Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 01:02 AM EST

PDB ID	:	4DJE
Title	:	Crystal structure of folate-bound corrinoid iron-sulfur protein (CFeSP) in complex with its methyltransferase (MeTr), co-crystallized with folate
Authors	:	Kung, Y.; Drennan, C.L.
Deposited on	:	2012-02-01
Resolution	:	3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

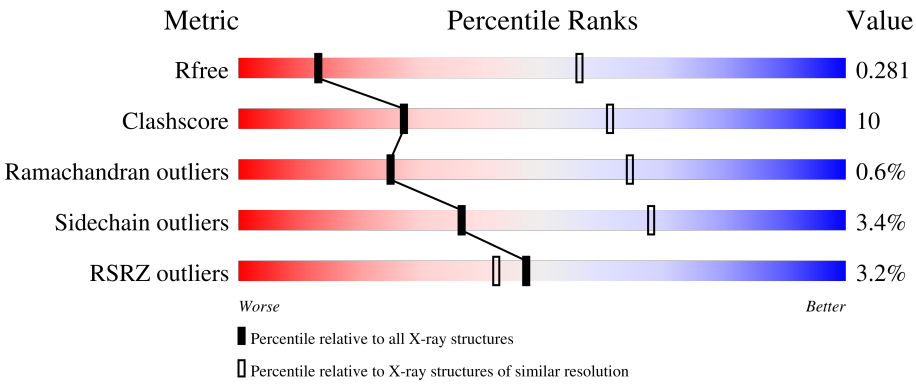
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	262	79% 20% •
1	B	262	82% 18%
2	C	446	4% 74% 21% • •
2	E	446	10% 76% 21% • •
3	D	323	84% 15% •

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Mol	Chain	Length	Quality of chain
3	F	323	85% 15%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SF4	E	501	-	-	X	-
7	B12	E	502	-	-	-	X

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 15367 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
			Total	C	N	O	S			
1	A	262	1997	1252	344	384	17	0	0	0
1	B	262	1997	1252	344	384	17	0	0	0

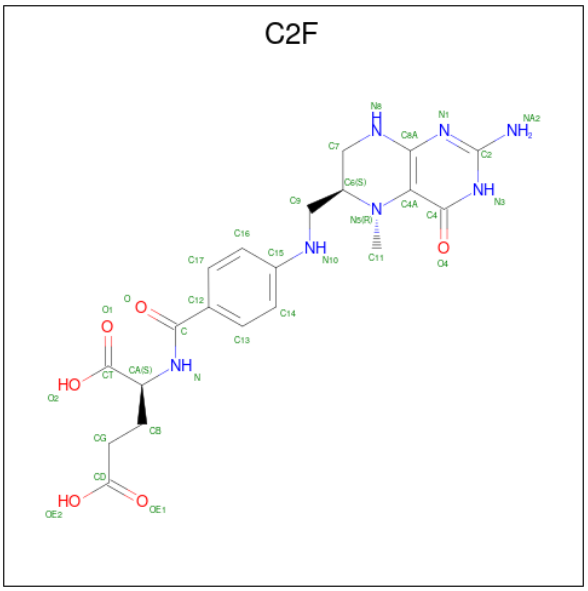
- Molecule 2 is a protein called Corrinoid/iron-sulfur protein large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	C	441	3139	1975	545	609	10	0	0	0
2	E	441	3034	1910	535	580	9	0	0	0

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

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

- Molecule 4 is 5-METHYL-5,6,7,8-TETRAHYDROFOLIC ACID (three-letter code: C2F) (formula: $C_{20}H_{25}N_7O_6$).

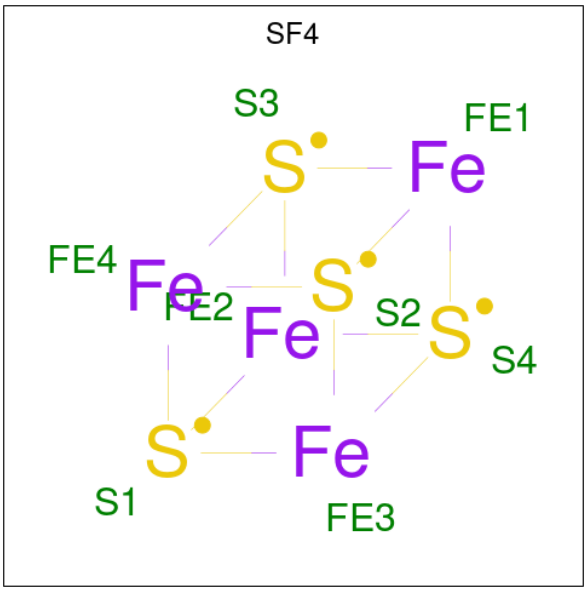


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			33	20	7	6		
4	B	1	Total	C	N	O	0	0
			33	20	7	6		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

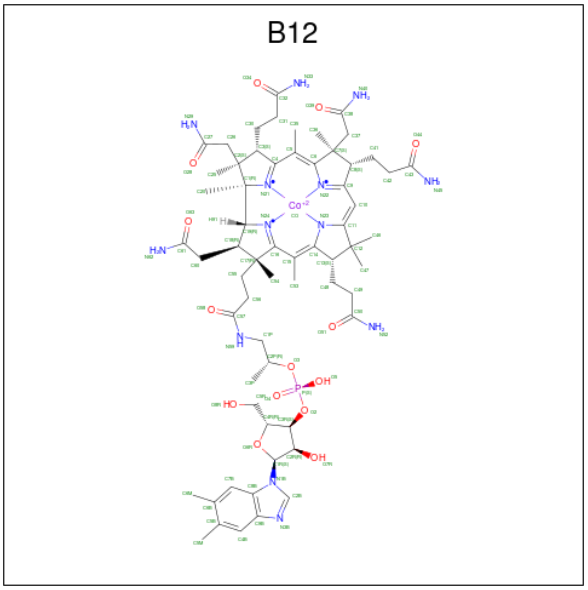
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	B	1	Total	Ca	0	0
			1	1		

- Molecule 6 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).



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

- Molecule 7 is COBALAMIN (three-letter code: B12) (formula: $C_{62}H_{89}CoN_{13}O_{14}P$).



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

- Molecule 8 is water.

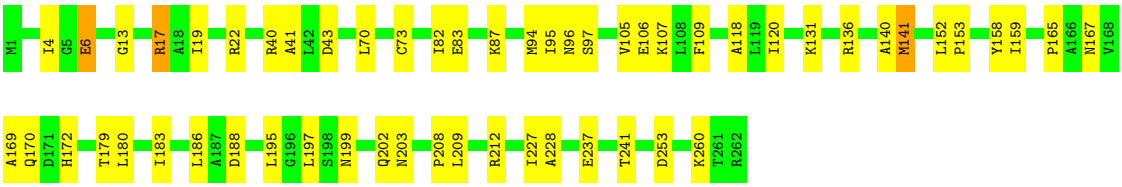
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	3	Total O 3 3	0	0
8	B	3	Total O 3 3	0	0
8	D	2	Total O 2 2	0	0
8	E	1	Total O 1 1	0	0
8	F	3	Total O 3 3	0	0

3 Residue-property plots (i)

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

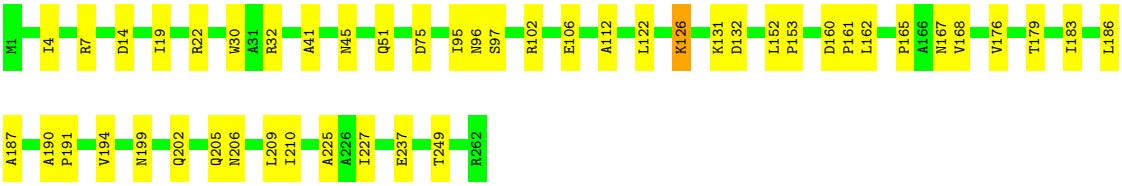
• Molecule 1: 5-methyltetrahydrofolate corrinoid/iron sulfur protein methyltransferase

Chain A:



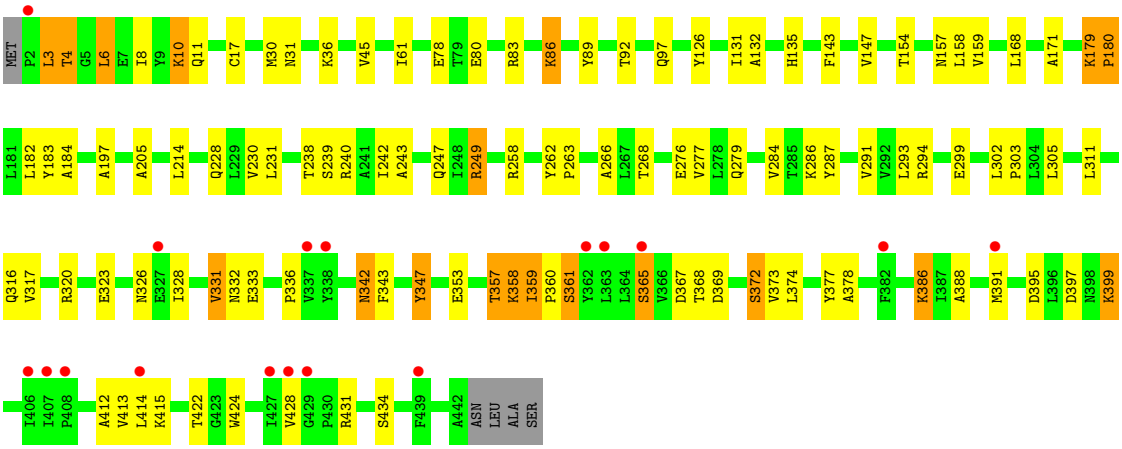
• Molecule 1: 5-methyltetrahydrofolate corrinoid/iron sulfur protein methyltransferase

Chain B:



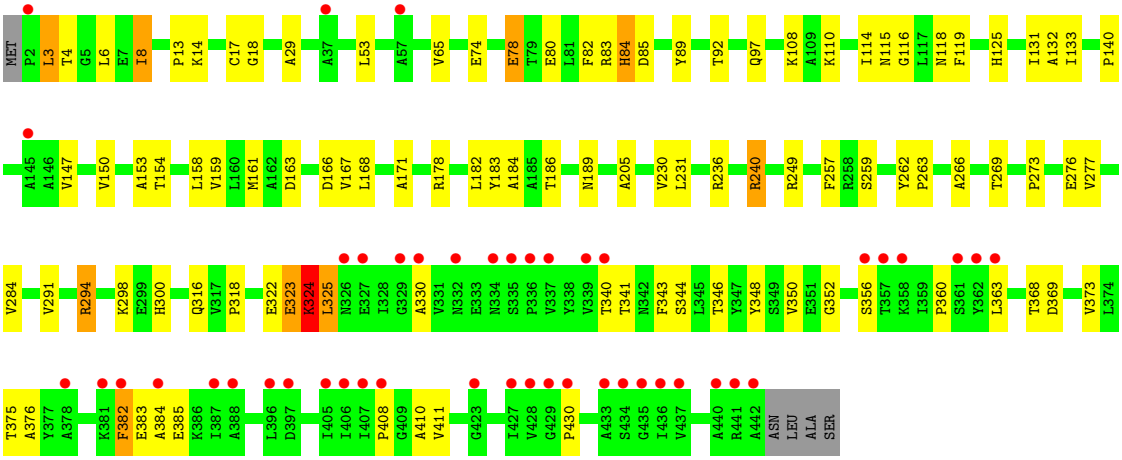
• Molecule 2: Corrinoid/iron-sulfur protein large subunit

Chain C:



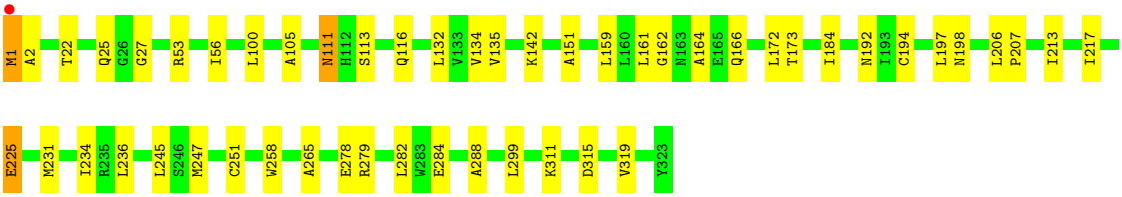
• Molecule 2: Corrinoid/iron-sulfur protein large subunit

Chain E:



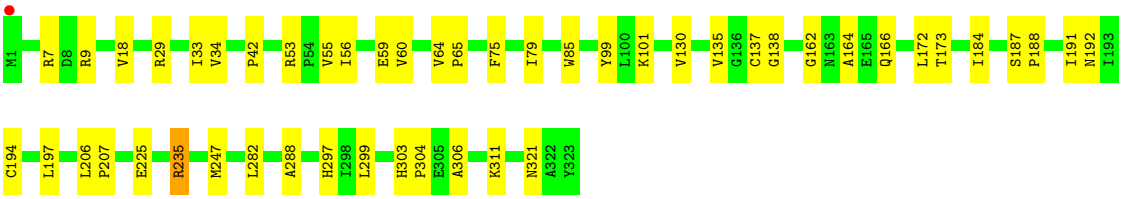
• Molecule 3: Corrinoid/iron-sulfur protein small subunit

Chain D:



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

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	136.42Å 250.66Å 82.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.46 – 3.50 48.46 – 3.50	Depositor EDS
% Data completeness (in resolution range)	95.6 (48.46-3.50) 95.4 (48.46-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.71 (at 3.48Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.240 , 0.289 0.232 , 0.281	Depositor DCC
R_{free} test set	1778 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	97.3	Xtriage
Anisotropy	0.809	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 85.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	15367	wwPDB-VP
Average B, all atoms (Å^2)	131.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: B12, SF4, CA, C2F

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	0.20	0/2023	0.36	0/2738
1	B	0.20	0/2023	0.37	0/2738
2	C	0.41	0/3195	0.50	0/4366
2	E	0.34	0/3084	0.46	1/4224 (0.0%)
3	D	0.19	0/2507	0.37	0/3408
3	F	0.19	0/2507	0.36	0/3408
All	All	0.28	0/15339	0.42	1/20882 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	384	ALA	N-CA-CB	-5.44	102.48	110.10

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	1997	0	2039	38	0
1	B	1997	0	2039	33	0
2	C	3139	0	2906	97	0
2	E	3034	0	2760	76	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	2461	0	2461	30	0
3	F	2461	0	2461	26	0
4	A	33	0	23	1	0
4	B	33	0	23	2	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	C	8	0	0	0	0
6	E	8	0	0	2	0
7	C	91	0	87	17	0
7	E	91	0	88	20	0
8	A	3	0	0	0	0
8	B	3	0	0	0	0
8	D	2	0	0	0	0
8	E	1	0	0	0	0
8	F	3	0	0	0	0
All	All	15367	0	14887	305	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 10.

All (305) 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:C:331:VAL:H	2:C:360:PRO:CB	1.56	1.17
2:E:350:VAL:HG11	2:E:363:LEU:HD11	1.14	1.13
2:C:331:VAL:N	2:C:360:PRO:HB3	1.62	1.11
2:C:331:VAL:HA	2:C:360:PRO:HB2	1.39	1.05
2:E:350:VAL:HG11	2:E:363:LEU:CD1	1.89	1.02
2:E:350:VAL:CG1	2:E:363:LEU:HD11	1.88	1.02
2:E:325:LEU:HD23	2:E:325:LEU:H	1.35	0.91
2:E:325:LEU:HD23	2:E:325:LEU:N	1.86	0.90
2:C:331:VAL:H	2:C:360:PRO:HB3	0.76	0.90
2:C:336:PRO:HG2	2:C:361:SER:OG	1.75	0.86
2:C:422:THR:O	2:C:424:TRP:CE3	2.30	0.84
2:C:331:VAL:N	2:C:360:PRO:CB	2.30	0.84
2:E:411:VAL:HG12	2:E:411:VAL:O	1.75	0.84
2:E:376:ALA:HB1	2:E:382:PHE:HB2	1.58	0.83
2:C:331:VAL:CA	2:C:360:PRO:HB2	2.10	0.81
2:E:376:ALA:CB	2:E:382:PHE:HB2	2.12	0.79
7:C:502:B12:H533	7:C:502:B12:H491	1.63	0.78
2:E:346:THR:HA	7:E:502:B12:H3P1	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:368:THR:O	2:C:369:ASP:HB2	1.86	0.74
7:E:502:B12:H533	7:E:502:B12:H491	1.71	0.72
2:C:422:THR:O	2:C:424:TRP:HE3	1.73	0.72
2:C:412:ALA:HB1	2:C:428:VAL:CB	2.20	0.70
2:C:320:ARG:HB2	2:C:342:ASN:ND2	2.08	0.69
3:D:164:ALA:HB2	3:D:172:LEU:HD23	1.75	0.69
2:E:330:ALA:O	2:E:360:PRO:HB3	1.94	0.68
1:A:136:ARG:HH22	1:A:172:HIS:HD1	1.40	0.68
2:C:413:VAL:C	2:C:415:LYS:H	1.97	0.68
2:C:378:ALA:HB2	7:C:502:B12:H331	1.60	0.67
2:C:331:VAL:HA	2:C:360:PRO:CB	2.22	0.66
2:E:430:PRO:HG2	7:E:502:B12:HM61	1.77	0.66
2:C:320:ARG:HB2	2:C:342:ASN:HD22	1.61	0.66
2:C:331:VAL:CA	2:C:360:PRO:CB	2.73	0.66
3:F:164:ALA:HB2	3:F:172:LEU:HD23	1.78	0.66
7:E:502:B12:O39	7:E:502:B12:H361	1.94	0.65
2:E:330:ALA:O	2:E:360:PRO:CB	2.45	0.65
7:C:502:B12:H531	7:C:502:B12:H543	1.79	0.65
7:E:502:B12:H531	7:E:502:B12:H561	1.79	0.64
1:B:132:ASP:OD1	2:C:86:LYS:NZ	2.30	0.64
2:E:266:ALA:HB3	2:E:291:VAL:HG12	1.79	0.64
3:D:56:ILE:HD12	3:D:311:LYS:HG2	1.79	0.64
7:C:502:B12:N33	7:C:502:B12:H353	2.13	0.63
7:E:502:B12:H561	7:E:502:B12:C53	2.27	0.63
2:C:357:THR:O	2:C:358:LYS:CB	2.47	0.63
1:A:167:ASN:O	3:F:192:ASN:ND2	2.32	0.62
2:C:413:VAL:O	2:C:415:LYS:N	2.31	0.62
2:E:230:VAL:HG12	2:E:263:PRO:HG2	1.81	0.62
2:C:332:ASN:O	2:C:333:GLU:CB	2.47	0.62
1:A:141:MET:HG2	1:A:186:LEU:HG	1.82	0.61
2:C:266:ALA:HB3	2:C:291:VAL:HG12	1.82	0.61
2:C:277:VAL:HG11	3:D:282:LEU:HD21	1.82	0.61
2:C:395:ASP:O	2:C:395:ASP:CG	2.39	0.61
2:C:326:ASN:CB	2:C:347:TYR:OH	2.48	0.61
2:C:374:LEU:HB3	7:C:502:B12:H203	1.83	0.60
2:E:131:ILE:HD12	2:E:154:THR:HG21	1.82	0.60
3:D:194:CYS:O	3:D:198:ASN:ND2	2.32	0.60
3:D:53:ARG:NH1	3:D:315:ASP:OD1	2.34	0.59
3:D:217:ILE:HD13	3:D:251:CYS:HB3	1.83	0.59
1:B:152:LEU:HD12	1:B:153:PRO:HD2	1.84	0.59
2:C:179:LYS:N	2:C:180:PRO:HD2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:ILE:O	1:B:22:ARG:NH1	2.30	0.59
2:E:340:THR:OG1	2:E:341:THR:N	2.35	0.59
3:D:22:THR:H	3:D:25:GLN:HB2	1.67	0.59
1:B:199:ASN:ND2	4:B:302:C2F:O4	2.36	0.58
2:E:8:ILE:HD11	2:E:29:ALA:HA	1.83	0.58
3:D:206:LEU:HD12	3:D:207:PRO:HD2	1.86	0.58
2:E:325:LEU:N	2:E:325:LEU:CD2	2.59	0.58
2:C:422:THR:O	2:C:424:TRP:CZ3	2.55	0.58
3:F:288:ALA:HB1	3:F:299:LEU:HD13	1.85	0.58
3:D:132:LEU:HB2	3:D:159:LEU:HD22	1.84	0.58
2:E:231:LEU:HD13	2:E:262:TYR:HB2	1.86	0.58
2:C:386:LYS:O	2:C:386:LYS:HD3	2.03	0.57
1:A:199:ASN:ND2	4:A:300:C2F:O4	2.37	0.57
1:B:168:VAL:HG21	7:C:502:B12:H532	1.85	0.57
2:C:347:TYR:HD1	2:C:347:TYR:C	2.07	0.57
2:E:115:ASN:O	2:E:118:ASN:ND2	2.36	0.57
1:A:253:ASP:O	1:B:205:GLN:NE2	2.37	0.57
7:C:502:B12:H362	7:C:502:B12:H351	1.86	0.57
2:C:358:LYS:O	2:C:359:ILE:CB	2.52	0.57
2:C:92:THR:HG21	2:C:284:VAL:HG12	1.86	0.57
2:C:6:LEU:HD22	2:C:10:LYS:HE2	1.86	0.57
1:A:131:LYS:NZ	2:E:85:ASP:O	2.37	0.56
1:B:75:ASP:OD1	1:B:96:ASN:ND2	2.37	0.56
2:E:411:VAL:O	2:E:411:VAL:CG1	2.48	0.56
2:C:157:ASN:HA	2:C:179:LYS:HG3	1.87	0.56
2:C:347:TYR:C	2:C:347:TYR:CD1	2.79	0.56
2:C:230:VAL:HG12	2:C:263:PRO:HG2	1.87	0.56
2:E:277:VAL:HG11	3:F:282:LEU:HD21	1.88	0.56
3:F:59:GLU:HA	3:F:99:TYR:HB3	1.86	0.56
1:B:160:ASP:OD2	4:B:302:C2F:NA2	2.38	0.56
2:C:158:LEU:HB2	2:C:180:PRO:HD3	1.89	0.55
2:E:168:LEU:HD21	2:E:182:LEU:HD22	1.89	0.55
2:C:231:LEU:HD13	2:C:262:TYR:HB2	1.89	0.55
2:E:65:VAL:HG22	2:E:74:GLU:HG2	1.89	0.54
2:E:368:THR:O	2:E:369:ASP:CB	2.55	0.54
2:C:373:VAL:O	2:C:377:TYR:HB2	2.08	0.54
3:F:162:GLY:HA2	3:F:184:ILE:HB	1.90	0.54
2:E:375:THR:HG23	7:E:502:B12:H412	1.89	0.54
2:C:326:ASN:CG	2:C:347:TYR:OH	2.47	0.54
1:B:187:ALA:HB3	1:B:191:PRO:HD3	1.90	0.54
1:A:19:ILE:O	1:A:22:ARG:NH1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLN:HG3	1:A:203:ASN:ND2	2.24	0.53
2:C:328:ILE:O	2:C:360:PRO:HA	2.09	0.53
1:B:126:LYS:HD3	1:B:126:LYS:H	1.73	0.53
2:C:413:VAL:C	2:C:415:LYS:N	2.59	0.53
3:D:265:ALA:O	3:D:279:ARG:NH2	2.40	0.53
2:E:166:ASP:OD1	2:E:166:ASP:N	2.40	0.53
1:B:165:PRO:HG3	1:B:202:GLN:HB3	1.90	0.53
3:D:100:LEU:HB3	3:D:134:VAL:HG22	1.91	0.52
3:D:166:GLN:HA	3:D:197:LEU:HD13	1.91	0.52
2:E:383:GLU:O	2:E:385:GLU:N	2.43	0.52
2:E:92:THR:HG21	2:E:284:VAL:HG12	1.92	0.52
3:F:29:ARG:NH2	3:F:130:VAL:O	2.42	0.52
2:C:353:GLU:HG2	2:C:434:SER:HA	1.92	0.52
3:D:213:ILE:HG13	3:D:247:MET:HB2	1.91	0.52
2:C:317:VAL:HG13	2:C:320:ARG:HH22	1.74	0.51
7:E:502:B12:H291	7:E:502:B12:H3	1.74	0.51
2:E:163:ASP:O	2:E:189:ASN:ND2	2.44	0.51
2:E:276:GLU:OE2	2:E:294:ARG:N	2.35	0.51
2:C:242:ILE:HG12	2:C:286:LYS:HG3	1.93	0.51
2:E:344:SER:O	2:E:348:TYR:HB2	2.11	0.51
7:E:502:B12:H353	7:E:502:B12:C32	2.40	0.51
3:D:247:MET:SD	3:D:247:MET:N	2.84	0.50
1:A:197:LEU:HB3	1:A:228:ALA:HB2	1.92	0.50
2:C:147:VAL:HG11	2:C:171:ALA:HB1	1.93	0.50
2:E:376:ALA:HB3	2:E:382:PHE:HB2	1.93	0.50
2:C:3:LEU:HD12	2:C:8:ILE:HG13	1.92	0.50
2:C:374:LEU:HB3	7:C:502:B12:C20	2.41	0.50
1:A:40:ARG:NH2	1:A:260:LYS:O	2.45	0.50
1:A:165:PRO:HG3	1:A:202:GLN:HB3	1.94	0.50
1:A:180:LEU:HD11	1:A:195:LEU:HD11	1.94	0.50
7:E:502:B12:H351	7:E:502:B12:H362	1.94	0.49
3:D:151:ALA:HB2	3:D:161:LEU:HD21	1.93	0.49
2:E:132:ALA:HA	2:E:159:VAL:HG13	1.95	0.49
2:C:342:ASN:OD1	2:C:367:ASP:HA	2.12	0.49
2:E:330:ALA:O	2:E:360:PRO:HB2	2.13	0.49
1:B:4:ILE:HB	1:B:227:ILE:HG12	1.95	0.49
3:D:258:TRP:NE1	3:D:284:GLU:OE1	2.41	0.49
7:E:502:B12:H363	7:E:502:B12:H411	1.66	0.49
2:C:374:LEU:HD13	7:C:502:B12:H253	1.95	0.49
7:C:502:B12:O39	7:C:502:B12:H361	2.13	0.49
1:A:4:ILE:HD12	1:A:227:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:502:B12:H533	7:E:502:B12:C49	2.42	0.48
3:D:113:SER:HB3	3:D:116:GLN:HG3	1.94	0.48
1:A:43:ASP:HA	1:A:73:CYS:HB3	1.95	0.48
1:A:82:ILE:HG21	1:A:95:ILE:HG23	1.96	0.48
2:E:17:CYS:N	6:E:501:SF4:S3	2.86	0.48
2:E:186:THR:OG1	2:E:189:ASN:OD1	2.24	0.48
1:B:122:LEU:HD22	1:B:162:LEU:HD21	1.95	0.48
1:A:6:GLU:HB3	1:A:227:ILE:HG22	1.94	0.48
3:D:234:ILE:HG23	3:D:245:LEU:HB3	1.96	0.48
1:B:95:ILE:HD11	1:B:112:ALA:HB2	1.95	0.48
2:C:78:GLU:HG2	2:C:249:ARG:NH2	2.29	0.48
2:C:397:ASP:CB	2:C:424:TRP:HZ2	2.27	0.48
3:D:173:THR:HG23	3:D:206:LEU:HD22	1.96	0.48
1:B:7:ARG:NH2	1:B:14:ASP:OD2	2.47	0.48
2:E:183:TYR:CG	2:E:184:ALA:HB2	2.49	0.48
1:A:152:LEU:HD12	1:A:153:PRO:HD2	1.95	0.48
1:B:96:ASN:HA	1:B:97:SER:HA	1.61	0.47
2:C:395:ASP:O	2:C:395:ASP:OD1	2.30	0.47
2:E:116:GLY:O	2:E:298:LYS:NZ	2.46	0.47
1:A:106:GLU:HG3	1:A:107:LYS:HG3	1.95	0.47
1:A:241:THR:HG23	1:B:210:ILE:HD13	1.96	0.47
2:C:97:GLN:HA	2:C:132:ALA:HB3	1.96	0.47
2:E:147:VAL:HG11	2:E:171:ALA:HB1	1.95	0.47
1:A:179:THR:O	1:A:183:ILE:HG13	2.14	0.47
1:A:83:GLU:HG2	1:A:87:LYS:HE3	1.97	0.47
7:E:502:B12:H531	7:E:502:B12:C56	2.43	0.47
2:C:131:ILE:HD12	2:C:154:THR:HG21	1.95	0.47
2:C:183:TYR:CG	2:C:184:ALA:HB2	2.49	0.47
7:C:502:B12:H91	7:C:502:B12:H262	1.68	0.47
1:A:40:ARG:HA	1:A:70:LEU:HD22	1.97	0.46
2:C:299:GLU:OE1	2:C:299:GLU:N	2.45	0.46
2:E:236:ARG:HD3	2:E:269:THR:HG21	1.98	0.46
2:E:323:GLU:O	2:E:324:LYS:CB	2.63	0.46
1:B:45:ASN:ND2	1:B:75:ASP:OD2	2.47	0.46
2:E:430:PRO:HD2	7:E:502:B12:HM63	1.98	0.46
2:C:388:ALA:O	2:C:391:MET:HB2	2.15	0.46
7:E:502:B12:H531	7:E:502:B12:C55	2.46	0.46
1:B:179:THR:O	1:B:183:ILE:HG13	2.15	0.46
2:E:140:PRO:HB3	2:E:167:VAL:HG22	1.97	0.46
1:A:140:ALA:HB1	1:A:159:ILE:HD13	1.97	0.46
2:C:372:SER:OG	7:C:502:B12:H2P	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:80:GLU:O	2:E:249:ARG:NH2	2.48	0.46
2:C:343:PHE:HD2	2:C:372:SER:HG	1.64	0.46
2:C:168:LEU:HD21	2:C:182:LEU:HD22	1.97	0.46
2:C:399:LYS:HA	2:C:399:LYS:HD3	1.58	0.46
2:C:183:TYR:CD2	2:C:184:ALA:HB2	2.50	0.45
1:A:208:PRO:O	1:A:212:ARG:HG2	2.16	0.45
7:C:502:B12:H531	7:C:502:B12:H552	1.98	0.45
2:E:133:ILE:HD11	2:E:150:VAL:HG11	1.98	0.45
2:C:126:TYR:HB3	2:C:305:LEU:HD23	1.98	0.45
2:E:257:PHE:CE2	2:E:259:SER:HB2	2.52	0.45
2:E:323:GLU:O	2:E:324:LYS:HD3	2.17	0.45
2:C:238:THR:HB	2:C:279:GLN:HG3	1.98	0.45
2:C:378:ALA:CB	7:C:502:B12:H331	2.27	0.45
7:C:502:B12:H543	7:C:502:B12:C53	2.46	0.45
3:D:1:MET:SD	3:D:2:ALA:N	2.90	0.45
2:E:183:TYR:CD2	2:E:184:ALA:HB2	2.52	0.45
2:C:132:ALA:HA	2:C:159:VAL:HG13	1.99	0.45
7:C:502:B12:H201	7:C:502:B12:H18	1.80	0.45
7:E:502:B12:H262	7:E:502:B12:H91	1.89	0.45
3:F:206:LEU:HD12	3:F:207:PRO:HD2	1.99	0.45
2:C:182:LEU:HD12	2:C:197:ALA:HB2	1.98	0.44
2:E:373:VAL:HG11	2:E:408:PRO:HG2	1.99	0.44
2:C:268:THR:HG21	2:C:293:LEU:HD23	1.99	0.44
2:E:352:GLY:O	2:E:356:SER:CB	2.65	0.44
1:A:188:ASP:HB2	2:C:4:THR:HG21	1.99	0.44
3:D:162:GLY:HA2	3:D:184:ILE:HB	1.99	0.44
3:D:288:ALA:HB1	3:D:299:LEU:HD13	1.97	0.44
2:E:343:PHE:CD1	2:E:344:SER:N	2.86	0.44
1:A:170:GLN:NE2	1:B:249:THR:O	2.40	0.44
2:C:353:GLU:OE1	2:C:353:GLU:HA	2.18	0.44
1:B:4:ILE:HG12	1:B:41:ALA:HB3	1.99	0.44
3:D:231:MET:HB3	3:D:231:MET:HE2	1.85	0.44
3:F:303:HIS:HD2	3:F:306:ALA:H	1.66	0.44
2:C:80:GLU:HG3	2:C:86:LYS:HB3	2.00	0.43
2:E:119:PHE:O	2:E:125:HIS:ND1	2.50	0.43
3:F:75:PHE:O	3:F:79:ILE:N	2.51	0.43
1:A:94:MET:HG2	1:A:118:ALA:HB3	2.00	0.43
3:F:7:ARG:HD3	3:F:9:ARG:HH12	1.82	0.43
1:A:253:ASP:HB3	1:B:205:GLN:HE21	1.81	0.43
3:F:173:THR:HG23	3:F:206:LEU:HD22	1.99	0.43
2:E:158:LEU:HD13	2:E:178:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:316:GLN:O	2:E:318:PRO:HD3	2.19	0.43
2:C:238:THR:HB	2:C:279:GLN:HE21	1.83	0.43
2:C:276:GLU:OE2	2:C:294:ARG:N	2.50	0.43
2:C:135:HIS:HD2	2:C:143:PHE:HB2	1.83	0.43
2:C:323:GLU:HA	2:C:365:SER:O	2.19	0.43
2:E:183:TYR:HA	2:E:205:ALA:HB3	2.00	0.43
3:F:42:PRO:HD3	3:F:235:ARG:HG2	1.99	0.43
3:F:56:ILE:HD12	3:F:311:LYS:HG3	2.00	0.43
3:F:191:ILE:HA	3:F:194:CYS:HB3	1.99	0.43
2:C:83:ARG:HD2	2:C:311:LEU:HD12	2.00	0.43
2:E:161:MET:HG2	2:E:183:TYR:HB3	2.01	0.43
1:A:169:ALA:HB1	1:A:172:HIS:CD2	2.54	0.43
1:B:161:PRO:HB2	1:B:176:VAL:HG13	2.00	0.43
2:C:183:TYR:HA	2:C:205:ALA:HB3	1.99	0.43
2:C:299:GLU:HB3	3:D:278:GLU:HB2	2.01	0.43
3:F:303:HIS:HA	3:F:304:PRO:HD3	1.87	0.43
2:E:82:PHE:HB3	2:E:84:HIS:CD2	2.54	0.43
2:C:6:LEU:O	2:C:10:LYS:HG2	2.19	0.42
2:C:61:ILE:HB	2:C:78:GLU:H	1.84	0.42
3:F:166:GLN:HA	3:F:197:LEU:HD13	2.01	0.42
3:F:65:PRO:HD2	3:F:79:ILE:HD11	2.01	0.42
2:C:183:TYR:HA	2:C:184:ALA:HA	1.72	0.42
2:C:317:VAL:CG1	2:C:320:ARG:HH12	2.32	0.42
3:F:137:CYS:SG	3:F:138:GLY:N	2.93	0.42
1:A:13:GLY:O	1:A:17:ARG:HD3	2.19	0.42
2:E:118:ASN:HB3	2:E:125:HIS:CE1	2.54	0.42
1:B:190:ALA:HA	1:B:191:PRO:HD3	1.88	0.42
3:D:105:ALA:O	3:D:142:LYS:NZ	2.44	0.42
3:F:18:VAL:HG22	3:F:34:VAL:HG22	2.00	0.42
2:E:18:GLY:N	6:E:501:SF4:S3	2.82	0.42
1:A:209:LEU:HD21	1:B:237:GLU:HB3	2.01	0.42
2:C:31:ASN:O	2:C:36:LYS:N	2.50	0.42
2:E:240:ARG:NH2	3:F:321:ASN:O	2.48	0.42
2:E:343:PHE:CE2	7:E:502:B12:N52	2.88	0.42
1:A:96:ASN:HA	1:A:97:SER:HA	1.67	0.42
2:E:346:THR:HG23	7:E:502:B12:O2	2.20	0.42
1:A:237:GLU:HB3	1:B:209:LEU:HD21	2.00	0.42
3:D:111:ASN:O	3:D:111:ASN:ND2	2.45	0.42
1:B:102:ARG:O	1:B:106:GLU:HG2	2.20	0.42
2:C:86:LYS:HE3	2:C:89:TYR:OH	2.20	0.41
2:C:258:ARG:HD3	2:C:258:ARG:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:22:THR:O	3:D:27:GLY:N	2.45	0.41
2:E:183:TYR:HA	2:E:184:ALA:HA	1.67	0.41
2:E:346:THR:HG21	2:E:373:VAL:HG23	2.01	0.41
3:F:235:ARG:HH12	3:F:297:HIS:HE1	1.67	0.41
1:A:120:ILE:HG12	1:A:158:TYR:HB2	2.01	0.41
2:C:243:ALA:O	2:C:247:GLN:HG2	2.20	0.41
2:C:374:LEU:HD23	2:C:374:LEU:HA	1.92	0.41
1:A:183:ILE:HA	1:A:186:LEU:HD13	2.02	0.41
1:B:131:LYS:HB2	2:C:316:GLN:HG2	2.01	0.41
2:E:110:LYS:O	2:E:114:ILE:HG13	2.21	0.41
2:E:346:THR:HA	7:E:502:B12:C3P	2.43	0.41
2:C:357:THR:CG2	2:C:358:LYS:N	2.83	0.41
2:E:161:MET:HA	2:E:183:TYR:O	2.20	0.41
2:E:350:VAL:CG1	2:E:363:LEU:CD1	2.71	0.41
2:E:408:PRO:C	2:E:410:ALA:H	2.24	0.41
2:E:97:GLN:HA	2:E:132:ALA:HB3	2.03	0.41
2:C:214:LEU:HD11	2:C:231:LEU:HG	2.02	0.41
1:B:194:VAL:HA	1:B:225:ALA:O	2.20	0.41
2:C:239:SER:OG	3:D:319:VAL:O	2.26	0.41
2:E:108:LYS:HE2	2:E:153:ALA:HB2	2.03	0.41
1:B:7:ARG:HG2	1:B:30:TRP:CE3	2.56	0.41
3:F:187:SER:HA	3:F:188:PRO:HD3	1.81	0.41
3:F:101:LYS:HD2	3:F:135:VAL:HG13	2.03	0.40
1:A:105:VAL:HG13	1:A:109:PHE:CD1	2.56	0.40
1:B:167:ASN:O	3:D:192:ASN:ND2	2.54	0.40
1:B:167:ASN:OD1	1:B:168:VAL:N	2.54	0.40
2:C:249:ARG:NH1	2:C:287:TYR:HB3	2.36	0.40
2:C:302:LEU:HB3	2:C:303:PRO:HD3	2.02	0.40
1:A:141:MET:HG3	2:C:30:MET:SD	2.60	0.40
2:C:342:ASN:OD1	2:C:368:THR:N	2.53	0.40
2:E:343:PHE:HD1	2:E:344:SER:H	1.69	0.40
3:F:33:ILE:HG21	3:F:55:VAL:HG11	2.03	0.40
3:F:60:VAL:HG13	3:F:85:TRP:CD2	2.55	0.40
2:C:286:LYS:HD3	2:C:286:LYS:HA	1.90	0.40
3:D:225:GLU:H	3:D:225:GLU:HG3	1.52	0.40
1:A:4:ILE:HG12	1:A:41:ALA:HB3	2.02	0.40
1:B:183:ILE:O	1:B:186:LEU:HG	2.22	0.40
7:C:502:B12:H411	7:C:502:B12:H363	1.63	0.40
2:E:78:GLU:OE2	2:E:89:TYR:N	2.55	0.40
2:E:273:PRO:HB2	2:E:300:HIS:CE1	2.56	0.40
7:E:502:B12:H301	7:E:502:B12:H253	1.89	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
1	B	260/262 (99%)	249 (96%)	11 (4%)	0	100	100
2	C	439/446 (98%)	412 (94%)	19 (4%)	8 (2%)	8	41
2	E	439/446 (98%)	413 (94%)	22 (5%)	4 (1%)	17	56
3	D	321/323 (99%)	307 (96%)	14 (4%)	0	100	100
3	F	321/323 (99%)	306 (95%)	15 (5%)	0	100	100
All	All	2040/2062 (99%)	1936 (95%)	92 (4%)	12 (1%)	25	64

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	45	VAL
2	C	180	PRO
2	C	414	LEU
2	E	13	PRO
2	E	324	LYS
2	C	358	LYS
2	C	228	GLN
2	E	14	LYS
2	C	86	LYS
2	C	331	VAL
2	E	3	LEU
2	C	359	ILE

5.3.2 Protein sidechains (i)

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	214/214 (100%)	211 (99%)	3 (1%)	67	85
1	B	214/214 (100%)	210 (98%)	4 (2%)	57	80
2	C	282/356 (79%)	264 (94%)	18 (6%)	17	50
2	E	256/356 (72%)	241 (94%)	15 (6%)	19	53
3	D	261/261 (100%)	256 (98%)	5 (2%)	57	80
3	F	261/261 (100%)	256 (98%)	5 (2%)	57	80
All	All	1488/1662 (90%)	1438 (97%)	50 (3%)	37	68

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	17	ARG
1	A	141	MET
1	B	32	ARG
1	B	51	GLN
1	B	126	LYS
1	B	206	ASN
2	C	3	LEU
2	C	4	THR
2	C	6	LEU
2	C	10	LYS
2	C	11	GLN
2	C	17	CYS
2	C	179	LYS
2	C	240	ARG
2	C	249	ARG
2	C	342	ASN
2	C	347	TYR
2	C	357	THR
2	C	361	SER
2	C	365	SER
2	C	372	SER
2	C	386	LYS
2	C	399	LYS
2	C	431	ARG
3	D	1	MET

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Mol	Chain	Res	Type
3	D	111	ASN
3	D	135	VAL
3	D	225	GLU
3	D	236	LEU
2	E	3	LEU
2	E	4	THR
2	E	6	LEU
2	E	8	ILE
2	E	53	LEU
2	E	78	GLU
2	E	83	ARG
2	E	84	HIS
2	E	240	ARG
2	E	294	ARG
2	E	322	GLU
2	E	323	GLU
2	E	324	LYS
2	E	325	LEU
2	E	382	PHE
3	F	53	ARG
3	F	64	VAL
3	F	225	GLU
3	F	235	ARG
3	F	247	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	199	ASN
1	A	211	ASN
1	B	20	GLN
1	B	51	GLN
1	B	199	ASN
1	B	205	GLN
1	B	206	ASN
1	B	211	ASN
2	C	135	HIS
2	C	279	GLN
2	C	316	GLN
2	C	326	ASN
3	D	15	GLN
3	D	61	GLN

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Mol	Chain	Res	Type
3	D	80	ASN
3	D	116	GLN
3	D	126	GLN
3	D	168	ASN
3	D	210	HIS
3	D	303	HIS
2	E	97	GLN
2	E	135	HIS
2	E	316	GLN
3	F	15	GLN
3	F	61	GLN
3	F	116	GLN
3	F	126	GLN
3	F	303	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
4	C2F	A	300	-	33,35,35	2.34	5 (15%)	35,49,49	1.63	7 (20%)
7	B12	C	502	-	90,101,101	1.35	15 (16%)	137,166,166	2.04	37 (27%)
4	C2F	B	302	-	33,35,35	2.34	5 (15%)	35,49,49	1.62	7 (20%)
6	SF4	E	501	2	0,12,12	-	-	-		
7	B12	E	502	-	90,101,101	1.20	7 (7%)	137,166,166	1.97	30 (21%)
6	SF4	C	501	2	0,12,12	-	-	-		

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
6	SF4	E	501	2	-	-	0/6/5/5
4	C2F	A	300	-	-	2/22/35/35	0/3/3/3
7	B12	C	502	-	-	14/52/223/223	0/3/11/11
4	C2F	B	302	-	-	6/22/35/35	0/3/3/3
7	B12	E	502	-	-	22/52/223/223	0/3/11/11
6	SF4	C	501	2	-	-	0/6/5/5

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	300	C2F	C2-NA2	8.74	1.51	1.33
4	B	302	C2F	C2-NA2	8.73	1.51	1.33
4	B	302	C2F	O4-C4	5.62	1.38	1.24
4	A	300	C2F	O4-C4	5.60	1.38	1.24
4	B	302	C2F	C-N	5.38	1.45	1.34
4	A	300	C2F	C-N	5.35	1.45	1.34
7	C	502	B12	O6R-C1R	-3.74	1.35	1.41
7	C	502	B12	C54-C17	3.38	1.60	1.54
7	E	502	B12	C2R-C1R	3.38	1.58	1.53
7	E	502	B12	C54-C17	3.21	1.60	1.54
4	A	300	C2F	C7-C6	3.18	1.55	1.52
4	A	300	C2F	C15-N10	3.15	1.47	1.38
4	B	302	C2F	C15-N10	3.14	1.47	1.38
4	B	302	C2F	C7-C6	3.10	1.55	1.52
7	E	502	B12	O6R-C1R	-3.02	1.36	1.41
7	C	502	B12	O7R-C2R	-2.99	1.35	1.43
7	C	502	B12	C9-N22	2.98	1.38	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	502	B12	C13-C14	-2.76	1.47	1.52
7	C	502	B12	C2R-C1R	2.67	1.57	1.53
7	C	502	B12	C14-N23	2.49	1.38	1.35
7	C	502	B12	O44-C43	2.49	1.31	1.24
7	C	502	B12	C30-C31	2.38	1.60	1.52
7	E	502	B12	O7R-C2R	-2.33	1.37	1.43
7	C	502	B12	C36-C7	2.31	1.58	1.54
7	C	502	B12	C48-C49	2.25	1.59	1.52
7	E	502	B12	C41-C8	2.23	1.59	1.54
7	E	502	B12	O44-C43	2.16	1.30	1.24
7	C	502	B12	O51-C50	2.16	1.30	1.24
7	C	502	B12	C55-C56	2.11	1.58	1.53
7	C	502	B12	C6B-C5B	2.09	1.46	1.40
7	C	502	B12	C13-C14	-2.08	1.48	1.52
7	C	502	B12	C55-C17	-2.07	1.49	1.54

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	502	B12	C20-C1-C19	-9.40	100.30	109.36
7	C	502	B12	C20-C1-C19	-7.81	101.83	109.36
7	E	502	B12	C18-C17-C16	7.26	109.49	100.67
7	C	502	B12	C7B-C8B-C9B	7.19	127.65	120.54
7	C	502	B12	C18-C17-C16	6.11	108.10	100.67
7	E	502	B12	C7B-C8B-C9B	4.90	125.39	120.54
4	A	300	C2F	C8A-C4A-C4	4.87	118.25	114.44
4	B	302	C2F	C8A-C4A-C4	4.78	118.18	114.44
7	C	502	B12	C17-C16-N24	-4.55	104.14	111.15
7	C	502	B12	C15-C16-N24	4.55	128.97	122.42
7	E	502	B12	C15-C16-N24	4.40	128.76	122.42
7	E	502	B12	C18-C19-N24	4.25	108.78	102.31
7	E	502	B12	C55-C17-C16	4.21	124.96	116.65
7	C	502	B12	C25-C2-C1	-4.17	107.49	113.78
7	E	502	B12	C17-C16-N24	-4.17	104.73	111.15
7	E	502	B12	C54-C17-C16	-4.15	90.87	112.40
7	C	502	B12	C16-C15-C14	-4.05	115.11	121.25
7	C	502	B12	C5M-C5B-C6B	-3.77	113.01	120.74
7	C	502	B12	C5B-C4B-C9B	-3.72	115.95	121.22
7	C	502	B12	C4B-C5B-C6B	3.66	126.07	119.91
7	E	502	B12	C5B-C4B-C9B	-3.63	116.08	121.22
7	C	502	B12	C1-C2-C3	-3.60	97.00	101.60
7	C	502	B12	C7-C8-C9	3.58	105.48	100.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	E	502	B12	C16-C15-C14	-3.58	115.82	121.25
7	C	502	B12	C54-C17-C16	-3.34	95.04	112.40
7	C	502	B12	C41-C8-C9	-3.34	105.31	111.19
7	C	502	B12	C4B-C9B-C8B	-3.31	117.71	121.10
7	C	502	B12	C54-C17-C55	-3.20	103.98	109.25
7	E	502	B12	C5M-C5B-C6B	-3.19	114.20	120.74
7	E	502	B12	C1-C2-C3	-3.17	97.55	101.60
7	E	502	B12	C2P-C1P-N59	-3.16	108.28	112.93
7	C	502	B12	C55-C56-C57	-3.08	104.52	111.23
7	C	502	B12	C2P-C1P-N59	-3.06	108.42	112.93
7	E	502	B12	C4B-C5B-C6B	3.05	125.05	119.91
7	E	502	B12	O44-C43-N45	2.93	130.50	122.50
7	E	502	B12	C55-C56-C57	-2.89	104.92	111.23
7	E	502	B12	C25-C2-C1	-2.86	109.47	113.78
7	C	502	B12	C55-C17-C16	2.82	122.22	116.65
7	E	502	B12	C17-C18-C19	-2.76	98.14	102.36
4	B	302	C2F	C2-N3-C4	2.75	120.30	115.93
4	B	302	C2F	CG-CB-CA	2.74	118.28	113.16
4	A	300	C2F	C2-N3-C4	2.74	120.28	115.93
7	C	502	B12	C12-C11-N23	-2.70	108.06	111.83
7	C	502	B12	C31-C30-C3	-2.68	106.99	114.73
4	A	300	C2F	CG-CB-CA	2.67	118.15	113.16
7	E	502	B12	O51-C50-C49	-2.61	113.40	121.07
4	B	302	C2F	C2-N1-C8A	2.60	120.37	114.54
4	A	300	C2F	C2-N1-C8A	2.59	120.35	114.54
7	E	502	B12	C19-C1-N21	2.55	104.77	102.16
4	B	302	C2F	C11-N5-C4A	-2.53	109.86	113.30
7	C	502	B12	C12-C11-C10	2.52	126.65	123.37
4	A	300	C2F	C11-N5-C4A	-2.50	109.90	113.30
7	C	502	B12	C25-C2-C26	2.50	114.76	109.71
7	E	502	B12	C2-C3-C4	2.49	104.46	101.63
7	E	502	B12	C26-C2-C3	2.48	111.80	107.41
7	C	502	B12	C37-C7-C8	-2.47	101.77	108.39
7	C	502	B12	O34-C32-N33	-2.45	115.80	122.50
7	E	502	B12	O63-C61-N62	-2.44	115.85	122.50
7	C	502	B12	O6R-C1R-C2R	-2.43	103.37	106.93
7	E	502	B12	C42-C43-N45	-2.42	108.97	116.51
7	C	502	B12	C5-C4-N21	-2.41	120.28	124.19
7	C	502	B12	C15-C14-N23	2.40	129.19	126.26
7	C	502	B12	O28-C27-N29	2.39	129.03	122.50
7	C	502	B12	C7B-C6B-C5B	-2.39	115.89	119.91
7	C	502	B12	C2-C1-N21	2.37	105.07	101.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	302	C2F	N1-C2-N3	-2.36	121.72	125.42
4	A	300	C2F	N1-C2-N3	-2.36	121.72	125.42
7	E	502	B12	C2-C1-N21	2.35	105.04	101.77
7	E	502	B12	O2-C3R-C2R	2.33	120.12	111.68
7	E	502	B12	C54-C17-C55	-2.32	105.42	109.25
4	A	300	C2F	C6-C9-N10	2.30	118.23	112.23
7	E	502	B12	C5-C6-N22	-2.26	120.43	123.88
7	C	502	B12	C2-C3-C4	2.24	104.17	101.63
7	C	502	B12	O2-C3R-C2R	2.21	119.69	111.68
7	C	502	B12	C53-C15-C16	2.15	124.08	120.38
7	C	502	B12	C20-C1-C2	2.13	116.84	113.28
4	B	302	C2F	C6-C9-N10	2.12	117.75	112.23
7	E	502	B12	C7-C8-C9	2.10	103.59	100.90
7	E	502	B12	O63-C61-C60	2.08	125.24	120.87
7	C	502	B12	O44-C43-N45	2.03	128.05	122.50
7	C	502	B12	C26-C27-N29	-2.00	110.17	116.52

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	302	C2F	N5-C6-C9-N10
7	C	502	B12	C3-C2-C26-C27
7	C	502	B12	C38-C37-C7-C36
7	C	502	B12	C38-C37-C7-C8
7	E	502	B12	C38-C37-C7-C36
7	E	502	B12	C38-C37-C7-C8
7	E	502	B12	C12-C13-C48-C49
7	E	502	B12	C14-C13-C48-C49
7	E	502	B12	C54-C17-C55-C56
7	E	502	B12	C18-C17-C55-C56
7	E	502	B12	C3R-C4R-C5R-O8R
4	B	302	C2F	N-CA-CB-CG
7	E	502	B12	O6R-C4R-C5R-O8R
7	E	502	B12	C42-C41-C8-C7
7	C	502	B12	C3R-C4R-C5R-O8R
7	C	502	B12	O6R-C4R-C5R-O8R
4	A	300	C2F	N-CA-CB-CG
4	A	300	C2F	CT-CA-CB-CG
4	B	302	C2F	CT-CA-CB-CG
7	C	502	B12	C14-C13-C48-C49
7	E	502	B12	C42-C41-C8-C9

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Mol	Chain	Res	Type	Atoms
7	E	502	B12	C2-C26-C27-N29
7	E	502	B12	C2-C26-C27-O28
7	C	502	B12	C12-C13-C48-C49
7	E	502	B12	C18-C60-C61-O63
7	E	502	B12	C18-C60-C61-N62
7	C	502	B12	C38-C37-C7-C6
7	E	502	B12	C38-C37-C7-C6
7	C	502	B12	C41-C42-C43-O44
4	B	302	C2F	C14-C15-N10-C9
7	E	502	B12	C1P-C2P-O3-P
7	E	502	B12	C3P-C2P-O3-P
7	C	502	B12	C41-C42-C43-N45
4	B	302	C2F	C16-C15-N10-C9
7	C	502	B12	C30-C31-C32-O34
7	C	502	B12	C2P-O3-P-O2
4	B	302	C2F	C7-C6-C9-N10
7	C	502	B12	C30-C31-C32-N33
7	E	502	B12	C13-C48-C49-C50
7	E	502	B12	C4-C3-C30-C31
7	E	502	B12	C55-C56-C57-O58
7	E	502	B12	C2P-O3-P-O2
7	C	502	B12	C3-C30-C31-C32
7	E	502	B12	C55-C56-C57-N59

There are no ring outliers.

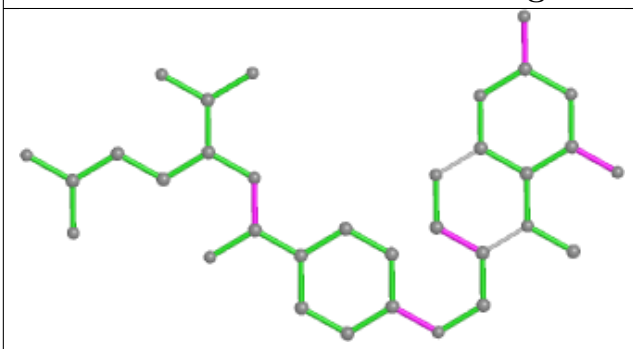
5 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	300	C2F	1	0
7	C	502	B12	17	0
4	B	302	C2F	2	0
6	E	501	SF4	2	0
7	E	502	B12	20	0

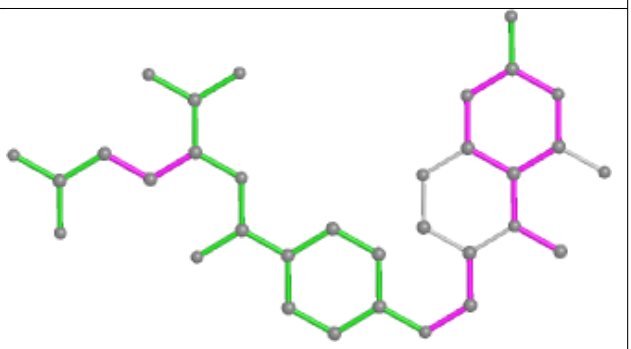
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

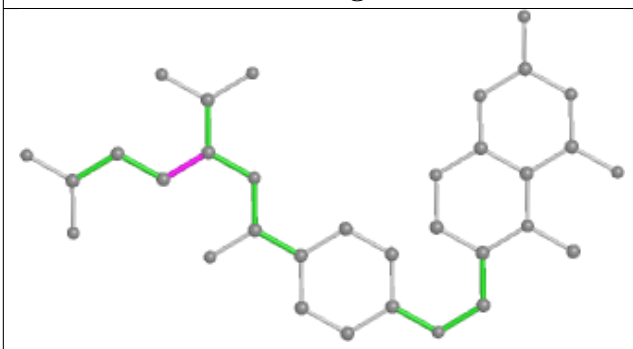
Ligand C2F A 300



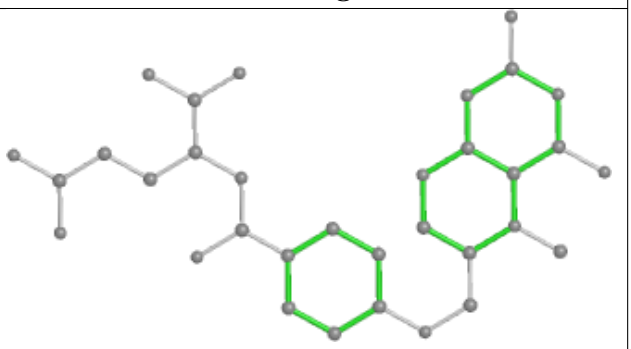
Bond lengths



Bond angles

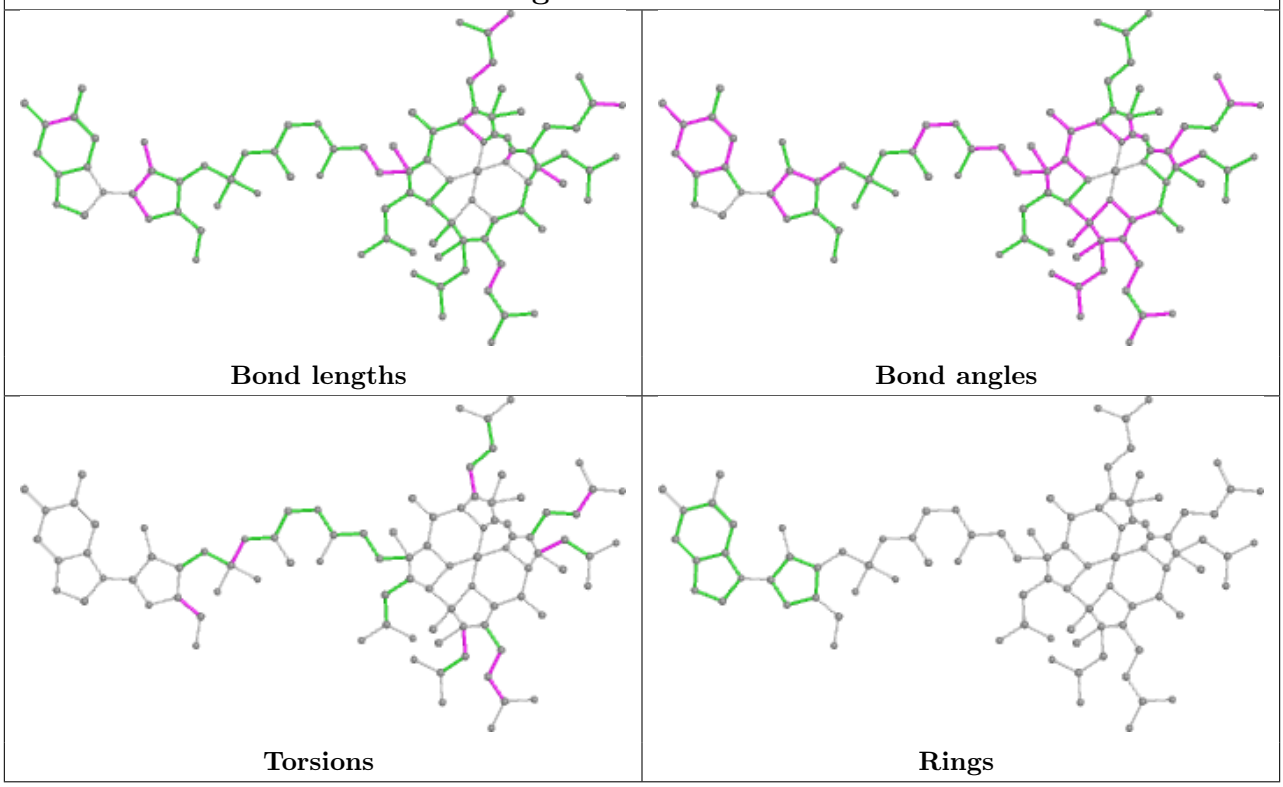


Torsions

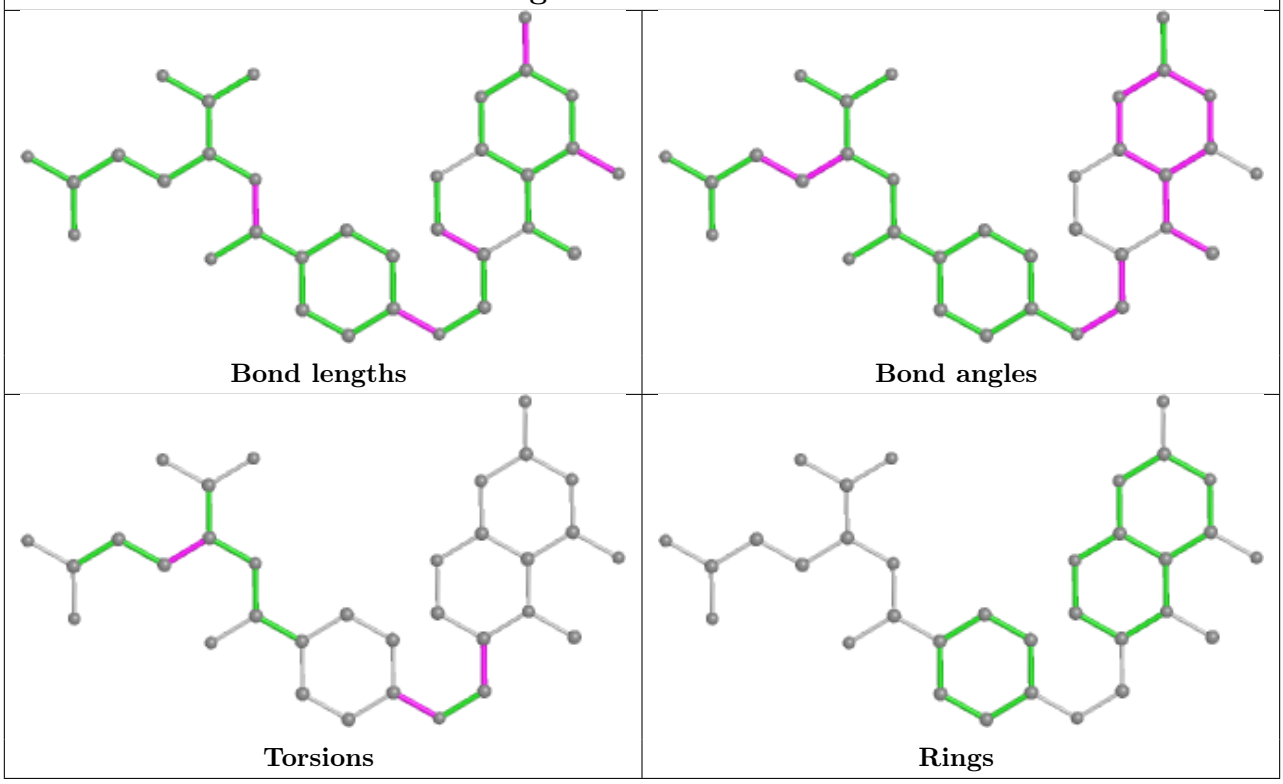


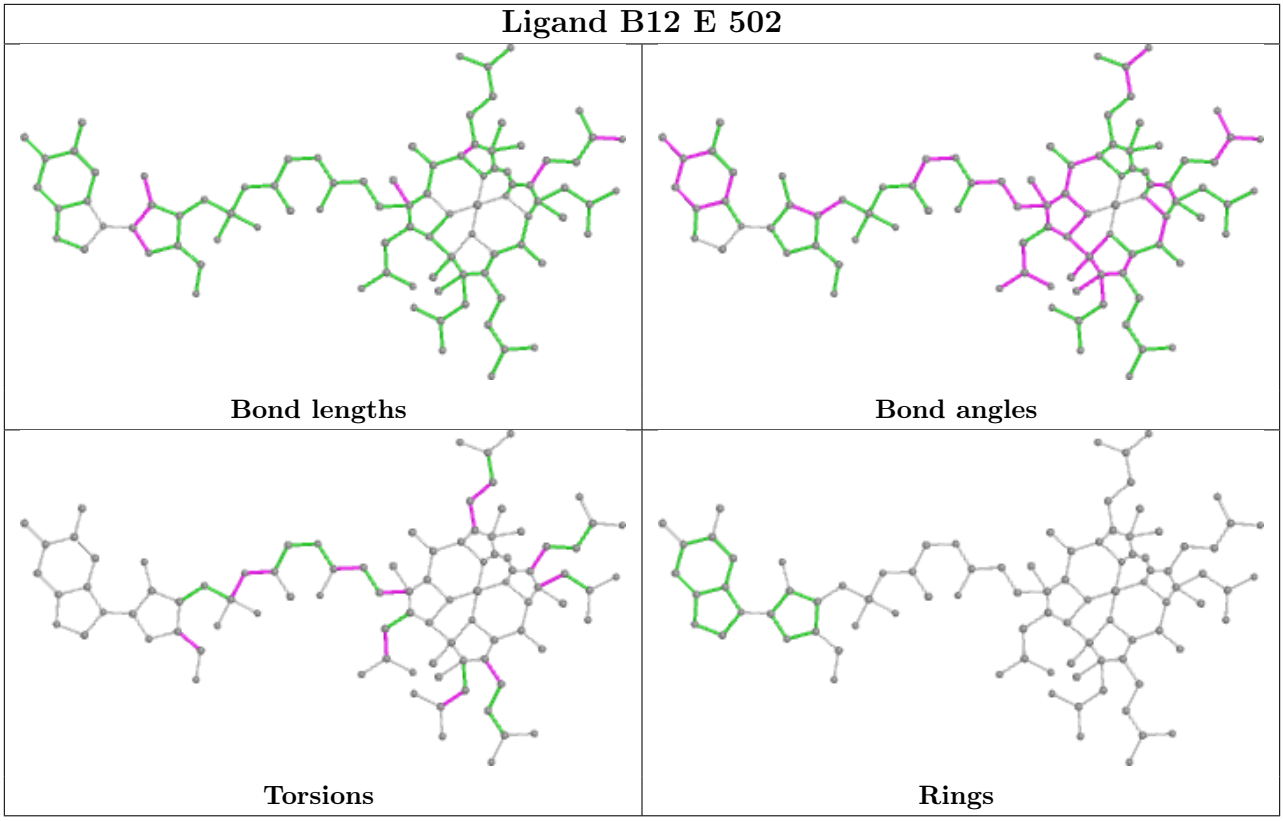
Rings

Ligand B12 C 502



Ligand C2F B 302





5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	262/262 (100%)	-0.20	0 100 100	58, 106, 152, 218	0
1	B	262/262 (100%)	-0.11	0 100 100	61, 136, 201, 258	0
2	C	441/446 (98%)	0.06	17 (3%) 39 35	54, 147, 229, 365	3 (0%)
2	E	441/446 (98%)	0.40	46 (10%) 6 7	79, 159, 279, 472	3 (0%)
3	D	323/323 (100%)	-0.30	1 (0%) 94 91	55, 96, 142, 311	0
3	F	323/323 (100%)	-0.30	1 (0%) 94 91	58, 105, 149, 207	0
All	All	2052/2062 (99%)	-0.04	65 (3%) 47 42	54, 124, 225, 472	6 (0%)

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	428	VAL	17.0
3	D	1	MET	6.9
2	E	433	ALA	6.7
2	E	406	ILE	6.5
2	E	396	LEU	6.3
2	E	429	GLY	6.2
2	E	434	SER	6.0
2	E	407	ILE	5.8
2	E	336	PRO	5.7
2	C	428	VAL	4.8
2	E	405	ILE	4.8
2	E	339	VAL	4.4
2	E	335	SER	4.3
2	E	437	VAL	4.0
2	E	382	PHE	3.9
2	E	427	ILE	3.9
2	E	363	LEU	3.7
2	E	436	ILE	3.7
2	E	384	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
2	C	406	ILE	3.6
2	E	340	THR	3.6
2	E	435	GLY	3.5
2	E	358	LYS	3.4
2	C	407	ILE	3.4
2	E	327	GLU	3.4
2	E	408	PRO	3.4
2	C	338	TYR	3.3
2	E	332	ASN	3.2
2	E	441	ARG	3.2
2	E	329	GLY	3.2
2	E	57	ALA	3.1
2	C	382	PHE	3.1
2	E	326	ASN	3.1
2	E	145	ALA	3.0
2	E	430	PRO	3.0
2	E	362	TYR	2.9
2	C	427	ILE	2.8
2	E	397	ASP	2.8
2	C	391	MET	2.7
2	C	327	GLU	2.6
2	E	330	ALA	2.6
3	F	1	MET	2.6
2	C	414	LEU	2.6
2	E	357	THR	2.5
2	E	337	VAL	2.5
2	E	440	ALA	2.5
2	C	2	PRO	2.4
2	E	334	ASN	2.4
2	E	356	SER	2.4
2	E	388	ALA	2.3
2	E	442	ALA	2.3
2	E	37	ALA	2.3
2	E	423	GLY	2.3
2	C	362	TYR	2.3
2	E	378	ALA	2.3
2	C	337	VAL	2.3
2	E	381	LYS	2.2
2	E	361	SER	2.2
2	C	429	GLY	2.2
2	C	439	PHE	2.2
2	C	363	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	365	SER	2.2
2	E	387	ILE	2.2
2	E	2	PRO	2.1
2	C	408	PRO	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 monosaccharides in this entry.

6.4 Ligands (i)

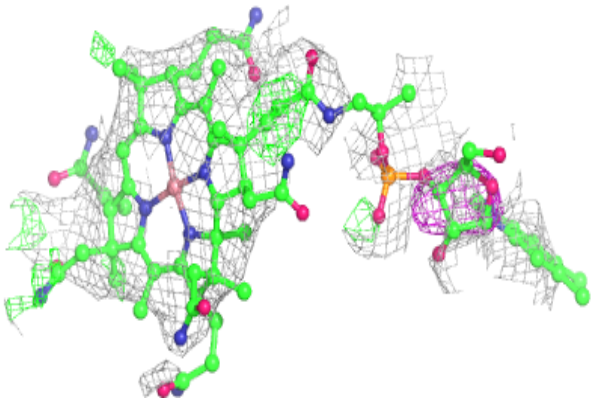
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

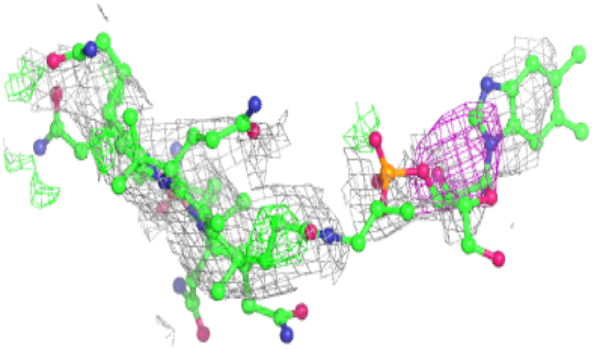
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	B12	E	502	91/91	0.71	0.41	205,205,205,205	0
5	CA	A	301	1/1	0.80	0.20	30,30,30,30	0
7	B12	C	502	91/91	0.81	0.34	165,165,165,165	0
4	C2F	A	300	33/33	0.88	0.34	92,92,92,92	0
4	C2F	B	302	33/33	0.89	0.25	103,103,103,103	0
5	CA	B	301	1/1	0.92	0.25	30,30,30,30	0
6	SF4	E	501	8/8	0.94	0.10	165,165,165,165	0
6	SF4	C	501	8/8	0.96	0.09	168,168,168,168	0

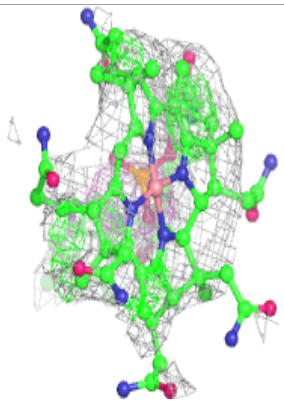
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

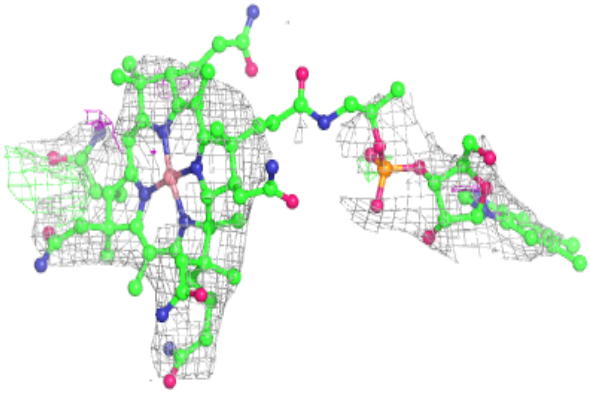


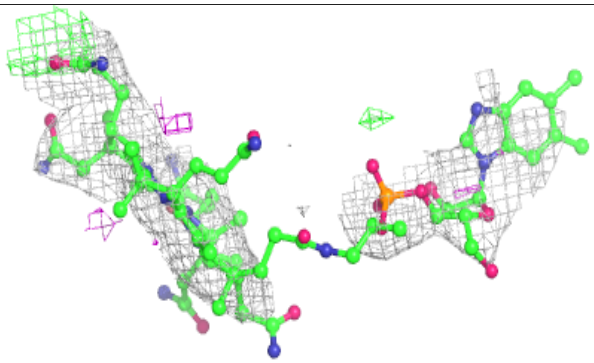


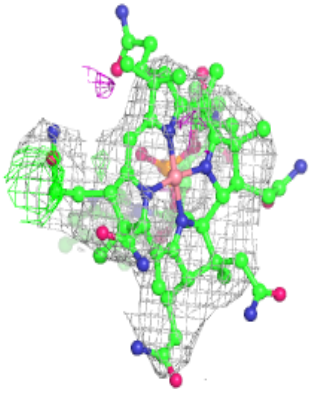


Electron density around B12 C 502:

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

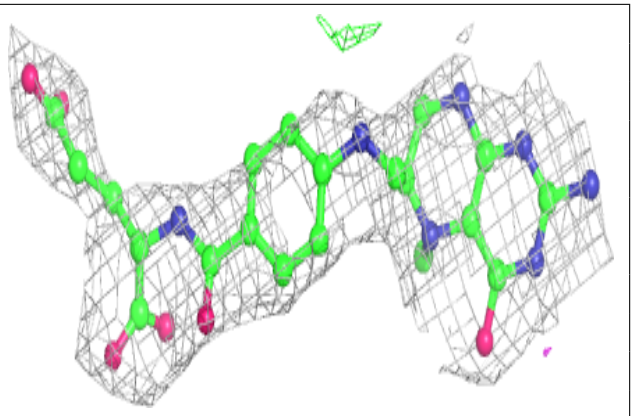


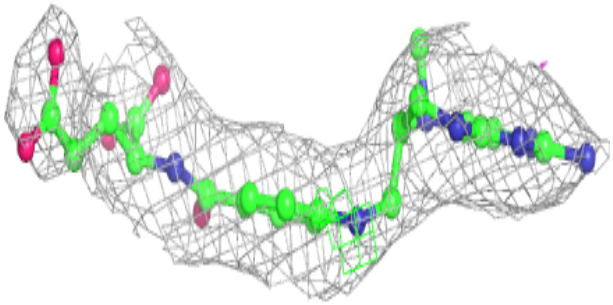


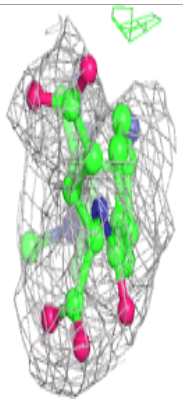


Electron density around C2F A 300:

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

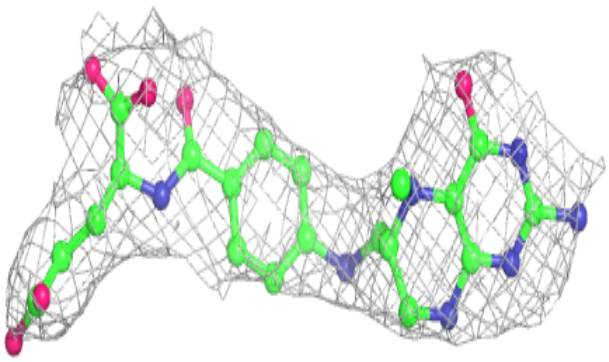


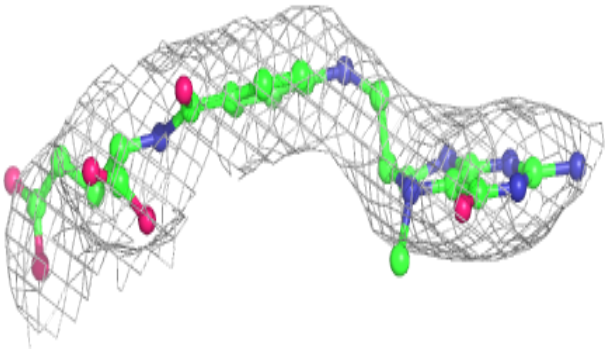


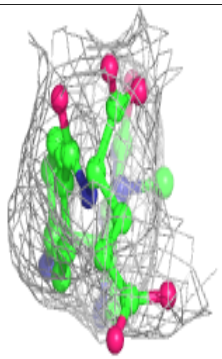


Electron density around C2F B 302:

$2mF_o$-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.