Full wwPDB X-ray Structure Validation Report (i)

Aug 4, 2026 – 07:34 PM EDT

PDB ID	:	3ABR / pdb_00003abr
Title	:	Crystal structure of ethanolamine ammonia-lyase from Escherichia coli complexed with CN-Cbl (substrate-free form)
Authors	:	Shibata, N.
Deposited on	:	2009-12-21
Resolution	:	2.10 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 (i) 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 (i)) were used in the production of this report:

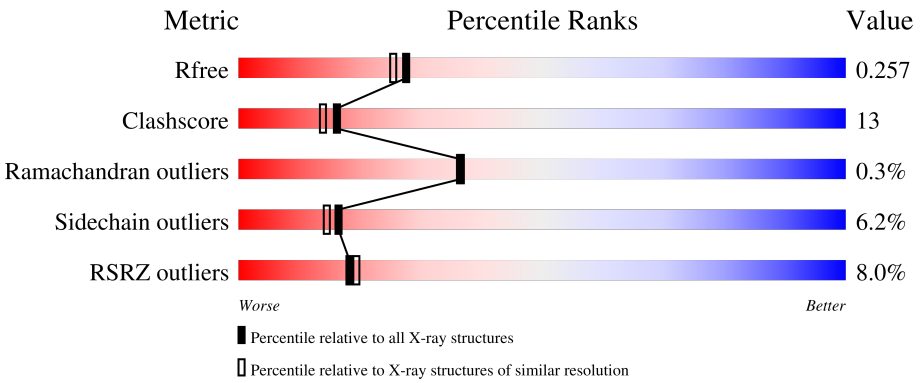
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	453	85% 13% •
1	C	453	85% 13% •
2	B	306	10% 57% 23% • 18%
2	D	306	26% 51% 25% 5% • 18%

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
5	B12	B	601	-	-	X	-
5	B12	D	601	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 11985 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
			Total	C	N	O	S			
1	A	453	3464	2170	593	679	22	0	0	0
1	C	453	3464	2170	593	679	22	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	252	1916	1197	347	362	10	0	0	0
2	D	252	1916	1197	347	362	10	0	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	expression tag	UNP P19636
B	-9	ASP	-	expression tag	UNP P19636
B	-8	GLN	-	expression tag	UNP P19636
B	-7	SER	-	expression tag	UNP P19636
B	-6	SER	-	expression tag	UNP P19636
B	-5	HIS	-	expression tag	UNP P19636
B	-4	HIS	-	expression tag	UNP P19636
B	-3	HIS	-	expression tag	UNP P19636
B	-2	HIS	-	expression tag	UNP P19636
B	-1	HIS	-	expression tag	UNP P19636
B	0	HIS	-	expression tag	UNP P19636
D	-10	MET	-	expression tag	UNP P19636
D	-9	ASP	-	expression tag	UNP P19636
D	-8	GLN	-	expression tag	UNP P19636
D	-7	SER	-	expression tag	UNP P19636
D	-6	SER	-	expression tag	UNP P19636

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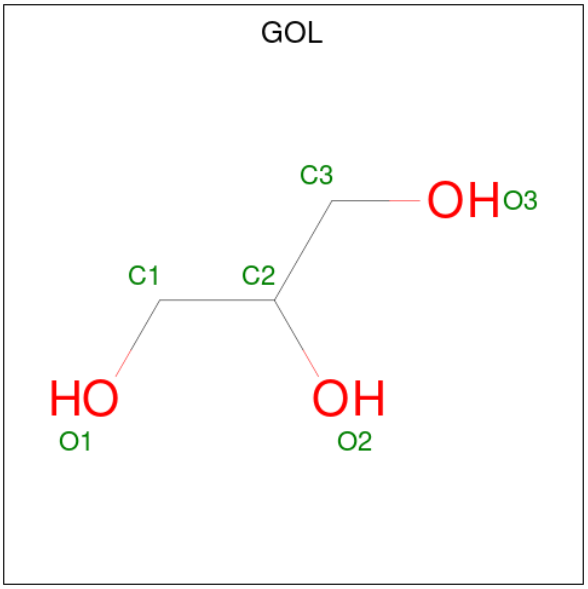
Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	HIS	-	expression tag	UNP P19636
D	-4	HIS	-	expression tag	UNP P19636
D	-3	HIS	-	expression tag	UNP P19636
D	-2	HIS	-	expression tag	UNP P19636
D	-1	HIS	-	expression tag	UNP P19636
D	0	HIS	-	expression tag	UNP P19636

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).

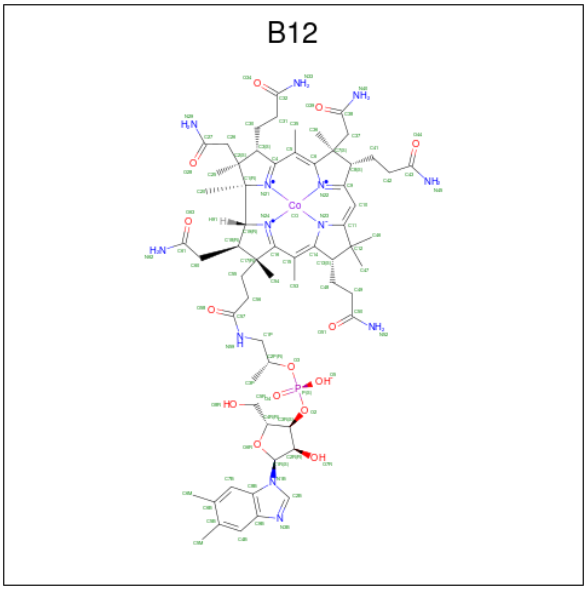


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O			
3	A	1	6	3	3		0	0
			Total	C	O			
3	A	1	6	3	3		0	0
			Total	C	O			
3	A	1	6	3	3		0	0
			Total	C	O			
3	C	1	6	3	3		0	0
			Total	C	O			
3	C	1	6	3	3		0	0
			Total	C	O			
3	C	1	6	3	3		0	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Na		
4	A	3	3	3	0	0
4	B	1	1	1	0	0
4	C	1	1	1	0	0
4	D	2	2	2	0	0

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



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	421	421	421	0	0
6	B	129	129	129	0	0
6	C	349	349	349	0	0
6	D	101	101	101	0	0

3 Residue-property plots (i)

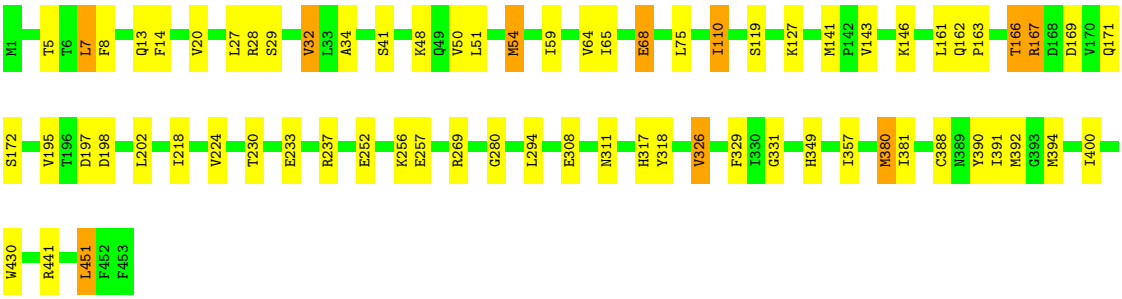
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

Chain A:

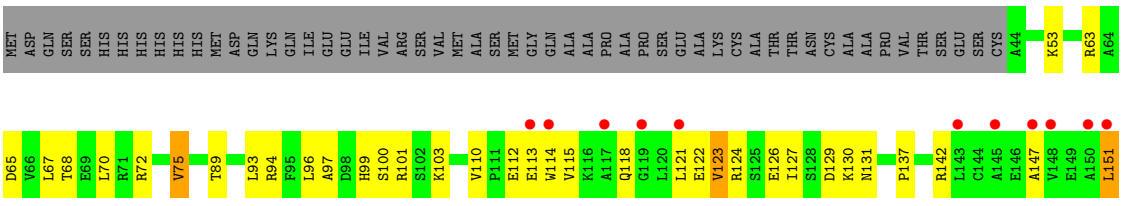
• Molecule 1: Ethanolamine ammonia-lyase heavy chain

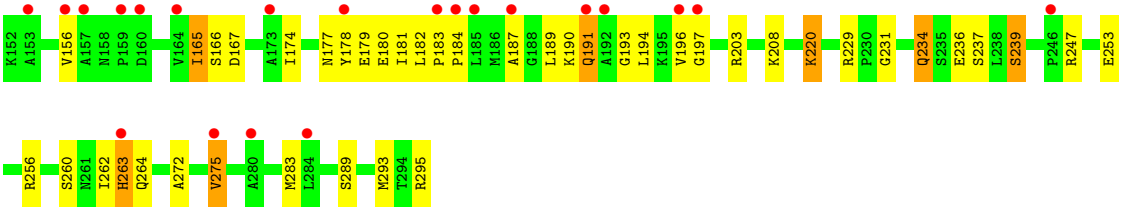
Chain C:



• Molecule 2: Ethanolamine ammonia-lyase light chain

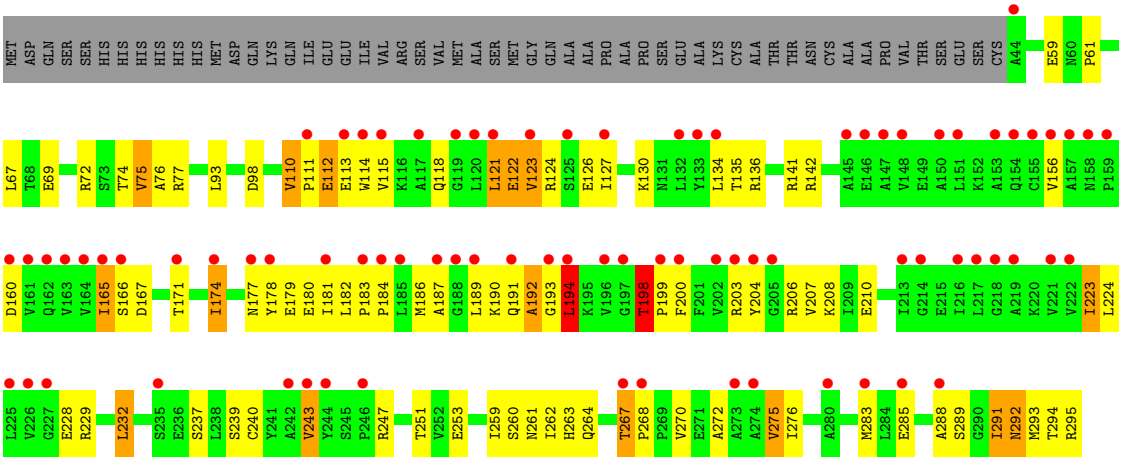
Chain B:





• Molecule 2: Ethanolamine ammonia-lyase light chain

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 63	Depositor
Cell constants a, b, c, α, β, γ	244.12Å 244.12Å 77.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.29 – 2.10 42.29 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.5 (42.29-2.10) 94.5 (42.29-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.5.0087	Depositor
R, R_{free}	0.248 , 0.285 0.238 , 0.257	Depositor DCC
R_{free} test set	7300 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 24.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.36$, $< L^2 > = 0.18$	Xtriage
Estimated twinning fraction	0.109 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	11985	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.03% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B12, NA, GOL

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	0.45	0/3518	0.73	0/4764
1	C	0.45	0/3518	0.74	2/4764 (0.0%)
2	B	0.39	0/1943	0.74	0/2633
2	D	0.37	0/1943	0.76	4/2633 (0.2%)
All	All	0.42	0/10922	0.74	6/14794 (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	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	331	GLY	CA-C-N	5.45	125.12	119.56
1	C	331	GLY	C-N-CA	5.45	125.12	119.56
2	D	268	PRO	CA-C-N	5.38	124.83	119.24
2	D	268	PRO	C-N-CA	5.38	124.83	119.24
2	D	198	THR	CA-C-N	5.16	125.07	119.85
2	D	198	THR	C-N-CA	5.16	125.07	119.85

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	VAL	Peptide
1	C	326	VAL	Peptide

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	3464	0	3418	51	0
1	C	3464	0	3419	57	0
2	B	1916	0	1973	61	0
2	D	1916	0	1973	77	0
3	A	18	0	24	2	0
3	C	18	0	24	2	0
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
5	B	91	0	88	22	0
5	D	91	0	88	27	0
6	A	421	0	0	7	1
6	B	129	0	0	5	0
6	C	349	0	0	4	1
6	D	101	0	0	4	0
All	All	11985	0	11007	288	1

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 (288) 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)
5:D:601:B12:H533	5:D:601:B12:N52	1.32	1.38
5:D:601:B12:H521	5:D:601:B12:C53	1.49	1.24
1:C:269:ARG:NH2	1:C:318:TYR:O	1.81	1.14
2:B:239:SER:HB3	2:B:260:SER:HA	1.30	1.12
2:B:165:ILE:HD11	2:B:174:ILE:HG23	1.28	1.07
2:D:167:ASP:HA	2:D:174:ILE:HD11	1.32	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:LEU:O	1:C:451:LEU:HD12	1.55	1.05
1:C:202:LEU:CD1	1:C:230:THR:HG22	1.89	1.02
5:D:601:B12:H531	5:D:601:B12:H552	1.42	1.01
5:B:601:B12:H531	5:B:601:B12:H552	1.42	1.00
5:B:601:B12:H362	5:B:601:B12:H351	1.40	1.00
1:C:202:LEU:HD12	1:C:230:THR:HG22	1.43	1.00
5:D:601:B12:H4R	5:D:601:B12:H491	1.49	0.94
5:D:601:B12:H362	5:D:601:B12:H351	1.50	0.93
2:D:74:THR:HG22	2:D:76:ALA:H	1.28	0.93
2:D:247:ARG:O	2:D:251:THR:HG22	1.70	0.92
2:B:189:LEU:O	2:B:193:GLY:HA3	1.70	0.92
2:B:110:VAL:O	2:B:203:ARG:NH2	2.03	0.92
1:C:202:LEU:HD22	1:C:224:VAL:HG11	1.52	0.91
2:D:110:VAL:O	2:D:203:ARG:NH2	2.06	0.88
2:D:240:CYS:HB3	2:D:259:ILE:HG22	1.57	0.86
2:D:167:ASP:HA	2:D:174:ILE:CD1	2.07	0.84
1:A:51:LEU:HD12	1:A:54:MET:HE3	1.59	0.84
2:D:141:ARG:NH2	5:D:601:B12:O8R	2.12	0.83
2:B:165:ILE:HD11	2:B:174:ILE:CG2	2.11	0.78
5:D:601:B12:H363	5:D:601:B12:H421	1.67	0.77
1:A:197:ASP:OD1	1:A:226:ALA:HB1	1.86	0.76
2:D:174:ILE:O	2:D:178:TYR:HB2	1.84	0.76
2:D:223:ILE:HD12	2:D:276:ILE:HG21	1.66	0.75
1:C:269:ARG:NH2	1:C:318:TYR:C	2.45	0.74
1:C:202:LEU:CD1	1:C:230:THR:CG2	2.64	0.74
5:B:601:B12:H362	5:B:601:B12:C35	2.17	0.74
1:A:326:VAL:HG12	1:A:329:PHE:HB2	1.69	0.74
2:D:223:ILE:HD12	2:D:276:ILE:CG2	2.18	0.73
1:C:202:LEU:HD11	1:C:230:THR:CG2	2.19	0.73
1:A:193:ASN:O	1:A:401:MET:HE1	1.89	0.72
1:C:202:LEU:CD2	1:C:224:VAL:HG11	2.18	0.72
1:C:202:LEU:HD22	1:C:224:VAL:CG1	2.19	0.72
5:D:601:B12:N52	5:D:601:B12:C53	2.26	0.72
1:C:29:SER:O	1:C:32:VAL:HG22	1.90	0.71
2:B:272:ALA:O	2:B:275:VAL:HG12	1.89	0.71
2:D:240:CYS:HB3	2:D:259:ILE:CG2	2.20	0.71
1:C:202:LEU:HD11	1:C:230:THR:HG22	1.73	0.70
2:D:191:GLN:O	2:D:192:ALA:HB3	1.91	0.70
1:A:200:GLU:HB2	6:A:740:HOH:O	1.91	0.70
5:D:601:B12:H491	5:D:601:B12:C4R	2.23	0.69
1:C:172:SER:OG	2:D:74:THR:HG23	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:283:MET:HE3	2:D:289:SER:HB3	1.75	0.68
2:D:182:LEU:HB3	2:D:183:PRO:HD3	1.76	0.67
1:A:4:LYS:HD3	1:A:13:GLN:OE1	1.95	0.66
2:B:101:ARG:NH1	6:B:317:HOH:O	2.24	0.65
5:B:601:B12:H552	5:B:601:B12:C53	2.20	0.65
5:D:601:B12:H202	5:D:601:B12:N3B	2.12	0.65
5:D:601:B12:C53	5:D:601:B12:H552	2.22	0.64
1:C:7:LEU:HD22	1:C:8:PHE:CD1	2.33	0.63
1:C:257:GLU:CD	2:D:253:GLU:HB2	2.23	0.63
1:C:5:THR:HG23	1:C:50:VAL:HG22	1.81	0.63
5:B:601:B12:H301	5:B:601:B12:H203	1.80	0.62
2:B:179:GLU:OE1	2:B:179:GLU:HA	1.99	0.62
2:B:187:ALA:O	2:B:191:GLN:HB2	2.00	0.61
2:D:156:VAL:HG13	2:D:198:THR:HG22	1.82	0.61
1:A:187:ASP:HB3	1:A:427:PHE:CG	2.36	0.60
1:C:166:THR:O	1:C:195:VAL:HG21	2.01	0.60
2:D:98:ASP:HB3	2:D:232:LEU:HD22	1.83	0.60
1:C:51:LEU:HA	1:C:54:MET:HG3	1.82	0.60
2:B:234:GLN:NE2	2:B:236:GLU:H	2.00	0.60
1:A:51:LEU:HA	1:A:54:MET:HE2	1.83	0.60
2:D:259:ILE:HG23	2:D:259:ILE:O	2.02	0.60
2:B:182:LEU:HB3	2:B:183:PRO:HD3	1.82	0.60
2:B:283:MET:HE2	2:B:289:SER:HB3	1.84	0.60
1:C:68:GLU:H	1:C:68:GLU:CD	2.08	0.59
1:C:110:ILE:HD12	1:C:141:MET:HG2	1.83	0.59
2:B:283:MET:HE2	2:B:289:SER:CB	2.31	0.59
2:B:123:VAL:CG1	2:B:147:ALA:HB1	2.32	0.59
5:B:601:B12:H351	5:B:601:B12:C36	2.18	0.59
5:B:601:B12:H401	5:B:601:B12:H8	1.66	0.59
2:D:288:ALA:HB1	2:D:292:ASN:HB2	1.83	0.59
2:B:53:LYS:HG2	2:B:94:ARG:NH1	2.18	0.58
1:C:326:VAL:HG12	1:C:329:PHE:HB2	1.84	0.58
1:A:20:VAL:HG11	1:A:54:MET:HE2	1.86	0.58
1:A:51:LEU:CD1	1:A:54:MET:HE3	2.33	0.58
5:B:601:B12:H492	5:B:601:B12:H533	1.84	0.58
1:A:198:ASP:OD1	6:A:841:HOH:O	2.17	0.58
1:C:167:ARG:NH1	6:C:875:HOH:O	2.36	0.58
2:D:191:GLN:O	2:D:192:ALA:CB	2.52	0.58
2:B:190:LYS:HG2	2:B:196:VAL:HG21	1.86	0.57
1:C:169:ASP:OD2	1:C:171:GLN:HB2	2.04	0.57
5:D:601:B12:H351	5:D:601:B12:C36	2.28	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:SER:OG	5:B:601:B12:N40	2.38	0.56
2:B:123:VAL:HG11	2:B:147:ALA:HB1	1.88	0.56
2:D:135:THR:HG23	2:D:136:ARG:HG2	1.86	0.56
1:A:401:MET:O	1:A:401:MET:HG2	2.05	0.56
5:D:601:B12:H262	5:D:601:B12:H601	1.88	0.55
1:A:59:ILE:HD12	1:A:93:ILE:HD11	1.89	0.55
1:A:110:ILE:HD12	1:A:141:MET:HG2	1.87	0.55
2:B:112:GLU:CD	2:B:112:GLU:H	2.13	0.55
5:D:601:B12:H301	5:D:601:B12:H203	1.88	0.55
1:A:372:ASP:HB2	6:A:538:HOH:O	2.06	0.55
2:B:147:ALA:O	2:B:151:LEU:HD13	2.07	0.55
2:D:228:GLU:HG2	2:D:237:SER:O	2.07	0.55
2:B:234:GLN:OE1	2:B:237:SER:HB2	2.06	0.54
2:B:190:LYS:HG2	2:B:196:VAL:CG2	2.37	0.54
1:C:143:VAL:HG13	3:C:2004:GOL:H12	1.89	0.54
2:B:262:ILE:O	2:B:263:HIS:HB3	2.06	0.54
1:C:349:HIS:CE1	1:C:388:CYS:HA	2.43	0.54
5:D:601:B12:C4	5:D:601:B12:H4B	2.37	0.54
1:C:441:ARG:NH1	6:C:703:HOH:O	2.41	0.53
2:B:123:VAL:HG13	2:B:147:ALA:CB	2.38	0.53
1:A:277:ARG:HB3	3:A:2006:GOL:H31	1.90	0.53
2:D:223:ILE:CD1	2:D:276:ILE:HG21	2.36	0.53
1:A:51:LEU:HD12	1:A:54:MET:CE	2.34	0.53
2:B:114:TRP:O	2:B:118:GLN:HG2	2.09	0.53
1:C:451:LEU:HD12	1:C:451:LEU:C	2.28	0.53
2:D:61:PRO:HB3	2:D:67:LEU:HD11	1.91	0.53
2:D:166:SER:O	2:D:174:ILE:HD12	2.08	0.53
2:D:285:GLU:HB3	6:D:815:HOH:O	2.07	0.53
2:B:220:LYS:HD3	2:B:220:LYS:N	2.24	0.53
5:D:601:B12:H362	5:D:601:B12:C35	2.32	0.53
2:B:99:HIS:O	2:B:103:LYS:HG2	2.09	0.53
2:B:123:VAL:CG1	2:B:124:ARG:N	2.72	0.52
1:C:162:GLN:O	1:C:394:MET:HE3	2.09	0.52
1:C:391:ILE:C	1:C:392:MET:HE2	2.33	0.52
2:B:234:GLN:HE22	2:B:236:GLU:N	2.08	0.52
1:C:218:ILE:HG12	1:C:430:TRP:CZ2	2.44	0.52
1:C:308:GLU:O	1:C:311:ASN:HB2	2.10	0.52
2:B:65:ASP:OD2	2:B:65:ASP:N	2.43	0.52
2:D:187:ALA:O	2:D:191:GLN:HB2	2.10	0.52
1:C:451:LEU:O	1:C:451:LEU:CD1	2.45	0.51
2:B:234:GLN:HE22	2:B:236:GLU:H	1.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:601:B12:H531	5:B:601:B12:C55	2.23	0.51
2:D:224:LEU:O	2:D:240:CYS:HA	2.11	0.51
5:B:601:B12:H2B	5:B:601:B12:O7R	2.11	0.51
1:A:368:HIS:H	1:A:368:HIS:CD2	2.29	0.51
2:D:114:TRP:O	2:D:118:GLN:HG2	2.11	0.50
2:D:165:ILE:HG22	2:D:200:PHE:O	2.11	0.50
1:A:64:VAL:HG23	1:A:65:ILE:HG13	1.94	0.50
1:C:75:LEU:HD21	1:C:317:HIS:CB	2.42	0.50
1:A:187:ASP:HB3	1:A:427:PHE:CD1	2.47	0.49
2:D:123:VAL:HG13	2:D:124:ARG:N	2.26	0.49
1:C:75:LEU:HD21	1:C:317:HIS:HB2	1.95	0.49
2:D:177:ASN:O	2:D:181:ILE:HG22	2.12	0.49
2:B:177:ASN:O	2:B:181:ILE:HG22	2.12	0.49
1:C:167:ARG:NH2	6:C:678:HOH:O	2.46	0.49
5:B:601:B12:H8	5:B:601:B12:N40	2.28	0.48
1:C:27:LEU:HD13	1:C:27:LEU:C	2.38	0.48
2:D:110:VAL:HG12	2:D:203:ARG:HH22	1.78	0.48
1:A:34:ALA:HB2	1:A:294:LEU:HD22	1.95	0.48
1:A:391:ILE:C	1:A:392:MET:HE2	2.38	0.48
2:B:112:GLU:OE2	6:B:325:HOH:O	2.20	0.48
2:D:267:THR:HG23	2:D:272:ALA:HB2	1.95	0.48
5:D:601:B12:H363	5:D:601:B12:C42	2.35	0.48
1:C:54:MET:HE3	1:C:59:ILE:HD11	1.95	0.48
1:A:166:THR:O	1:A:195:VAL:HG21	2.13	0.48
2:B:234:GLN:C	2:B:234:GLN:CD	2.81	0.48
1:C:202:LEU:HD11	1:C:230:THR:HG21	1.95	0.48
2:D:121:LEU:HD22	2:D:122:GLU:N	2.29	0.48
5:D:601:B12:O34	5:D:601:B12:HM52	2.14	0.48
1:A:199:VAL:HG21	1:A:237:ARG:HH11	1.79	0.48
2:B:247:ARG:NH2	6:B:823:HOH:O	2.47	0.48
1:C:202:LEU:HD12	1:C:230:THR:CG2	2.27	0.48
1:A:322:ILE:HB	1:A:390:TYR:CE1	2.49	0.47
2:D:180:GLU:HG2	2:D:270:VAL:HG23	1.96	0.47
1:A:326:VAL:CG1	1:A:329:PHE:HB2	2.40	0.47
5:B:601:B12:H473	5:B:601:B12:H481	1.52	0.47
2:D:112:GLU:CD	2:D:112:GLU:H	2.22	0.47
5:B:601:B12:O7R	5:B:601:B12:C2B	2.62	0.47
1:A:169:ASP:OD2	1:A:171:GLN:HB2	2.15	0.47
2:B:156:VAL:CG2	2:B:197:GLY:HA2	2.45	0.47
2:D:203:ARG:HG2	2:D:204:TYR:CD2	2.50	0.47
1:A:1:MET:HE1	1:A:17:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:GLN:HG3	1:A:14:PHE:N	2.29	0.47
2:B:97:ALA:O	2:B:100:SER:OG	2.30	0.47
1:C:20:VAL:HG11	1:C:54:MET:HE2	1.97	0.47
1:C:34:ALA:HB2	1:C:294:LEU:HD22	1.95	0.47
2:D:239:SER:OG	2:D:260:SER:HA	2.14	0.47
5:D:601:B12:H4B	5:D:601:B12:H302	1.95	0.47
1:C:64:VAL:HG23	1:C:65:ILE:HG13	1.97	0.47
1:C:161:LEU:O	1:C:163:PRO:HD3	2.15	0.47
5:D:601:B12:H531	5:D:601:B12:C55	2.21	0.47
2:D:295:ARG:NH1	2:D:295:ARG:HB3	2.30	0.47
1:C:48:LYS:NZ	1:C:127:LYS:O	2.48	0.47
2:D:267:THR:O	2:D:267:THR:CG2	2.63	0.47
5:D:601:B12:H301	5:D:601:B12:H253	1.66	0.47
1:A:333:GLU:HG3	2:B:137:PRO:HG3	1.97	0.46
2:D:110:VAL:HG23	2:D:171:THR:HG23	1.97	0.46
2:D:189:LEU:O	2:D:193:GLY:HA3	2.15	0.46
2:D:160:ASP:OD1	2:D:194:LEU:HB3	2.14	0.46
2:D:291:ILE:O	2:D:291:ILE:HG23	2.15	0.46
2:B:126:GLU:OE1	2:B:142:ARG:NH1	2.48	0.46
2:D:111:PRO:HG2	2:D:114:TRP:HB2	1.96	0.46
1:A:277:ARG:NH2	6:A:546:HOH:O	2.49	0.46
2:B:89:THR:O	2:B:93:LEU:HG	2.14	0.46
1:C:218:ILE:HG12	1:C:430:TRP:CE2	2.50	0.46
5:B:601:B12:H533	5:B:601:B12:C49	2.46	0.46
1:C:326:VAL:CG1	1:C:329:PHE:HB2	2.44	0.46
1:C:390:TYR:CE2	1:C:392:MET:HE1	2.50	0.46
2:D:77:ARG:NH2	2:D:232:LEU:HD13	2.31	0.46
1:A:51:LEU:CD1	1:A:54:MET:CE	2.93	0.46
1:A:63:PRO:HD2	6:A:693:HOH:O	2.15	0.46
2:D:207:VAL:O	2:D:210:GLU:HG2	2.16	0.46
2:D:262:ILE:O	2:D:263:HIS:HB3	2.16	0.46
2:B:166:SER:O	2:B:174:ILE:HD11	2.16	0.46
1:A:364:CYS:HB2	1:A:404:TYR:CD2	2.52	0.45
2:B:247:ARG:HG3	6:B:550:HOH:O	2.15	0.45
2:D:112:GLU:HA	2:D:115:VAL:HG22	1.98	0.45
2:B:178:TYR:C	2:B:180:GLU:H	2.23	0.45
1:C:197:ASP:OD1	1:C:230:THR:HG21	2.17	0.45
1:C:143:VAL:HG11	1:C:357:ILE:C	2.42	0.45
1:A:30:GLY:HA3	1:A:304:GLN:OE1	2.17	0.45
3:C:2003:GOL:H12	6:C:936:HOH:O	2.17	0.45
2:D:295:ARG:HB3	2:D:295:ARG:CZ	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:CYS:HB2	1:A:404:TYR:CE2	2.52	0.45
2:B:208:LYS:HG2	2:B:256:ARG:HH21	1.82	0.45
2:B:165:ILE:HG13	2:B:166:SER:N	2.31	0.44
2:D:259:ILE:HD13	2:D:275:VAL:HG21	1.99	0.44
2:D:126:GLU:OE1	2:D:142:ARG:NH1	2.50	0.44
2:D:179:GLU:OE1	2:D:179:GLU:HA	2.17	0.44
2:B:129:ASP:OD1	2:B:131:ASN:HB2	2.16	0.44
2:B:208:LYS:HE2	5:B:601:B12:O8R	2.17	0.44
1:C:27:LEU:HD13	1:C:28:ARG:N	2.32	0.44
1:A:368:HIS:H	1:A:368:HIS:HD2	1.64	0.44
1:A:1:MET:HB3	1:A:58:ASP:OD2	2.18	0.44
1:C:34:ALA:HB2	1:C:294:LEU:CD2	2.47	0.44
5:D:601:B12:O7R	5:D:601:B12:C2B	2.65	0.44
1:A:380:MET:SD	1:A:411:ASP:HB3	2.58	0.44
5:D:601:B12:O7R	5:D:601:B12:H2B	2.17	0.44
2:D:124:ARG:HD2	2:D:127:ILE:O	2.17	0.44
2:B:123:VAL:HG13	2:B:124:ARG:N	2.33	0.43
5:B:601:B12:N40	5:B:601:B12:C8	2.81	0.43
1:C:13:GLN:HG3	1:C:14:PHE:N	2.33	0.43
5:B:601:B12:H301	5:B:601:B12:H253	1.76	0.43
2:B:123:VAL:HG13	2:B:147:ALA:HB1	1.99	0.43
2:D:74:THR:HG21	2:D:76:ALA:HB3	1.99	0.43
1:A:168:ASP:CG	1:A:195:VAL:H	2.26	0.43
2:B:123:VAL:HG13	2:B:147:ALA:HB2	2.01	0.43
2:B:253:GLU:CD	5:B:601:B12:H5R1	2.43	0.43
2:D:141:ARG:HG2	2:D:208:LYS:HB2	2.00	0.43
2:D:186:MET:HE1	2:D:199:PRO:HD3	1.99	0.43
2:D:261:ASN:ND2	6:D:410:HOH:O	2.15	0.43
2:B:183:PRO:N	2:B:184:PRO:HD2	2.33	0.43
1:C:252:GLU:O	1:C:256:LYS:HG3	2.19	0.43
1:C:380:MET:HG2	1:C:381:ILE:N	2.33	0.43
2:D:110:VAL:HG13	2:D:111:PRO:O	2.19	0.43
2:B:72:ARG:HE	2:B:72:ARG:HB2	1.45	0.43
1:C:400:ILE:HG21	2:D:75:VAL:HG12	2.00	0.42
2:B:178:TYR:C	2:B:180:GLU:N	2.76	0.42
1:A:451:LEU:C	1:A:451:LEU:HD23	2.45	0.42
2:D:171:THR:O	2:D:174:ILE:HG12	2.20	0.42
1:A:277:ARG:HE	3:A:2006:GOL:H31	1.85	0.42
2:B:124:ARG:HD2	2:B:127:ILE:O	2.20	0.42
1:A:162:GLN:HB3	1:A:394:MET:HG2	2.02	0.42
2:D:183:PRO:N	2:D:184:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:VAL:HG11	1:A:357:ILE:C	2.45	0.42
1:A:397:GLY:O	1:A:405:GLN:HA	2.20	0.42
5:B:601:B12:H481	5:B:601:B12:H521	1.20	0.42
2:D:123:VAL:CG1	2:D:124:ARG:N	2.83	0.42
2:D:210:GLU:OE2	2:D:243:VAL:HG22	2.20	0.42
2:D:237:SER:OG	2:D:261:ASN:HA	2.20	0.42
6:A:661:HOH:O	2:B:231:GLY:HA3	2.19	0.42
2:D:259:ILE:CG2	2:D:259:ILE:O	2.68	0.42
5:D:601:B12:O28	5:D:601:B12:H3	2.19	0.42
2:B:167:ASP:HA	2:B:174:ILE:HG13	2.02	0.41
2:D:59:GLU:HG3	6:D:669:HOH:O	2.19	0.41
2:D:289:SER:HA	2:D:293:MET:SD	2.61	0.41
5:D:601:B12:H482	5:D:601:B12:H473	1.70	0.41
1:A:97:ARG:HD2	1:A:128:ILE:HG13	2.02	0.41
5:B:601:B12:H351	5:B:601:B12:H371	2.01	0.41
1:C:233:GLU:O	1:C:237:ARG:HG3	2.20	0.41
2:B:220:LYS:HE2	6:B:719:HOH:O	2.19	0.41
1:A:129:CYS:HB3	1:A:133:ASP:HB2	2.03	0.41
1:C:146:LYS:HG3	1:C:280:GLY:HA3	2.03	0.41
2:D:75:VAL:O	2:D:75:VAL:CG1	2.65	0.41
2:B:75:VAL:O	2:B:75:VAL:CG1	2.69	0.41
2:D:180:GLU:HG2	2:D:270:VAL:CG2	2.50	0.41
2:D:203:ARG:HG2	2:D:204:TYR:CE2	2.56	0.41
2:B:283:MET:CE	2:B:289:SER:HB3	2.50	0.41
2:D:115:VAL:HG21	2:D:122:GLU:OE2	2.22	0.40
2:D:207:VAL:HG23	2:D:208:LYS:N	2.36	0.40
1:A:326:VAL:HA	1:A:362:ASP:HB3	2.02	0.40
2:B:67:LEU:HD23	2:B:67:LEU:HA	1.91	0.40
5:D:601:B12:H541	5:D:601:B12:H602	1.83	0.40
1:A:294:LEU:O	1:A:294:LEU:HD12	2.21	0.40
2:B:289:SER:HA	2:B:293:MET:SD	2.62	0.40
5:B:601:B12:H203	5:B:601:B12:C30	2.48	0.40
2:D:206:ARG:HD2	6:D:321:HOH:O	2.20	0.40
2:D:294:THR:O	2:D:295:ARG:C	2.65	0.40
5:D:601:B12:H2B	5:D:601:B12:H492	2.02	0.40
1:A:297:GLY:HA2	6:A:611:HOH:O	2.20	0.40

All (1) 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)
6:A:763:HOH:O	6:C:562:HOH:O[2_545]	2.11	0.09

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	451/453 (100%)	433 (96%)	18 (4%)	0	100	100
1	C	451/453 (100%)	437 (97%)	14 (3%)	0	100	100
2	B	250/306 (82%)	240 (96%)	8 (3%)	2 (1%)	16	12
2	D	250/306 (82%)	237 (95%)	11 (4%)	2 (1%)	16	12
All	All	1402/1518 (92%)	1347 (96%)	51 (4%)	4 (0%)	36	36

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	63	ARG
2	B	263	HIS
2	D	194	LEU
2	D	192	ALA

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	370/370 (100%)	358 (97%)	12 (3%)	34	38
1	C	370/370 (100%)	358 (97%)	12 (3%)	34	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	B	206/251 (82%)	185 (90%)	21 (10%)	7 4
2	D	206/251 (82%)	180 (87%)	26 (13%)	4 2
All	All	1152/1242 (93%)	1081 (94%)	71 (6%)	16 14

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	ILE
1	A	110	ILE
1	A	198	ASP
1	A	247	SER
1	A	262	LEU
1	A	269	ARG
1	A	294	LEU
1	A	314	LEU
1	A	375	LEU
1	A	401	MET
1	A	433	SER
1	A	451	LEU
2	B	68	THR
2	B	70	LEU
2	B	75	VAL
2	B	96	LEU
2	B	113	GLU
2	B	115	VAL
2	B	121	LEU
2	B	122	GLU
2	B	123	VAL
2	B	130	LYS
2	B	151	LEU
2	B	165	ILE
2	B	191	GLN
2	B	194	LEU
2	B	220	LYS
2	B	229	ARG
2	B	234	GLN
2	B	239	SER
2	B	264	GLN
2	B	275	VAL
2	B	295	ARG
1	C	7	LEU

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Mol	Chain	Res	Type
1	C	32	VAL
1	C	41	SER
1	C	54	MET
1	C	68	GLU
1	C	110	ILE
1	C	119	SER
1	C	166	THR
1	C	167	ARG
1	C	198	ASP
1	C	380	MET
1	C	451	LEU
2	D	69	GLU
2	D	72	ARG
2	D	75	VAL
2	D	93	LEU
2	D	110	VAL
2	D	112	GLU
2	D	113	GLU
2	D	121	LEU
2	D	122	GLU
2	D	123	VAL
2	D	130	LYS
2	D	134	LEU
2	D	165	ILE
2	D	174	ILE
2	D	190	LYS
2	D	194	LEU
2	D	198	THR
2	D	223	ILE
2	D	229	ARG
2	D	232	LEU
2	D	243	VAL
2	D	264	GLN
2	D	267	THR
2	D	275	VAL
2	D	291	ILE
2	D	292	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	171	GLN
1	A	368	HIS
2	B	158	ASN
2	B	177	ASN
2	B	234	GLN
1	C	10	ASN
1	C	349	HIS
2	D	62	HIS

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)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	B12	D	601	-	94,101,101	1.42	11 (11%)	149,166,166	1.62	32 (21%)
3	GOL	A	2006	-	5,5,5	0.17	0	5,5,5	0.49	0
3	GOL	A	2002	-	5,5,5	0.29	0	5,5,5	0.70	0
3	GOL	A	2001	-	5,5,5	0.29	0	5,5,5	0.57	0
5	B12	B	601	-	94,101,101	1.47	12 (12%)	149,166,166	1.42	24 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	GOL	C	2004	-	5,5,5	0.28	0	5,5,5	1.08	0
3	GOL	C	2003	-	5,5,5	0.38	0	5,5,5	0.50	0
3	GOL	C	2005	-	5,5,5	0.31	0	5,5,5	0.67	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
5	B12	D	601	-	-	16/56/223/223	0/3/11/11
3	GOL	A	2006	-	-	4/4/4/4	-
3	GOL	A	2002	-	-	2/4/4/4	-
3	GOL	A	2001	-	-	2/4/4/4	-
5	B12	B	601	-	-	23/56/223/223	0/3/11/11
3	GOL	C	2004	-	-	4/4/4/4	-
3	GOL	C	2003	-	-	4/4/4/4	-
3	GOL	C	2005	-	-	3/4/4/4	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	B12	C19-N24	-5.80	1.41	1.49
5	B	601	B12	C19-N24	-5.69	1.42	1.49
5	B	601	B12	C8B-C9B	4.98	1.48	1.40
5	D	601	B12	C8B-C9B	4.81	1.48	1.40
5	B	601	B12	C14-N23	4.80	1.41	1.35
5	B	601	B12	C9-N22	4.52	1.41	1.30
5	D	601	B12	C14-N23	4.34	1.40	1.35
5	D	601	B12	C9-N22	4.09	1.40	1.30
5	B	601	B12	C16-C15	-3.61	1.34	1.44
5	B	601	B12	C6B-C5B	3.54	1.49	1.40
5	D	601	B12	C16-C15	-3.49	1.34	1.44
5	D	601	B12	C6B-C5B	3.31	1.48	1.40
5	B	601	B12	C8B-N1B	-2.85	1.33	1.39
5	D	601	B12	C2B-N3B	2.70	1.36	1.31
5	D	601	B12	C10-C9	2.67	1.46	1.39
5	B	601	B12	C10-C9	2.63	1.46	1.39
5	B	601	B12	C2B-N3B	2.62	1.36	1.31
5	B	601	B12	C11-N23	2.51	1.41	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	601	B12	C1-C2	-2.50	1.53	1.58
5	D	601	B12	C12-C11	-2.47	1.47	1.52
5	B	601	B12	C9B-N3B	-2.46	1.35	1.39
5	B	601	B12	C1-C2	-2.15	1.53	1.58
5	D	601	B12	C8B-N1B	-2.15	1.35	1.39

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	601	B12	C47-C12-C46	7.12	121.20	109.41
5	B	601	B12	C19-N24-C16	4.42	112.12	107.29
5	D	601	B12	C2-C1-C19	4.16	125.08	118.61
5	B	601	B12	C2-C1-C19	4.13	125.03	118.61
5	D	601	B12	C54-C17-C18	-4.12	107.07	112.99
5	D	601	B12	C19-N24-C16	4.06	111.73	107.29
5	D	601	B12	C8B-C9B-N3B	-3.77	105.93	110.00
5	B	601	B12	C46-C12-C13	-3.33	99.25	112.74
5	D	601	B12	C20-C1-C2	-3.32	107.81	113.28
5	B	601	B12	C8B-C9B-N3B	-3.30	106.43	110.00
5	B	601	B12	C7-C6-C5	-3.16	123.14	128.07
5	D	601	B12	C19-C1-N21	3.12	105.36	102.14
5	D	601	B12	C30-C3-C2	-3.09	112.17	119.00
5	D	601	B12	C9B-C8B-N1B	3.04	106.65	105.30
5	D	601	B12	C20-C1-C19	-3.03	106.43	109.35
5	B	601	B12	C20-C1-C19	-2.99	106.47	109.35
5	D	601	B12	C15-C14-N23	-2.98	122.67	126.26
5	B	601	B12	C47-C12-C11	2.94	120.60	110.08
5	B	601	B12	C9B-C8B-N1B	2.94	106.61	105.30
5	B	601	B12	C54-C17-C18	-2.91	108.81	112.99
5	D	601	B12	C48-C13-C12	-2.85	108.37	116.52
5	D	601	B12	C9B-N3B-C2B	2.84	107.88	104.40
5	D	601	B12	C26-C2-C3	2.83	112.36	107.42
5	B	601	B12	C47-C12-C46	2.80	114.04	109.41
5	D	601	B12	C1-C2-C3	2.78	105.10	101.60
5	D	601	B12	C3-C4-N21	-2.78	108.52	111.98
5	D	601	B12	C25-C2-C1	-2.77	109.61	113.75
5	B	601	B12	C3-C4-N21	-2.76	108.55	111.98
5	B	601	B12	C9-C10-C11	-2.73	122.06	125.97
5	D	601	B12	C55-C17-C18	2.67	116.22	111.12
5	D	601	B12	C12-C11-C10	-2.65	119.98	123.40
5	B	601	B12	C55-C56-C57	-2.62	105.41	111.25
5	B	601	B12	C1-C2-C3	2.60	104.87	101.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	601	B12	C30-C3-C2	-2.60	113.27	119.00
5	D	601	B12	C7B-C8B-C9B	-2.51	119.46	122.47
5	B	601	B12	C8-C7-C6	2.51	105.18	100.92
5	D	601	B12	C9-C10-C11	-2.47	122.44	125.97
5	D	601	B12	C37-C7-C8	-2.38	102.09	108.37
5	D	601	B12	C9-N22-C6	2.35	108.11	105.28
5	B	601	B12	C18-C17-C16	2.35	103.52	100.69
5	B	601	B12	C17-C16-N24	-2.34	107.59	111.17
5	D	601	B12	C13-C12-C11	-2.34	98.36	100.97
5	D	601	B12	C17-C16-N24	-2.34	107.60	111.17
5	D	601	B12	C8B-N1B-C2B	2.33	108.37	106.26
5	B	601	B12	C9B-N3B-C2B	2.32	107.24	104.40
5	B	601	B12	C20-C1-C2	-2.27	109.53	113.28
5	D	601	B12	C46-C12-C11	2.26	118.15	110.08
5	D	601	B12	C8-C7-C6	2.24	104.72	100.92
5	D	601	B12	C2P-C1P-N59	-2.22	109.66	112.92
5	B	601	B12	C5R-C4R-C3R	-2.20	107.91	114.84
5	B	601	B12	C55-C17-C18	2.20	115.32	111.12
5	B	601	B12	C8B-N1B-C2B	2.14	108.21	106.26
5	D	601	B12	C18-C17-C16	2.14	103.26	100.69
5	D	601	B12	C47-C12-C11	-2.04	102.77	110.08
5	B	601	B12	C1-C19-N24	2.04	108.51	106.25
5	D	601	B12	C13-C14-C15	2.00	127.36	124.32

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2002	GOL	C1-C2-C3-O3
3	A	2006	GOL	O1-C1-C2-C3
3	C	2004	GOL	C1-C2-C3-O3
3	C	2005	GOL	O1-C1-C2-O2
3	C	2005	GOL	O1-C1-C2-C3
5	B	601	B12	C2P-O3-P-O5
5	B	601	B12	C2P-O3-P-O2
5	B	601	B12	O6R-C1R-N1B-C8B
5	D	601	B12	C38-C37-C7-C6
5	D	601	B12	C38-C37-C7-C36
5	D	601	B12	C38-C37-C7-C8
5	D	601	B12	C2P-O3-P-O5
5	D	601	B12	O6R-C1R-N1B-C8B
5	D	601	B12	O6R-C4R-C5R-O8R

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Mol	Chain	Res	Type	Atoms
5	B	601	B12	O6R-C4R-C5R-O8R
5	B	601	B12	C3R-C4R-C5R-O8R
5	D	601	B12	C3R-C4R-C5R-O8R
5	B	601	B12	C13-C48-C49-C50
5	B	601	B12	C42-C41-C8-C9
3	C	2004	GOL	O2-C2-C3-O3
5	B	601	B12	C18-C17-C55-C56
5	B	601	B12	C16-C17-C55-C56
5	D	601	B12	C16-C17-C55-C56
5	B	601	B12	C14-C13-C48-C49
5	D	601	B12	C25-C2-C26-C27
3	A	2006	GOL	C1-C2-C3-O3
3	C	2003	GOL	O1-C1-C2-C3
3	C	2003	GOL	C1-C2-C3-O3
3	C	2004	GOL	O1-C1-C2-C3
5	B	601	B12	C2R-C1R-N1B-C8B
5	D	601	B12	C2R-C1R-N1B-C8B
3	A	2006	GOL	O1-C1-C2-O2
3	A	2006	GOL	O2-C2-C3-O3
5	B	601	B12	C48-C49-C50-O51
3	C	2003	GOL	O1-C1-C2-O2
3	C	2004	GOL	O1-C1-C2-O2
5	D	601	B12	C18-C17-C55-C56
5	B	601	B12	C48-C49-C50-N52
5	B	601	B12	C12-C13-C48-C49
3	A	2002	GOL	O2-C2-C3-O3
5	B	601	B12	C2-C3-C30-C31
3	A	2001	GOL	O1-C1-C2-O2
5	B	601	B12	C1P-C2P-O3-P
5	B	601	B12	C3P-C2P-O3-P
5	D	601	B12	C3-C2-C26-C27
5	D	601	B12	C2-C3-C30-C31
5	B	601	B12	C38-C37-C7-C36
5	D	601	B12	C2P-O3-P-O4
3	C	2003	GOL	O2-C2-C3-O3
3	A	2001	GOL	C1-C2-C3-O3
5	B	601	B12	C7-C37-C38-N40
5	B	601	B12	C4-C3-C30-C31
5	B	601	B12	C7-C37-C38-O39
3	C	2005	GOL	O2-C2-C3-O3
5	B	601	B12	C18-C60-C61-O63
5	B	601	B12	C2P-O3-P-O4

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Mol	Chain	Res	Type	Atoms
5	D	601	B12	C3R-O2-P-O5
5	D	601	B12	C1P-C2P-O3-P

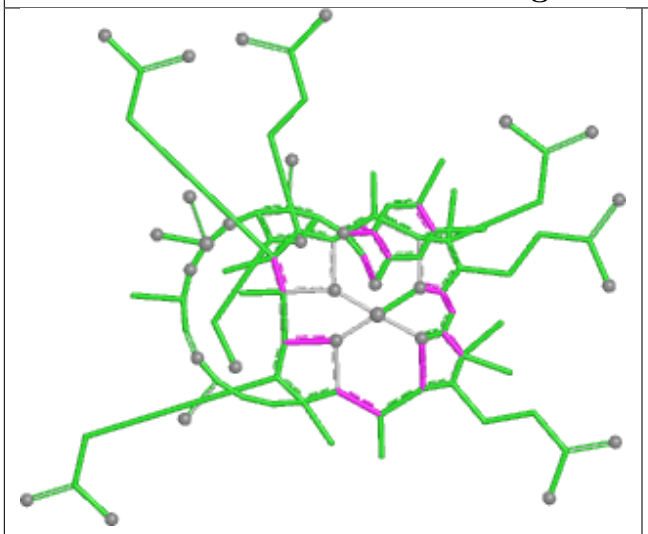
There are no ring outliers.

5 monomers are involved in 53 short contacts:

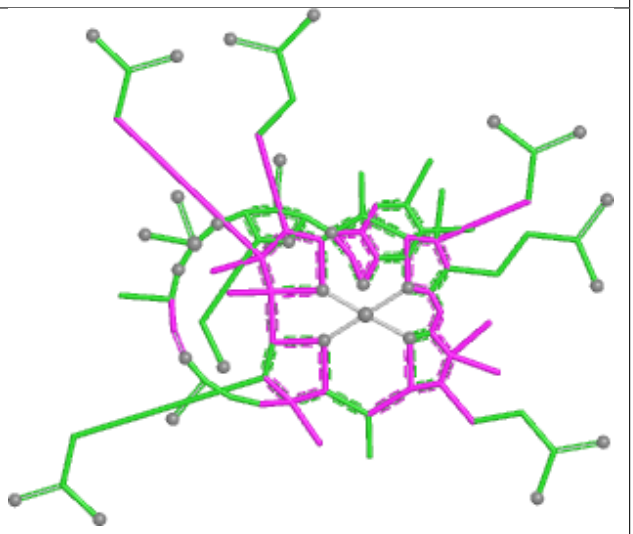
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	601	B12	27	0
3	A	2006	GOL	2	0
5	B	601	B12	22	0
3	C	2004	GOL	1	0
3	C	2003	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

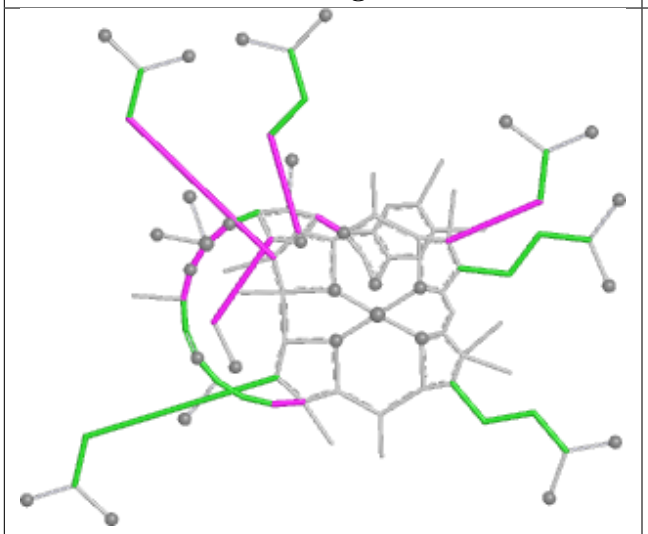
Ligand B12 D 601



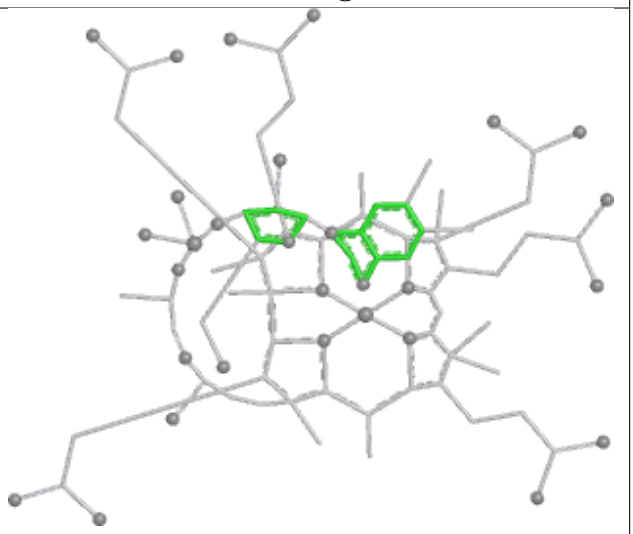
Bond lengths



Bond angles



Torsions



Rings

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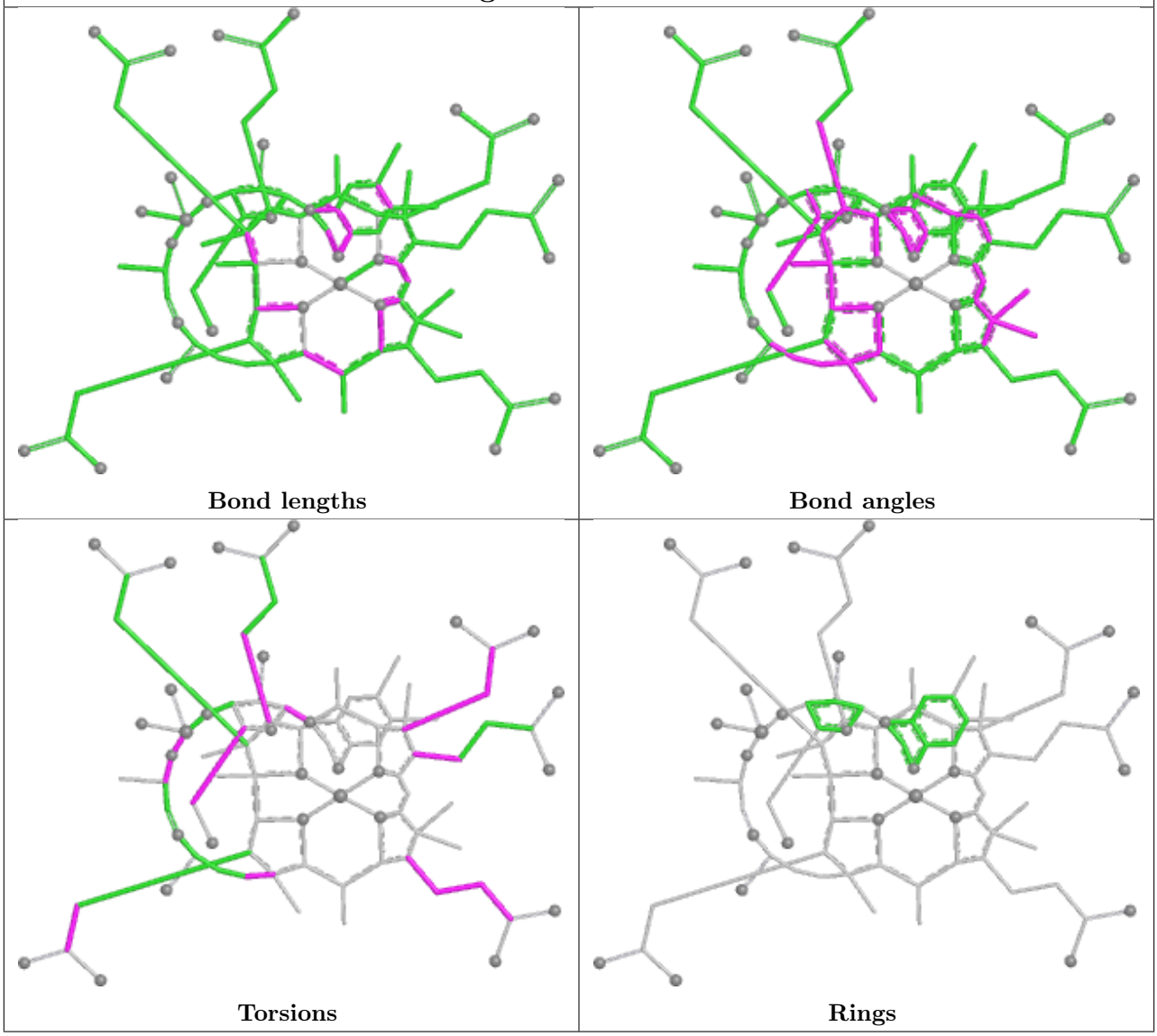

5.7 Other polymers (i)

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%)	-0.98	0	100	100	15, 27, 41, 50	0
1	C	453/453 (100%)	-0.96	0	100	100	15, 26, 44, 63	0
2	B	252/306 (82%)	0.54	32 (12%)	8	8	25, 50, 73, 82	0
2	D	252/306 (82%)	1.28	81 (32%)	1	1	19, 63, 105, 118	0
All	All	1410/1518 (92%)	-0.30	113 (8%)	18	19	15, 33, 80, 118	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	205	GLY	7.3
2	D	148	VAL	5.9
2	D	153	ALA	5.7
2	D	187	ALA	5.0
2	D	193	GLY	4.9
2	D	114	TRP	4.8
2	D	158	ASN	4.7
2	D	202	VAL	4.7
2	D	243	VAL	4.6
2	D	123	VAL	4.5
2	D	156	VAL	4.4
2	D	145	ALA	4.2
2	D	120	LEU	4.1
2	D	219	ALA	4.0
2	B	191	GLN	4.0
2	D	121	LEU	3.8
2	D	235	SER	3.8
2	D	161	VAL	3.8
2	D	213	ILE	3.7
2	B	143	LEU	3.6
2	D	204	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
2	D	164	VAL	3.6
2	D	111	PRO	3.6
2	D	150	ALA	3.5
2	D	196	VAL	3.5
2	D	151	LEU	3.5
2	D	119	GLY	3.4
2	B	178	TYR	3.4
2	D	200	PHE	3.4
2	B	147	ALA	3.3
2	D	273	ALA	3.3
2	B	119	GLY	3.3
2	D	117	ALA	3.3
2	B	164	VAL	3.2
2	D	159	PRO	3.1
2	D	214	GLY	3.0
2	D	113	GLU	3.0
2	B	275	VAL	3.0
2	D	154	GLN	2.9
2	D	181	ILE	2.9
2	D	160	ASP	2.9
2	D	191	GLN	2.9
2	D	178	TYR	2.9
2	B	151	LEU	2.9
2	D	218	GLY	2.9
2	D	267	THR	2.9
2	D	185	LEU	2.9
2	D	125	SER	2.9
2	D	217	LEU	2.8
2	B	121	LEU	2.8
2	B	197	GLY	2.8
2	D	197	GLY	2.8
2	D	199	PRO	2.8
2	D	227	GLY	2.7
2	D	268	PRO	2.7
2	D	242	ALA	2.7
2	D	165	ILE	2.7
2	D	188	GLY	2.6
2	B	150	ALA	2.6
2	D	194	LEU	2.6
2	D	115	VAL	2.6
2	D	221	VAL	2.6
2	B	157	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	187	ALA	2.6
2	B	159	PRO	2.6
2	D	183	PRO	2.6
2	B	114	TRP	2.6
2	B	160	ASP	2.5
2	D	44	ALA	2.5
2	D	246	PRO	2.5
2	D	222	VAL	2.5
2	D	133	TYR	2.5
2	D	163	VAL	2.4
2	D	155	CYS	2.4
2	D	189	LEU	2.4
2	B	145	ALA	2.4
2	B	185	LEU	2.3
2	D	225	LEU	2.3
2	D	285	GLU	2.3
2	D	157	ALA	2.3
2	D	274	ALA	2.3
2	D	203	ARG	2.3
2	D	127	ILE	2.3
2	B	196	VAL	2.3
2	B	246	PRO	2.3
2	D	147	ALA	2.3
2	D	244	TYR	2.3
2	D	174	ILE	2.3
2	B	280	ALA	2.2
2	D	280	ALA	2.2
2	B	113	GLU	2.2
2	D	162	GLN	2.2
2	B	184	PRO	2.2
2	B	284	LEU	2.2
2	B	183	PRO	2.2
2	B	173	ALA	2.2
2	B	263	HIS	2.2
2	D	226	VAL	2.1
2	B	117	ALA	2.1
2	D	288	ALA	2.1
2	B	153	ALA	2.1
2	D	134	LEU	2.1
2	D	146	GLU	2.1
2	B	192	ALA	2.1
2	D	166	SER	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	283	MET	2.1
2	D	171	THR	2.1
2	D	184	PRO	2.1
2	B	148	VAL	2.1
2	B	156	VAL	2.1
2	D	132	LEU	2.0
2	D	177	ASN	2.0
2	D	216	ILE	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)

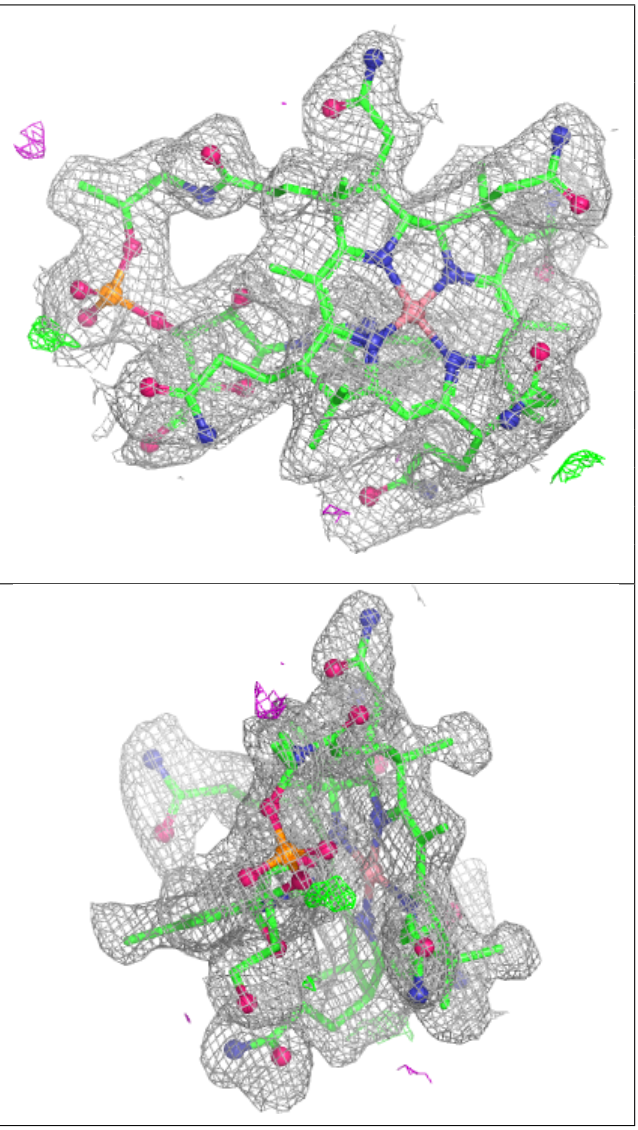
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	NA	C	3007	1/1	0.94	0.06	24,24,24,24	0
3	GOL	A	2006	6/6	0.97	0.10	21,21,21,21	0
3	GOL	C	2005	6/6	0.98	0.05	20,20,20,21	0
3	GOL	C	2003	6/6	0.98	0.08	20,20,20,20	0
3	GOL	C	2004	6/6	0.99	0.05	20,20,21,21	0
3	GOL	A	2001	6/6	0.99	0.05	19,19,20,20	0
4	NA	A	3001	1/1	0.99	0.08	20,20,20,20	0
4	NA	A	3004	1/1	0.99	0.03	19,19,19,19	0
4	NA	A	3005	1/1	0.99	0.07	22,22,22,22	0
4	NA	B	3002	1/1	0.99	0.05	20,20,20,20	0
3	GOL	A	2002	6/6	0.99	0.05	19,19,19,19	0
4	NA	D	3003	1/1	0.99	0.04	21,21,21,21	0
4	NA	D	3006	1/1	0.99	0.07	20,20,20,20	0
5	B12	B	601	91/91	0.99	0.04	17,18,18,19	0
5	B12	D	601	91/91	0.99	0.04	18,18,19,19	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.

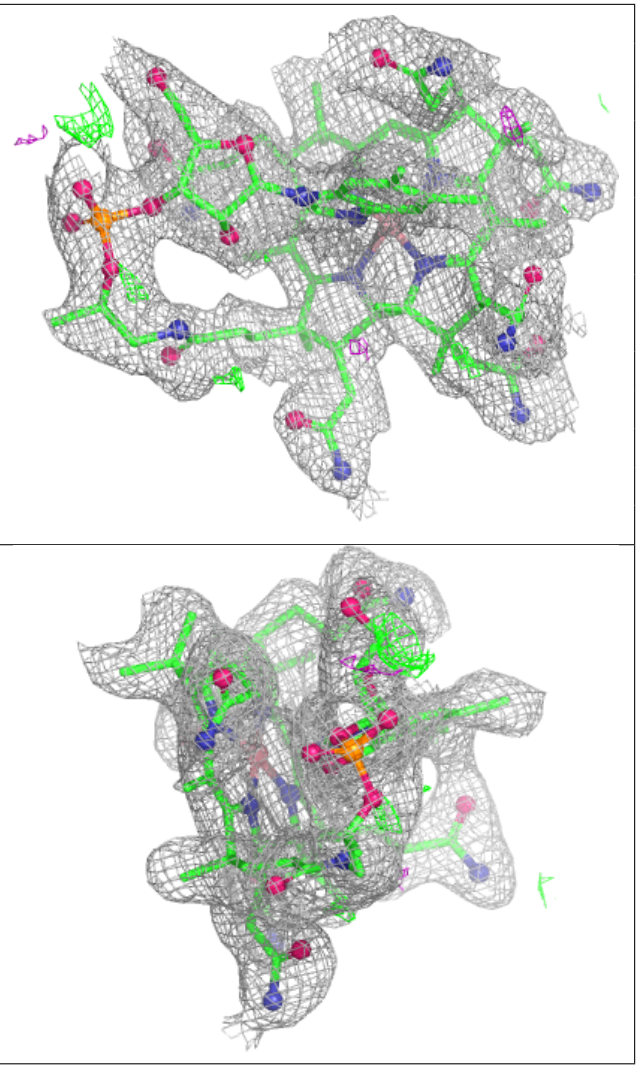
Electron density around B12 B 601:

$2mF_o$-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.