



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 08:23 PM EDT

PDB ID : 4DJJ / pdb_00004djd
Title : Crystal structure of folate-free corrinoid iron-sulfur protein (CFeSP) in complex with its methyltransferase (MeTr)
Authors : Kung, Y.; Doukov, T.I.; Blasiak, L.C.; Drennan, C.L.
Deposited on : 2012-02-01
Resolution : 2.38 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	:	9.0.015 (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

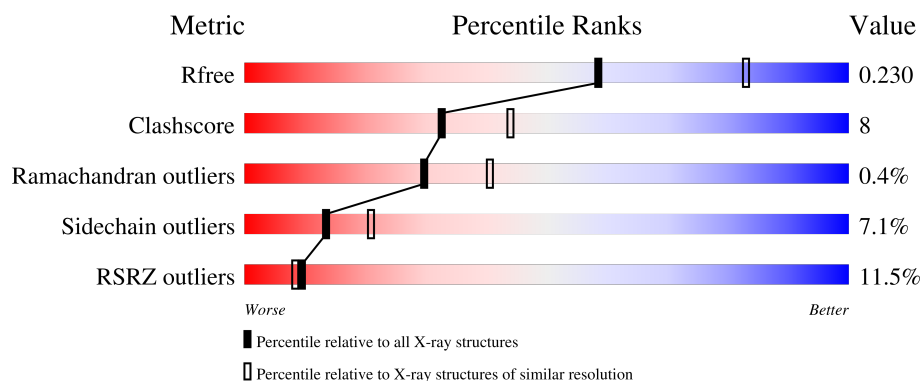
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.38 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	7164 (2.40-2.36)
Clashscore	190562	7722 (2.40-2.36)
Ramachandran outliers	187476	7626 (2.40-2.36)
Sidechain outliers	187428	7627 (2.40-2.36)
RSRZ outliers	180081	7170 (2.40-2.36)

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	262	4% 87% 12% .
1	B	262	3% 84% 16%
2	C	446	22% 75% 22% ..
2	E	446	25% 79% 17% ..
3	D	323	% 87% 11% .

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Mol	Chain	Length	Quality of chain
3	F	323	% 88% 10%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 15832 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 5-methyltetrahydrofolate corrinoid/iron sulfur protein methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			1993	1249	343	384	17			
1	B	262	Total	C	N	O	S	0	0	0
			1993	1249	343	384	17			

- Molecule 2 is a protein called Corrinoid/iron-sulfur protein large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	441	Total	C	N	O	S	0	0	0
			3149	1993	544	602	10			
2	E	441	Total	C	N	O	S	0	0	0
			3105	1955	536	604	10			

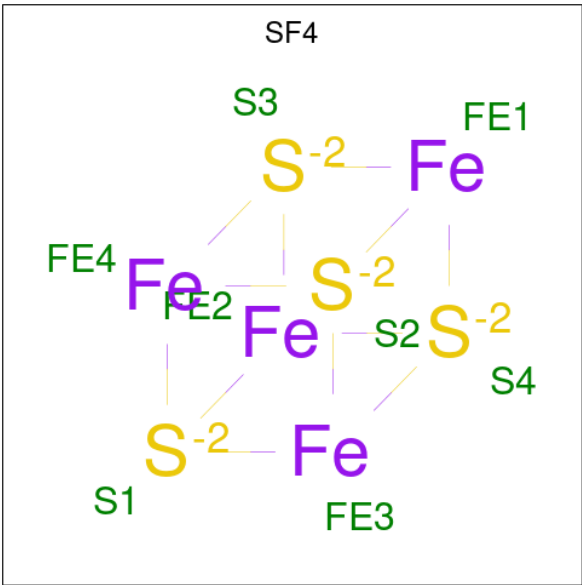
- Molecule 3 is a protein called Corrinoid/iron-sulfur protein small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	323	Total	C	N	O	S	0	0	0
			2461	1553	426	467	15			
3	F	323	Total	C	N	O	S	0	1	0
			2470	1561	426	468	15			

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

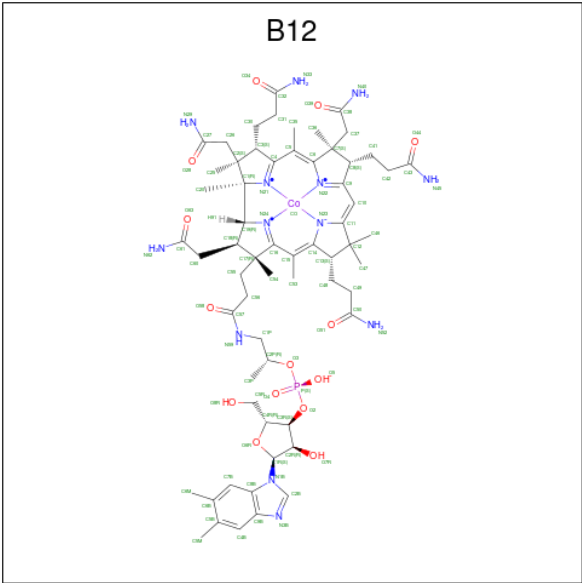
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	B	1	Total	Ca	0	0
			1	1		

- Molecule 5 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄).



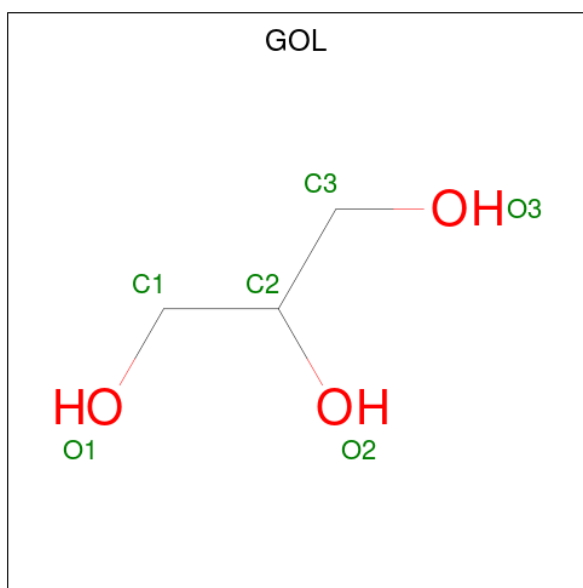
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	Fe	S	0	0
			8	4	4		
5	E	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 6 is COBALAMIN (CCD ID: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	D	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	E	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		
7	F	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	33	Total	O	0	0
			33	33		

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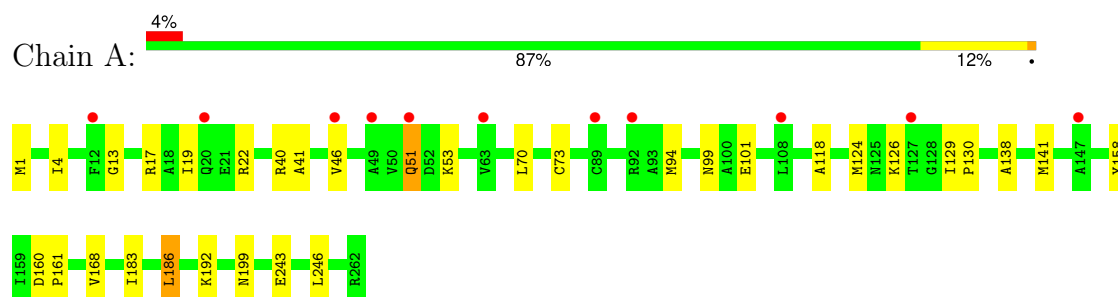
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	34	Total 34	O 34	0	0
8	C	39	Total 39	O 39	0	0
8	D	121	Total 121	O 121	0	0
8	E	63	Total 63	O 63	0	0
8	F	111	Total 111	O 111	0	0

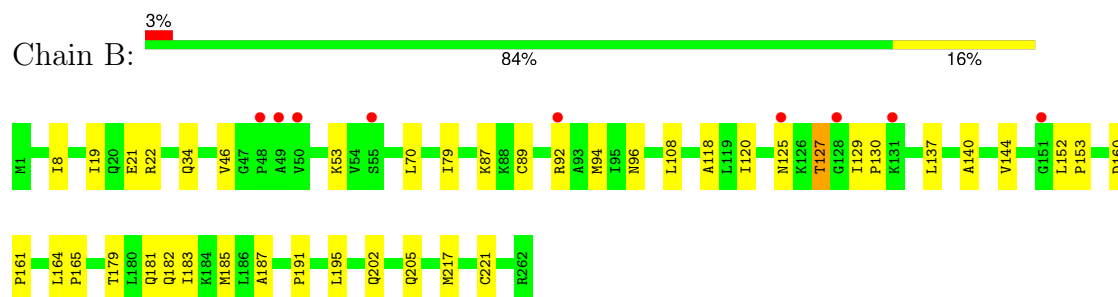
3 Residue-property plots

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

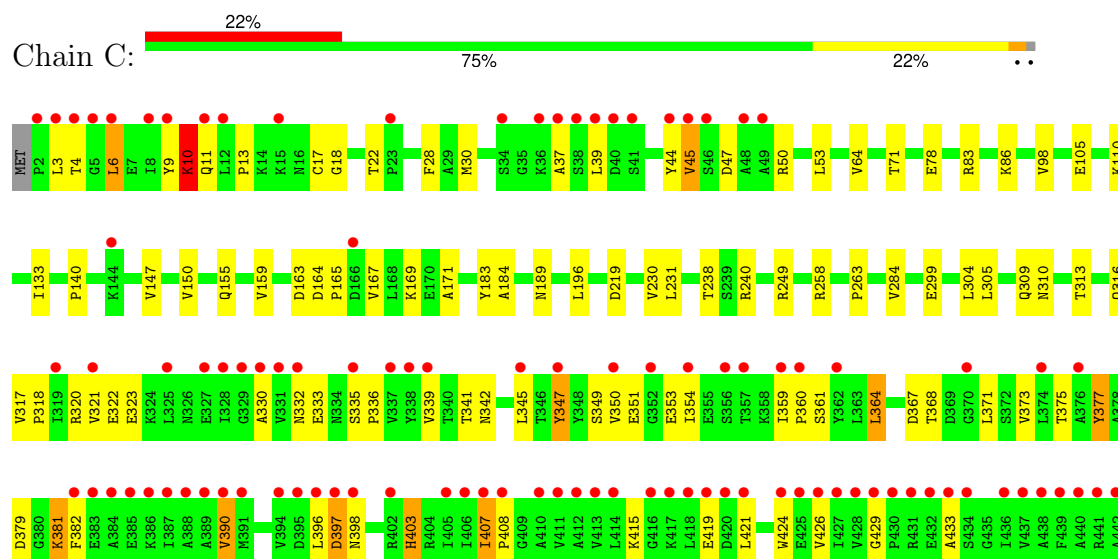
- Molecule 1: 5-methyltetrahydrofolate corrinoid/iron sulfur protein methyltransferase



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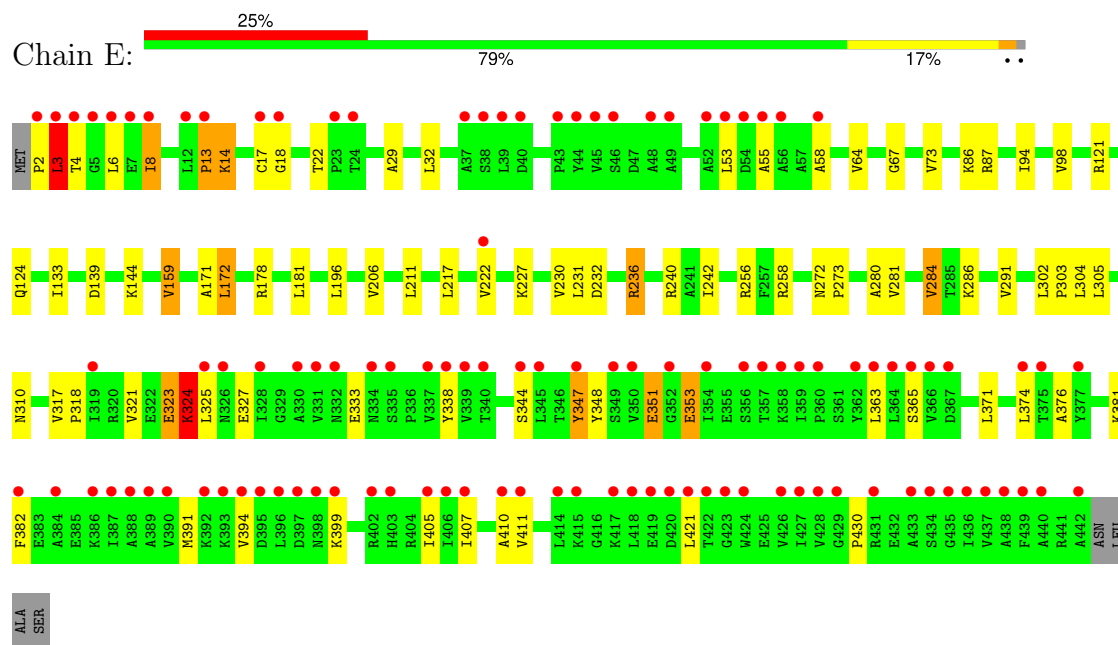


- Molecule 2: Corrinoid/iron-sulfur protein large subunit

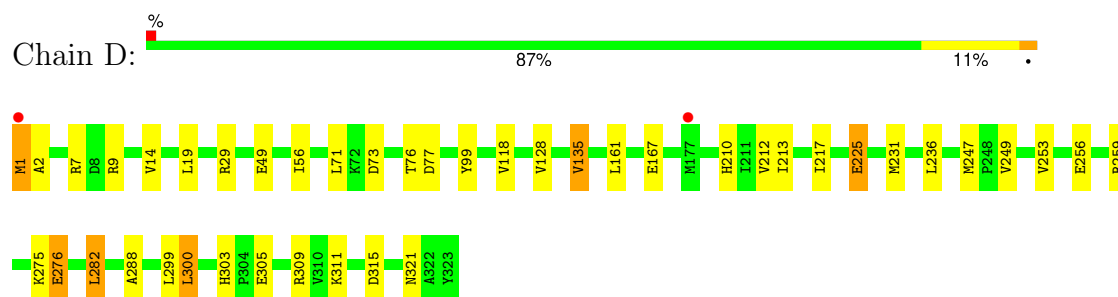


ASN
LEU
ALA
SER

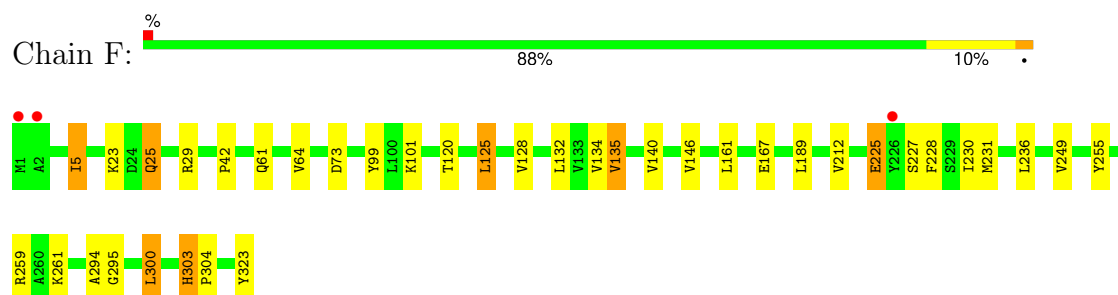
• Molecule 2: Corrinoide/iron-sulfur protein large subunit



• Molecule 3: Corrinoide/iron-sulfur protein small subunit



• Molecule 3: Corrinoide/iron-sulfur protein small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	125.61Å 242.84Å 79.67Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.83 – 2.38 39.83 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.83-2.38) 98.9 (39.83-2.38)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.37Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.187 , 0.229 0.189 , 0.230	Depositor DCC
R_{free} test set	4866 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	45.6	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	15832	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: CA, B12, GOL, SF4

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	0.34	0/2019	0.71	0/2734
1	B	0.33	0/2019	0.73	0/2734
2	C	0.33	0/3205	0.82	3/4383 (0.1%)
2	E	0.37	0/3157	0.80	2/4317 (0.0%)
3	D	0.38	0/2507	0.75	2/3408 (0.1%)
3	F	0.37	0/2520	0.73	2/3426 (0.1%)
All	All	0.35	0/15427	0.76	9/21002 (0.0%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	303	HIS	CA-C-N	5.74	125.42	119.05
3	D	303	HIS	C-N-CA	5.74	125.42	119.05
3	F	303	HIS	CA-C-N	5.67	125.34	119.05
3	F	303	HIS	C-N-CA	5.67	125.34	119.05
2	E	324	LYS	N-CA-C	-5.46	99.16	110.80
2	C	429	GLY	CA-C-N	5.43	125.38	119.78
2	C	429	GLY	C-N-CA	5.43	125.38	119.78
2	E	421	LEU	N-CA-C	5.11	116.93	111.36
2	C	403	HIS	CB-CA-C	-5.03	103.04	111.13

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	1993	0	2028	18	0
1	B	1993	0	2028	20	0
2	C	3149	0	2976	72	0
2	E	3105	0	2878	77	0
3	D	2461	0	2461	24	0
3	F	2470	0	2470	20	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	C	8	0	0	0	0
5	E	8	0	0	1	0
6	C	91	0	87	13	0
6	E	91	0	87	12	0
7	D	30	0	40	0	0
7	E	12	0	16	3	0
7	F	18	0	24	2	0
8	A	33	0	0	0	0
8	B	34	0	0	0	0
8	C	39	0	0	1	0
8	D	121	0	0	1	0
8	E	63	0	0	1	0
8	F	111	0	0	0	0
All	All	15832	0	15095	240	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 8.

All (240) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:324:LYS:HE3	2:E:324:LYS:HA	1.20	1.16
2:E:391:MET:SD	2:E:405:ILE:HD13	1.90	1.12
2:C:347:TYR:HD1	2:C:347:TYR:O	1.33	1.10
2:E:321:VAL:HG11	2:E:347:TYR:CD2	1.94	1.02
2:E:353:GLU:OE1	2:E:353:GLU:HA	1.59	0.99
2:E:321:VAL:HG11	2:E:347:TYR:CE2	1.97	0.99
2:C:347:TYR:HD1	2:C:347:TYR:C	1.74	0.95
2:C:347:TYR:C	2:C:347:TYR:CD1	2.42	0.92
2:E:391:MET:SD	2:E:405:ILE:CD1	2.57	0.92
2:E:324:LYS:HA	2:E:324:LYS:CE	1.94	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:415:LYS:CB	2:C:426:VAL:HG11	2.01	0.90
2:C:364:LEU:HD11	2:C:390:VAL:CG1	2.01	0.89
2:E:324:LYS:HE3	2:E:324:LYS:CA	2.03	0.89
2:C:347:TYR:O	2:C:347:TYR:CD1	2.25	0.89
2:E:347:TYR:C	2:E:347:TYR:HD1	1.79	0.88
2:E:347:TYR:HD1	2:E:347:TYR:O	1.57	0.88
2:E:347:TYR:C	2:E:347:TYR:CD1	2.50	0.86
2:E:347:TYR:HE1	2:E:351:GLU:CG	1.90	0.85
2:C:321:VAL:HG11	2:C:347:TYR:HE2	1.44	0.83
2:C:321:VAL:HG11	2:C:347:TYR:CE2	2.15	0.82
2:E:347:TYR:HE1	2:E:351:GLU:HG3	1.46	0.81
2:E:347:TYR:CE1	2:E:351:GLU:HG3	2.15	0.80
2:E:391:MET:CE	2:E:405:ILE:HD13	2.13	0.78
2:E:3:LEU:HD13	2:E:4:THR:H	1.47	0.78
2:E:353:GLU:OE1	2:E:353:GLU:CA	2.32	0.76
6:C:502:B12:H252	6:C:502:B12:H602	1.66	0.76
2:E:411:VAL:HG12	2:E:411:VAL:O	1.84	0.76
2:C:364:LEU:HD11	2:C:390:VAL:HG11	1.67	0.75
2:E:382:PHE:HE2	2:E:411:VAL:HG21	1.51	0.75
2:E:321:VAL:HG21	2:E:347:TYR:CD2	2.21	0.75
6:C:502:B12:H552	6:C:502:B12:H531	1.67	0.75
6:E:502:B12:H531	6:E:502:B12:H552	1.67	0.74
2:C:379:ASP:OD2	2:C:381:LYS:HE3	1.87	0.74
3:F:295:GLY:HA2	7:F:401:GOL:H32	1.70	0.74
6:E:502:B12:H252	6:E:502:B12:H602	1.70	0.73
2:E:323:GLU:O	2:E:324:LYS:HG2	1.88	0.72
2:E:8:ILE:HD13	2:E:32:LEU:HD12	1.70	0.72
2:E:211:LEU:H	7:E:503:GOL:H31	1.53	0.72
2:E:321:VAL:HG11	2:E:347:TYR:HD2	1.50	0.70
2:C:321:VAL:HG21	2:C:347:TYR:CD2	2.28	0.69
2:E:240:ARG:HD2	7:E:504:GOL:H31	1.73	0.68
2:C:415:LYS:CB	2:C:426:VAL:CG1	2.73	0.67
2:C:240:ARG:NH2	3:D:321:ASN:O	2.28	0.66
2:E:2:PRO:O	2:E:3:LEU:HB2	1.94	0.66
2:C:377:TYR:HD1	2:C:377:TYR:C	2.04	0.66
2:E:321:VAL:HG11	2:E:347:TYR:HE2	1.58	0.64
2:E:321:VAL:HG23	2:E:344:SER:HA	1.79	0.64
3:F:125:LEU:HD13	3:F:132:LEU:HD22	1.80	0.64
1:A:94:MET:HB3	1:A:118:ALA:HB3	1.80	0.63
2:C:377:TYR:C	2:C:377:TYR:CD1	2.77	0.63
2:E:2:PRO:O	2:E:3:LEU:CB	2.46	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:353:GLU:HG2	2:C:433:ALA:O	1.99	0.62
2:C:345:LEU:CD1	6:C:502:B12:H3P3	2.29	0.62
2:E:391:MET:CE	2:E:405:ILE:CD1	2.75	0.62
2:C:332:ASN:O	2:C:333:GLU:CB	2.49	0.61
2:E:310:ASN:HB3	3:F:225:GLU:HG3	1.82	0.61
2:E:310:ASN:O	3:F:225:GLU:HG2	2.00	0.61
2:C:98:VAL:HG23	2:C:110:LYS:HD3	1.83	0.61
2:C:147:VAL:HG11	2:C:171:ALA:HB1	1.83	0.60
3:D:56:ILE:HD12	3:D:311:LYS:HG2	1.83	0.60
2:C:415:LYS:O	2:C:419:GLU:N	2.26	0.60
2:E:121:ARG:NH2	8:E:624:HOH:O	2.30	0.60
2:E:324:LYS:CE	2:E:324:LYS:CA	2.68	0.60
2:E:325:LEU:HA	2:E:363:LEU:O	2.01	0.59
2:E:371:LEU:HB2	2:E:376:ALA:HB2	1.84	0.59
3:D:7:ARG:HD3	3:D:9:ARG:HH12	1.68	0.59
2:E:333:GLU:HG2	2:E:399:LYS:O	2.01	0.59
2:C:310:ASN:HB3	3:D:225:GLU:HG3	1.85	0.58
2:C:350:VAL:O	2:C:354:ILE:HG13	2.03	0.58
3:F:29:ARG:NH2	3:F:128:VAL:O	2.35	0.58
6:C:502:B12:H301	6:C:502:B12:H203	1.86	0.58
2:E:3:LEU:HD13	2:E:4:THR:N	2.16	0.58
2:C:163:ASP:O	2:C:189:ASN:ND2	2.35	0.58
3:D:99:TYR:HE1	3:D:135:VAL:HG13	1.69	0.57
1:B:152:LEU:HD12	1:B:153:PRO:HD2	1.85	0.57
6:E:502:B12:H301	6:E:502:B12:H203	1.86	0.57
6:C:502:B12:H3	6:C:502:B12:H291	1.70	0.57
1:A:101:GLU:HG3	1:A:126:LYS:HD3	1.86	0.57
6:E:502:B12:H291	6:E:502:B12:H3	1.70	0.57
2:C:169:LYS:HB3	2:C:196:LEU:HD11	1.86	0.57
2:C:336:PRO:O	2:C:361:SER:HB3	2.04	0.57
2:E:321:VAL:CG1	2:E:347:TYR:HD2	2.18	0.56
2:C:310:ASN:O	3:D:225:GLU:HG2	2.06	0.56
2:C:403:HIS:O	2:C:424:TRP:HB3	2.06	0.55
6:C:502:B12:H3	6:C:502:B12:N29	2.21	0.55
2:C:396:LEU:O	2:C:398:ASN:N	2.40	0.55
2:E:382:PHE:CE2	2:E:411:VAL:HG21	2.37	0.55
6:E:502:B12:H3	6:E:502:B12:N29	2.22	0.55
2:E:391:MET:SD	2:E:405:ILE:HD11	2.45	0.54
2:E:374:LEU:HD21	2:E:410:ALA:HB1	1.90	0.54
2:C:342:ASN:HB2	2:C:368:THR:H	1.73	0.54
2:E:321:VAL:CG1	2:E:347:TYR:CD2	2.81	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:347:TYR:HE1	2:E:351:GLU:HG2	1.68	0.53
1:A:19:ILE:O	1:A:22:ARG:NH1	2.41	0.53
2:E:8:ILE:HD11	2:E:29:ALA:HA	1.89	0.53
2:E:323:GLU:HA	2:E:365:SER:OG	2.09	0.53
2:E:17:CYS:N	5:E:501:SF4:S3	2.81	0.52
2:C:140:PRO:HB3	2:C:167:VAL:HG22	1.91	0.52
2:C:230:VAL:HG12	2:C:263:PRO:HG2	1.91	0.52
3:F:189:LEU:HD21	3:F:227:SER:HB3	1.91	0.52
2:C:39:LEU:HD23	2:C:39:LEU:H	1.74	0.52
3:F:231:MET:HE3	3:F:249:VAL:HG11	1.91	0.52
2:E:222:VAL:HG23	2:E:227:LYS:HG2	1.92	0.52
1:A:46:VAL:HG21	1:A:53:LYS:HD2	1.92	0.52
2:E:430:PRO:HD2	6:E:502:B12:C6M	2.40	0.51
2:E:411:VAL:O	2:E:411:VAL:CG1	2.54	0.51
2:E:280:ALA:O	2:E:284:VAL:HG13	2.10	0.51
2:C:28:PHE:HE1	2:C:37:ALA:HB3	1.76	0.51
3:F:42:PRO:HB3	7:F:401:GOL:H31	1.93	0.51
2:C:78:GLU:HG2	2:C:249:ARG:NH2	2.27	0.50
3:F:29:ARG:HD2	3:F:29:ARG:N	2.26	0.50
2:C:321:VAL:HG12	2:C:322:GLU:N	2.26	0.50
6:C:502:B12:H531	6:C:502:B12:C55	2.41	0.50
2:E:323:GLU:O	2:E:324:LYS:CG	2.58	0.50
2:C:407:ILE:HD12	2:C:426:VAL:HG11	1.92	0.49
2:E:144:LYS:HD3	2:E:171:ALA:HA	1.94	0.49
2:C:321:VAL:HG21	2:C:347:TYR:HD2	1.77	0.49
2:C:335:SER:HB2	2:C:361:SER:HA	1.95	0.49
2:C:364:LEU:CD1	2:C:390:VAL:HG11	2.41	0.49
2:C:345:LEU:HD12	6:C:502:B12:H3P3	1.93	0.49
3:F:101:LYS:HD2	3:F:135:VAL:HG22	1.95	0.48
1:A:138:ALA:HA	2:C:30:MET:HE1	1.95	0.48
2:C:318:PRO:HD2	2:C:320:ARG:NH1	2.28	0.48
6:C:502:B12:H362	6:C:502:B12:H351	1.95	0.48
2:E:321:VAL:HG21	2:E:347:TYR:HD2	1.75	0.48
2:C:396:LEU:O	2:C:397:ASP:C	2.57	0.48
1:A:158:TYR:CZ	1:A:192:LYS:HD3	2.49	0.48
2:C:321:VAL:HG12	2:C:322:GLU:H	1.79	0.48
2:E:18:GLY:HA2	2:E:22:THR:O	2.14	0.48
3:F:99:TYR:CD2	3:F:300:LEU:HG	2.49	0.48
2:E:55:ALA:HB2	2:E:258:ARG:HD3	1.96	0.48
2:E:348:TYR:HA	2:E:351:GLU:HB2	1.94	0.48
2:C:309:GLN:O	2:C:313:THR:HG23	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:347:TYR:CE1	2:E:351:GLU:CG	2.78	0.47
3:F:255:TYR:O	3:F:259:ARG:HG3	2.15	0.47
2:C:407:ILE:HG23	2:C:408:PRO:HD2	1.96	0.47
6:E:502:B12:H351	6:E:502:B12:H362	1.95	0.47
2:C:323:GLU:CD	2:C:367:ASP:HB2	2.39	0.47
2:C:9:TYR:C	2:C:11:GLN:H	2.22	0.47
3:D:73:ASP:HA	3:D:76:THR:HG23	1.96	0.47
3:D:77:ASP:OD1	3:D:77:ASP:N	2.46	0.47
3:D:213:ILE:HG13	3:D:247:MET:HB2	1.96	0.47
1:B:187:ALA:HB3	1:B:191:PRO:HD3	1.97	0.46
6:C:502:B12:H351	6:C:502:B12:C36	2.45	0.46
1:A:73:CYS:HA	1:A:94:MET:HG3	1.98	0.46
2:C:371:LEU:HD13	2:C:375:THR:HG22	1.97	0.46
1:B:137:LEU:HD12	1:B:179:THR:HG23	1.97	0.46
3:D:210:HIS:HD2	8:D:547:HOH:O	1.98	0.46
1:B:19:ILE:O	1:B:22:ARG:NH1	2.49	0.46
3:D:29:ARG:NH2	3:D:128:VAL:O	2.46	0.45
1:B:161:PRO:HD2	1:B:195:LEU:HD23	1.99	0.45
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.83	0.45
2:C:341:THR:HG21	2:C:373:VAL:HA	1.98	0.45
2:E:159:VAL:HB	2:E:181:LEU:HB3	1.99	0.45
6:E:502:B12:H351	6:E:502:B12:C36	2.45	0.45
1:B:8:ILE:HG13	1:B:34:GLN:HE22	1.82	0.45
2:C:133:ILE:HD11	2:C:150:VAL:HG11	1.98	0.45
2:C:330:ALA:N	2:C:360:PRO:HB3	2.31	0.45
3:D:276:GLU:H	3:D:276:GLU:CD	2.24	0.45
1:B:182:GLN:HA	1:B:185:MET:HE2	1.99	0.45
2:E:321:VAL:CB	2:E:347:TYR:HD2	2.29	0.45
3:D:1:MET:SD	3:D:1:MET:N	2.83	0.45
2:E:242:ILE:HG23	2:E:286:LYS:HG3	1.98	0.45
3:F:99:TYR:HE1	3:F:135:VAL:HG13	1.81	0.45
3:D:256:GLU:O	3:D:259:ARG:HG2	2.17	0.45
1:A:13:GLY:O	1:A:17:ARG:HD3	2.17	0.44
2:E:232:ASP:OD1	2:E:236:ARG:NH2	2.50	0.44
3:D:99:TYR:CD2	3:D:300:LEU:HG	2.53	0.44
1:B:46:VAL:HG21	1:B:53:LYS:HG3	1.99	0.44
1:A:168:VAL:HG21	6:E:502:B12:H401	1.81	0.44
2:C:364:LEU:HD11	2:C:390:VAL:HG13	1.91	0.44
2:C:299:GLU:CD	2:C:299:GLU:H	2.26	0.43
2:E:324:LYS:NZ	2:E:394:VAL:HA	2.33	0.43
2:E:338:TYR:HB3	6:E:502:B12:HM52	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:299:GLU:HG3	3:D:275:LYS:N	2.33	0.43
2:C:396:LEU:C	2:C:398:ASN:N	2.76	0.43
2:E:240:ARG:HH11	7:E:504:GOL:H31	1.84	0.43
6:E:502:B12:H533	6:E:502:B12:H491	2.00	0.43
2:C:219:ASP:OD2	3:D:1:MET:N	2.44	0.43
2:E:317:VAL:HA	2:E:318:PRO:HD3	1.88	0.43
3:F:228:PHE:CD1	3:F:294:ALA:HB2	2.53	0.43
2:C:45:VAL:O	2:C:50:ARG:NH2	2.52	0.43
2:C:6:LEU:O	2:C:10:LYS:HG2	2.19	0.43
2:E:371:LEU:HD12	2:E:381:LYS:NZ	2.33	0.43
1:B:140:ALA:O	1:B:144:VAL:HG23	2.19	0.43
2:C:354:ILE:HG22	2:C:359:ILE:O	2.19	0.43
6:C:502:B12:H533	6:C:502:B12:H491	2.00	0.43
2:C:18:GLY:HA2	2:C:22:THR:O	2.19	0.43
2:C:164:ASP:HA	2:C:165:PRO:HD3	1.91	0.43
2:E:272:ASN:HA	2:E:273:PRO:HD3	1.92	0.43
2:C:13:PRO:HG2	2:C:44:TYR:HB2	2.01	0.42
2:E:67:GLY:HA2	2:E:178:ARG:O	2.18	0.42
2:E:172:LEU:HD12	2:E:172:LEU:HA	1.89	0.42
3:F:25:GLN:HE21	3:F:25:GLN:HB3	1.62	0.42
1:A:40:ARG:HA	1:A:70:LEU:HD22	2.01	0.42
3:D:1:MET:HB2	3:D:2:ALA:H	1.68	0.42
1:A:4:ILE:HG12	1:A:41:ALA:HB3	2.01	0.42
1:A:51:GLN:H	1:A:51:GLN:CD	2.28	0.42
2:C:6:LEU:HD22	2:C:10:LYS:HE2	2.01	0.42
1:A:1:MET:N	1:A:243:GLU:OE2	2.48	0.42
1:A:246:LEU:HG	1:B:217:MET:HE1	2.02	0.42
1:B:92:ARG:HD2	1:B:92:ARG:HA	1.91	0.42
2:C:78:GLU:HG3	8:C:625:HOH:O	2.19	0.42
2:E:58:ALA:O	2:E:256:ARG:NH1	2.48	0.42
1:B:165:PRO:HG3	1:B:202:GLN:HB3	2.02	0.42
2:E:391:MET:HE1	2:E:405:ILE:HD13	1.98	0.42
6:E:502:B12:H353	6:E:502:B12:H302	2.02	0.42
3:F:61:GLN:HG2	3:F:101:LYS:HB3	2.02	0.42
2:C:258:ARG:HD3	2:C:258:ARG:HA	1.77	0.42
2:E:391:MET:HE2	2:E:391:MET:HB2	1.97	0.42
1:B:94:MET:HG3	1:B:118:ALA:HB3	2.01	0.42
3:D:305:GLU:OE2	3:D:309:ARG:NH1	2.42	0.42
1:A:99:ASN:HB2	1:A:124:MET:O	2.20	0.41
1:A:160:ASP:HA	1:A:161:PRO:HD3	1.83	0.41
1:B:160:ASP:HA	1:B:161:PRO:HD3	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:421:LEU:HD23	2:C:421:LEU:O	2.20	0.41
1:B:125:ASN:HB3	1:B:127:THR:HG23	2.03	0.41
1:B:181:GLN:HG3	1:B:221:CYS:HB3	2.01	0.41
6:C:502:B12:H302	6:C:502:B12:H353	2.02	0.41
3:D:288:ALA:HB1	3:D:299:LEU:HD13	2.02	0.41
2:E:2:PRO:HB2	2:E:3:LEU:H	1.61	0.41
2:E:13:PRO:HB2	2:E:14:LYS:H	1.61	0.41
3:F:189:LEU:HD22	3:F:230:ILE:HD12	2.02	0.41
1:B:79:ILE:HD12	1:B:108:LEU:HD21	2.02	0.41
3:D:7:ARG:HD3	3:D:9:ARG:NH1	2.35	0.41
1:A:183:ILE:HA	1:A:186:LEU:HD22	2.01	0.41
3:D:282:LEU:HD12	3:D:282:LEU:HA	1.91	0.41
3:F:5:ILE:HD13	3:F:323:TYR:CD2	2.56	0.41
1:A:129:ILE:HA	1:A:130:PRO:HD3	1.96	0.41
1:B:96:ASN:HB2	1:B:120:ILE:HD12	2.03	0.41
3:D:231:MET:HE3	3:D:249:VAL:HG11	2.02	0.41
2:E:302:LEU:HB3	2:E:303:PRO:HD3	2.03	0.41
3:D:71:LEU:HD12	3:D:71:LEU:HA	1.88	0.40
1:B:129:ILE:HA	1:B:130:PRO:HD3	1.94	0.40
2:C:345:LEU:HD13	6:C:502:B12:H3P3	2.03	0.40
3:F:303:HIS:HA	3:F:304:PRO:HD3	1.82	0.40
2:C:183:TYR:HA	2:C:184:ALA:HA	1.76	0.40
2:C:377:TYR:HD1	2:C:377:TYR:O	2.03	0.40
1:B:129:ILE:HD13	1:B:164:LEU:HD21	2.02	0.40
2:E:310:ASN:HB3	3:F:225:GLU:CG	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/262 (99%)	250 (96%)	10 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
2	C	439/446 (98%)	421 (96%)	14 (3%)	4 (1%)	14	20
2	E	439/446 (98%)	421 (96%)	13 (3%)	5 (1%)	11	16
3	D	321/323 (99%)	314 (98%)	7 (2%)	0	100	100
3	F	322/323 (100%)	312 (97%)	10 (3%)	0	100	100
All	All	2041/2062 (99%)	1969 (96%)	63 (3%)	9 (0%)	30	40

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	13	PRO
2	E	14	LYS
2	E	324	LYS
2	C	45	VAL
2	C	397	ASP
2	E	3	LEU
2	C	10	LYS
2	C	86	LYS
2	E	86	LYS

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	213/214 (100%)	209 (98%)	4 (2%)	50	69
1	B	213/214 (100%)	206 (97%)	7 (3%)	33	52
2	C	290/356 (82%)	261 (90%)	29 (10%)	7	10
2	E	278/356 (78%)	246 (88%)	32 (12%)	5	7
3	D	261/261 (100%)	244 (94%)	17 (6%)	15	24
3	F	262/261 (100%)	244 (93%)	18 (7%)	14	22
All	All	1517/1662 (91%)	1410 (93%)	107 (7%)	13	21

All (107) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	141	MET
1	A	186	LEU
1	A	199	ASN
1	B	21	GLU
1	B	70	LEU
1	B	87	LYS
1	B	89	CYS
1	B	127	THR
1	B	183	ILE
1	B	205	GLN
2	C	3	LEU
2	C	4	THR
2	C	6	LEU
2	C	10	LYS
2	C	17	CYS
2	C	47	ASP
2	C	53	LEU
2	C	64	VAL
2	C	71	THR
2	C	83	ARG
2	C	105	GLU
2	C	155	GLN
2	C	159	VAL
2	C	231	LEU
2	C	238	THR
2	C	284	VAL
2	C	304	LEU
2	C	305	LEU
2	C	316	GLN
2	C	339	VAL
2	C	347	TYR
2	C	349	SER
2	C	351	GLU
2	C	364	LEU
2	C	377	TYR
2	C	381	LYS
2	C	382	PHE
2	C	390	VAL
2	C	407	ILE
3	D	1	MET
3	D	14	VAL

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Mol	Chain	Res	Type
3	D	19	LEU
3	D	49	GLU
3	D	118	VAL
3	D	135	VAL
3	D	161	LEU
3	D	167	GLU
3	D	212	VAL
3	D	217	ILE
3	D	225	GLU
3	D	236	LEU
3	D	253	VAL
3	D	276	GLU
3	D	282	LEU
3	D	300	LEU
3	D	315	ASP
2	E	3	LEU
2	E	6	LEU
2	E	8	ILE
2	E	53	LEU
2	E	64	VAL
2	E	73	VAL
2	E	87	ARG
2	E	94	ILE
2	E	98	VAL
2	E	124	GLN
2	E	133	ILE
2	E	139	ASP
2	E	159	VAL
2	E	172	LEU
2	E	196	LEU
2	E	206	VAL
2	E	217	LEU
2	E	230	VAL
2	E	231	LEU
2	E	236	ARG
2	E	281	VAL
2	E	284	VAL
2	E	291	VAL
2	E	304	LEU
2	E	305	LEU
2	E	323	GLU
2	E	324	LYS

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Mol	Chain	Res	Type
2	E	327	GLU
2	E	347	TYR
2	E	351	GLU
2	E	353	GLU
2	E	407	ILE
3	F	5	ILE
3	F	23	LYS
3	F	25	GLN
3	F	64	VAL
3	F	73	ASP
3	F	120	THR
3	F	125	LEU
3	F	134	VAL
3	F	135	VAL
3	F	140	VAL
3	F	146	VAL
3	F	161	LEU
3	F	167	GLU
3	F	212	VAL
3	F	225	GLU
3	F	236	LEU
3	F	261	LYS
3	F	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	A	206	ASN
1	A	211	ASN
1	B	20	GLN
1	B	182	GLN
1	B	206	ASN
2	C	84	HIS
2	C	155	GLN
2	C	282	ASN
3	D	52	ASN
3	D	163	ASN
3	D	166	GLN
2	E	228	GLN
3	F	25	GLN
3	F	179	HIS

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Mol	Chain	Res	Type
3	F	293	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 2 are monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	GOL	D	401	-	5,5,5	0.42	0	5,5,5	0.34	0
7	GOL	E	504	-	5,5,5	0.37	0	5,5,5	0.21	0
7	GOL	E	503	-	5,5,5	0.39	0	5,5,5	0.19	0
7	GOL	D	403	-	5,5,5	0.37	0	5,5,5	0.19	0
7	GOL	F	401	-	5,5,5	0.42	0	5,5,5	0.29	0
6	B12	C	502	-	94,101,101	1.51	14 (14%)	149,166,166	2.10	40 (26%)
7	GOL	D	405	-	5,5,5	0.36	0	5,5,5	0.24	0
5	SF4	C	501	2	0,12,12	-	-	-	-	-
7	GOL	D	404	-	5,5,5	0.41	0	5,5,5	0.27	0
7	GOL	D	402	-	5,5,5	0.37	0	5,5,5	0.34	0
7	GOL	F	402	-	5,5,5	0.34	0	5,5,5	0.39	0
6	B12	E	502	-	94,101,101	1.50	15 (15%)	149,166,166	2.11	40 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	SF4	E	501	2	0,12,12	-	-	-		
7	GOL	F	403	-	5,5,5	0.37	0	5,5,5	0.31	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
7	GOL	D	401	-	-	2/4/4/4	-
7	GOL	E	504	-	-	2/4/4/4	-
7	GOL	F	401	-	-	4/4/4/4	-
7	GOL	D	403	-	-	3/4/4/4	-
5	SF4	E	501	2	-	-	0/6/5/5
6	B12	C	502	-	-	12/56/223/223	0/3/11/11
7	GOL	D	405	-	-	2/4/4/4	-
5	SF4	C	501	2	-	-	0/6/5/5
7	GOL	D	404	-	-	4/4/4/4	-
7	GOL	D	402	-	-	4/4/4/4	-
7	GOL	F	402	-	-	4/4/4/4	-
6	B12	E	502	-	-	12/56/223/223	0/3/11/11
7	GOL	E	503	-	-	4/4/4/4	-
7	GOL	F	403	-	-	2/4/4/4	-

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	502	B12	C7B-C6B	4.66	1.46	1.39
6	E	502	B12	C7B-C6B	4.66	1.46	1.39
6	C	502	B12	C41-C8	4.24	1.64	1.54
6	E	502	B12	C41-C8	4.22	1.64	1.54
6	C	502	B12	C14-N23	4.04	1.40	1.35
6	E	502	B12	C14-N23	3.91	1.40	1.35
6	C	502	B12	C6B-C5B	3.70	1.49	1.40
6	E	502	B12	C6B-C5B	3.50	1.49	1.40
6	E	502	B12	C55-C56	3.02	1.59	1.53
6	C	502	B12	C55-C56	2.97	1.59	1.53
6	C	502	B12	C1P-C2P	2.87	1.58	1.51
6	E	502	B12	C1P-C2P	2.66	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	502	B12	C35-C5	2.63	1.56	1.50
6	E	502	B12	C54-C17	2.54	1.58	1.54
6	E	502	B12	C60-C18	-2.54	1.48	1.54
6	C	502	B12	O58-C57	2.52	1.28	1.23
6	C	502	B12	C54-C17	2.51	1.58	1.54
6	E	502	B12	C35-C5	2.51	1.55	1.50
6	C	502	B12	C60-C18	-2.45	1.48	1.54
6	E	502	B12	O58-C57	2.42	1.28	1.23
6	E	502	B12	C11-N23	2.31	1.41	1.36
6	C	502	B12	C25-C2	-2.19	1.50	1.54
6	E	502	B12	C25-C2	-2.15	1.50	1.54
6	E	502	B12	C1P-N59	2.09	1.52	1.46
6	C	502	B12	C11-N23	2.09	1.40	1.36
6	C	502	B12	C3P-C2P	-2.07	1.43	1.51
6	E	502	B12	C3P-C2P	-2.04	1.43	1.51
6	C	502	B12	C8B-C9B	2.02	1.43	1.40
6	E	502	B12	C3-C4	2.01	1.56	1.51

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	502	B12	O2-P-O3	8.26	125.93	102.87
6	C	502	B12	O2-P-O3	8.21	125.81	102.87
6	E	502	B12	C18-C60-C61	7.56	133.26	114.04
6	C	502	B12	C18-C60-C61	7.46	133.00	114.04
6	E	502	B12	O2-P-O4	-5.70	91.58	109.81
6	C	502	B12	O2-P-O4	-5.67	91.69	109.81
6	E	502	B12	C20-C1-N21	-5.64	100.94	110.26
6	C	502	B12	C20-C1-N21	-5.57	101.05	110.26
6	C	502	B12	O7R-C2R-C3R	5.36	126.20	111.19
6	E	502	B12	O7R-C2R-C3R	5.36	126.19	111.19
6	E	502	B12	C60-C61-N62	5.08	128.36	116.19
6	C	502	B12	C60-C61-N62	5.07	128.34	116.19
6	C	502	B12	C60-C18-C17	4.80	128.97	115.82
6	E	502	B12	C60-C18-C17	4.73	128.77	115.82
6	E	502	B12	C48-C13-C12	-4.52	103.59	116.52
6	C	502	B12	C48-C13-C12	-4.48	103.72	116.52
6	E	502	B12	C3R-C2R-C1R	4.07	108.84	99.89
6	C	502	B12	C3R-C2R-C1R	4.07	108.84	99.89
6	E	502	B12	C41-C8-C9	-3.83	104.50	111.19
6	C	502	B12	C41-C8-C9	-3.77	104.61	111.19
6	E	502	B12	C20-C1-C19	-3.59	105.90	109.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	502	B12	C55-C17-C18	-3.56	104.31	111.12
6	C	502	B12	C55-C17-C18	-3.54	104.36	111.12
6	C	502	B12	C20-C1-C19	-3.45	106.03	109.35
6	C	502	B12	C9-N22-C6	3.32	109.27	105.28
6	C	502	B12	O63-C61-C60	-3.32	113.94	120.87
6	E	502	B12	C9-N22-C6	3.31	109.27	105.28
6	E	502	B12	O6R-C1R-N1B	-3.27	101.80	108.09
6	E	502	B12	O63-C61-C60	-3.27	114.04	120.87
6	C	502	B12	C2R-C1R-N1B	3.19	121.23	113.30
6	C	502	B12	O6R-C1R-N1B	-3.19	101.96	108.09
6	E	502	B12	C2R-C1R-N1B	3.18	121.21	113.30
6	E	502	B12	C2-C1-C19	3.18	123.56	118.61
6	C	502	B12	C2-C1-C19	3.14	123.50	118.61
6	E	502	B12	O58-C57-C56	-3.09	116.42	122.02
6	C	502	B12	O58-C57-C56	-3.08	116.43	122.02
6	C	502	B12	C47-C12-C46	-3.02	104.41	109.41
6	E	502	B12	C47-C12-C46	-2.93	104.55	109.41
6	C	502	B12	O8R-C5R-C4R	2.88	121.13	111.33
6	E	502	B12	O8R-C5R-C4R	2.87	121.12	111.33
6	E	502	B12	O58-C57-N59	2.80	128.52	123.03
6	C	502	B12	C7-C8-C9	2.78	104.41	100.89
6	C	502	B12	O58-C57-N59	2.77	128.46	123.03
6	E	502	B12	C47-C12-C13	2.73	123.81	112.74
6	E	502	B12	O6R-C4R-C3R	2.72	110.65	104.92
6	E	502	B12	C37-C7-C8	-2.70	101.23	108.37
6	C	502	B12	O6R-C4R-C3R	2.70	110.61	104.92
6	C	502	B12	C47-C12-C13	2.67	123.56	112.74
6	C	502	B12	C37-C7-C8	-2.67	101.33	108.37
6	E	502	B12	C7-C8-C9	2.63	104.23	100.89
6	E	502	B12	C8-C9-C10	-2.63	117.74	123.33
6	E	502	B12	C46-C12-C11	-2.55	100.95	110.08
6	C	502	B12	C8-C9-C10	-2.54	117.91	123.33
6	E	502	B12	C19-C1-N21	2.53	104.75	102.14
6	C	502	B12	C1-C2-C3	-2.53	98.41	101.60
6	E	502	B12	C2P-C1P-N59	2.53	116.64	112.92
6	E	502	B12	C1-C2-C3	-2.50	98.46	101.60
6	C	502	B12	C2P-C1P-N59	2.49	116.58	112.92
6	C	502	B12	C46-C12-C11	-2.48	101.21	110.08
6	C	502	B12	C49-C48-C13	2.45	121.60	114.65
6	C	502	B12	C25-C2-C1	-2.45	110.09	113.75
6	C	502	B12	O6R-C1R-C2R	-2.45	101.38	106.62
6	C	502	B12	C19-C1-N21	2.43	104.65	102.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	502	B12	O6R-C1R-C2R	-2.41	101.45	106.62
6	E	502	B12	C25-C2-C1	-2.41	110.15	113.75
6	E	502	B12	C49-C48-C13	2.41	121.48	114.65
6	E	502	B12	C12-C13-C14	2.32	106.07	102.26
6	C	502	B12	C25-C2-C3	2.17	118.44	112.91
6	C	502	B12	C12-C13-C14	2.15	105.80	102.26
6	E	502	B12	C25-C2-C3	2.15	118.37	112.91
6	E	502	B12	P-O3-C2P	2.13	128.39	121.10
6	C	502	B12	P-O3-C2P	2.12	128.35	121.10
6	E	502	B12	C26-C2-C1	2.12	113.28	110.00
6	C	502	B12	C54-C17-C18	2.11	116.02	112.99
6	C	502	B12	C26-C2-C1	2.09	113.23	110.00
6	E	502	B12	C10-C9-N22	2.03	128.06	125.74
6	C	502	B12	C47-C12-C11	2.03	117.33	110.08
6	C	502	B12	C1P-N59-C57	2.03	127.05	122.69
6	E	502	B12	C47-C12-C11	2.02	117.28	110.08
6	E	502	B12	C54-C17-C18	2.01	115.87	112.99

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	502	B12	C17-C18-C60-C61
6	C	502	B12	C1P-C2P-O3-P
6	C	502	B12	C3P-C2P-O3-P
6	E	502	B12	C17-C18-C60-C61
6	E	502	B12	C1P-C2P-O3-P
6	E	502	B12	C3P-C2P-O3-P
7	D	401	GOL	O1-C1-C2-O2
7	D	401	GOL	O1-C1-C2-C3
7	D	402	GOL	O1-C1-C2-C3
7	D	404	GOL	C1-C2-C3-O3
7	E	503	GOL	O1-C1-C2-C3
7	E	504	GOL	O1-C1-C2-C3
7	F	401	GOL	O1-C1-C2-C3
7	F	402	GOL	O1-C1-C2-C3
7	D	404	GOL	O2-C2-C3-O3
7	D	405	GOL	O1-C1-C2-O2
7	D	403	GOL	O1-C1-C2-C3
7	D	404	GOL	O1-C1-C2-C3
7	D	405	GOL	O1-C1-C2-C3
7	E	503	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
7	F	401	GOL	C1-C2-C3-O3
7	F	402	GOL	C1-C2-C3-O3
7	F	403	GOL	O1-C1-C2-C3
6	C	502	B12	O6R-C1R-N1B-C8B
6	E	502	B12	O6R-C1R-N1B-C8B
7	E	503	GOL	O1-C1-C2-O2
7	E	504	GOL	O1-C1-C2-O2
7	F	401	GOL	O1-C1-C2-O2
7	F	401	GOL	O2-C2-C3-O3
7	F	402	GOL	O1-C1-C2-O2
7	F	402	GOL	O2-C2-C3-O3
7	D	402	GOL	O1-C1-C2-O2
7	F	403	GOL	O1-C1-C2-O2
6	C	502	B12	C41-C42-C43-O44
6	E	502	B12	C41-C42-C43-O44
6	C	502	B12	C41-C42-C43-N45
6	E	502	B12	C41-C42-C43-N45
7	D	402	GOL	O2-C2-C3-O3
7	D	402	GOL	C1-C2-C3-O3
6	C	502	B12	C3-C30-C31-C32
6	E	502	B12	C3-C30-C31-C32
6	E	502	B12	C18-C60-C61-O63
6	E	502	B12	C18-C60-C61-N62
7	D	404	GOL	O1-C1-C2-O2
6	C	502	B12	C2R-C1R-N1B-C8B
6	E	502	B12	C2R-C1R-N1B-C8B
6	C	502	B12	C2R-C1R-N1B-C2B
6	E	502	B12	C2R-C1R-N1B-C2B
7	E	503	GOL	O2-C2-C3-O3
6	C	502	B12	C18-C60-C61-N62
7	D	403	GOL	C1-C2-C3-O3
6	E	502	B12	C19-C18-C60-C61
7	D	403	GOL	O1-C1-C2-O2
6	C	502	B12	C18-C60-C61-O63
6	C	502	B12	C19-C18-C60-C61

There are no ring outliers.

6 monomers are involved in 31 short contacts:

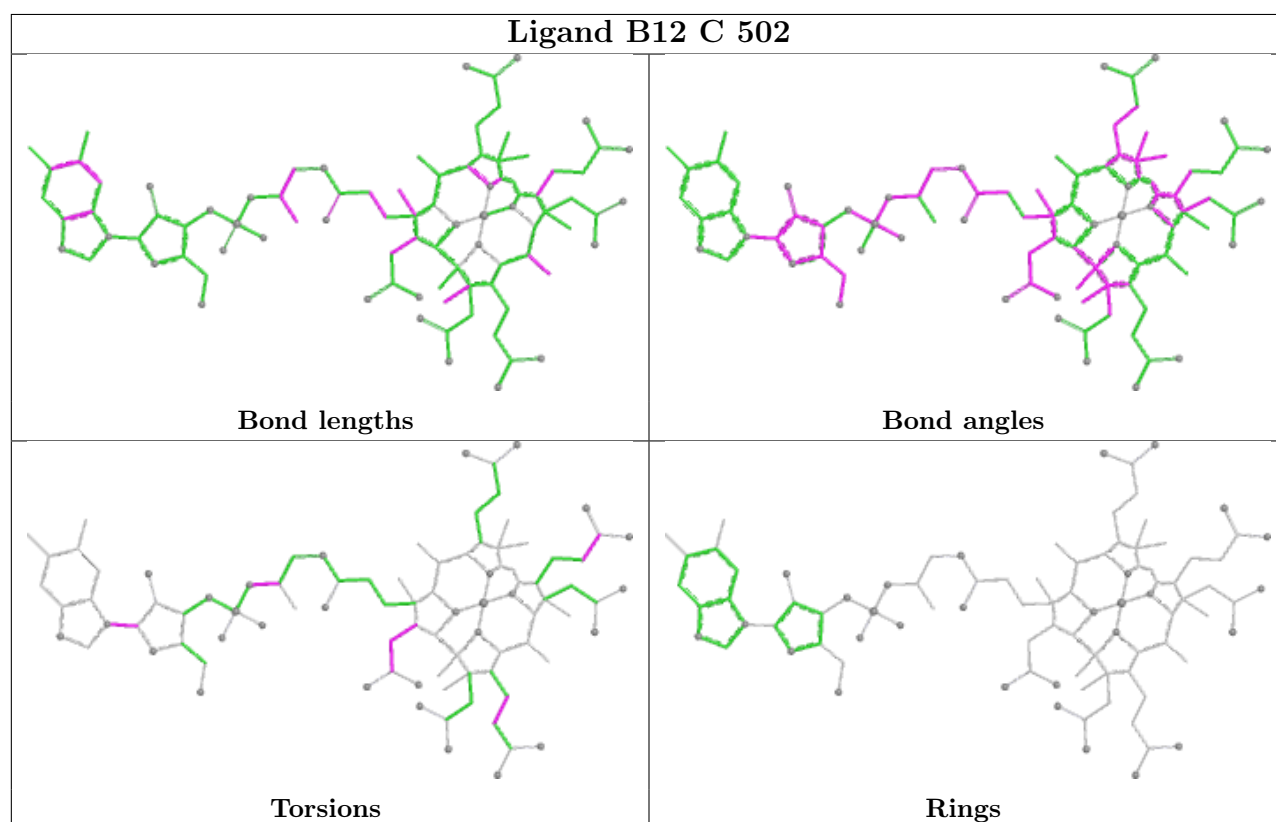
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	E	504	GOL	2	0
7	E	503	GOL	1	0

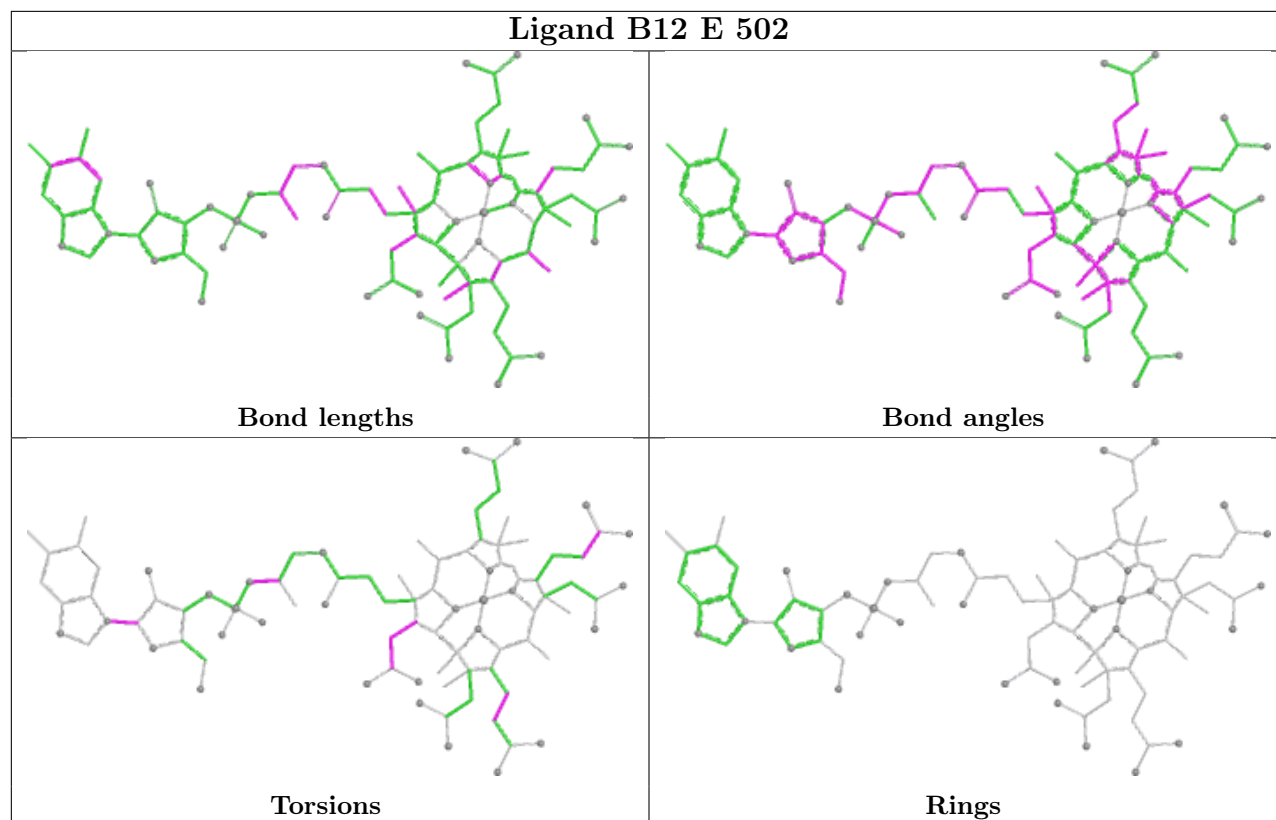
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	401	GOL	2	0
6	C	502	B12	13	0
6	E	502	B12	12	0
5	E	501	SF4	1	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	262/262 (100%)	0.31	11 (4%) 40 40	33, 68, 118, 165	0
1	B	262/262 (100%)	0.31	9 (3%) 48 48	35, 71, 115, 146	0
2	C	441/446 (98%)	1.10	100 (22%) 2 2	36, 87, 193, 226	3 (0%)
2	E	441/446 (98%)	0.85	110 (24%) 2 1	32, 59, 201, 248	3 (0%)
3	D	323/323 (100%)	-0.40	2 (0%) 85 85	27, 38, 66, 119	0
3	F	323/323 (100%)	-0.31	3 (0%) 81 80	27, 43, 68, 112	1 (0%)
All	All	2052/2062 (99%)	0.39	235 (11%) 9 8	27, 56, 176, 248	7 (0%)

All (235) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	414	LEU	5.8
2	C	412	ALA	5.7
2	E	362	TYR	5.6
2	E	354	ILE	5.6
2	C	427	ILE	5.4
2	E	39	LEU	5.4
2	E	382	PHE	5.2
2	E	442	ALA	5.1
2	C	428	VAL	5.0
2	E	5	GLY	4.9
2	C	410	ALA	4.9
2	E	350	VAL	4.8
2	E	439	PHE	4.7
2	C	390	VAL	4.6
2	C	362	TYR	4.5
2	C	39	LEU	4.5
2	E	394	VAL	4.5
2	C	406	ILE	4.4
2	C	331	VAL	4.3

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Mol	Chain	Res	Type	RSRZ
2	C	411	VAL	4.3
2	C	437	VAL	4.2
2	E	326	ASN	4.2
2	E	45	VAL	4.2
2	E	4	THR	4.2
2	E	332	ASN	4.2
2	E	434	SER	4.2
2	E	53	LEU	4.2
2	C	350	VAL	4.1
2	E	437	VAL	4.1
2	C	2	PRO	4.0
2	C	37	ALA	4.0
2	C	396	LEU	4.0
2	E	357	THR	4.0
2	C	439	PHE	4.0
2	C	332	ASN	4.0
2	E	52	ALA	3.9
2	C	385	GLU	3.9
2	C	359	ILE	3.8
2	C	45	VAL	3.8
2	C	405	ILE	3.8
2	E	396	LEU	3.8
2	C	357	THR	3.8
2	E	340	THR	3.8
2	C	388	ALA	3.7
2	C	440	ALA	3.7
2	E	56	ALA	3.7
2	C	38	SER	3.7
2	E	44	TYR	3.6
2	C	426	VAL	3.6
2	C	433	ALA	3.6
2	E	8	ILE	3.5
2	E	403	HIS	3.5
2	C	383	GLU	3.5
2	C	360	PRO	3.5
3	D	1	MET	3.5
2	E	46	SER	3.5
2	C	328	ILE	3.5
2	E	397	ASP	3.5
2	E	414	LEU	3.5
2	C	356	SER	3.4
2	E	330	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
2	E	410	ALA	3.4
2	E	424	TRP	3.4
2	C	389	ALA	3.4
2	C	5	GLY	3.4
2	C	354	ILE	3.4
2	E	421	LEU	3.4
2	E	347	TYR	3.4
2	C	413	VAL	3.4
2	C	397	ASP	3.4
2	E	2	PRO	3.3
2	C	438	ALA	3.3
2	E	366	VAL	3.3
2	E	405	ILE	3.3
2	C	382	PHE	3.3
2	C	376	ALA	3.3
2	E	49	ALA	3.3
2	C	325	LEU	3.3
2	C	394	VAL	3.3
2	E	398	ASN	3.3
2	C	8	ILE	3.3
2	E	48	ALA	3.2
2	E	55	ALA	3.2
2	E	388	ALA	3.2
2	E	344	SER	3.2
2	C	374	LEU	3.2
2	E	440	ALA	3.2
2	E	7	GLU	3.2
2	E	363	LEU	3.2
2	E	406	ILE	3.2
2	E	359	ILE	3.2
2	E	438	ALA	3.1
2	E	426	VAL	3.1
2	C	12	LEU	3.1
2	E	395	ASP	3.1
3	F	2	ALA	3.1
2	C	34	SER	3.1
2	E	436	ILE	3.0
2	C	425	GLU	3.0
2	E	407	ILE	3.0
2	C	420	ASP	3.0
2	E	37	ALA	3.0
2	E	319	ILE	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	402	ARG	3.0
2	E	334	ASN	3.0
2	E	360	PRO	3.0
2	C	442	ALA	2.9
2	E	345	LEU	2.9
2	C	41	SER	2.9
2	E	433	ALA	2.9
2	E	428	VAL	2.9
2	C	338	TYR	2.9
2	E	356	SER	2.9
2	E	364	LEU	2.9
2	C	345	LEU	2.9
2	E	339	VAL	2.9
2	E	24	THR	2.9
3	F	1	MET	2.9
2	C	441	ARG	2.8
2	E	23	PRO	2.8
2	E	325	LEU	2.8
2	C	337	VAL	2.8
2	E	374	LEU	2.8
1	B	49	ALA	2.8
2	E	399	LYS	2.8
2	C	46	SER	2.8
2	E	384	ALA	2.8
1	B	50	VAL	2.7
2	E	331	VAL	2.7
2	E	427	ILE	2.7
2	C	391	MET	2.7
2	E	390	VAL	2.7
2	C	327	GLU	2.7
2	E	349	SER	2.7
2	E	365	SER	2.7
2	E	367	ASP	2.7
2	C	436	ILE	2.7
2	C	6	LEU	2.7
2	C	384	ALA	2.6
2	E	422	THR	2.6
2	E	328	ILE	2.6
2	E	3	LEU	2.6
2	C	329	GLY	2.6
2	E	13	PRO	2.6
2	C	434	SER	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	335	SER	2.6
1	A	20	GLN	2.6
2	C	40	ASP	2.6
2	C	387	ILE	2.6
2	E	12	LEU	2.6
1	A	49	ALA	2.6
2	C	4	THR	2.6
2	C	335	SER	2.6
2	C	421	LEU	2.5
1	B	48	PRO	2.5
2	E	43	PRO	2.5
2	E	337	VAL	2.5
2	C	402	ARG	2.5
2	E	40	ASP	2.5
2	C	429	GLY	2.5
2	E	386	LYS	2.5
1	A	63	VAL	2.5
2	E	222	VAL	2.5
2	C	23	PRO	2.5
2	E	352	GLY	2.5
1	A	46	VAL	2.5
2	E	411	VAL	2.5
3	F	226[A]	TYR	2.5
2	C	166	ASP	2.5
2	C	430	PRO	2.5
2	C	339	VAL	2.4
1	B	131	LYS	2.4
2	E	420	ASP	2.4
2	C	419	GLU	2.4
2	E	435	GLY	2.4
2	E	38	SER	2.4
2	E	418	LEU	2.4
2	E	17	CYS	2.4
3	D	177	MET	2.4
2	C	330	ALA	2.3
2	E	393	LYS	2.3
2	C	319	ILE	2.3
2	E	387	ILE	2.3
2	C	352	GLY	2.3
2	E	58	ALA	2.3
1	B	125	ASN	2.3
2	C	424	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	147	ALA	2.3
1	B	55	SER	2.3
2	E	417	LYS	2.3
1	B	151	GLY	2.3
2	E	431	ARG	2.3
2	E	415	LYS	2.3
2	C	395	ASP	2.2
2	E	423	GLY	2.2
2	C	144	LYS	2.2
2	E	338	TYR	2.2
2	E	377	TYR	2.2
2	C	398	ASN	2.2
2	E	429	GLY	2.2
2	C	15	LYS	2.2
2	C	347	TYR	2.2
1	B	92	ARG	2.2
2	E	392	LYS	2.2
2	C	11	GLN	2.2
2	E	389	ALA	2.2
2	C	418	LEU	2.1
2	E	6	LEU	2.1
1	A	89	CYS	2.1
2	C	49	ALA	2.1
2	E	375	THR	2.1
2	C	407	ILE	2.1
2	E	419	GLU	2.1
1	A	127	THR	2.1
2	C	48	ALA	2.1
2	C	3	LEU	2.1
2	C	370	GLY	2.1
2	C	416	GLY	2.1
2	C	431	ARG	2.1
2	C	386	LYS	2.1
2	E	358	LYS	2.1
1	A	108	LEU	2.1
2	E	54	ASP	2.1
2	C	321	VAL	2.1
1	A	12	PHE	2.1
2	E	18	GLY	2.1
2	C	36	LYS	2.0
1	A	51	GLN	2.0
2	C	408	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
2	C	9	TYR	2.0
2	C	44	TYR	2.0
1	B	128	GLY	2.0
2	C	432	GLU	2.0
1	A	92	ARG	2.0
2	C	417	LYS	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](#)

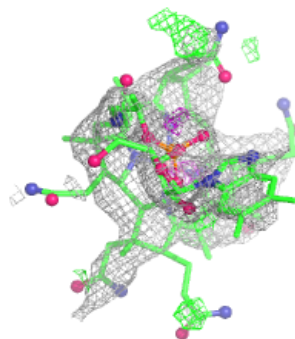
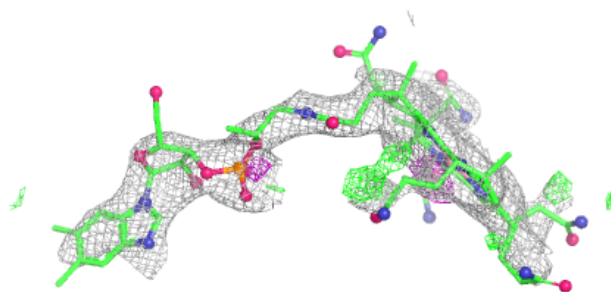
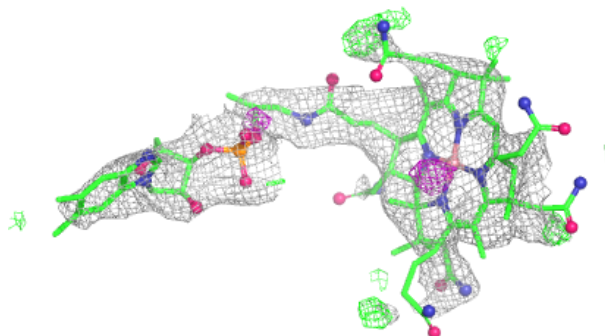
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	GOL	D	405	6/6	0.78	0.21	66,77,84,86	0
7	GOL	E	504	6/6	0.78	0.21	61,81,88,90	0
4	CA	B	301	1/1	0.80	0.14	76,76,76,76	0
6	B12	E	502	91/91	0.82	0.16	81,134,181,183	0
6	B12	C	502	91/91	0.85	0.15	57,106,145,159	0
7	GOL	E	503	6/6	0.86	0.15	70,75,76,84	0
7	GOL	D	402	6/6	0.86	0.12	70,73,77,78	0
7	GOL	F	402	6/6	0.86	0.16	48,50,68,71	0
4	CA	A	301	1/1	0.88	0.18	70,70,70,70	0
7	GOL	D	404	6/6	0.88	0.16	50,67,73,75	0
7	GOL	F	403	6/6	0.90	0.13	62,80,85,89	0
7	GOL	D	401	6/6	0.93	0.15	37,54,60,63	0
5	SF4	E	501	8/8	0.93	0.07	132,148,168,242	0
7	GOL	F	401	6/6	0.94	0.14	41,49,52,53	0
5	SF4	C	501	8/8	0.95	0.07	110,118,140,229	0
7	GOL	D	403	6/6	0.97	0.06	44,46,53,65	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.

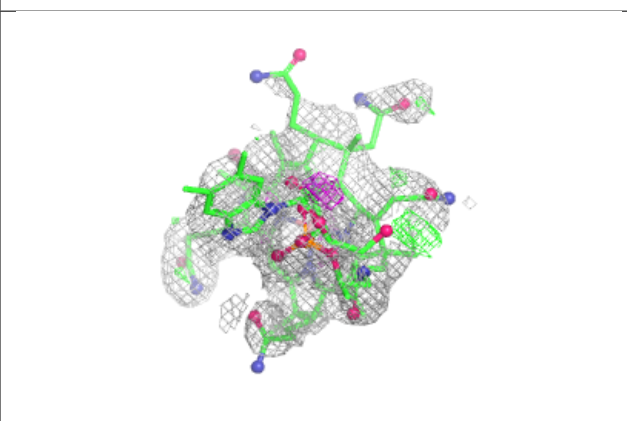
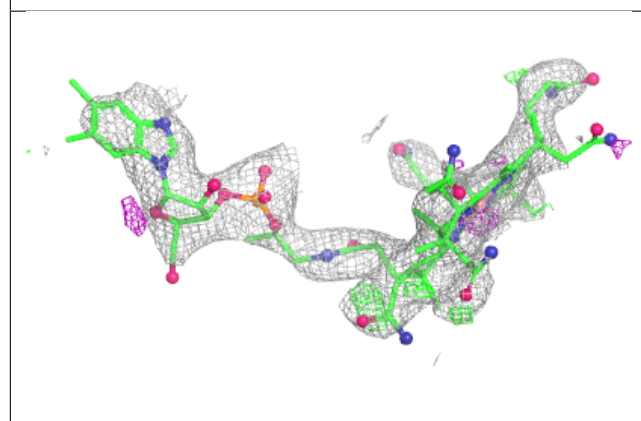
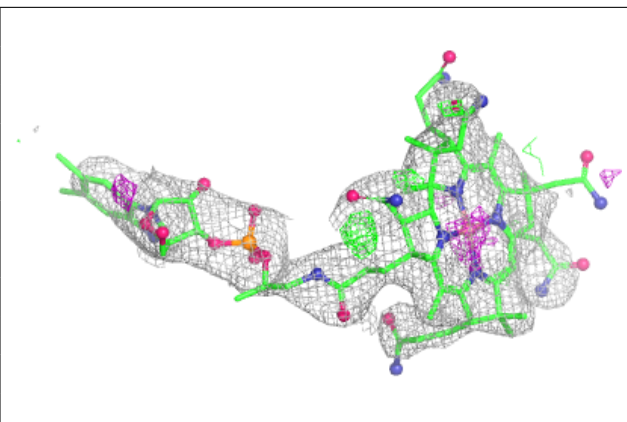
Electron density around B12 E 502:

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



Electron density around B12 C 502:

$2mF_o-DF_c$ (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.