



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:59 am BST

PDB ID : 4DJJ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

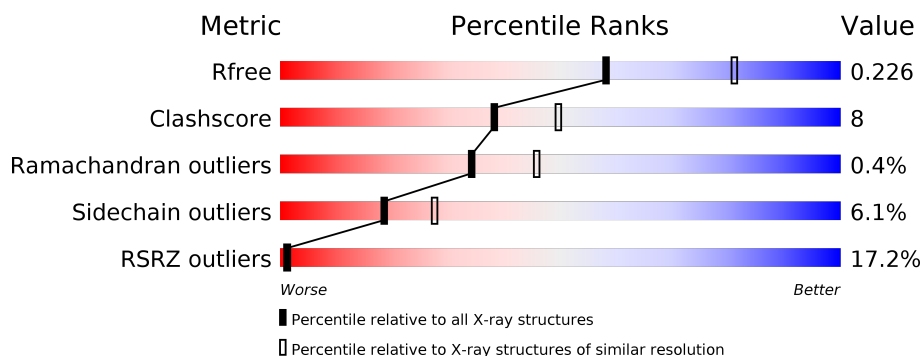
1 Overall quality at a glance

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}	130704	5509 (2.40-2.36)
Clashscore	141614	6082 (2.40-2.36)
Ramachandran outliers	138981	5973 (2.40-2.36)
Sidechain outliers	138945	5975 (2.40-2.36)
RSRZ outliers	127900	5397 (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 on 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	<div> <div>10%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>
1	B	262	<div> <div>11%</div> <div>85%</div> <div>14%</div> <div>.</div> </div>
2	C	446	<div> <div>34%</div> <div>76%</div> <div>21%</div> <div>..</div> </div>
2	E	446	<div> <div>31%</div> <div>81%</div> <div>15%</div> <div>..</div> </div>
3	D	323	<div> <div>88%</div> <div>10%</div> <div>.</div> </div>
3	F	323	<div> <div>2%</div> <div>89%</div> <div>10%</div> <div>.</div> </div>

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			

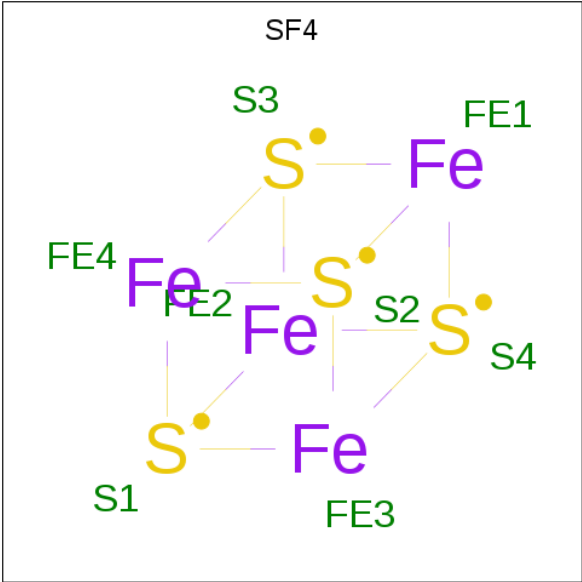
- Molecule 3 is a protein called Corrinoid/iron-sulfur protein small subunit.

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 (three-letter code: CA) (formula: Ca).

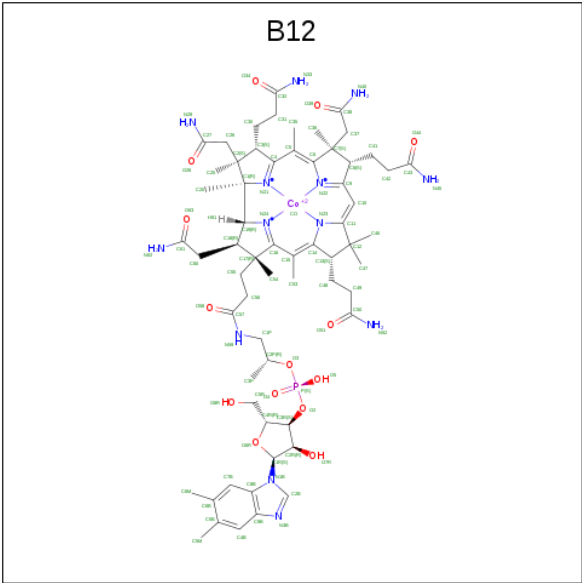
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is IRON/SULFUR CLUSTER (three-letter code: 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 (three-letter code: B12) (formula: C₆₂H₈₉CoN₁₃O₁₄P).



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 (three-letter code: 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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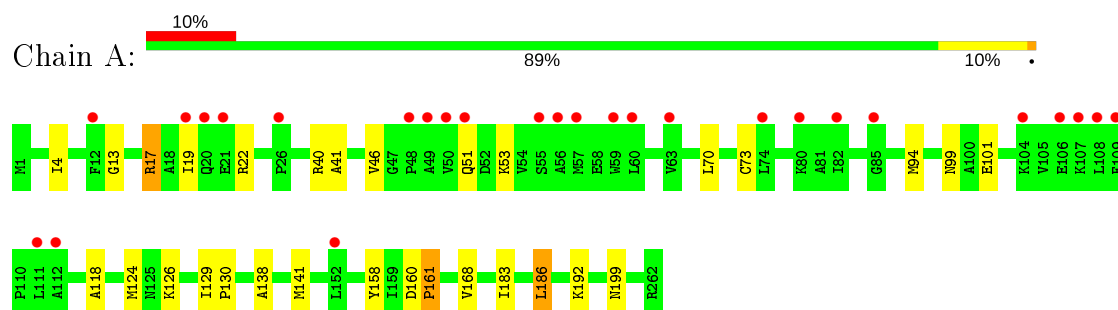
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	34	Total 34	O 34	0	0
8	C	39	Total 39	O 39	0	0
8	D	121	Total 121	O 121	0	0
8	E	63	Total 63	O 63	0	0
8	F	111	Total 111	O 111	0	0

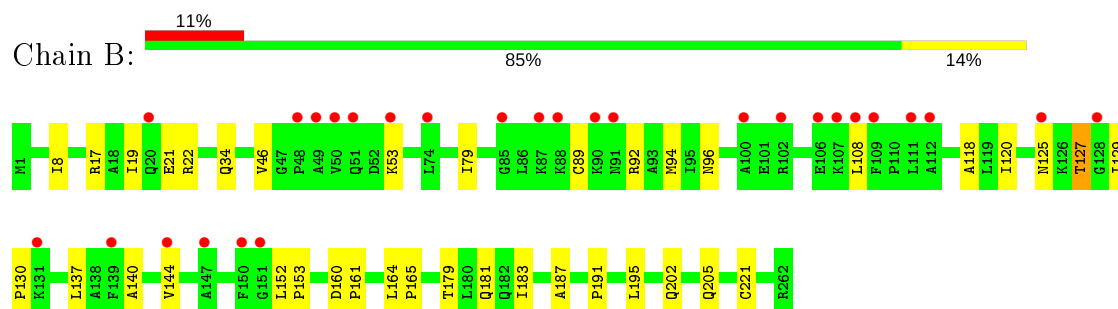
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

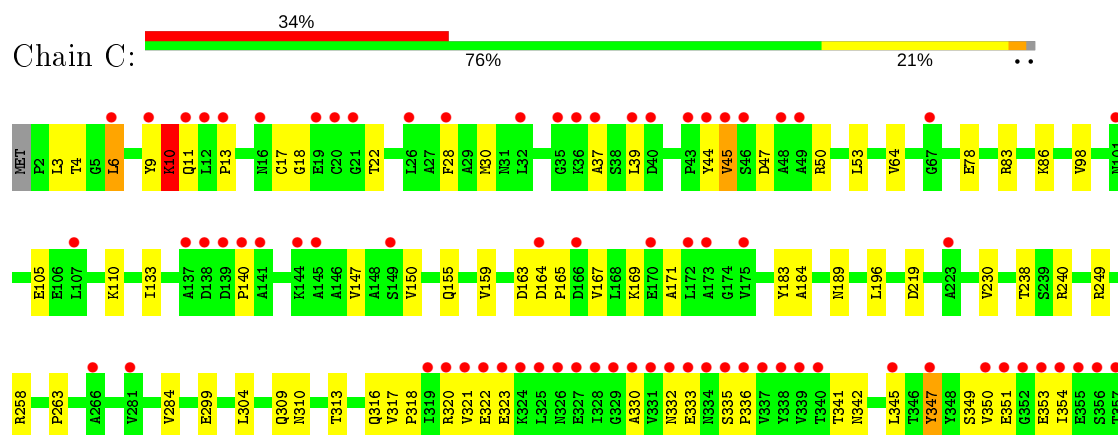
- Molecule 1: 5-methyltetrahydrofolate corrinoid/iron sulfur protein methyltransferase

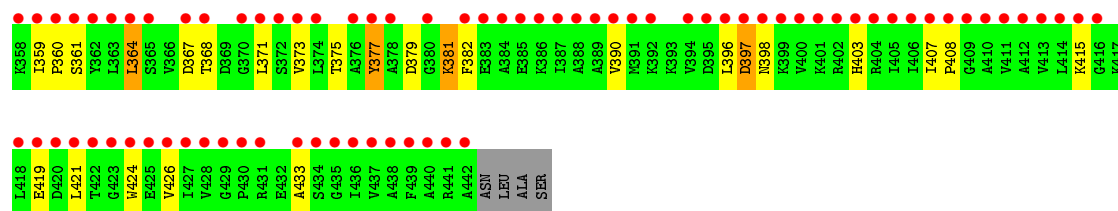


- Molecule 1: 5-methyltetrahydrofolate corrinoid/iron sulfur protein methyltransferase

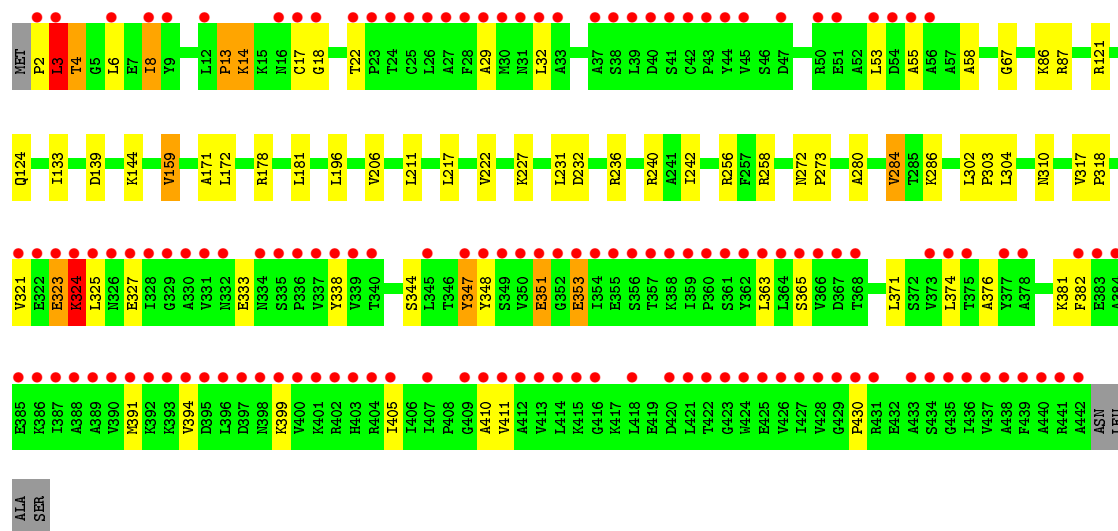
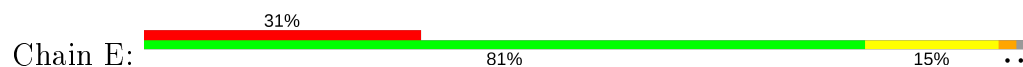


- Molecule 2: Corrinoid/iron-sulfur protein large subunit

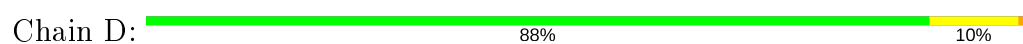




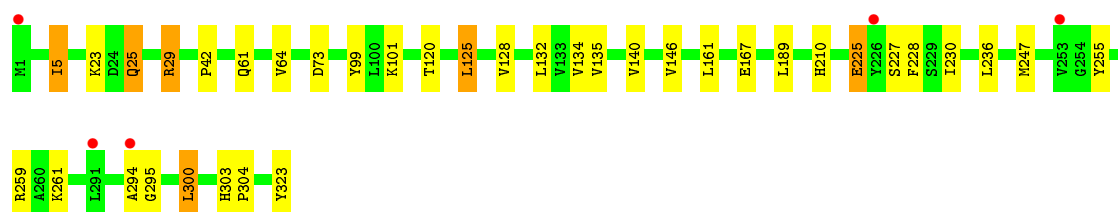
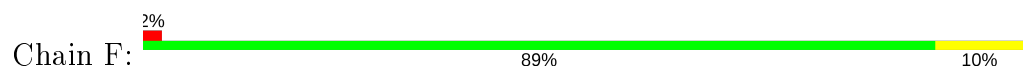
● Molecule 2: Corrinoid/iron-sulfur protein large subunit



● Molecule 3: Corrinoid/iron-sulfur protein small subunit



● Molecule 3: Corrinoid/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 48.34 – 2.38	Depositor EDS
% Data completeness (in resolution range)	99.0 (39.83-2.38) 99.0 (48.34-2.38)	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 0.184 , 0.226	Depositor DCC
R_{free} test set	4866 reflections (4.99%)	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 , 65.1	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: GOL, SF4, B12, CA

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	0/2019	0.43	0/2734
1	B	0.24	0/2019	0.43	0/2734
2	C	0.24	0/3205	0.44	0/4383
2	E	0.26	0/3157	0.46	0/4317
3	D	0.27	0/2507	0.46	0/3408
3	F	0.27	0/2520	0.45	0/3426
All	All	0.25	0/15427	0.45	0/21002

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1993	0	2028	15	0
1	B	1993	0	2028	18	0
2	C	3149	0	2976	70	0
2	E	3105	0	2878	78	0
3	D	2461	0	2461	22	0
3	F	2470	0	2470	19	0
4	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	232	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 (232) 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:E:391:MET:SD	2:E:405:ILE:CD1	2.57	0.92
2:E:324:LYS:CE	2:E:324:LYS:HA	1.94	0.91
2:C:415:LYS:CB	2:C:426:VAL:HG11	2.01	0.90
2:C:347:TYR:C	2:C:347:TYR:HD1	1.74	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:CD1	2:C:347:TYR:O	2.25	0.89
2:E:347:TYR:O	2:E:347:TYR:HD1	1.57	0.88
2:C:347:TYR:C	2:C:347:TYR:CD1	2.42	0.88
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:E:347:TYR:C	2:E:347:TYR:HD1	1.79	0.83
2:C:321:VAL:HG11	2:C:347:TYR:CE2	2.15	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:347:TYR:CD1	2:E:347:TYR:C	2.50	0.81
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:H602	6:C:502:B12:H252	1.66	0.76
2:E:411:VAL:O	2:E:411:VAL:HG12	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:H552	6:E:502:B12:H531	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:H602	6:E:502:B12:H252	1.70	0.73
2:E:323:GLU:O	2:E:324:LYS:HG2	1.88	0.72
6:C:502:B12:H362	6:C:502:B12:H351	1.71	0.72
2:E:211:LEU:H	7:E:503:GOL:H31	1.53	0.72
2:E:8:ILE:HD13	2:E:32:LEU:HD12	1.70	0.72
2:E:321:VAL:HG11	2:E:347:TYR:HD2	1.50	0.70
6:E:502:B12:H351	6:E:502:B12:H362	1.72	0.69
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:E:338:TYR:HB3	6:E:502:B12:HM52	1.77	0.66
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:E:391:MET:HE1	2:E:405:ILE:HD13	1.78	0.65
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:E:2:PRO:O	2:E:3:LEU:CB	2.46	0.63
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:377:TYR:C	2:C:377:TYR:HD1	2.04	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
2:C:377:TYR:C	2:C:377:TYR:CD1	2.77	0.58
6:C:502:B12:H203	6:C:502:B12:H301	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:H291	6:C:502:B12:H3	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
1:A:138:ALA:HA	2:C:30:MET:HE1	1.86	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:N29	6:E:502:B12:H3	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:391:MET:HE1	2:E:405:ILE:CD1	2.38	0.52
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:H	2:C:39:LEU:HD23	1.74	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:N	3:F:29:ARG:HD2	2.26	0.50
2:C:321:VAL:HG12	2:C:322:GLU:N	2.26	0.50
6:C:502:B12:C55	6:C:502:B12:H531	2.41	0.50
2:C:219:ASP:OD2	3:D:1:MET:N	2.44	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
2:C:318:PRO:HD2	2:C:320:ARG:NH1	2.28	0.48
2:E:321:VAL:HG21	2:E:347:TYR:HD2	1.75	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
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
3:D:73:ASP:HA	3:D:76:THR:HG23	1.96	0.47
3:D:213:ILE:HG13	3:D:247:MET:HB2	1.96	0.47
3:D:77:ASP:N	3:D:77:ASP:OD1	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:ALA:HB3	1:B:191:PRO:HD3	1.97	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
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
2:E:321:VAL:CB	2:E:347:TYR:HD2	2.29	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:E:324:LYS:NZ	2:E:394:VAL:HA	2.33	0.43
2:C:299:GLU:HG3	3:D:275:LYS:N	2.33	0.43
2:C:396:LEU:O	2:C:397:ASP:C	2.57	0.43
6:E:502:B12:H533	6:E:502:B12:H491	2.00	0.43
2:E:240:ARG:HH11	7:E:504:GOL:H31	1.84	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:164:ASP:HA	2:C:165:PRO:HD3	1.91	0.43
2:C:18:GLY:HA2	2:C:22:THR:O	2.19	0.43
2:E:272:ASN:HA	2:E:273:PRO:HD3	1.92	0.43
2:C:323:GLU:CD	2:C:367:ASP:HB2	2.39	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	2:E:172:LEU:HD12	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
2:C:9:TYR:C	2:C:11:GLN:H	2.22	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
2:C:6:LEU:HD22	2:C:10:LYS:HE2	2.01	0.42
1:B:92:ARG:HA	1:B:92:ARG:HD2	1.91	0.42
6:C:502:B12:H363	6:C:502:B12:H411	1.80	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
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:HA	2:C:258:ARG:HD3	1.77	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
2:C:421:LEU:O	2:C:421:LEU:HD23	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:324:LYS:HZ2	2:E:394:VAL:HA	1.85	0.41
2:E:13:PRO:HB2	2:E:14:LYS:H	1.61	0.41
2:E:2:PRO:HB2	2:E:3:LEU:H	1.61	0.41
6:E:502:B12:H363	6:E:502:B12:H411	1.80	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:HA	3:D:282:LEU:HD12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:276:GLU:CD	3:D:276:GLU:H	2.24	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
1	B	260/262 (99%)	251 (96%)	9 (4%)	0	100	100
2	C	439/446 (98%)	421 (96%)	14 (3%)	4 (1%)	17	23
2	E	439/446 (98%)	421 (96%)	13 (3%)	5 (1%)	14	18
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%)	34	46

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

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Mol	Chain	Res	Type
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%)	207 (97%)	6 (3%)	43	61
1	B	213/214 (100%)	207 (97%)	6 (3%)	43	61
2	C	290/356 (82%)	267 (92%)	23 (8%)	12	17
2	E	278/356 (78%)	256 (92%)	22 (8%)	12	17
3	D	261/261 (100%)	245 (94%)	16 (6%)	18	27
3	F	262/261 (100%)	243 (93%)	19 (7%)	14	20
All	All	1517/1662 (91%)	1425 (94%)	92 (6%)	18	27

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	ARG
1	A	51	GLN
1	A	141	MET
1	A	161	PRO
1	A	186	LEU
1	A	199	ASN
1	B	17	ARG
1	B	21	GLU
1	B	89	CYS
1	B	127	THR
1	B	183	ILE
1	B	205	GLN
2	C	3	LEU

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Mol	Chain	Res	Type
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	83	ARG
2	C	105	GLU
2	C	155	GLN
2	C	159	VAL
2	C	238	THR
2	C	284	VAL
2	C	304	LEU
2	C	316	GLN
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
3	D	1	MET
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	210	HIS
3	D	212	VAL
3	D	217	ILE
3	D	225	GLU
3	D	236	LEU
3	D	247	MET
3	D	282	LEU
3	D	300	LEU
3	D	315	ASP
2	E	3	LEU
2	E	4	THR
2	E	6	LEU
2	E	8	ILE

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Mol	Chain	Res	Type
2	E	53	LEU
2	E	87	ARG
2	E	124	GLN
2	E	133	ILE
2	E	139	ASP
2	E	159	VAL
2	E	196	LEU
2	E	206	VAL
2	E	217	LEU
2	E	231	LEU
2	E	284	VAL
2	E	304	LEU
2	E	323	GLU
2	E	324	LYS
2	E	327	GLU
2	E	347	TYR
2	E	351	GLU
2	E	353	GLU
3	F	5	ILE
3	F	23	LYS
3	F	25	GLN
3	F	29	ARG
3	F	64	VAL
3	F	73	ASP
3	F	120	THR
3	F	125	LEU
3	F	134	VAL
3	F	140	VAL
3	F	146	VAL
3	F	161	LEU
3	F	167	GLU
3	F	210	HIS
3	F	225	GLU
3	F	236	LEU
3	F	247	MET
3	F	261	LYS
3	F	300	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

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 carbohydrates 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	404	-	5,5,5	0.40	0	5,5,5	0.24	0
6	B12	E	502	-	80,101,101	1.34	11 (13%)	101,166,166	2.17	26 (25%)
7	GOL	E	504	-	5,5,5	0.36	0	5,5,5	0.18	0
5	SF4	C	501	2	0,12,12	0.00	-	-		
7	GOL	D	403	-	5,5,5	0.36	0	5,5,5	0.16	0
7	GOL	F	403	-	5,5,5	0.36	0	5,5,5	0.28	0
7	GOL	E	503	-	5,5,5	0.38	0	5,5,5	0.16	0
5	SF4	E	501	2	0,12,12	0.00	-	-		
7	GOL	F	401	-	5,5,5	0.41	0	5,5,5	0.26	0
7	GOL	F	402	-	5,5,5	0.33	0	5,5,5	0.35	0
7	GOL	D	405	-	5,5,5	0.35	0	5,5,5	0.21	0
7	GOL	D	402	-	5,5,5	0.36	0	5,5,5	0.30	0
7	GOL	D	401	-	5,5,5	0.41	0	5,5,5	0.32	0
6	B12	C	502	-	80,101,101	1.36	11 (13%)	101,166,166	2.16	28 (27%)

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	404	-	-	4/4/4/4	-
6	B12	E	502	-	-	9/51/223/223	0/3/11/11
7	GOL	E	504	-	-	2/4/4/4	-
7	GOL	D	403	-	-	3/4/4/4	-
7	GOL	F	403	-	-	2/4/4/4	-
5	SF4	C	501	2	-	-	0/6/5/5
7	GOL	E	503	-	-	4/4/4/4	-
5	SF4	E	501	2	-	-	0/6/5/5
7	GOL	F	401	-	-	4/4/4/4	-
7	GOL	F	402	-	-	4/4/4/4	-
7	GOL	D	405	-	-	2/4/4/4	-
7	GOL	D	402	-	-	4/4/4/4	-
7	GOL	D	401	-	-	2/4/4/4	-
6	B12	C	502	-	-	9/51/223/223	0/3/11/11

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	502	B12	C11-C10	-4.03	1.34	1.40
6	E	502	B12	C11-C10	-3.92	1.34	1.40
6	C	502	B12	C6B-C5B	3.59	1.49	1.40
6	E	502	B12	C6B-C5B	3.40	1.49	1.40
6	E	502	B12	C7B-C6B	3.24	1.46	1.37
6	C	502	B12	C7B-C6B	3.24	1.46	1.37
6	E	502	B12	C55-C56	2.94	1.59	1.53
6	C	502	B12	C55-C56	2.88	1.59	1.53
6	C	502	B12	C1P-C2P	2.83	1.58	1.51
6	E	502	B12	P-O3	-2.78	1.53	1.60
6	C	502	B12	P-O3	-2.69	1.53	1.60
6	E	502	B12	C1P-C2P	2.62	1.58	1.51
6	E	502	B12	C60-C18	-2.45	1.48	1.54
6	C	502	B12	O58-C57	2.45	1.28	1.23
6	C	502	B12	C60-C18	-2.37	1.48	1.54
6	E	502	B12	O58-C57	2.36	1.28	1.23
6	C	502	B12	C25-C2	-2.06	1.50	1.54
6	C	502	B12	C35-C5	2.06	1.56	1.52
6	E	502	B12	C1P-N59	2.06	1.52	1.46
6	C	502	B12	C3P-C2P	-2.04	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	502	B12	C25-C2	-2.03	1.50	1.54
6	E	502	B12	C3P-C2P	-2.02	1.43	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	E	502	B12	C18-C60-C61	7.73	133.26	113.97
6	C	502	B12	C18-C60-C61	7.63	133.00	113.97
6	C	502	B12	C60-C18-C17	5.48	128.97	115.74
6	E	502	B12	C60-C18-C17	5.39	128.77	115.74
6	C	502	B12	O7R-C2R-C3R	5.29	126.20	111.17
6	E	502	B12	O7R-C2R-C3R	5.29	126.19	111.17
6	E	502	B12	C60-C61-N62	5.04	128.36	116.21
6	C	502	B12	C60-C61-N62	5.04	128.34	116.21
6	E	502	B12	O2-P-O4	-4.77	91.58	109.47
6	C	502	B12	O2-P-O4	-4.74	91.69	109.47
6	E	502	B12	C48-C13-C12	-4.68	103.59	116.59
6	C	502	B12	C48-C13-C12	-4.63	103.72	116.59
6	E	502	B12	C3R-C2R-C1R	4.04	108.84	99.89
6	C	502	B12	C3R-C2R-C1R	4.04	108.84	99.89
6	C	502	B12	O6R-C1R-C2R	-3.80	101.38	106.93
6	E	502	B12	O6R-C1R-C2R	-3.75	101.45	106.93
6	E	502	B12	C20-C1-C19	-3.59	105.90	109.36
6	E	502	B12	C55-C17-C18	-3.53	104.31	111.14
6	C	502	B12	C55-C17-C18	-3.51	104.36	111.14
6	C	502	B12	C20-C1-C19	-3.45	106.03	109.36
6	C	502	B12	O63-C61-C60	-3.29	113.94	120.87
6	E	502	B12	O63-C61-C60	-3.24	114.04	120.87
6	E	502	B12	C2-C1-C19	3.14	123.56	118.60
6	E	502	B12	C16-C15-C14	-3.12	119.40	124.27
6	C	502	B12	C2-C1-C19	3.10	123.50	118.60
6	C	502	B12	C16-C15-C14	-3.08	119.47	124.27
6	E	502	B12	O58-C57-C56	-3.06	116.42	122.02
6	C	502	B12	O58-C57-C56	-3.05	116.43	122.02
6	E	502	B12	O58-C57-N59	2.92	128.52	123.01
6	C	502	B12	O58-C57-N59	2.89	128.46	123.01
6	C	502	B12	O8R-C5R-C4R	2.87	121.13	111.29
6	E	502	B12	O8R-C5R-C4R	2.86	121.12	111.29
6	E	502	B12	O6R-C4R-C3R	2.70	110.65	104.87
6	C	502	B12	O6R-C4R-C3R	2.68	110.61	104.87
6	E	502	B12	C37-C7-C8	-2.66	101.23	108.37
6	C	502	B12	C37-C7-C8	-2.63	101.33	108.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	502	B12	C47-C12-C46	-2.54	104.41	109.73
6	C	502	B12	C1-C2-C3	-2.53	98.41	101.59
6	E	502	B12	C19-C1-N21	2.52	104.75	102.16
6	E	502	B12	C2P-C1P-N59	2.51	116.64	112.93
6	C	502	B12	C25-C2-C1	-2.50	110.09	113.80
6	E	502	B12	C1-C2-C3	-2.50	98.46	101.59
6	C	502	B12	C2P-C1P-N59	2.47	116.58	112.93
6	E	502	B12	C47-C12-C46	-2.47	104.55	109.73
6	E	502	B12	C25-C2-C1	-2.46	110.15	113.80
6	E	502	B12	C8-C9-N22	2.45	114.19	111.12
6	C	502	B12	C19-C1-N21	2.42	104.65	102.16
6	C	502	B12	C8-C9-N22	2.42	114.14	111.12
6	C	502	B12	C4B-C9B-C8B	-2.37	118.67	121.10
6	E	502	B12	C4B-C9B-C8B	-2.33	118.71	121.10
6	E	502	B12	C26-C2-C1	2.10	113.28	110.02
6	C	502	B12	C26-C2-C1	2.06	113.23	110.02
6	C	502	B12	C54-C17-C18	2.06	116.02	112.98
6	C	502	B12	C1P-N59-C57	2.00	127.05	122.69

There are no chirality outliers.

All (49) torsion outliers are listed below:

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

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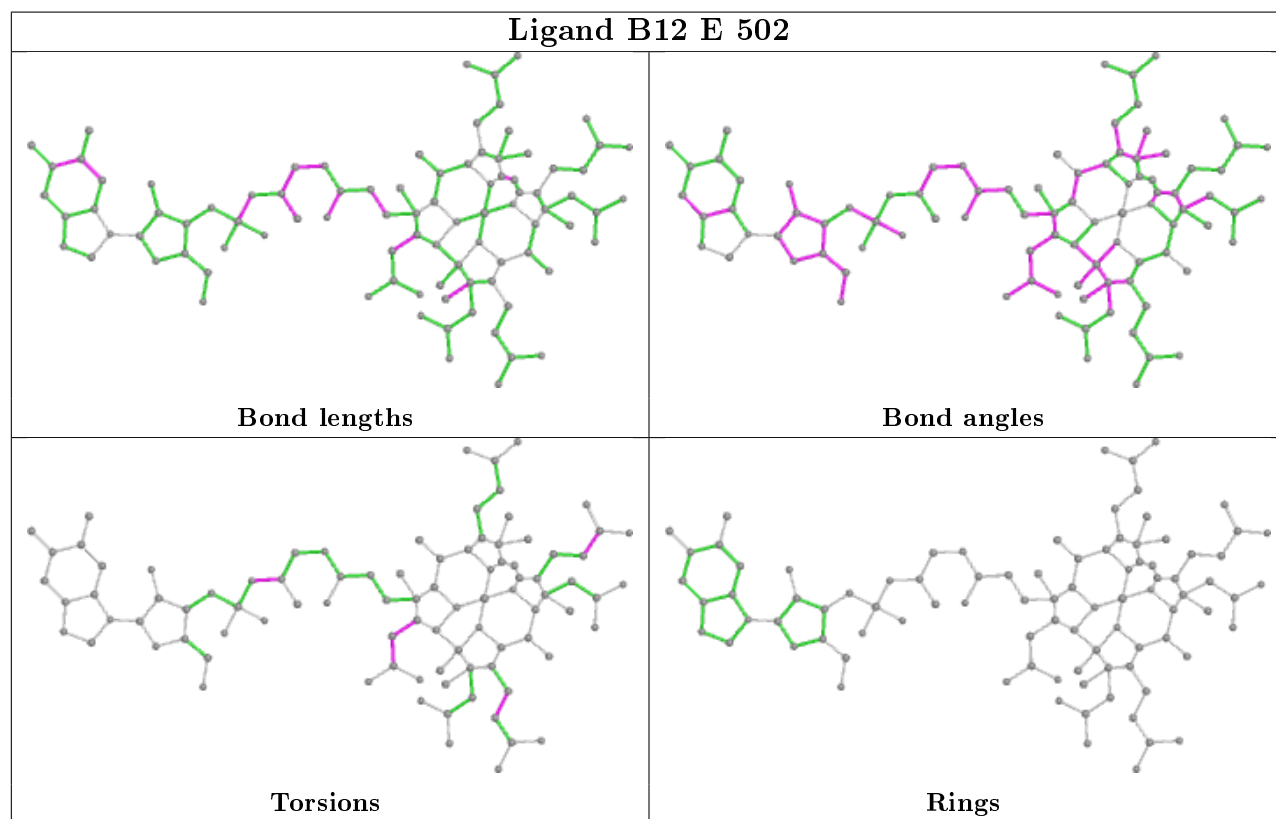
Mol	Chain	Res	Type	Atoms
7	F	401	GOL	C1-C2-C3-O3
7	F	402	GOL	C1-C2-C3-O3
7	D	405	GOL	O1-C1-C2-C3
7	D	402	GOL	C1-C2-C3-O3
7	F	403	GOL	O1-C1-C2-C3
7	E	504	GOL	O1-C1-C2-O2
7	E	503	GOL	O1-C1-C2-O2
7	F	401	GOL	O1-C1-C2-O2
7	F	401	GOL	O2-C2-C3-O3
7	F	402	GOL	O1-C1-C2-O2
7	F	402	GOL	O2-C2-C3-O3
7	D	402	GOL	O1-C1-C2-O2
7	F	403	GOL	O1-C1-C2-O2
6	E	502	B12	C41-C42-C43-O44
6	C	502	B12	C41-C42-C43-O44
6	E	502	B12	C41-C42-C43-N45
6	C	502	B12	C41-C42-C43-N45
6	E	502	B12	C3-C30-C31-C32
6	C	502	B12	C3-C30-C31-C32
7	D	402	GOL	O2-C2-C3-O3
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	C18-C60-C61-O63
6	C	502	B12	C18-C60-C61-N62
7	E	503	GOL	O2-C2-C3-O3
6	E	502	B12	C19-C18-C60-C61
7	D	403	GOL	O1-C1-C2-O2
7	D	403	GOL	C1-C2-C3-O3
6	C	502	B12	C19-C18-C60-C61

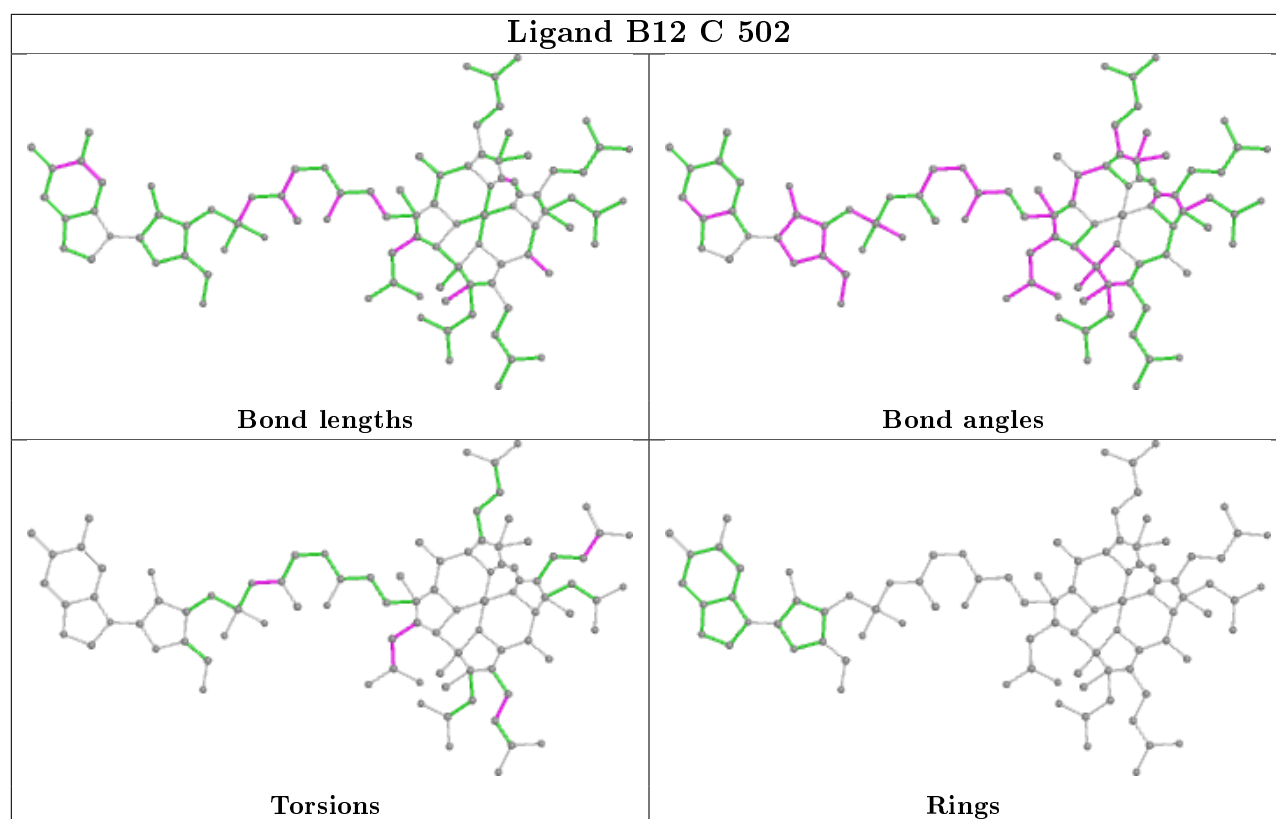
There are no ring outliers.

6 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	502	B12	12	0
7	E	504	GOL	2	0
7	E	503	GOL	1	0
5	E	501	SF4	1	0
7	F	401	GOL	2	0
6	C	502	B12	13	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%)	0.61	27 (10%) 6 7	33, 68, 118, 165	0
1	B	262/262 (100%)	0.57	28 (10%) 6 6	35, 71, 115, 146	0
2	C	441/446 (98%)	2.27	152 (34%) 0 0	36, 87, 193, 226	3 (0%)
2	E	441/446 (98%)	1.88	140 (31%) 0 0	32, 60, 201, 248	3 (0%)
3	D	323/323 (100%)	0.15	1 (0%) 94 94	27, 38, 66, 119	0
3	F	323/323 (100%)	0.31	5 (1%) 73 75	30, 43, 68, 112	0
All	All	2052/2062 (99%)	1.12	353 (17%) 1 1	27, 56, 176, 248	6 (0%)

All (353) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	440	ALA	20.2
2	C	427	ILE	17.3
2	E	396	LEU	16.6
2	E	357	THR	16.0
2	E	326	ASN	15.5
2	C	433	ALA	15.2
2	C	428	VAL	14.8
2	E	394	VAL	13.3
2	E	359	ILE	13.2
2	C	356	SER	13.2
2	E	356	SER	12.6
2	C	390	VAL	11.8
2	C	383	GLU	11.7
2	C	413	VAL	11.7
2	C	331	VAL	11.4
2	C	357	THR	11.4
2	E	43	PRO	11.2
2	C	394	VAL	11.0
2	E	330	ALA	10.9

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Mol	Chain	Res	Type	RSRZ
2	E	400	VAL	10.8
2	C	396	LEU	10.7
2	E	395	ASP	10.7
2	C	359	ILE	10.7
2	C	406	ILE	10.7
2	C	426	VAL	10.5
2	E	329	GLY	10.3
2	C	328	ILE	10.3
2	C	330	ALA	10.3
2	C	350	VAL	10.2
2	E	39	LEU	10.1
2	E	335	SER	10.1
2	E	426	VAL	9.8
2	C	407	ILE	9.8
2	E	415	LYS	9.7
2	E	440	ALA	9.7
2	E	418	LEU	9.7
2	C	405	ILE	9.5
2	E	401	LYS	9.5
2	E	433	ALA	9.4
2	E	336	PRO	9.4
2	E	405	ILE	9.3
2	E	352	GLY	9.3
2	C	388	ALA	8.9
2	E	399	LYS	8.8
2	C	430	PRO	8.7
2	C	336	PRO	8.6
2	C	409	GLY	8.6
2	E	416	GLY	8.5
2	C	339	VAL	8.5
2	C	436	ILE	8.5
2	C	441	ARG	8.4
2	E	382	PHE	8.1
2	E	37	ALA	8.1
3	F	1	MET	7.9
2	C	45	VAL	7.9
2	C	418	LEU	7.9
2	C	410	ALA	7.9
2	C	360	PRO	7.9
2	C	384	ALA	7.9
2	E	361	SER	7.9
2	C	352	GLY	7.9

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Mol	Chain	Res	Type	RSRZ
2	E	439	PHE	7.8
2	C	362	TYR	7.7
2	C	325	LEU	7.7
2	C	439	PHE	7.7
2	E	414	LEU	7.6
2	E	402	ARG	7.6
2	C	363	LEU	7.6
2	C	376	ALA	7.4
2	C	392	LYS	7.3
2	C	44	TYR	7.3
2	C	389	ALA	7.3
2	E	362	TYR	7.2
2	E	436	ILE	7.2
2	E	427	ILE	7.1
2	C	385	GLU	7.1
2	E	404	ARG	7.1
2	E	40	ASP	7.0
2	E	32	LEU	6.9
2	C	39	LEU	6.9
2	C	415	LYS	6.9
2	C	335	SER	6.9
2	E	388	ALA	6.8
2	C	12	LEU	6.7
2	C	425	GLU	6.6
2	C	338	TYR	6.6
2	C	435	GLY	6.6
2	E	355	GLU	6.6
2	E	28	PHE	6.5
2	E	339	VAL	6.4
2	E	55	ALA	6.4
2	C	397	ASP	6.3
2	E	322	GLU	6.3
2	C	424	TRP	6.2
2	E	340	THR	6.2
2	E	337	VAL	6.2
2	E	338	TYR	6.2
2	C	414	LEU	5.9
2	E	431	ARG	5.9
2	C	347	TYR	5.8
2	E	367	ASP	5.8
2	C	358	LYS	5.7
2	C	386	LYS	5.7

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Mol	Chain	Res	Type	RSRZ
2	E	422	THR	5.6
2	C	326	ASN	5.5
2	C	391	MET	5.5
2	E	354	ILE	5.5
2	E	324	LYS	5.5
2	C	355	GLU	5.5
2	C	364	LEU	5.5
2	E	22	THR	5.4
2	C	416	GLY	5.4
2	E	323	GLU	5.4
2	E	358	LYS	5.4
2	C	48	ALA	5.4
2	E	2	PRO	5.4
2	C	380	GLY	5.3
2	C	323	GLU	5.3
2	E	350	VAL	5.3
2	E	384	ALA	5.3
2	C	404	ARG	5.3
2	C	144	LYS	5.3
2	E	360	PRO	5.3
2	C	399	LYS	5.3
2	E	349	SER	5.3
2	E	423	GLY	5.3
2	E	391	MET	5.2
2	C	434	SER	5.2
2	E	334	ASN	5.2
2	C	398	ASN	5.2
2	C	382	PHE	5.2
2	E	407	ILE	5.2
1	A	51	GLN	5.1
2	E	44	TYR	5.1
2	E	430	PRO	5.1
2	C	332	ASN	5.1
2	E	9	TYR	5.1
2	E	325	LEU	5.0
2	E	397	ASP	5.0
2	E	56	ALA	4.9
2	E	50	ARG	4.9
2	E	390	VAL	4.9
2	C	395	ASP	4.9
2	E	421	LEU	4.9
2	E	387	ILE	4.8

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Mol	Chain	Res	Type	RSRZ
2	E	363	LEU	4.7
2	C	43	PRO	4.7
2	C	37	ALA	4.7
2	E	383	GLU	4.7
2	E	26	LEU	4.6
2	C	324	LYS	4.6
2	C	354	ILE	4.6
2	C	334	ASN	4.6
2	E	392	LYS	4.6
2	E	411	VAL	4.5
2	C	412	ALA	4.5
2	E	17	CYS	4.5
2	E	24	THR	4.5
2	C	145	ALA	4.4
1	B	90	LYS	4.4
2	C	377	TYR	4.4
2	C	107	LEU	4.4
3	F	226[A]	TYR	4.3
2	C	21	GLY	4.3
1	B	87	LYS	4.3
2	E	45	VAL	4.3
2	C	340	THR	4.3
1	B	48	PRO	4.3
2	C	13	PRO	4.3
2	E	393	LYS	4.3
2	E	365	SER	4.2
2	C	419	GLU	4.2
2	C	442	ALA	4.2
2	C	361	SER	4.2
2	C	49	ALA	4.1
2	E	420	ASP	4.1
2	C	401	LYS	4.1
2	E	51	GLU	4.1
2	E	398	ASN	4.1
2	C	378	ALA	4.1
2	E	364	LEU	4.1
2	E	23	PRO	4.1
1	B	151	GLY	4.0
2	E	328	ILE	4.0
2	C	173	ALA	4.0
2	E	351	GLU	4.0
2	E	347	TYR	4.0

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Mol	Chain	Res	Type	RSRZ
2	C	170	GLU	4.0
2	E	29	ALA	4.0
2	C	373	VAL	4.0
2	E	377	TYR	4.0
2	E	12	LEU	4.0
2	C	423	GLY	4.0
2	C	137	ALA	3.9
2	E	412	ALA	3.8
1	A	63	VAL	3.8
2	C	353	GLU	3.8
2	E	31	ASN	3.8
2	C	321	VAL	3.8
2	E	425	GLU	3.7
2	C	175	VAL	3.7
2	C	403	HIS	3.7
2	C	429	GLY	3.7
2	C	438	ALA	3.7
2	C	329	GLY	3.7
2	E	41	SER	3.6
2	C	400	VAL	3.6
2	E	321	VAL	3.6
1	A	20	GLN	3.5
2	C	138	ASP	3.5
2	C	139	ASP	3.5
2	C	431	ARG	3.5
2	E	435	GLY	3.5
2	C	337	VAL	3.5
1	A	112	ALA	3.5
1	A	107	LYS	3.4
1	A	26	PRO	3.4
2	C	11	GLN	3.4
1	B	91	ASN	3.4
2	E	332	ASN	3.4
2	E	442	ALA	3.4
2	E	366	VAL	3.4
2	C	421	LEU	3.4
2	E	6	LEU	3.3
2	E	353	GLU	3.3
2	E	437	VAL	3.3
2	E	413	VAL	3.3
2	E	38	SER	3.3
2	C	422	THR	3.3

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Mol	Chain	Res	Type	RSRZ
2	E	386	LYS	3.3
1	A	49	ALA	3.3
2	C	387	ILE	3.3
2	C	9	TYR	3.3
2	E	348	TYR	3.3
1	A	109	PHE	3.3
2	E	3	LEU	3.2
2	C	411	VAL	3.2
2	C	365	SER	3.2
1	A	50	VAL	3.2
1	B	49	ALA	3.1
1	B	109	PHE	3.1
2	E	33	ALA	3.1
2	E	331	VAL	3.1
1	A	111	LEU	3.1
2	C	26	LEU	3.1
1	A	108	LEU	3.0
2	C	402	ARG	3.0
2	E	441	ARG	3.0
1	A	85	GLY	3.0
2	C	32	LEU	3.0
3	D	1	MET	3.0
2	E	438	ALA	3.0
2	E	16	ASN	2.9
2	E	8	ILE	2.9
1	A	80	LYS	2.9
2	C	164	ASP	2.9
2	E	25	CYS	2.9
2	C	40	ASP	2.9
2	C	374	LEU	2.8
2	E	410	ALA	2.8
1	B	150	PHE	2.8
2	E	42	CYS	2.8
2	E	374	LEU	2.8
2	C	333	GLU	2.8
1	A	82	ILE	2.8
2	E	327	GLU	2.8
2	C	101	ASN	2.8
2	C	20	CYS	2.8
2	C	351	GLU	2.8
2	C	437	VAL	2.7
2	E	345	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	55	SER	2.7
2	C	19	GLU	2.7
1	B	139	PHE	2.7
2	E	54	ASP	2.7
1	B	144	VAL	2.7
1	B	125	ASN	2.6
2	C	322	GLU	2.6
2	E	18	GLY	2.6
2	C	327	GLU	2.6
1	A	57	MET	2.6
2	E	47	ASP	2.6
2	E	389	ALA	2.6
1	B	50	VAL	2.6
1	A	19	ILE	2.6
2	E	373	VAL	2.6
2	C	36	LYS	2.6
1	B	128	GLY	2.6
1	B	106	GLU	2.6
2	C	140	PRO	2.5
1	B	108	LEU	2.5
2	E	424	TRP	2.5
2	C	320	ARG	2.4
1	B	53	LYS	2.4
1	B	107	LYS	2.4
2	E	403	HIS	2.4
2	C	149	SER	2.4
2	C	281	VAL	2.4
1	B	20	GLN	2.4
2	C	16	ASN	2.4
1	B	112	ALA	2.4
2	C	35	GLY	2.4
1	A	12	PHE	2.4
2	E	409	GLY	2.3
1	A	21	GLU	2.3
3	F	291	LEU	2.3
3	F	253	VAL	2.3
1	B	88	LYS	2.3
3	F	294	ALA	2.3
2	C	166	ASP	2.3
1	B	111	LEU	2.3
2	C	6	LEU	2.3
2	E	428	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	C	367	ASP	2.3
2	E	434	SER	2.3
1	A	106	GLU	2.3
2	C	345	LEU	2.2
2	C	408	PRO	2.2
1	B	147	ALA	2.2
1	B	85	GLY	2.2
2	E	385	GLU	2.2
2	E	27	ALA	2.2
1	A	48	PRO	2.2
1	A	104	LYS	2.2
2	E	429	GLY	2.2
1	B	51	GLN	2.2
2	C	266	ALA	2.2
1	A	59	TRP	2.2
1	A	74	LEU	2.2
1	B	74	LEU	2.2
2	C	370	GLY	2.2
1	B	102	ARG	2.1
2	C	28	PHE	2.1
2	C	319	ILE	2.1
2	E	53	LEU	2.1
1	B	100	ALA	2.1
2	C	46	SER	2.1
1	A	60	LEU	2.1
1	A	152	LEU	2.1
2	E	30	MET	2.1
2	C	141	ALA	2.1
2	C	368	THR	2.1
2	C	172	LEU	2.1
2	C	371	LEU	2.1
1	B	131	LYS	2.0
2	E	368	THR	2.0
2	C	223	ALA	2.0
2	C	420	ASP	2.0
2	E	375	THR	2.0
2	C	67	GLY	2.0
2	C	372	SER	2.0
1	A	56	ALA	2.0
2	E	378	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

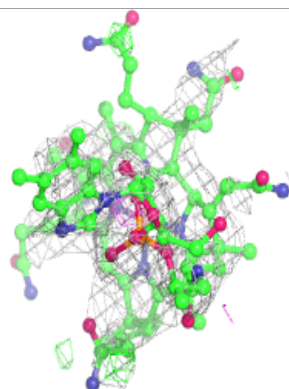
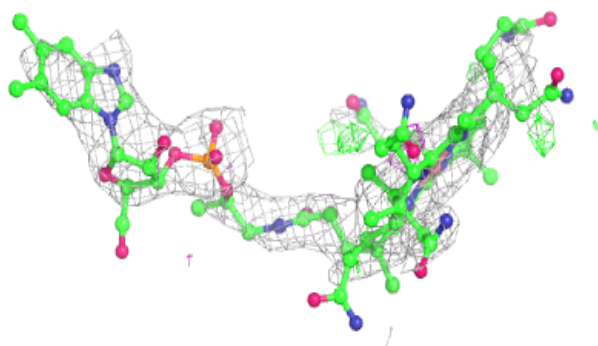
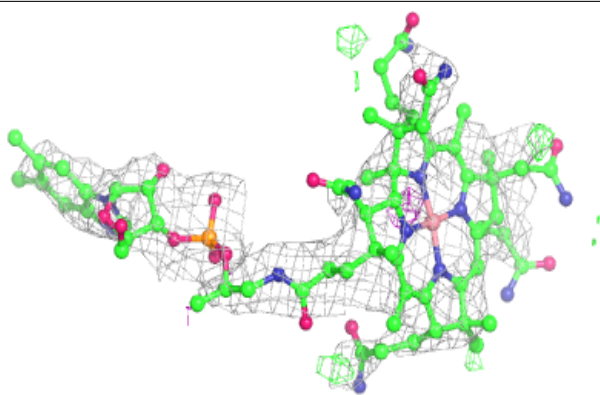
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	GOL	D	405	6/6	0.59	0.23	66,77,84,86	0
4	CA	B	301	1/1	0.77	0.21	76,76,76,76	0
7	GOL	D	404	6/6	0.83	0.21	50,67,73,75	0
7	GOL	E	504	6/6	0.83	0.23	61,81,88,90	0
7	GOL	E	503	6/6	0.84	0.20	70,75,76,84	0
6	B12	E	502	91/91	0.85	0.25	81,134,181,183	0
7	GOL	F	402	6/6	0.87	0.22	48,50,68,71	0
6	B12	C	502	91/91	0.88	0.25	57,106,145,159	0
7	GOL	D	401	6/6	0.90	0.25	37,54,60,63	0
7	GOL	F	403	6/6	0.90	0.25	62,80,85,89	0
7	GOL	D	402	6/6	0.92	0.21	70,73,77,78	0
4	CA	A	301	1/1	0.92	0.32	70,70,70,70	0
7	GOL	F	401	6/6	0.94	0.17	41,49,52,53	0
5	SF4	E	501	8/8	0.96	0.07	132,148,168,242	0
5	SF4	C	501	8/8	0.97	0.08	110,118,140,229	0
7	GOL	D	403	6/6	0.98	0.16	44,46,53,65	0

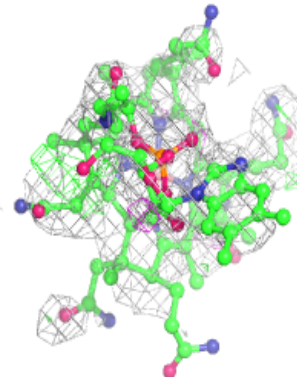
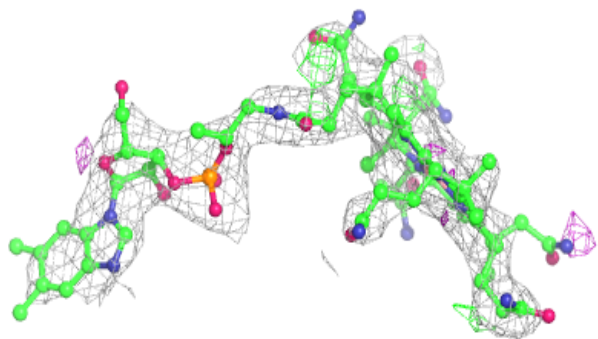
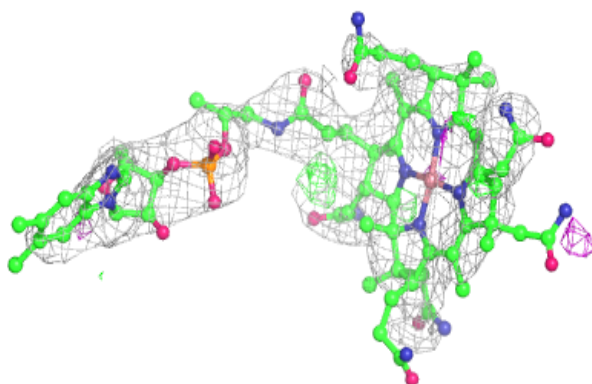
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

There are no such residues in this entry.