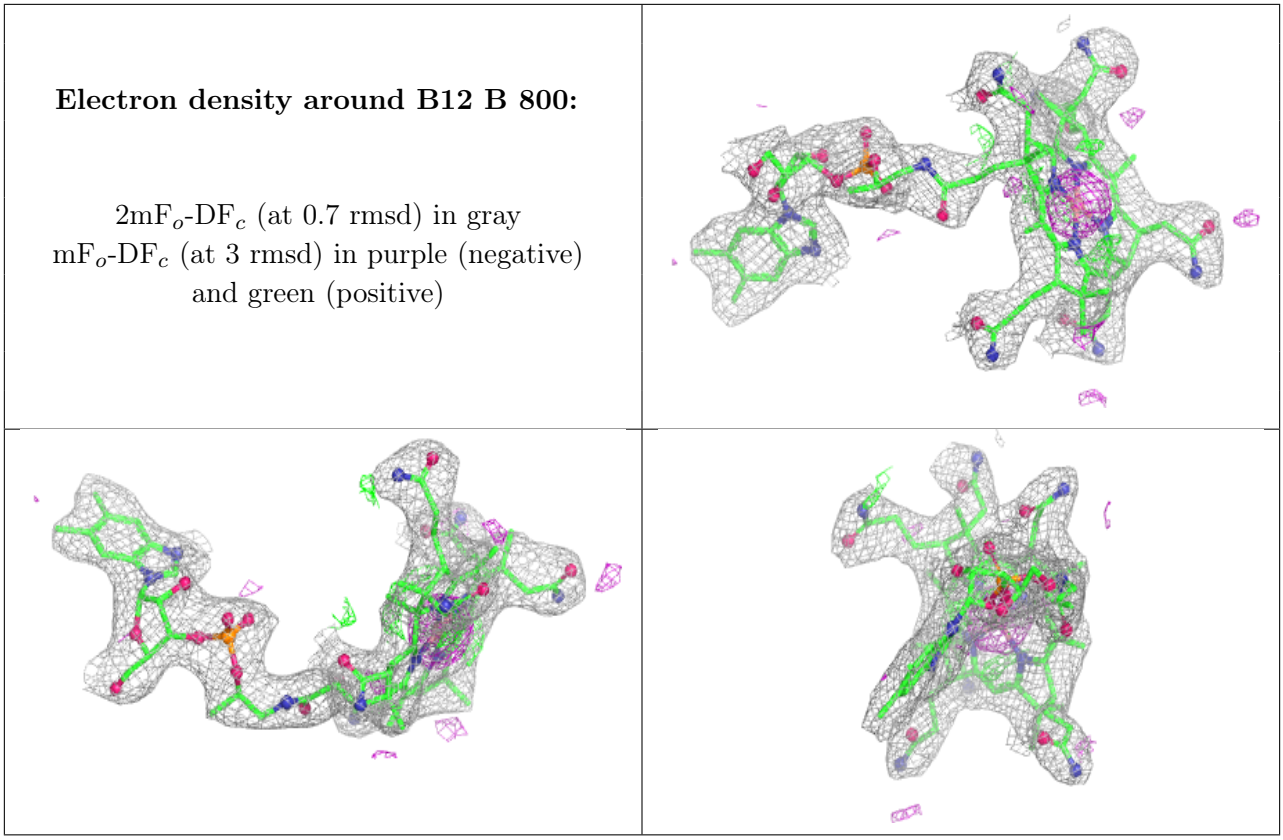






Electron density around B12 B 800:

$2mF_o$-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.