Full wwPDB X-ray Structure Validation Report (i)

Sep 14, 2023 – 04:51 AM EDT

PDB ID	:	5REQ
Title	:	Methylmalonyl-COA MUTASE, Y89F Mutant, substrate complex
Authors	:	Evans, P.R.; Thomae, N.H.
Deposited on	:	1998-08-03
Resolution	:	2.20 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:

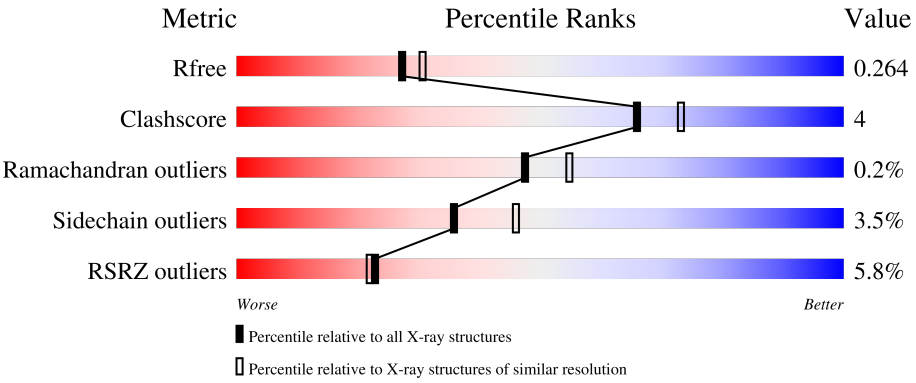
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	727	2% 84% 14%
1	C	727	5% 84% 14%
2	B	637	6% 83% 13%
2	D	637	10% 84% 11%

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	GOL	B	3002	-	-	-	X
6	GOL	D	3004	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 22112 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 PROTEIN (METHYLMALONYL-COA MUTASE ALPHA-SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	725	5574	3526	966	1058	24	0	0	0
1	C	725	Total 5574	C 3526	N 966	O 1058	S 24	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	89	PHE	TYR	engineered mutation	UNP P11653
C	89	PHE	TYR	engineered mutation	UNP P11653

- Molecule 2 is a protein called PROTEIN (METHYLMALONYL-COA MUTASE BETA-SUBUNIT).

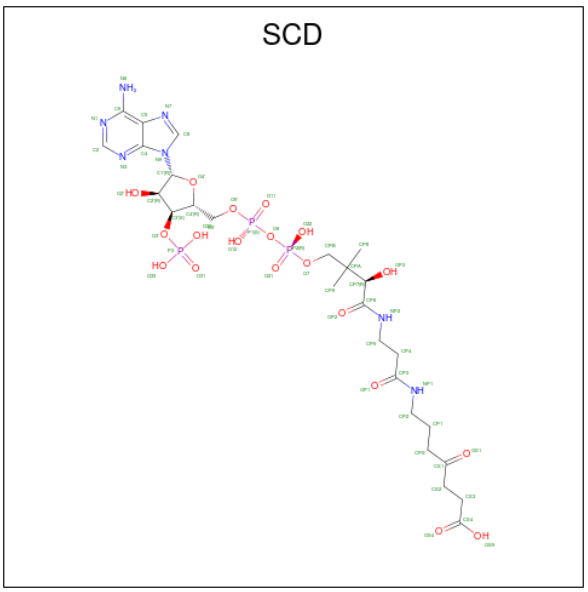
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	619	4722	2976	821	912	13	0	0	0
2	D	619	Total 4722	C 2976	N 821	O 912	S 13	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	203	GLY	ALA	SEE REMARK 999	UNP P11652
D	203	GLY	ALA	SEE REMARK 999	UNP P11652
B	330	GLU	ASP	SEE REMARK 999	UNP P11652
D	330	GLU	ASP	SEE REMARK 999	UNP P11652
B	331	LEU	VAL	SEE REMARK 999	UNP P11652
D	331	LEU	VAL	SEE REMARK 999	UNP P11652

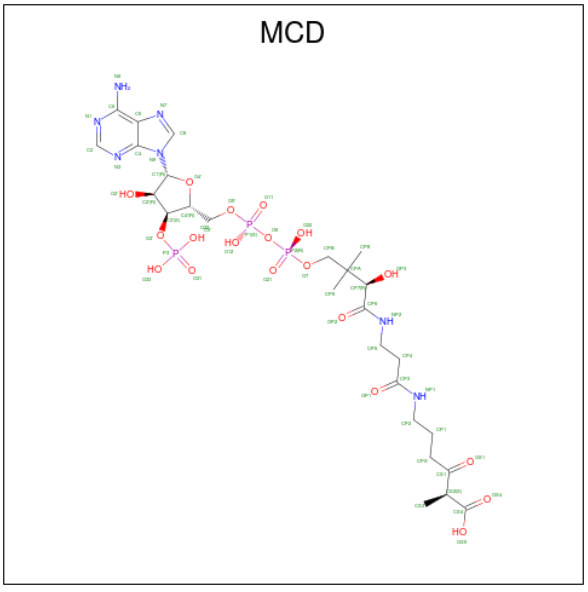
- Molecule 3 is SUCCINYL(CARBADETHIA)-COENZYME A (three-letter code: SCD)

(formula: $C_{26}H_{42}N_7O_{19}P_3$).



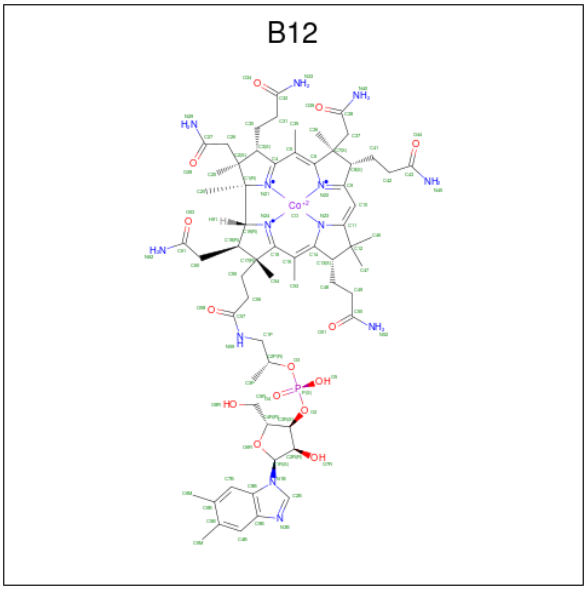
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	1
			55	26	7	19	3		
3	C	1	Total	C	N	O	P	0	1
			55	26	7	19	3		

- Molecule 4 is METHYLMALONYL(CARBADETHIA)-COENZYME A (three-letter code: MCD) (formula: $C_{26}H_{42}N_7O_{19}P_3$).



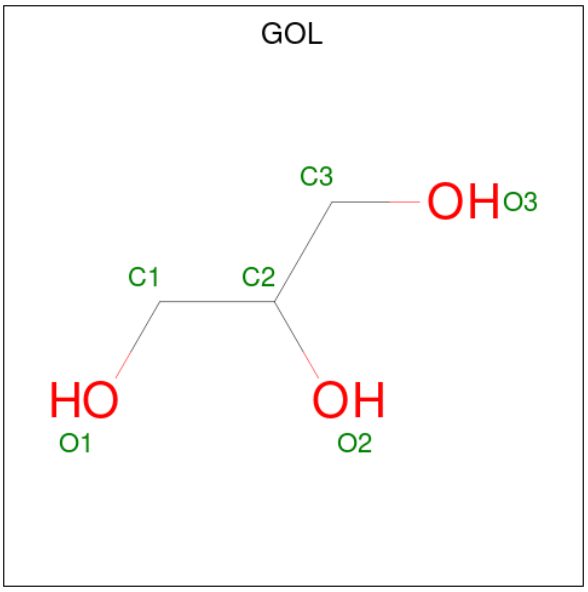
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	1
			55	26	7	19	3		
4	C	1	Total	C	N	O	P	0	1
			55	26	7	19	3		

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



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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 7 is water.

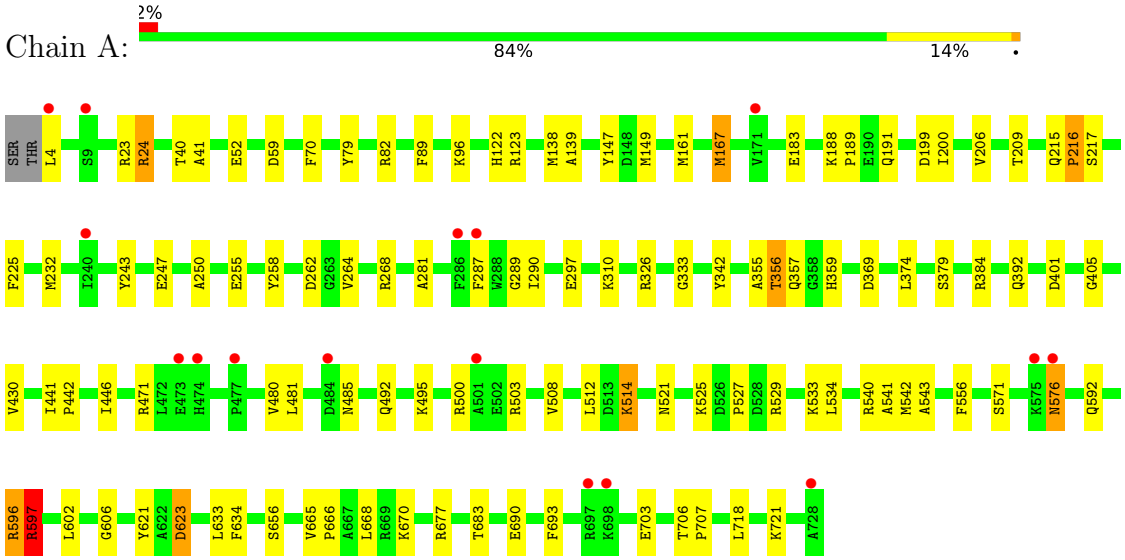
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	356	Total O 356 356	0	0
7	B	192	Total O 192 192	0	0
7	C	353	Total O 353 353	0	0
7	D	193	Total O 193 193	0	0

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.

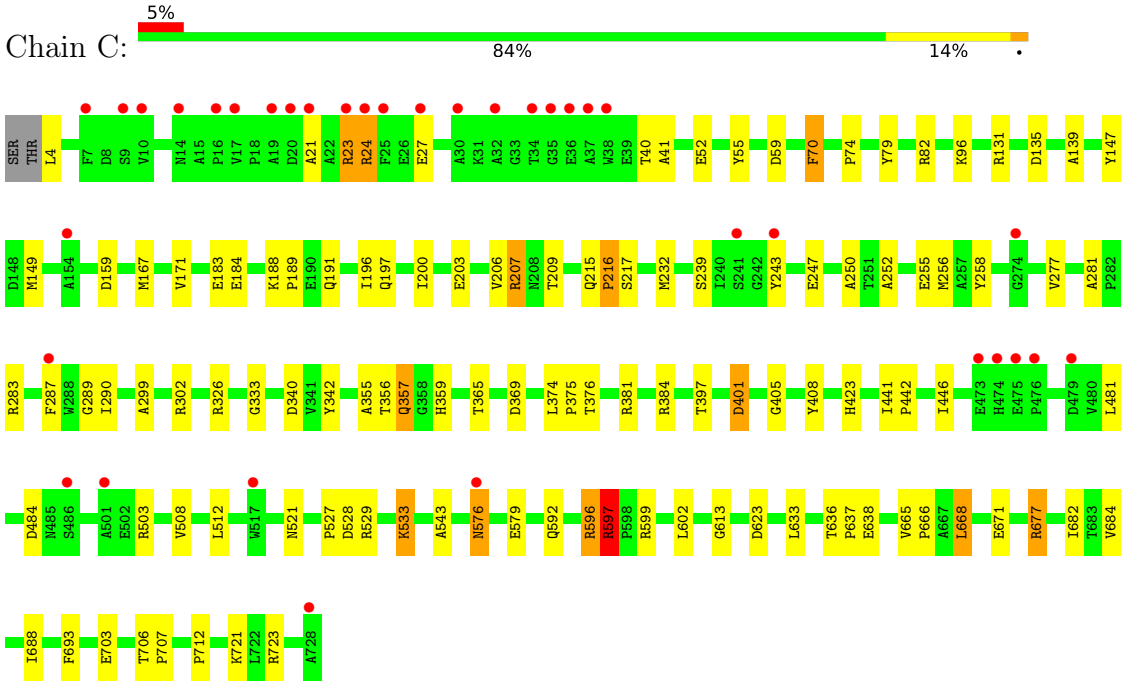
• Molecule 1: PROTEIN (METHYLMALONYL-COA MUTASE ALPHA-SUBUNIT)

Chain A:



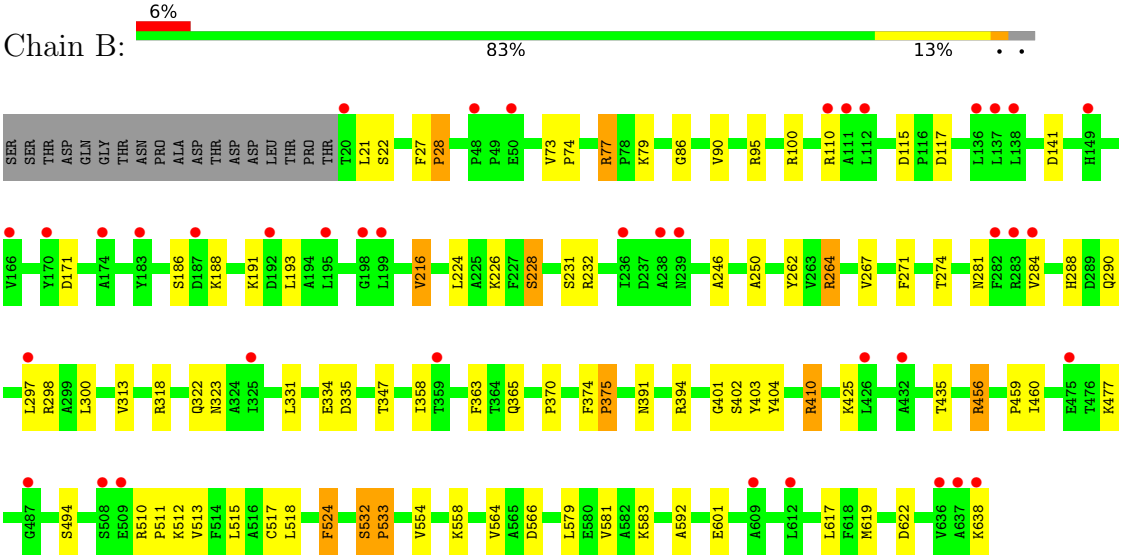
• Molecule 1: PROTEIN (METHYLMALONYL-COA MUTASE ALPHA-SUBUNIT)

Chain C:



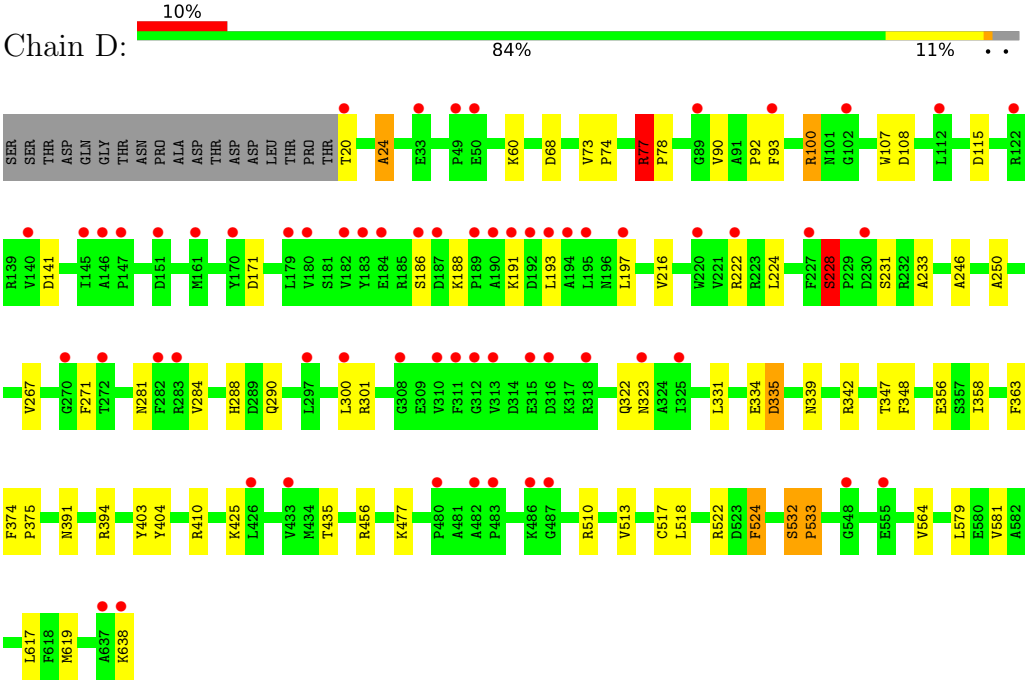
• Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE BETA-SUBUNIT)

Chain B:



• Molecule 2: PROTEIN (METHYLMALONYL-COA MUTASE BETA-SUBUNIT)

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	120.20Å 161.89Å 88.70Å 90.00° 104.88° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 32.62 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-2.20) 99.9 (32.62-2.20)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	3.88 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.246 , 0.292 0.230 , 0.264	Depositor DCC
R_{free} test set	8387 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å^2)	34.4	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 49.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22112	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.66% 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: SCD, GOL, B12, MCD

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	0.49	0/5691	1.54	49/7728 (0.6%)
1	C	0.50	0/5691	1.55	61/7728 (0.8%)
2	B	0.45	0/4812	1.42	37/6533 (0.6%)
2	D	0.44	0/4812	1.41	27/6533 (0.4%)
All	All	0.47	0/21006	1.49	174/28522 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	C	0	12
2	B	0	2
2	D	0	4
All	All	0	27

There are no bond length outliers.

All (174) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	23	ARG	CD-NE-CZ	18.94	150.12	123.60
1	C	597	ARG	NE-CZ-NH1	13.00	126.80	120.30
1	C	384	ARG	CD-NE-CZ	12.95	141.72	123.60
2	B	77	ARG	CD-NE-CZ	12.60	141.24	123.60
2	D	77	ARG	CD-NE-CZ	11.89	140.24	123.60
1	C	597	ARG	CD-NE-CZ	11.87	140.22	123.60
1	A	597	ARG	CD-NE-CZ	11.75	140.05	123.60
1	A	597	ARG	NE-CZ-NH1	11.18	125.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	77	ARG	NE-CZ-NH1	10.59	125.59	120.30
1	C	596	ARG	CD-NE-CZ	10.49	138.29	123.60
2	B	264	ARG	NE-CZ-NH2	-9.95	115.33	120.30
2	D	404	TYR	CB-CG-CD1	9.58	126.75	121.00
1	A	79	TYR	CB-CG-CD2	-9.29	115.43	121.00
2	B	95	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	A	384	ARG	CD-NE-CZ	8.85	135.98	123.60
1	A	79	TYR	CB-CG-CD1	8.76	126.25	121.00
1	A	147	TYR	CB-CG-CD1	8.74	126.24	121.00
2	B	77	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	A	596	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	C	79	TYR	CB-CG-CD2	-8.28	116.03	121.00
2	B	404	TYR	CB-CG-CD1	8.27	125.96	121.00
1	C	159	ASP	CB-CG-OD1	8.25	125.72	118.30
2	B	264	ARG	NE-CZ-NH1	8.17	124.39	120.30
2	D	404	TYR	CB-CG-CD2	-8.12	116.13	121.00
1	A	82	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	C	596	ARG	NE-CZ-NH1	8.04	124.32	120.30
2	D	335	ASP	CB-CG-OD1	7.96	125.47	118.30
1	C	596	ARG	NE-CZ-NH2	-7.91	116.34	120.30
1	C	147	TYR	CB-CG-CD1	7.88	125.73	121.00
1	C	79	TYR	CB-CG-CD1	7.75	125.65	121.00
2	D	264	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	A	500	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	B	298	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	C	82	ARG	CD-NE-CZ	7.64	134.30	123.60
2	D	403	TYR	CB-CG-CD1	7.62	125.57	121.00
1	C	24	ARG	CD-NE-CZ	7.45	134.03	123.60
1	C	283	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	C	41	ALA	C-N-CA	7.40	140.21	121.70
2	B	262	TYR	CB-CG-CD1	7.25	125.35	121.00
1	C	287	PHE	CB-CG-CD1	7.24	125.87	120.80
2	B	115	ASP	CB-CG-OD1	7.15	124.73	118.30
2	D	524	PHE	CB-CG-CD1	7.09	125.77	120.80
1	A	41	ALA	C-N-CA	6.97	139.12	121.70
1	C	384	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	B	524	PHE	CB-CG-CD1	6.92	125.64	120.80
1	A	621	TYR	CB-CG-CD1	6.89	125.13	121.00
2	B	100	ARG	NE-CZ-NH1	6.87	123.74	120.30
1	C	369	ASP	CB-CG-OD1	6.85	124.47	118.30
1	A	326	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	B	117	ASP	CB-CG-OD1	6.82	124.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	95	ARG	CG-CD-NE	6.80	126.08	111.80
2	D	68	ASP	CB-CG-OD1	6.75	124.38	118.30
1	A	82	ARG	CD-NE-CZ	6.74	133.03	123.60
2	B	601	GLU	C-N-CA	6.71	138.49	121.70
1	C	55	TYR	CB-CG-CD1	6.69	125.02	121.00
1	C	258	TYR	CB-CG-CD1	6.69	125.01	121.00
1	A	258	TYR	CB-CG-CD1	6.64	124.98	121.00
2	D	617	LEU	CA-CB-CG	6.64	130.58	115.30
1	C	333	GLY	O-C-N	-6.63	112.09	122.70
2	B	404	TYR	CB-CG-CD2	-6.58	117.06	121.00
2	D	510	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	C	677	ARG	CA-CB-CG	6.54	127.79	113.40
2	B	232	ARG	CD-NE-CZ	6.53	132.75	123.60
2	B	335	ASP	CB-CG-OD1	6.53	124.18	118.30
1	C	693	PHE	CB-CG-CD1	6.47	125.33	120.80
2	B	264	ARG	CD-NE-CZ	6.36	132.50	123.60
2	D	262	TYR	CB-CG-CD1	6.34	124.80	121.00
1	C	401	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	287	PHE	CB-CG-CD1	6.31	125.22	120.80
1	A	147	TYR	CB-CG-CD2	-6.27	117.24	121.00
1	A	326	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	500	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	C	209	THR	N-CA-CB	6.15	121.99	110.30
1	A	59	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	207	ARG	NE-CZ-NH2	-6.11	117.24	120.30
2	B	262	TYR	CB-CG-CD2	-6.09	117.35	121.00
1	A	206	VAL	CB-CA-C	-6.07	99.87	111.40
2	B	100	ARG	NE-CZ-NH2	-6.06	117.27	120.30
1	C	232	MET	CA-CB-CG	6.06	123.60	113.30
1	C	484	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	24	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	A	621	TYR	CB-CG-CD2	-6.02	117.39	121.00
2	D	403	TYR	CB-CG-CD2	-6.01	117.39	121.00
2	D	533	PRO	N-CA-CB	6.00	110.50	103.30
2	D	601	GLU	C-N-CA	5.97	136.62	121.70
1	C	255	GLU	OE1-CD-OE2	-5.93	116.18	123.30
2	D	115	ASP	CB-CG-OD1	5.91	123.62	118.30
1	A	24	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	B	456	ARG	O-C-N	-5.88	113.29	122.70
1	A	225	PHE	CB-CG-CD1	5.88	124.91	120.80
1	C	41	ALA	O-C-N	-5.87	113.31	122.70
1	A	209	THR	N-CA-CB	5.86	121.43	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	147	TYR	CB-CG-CD2	-5.78	117.53	121.00
1	C	82	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	C	597	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	A	693	PHE	CB-CG-CD1	5.75	124.83	120.80
1	A	633	LEU	O-C-N	-5.72	113.55	122.70
1	A	690	GLU	C-N-CA	5.70	135.94	121.70
1	C	340	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	333	GLY	O-C-N	-5.68	113.61	122.70
2	B	510	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	B	363	PHE	C-N-CA	5.65	135.82	121.70
1	A	297	GLU	OE1-CD-OE2	-5.64	116.53	123.30
2	D	77	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	623	ASP	CB-CG-OD1	5.61	123.35	118.30
2	D	264	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	D	108	ASP	CB-CG-OD1	5.60	123.34	118.30
1	C	599	ARG	NE-CZ-NH1	5.57	123.08	120.30
1	A	703	GLU	CA-CB-CG	5.57	125.64	113.40
1	C	703	GLU	CA-CB-CG	5.55	125.61	113.40
2	D	100	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	677	ARG	CA-CB-CG	5.51	125.52	113.40
1	C	52	GLU	O-C-N	-5.50	113.89	122.70
1	A	596	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	B	410	ARG	NE-CZ-NH1	5.47	123.04	120.30
1	C	381	ARG	NE-CZ-NH2	5.47	123.04	120.30
2	D	262	TYR	CB-CG-CD2	-5.47	117.72	121.00
2	D	264	ARG	CD-NE-CZ	5.47	131.26	123.60
2	B	617	LEU	CA-CB-CG	5.44	127.81	115.30
1	C	206	VAL	CB-CA-C	-5.42	101.10	111.40
1	A	199	ASP	CB-CG-OD1	5.40	123.16	118.30
1	C	183	GLU	O-C-N	-5.40	114.06	122.70
1	C	59	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	384	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	C	216	PRO	N-CA-CB	5.36	109.73	103.30
1	A	369	ASP	O-C-N	-5.35	114.14	122.70
1	A	356	THR	CA-CB-CG2	-5.34	104.93	112.40
1	C	633	LEU	C-N-CA	5.31	134.96	121.70
1	A	527	PRO	N-CA-CB	5.30	109.67	103.30
1	A	41	ALA	O-C-N	-5.30	114.23	122.70
1	C	633	LEU	O-C-N	-5.28	114.25	122.70
1	C	184	GLU	C-N-CA	5.25	134.84	121.70
2	B	297	LEU	CA-CB-CG	5.25	127.37	115.30
1	C	527	PRO	N-CA-CB	5.25	109.59	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	556	PHE	CB-CG-CD1	5.24	124.47	120.80
2	B	90	VAL	CA-CB-CG2	5.24	118.75	110.90
1	A	258	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	C	423	HIS	CA-CB-CG	5.21	122.46	113.60
2	B	622	ASP	CB-CG-OD1	5.20	122.98	118.30
2	D	24	ALA	O-C-N	-5.20	114.37	123.20
2	B	86	GLY	O-C-N	-5.19	114.39	122.70
1	C	302	ARG	NE-CZ-NH1	5.19	122.90	120.30
2	D	363	PHE	C-N-CA	5.18	134.65	121.70
1	A	255	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	C	326	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	C	375	PRO	N-CA-CB	5.18	109.51	103.30
2	D	510	ARG	CD-NE-CZ	5.16	130.83	123.60
1	C	397	THR	O-C-N	-5.16	114.45	122.70
1	C	23	ARG	CD-NE-CZ	5.15	130.81	123.60
1	A	232	MET	CA-CB-CG	5.14	122.04	113.30
2	B	533	PRO	N-CA-CB	5.14	109.47	103.30
2	B	110	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	C	299	ALA	N-CA-CB	-5.13	102.92	110.10
2	B	511	PRO	N-CA-CB	5.11	109.44	103.30
2	B	318	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	135	ASP	CB-CG-OD1	5.11	122.90	118.30
1	A	161	MET	CA-CB-CG	5.09	121.96	113.30
1	C	287	PHE	CB-CG-CD2	-5.09	117.23	120.80
1	A	52	GLU	O-C-N	-5.08	114.57	122.70
2	B	110	ARG	CD-NE-CZ	5.08	130.72	123.60
1	C	70	PHE	O-C-N	-5.08	114.58	122.70
2	B	375	PRO	N-CA-CB	5.08	109.39	103.30
1	C	723	ARG	NE-CZ-NH1	5.07	122.84	120.30
1	A	262	ASP	CB-CG-OD2	5.07	122.86	118.30
2	D	222	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	A	216	PRO	N-CA-CB	5.06	109.37	103.30
1	A	24	ARG	CD-NE-CZ	5.05	130.67	123.60
1	C	408	TYR	CB-CG-CD1	5.05	124.03	121.00
1	A	623	ASP	CB-CG-OD1	5.05	122.84	118.30
2	B	403	TYR	CB-CG-CD1	5.04	124.03	121.00
2	B	28	PRO	N-CA-CB	5.03	109.33	103.30
1	C	131	ARG	NE-CZ-NH2	-5.02	117.79	120.30
2	D	301	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	C	206	VAL	CA-CB-CG1	5.00	118.40	110.90

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	167	MET	Mainchain
1	A	183	GLU	Mainchain
1	A	281	ALA	Mainchain
1	A	342	TYR	Mainchain
1	A	356	THR	Mainchain
1	A	40	THR	Mainchain
1	A	405	GLY	Mainchain
1	A	540	ARG	Mainchain
1	A	70	PHE	Mainchain
2	B	401	GLY	Mainchain
2	B	456	ARG	Mainchain
1	C	167	MET	Mainchain
1	C	277	VAL	Mainchain
1	C	281	ALA	Mainchain
1	C	342	TYR	Mainchain
1	C	356	THR	Mainchain
1	C	357	GLN	Mainchain
1	C	376	THR	Mainchain
1	C	40	THR	Mainchain
1	C	405	GLY	Mainchain
1	C	677	ARG	Mainchain
1	C	70	PHE	Mainchain
1	C	74	PRO	Mainchain
2	D	228	SER	Mainchain
2	D	24	ALA	Mainchain
2	D	348	PHE	Mainchain
2	D	456	ARG	Mainchain

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	5574	0	5486	37	2
1	C	5574	0	5486	40	0
2	B	4722	0	4642	31	0
2	D	4722	0	4642	33	2
3	A	55	0	37	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	55	0	37	1	0
4	A	55	0	37	3	0
4	C	55	0	37	2	0
5	A	91	0	88	17	0
5	C	91	0	88	16	0
6	B	12	0	16	1	0
6	D	12	0	16	3	0
7	A	356	0	0	0	0
7	B	192	0	0	1	0
7	C	353	0	0	4	0
7	D	193	0	0	0	0
All	All	22112	0	20612	166	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (166) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1800:B12:H531	5:A:1800:B12:H552	1.46	0.96
5:A:1800:B12:H421	5:A:1800:B12:H363	1.46	0.95
1:C:21:ALA:HB3	7:C:4310:HOH:O	1.72	0.89
1:A:357:GLN:HE22	2:B:290:GLN:HE22	1.24	0.85
5:C:2800:B12:H552	5:C:2800:B12:H531	1.64	0.80
1:C:357:GLN:HE22	2:D:290:GLN:HE22	1.32	0.77
5:C:2800:B12:H353	5:C:2800:B12:H302	1.67	0.77
1:A:290:ILE:HG13	1:A:355:ALA:HB2	1.65	0.76
1:C:27:GLU:HB2	7:C:4284:HOH:O	1.84	0.75
6:B:3002:GOL:O3	6:B:3002:GOL:O1	1.99	0.75
2:B:370:PRO:HB3	2:B:375:PRO:HG2	1.69	0.74
1:C:290:ILE:HG13	1:C:355:ALA:HB2	1.69	0.74
1:A:247:GLU:HB3	5:A:1800:B12:H532	1.71	0.73
1:C:706:THR:HB	1:C:707:PRO:HD2	1.71	0.72
2:D:281:ASN:HD22	2:D:323:ASN:HD21	1.36	0.72
1:A:706:THR:HB	1:A:707:PRO:HD2	1.73	0.71
5:A:1800:B12:H363	5:A:1800:B12:C42	2.11	0.70
1:C:4:LEU:HB3	2:D:264:ARG:HG2	1.76	0.68
2:B:73:VAL:HB	2:B:74:PRO:HD2	1.77	0.67
2:B:281:ASN:HD22	2:B:323:ASN:HD21	1.43	0.66
1:C:188:LYS:H	1:C:191:GLN:NE2	1.93	0.66
1:C:215:GLN:HB3	1:C:216:PRO:HD3	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:247:GLU:HB3	5:C:2800:B12:H532	1.77	0.66
5:A:1800:B12:H353	5:A:1800:B12:H302	1.76	0.65
2:D:370:PRO:HB3	2:D:375:PRO:HG2	1.79	0.65
1:A:200:ILE:HG21	1:A:217:SER:HB3	1.79	0.64
2:D:564:VAL:HG22	2:D:592:ALA:HB3	1.78	0.64
3:A:1801[A]:SCD:OP2	3:A:1801[A]:SCD:HPB1	1.97	0.64
2:B:564:VAL:HG22	2:B:592:ALA:HB3	1.78	0.64
2:B:224:LEU:HD21	2:B:231:SER:HB3	1.80	0.64
1:C:23:ARG:HD2	7:C:4304:HOH:O	1.99	0.62
2:D:374:PHE:HB3	2:D:375:PRO:HD3	1.81	0.62
1:A:441:ILE:HB	1:A:442:PRO:HD3	1.81	0.62
2:D:197:LEU:HB2	2:D:233:ALA:HA	1.81	0.62
1:A:188:LYS:H	1:A:191:GLN:NE2	1.99	0.61
5:C:2800:B12:H531	5:C:2800:B12:C55	2.30	0.61
3:C:2801[A]:SCD:HPB1	3:C:2801[A]:SCD:OP2	1.99	0.60
5:A:1800:B12:H531	5:A:1800:B12:C55	2.28	0.59
2:D:73:VAL:HB	2:D:74:PRO:HD2	1.85	0.59
2:B:532:SER:HB3	2:B:533:PRO:HD3	1.85	0.58
2:D:197:LEU:HD12	2:D:233:ALA:CB	2.34	0.58
2:D:532:SER:HB3	2:D:533:PRO:HD3	1.85	0.58
2:B:284:VAL:HG11	2:B:322:GLN:HE21	1.68	0.57
2:D:284:VAL:HG11	2:D:322:GLN:HE21	1.69	0.57
2:B:374:PHE:HB3	2:B:375:PRO:HD3	1.87	0.57
2:B:391:ASN:HD22	2:B:394:ARG:HE	1.52	0.57
1:A:4:LEU:HB3	2:B:264:ARG:HG2	1.85	0.57
5:A:1800:B12:H312	5:A:1800:B12:H251	1.88	0.56
1:C:441:ILE:HB	1:C:442:PRO:HD3	1.87	0.56
4:C:2802[B]:MCD:HPB1	4:C:2802[B]:MCD:OP2	2.05	0.56
5:A:1800:B12:H2B	5:A:1800:B12:O7R	2.06	0.56
1:C:374:LEU:HB2	1:C:481:LEU:HD23	1.87	0.56
2:D:356:GLU:HA	6:D:3004:GOL:H2	1.89	0.55
5:C:2800:B12:H301	5:C:2800:B12:H203	1.87	0.55
5:A:1800:B12:H203	5:A:1800:B12:H301	1.89	0.55
5:A:1800:B12:H312	5:A:1800:B12:C25	2.37	0.54
1:C:638:GLU:HA	1:C:671:GLU:HG3	1.89	0.54
2:B:347:THR:HG23	2:B:358:ILE:HG21	1.89	0.54
2:B:391:ASN:ND2	2:B:394:ARG:HE	2.05	0.54
2:D:281:ASN:ND2	2:D:323:ASN:HD21	2.05	0.53
1:A:215:GLN:HB3	1:A:216:PRO:HD3	1.89	0.53
2:B:216:VAL:HG23	7:B:5409:HOH:O	2.07	0.53
1:C:706:THR:HB	1:C:707:PRO:CD	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:224:LEU:HD21	2:D:231:SER:HB3	1.89	0.53
2:D:513:VAL:HG13	2:D:564:VAL:HG12	1.92	0.52
4:A:1802[B]:MCD:NP2	4:A:1802[B]:MCD:HP92	2.21	0.52
1:A:512:LEU:HD21	1:A:543:ALA:HB1	1.92	0.52
1:C:512:LEU:HD21	1:C:543:ALA:HB1	1.92	0.52
1:C:357:GLN:HE22	2:D:290:GLN:NE2	2.05	0.51
1:C:528:ASP:HA	1:C:533:LYS:HE3	1.92	0.51
4:A:1802[B]:MCD:HPB1	4:A:1802[B]:MCD:OP2	2.11	0.51
1:C:200:ILE:HG21	1:C:217:SER:HB3	1.93	0.51
2:B:513:VAL:HG13	2:B:564:VAL:HG12	1.93	0.51
1:A:250:ALA:HB2	1:A:446:ILE:HG12	1.92	0.50
5:C:2800:B12:H372	5:C:2800:B12:H351	1.94	0.50
1:C:684:VAL:HG12	1:C:688:ILE:HD11	1.94	0.50
2:D:77:ARG:HB3	2:D:78:PRO:HD2	1.93	0.50
2:B:554:VAL:HG12	2:B:558:LYS:HD2	1.93	0.49
1:C:250:ALA:HB2	1:C:446:ILE:HG12	1.95	0.49
5:C:2800:B12:C25	5:C:2800:B12:H312	2.43	0.49
6:D:3004:GOL:O3	6:D:3004:GOL:O1	2.22	0.49
1:C:665:VAL:N	1:C:666:PRO:HD2	2.27	0.49
5:C:2800:B12:H312	5:C:2800:B12:H251	1.95	0.49
1:A:706:THR:HB	1:A:707:PRO:CD	2.41	0.48
1:A:359:HIS:CE1	1:A:401:ASP:H	2.32	0.48
2:D:391:ASN:ND2	2:D:394:ARG:HE	2.10	0.48
1:C:359:HIS:CE1	1:C:401:ASP:H	2.31	0.48
2:D:391:ASN:HD22	2:D:394:ARG:HE	1.62	0.48
1:C:139:ALA:HB1	5:C:2800:B12:H362	1.96	0.48
1:A:243:TYR:HD1	1:A:289:GLY:HA2	1.79	0.48
1:A:503:ARG:HD2	1:A:508:VAL:HG21	1.95	0.48
1:C:188:LYS:HB3	1:C:189:PRO:HD2	1.95	0.48
5:C:2800:B12:H353	5:C:2800:B12:C30	2.40	0.47
5:A:1800:B12:H372	5:A:1800:B12:H351	1.97	0.47
2:B:27:PHE:HB3	2:B:28:PRO:HD2	1.97	0.47
2:B:331:LEU:HD13	2:B:365:GLN:HB3	1.97	0.47
1:C:597:ARG:HG2	1:C:597:ARG:HH11	1.80	0.47
5:A:1800:B12:O7R	5:A:1800:B12:C2B	2.63	0.46
4:C:2802[B]:MCD:NP2	4:C:2802[B]:MCD:HP92	2.28	0.46
2:D:347:THR:HG23	2:D:358:ILE:HG21	1.97	0.46
1:A:597:ARG:HH11	1:A:597:ARG:HG2	1.81	0.46
1:A:514:LYS:HD3	1:A:534:LEU:HD22	1.98	0.46
1:A:665:VAL:N	1:A:666:PRO:CD	2.79	0.46
2:D:339:ASN:HA	2:D:342:ARG:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:100:ARG:HE	6:D:3004:GOL:HO1	1.64	0.45
5:C:2800:B12:C42	5:C:2800:B12:H363	2.47	0.45
2:B:518:LEU:HD21	2:B:581:VAL:HG11	1.98	0.45
2:D:246:ALA:HB1	2:D:250:ALA:HB3	1.98	0.45
1:C:21:ALA:HA	2:D:90:VAL:HG11	1.98	0.45
2:B:274:THR:HA	2:B:313:VAL:HG13	1.97	0.45
5:C:2800:B12:H2B	5:C:2800:B12:O2	2.16	0.45
2:D:92:PRO:O	2:D:93:PHE:HB2	2.17	0.45
2:B:281:ASN:ND2	2:B:323:ASN:HD21	2.14	0.44
1:C:668:LEU:HD13	1:C:682:ILE:HG12	1.99	0.44
1:A:264:VAL:HG12	1:A:268:ARG:HH21	1.81	0.44
1:A:357:GLN:HE22	2:B:290:GLN:NE2	2.03	0.44
1:A:122:HIS:HA	1:A:167:MET:HE1	2.00	0.44
1:A:310:LYS:HE2	2:B:21:LEU:HD11	2.00	0.44
2:B:532:SER:CB	2:B:533:PRO:HD3	2.47	0.44
1:A:188:LYS:HB3	1:A:189:PRO:HD2	1.98	0.44
1:A:665:VAL:N	1:A:666:PRO:HD2	2.34	0.43
2:D:579:LEU:HG	2:D:583:LYS:HE3	2.01	0.43
1:A:139:ALA:HB1	5:A:1800:B12:H362	2.01	0.43
1:C:203:GLU:OE2	1:C:207:ARG:HD3	2.19	0.43
2:B:517:CYS:HB3	2:B:524:PHE:CG	2.54	0.43
2:B:515:LEU:HD23	2:B:566:ASP:HB3	2.01	0.42
2:B:579:LEU:HG	2:B:583:LYS:HE3	2.00	0.42
1:A:492:GLN:HE22	1:A:495:LYS:NZ	2.17	0.42
1:A:541:ALA:O	1:A:542:MET:HB2	2.19	0.42
2:B:246:ALA:HB1	2:B:250:ALA:HB3	2.00	0.42
1:C:197:GLN:HA	1:C:239:SER:HB3	2.02	0.42
1:A:138:MET:SD	1:A:485:ASN:HB2	2.59	0.42
1:C:215:GLN:HB3	1:C:216:PRO:CD	2.46	0.42
1:C:636:THR:HB	1:C:637:PRO:HD2	2.01	0.42
5:A:1800:B12:H2B	5:A:1800:B12:O2	2.19	0.42
1:C:23:ARG:CD	7:C:4304:HOH:O	2.62	0.42
2:D:517:CYS:HB3	2:D:524:PHE:CG	2.55	0.42
1:C:252:ALA:O	1:C:256:MET:HG3	2.20	0.42
5:C:2800:B12:H363	5:C:2800:B12:H421	2.02	0.42
2:D:267:VAL:HA	2:D:271:PHE:O	2.20	0.42
1:A:571:SER:HB3	1:A:623:ASP:HB3	2.02	0.42
1:A:602:LEU:HD22	5:A:1800:B12:HM52	2.01	0.42
1:C:171:VAL:HG23	1:C:196:ILE:HG12	2.01	0.42
1:C:521:ASN:O	1:C:529:ARG:HD3	2.19	0.42
1:C:243:TYR:HD1	1:C:289:GLY:HA2	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:602:LEU:HD22	5:C:2800:B12:HM52	2.02	0.41
1:A:521:ASN:O	1:A:529:ARG:HD3	2.21	0.41
1:C:579:GLU:HB3	1:C:712:PRO:HB2	2.01	0.41
2:D:107:TRP:CD1	2:D:358:ILE:HD12	2.56	0.41
1:A:392:GLN:HB3	2:B:459:PRO:HG2	2.02	0.41
5:A:1800:B12:H262	5:A:1800:B12:H91	1.97	0.41
2:D:331:LEU:HD13	2:D:365:GLN:HB3	2.03	0.41
2:D:518:LEU:HD21	2:D:581:VAL:HG11	2.02	0.41
1:A:89:PHE:CE2	3:A:1801[A]:SCD:HS21	2.55	0.41
1:A:683:THR:HG21	1:A:718:LEU:HD13	2.02	0.41
2:B:267:VAL:HA	2:B:271:PHE:O	2.21	0.41
5:C:2800:B12:C61	5:C:2800:B12:H551	2.50	0.41
2:D:374:PHE:CB	2:D:375:PRO:HD3	2.50	0.41
1:A:374:LEU:HB2	1:A:481:LEU:HD23	2.03	0.41
1:C:503:ARG:HD2	1:C:508:VAL:HG21	2.03	0.41
1:A:606:GLY:O	1:A:634:PHE:HA	2.20	0.40
5:A:1800:B12:H601	5:A:1800:B12:H252	2.03	0.40
1:A:89:PHE:CE2	4:A:1802[B]:MCD:HS2	2.57	0.40
1:C:613:GLY:HA2	5:C:2800:B12:H3P1	2.03	0.40
2:D:197:LEU:HD12	2:D:233:ALA:HB1	2.03	0.40
2:B:460:ILE:HD13	2:B:494:SER:HB3	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:LYS:NZ	2:D:20:THR:OG1[2_646]	1.69	0.51
1:A:670:LYS:CD	2:D:20:THR:O[2_646]	2.02	0.18

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	723/727 (99%)	695 (96%)	27 (4%)	1 (0%)	51	60
1	C	723/727 (99%)	693 (96%)	29 (4%)	1 (0%)	51	60
2	B	617/637 (97%)	594 (96%)	21 (3%)	2 (0%)	41	46
2	D	617/637 (97%)	596 (97%)	19 (3%)	2 (0%)	41	46
All	All	2680/2728 (98%)	2578 (96%)	96 (4%)	6 (0%)	47	55

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	576	ASN
2	D	171	ASP
1	A	576	ASN
2	B	171	ASP
2	D	228	SER
2	B	228	SER

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	573/590 (97%)	555 (97%)	18 (3%)	40	51
1	C	573/590 (97%)	562 (98%)	11 (2%)	57	71
2	B	481/509 (94%)	458 (95%)	23 (5%)	25	32
2	D	481/509 (94%)	460 (96%)	21 (4%)	28	35
All	All	2108/2198 (96%)	2035 (96%)	73 (4%)	36	46

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	96	LYS
1	A	123	ARG
1	A	149	MET
1	A	379	SER

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Mol	Chain	Res	Type
1	A	430	VAL
1	A	471	ARG
1	A	480	VAL
1	A	514	LYS
1	A	525	LYS
1	A	533	LYS
1	A	576	ASN
1	A	592	GLN
1	A	596	ARG
1	A	597	ARG
1	A	656	SER
1	A	668	LEU
1	A	721	LYS
2	B	22	SER
2	B	77	ARG
2	B	79	LYS
2	B	141	ASP
2	B	186	SER
2	B	188	LYS
2	B	191	LYS
2	B	193	LEU
2	B	216	VAL
2	B	226	LYS
2	B	228	SER
2	B	288	HIS
2	B	300	LEU
2	B	334	GLU
2	B	402	SER
2	B	410	ARG
2	B	425	LYS
2	B	435	THR
2	B	477	LYS
2	B	512	LYS
2	B	532	SER
2	B	619	MET
2	B	638	LYS
1	C	24	ARG
1	C	96	LYS
1	C	149	MET
1	C	365	THR
1	C	533	LYS
1	C	576	ASN

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Mol	Chain	Res	Type
1	C	592	GLN
1	C	596	ARG
1	C	597	ARG
1	C	668	LEU
1	C	721	LYS
2	D	60	LYS
2	D	77	ARG
2	D	141	ASP
2	D	186	SER
2	D	188	LYS
2	D	191	LYS
2	D	193	LEU
2	D	216	VAL
2	D	228	SER
2	D	288	HIS
2	D	300	LEU
2	D	334	GLU
2	D	335	ASP
2	D	410	ARG
2	D	425	LYS
2	D	435	THR
2	D	477	LYS
2	D	522	ARG
2	D	532	SER
2	D	619	MET
2	D	638	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	191	GLN
1	A	198	ASN
1	A	246	GLN
1	A	359	HIS
1	A	385	ASN
1	A	492	GLN
1	A	635	GLN
1	A	643	GLN
2	B	290	GLN
2	B	322	GLN
2	B	323	ASN
2	B	391	ASN

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Mol	Chain	Res	Type
1	C	191	GLN
1	C	198	ASN
1	C	246	GLN
1	C	359	HIS
1	C	385	ASN
1	C	454	GLN
1	C	492	GLN
1	C	635	GLN
1	C	643	GLN
2	D	290	GLN
2	D	322	GLN
2	D	323	ASN
2	D	391	ASN

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 monosaccharides in this entry.

5.6 Ligand geometry

10 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MCD	A	1802[B]	-	48,57,57	1.17	4 (8%)	59,85,85	1.49	10 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	B12	A	1800	1	90,101,101	0.93	2 (2%)	137,166,166	1.63	28 (20%)
3	SCD	A	1801[A]	-	49,57,57	1.15	4 (8%)	62,84,84	1.59	13 (20%)
4	MCD	C	2802[B]	-	48,57,57	1.15	4 (8%)	59,85,85	1.46	9 (15%)
6	GOL	B	3001	-	5,5,5	0.22	0	5,5,5	0.33	0
3	SCD	C	2801[A]	-	49,57,57	1.11	4 (8%)	62,84,84	1.56	11 (17%)
6	GOL	B	3002	-	5,5,5	0.29	0	5,5,5	0.90	0
5	B12	C	2800	1	90,101,101	0.96	4 (4%)	137,166,166	1.54	25 (18%)
6	GOL	D	3003	-	5,5,5	0.21	0	5,5,5	0.41	0
6	GOL	D	3004	-	5,5,5	0.29	0	5,5,5	0.62	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MCD	A	1802[B]	-	-	3/55/75/75	0/3/3/3
5	B12	A	1800	1	-	6/52/223/223	0/3/11/11
3	SCD	A	1801[A]	-	-	4/52/72/72	0/3/3/3
4	MCD	C	2802[B]	-	-	2/55/75/75	0/3/3/3
6	GOL	B	3001	-	-	4/4/4/4	-
3	SCD	C	2801[A]	-	-	6/52/72/72	0/3/3/3
6	GOL	B	3002	-	-	2/4/4/4	-
5	B12	C	2800	1	-	6/52/223/223	0/3/11/11
6	GOL	D	3003	-	-	4/4/4/4	-
6	GOL	D	3004	-	-	2/4/4/4	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1802[B]	MCD	CP2-NP1	3.61	1.54	1.46
3	A	1801[A]	SCD	CP2-NP1	3.57	1.54	1.46
4	A	1802[B]	MCD	CP5-NP2	3.45	1.54	1.46
4	C	2802[B]	MCD	CP5-NP2	3.39	1.53	1.46
4	C	2802[B]	MCD	CP2-NP1	3.26	1.53	1.46
3	A	1801[A]	SCD	CP5-NP2	3.24	1.53	1.46
3	C	2801[A]	SCD	CP2-NP1	3.09	1.53	1.46
3	C	2801[A]	SCD	CP5-NP2	3.05	1.53	1.46
5	A	1800	B12	C14-N23	3.03	1.39	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1801[A]	SCD	P2-O7	-2.99	1.47	1.59
4	A	1802[B]	MCD	P2-O7	-2.85	1.47	1.59
3	C	2801[A]	SCD	P2-O7	-2.80	1.48	1.59
4	C	2802[B]	MCD	P2-O7	-2.70	1.48	1.59
5	C	2800	B12	C14-N23	2.58	1.38	1.35
5	C	2800	B12	P-O2	2.27	1.66	1.60
4	A	1802[B]	MCD	OS4-CS4	2.18	1.28	1.22
5	C	2800	B12	C30-C3	2.15	1.59	1.54
3	A	1801[A]	SCD	OS4-CS4	2.11	1.29	1.22
5	C	2800	B12	C35-C5	2.10	1.55	1.50
4	C	2802[B]	MCD	OS4-CS4	2.07	1.28	1.22
3	C	2801[A]	SCD	C2-N1	2.05	1.37	1.33
5	A	1800	B12	P-O2	2.01	1.65	1.60

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1800	B12	C7B-C8B-C9B	5.65	126.13	120.54
5	C	2800	B12	C7B-C8B-C9B	4.99	125.48	120.54
5	A	1800	B12	C16-C15-C14	-4.87	113.86	121.25
3	C	2801[A]	SCD	CP8-CPA-CPB	4.73	115.95	108.23
4	A	1802[B]	MCD	CP5-NP2-CP6	-4.72	114.17	122.59
3	A	1801[A]	SCD	CP8-CPA-CPB	4.44	115.47	108.23
4	C	2802[B]	MCD	CP5-NP2-CP6	-4.42	114.70	122.59
3	C	2801[A]	SCD	CP5-NP2-CP6	-4.28	114.95	122.59
3	A	1801[A]	SCD	CP5-NP2-CP6	-4.25	115.01	122.59
5	C	2800	B12	C20-C1-C19	4.16	113.36	109.36
5	C	2800	B12	C16-C15-C14	-4.01	115.16	121.25
4	C	2802[B]	MCD	CP8-CPA-CPB	3.97	114.71	108.23
5	A	1800	B12	C54-C17-C16	-3.88	92.26	112.40
5	C	2800	B12	C54-C17-C16	-3.80	92.66	112.40
4	A	1802[B]	MCD	CP8-CPA-CPB	3.69	114.25	108.23
3	A	1801[A]	SCD	O7-CPB-CPA	-3.67	104.65	110.55
4	C	2802[B]	MCD	O7-CPB-CPA	-3.60	104.75	110.55
5	A	1800	B12	C55-C17-C18	3.57	118.05	111.15
5	A	1800	B12	C13-C14-C15	-3.54	118.90	124.32
4	A	1802[B]	MCD	O7-CPB-CPA	-3.54	104.85	110.55
5	C	2800	B12	C55-C17-C16	3.49	123.54	116.65
3	C	2801[A]	SCD	CS3-CS2-CS1	-3.47	109.22	113.61
3	C	2801[A]	SCD	C5-C6-N6	3.40	125.52	120.35
3	C	2801[A]	SCD	O7-CPB-CPA	-3.35	105.16	110.55
5	A	1800	B12	C12-C11-C10	-3.35	119.01	123.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	2802[B]	MCD	C5-C6-N6	3.31	125.39	120.35
3	A	1801[A]	SCD	C5-C6-N6	3.16	125.15	120.35
3	C	2801[A]	SCD	CP9-CPA-CPB	3.09	113.27	108.23
3	A	1801[A]	SCD	CP2-NP1-CP3	-3.07	117.13	122.84
4	A	1802[B]	MCD	C5-C6-N6	3.04	124.98	120.35
4	C	2802[B]	MCD	CP9-CPA-CPB	3.04	113.19	108.23
5	C	2800	B12	C55-C17-C18	3.00	116.95	111.15
5	A	1800	B12	C55-C56-C57	-2.98	104.72	111.23
5	C	2800	B12	O51-C50-C49	-2.96	112.36	121.07
3	A	1801[A]	SCD	OS5-CS4-CS3	2.96	123.54	114.03
5	A	1800	B12	C13-C14-N23	2.86	113.00	109.10
4	A	1802[B]	MCD	CP1-CP2-NP1	-2.86	104.03	112.21
4	C	2802[B]	MCD	CP9-CPA-CP7	-2.85	103.87	108.82
5	A	1800	B12	C5B-C4B-C9B	-2.80	117.26	121.22
5	C	2800	B12	O6R-C1R-C2R	-2.79	102.85	106.93
5	A	1800	B12	C5-C6-N22	-2.72	119.72	123.88
5	A	1800	B12	C5M-C5B-C6B	-2.71	115.18	120.74
5	A	1800	B12	O51-C50-C49	-2.71	113.12	121.07
5	A	1800	B12	C10-C11-N23	2.65	128.97	124.43
5	C	2800	B12	C18-C19-N24	2.60	106.27	102.31
5	C	2800	B12	C2P-C1P-N59	-2.59	109.11	112.93
5	A	1800	B12	C20-C1-C2	-2.59	108.96	113.28
3	C	2801[A]	SCD	OS5-CS4-CS3	2.58	122.31	114.03
5	A	1800	B12	O5-P-O4	2.56	124.89	112.24
5	C	2800	B12	C5B-C4B-C9B	-2.51	117.67	121.22
3	C	2801[A]	SCD	CP1-CP2-NP1	-2.51	105.04	112.21
4	C	2802[B]	MCD	CP1-CP2-NP1	-2.48	105.13	112.21
5	A	1800	B12	C55-C17-C16	2.47	121.53	116.65
5	C	2800	B12	C3-C4-C5	-2.45	119.68	123.81
5	A	1800	B12	C18-C19-N24	2.45	106.04	102.31
3	A	1801[A]	SCD	CP1-CP2-NP1	-2.44	105.23	112.21
5	C	2800	B12	C54-C17-C55	-2.41	105.28	109.25
4	A	1802[B]	MCD	CP2-NP1-CP3	-2.39	118.41	122.84
5	C	2800	B12	C35-C5-C4	-2.38	111.93	116.79
3	C	2801[A]	SCD	OS5-CS4-OS4	-2.38	117.38	123.30
3	A	1801[A]	SCD	OP2-CP6-NP2	2.37	128.08	122.99
5	A	1800	B12	C1P-N59-C57	-2.36	117.56	122.69
4	C	2802[B]	MCD	OS1-CS1-CPS	2.35	125.88	121.70
5	C	2800	B12	C1P-N59-C57	-2.34	117.59	122.69
5	A	1800	B12	C53-C15-C16	2.33	124.39	120.38
5	A	1800	B12	C42-C43-N45	2.33	123.76	116.51
5	C	2800	B12	C1-C2-C3	-2.33	98.62	101.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	1800	B12	C3-C4-C5	-2.33	119.89	123.81
5	C	2800	B12	C2-C1-C19	-2.31	114.96	118.60
5	C	2800	B12	C15-C16-N24	2.30	125.73	122.42
5	A	1800	B12	C4B-C9B-C8B	-2.29	118.76	121.10
5	A	1800	B12	C2-C1-N21	2.29	104.95	101.77
3	A	1801[A]	SCD	CS3-CS2-CS1	-2.28	110.72	113.61
5	C	2800	B12	C2-C1-N21	2.27	104.94	101.77
3	C	2801[A]	SCD	OP2-CP6-NP2	2.25	127.82	122.99
4	A	1802[B]	MCD	C2'-C3'-C4'	-2.24	99.25	103.22
5	C	2800	B12	C55-C56-C57	-2.24	106.35	111.23
5	A	1800	B12	C1-C2-C3	-2.23	98.75	101.60
4	C	2802[B]	MCD	C2'-C3'-C4'	-2.20	99.33	103.22
4	A	1802[B]	MCD	CP9-CPA-CP7	-2.20	105.01	108.82
5	A	1800	B12	C41-C8-C9	-2.19	107.33	111.19
5	C	2800	B12	C13-C14-C15	-2.18	120.98	124.32
5	C	2800	B12	O5-P-O4	2.18	123.01	112.24
3	C	2801[A]	SCD	C2'-C3'-C4'	-2.17	99.38	103.22
5	C	2800	B12	C4B-C9B-C8B	-2.16	118.89	121.10
5	A	1800	B12	C2P-C1P-N59	-2.15	109.76	112.93
5	A	1800	B12	C54-C17-C18	-2.15	109.81	112.98
4	A	1802[B]	MCD	C5-C6-N1	-2.15	115.48	120.35
4	A	1802[B]	MCD	OP2-CP6-CP7	-2.14	114.53	121.06
3	A	1801[A]	SCD	C5-C6-N1	-2.13	115.52	120.35
3	A	1801[A]	SCD	C2'-C3'-C4'	-2.11	99.48	103.22
5	A	1800	B12	C4B-C5B-C6B	2.11	123.46	119.91
3	A	1801[A]	SCD	CP9-CPA-CPB	2.10	111.66	108.23
5	C	2800	B12	C30-C31-C32	2.05	119.56	112.59
5	C	2800	B12	O58-C57-N59	2.03	126.84	123.01
3	A	1801[A]	SCD	O4'-C1'-C2'	-2.01	103.99	106.93

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	2801[A]	SCD	P1-O6-P2-O7
4	A	1802[B]	MCD	P1-O6-P2-O7
4	C	2802[B]	MCD	P1-O6-P2-O7
6	B	3001	GOL	O1-C1-C2-C3
6	B	3001	GOL	C1-C2-C3-O3
6	B	3002	GOL	C1-C2-C3-O3
6	D	3003	GOL	O1-C1-C2-C3
6	D	3003	GOL	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
6	D	3004	GOL	C1-C2-C3-O3
5	C	2800	B12	C42-C41-C8-C9
6	B	3001	GOL	O1-C1-C2-O2
6	B	3002	GOL	O2-C2-C3-O3
5	A	1800	B12	C16-C17-C55-C56
6	B	3001	GOL	O2-C2-C3-O3
6	D	3003	GOL	O1-C1-C2-O2
6	D	3004	GOL	O2-C2-C3-O3
6	D	3003	GOL	O2-C2-C3-O3
5	A	1800	B12	C41-C42-C43-O44
5	A	1800	B12	C41-C42-C43-N45
5	C	2800	B12	C2P-O3-P-O2
3	A	1801[A]	SCD	P1-O6-P2-O7
5	A	1800	B12	C2P-O3-P-O2
3	A	1801[A]	SCD	P2-O6-P1-O12
3	C	2801[A]	SCD	P2-O6-P1-O12
4	C	2802[B]	MCD	P2-O6-P1-O12
4	A	1802[B]	MCD	P2-O6-P1-O12
3	A	1801[A]	SCD	CP8-CPA-CPB-O7
3	C	2801[A]	SCD	CP8-CPA-CPB-O7
4	A	1802[B]	MCD	CPS-CS1-CS2-CS4
5	C	2800	B12	C55-C56-C57-O58
5	C	2800	B12	C30-C31-C32-N33
5	A	1800	B12	C30-C31-C32-N33
3	C	2801[A]	SCD	P2-O6-P1-O11
3	A	1801[A]	SCD	CS2-CS3-CS4-OS4
5	C	2800	B12	C55-C56-C57-N59
5	C	2800	B12	C30-C31-C32-O34
3	C	2801[A]	SCD	CS2-CS3-CS4-OS5
5	A	1800	B12	C30-C31-C32-O34
3	C	2801[A]	SCD	CS2-CS3-CS4-OS4

There are no ring outliers.

8 monomers are involved in 45 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1802[B]	MCD	3	0
5	A	1800	B12	17	0
3	A	1801[A]	SCD	2	0
4	C	2802[B]	MCD	2	0
3	C	2801[A]	SCD	1	0
6	B	3002	GOL	1	0

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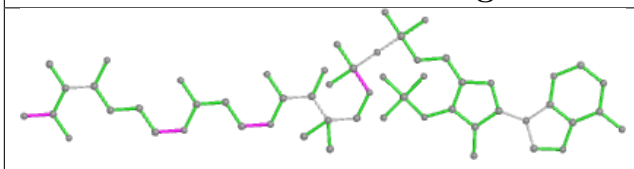
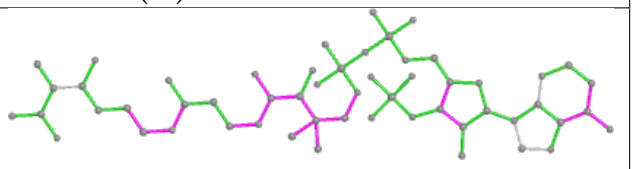
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2800	B12	16	0
6	D	3004	GOL	3	0

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.

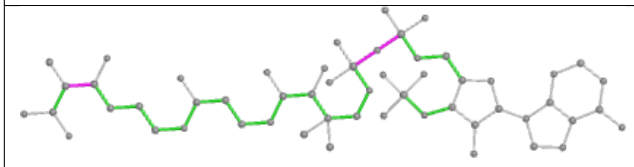
Ligand MCD A 1802 (B)



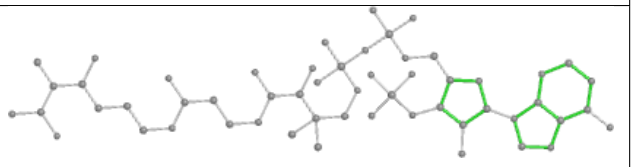
Bond lengths



Bond angles

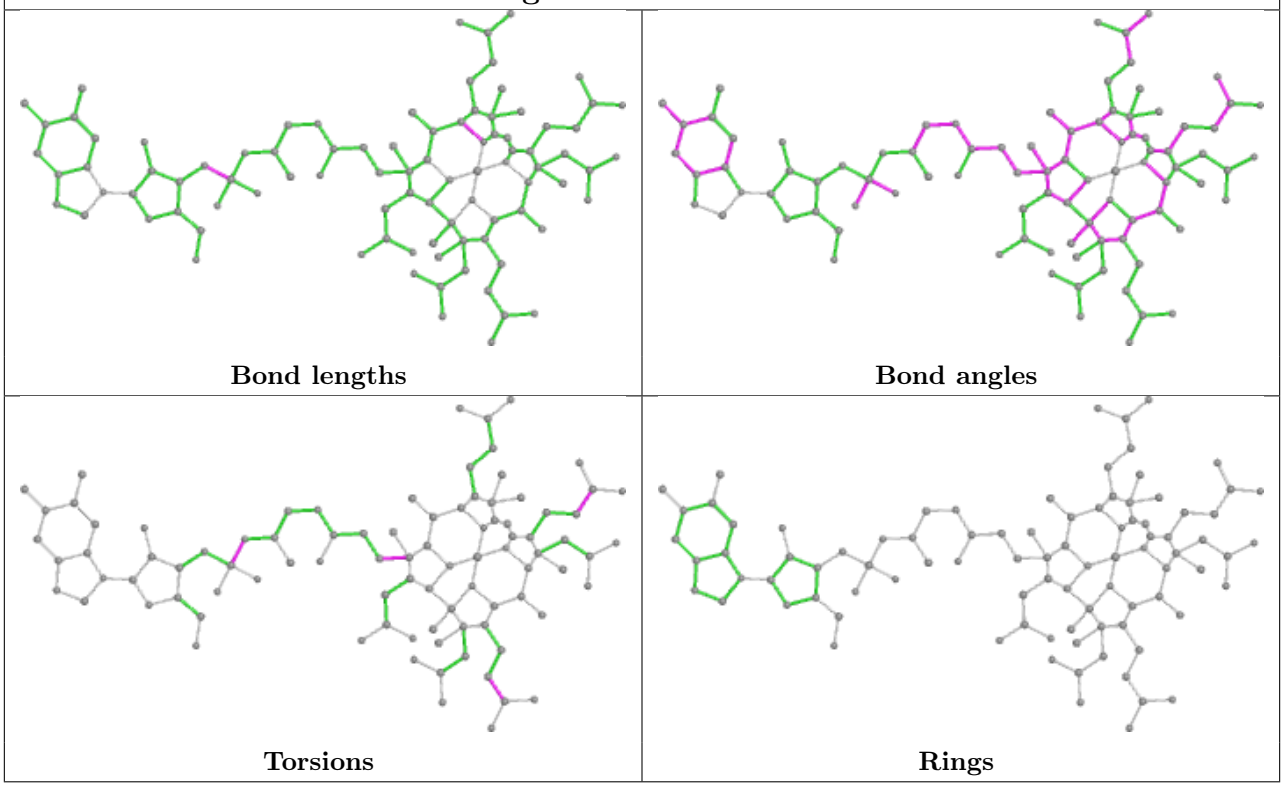


Torsions

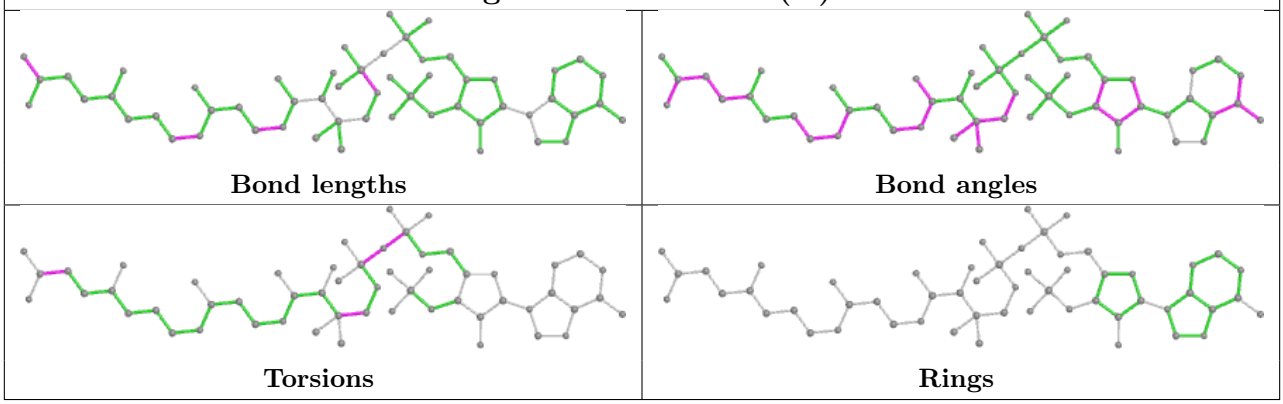


Rings

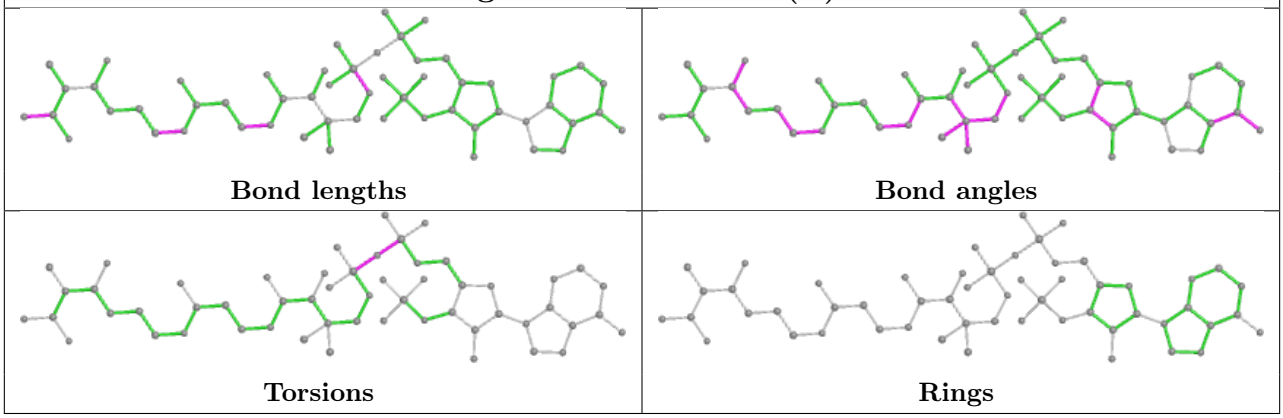
Ligand B12 A 1800



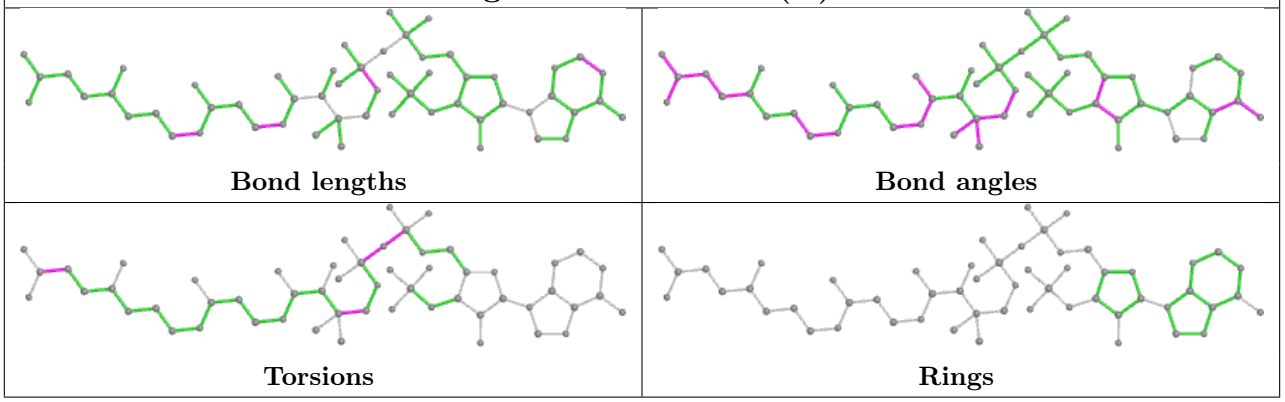
Ligand SCD A 1801 (A)



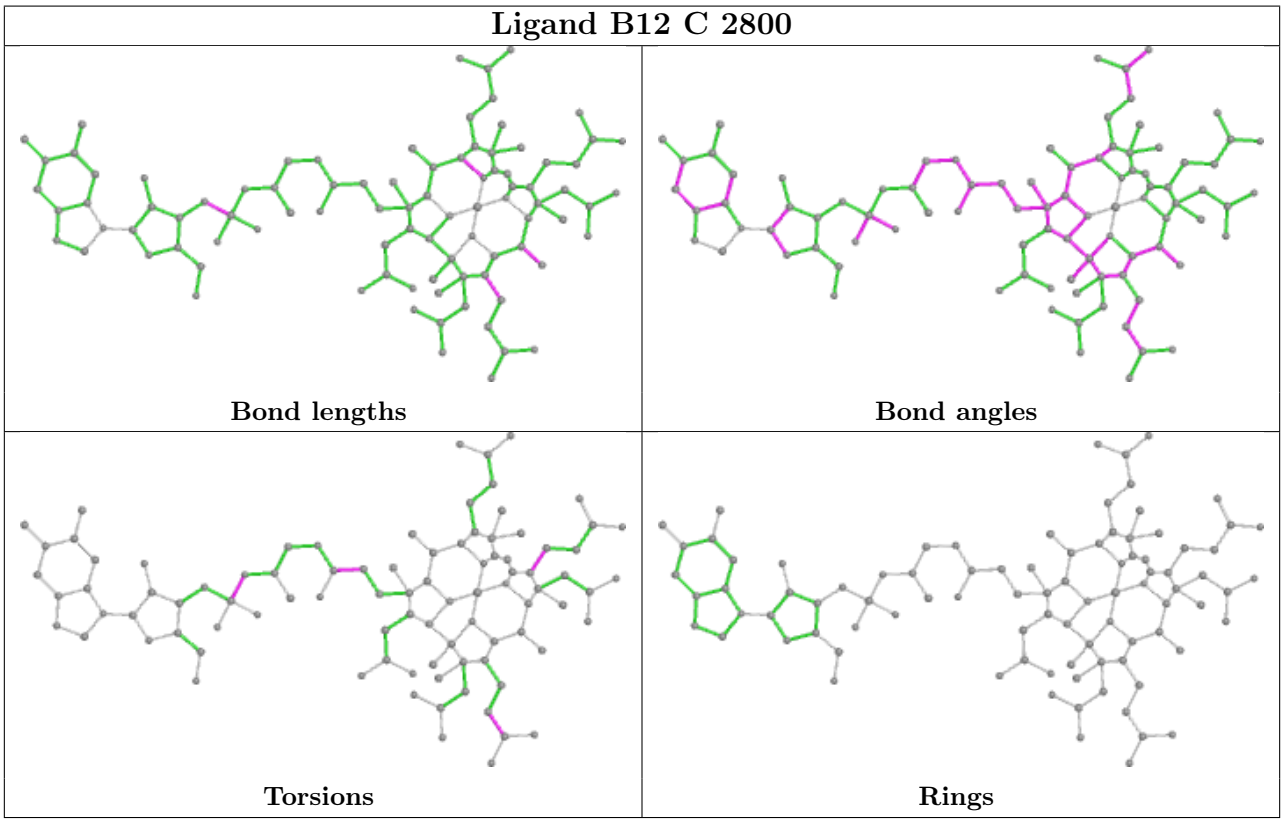
Ligand MCD C 2802 (B)



Ligand SCD C 2801 (A)



Ligand B12 C 2800



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	725/727 (99%)	0.07	16 (2%) 62 59	17, 36, 60, 80	0
1	C	725/727 (99%)	0.27	35 (4%) 30 29	17, 36, 60, 81	0
2	B	619/637 (97%)	0.37	39 (6%) 20 19	24, 49, 73, 89	0
2	D	619/637 (97%)	0.60	66 (10%) 6 5	26, 50, 73, 89	0
All	All	2688/2728 (98%)	0.32	156 (5%) 23 22	17, 42, 70, 89	0

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	501	ALA	6.5
2	D	183	TYR	6.4
2	D	192	ASP	6.2
1	C	23	ARG	6.1
2	D	20	THR	5.1
1	C	576	ASN	4.9
2	D	638	LYS	4.7
2	B	638	LYS	4.7
1	A	477	PRO	4.5
1	A	576	ASN	4.4
1	C	9	SER	4.4
2	D	186	SER	4.4
1	A	473	GLU	4.3
1	C	474	HIS	4.3
1	A	728	ALA	4.3
2	D	548	GLY	4.2
2	D	426	LEU	4.1
2	D	170	TYR	4.1
1	C	728	ALA	4.1
1	C	25	PHE	3.9
2	D	272	THR	3.9

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Mol	Chain	Res	Type	RSRZ
1	C	476	PRO	3.8
2	B	137	LEU	3.7
1	C	473	GLU	3.6
2	D	126	LEU	3.6
1	C	19	ALA	3.6
2	D	189	PRO	3.6
2	D	187	ASP	3.6
1	C	14	ASN	3.6
2	D	312	GLY	3.5
2	B	612	LEU	3.5
2	D	194	ALA	3.5
2	D	311	PHE	3.5
1	C	27	GLU	3.5
2	D	193	LEU	3.4
1	A	240	ILE	3.3
1	A	474	HIS	3.3
2	B	170	TYR	3.3
1	C	16	PRO	3.3
2	D	140	VAL	3.3
2	B	637	ALA	3.3
2	D	191	LYS	3.3
1	C	486	SER	3.2
1	C	30	ALA	3.2
2	D	161	MET	3.2
1	C	20	ASP	3.1
2	D	316	ASP	3.1
1	C	24	ARG	3.1
1	C	21	ALA	3.0
2	B	609	ALA	3.0
2	D	308	GLY	3.0
2	D	151	ASP	3.0
2	D	50	GLU	2.9
2	D	313	VAL	2.9
1	C	35	GLY	2.9
2	B	282	PHE	2.9
2	D	318	ARG	2.9
2	D	182	VAL	2.9
1	A	4	LEU	2.9
1	A	501	ALA	2.9
2	B	198	GLY	2.8
2	D	555	GLU	2.7
2	D	270	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	B	136	LEU	2.7
2	D	325	ILE	2.7
1	C	154	ALA	2.7
2	D	49	PRO	2.6
1	C	36	GLU	2.6
2	B	112	LEU	2.6
2	D	184	GLU	2.6
2	D	122	ARG	2.6
2	B	166	VAL	2.6
2	D	282	PHE	2.6
1	C	32	ALA	2.6
2	D	146	ALA	2.6
2	B	174	ALA	2.5
1	C	475	GLU	2.5
2	B	138	LEU	2.5
1	C	7	PHE	2.5
2	B	636	VAL	2.5
2	B	192	ASP	2.5
2	B	508	SER	2.5
2	D	180	VAL	2.5
2	D	310	VAL	2.5
1	C	274	GLY	2.5
2	B	283	ARG	2.4
2	B	195	LEU	2.4
1	A	286	PHE	2.4
1	C	10	VAL	2.4
2	D	433	VAL	2.4
1	C	243	TYR	2.4
2	B	187	ASP	2.4
2	B	426	LEU	2.4
1	C	37	ALA	2.4
2	B	238	ALA	2.4
2	D	482	ALA	2.4
2	D	487	GLY	2.4
2	D	486	LYS	2.4
1	C	479	ASP	2.3
2	D	112	LEU	2.3
2	D	315	GLU	2.3
2	D	297	LEU	2.3
1	A	697	ARG	2.3
2	D	93	PHE	2.3
2	D	483	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	38	TRP	2.3
2	D	220	TRP	2.3
2	D	283	ARG	2.3
2	D	147	PRO	2.3
1	C	34	THR	2.3
2	D	260	ALA	2.3
2	B	487	GLY	2.2
2	D	230	ASP	2.2
1	C	287	PHE	2.2
1	C	517	TRP	2.2
2	B	20	THR	2.2
2	D	102	GLY	2.2
2	B	284	VAL	2.2
2	D	190	ALA	2.2
2	D	138	LEU	2.2
2	D	480	PRO	2.2
1	A	9	SER	2.2
1	C	17	VAL	2.2
2	B	149	HIS	2.2
2	D	89	GLY	2.2
1	A	287	PHE	2.1
2	B	475	GLU	2.1
2	B	297	LEU	2.1
2	D	222	ARG	2.1
1	C	241	SER	2.1
2	D	145	ILE	2.1
2	B	239	ASN	2.1
2	D	227	PHE	2.1
2	B	48	PRO	2.1
2	B	325	ILE	2.1
1	A	484	ASP	2.1
2	B	110	ARG	2.1
2	B	111	ALA	2.1
2	B	183	TYR	2.1
2	D	179	LEU	2.1
2	D	197	LEU	2.1
2	B	509	GLU	2.1
2	D	137	LEU	2.0
2	B	359	THR	2.0
2	B	432	ALA	2.0
2	B	50	GLU	2.0
1	A	698	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	199	LEU	2.0
2	D	300	LEU	2.0
2	D	637	ALA	2.0
1	A	171	VAL	2.0
1	A	575	LYS	2.0
2	D	323	ASN	2.0
2	B	236	ILE	2.0
2	D	33	GLU	2.0
2	D	195	LEU	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, 95^{th} 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.

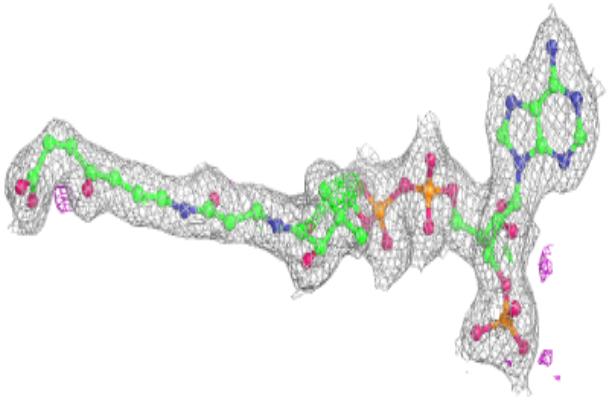
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	GOL	D	3003	6/6	0.43	0.24	94,95,95,95	0
6	GOL	D	3004	6/6	0.51	0.52	84,84,85,86	0
6	GOL	B	3001	6/6	0.75	0.15	95,95,95,95	0
6	GOL	B	3002	6/6	0.78	0.42	82,83,84,84	0
3	SCD	C	2801[A]	55/55	0.95	0.14	15,21,27,28	55
4	MCD	C	2802[B]	55/55	0.95	0.14	19,24,35,37	55
3	SCD	A	1801[A]	55/55	0.96	0.13	15,22,26,27	55
5	B12	A	1800	91/91	0.96	0.17	16,27,34,37	0
4	MCD	A	1802[B]	55/55	0.96	0.13	21,24,36,39	55
5	B12	C	2800	91/91	0.97	0.18	18,26,32,36	0

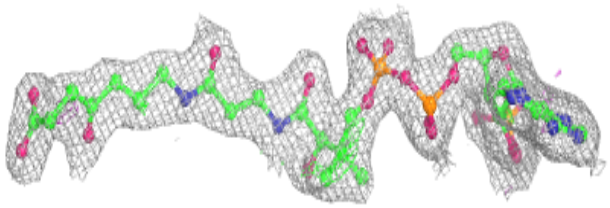
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

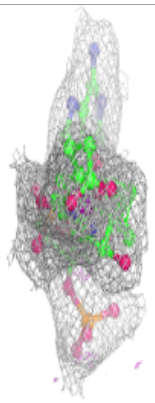
orientation to approximate a three-dimensional view.

Electron density around SCD C 2801 (A):

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

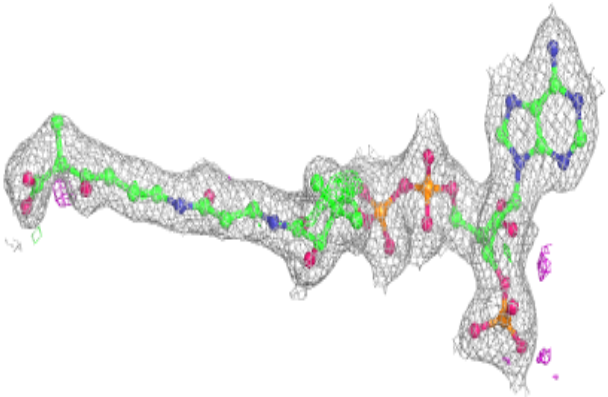


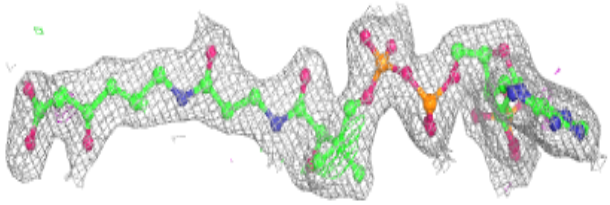


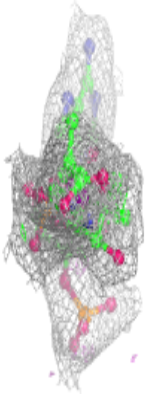


Electron density around MCD C 2802 (B):

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

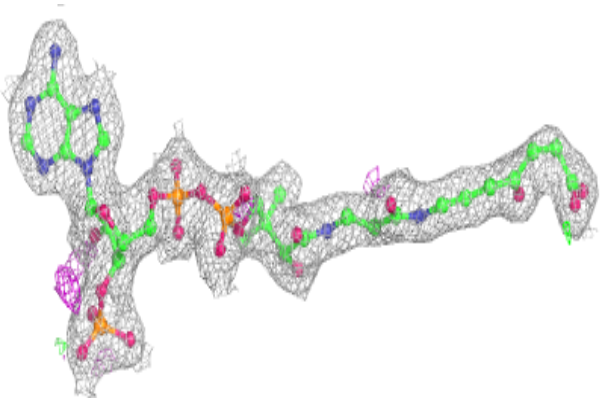


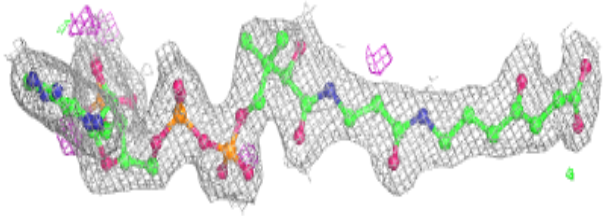


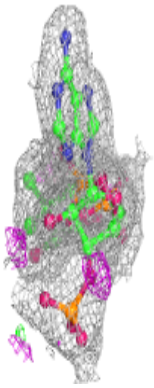


Electron density around SCD A 1801 (A):

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

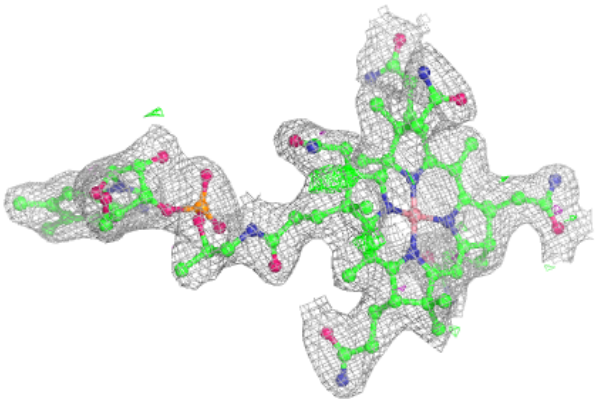


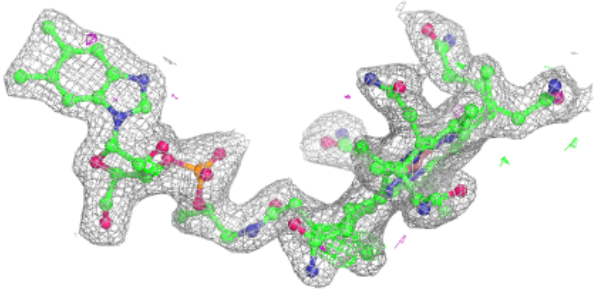


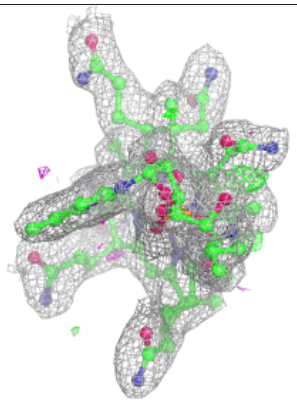


Electron density around B12 A 1800:

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

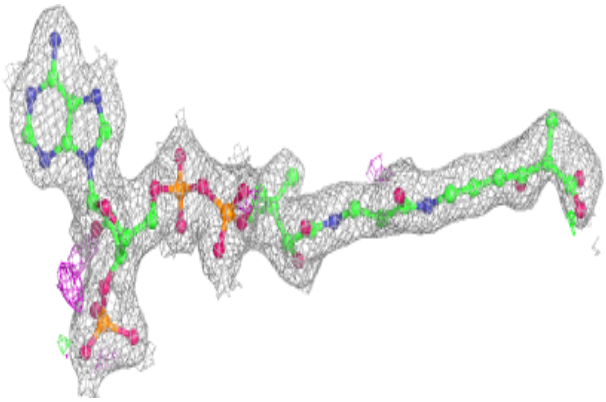


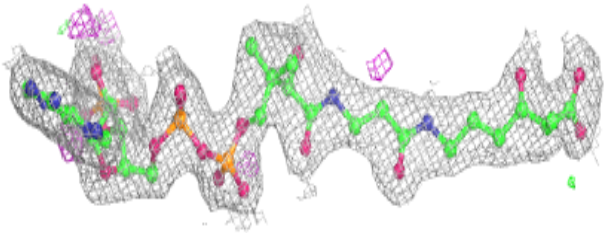


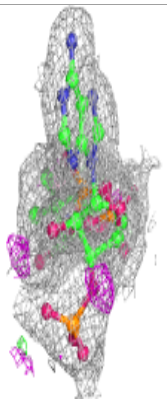


Electron density around MCD A 1802 (B):

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

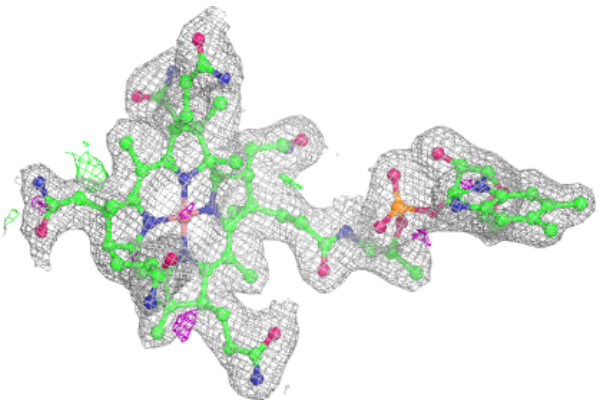


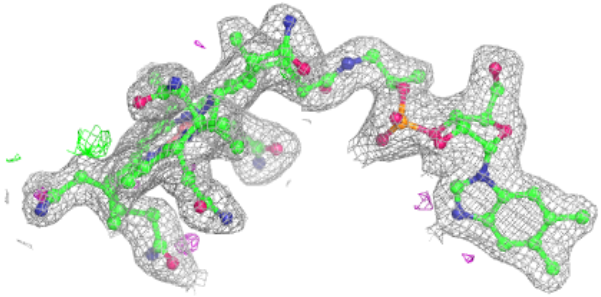


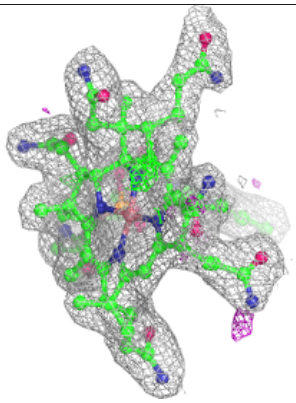


Electron density around B12 C 2800:

$2mF_o$-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.