



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:32 PM UTC

PDB ID : 5YSR / pdb_00005ysr
Title : Ethanolamine ammonia-lyase, AdoCbl/2-amino-1-propanol
Authors : Shibata, N.
Deposited on : 2017-11-14
Resolution : 2.05 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

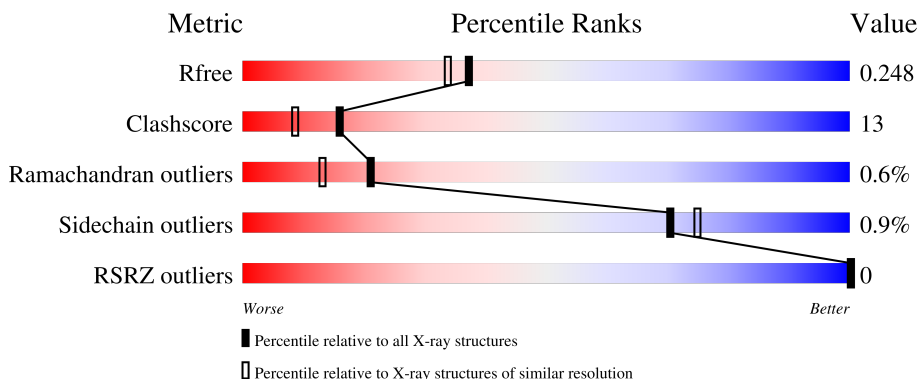
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	2260 (2.04-2.04)
Clashscore	190562	2333 (2.04-2.04)
Ramachandran outliers	187476	2318 (2.04-2.04)
Sidechain outliers	187428	2318 (2.04-2.04)
RSRZ outliers	180081	2260 (2.04-2.04)

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	453	
1	C	453	
2	B	295	
2	D	295	

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 11749 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.

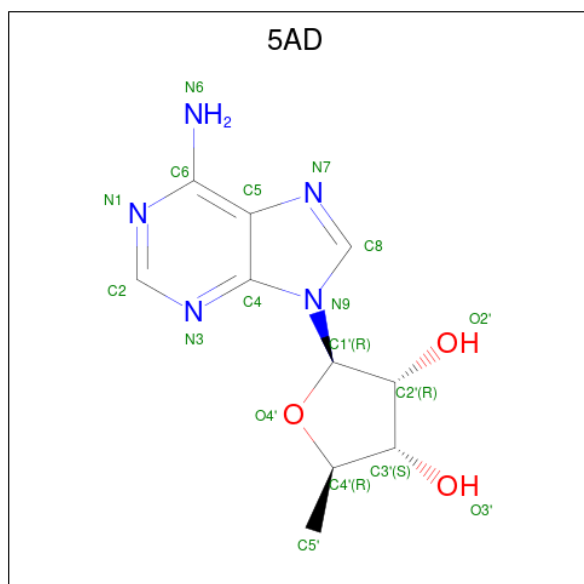
- Molecule 1 is a protein called Ethanolamine ammonia-lyase heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	453	Total	C	N	O	S	0	5	0
			3492	2188	598	684	22			
1	C	453	Total	C	N	O	S	0	3	0
			3486	2184	599	681	22			

- Molecule 2 is a protein called Ethanolamine ammonia-lyase light chain.

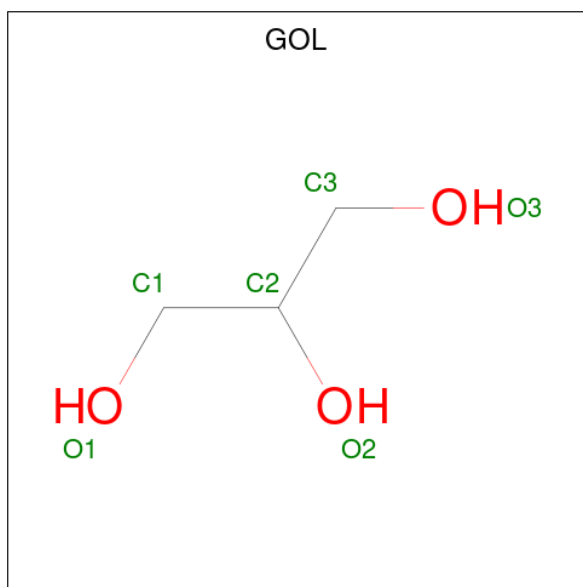
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	1	0
			1924	1202	350	362	10			
2	D	251	Total	C	N	O	S	0	2	0
			1919	1200	347	362	10			

- Molecule 3 is 5'-DEOXYADENOSINE (CCD ID: 5AD) (formula: $C_{10}H_{13}N_5O_3$).



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

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



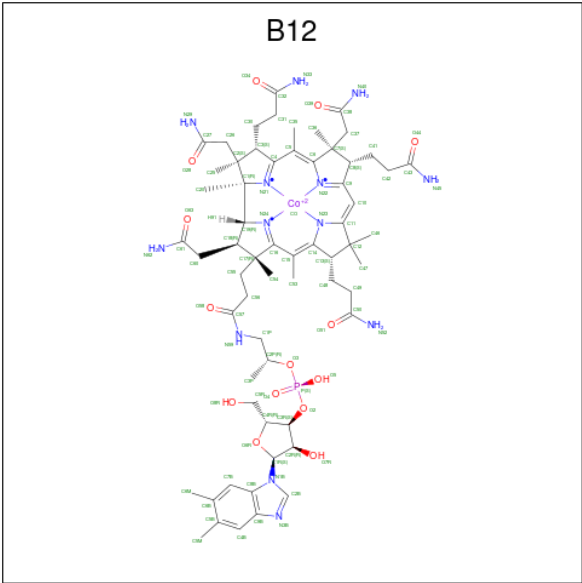
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		
4	C	1	Total	C	O	0	0
			6	3	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	269	Total	O	0	0
			269	269		
6	B	77	Total	O	0	0
			77	77		
6	C	244	Total	O	0	0
			244	244		
6	D	54	Total	O	0	0
			54	54		

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.

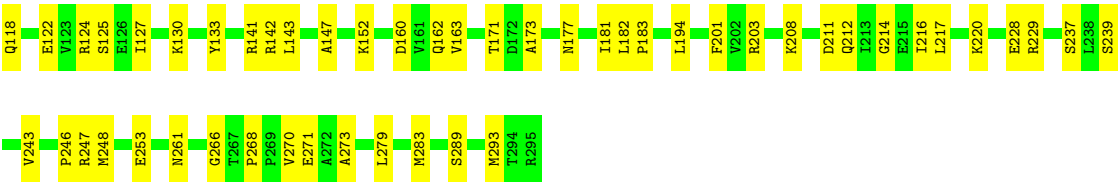
- Chain A: 79% 21%

Position	Amino Acid
1	L354
2	S355
3	M359
4	D362
5	Y365
6	D372
7	E377
8	M380
9	I381
10	T385
11	Y390
12	I391
13	N392
14	G393
15	M394
16	P395
17	L396
18	M401
19	L402
20	M403
21	Y404
22	Q405
23	A408
24	F409
25	F427
26	M434
27	L442
28	T443
29	A446
30	F452
31	F453
32	D197
33	N201
34	S203
35	R204
36	V224
37	Q231
38	I232
39	E233
40	R237
41	G242
42	F245
43	E252
44	K256
45	E267
46	V271
47	G272
48	N276
49	N282
50	Y285
51	Q290
52	E308
53	N311
54	Y312
55	G313
56	D319
57	P320
58	F321
59	V326
60	F329
61	I330
62	G331
63	P332
64	F333
65	Y334
66	L335
67	R339
68	G352
69	V353
70	M1
71	K2
72	Q13
73	F14
74	L21
75	A22
76	V36
77	V45
78	T55
79	R60
80	V64
81	I65
82	Q77
83	S92
84	I93
85	I110
86	K115
87	V122
88	A123
89	A124
90	K127
91	I128
92	M141
93	R160
94	L161
95	Q162
96	P163
97	N164
98	D165
99	T166
100	R167
101	D168
102	I177
103	V185
104	G186
105	D187
106	I190
107	N193
108	P194
109	V195
110	T196

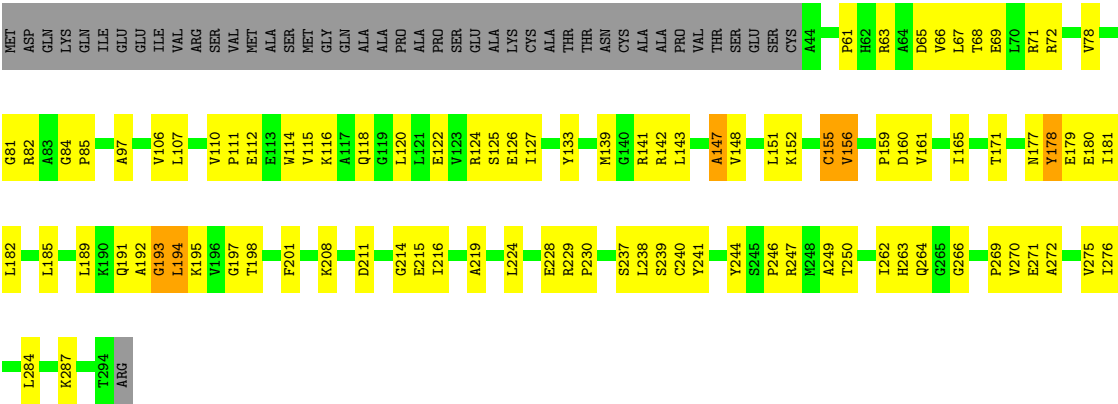
- Chain C: 74% 26%

Row	Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	Col 7	Col 8	Col 9	Col 10	Col 11	Col 12	Col 13	Col 14	Col 15
1	M1	R2	L3	K15	D16	V17	K18	E19	V20	A22	L21	K23	L27	R28	S29
2	E120	V121	V122	A123	K127	D133	L134	I135	M141	K146	T150	R160	L161	Q162	P163
3	L284	Y285	L294	A302	E308	A309	R310	N311	L314	I322	V323	N324	T325	V326	I330
4	M401	Y404	T407	A408	F409	H410	D411	Q417	P425	E426	F427	E428	R429	W430	L431
5	G435	I436	L442	T443	K444	R445	S450	F453	H349	F350	M351	G352	K353	L354	M359
6	D362	N367	H368	A369	D370	E377	M380	I381	L382	L383	A386	C388	N389	Y390	F391
7	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92	E95	L96	R97	D109	I110
8	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
9	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
10	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
11	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
12	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
13	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
14	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
15	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
16	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
17	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
18	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
19	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
20	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
21	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
22	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
23	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
24	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
25	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
26	R44	K48	Q49	V50	L51	M54	R60	V64	E68	V72	Q77	E82	T83	Q87	S92
27	R44	K48	Q49	V50											

- Chain B:  66% 20% 15%
- | Residue | Category |
|---------|----------|
| MET | Green |
| ASP | Green |
| GLN | Green |
| LYS | Green |
| GLN | Green |
| ILE | Green |
| GLU | Green |
| GLU | Green |
| ILE | Green |
| VAL | Green |
| ARG | Green |
| SER | Green |
| VAL | Green |
| MET | Green |
| SER | Green |
| GLY | Green |
| GLN | Green |
| ALA | Green |
| ALA | Green |
| ALA | Green |
| ALA | Green |
| SER | Green |
| GLU | Green |
| LYS | Green |
| CYS | Green |
| ALA | Green |
| THR | Green |
| THR | Green |
| ASN | Green |
| CYS | Green |
| ALA | Green |
| ALA | Green |
| PRO | Green |
| VAL | Green |
| THR | Green |
| SER | Green |
| GLU | Green |
| SER | Green |
| CYS | Green |
| ALA | Green |
| K44 | Yellow |
| K53 | Yellow |
| R77 | Yellow |
| R82 | Yellow |
| R86 | Yellow |
| R84 | Yellow |
| E109 | Grey |
| V110 | Grey |
| V114 | Grey |



• Molecule 2: Ethanolamine ammonia-lyase light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α , β , γ	242.50Å 242.50Å 77.02Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.00 – 2.05 48.00 – 2.05	Depositor EDS
% Data completeness (in resolution range)	95.2 (48.00-2.05) 98.2 (48.00-2.05)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.05Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.223 , 0.257 (Not available) , 0.248	Depositor DCC
R_{free} test set	8086 reflections (4.68%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.164	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 32.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.31$, $\langle L^2 \rangle = 0.14$	Xtriage
Estimated twinning fraction	0.168 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.750 for h,-h-k,-l	Depositor
Outliers	0 of 161639 reflections	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11749	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.05% 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: 5AD, GOL, B12

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	0.24	0/3561	0.43	0/4822
1	C	0.25	0/3549	0.42	0/4804
2	B	0.29	0/1954	0.50	0/2647
2	D	0.27	0/1952	0.54	2/2645 (0.1%)
All	All	0.26	0/11016	0.46	2/14918 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	193	GLY	CA-C-N	6.05	132.58	121.70
2	D	193	GLY	C-N-CA	6.05	132.58	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3492	0	3457	74	1
1	C	3486	0	3451	91	1
2	B	1924	0	1986	56	0
2	D	1919	0	1981	76	0
3	A	18	0	13	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	18	0	13	4	0
4	A	36	0	48	1	1
4	C	30	0	40	4	0
5	B	91	0	88	7	0
5	D	91	0	88	11	0
6	A	269	0	0	2	0
6	B	77	0	0	3	0
6	C	244	0	0	4	1
6	D	54	0	0	3	0
All	All	11749	0	11165	294	2

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 13.

All (294) 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:A:231:GLN:HE22	1:A:245:PHE:H	1.18	0.91
2:D:111:PRO:HB2	2:D:114:TRP:H	1.37	0.89
1:A:60:ARG:HE	1:A:77:GLN:HE22	1.16	0.87
2:D:193:GLY:HA3	2:D:194:LEU:HB2	1.59	0.83
1:C:273:ALA:HA	4:C:504:GOL:H11	1.61	0.81
2:D:156:VAL:HG11	2:D:197:GLY:HA2	1.62	0.81
1:C:377:GLU:HA	1:C:380:MET:HE3	1.65	0.78
2:B:208:LYS:NZ	2:B:253:GLU:OE2	2.16	0.77
1:C:211:GLY:HA3	4:C:505:GOL:H2	1.66	0.77
2:D:148:VAL:HA	2:D:151:LEU:HD23	1.67	0.76
2:B:246:PRO:O	2:B:247:ARG:NH2	2.18	0.76
2:D:214:GLY:HA3	2:D:246:PRO:HG2	1.67	0.75
2:B:268:PRO:HB2	2:B:270:VAL:HG12	1.69	0.75
2:B:173:ALA:O	2:B:177:ASN:ND2	2.21	0.72
2:B:122:GLU:HG3	2:B:201:PHE:HD2	1.56	0.71
2:D:124:ARG:NH1	2:D:125:SER:O	2.23	0.70
2:D:165:ILE:HD11	2:D:182:LEU:HD13	1.73	0.70
1:C:21:LEU:HB3	1:C:127:LYS:HE3	1.71	0.70
2:B:283:MET:HE3	2:B:289:SER:HB3	1.72	0.69
3:C:501:5AD:N1	6:C:602:HOH:O	2.25	0.69
2:B:86:ARG:NE	1:C:133:ASP:OD1	2.20	0.69
2:D:180:GLU:HG2	2:D:270:VAL:HG23	1.75	0.68
1:C:92:SER:OG	1:C:95:GLU:OE1	2.14	0.66
1:A:164:ASN:HD21	1:A:193:ASN:H	1.44	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ARG:HE	1:A:77:GLN:NE2	1.92	0.65
1:A:202:LEU:HB3	1:A:224:VAL:HG11	1.77	0.65
1:C:68:GLU:N	1:C:68:GLU:OE1	2.29	0.65
1:A:232:ILE:HG23	1:A:271:VAL:HG21	1.78	0.64
1:A:329:PHE:O	2:B:229:ARG:NH1	2.30	0.64
2:B:212:GLN:HG3	2:B:248:MET:SD	2.38	0.64
1:C:120:GLU:OE2	1:C:310:ARG:NH1	2.31	0.64
1:C:417:GLN:NE2	1:C:442:LEU:H	1.95	0.63
1:A:290:GLN:O	6:A:601:HOH:O	2.15	0.62
1:C:326:VAL:HA	1:C:362:ASP:HB3	1.80	0.62
1:C:443:THR:O	2:D:82:ARG:NH1	2.32	0.62
2:D:120:LEU:HD11	2:D:178:TYR:OH	1.98	0.62
1:C:401:MET:HE1	5:D:601:B12:H262	1.81	0.62
1:A:396:LEU:HD12	2:B:77:ARG:HD2	1.81	0.62
2:B:114:TRP:O	2:B:118:GLN:HG2	2.00	0.62
2:D:122:GLU:HG3	2:D:201:PHE:HD1	1.62	0.62
2:D:159:PRO:HG2	2:D:219:ALA:HB2	1.81	0.62
5:B:601:B12:H531	5:B:601:B12:H552	1.80	0.61
1:C:44:ARG:O	1:C:48:LYS:HG2	2.01	0.61
2:D:114:TRP:O	2:D:118:GLN:HG2	2.01	0.60
2:D:111:PRO:HG2	2:D:114:TRP:HB2	1.84	0.60
5:B:601:B12:H601	5:B:601:B12:H261	1.83	0.60
3:C:501:5AD:O3'	5:D:601:B12:O28	2.17	0.60
2:B:229:ARG:HG2	2:B:229:ARG:O	2.02	0.59
2:D:126:GLU:OE1	2:D:142:ARG:NH1	2.36	0.59
5:D:601:B12:H531	5:D:601:B12:H552	1.84	0.59
2:B:211:ASP:HA	2:B:246:PRO:HB2	1.85	0.58
1:C:141:MET:HE1	1:C:354:LEU:HD13	1.85	0.58
1:C:252:GLU:HG2	1:C:256:LYS:HE3	1.85	0.58
1:A:160:ARG:HD3	1:A:392:MET:SD	2.43	0.58
2:D:148:VAL:HA	2:D:151:LEU:CD2	2.34	0.58
2:D:194:LEU:HD21	2:D:284:LEU:HD11	1.86	0.58
2:D:228:GLU:HA	5:D:601:B12:H1P2	1.86	0.58
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.39	0.57
2:D:178:TYR:OH	2:D:182:LEU:HD22	2.03	0.57
1:A:64:VAL:HG23	1:A:65:ILE:HG13	1.86	0.57
1:C:380:MET:SD	1:C:411:ASP:HB3	2.44	0.57
2:D:122:GLU:HG3	2:D:201:PHE:CD1	2.40	0.57
1:C:135:ILE:HG23	1:C:386:ALA:HB2	1.86	0.57
1:A:252:GLU:HG2	1:A:256:LYS:HE3	1.85	0.56
2:D:193:GLY:HA3	2:D:194:LEU:CB	2.34	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:ILE:HG21	2:B:133:TYR:HB2	1.88	0.56
2:D:141:ARG:HD3	2:D:208:LYS:HD2	1.88	0.56
1:A:110:ILE:HD13	1:A:141:MET:HG2	1.87	0.56
2:B:247:ARG:HA	2:B:247:ARG:NE	2.21	0.56
1:A:308:GLU:O	1:A:311:ASN:HB2	2.06	0.55
1:A:231:GLN:NE2	1:A:245:PHE:H	1.97	0.55
1:A:196:THR:HB	1:A:201:ASN:HD22	1.71	0.55
2:B:246:PRO:O	2:B:247:ARG:CZ	2.54	0.55
1:C:110:ILE:HD13	1:C:141:MET:HG2	1.88	0.55
1:C:367:ASN:ND2	2:D:230:PRO:O	2.39	0.55
1:A:185:VAL:HG21	1:A:409:PHE:HD1	1.72	0.55
2:D:272:ALA:O	2:D:276:ILE:HG13	2.06	0.55
1:A:124:ALA:HA	1:A:127:LYS:HD2	1.89	0.54
2:B:109:GLU:HB3	2:B:203:ARG:HH21	1.72	0.54
1:A:164:ASN:ND2	1:A:193:ASN:H	2.06	0.54
1:C:232:ILE:HG23	1:C:271:VAL:HG21	1.89	0.54
1:C:308:GLU:O	1:C:311:ASN:HB2	2.07	0.54
2:D:148:VAL:O	2:D:152:LYS:NZ	2.31	0.54
1:C:1:MET:HE3	1:C:3:LEU:HD21	1.90	0.54
2:D:152:LYS:HE3	2:D:216:ILE:HG23	1.89	0.54
1:A:201:ASN:CG	1:A:204:ARG:HH11	2.16	0.53
2:D:155:CYS:SG	2:D:198:THR:HB	2.48	0.53
1:A:21:LEU:O	1:A:127:LYS:NZ	2.29	0.53
2:D:228:GLU:OE1	2:D:239:SER:OG	2.22	0.53
1:C:246:GLN:NE2	5:D:601:B12:O39	2.41	0.53
1:C:122:VAL:HG13	1:C:354:LEU:HD23	1.89	0.53
2:D:181:ILE:HB	2:D:269:PRO:HB3	1.89	0.53
1:C:29:SER:H	1:C:340:GLN:HE22	1.57	0.53
1:C:160:ARG:HD3	1:C:392:MET:SD	2.48	0.53
1:C:380:MET:HG3	1:C:381:ILE:N	2.24	0.52
1:C:259:GLY:O	1:C:264:MET:HE1	2.10	0.52
1:A:332:PRO:HA	1:A:335:LEU:O	2.10	0.52
1:A:381:ILE:O	1:A:385:THR:HG23	2.10	0.52
2:D:247:ARG:HG2	2:D:250:THR:HB	1.92	0.52
1:C:244:ILE:HG21	1:C:268:ALA:HB1	1.92	0.52
1:A:443:THR:O	2:B:82:ARG:NH1	2.42	0.52
1:C:60:ARG:NH2	1:C:82:GLU:OE1	2.32	0.52
1:A:330:ILE:HG21	1:A:334:TYR:HE2	1.74	0.51
2:B:143:LEU:HD22	2:B:147:ALA:HB1	1.92	0.51
1:C:72:VAL:HG22	1:C:314:LEU:HD13	1.91	0.51
1:C:431:LEU:HD22	1:C:436:ILE:HG21	1.92	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:GLU:OE1	2:B:237:SER:OG	2.22	0.51
2:B:229:ARG:NH2	5:B:601:B12:H543	2.26	0.51
2:B:160:ASP:HB2	2:B:194:LEU:HD12	1.93	0.51
1:C:245:PHE:HA	1:C:285:TYR:O	2.10	0.51
2:B:211:ASP:HA	2:B:246:PRO:CB	2.40	0.51
1:C:15:LYS:HG2	1:C:16:ASP:CG	2.36	0.51
1:C:435:GLY:O	1:C:445:ARG:NH2	2.41	0.51
2:D:284:LEU:O	2:D:287:LYS:HD2	2.10	0.51
2:D:66:VAL:O	2:D:69:GLU:HG2	2.11	0.51
1:A:352:GLY:HA3	1:A:359:MET:HG2	1.93	0.51
2:D:71:ARG:NH2	6:D:702:HOH:O	2.26	0.50
3:A:501:5AD:O2'	5:B:601:B12:H371	2.11	0.50
1:A:55:THR:HA	1:A:92:SER:HA	1.93	0.50
1:A:93:ILE:HG22	1:A:128:ILE:HD11	1.92	0.50
1:A:196:THR:HG22	1:A:197:ASP:H	1.76	0.50
1:C:380:MET:HE1	1:C:411:ASP:CG	2.36	0.50
2:D:127:ILE:HG21	2:D:133:TYR:HB2	1.92	0.50
2:D:238:LEU:HB3	2:D:262:ILE:HB	1.93	0.49
2:B:122:GLU:HG3	2:B:201:PHE:CD2	2.44	0.49
1:C:161:LEU:O	1:C:163:PRO:HD3	2.13	0.49
1:C:383:LEU:HB3	1:C:388:CYS:HB2	1.93	0.49
1:A:394:MET:O	1:A:408:ALA:HA	2.12	0.49
2:B:270:VAL:HG13	2:B:271:GLU:HG3	1.94	0.49
1:C:326:VAL:HG21	3:C:501:5AD:C8	2.42	0.49
1:C:114:ARG:HA	1:C:117:LEU:HD12	1.95	0.49
1:C:167[A]:ARG:NE	2:D:266:GLY:O	2.45	0.49
2:B:141:ARG:NH2	6:B:703:HOH:O	2.35	0.49
1:C:83:THR:O	1:C:87:GLN:HG3	2.13	0.49
1:C:401:MET:HE1	5:D:601:B12:C26	2.43	0.49
1:C:15:LYS:N	1:C:19:GLU:OE1	2.26	0.48
1:A:365:TYR:CE1	1:A:405:GLN:HB2	2.47	0.48
1:A:377:GLU:HA	1:A:380:MET:SD	2.53	0.48
1:A:313:GLY:O	6:A:602:HOH:O	2.20	0.48
2:B:53:LYS:HA	2:B:94:ARG:CZ	2.44	0.48
1:C:410:HIS:HE1	2:D:81:GLY:O	1.96	0.48
1:A:45:VAL:HG11	2:D:97:ALA:HB2	1.94	0.48
2:D:215:GLU:OE2	2:D:247:ARG:HD3	2.12	0.48
1:C:60:ARG:NE	1:C:77:GLN:OE1	2.37	0.48
5:D:601:B12:C4	5:D:601:B12:H4B	2.43	0.48
1:A:166[B]:THR:HA	1:A:401:MET:HG2	1.96	0.48
1:C:261:GLU:N	1:C:264:MET:SD	2.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:330:ILE:HG12	5:D:601:B12:H491	1.96	0.47
2:D:247:ARG:HG3	2:D:249:ALA:H	1.78	0.47
1:A:161:LEU:HD11	1:A:177:ILE:HA	1.96	0.47
2:B:216:ILE:HG22	2:B:217:LEU:HD23	1.96	0.47
1:A:2:LYS:HE3	1:A:2:LYS:HB2	1.73	0.47
1:A:161:LEU:HB3	1:A:190:ILE:HG23	1.95	0.47
1:A:194:PRO:HG3	1:A:224:VAL:HG22	1.96	0.47
2:B:124[B]:ARG:HB3	2:B:203:ARG:HB3	1.97	0.47
1:C:50:VAL:O	1:C:54:MET:HG3	2.14	0.47
1:C:187:ASP:OD1	1:C:187:ASP:N	2.47	0.47
1:C:17:VAL:O	1:C:21:LEU:HG	2.15	0.47
2:D:165:ILE:O	2:D:201:PHE:HA	2.14	0.47
1:A:403:ASN:HB2	2:B:229:ARG:HG2	1.96	0.47
1:C:408:ALA:N	1:C:411:ASP:OD2	2.47	0.47
2:D:65:ASP:OD1	2:D:65:ASP:N	2.48	0.47
5:D:601:B12:H253	5:D:601:B12:H301	1.72	0.47
1:A:442:LEU:HB3	1:A:446:ALA:HB3	1.97	0.46
5:D:601:B12:H601	5:D:601:B12:H261	1.96	0.46
2:D:224:LEU:O	2:D:240:CYS:HA	2.15	0.46
2:D:160:ASP:HB2	2:D:194:LEU:HD23	1.97	0.46
1:A:272:GLY:HA2	1:A:276:ASN:OD1	2.16	0.46
1:C:141:MET:HE1	1:C:354:LEU:CD1	2.46	0.46
2:D:143:LEU:HB3	2:D:147:ALA:CB	2.45	0.46
2:D:191:GLN:HA	2:D:192:ALA:HA	1.56	0.46
2:D:244:TYR:OH	2:D:287:LYS:HG3	2.16	0.46
1:A:60:ARG:NE	1:A:77:GLN:HE22	1.97	0.46
2:B:124[B]:ARG:CB	2:B:203:ARG:HB3	2.46	0.46
1:C:187:ASP:HB3	1:C:427:PHE:CG	2.51	0.46
2:D:148:VAL:CA	2:D:151:LEU:HD23	2.42	0.46
1:A:233:GLU:O	1:A:237:ARG:HB2	2.16	0.46
2:B:109:GLU:HB3	2:B:203:ARG:NH2	2.31	0.46
1:C:202:LEU:HG	1:C:224:VAL:HG11	1.98	0.46
1:C:417:GLN:HE21	1:C:442:LEU:H	1.62	0.46
1:A:13:GLN:HG3	1:A:14:PHE:N	2.29	0.45
1:C:227:HIS:HE1	1:C:264:MET:CE	2.29	0.45
2:B:243:VAL:HG13	2:B:246:PRO:HG3	1.97	0.45
1:A:326:VAL:HA	1:A:362:ASP:HB3	1.97	0.45
2:B:109:GLU:HG2	2:B:130:LYS:NZ	2.30	0.45
2:D:111:PRO:O	2:D:115:VAL:HG13	2.17	0.45
2:D:177:ASN:O	2:D:181:ILE:HG22	2.16	0.45
1:A:166[B]:THR:HG23	2:B:266:GLY:HA2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:228:GLU:OE2	2:B:239:SER:HB3	2.17	0.45
1:C:51:LEU:HA	1:C:54:MET:HE2	1.98	0.45
1:C:109:ASP:HA	6:C:607:HOH:O	2.16	0.45
1:C:332:PRO:HD2	1:C:368:HIS:CD2	2.52	0.45
2:B:124[A]:ARG:HB3	2:B:203:ARG:HB3	1.98	0.45
1:A:282:ASN:ND2	1:A:319:ASP:OD2	2.50	0.45
1:C:29:SER:H	1:C:340:GLN:NE2	2.14	0.45
1:C:401:MET:C	1:C:401:MET:HE2	2.42	0.45
1:C:23:LYS:HB3	1:C:38:ALA:HB2	1.98	0.45
1:C:273:ALA:HA	4:C:504:GOL:H32	1.99	0.45
2:B:160:ASP:HA	2:B:220:LYS:HB2	1.98	0.45
5:B:601:B12:H4B	5:B:601:B12:C4	2.47	0.45
3:C:501:5AD:O2'	5:D:601:B12:H371	2.17	0.45
2:D:106:VAL:HG12	2:D:107:LEU:HG	1.99	0.45
2:B:142:ARG:HE	2:B:142:ARG:HB2	1.65	0.44
5:B:601:B12:H531	5:B:601:B12:C55	2.47	0.44
1:C:35:GLY:HA3	4:C:506:GOL:H12	1.98	0.44
2:D:237:SER:HA	2:D:263:HIS:CD2	2.52	0.44
1:A:355:SER:HA	4:A:502:GOL:H32	1.99	0.44
2:B:253:GLU:HG2	6:B:711:HOH:O	2.17	0.44
2:D:112:GLU:O	2:D:115:VAL:HG22	2.16	0.44
2:B:237:SER:OG	2:B:261:ASN:HA	2.17	0.44
1:C:352:GLY:HA3	1:C:359:MET:HG2	2.00	0.44
1:A:232:ILE:HD13	1:A:267:GLU:HG2	1.99	0.44
1:A:403:ASN:HB2	2:B:229:ARG:CG	2.47	0.44
2:B:124[A]:ARG:CB	2:B:203:ARG:HB3	2.47	0.44
2:D:211:ASP:HA	2:D:246:PRO:HB2	1.99	0.44
1:A:245:PHE:HA	1:A:285:TYR:O	2.17	0.43
1:A:282:ASN:HB3	1:A:321:PHE:HA	2.00	0.43
2:B:162:GLN:NE2	2:B:163:VAL:O	2.51	0.43
2:D:127:ILE:CD1	2:D:139:MET:HB2	2.47	0.43
2:D:165:ILE:HD12	2:D:178:TYR:HE1	1.83	0.43
2:D:185:LEU:O	2:D:189:LEU:HD12	2.18	0.43
1:A:21:LEU:HD22	1:A:127:LYS:HE3	2.01	0.43
1:A:166[A]:THR:HA	1:A:401:MET:HG2	2.00	0.43
1:A:201:ASN:OD1	1:A:204:ARG:NE	2.49	0.43
1:C:425:PRO:O	1:C:429:ARG:HG3	2.19	0.43
1:C:64:VAL:HB	1:C:302:ALA:HB2	2.00	0.43
2:B:177:ASN:O	2:B:181:ILE:HG22	2.19	0.43
2:D:106:VAL:HG22	2:D:230:PRO:HG2	2.01	0.43
2:D:127:ILE:HD11	2:D:139:MET:HB2	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:LEU:HD12	2:B:77:ARG:CD	2.48	0.43
2:B:110:VAL:HG21	2:B:201:PHE:CZ	2.54	0.43
1:C:324:ASN:HB3	1:C:390:TYR:CZ	2.54	0.42
1:C:332:PRO:HG3	1:C:368:HIS:O	2.19	0.42
2:D:110:VAL:HB	2:D:171:THR:HG23	2.00	0.42
5:B:601:B12:H261	5:B:601:B12:H91	1.57	0.42
1:C:22:ALA:HB1	1:C:36:VAL:HB	2.00	0.42
1:C:380:MET:HE1	1:C:411:ASP:HB3	2.01	0.42
1:A:196:THR:CB	1:A:201:ASN:HD22	2.32	0.42
1:C:123:ALA:HA	1:C:351:MET:SD	2.59	0.42
1:C:380:MET:HE2	1:C:407:THR:HG22	2.01	0.42
2:D:241:TYR:OH	6:D:701:HOH:O	2.20	0.42
1:A:141:MET:HE1	1:A:354:LEU:HB2	2.02	0.42
2:D:141:ARG:HG2	2:D:208:LYS:HB2	2.02	0.42
1:A:434:MET:HE2	1:A:452:PHE:CE1	2.54	0.42
2:B:181:ILE:HG13	2:B:273:ALA:HB2	2.02	0.42
2:B:279:LEU:HD12	2:B:293:MET:HE1	2.02	0.42
1:C:227:HIS:HE1	1:C:264:MET:HE1	1.85	0.42
1:C:261:GLU:HB3	6:C:780:HOH:O	2.19	0.42
1:C:349:HIS:NE2	1:C:388:CYS:HA	2.35	0.42
2:D:182:LEU:HD12	2:D:185:LEU:HD23	2.02	0.42
1:A:122:VAL:HG13	1:A:354:LEU:HD23	2.01	0.42
1:A:329:PHE:CZ	3:A:501:5AD:H5'2	2.55	0.42
1:A:161:LEU:O	1:A:163:PRO:HD3	2.20	0.42
1:A:168:ASP:CG	1:A:195:VAL:HG12	2.45	0.42
1:C:353:LYS:HA	1:C:353:LYS:HD3	1.66	0.42
1:A:326:VAL:HG21	3:A:501:5AD:C8	2.50	0.41
1:C:146:LYS:HD3	1:C:150:THR:OG1	2.20	0.41
1:C:380:MET:HG3	1:C:381:ILE:HG13	2.02	0.41
1:C:450:SER:HB2	2:D:63:ARG:HB2	2.00	0.41
2:D:161:VAL:HG21	2:D:189:LEU:HD22	2.01	0.41
1:A:339:ARG:HH12	1:C:370:ASP:CG	2.28	0.41
1:A:390:TYR:CE2	1:A:392:MET:HE1	2.56	0.41
2:B:109:GLU:HG2	2:B:130:LYS:HZ3	1.85	0.41
2:B:214:GLY:HA3	2:B:246:PRO:HG2	2.02	0.41
1:C:252:GLU:O	1:C:256:LYS:HG3	2.19	0.41
1:C:15:LYS:HE3	6:C:764:HOH:O	2.20	0.41
2:D:84:GLY:HA3	2:D:85:PRO:HD3	1.93	0.41
2:D:126:GLU:HB2	2:D:139:MET:HB3	2.02	0.41
1:A:402:LEU:O	2:B:229:ARG:HD3	2.20	0.41
2:D:71:ARG:HD2	2:D:78:VAL:HG23	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:180:GLU:HB2	6:D:714:HOH:O	2.20	0.41
2:B:152:LYS:HB2	2:B:152:LYS:HE3	1.86	0.41
2:D:178:TYR:CZ	2:D:182:LEU:HD22	2.56	0.41
2:B:162:GLN:HG2	2:B:217:LEU:HD12	2.03	0.41
1:C:27:LEU:HD12	1:C:28:ARG:N	2.36	0.41
1:C:48:LYS:HG2	1:C:48:LYS:H	1.69	0.41
2:B:160:ASP:CB	2:B:194:LEU:HD12	2.51	0.41
1:C:97:ARG:HH11	1:C:97:ARG:HG2	1.86	0.41
1:C:285:TYR:CD1	1:C:322:ILE:HG13	2.56	0.41
1:C:294:LEU:HD23	1:C:334:TYR:HE1	1.86	0.41
2:D:68:THR:O	2:D:72[B]:ARG:HG2	2.21	0.41
2:D:116:LYS:HA	2:D:116:LYS:HD3	1.88	0.41
1:A:372:ASP:HB2	6:B:748:HOH:O	2.21	0.41
2:B:182:LEU:HB3	2:B:183:PRO:HD3	2.03	0.41
1:C:269:ARG:HG2	1:C:284:LEU:HD11	2.03	0.41
2:D:271:GLU:O	2:D:275:VAL:HG23	2.21	0.41
1:A:242:GLY:O	1:A:276:ASN:ND2	2.40	0.40
1:A:390:TYR:HE2	1:A:392:MET:HE1	1.86	0.40
1:A:1:MET:HE3	1:A:1:MET:HB2	1.90	0.40
2:D:178:TYR:O	2:D:180:GLU:N	2.55	0.40
1:A:22:ALA:HB1	1:A:36:VAL:HB	2.03	0.40
2:D:61:PRO:HB3	2:D:67:LEU:HD11	2.04	0.40
2:D:141:ARG:CD	2:D:208:LYS:HD2	2.49	0.40
1:C:332:PRO:HA	1:C:335:LEU:O	2.21	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:115:LYS:NZ	1:C:278:ILE:O[3_655]	2.14	0.06
4:A:504:GOL:O1	6:C:777:HOH:O[3_655]	2.14	0.06

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	456/453 (101%)	436 (96%)	19 (4%)	1 (0%)	43	37
1	C	454/453 (100%)	426 (94%)	27 (6%)	1 (0%)	43	37
2	B	251/295 (85%)	239 (95%)	11 (4%)	1 (0%)	30	22
2	D	251/295 (85%)	235 (94%)	10 (4%)	6 (2%)	4	1
All	All	1412/1496 (94%)	1336 (95%)	67 (5%)	9 (1%)	21	13

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	125	SER
2	D	194	LEU
2	D	179	GLU
2	D	195	LYS
1	A	163	PRO
2	D	178	TYR
1	C	163	PRO
2	D	147	ALA
2	D	156	VAL

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	375/370 (101%)	373 (100%)	2 (0%)	81	85
1	C	373/370 (101%)	369 (99%)	4 (1%)	65	68
2	B	207/240 (86%)	206 (100%)	1 (0%)	81	85
2	D	207/240 (86%)	203 (98%)	4 (2%)	50	50
All	All	1162/1220 (95%)	1151 (99%)	11 (1%)	70	75

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	326	VAL
1	A	404	TYR
2	B	171	THR
1	C	230	THR
1	C	326	VAL
1	C	401	MET
1	C	404	TYR
2	D	155	CYS
2	D	229	ARG
2	D	264[A]	GLN
2	D	264[B]	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	87	GLN
1	A	162	GLN
1	A	164	ASN
1	A	231	GLN
1	A	367	ASN
1	A	405	GLN
1	A	439	ASN
2	B	62	HIS
2	B	154	GLN
2	B	162	GLN
1	C	201	ASN
1	C	227	HIS
1	C	340	GLN
1	C	403	ASN
1	C	410	HIS
1	C	417	GLN
2	D	154	GLN
2	D	162	GLN
2	D	292	ASN

5.3.3 RNA ⓘ

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](#)

15 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	$\# Z > 2$
4	GOL	C	503	-	5,5,5	0.36	0	5,5,5	0.44	0
4	GOL	A	502	-	5,5,5	0.40	0	5,5,5	0.34	0
4	GOL	C	502	-	5,5,5	0.38	0	5,5,5	0.36	0
4	GOL	C	505	-	5,5,5	0.39	0	5,5,5	0.32	0
4	GOL	A	506	-	5,5,5	0.37	0	5,5,5	0.36	0
3	5AD	A	501	-	20,20,20	1.56	5 (25%)	28,30,30	2.25	10 (35%)
4	GOL	C	506	-	5,5,5	0.39	0	5,5,5	0.47	0
5	B12	D	601	-	94,101,101	2.27	16 (17%)	149,166,166	1.51	23 (15%)
4	GOL	A	504	-	5,5,5	0.40	0	5,5,5	0.34	0
4	GOL	A	507	-	5,5,5	0.37	0	5,5,5	0.47	0
4	GOL	C	504	-	5,5,5	0.38	0	5,5,5	0.33	0
5	B12	B	601	-	94,101,101	2.23	14 (14%)	149,166,166	1.57	25 (16%)
4	GOL	A	503	-	5,5,5	0.45	0	5,5,5	0.18	0
3	5AD	C	501	-	20,20,20	1.59	4 (20%)	28,30,30	2.40	11 (39%)
4	GOL	A	505	-	5,5,5	0.43	0	5,5,5	0.34	0

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
4	GOL	C	503	-	-	2/4/4/4	-
4	GOL	A	502	-	-	0/4/4/4	-
4	GOL	C	502	-	-	2/4/4/4	-
4	GOL	C	505	-	-	2/4/4/4	-
4	GOL	A	506	-	-	0/4/4/4	-
3	5AD	A	501	-	-	0/4/20/20	0/3/3/3
4	GOL	C	506	-	-	0/4/4/4	-
5	B12	D	601	-	-	15/56/223/223	0/3/11/11
4	GOL	A	504	-	-	2/4/4/4	-
4	GOL	A	507	-	-	0/4/4/4	-
4	GOL	C	504	-	-	4/4/4/4	-
5	B12	B	601	-	-	16/56/223/223	0/3/11/11
4	GOL	A	503	-	-	2/4/4/4	-
3	5AD	C	501	-	-	0/4/20/20	0/3/3/3
4	GOL	A	505	-	-	2/4/4/4	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	B12	C19-N24	-17.11	1.27	1.49
5	B	601	B12	C19-N24	-16.81	1.27	1.49
5	D	601	B12	C8B-C9B	5.38	1.49	1.40
5	D	601	B12	C14-N23	-5.28	1.28	1.35
5	B	601	B12	C14-N23	-5.22	1.28	1.35
5	B	601	B12	C8B-C9B	5.20	1.48	1.40
3	C	501	5AD	C5-C4	4.73	1.47	1.39
3	A	501	5AD	C5-C4	4.53	1.47	1.39
5	B	601	B12	C11-N23	3.88	1.44	1.36
5	D	601	B12	C11-N23	3.85	1.44	1.36
5	D	601	B12	C16-C15	-3.79	1.33	1.44
5	B	601	B12	C16-C15	-3.70	1.34	1.44
5	D	601	B12	C6B-C5B	3.49	1.49	1.40
5	B	601	B12	C6B-C5B	3.35	1.49	1.40
5	D	601	B12	C9B-N3B	-3.26	1.33	1.39
5	B	601	B12	C9B-N3B	-3.16	1.33	1.39
3	A	501	5AD	C5-C6	2.75	1.48	1.41
3	C	501	5AD	C5-C6	2.68	1.48	1.41
5	D	601	B12	C8B-N1B	-2.66	1.34	1.39
5	B	601	B12	C14-C15	2.66	1.49	1.38
5	D	601	B12	C14-C15	2.65	1.49	1.38
3	C	501	5AD	C8-N7	2.47	1.36	1.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	601	B12	C8B-N1B	-2.44	1.34	1.39
3	A	501	5AD	C8-N7	2.41	1.36	1.31
5	B	601	B12	C10-C9	2.31	1.45	1.39
5	D	601	B12	C12-C11	-2.31	1.48	1.52
5	B	601	B12	C1-C19	-2.26	1.50	1.55
5	D	601	B12	C1-C19	-2.18	1.50	1.55
5	B	601	B12	CO-N22	-2.18	1.86	1.96
5	D	601	B12	C1-C2	-2.17	1.53	1.58
3	A	501	5AD	C4-N9	-2.15	1.33	1.37
3	C	501	5AD	C5-N7	-2.14	1.35	1.39
5	D	601	B12	C10-C9	2.14	1.45	1.39
3	A	501	5AD	C5-N7	-2.14	1.35	1.39
5	D	601	B12	CO-N22	-2.11	1.86	1.96
5	B	601	B12	C10-C11	-2.09	1.31	1.37
5	D	601	B12	C2B-N3B	2.09	1.35	1.31
5	D	601	B12	C10-C11	-2.08	1.31	1.37
5	B	601	B12	C1-C2	-2.07	1.54	1.58

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	501	5AD	C5-C4-N3	-5.90	118.60	126.72
5	D	601	B12	C9B-C8B-N1B	5.66	107.81	105.30
5	B	601	B12	C8B-C9B-N3B	-5.63	103.91	110.00
5	B	601	B12	C18-C19-N24	5.54	110.66	102.33
3	A	501	5AD	C5-C4-N3	-5.48	119.17	126.72
5	D	601	B12	C8B-C9B-N3B	-5.36	104.20	110.00
5	B	601	B12	C9B-C8B-N1B	5.33	107.67	105.30
5	D	601	B12	C18-C19-N24	5.30	110.30	102.33
5	B	601	B12	C9B-N3B-C2B	4.84	110.33	104.40
5	B	601	B12	C20-C1-C19	-4.83	104.70	109.35
3	C	501	5AD	N3-C4-N9	4.60	134.99	127.17
5	D	601	B12	C9B-N3B-C2B	4.58	110.02	104.40
3	A	501	5AD	N3-C4-N9	4.32	134.51	127.17
5	D	601	B12	C20-C1-C19	-3.99	105.51	109.35
3	C	501	5AD	C5'-C4'-C3'	-3.97	111.53	115.70
3	C	501	5AD	C2-N3-C4	3.78	121.06	111.83
5	B	601	B12	C54-C17-C18	-3.68	107.70	112.99
3	A	501	5AD	C2-N3-C4	3.66	120.78	111.83
3	A	501	5AD	C4-C5-N7	-3.65	106.41	110.58
5	B	601	B12	C13-C14-N23	3.54	113.89	109.09
3	C	501	5AD	C4-C5-N7	-3.52	106.56	110.58

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	601	B12	C9-C10-C11	-3.36	121.17	125.97
3	A	501	5AD	N3-C2-N1	-3.31	123.58	128.58
5	D	601	B12	C9-C10-C11	-3.23	121.35	125.97
5	B	601	B12	C30-C3-C2	-3.22	111.90	119.00
3	A	501	5AD	C4-N9-C8	3.21	109.11	105.74
3	C	501	5AD	N3-C2-N1	-3.20	123.73	128.58
5	D	601	B12	C2P-C1P-N59	-3.19	108.24	112.92
5	D	601	B12	C13-C14-N23	3.15	113.36	109.09
5	B	601	B12	C4B-C9B-N3B	3.13	135.78	130.51
5	B	601	B12	C19-N24-C16	3.11	110.69	107.29
5	D	601	B12	C4B-C9B-N3B	3.06	135.67	130.51
5	B	601	B12	C17-C16-C15	3.00	131.00	126.26
5	B	601	B12	C20-C1-N21	2.97	115.17	110.26
5	D	601	B12	C8-C9-N22	2.86	116.41	110.77
5	B	601	B12	C17-C16-N24	-2.84	106.83	111.17
5	D	601	B12	C1-C19-N24	2.84	109.41	106.25
5	D	601	B12	C19-N24-C16	2.75	110.29	107.29
3	C	501	5AD	C3'-C2'-C1'	2.70	106.57	101.46
5	B	601	B12	C7-C8-C9	2.69	104.30	100.89
3	A	501	5AD	C5-N7-C8	2.67	107.65	103.45
5	D	601	B12	C8-C9-C10	-2.66	117.67	123.33
5	B	601	B12	C8-C9-C10	-2.65	117.68	123.33
3	C	501	5AD	C4-N9-C8	2.65	108.52	105.74
5	B	601	B12	C13-C14-C15	-2.64	120.31	124.32
5	B	601	B12	C1-C19-N24	2.64	109.18	106.25
5	B	601	B12	C8-C9-N22	2.63	115.97	110.77
5	B	601	B12	C53-C15-C16	2.63	124.82	120.36
5	D	601	B12	C7-C8-C9	2.61	104.20	100.89
5	D	601	B12	C20-C1-N21	2.60	114.56	110.26
5	D	601	B12	C13-C14-C15	-2.60	120.36	124.32
3	C	501	5AD	C2'-C1'-N9	-2.58	106.89	113.30
5	D	601	B12	C17-C16-C15	2.57	130.32	126.26
5	D	601	B12	C30-C3-C2	-2.56	113.34	119.00
5	D	601	B12	C48-C13-C14	2.56	114.87	108.51
3	A	501	5AD	C3'-C2'-C1'	2.52	106.23	101.46
5	B	601	B12	O3-C2P-C1P	2.45	111.79	106.94
3	C	501	5AD	C5-N7-C8	2.44	107.28	103.45
3	A	501	5AD	N9-C8-N7	-2.42	110.50	113.94
5	D	601	B12	C3R-C2R-C1R	2.41	105.19	99.89
3	A	501	5AD	C6-C5-N7	2.40	136.71	132.09
5	D	601	B12	N1B-C2B-N3B	-2.39	110.54	113.94
5	B	601	B12	N1B-C2B-N3B	-2.32	110.65	113.94

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	601	B12	C54-C17-C18	-2.28	109.71	112.99
3	C	501	5AD	C6-C5-N7	2.19	136.31	132.09
5	B	601	B12	C26-C2-C3	2.18	111.23	107.42
5	B	601	B12	C3R-C2R-C1R	2.13	104.57	99.89
5	D	601	B12	C53-C15-C16	2.05	123.84	120.36
5	B	601	B12	C7B-C8B-C9B	-2.01	120.07	122.47

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	GOL	O1-C1-C2-C3
4	C	503	GOL	C1-C2-C3-O3
4	C	504	GOL	C1-C2-C3-O3
4	C	504	GOL	O2-C2-C3-O3
4	C	505	GOL	C1-C2-C3-O3
4	C	505	GOL	O2-C2-C3-O3
5	B	601	B12	C1-C2-C26-C27
5	B	601	B12	C25-C2-C26-C27
5	B	601	B12	C3-C2-C26-C27
5	B	601	B12	C38-C37-C7-C36
5	B	601	B12	C2P-O3-P-O5
5	B	601	B12	C2R-C1R-N1B-C8B
5	B	601	B12	O6R-C1R-N1B-C8B
5	D	601	B12	C1-C2-C26-C27
5	D	601	B12	C25-C2-C26-C27
5	D	601	B12	C3-C2-C26-C27
5	D	601	B12	C2P-O3-P-O5
5	D	601	B12	C13-C48-C49-C50
4	A	505	GOL	O2-C2-C3-O3
5	B	601	B12	C42-C41-C8-C9
5	D	601	B12	C42-C41-C8-C9
5	B	601	B12	C13-C48-C49-C50
5	B	601	B12	C2-C3-C30-C31
4	A	504	GOL	C1-C2-C3-O3
4	A	505	GOL	C1-C2-C3-O3
4	C	502	GOL	O1-C1-C2-C3
4	C	504	GOL	O1-C1-C2-C3
5	D	601	B12	O6R-C1R-N1B-C8B
5	B	601	B12	C38-C37-C7-C8
4	A	503	GOL	O1-C1-C2-O2
4	C	503	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	601	B12	C4-C3-C30-C31
4	C	502	GOL	O1-C1-C2-O2
4	C	504	GOL	O1-C1-C2-O2
5	D	601	B12	C2R-C1R-N1B-C8B
5	D	601	B12	C2-C3-C30-C31
5	D	601	B12	C4-C3-C30-C31
5	D	601	B12	C38-C37-C7-C36
5	D	601	B12	C18-C60-C61-O63
5	B	601	B12	C38-C37-C7-C6
5	B	601	B12	C2P-O3-P-O4
5	B	601	B12	C3R-O2-P-O4
5	B	601	B12	C3R-O2-P-O5
5	D	601	B12	C2P-O3-P-O4
5	D	601	B12	C3R-O2-P-O4
5	D	601	B12	C3R-O2-P-O5
4	A	504	GOL	O1-C1-C2-O2

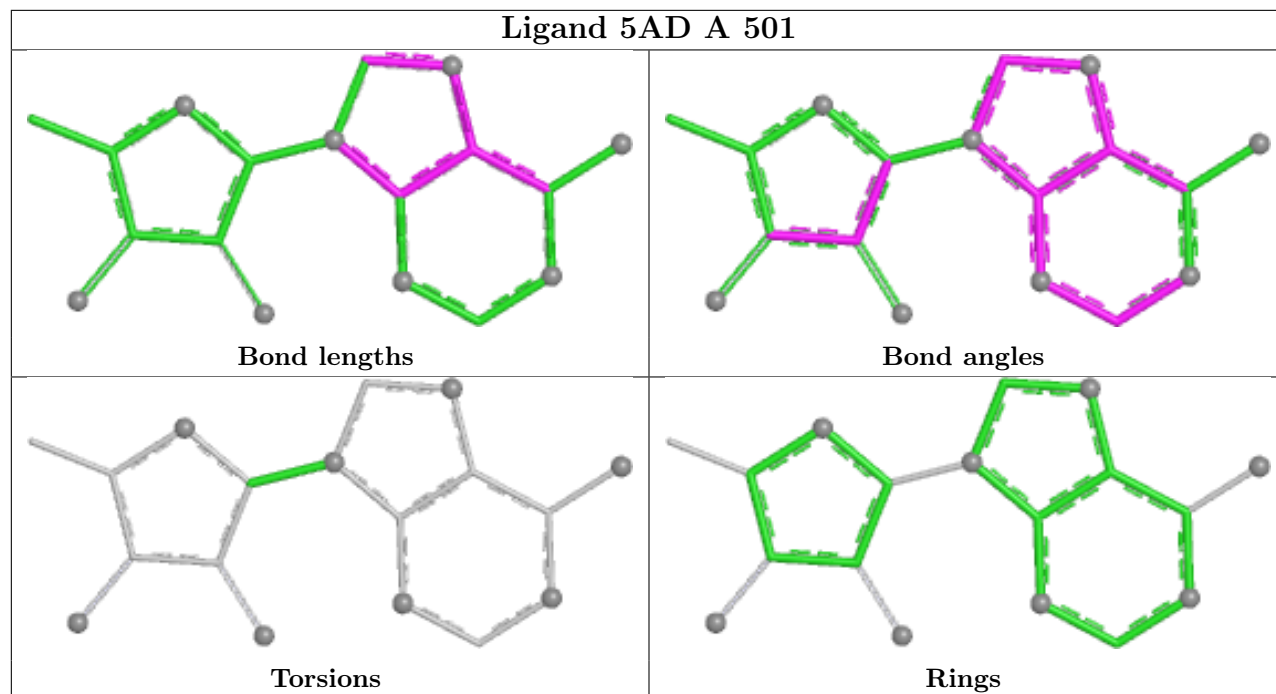
There are no ring outliers.

9 monomers are involved in 28 short contacts:

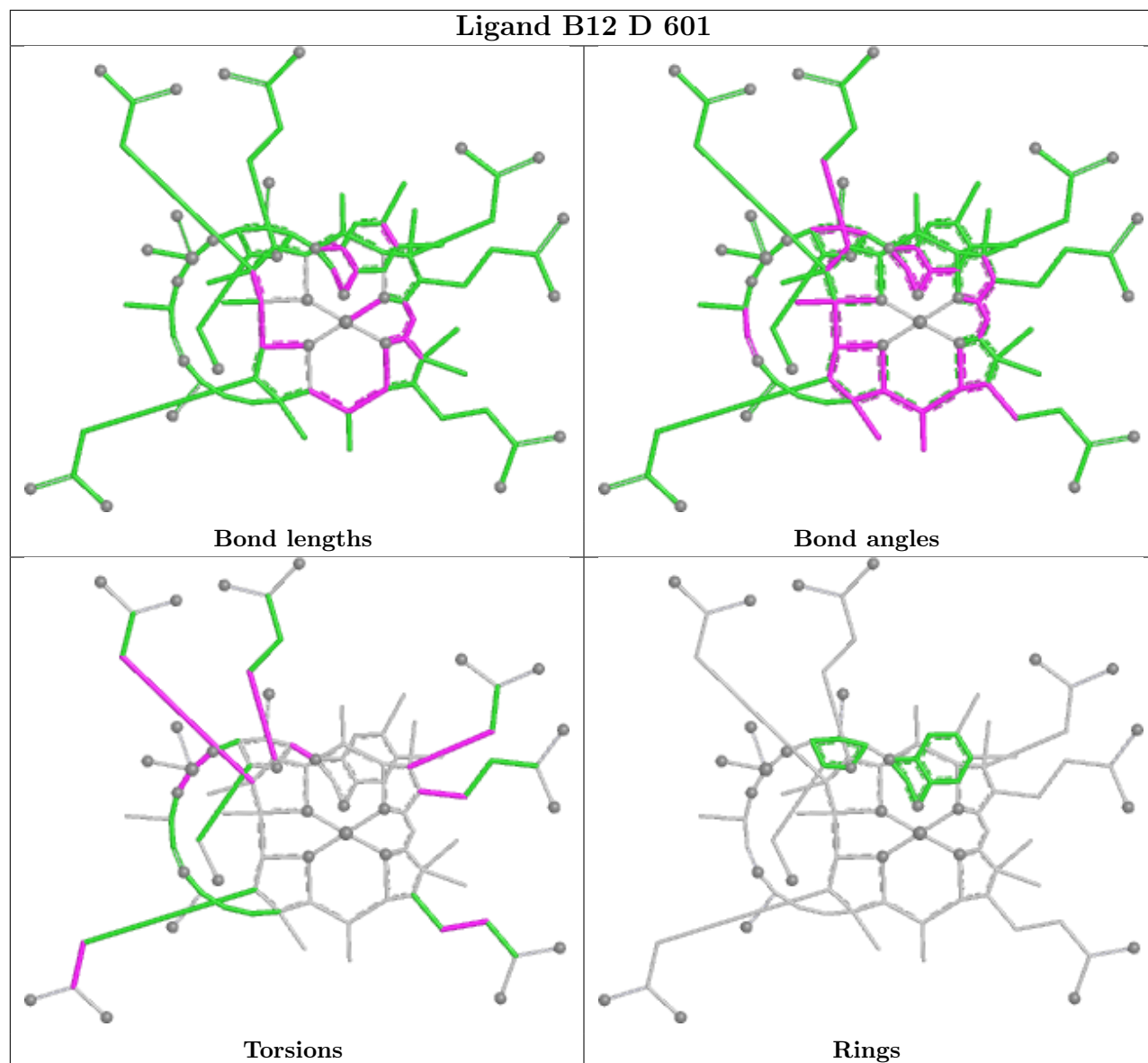
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	502	GOL	1	0
4	C	505	GOL	1	0
3	A	501	5AD	3	0
4	C	506	GOL	1	0
5	D	601	B12	11	0
4	A	504	GOL	0	1
4	C	504	GOL	2	0
5	B	601	B12	7	0
3	C	501	5AD	4	0

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

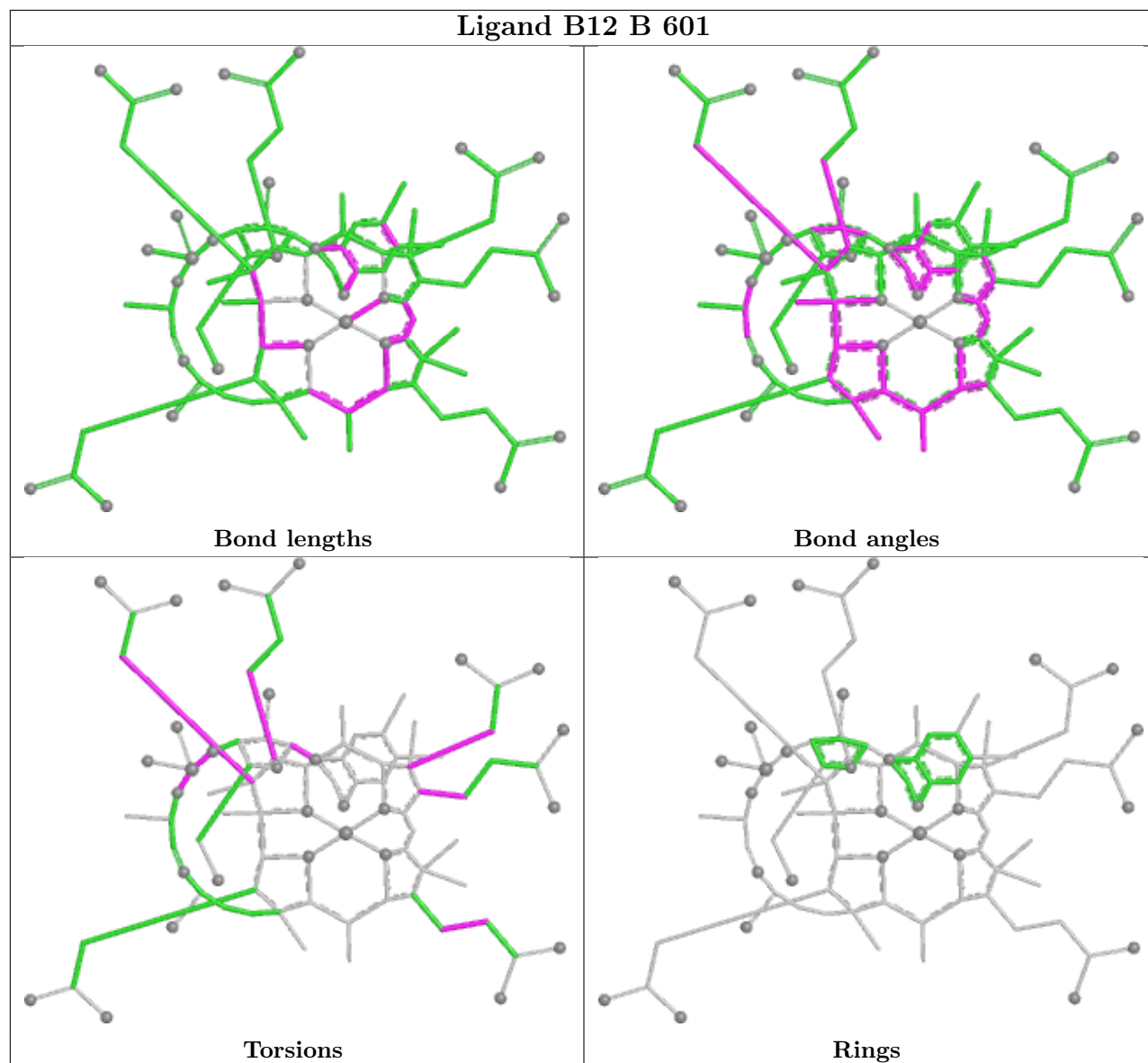
equivalents in the CSD to analyse the geometry.

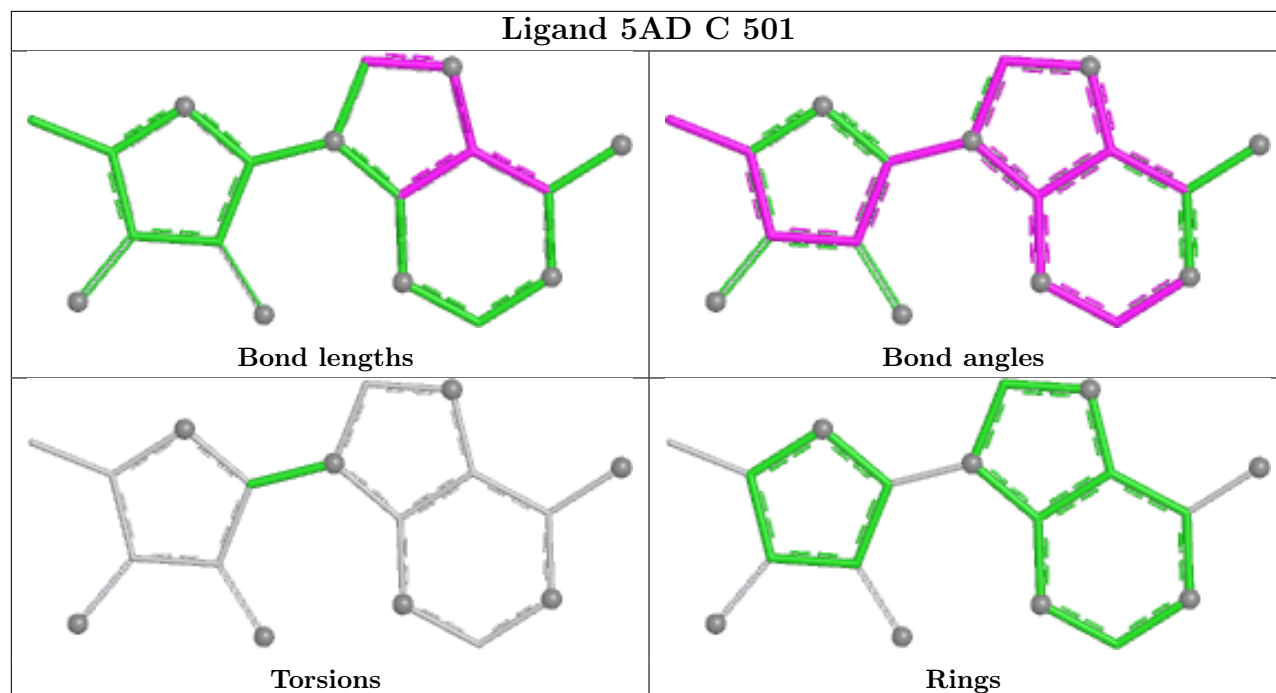


Ligand B12 D 601



Ligand B12 B 601





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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	453/453 (100%)	-1.29	0 100 100	10, 21, 31, 47	5 (1%)
1	C	453/453 (100%)	-1.27	0 100 100	10, 21, 33, 51	3 (0%)
2	B	252/295 (85%)	-0.75	0 100 100	15, 36, 50, 60	1 (0%)
2	D	251/295 (85%)	-0.86	0 100 100	13, 35, 53, 70	2 (0%)
All	All	1409/1496 (94%)	-1.11	0 100 100	10, 25, 47, 70	11 (0%)

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
4	GOL	A	507	6/6	0.98	0.06	28,36,38,39	0
4	GOL	C	502	6/6	0.98	0.05	16,20,28,40	0
4	GOL	C	504	6/6	0.98	0.04	13,16,19,24	0
4	GOL	A	503	6/6	0.99	0.04	19,23,26,32	0

Continued on next page...

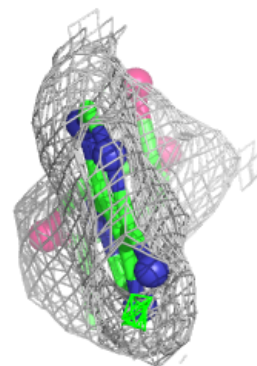
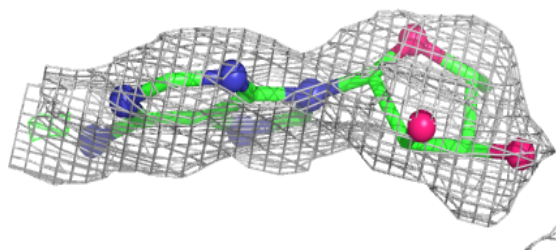
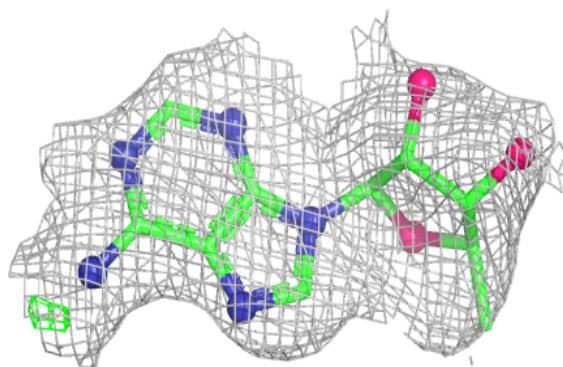
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	GOL	A	504	6/6	0.99	0.07	25,29,31,32	0
4	GOL	A	505	6/6	0.99	0.05	18,21,23,24	0
4	GOL	A	506	6/6	0.99	0.05	35,38,42,45	0
3	5AD	A	501	18/18	0.99	0.06	27,40,48,49	0
3	5AD	C	501	18/18	0.99	0.04	31,34,40,42	0
4	GOL	C	503	6/6	0.99	0.05	25,28,29,30	0
4	GOL	A	502	6/6	0.99	0.04	18,21,24,29	0
4	GOL	C	505	6/6	0.99	0.06	20,23,30,31	0
4	GOL	C	506	6/6	0.99	0.06	35,41,43,43	0
5	B12	B	601	91/91	0.99	0.04	17,23,33,39	0
5	B12	D	601	91/91	0.99	0.04	17,25,34,40	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.

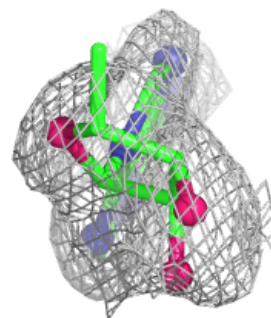
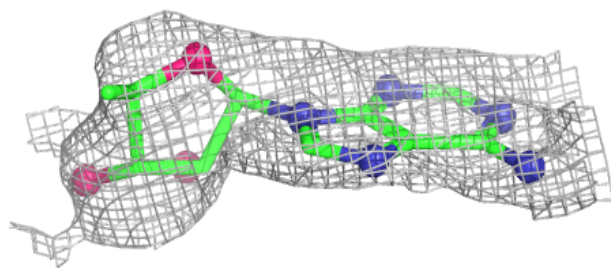
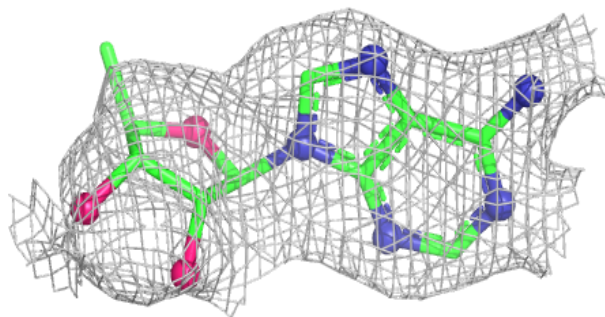
Electron density around 5AD A 501:

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



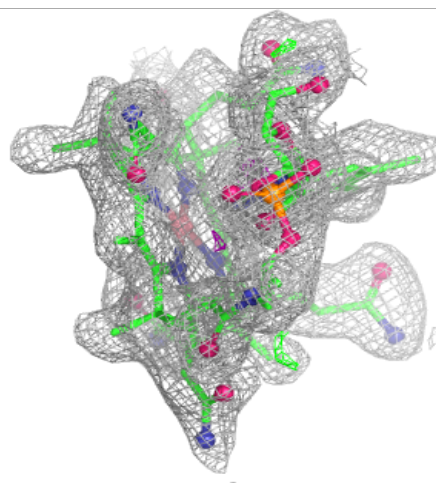
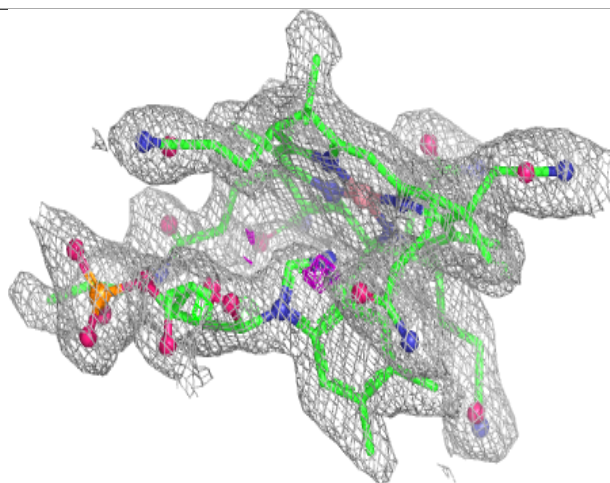
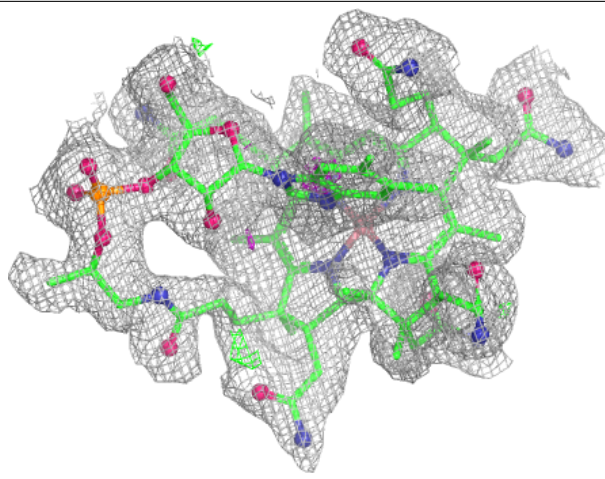
Electron density around 5AD C 501:

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



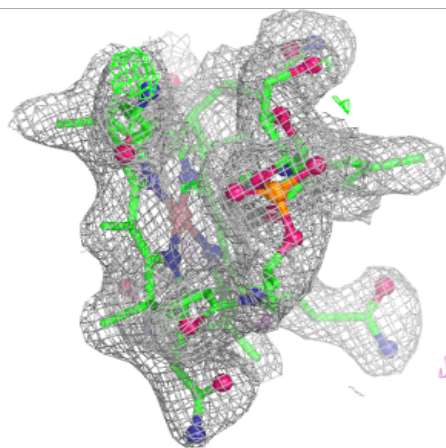
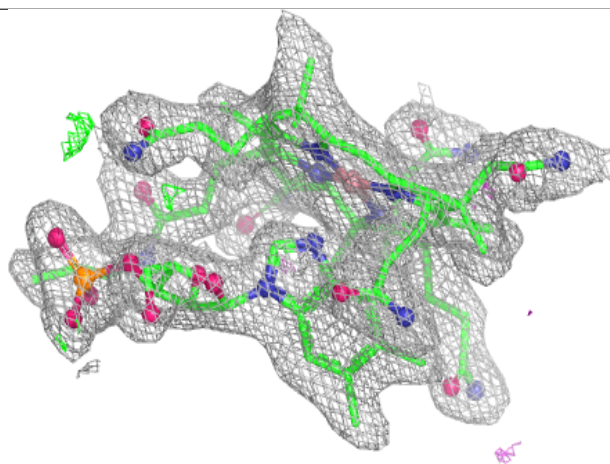
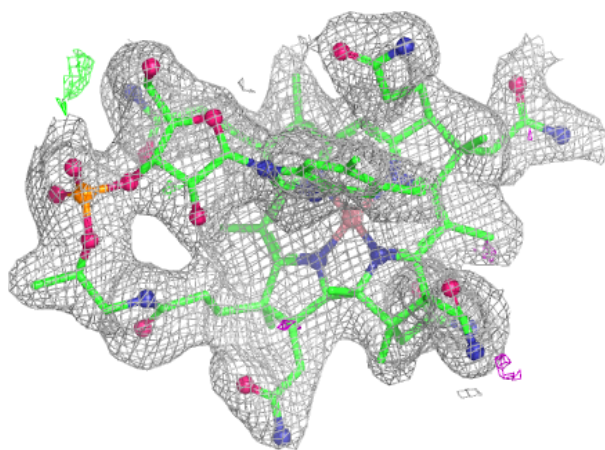
Electron density around B12 B 601:

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



Electron density around B12 D 601:

$2mF_o-DF_c$ (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.