Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2021 – 12:09 pm BST

PDB ID	:	4ZRP
Title	:	TC:CD320
Authors	:	Alam, A.; Locher, K.P.
Deposited on	:	2015-05-12
Resolution	:	2.10 Å(reported)

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

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

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

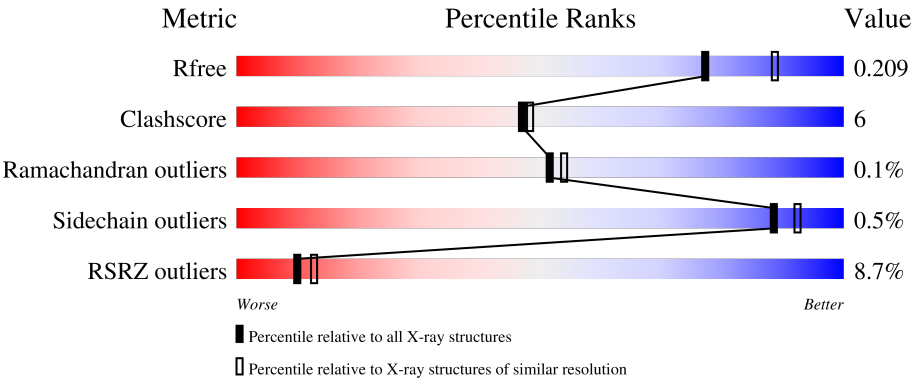
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.1

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 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	409	4% 91% 7% ·
1	B	409	3% 91% 6% ·
2	C	119	26% 48% 17% · 34%
2	D	119	18% 55% 10% ·· 34%

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
3	CNC	A	501	X	-	-	-
3	CNC	B	501	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8001 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 Transcobalamin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	0	0	0
			3103	1981	542	561	19			
1	B	399	Total	C	N	O	S	0	0	0
			3101	1978	543	561	19			

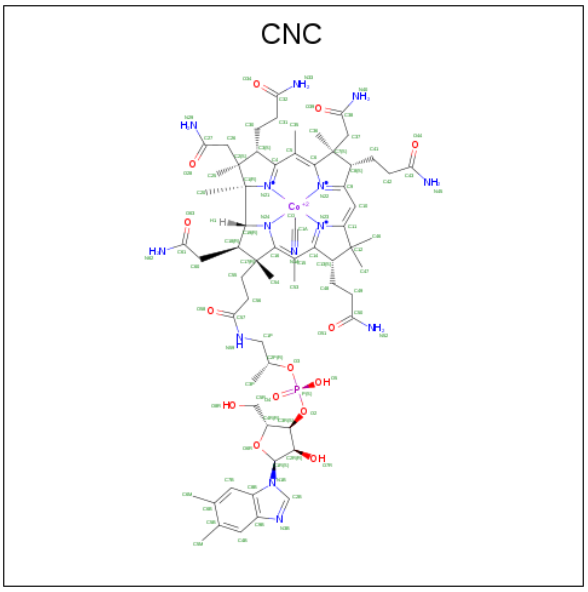
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	209	GLN	ARG	conflict	UNP P20062
B	209	GLN	ARG	conflict	UNP P20062

- Molecule 2 is a protein called CD320 antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	78	Total	C	N	O	S	0	0	0
			560	334	91	123	12			
2	D	79	Total	C	N	O	S	0	0	0
			565	336	91	126	12			

- Molecule 3 is CYANOCOBALAMIN (three-letter code: CNC) (formula: $C_{63}H_{89}CoN_{14}O_{14}P$).

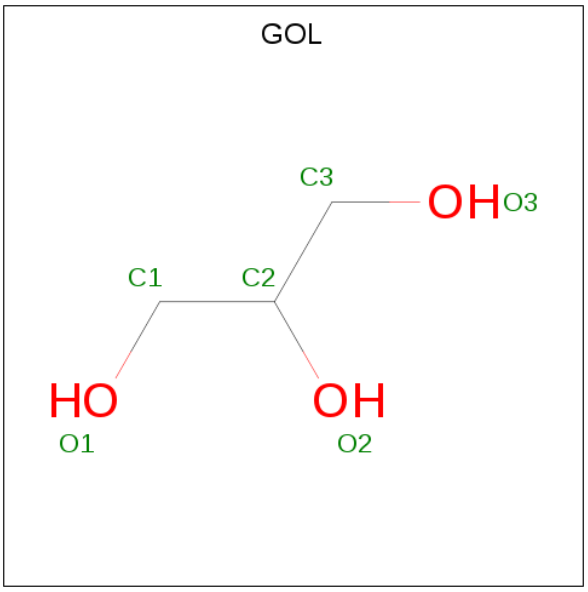


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		
3	B	1	Total	C	Co	N	O	P	0	0
			93	63	1	14	14	1		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		
4	D	2	Total	Ca	0	0
			2	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

- Molecule 6 is water.

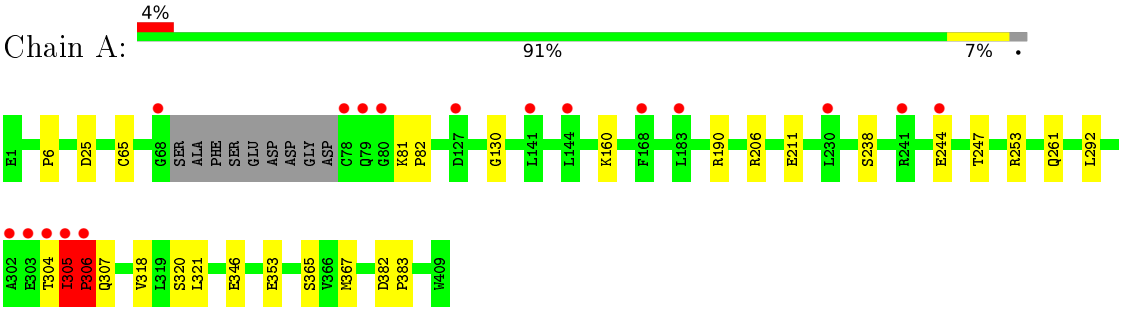
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	227	Total O 227 227	0	0
6	B	195	Total O 195 195	0	0
6	C	12	Total O 12 12	0	0
6	D	10	Total O 10 10	0	0

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.

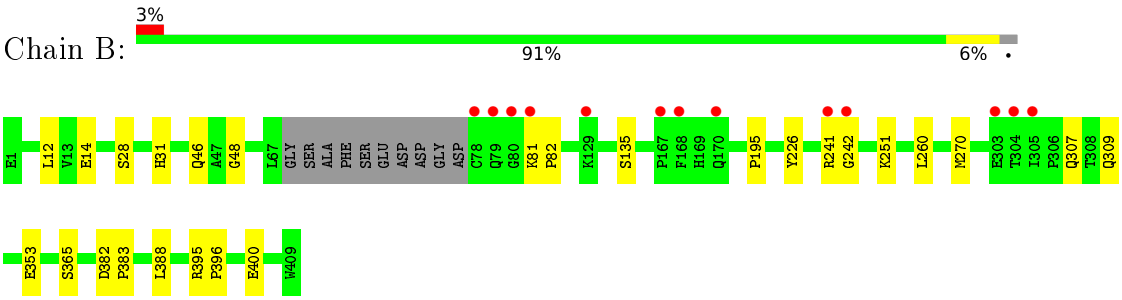
- Molecule 1: Transcobalamin-2

Chain A:



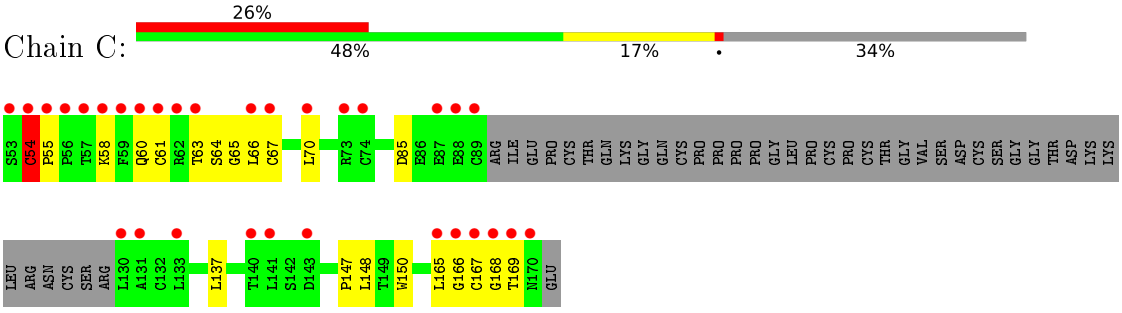
- Molecule 1: Transcobalamin-2

Chain B:



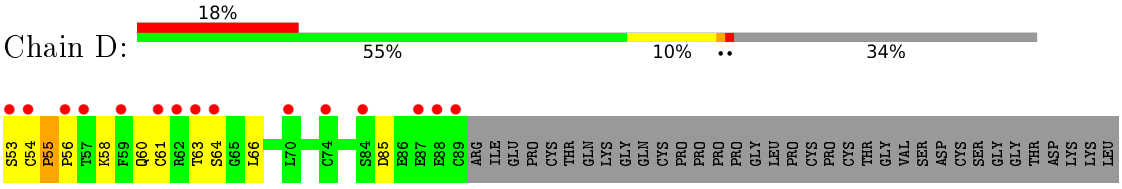
- Molecule 2: CD320 antigen

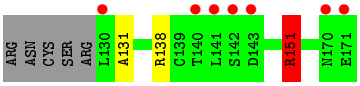
Chain C:



- Molecule 2: CD320 antigen

Chain D:




ARG
ASN
CYS
SER
ARG
L130
A131
R138
C139
T140
L141
S142
D143
R151
N170
E171

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	98.10Å 98.10Å 355.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.94 – 2.10 29.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (29.94-2.10) 86.4 (29.94-2.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.41 (at 2.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.184 , 0.207 0.188 , 0.209	Depositor DCC
R_{free} test set	2000 reflections (1.76%)	wwPDB-VP
Wilson B-factor (Å^2)	35.0	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 54.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	8001	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.63% 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

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.34	0/3171	0.48	1/4300 (0.0%)
1	B	0.32	0/3168	0.45	0/4295
2	C	0.68	1/570 (0.2%)	0.85	3/778 (0.4%)
2	D	0.43	0/575	0.79	1/786 (0.1%)
All	All	0.37	1/7484 (0.0%)	0.54	5/10159 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
2	C	0	1
2	D	0	1
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	67	CYS	CB-SG	10.44	2.00	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	67	CYS	CA-CB-SG	9.99	131.98	114.00
2	C	54	CYS	CA-CB-SG	6.13	125.04	114.00
2	C	168	GLY	N-CA-C	-5.85	98.47	113.10
1	A	306	PRO	N-CA-C	5.54	126.52	112.10
2	D	151	ARG	NE-CZ-NH1	5.21	122.91	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	305	ILE	Peptide
1	A	306	PRO	Peptide
2	C	54	CYS	Peptide
2	D	55	PRO	Peptide

5.2 Too-close contacts

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	3103	0	3115	27	0
1	B	3101	0	3122	18	0
2	C	560	0	477	16	0
2	D	565	0	472	13	0
3	A	93	0	84	11	0
3	B	93	0	84	8	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	A	30	0	40	4	0
5	B	6	0	8	0	0
6	A	227	0	0	12	1
6	B	195	0	0	7	0
6	C	12	0	0	0	0
6	D	10	0	0	1	0
All	All	8001	0	7402	93	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (93) 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)
3:A:501:CNC:C30	3:A:501:CNC:C31	1.88	1.49
3:A:501:CNC:C31	3:A:501:CNC:C3	1.91	1.30

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:501:CNC:C31	3:A:501:CNC:H3	1.52	1.28
1:B:31:HIS:ND1	6:B:601:HOH:O	1.88	1.03
1:A:130:GLY:O	6:A:602:HOH:O	1.93	0.86
1:A:306:PRO:HB3	1:A:307:GLN:HG3	1.53	0.86
2:D:60:GLN:NE2	2:D:61:CYS:O	2.08	0.86
1:A:261:GLN:OE1	6:A:603:HOH:O	1.94	0.86
1:A:307:GLN:O	6:A:601:HOH:O	1.92	0.85
2:C:60:GLN:NE2	2:C:61:CYS:O	2.11	0.84
2:D:54:CYS:HB2	2:D:55:PRO:HD3	1.64	0.80
2:C:54:CYS:HB2	2:C:55:PRO:HD3	1.62	0.79
3:A:501:CNC:H4B	3:A:501:CNC:C4	2.12	0.79
2:D:54:CYS:HB2	2:D:55:PRO:CD	2.14	0.78
3:B:501:CNC:H2B	3:B:501:CNC:C14	2.14	0.76
3:A:501:CNC:H2B	3:A:501:CNC:C14	2.17	0.75
3:A:501:CNC:H3	3:A:501:CNC:H311	1.66	0.74
1:A:305:ILE:N	1:A:306:PRO:HD3	2.03	0.74
1:A:304:THR:HG22	1:A:306:PRO:HD2	1.69	0.73
1:B:46:GLN:HG2	1:B:48:GLY:H	1.54	0.72
2:C:54:CYS:HB2	2:C:55:PRO:CD	2.19	0.71
1:B:14:GLU:OE2	6:B:602:HOH:O	2.10	0.70
3:B:501:CNC:H4B	3:B:501:CNC:C4	2.22	0.69
5:A:507:GOL:O1	6:A:604:HOH:O	2.12	0.67
1:A:382:ASP:HA	5:A:505:GOL:H2	1.77	0.66
1:B:28:SER:OG	6:B:601:HOH:O	2.12	0.66
1:B:395:ARG:NH1	6:B:606:HOH:O	2.28	0.66
1:A:346:GLU:OE2	6:A:606:HOH:O	2.13	0.65
1:A:25:ASP:OD2	6:A:605:HOH:O	2.13	0.65
1:B:195:PRO:O	6:B:604:HOH:O	2.14	0.65
2:C:58:LYS:HA	2:C:70:LEU:HG	1.79	0.65
2:C:137:LEU:HD23	2:C:148:LEU:HD23	1.79	0.64
1:A:244:GLU:OE1	6:A:607:HOH:O	2.15	0.64
1:B:12:LEU:HD21	1:B:260:LEU:HD13	1.79	0.63
1:A:304:THR:HG22	1:A:306:PRO:CD	2.29	0.62
1:A:65:CYS:HB3	1:A:81:LYS:HB2	1.83	0.61
1:A:244:GLU:OE1	1:A:247:THR:OG1	2.15	0.60
1:B:353:GLU:HB2	1:B:365:SER:HB3	1.84	0.58
2:D:55:PRO:HB2	2:D:56:PRO:O	2.04	0.58
2:C:166:GLY:O	2:C:169:THR:HG22	2.04	0.58
1:A:353:GLU:HB2	1:A:365:SER:HB3	1.85	0.57
1:A:206:ARG:HD3	6:A:621:HOH:O	2.05	0.56
3:B:501:CNC:C14	3:B:501:CNC:C2B	2.86	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:165:LEU:C	2:C:167:CYS:H	2.11	0.53
2:D:64:SER:O	2:D:66:LEU:N	2.41	0.53
3:A:501:CNC:N3B	3:A:501:CNC:N23	2.58	0.51
2:D:56:PRO:HA	2:D:58:LYS:H	1.76	0.51
2:D:54:CYS:CB	2:D:55:PRO:CD	2.85	0.50
1:B:400:GLU:OE2	6:B:605:HOH:O	2.20	0.50
1:A:6:PRO:HD2	1:A:253:ARG:HD2	1.94	0.50
3:A:501:CNC:N23	3:A:501:CNC:C2B	2.76	0.48
1:A:211:GLU:HG3	6:A:736:HOH:O	2.12	0.48
2:C:64:SER:O	2:C:66:LEU:N	2.47	0.48
1:A:238:SER:OG	6:A:609:HOH:O	2.20	0.47
3:B:501:CNC:H532	3:B:501:CNC:H13	1.69	0.47
3:A:501:CNC:C14	3:A:501:CNC:C2B	2.91	0.47
1:A:160:LYS:HE2	6:A:683:HOH:O	2.15	0.46
2:D:131:ALA:HA	2:D:138:ARG:HH22	1.81	0.46
3:B:501:CNC:H541	3:B:501:CNC:H602	1.78	0.46
2:C:54:CYS:CB	2:C:55:PRO:HD3	2.39	0.46
1:B:241:ARG:HA	1:B:242:GLY:HA2	1.73	0.46
2:C:165:LEU:O	2:C:167:CYS:N	2.48	0.46
2:C:85:ASP:OD1	2:C:85:ASP:N	2.49	0.46
1:A:304:THR:C	1:A:306:PRO:HD3	2.35	0.45
2:D:60:GLN:OE1	2:D:66:LEU:O	2.34	0.45
1:B:81:LYS:HB2	1:B:82:PRO:HD2	1.98	0.45
2:D:85:ASP:OD1	2:D:85:ASP:N	2.49	0.45
1:B:307:GLN:CD	1:B:309:GLN:HE22	2.20	0.44
2:D:54:CYS:HB2	2:D:55:PRO:HD2	1.94	0.44
3:A:501:CNC:H541	3:A:501:CNC:H602	1.76	0.44
1:B:388:LEU:O	3:B:501:CNC:H311	2.19	0.43
3:B:501:CNC:N3B	3:B:501:CNC:N23	2.67	0.43
1:B:382:ASP:HA	1:B:383:PRO:HA	1.81	0.43
2:C:63:THR:HG22	2:C:63:THR:O	2.19	0.42
1:B:395:ARG:HA	1:B:396:PRO:HD2	1.94	0.42
1:A:81:LYS:HB2	1:A:82:PRO:HD2	2.02	0.42
1:A:320:SER:O	1:A:321:LEU:HD23	2.20	0.41
1:A:318:VAL:HB	1:A:367:MET:HE1	2.02	0.41
3:A:501:CNC:H201	3:A:501:CNC:H18	1.86	0.41
1:A:383:PRO:HA	5:A:505:GOL:H2	2.03	0.41
3:B:501:CNC:H201	3:B:501:CNC:H18	1.80	0.41
1:B:226:TYR:O	1:B:270:MET:HE1	2.20	0.41
1:A:382:ASP:HA	1:A:383:PRO:HA	1.83	0.41
1:B:251:LYS:HE2	1:B:251:LYS:HB2	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HB2	5:A:504:GOL:O1	2.21	0.41
1:B:135:SER:HB2	6:B:689:HOH:O	2.20	0.41
2:C:60:GLN:NE2	2:C:65:GLY:HA2	2.36	0.41
2:C:147:PRO:HD2	2:C:150:TRP:CD2	2.55	0.41
2:D:151:ARG:HD2	6:D:301:HOH:O	2.19	0.41
2:C:58:LYS:HB3	2:C:58:LYS:HE2	1.82	0.40
2:D:63:THR:O	2:D:63:THR:HG22	2.22	0.40
1:A:190:ARG:NE	6:A:608:HOH:O	2.20	0.40
2:C:165:LEU:C	2:C:167:CYS:N	2.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:687:HOH:O	6:A:810:HOH:O[5_454]	2.17	0.03

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	396/409 (97%)	390 (98%)	5 (1%)	1 (0%)	41 41
1	B	395/409 (97%)	391 (99%)	4 (1%)	0	100 100
2	C	74/119 (62%)	59 (80%)	15 (20%)	0	100 100
2	D	75/119 (63%)	67 (89%)	8 (11%)	0	100 100
All	All	940/1056 (89%)	907 (96%)	32 (3%)	1 (0%)	51 54

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	332/348 (95%)	331 (100%)	1 (0%)	92 95
1	B	333/348 (96%)	333 (100%)	0	100 100
2	C	66/106 (62%)	65 (98%)	1 (2%)	65 71
2	D	66/106 (62%)	64 (97%)	2 (3%)	41 44
All	All	797/908 (88%)	793 (100%)	4 (0%)	88 92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	305	ILE
2	C	54	CYS
2	D	53	SER
2	D	151	ARG

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

Mol	Chain	Res	Type
1	B	309	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	CNC	B	501	-	77,103,103	3.87	34 (44%)	11,171,171	6.79	10 (90%)
5	GOL	A	508	-	5,5,5	0.32	0	5,5,5	0.24	0
5	GOL	A	505	-	5,5,5	0.34	0	5,5,5	0.34	0
3	CNC	A	501	-	77,103,103	3.69	35 (45%)	100,171,171	3.53	39 (39%)
5	GOL	A	506	-	5,5,5	0.36	0	5,5,5	0.33	0
5	GOL	A	507	-	5,5,5	0.34	0	5,5,5	0.27	0
5	GOL	B	502	-	5,5,5	0.35	0	5,5,5	0.28	0
5	GOL	A	504	-	5,5,5	0.36	0	5,5,5	0.19	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
3	CNC	B	501	-	2/2/36/38	-	-
5	GOL	A	508	-	-	3/4/4/4	-
5	GOL	A	505	-	-	2/4/4/4	-
3	CNC	A	501	-	2/2/36/38	5/51/235/235	0/3/11/11
5	GOL	A	506	-	-	4/4/4/4	-
5	GOL	A	507	-	-	2/4/4/4	-
5	GOL	B	502	-	-	2/4/4/4	-
5	GOL	A	504	-	-	2/4/4/4	-

All (69) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	501	CNC	C30-C31	14.03	1.96	1.52
3	B	501	CNC	C11-C10	12.36	1.61	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	CNC	C11-C10	11.40	1.59	1.40
3	A	501	CNC	C30-C31	11.29	1.88	1.52
3	B	501	CNC	C2R-C3R	-10.16	1.30	1.52
3	A	501	CNC	C2R-C3R	-9.91	1.30	1.52
3	A	501	CNC	C1-C19	8.86	1.74	1.55
3	B	501	CNC	C1-C19	8.78	1.74	1.55
3	A	501	CNC	C32-N33	8.75	1.61	1.32
3	B	501	CNC	C32-N33	8.58	1.60	1.32
3	A	501	CNC	O6R-C1R	6.82	1.50	1.41
3	A	501	CNC	C43-N45	6.82	1.54	1.32
3	B	501	CNC	C43-N45	6.69	1.54	1.32
3	B	501	CNC	O6R-C1R	6.51	1.50	1.41
3	A	501	CNC	C20-C1	6.43	1.66	1.53
3	B	501	CNC	C57-N59	6.35	1.47	1.33
3	A	501	CNC	C57-N59	6.00	1.47	1.33
3	B	501	CNC	C2-C3	5.81	1.68	1.58
3	B	501	CNC	C56-C57	5.76	1.62	1.51
3	B	501	CNC	O6R-C4R	-5.70	1.32	1.45
3	B	501	CNC	C20-C1	5.54	1.64	1.53
3	A	501	CNC	C56-C57	5.52	1.61	1.51
3	A	501	CNC	O6R-C4R	-5.38	1.33	1.45
3	A	501	CNC	C31-C32	5.37	1.72	1.51
3	B	501	CNC	C48-C49	-4.75	1.38	1.52
3	A	501	CNC	C48-C49	-4.74	1.38	1.52
3	B	501	CNC	C14-C15	4.45	1.57	1.40
3	B	501	CNC	C31-C32	4.41	1.68	1.51
3	B	501	CNC	C6-C5	4.32	1.59	1.41
3	A	501	CNC	C25-C2	-4.17	1.45	1.54
3	A	501	CNC	C14-C15	4.12	1.55	1.40
3	A	501	CNC	C6-C5	4.01	1.58	1.41
3	A	501	CNC	C36-C7	-3.77	1.48	1.55
3	B	501	CNC	C9-C10	3.68	1.60	1.41
3	B	501	CNC	C36-C7	-3.63	1.48	1.55
3	B	501	CNC	C54-C17	-3.48	1.48	1.55
3	A	501	CNC	C9-C10	3.48	1.59	1.41
3	B	501	CNC	C25-C2	-3.45	1.47	1.54
3	A	501	CNC	C41-C42	3.39	1.63	1.52
3	A	501	CNC	C54-C17	-3.34	1.49	1.55
3	B	501	CNC	C46-C12	3.34	1.67	1.53
3	B	501	CNC	C37-C7	-3.31	1.46	1.56
3	A	501	CNC	C46-C12	3.24	1.66	1.53
3	A	501	CNC	C38-N40	3.22	1.43	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	CNC	C55-C17	3.18	1.62	1.54
3	A	501	CNC	C37-C7	-3.16	1.46	1.56
3	A	501	CNC	C60-C61	-3.15	1.43	1.51
3	B	501	CNC	C60-C61	-3.14	1.43	1.51
3	B	501	CNC	C38-N40	3.14	1.43	1.32
3	B	501	CNC	C55-C17	3.13	1.62	1.54
3	B	501	CNC	C49-C50	-2.92	1.39	1.51
3	A	501	CNC	O7R-C2R	2.89	1.49	1.43
3	A	501	CNC	C49-C50	-2.83	1.40	1.51
3	B	501	CNC	C41-C42	2.83	1.61	1.52
3	B	501	CNC	O7R-C2R	2.70	1.49	1.43
3	A	501	CNC	C55-C56	2.59	1.59	1.53
3	A	501	CNC	C26-C27	2.59	1.60	1.51
3	A	501	CNC	C17-C18	2.56	1.57	1.54
3	B	501	CNC	C17-C18	2.50	1.57	1.54
3	B	501	CNC	C26-C27	2.46	1.59	1.51
3	B	501	CNC	C16-C15	2.34	1.50	1.41
3	A	501	CNC	C16-C15	2.25	1.49	1.41
3	B	501	CNC	C1P-C2P	-2.24	1.45	1.51
3	A	501	CNC	C1P-C2P	-2.21	1.45	1.51
3	A	501	CNC	C2R-C1R	2.17	1.57	1.53
3	A	501	CNC	O2-C3R	2.05	1.51	1.44
3	B	501	CNC	O2-C3R	2.05	1.51	1.44
3	A	501	CNC	C3R-C4R	2.04	1.58	1.52
3	B	501	CNC	C3R-C4R	2.01	1.58	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	501	CNC	C25-C2-C26	-13.83	81.75	109.71
3	A	501	CNC	C25-C2-C26	-12.94	83.56	109.71
3	A	501	CNC	C26-C2-C1	-11.82	91.64	110.02
3	A	501	CNC	C1-C19-C18	-10.52	104.53	121.93
3	B	501	CNC	C26-C2-C1	-10.15	94.24	110.02
3	B	501	CNC	C25-C2-C1	9.71	128.24	113.80
3	A	501	CNC	C25-C2-C1	9.66	128.16	113.80
3	A	501	CNC	C3-C4-C5	-8.23	101.82	131.68
3	A	501	CNC	C13-C14-C15	-7.61	104.06	131.68
3	A	501	CNC	C47-C12-C46	-7.12	94.80	109.73
3	A	501	CNC	C6-C5-C4	-7.07	113.24	124.27
3	A	501	CNC	C16-C15-C14	-6.66	113.87	124.27
3	B	501	CNC	C25-C2-C3	5.83	124.49	115.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	CNC	C1-C2-C3	5.62	108.63	101.59
3	A	501	CNC	C54-C17-C55	-5.40	100.33	109.26
3	A	501	CNC	C9-C10-C11	-5.14	112.97	130.91
3	A	501	CNC	C2-C3-C4	-5.08	96.35	101.67
3	A	501	CNC	C5M-C5B-C4B	-4.86	108.72	120.34
3	A	501	CNC	C5M-C5B-C6B	4.79	130.55	120.74
3	A	501	CNC	O6R-C1R-C2R	-4.78	99.94	106.93
3	A	501	CNC	O28-C27-N29	-4.76	109.50	122.50
3	A	501	CNC	C25-C2-C3	4.72	122.80	115.58
3	A	501	CNC	C20-C1-C19	4.66	113.84	109.36
3	B	501	CNC	C1-C2-C3	4.43	107.14	101.59
3	B	501	CNC	C26-C2-C3	-4.33	99.51	107.47
3	B	501	CNC	C20-C1-C19	3.92	113.14	109.36
3	A	501	CNC	C55-C17-C16	3.84	122.72	109.92
3	A	501	CNC	O63-C61-N62	-3.82	112.09	122.50
3	B	501	CNC	C2-C26-C27	3.77	125.83	115.22
3	A	501	CNC	C2-C26-C27	3.72	125.67	115.22
3	A	501	CNC	C15-C14-N23	-3.32	119.03	124.64
3	A	501	CNC	C26-C27-N29	3.28	126.92	116.52
3	A	501	CNC	O63-C61-C60	2.96	127.10	120.87
3	A	501	CNC	C36-C7-C37	-2.95	105.78	110.83
3	B	501	CNC	C19-C1-N21	-2.90	99.19	102.16
3	B	501	CNC	C20-C1-C2	-2.88	108.56	113.32
3	A	501	CNC	C30-C3-C2	-2.86	113.06	119.13
3	A	501	CNC	C20-C1-C2	-2.67	108.90	113.32
3	A	501	CNC	C3R-C2R-C1R	2.60	105.64	99.89
3	A	501	CNC	C60-C18-C17	-2.52	109.65	115.74
3	A	501	CNC	C26-C2-C3	-2.45	102.97	107.47
3	A	501	CNC	O34-C32-N33	-2.41	115.92	122.50
3	A	501	CNC	C5R-C4R-C3R	-2.38	107.27	114.85
3	A	501	CNC	O58-C57-N59	-2.36	118.57	123.01
3	A	501	CNC	C18-C60-C61	2.30	119.70	113.97
3	A	501	CNC	C55-C17-C18	-2.27	106.75	111.14
3	A	501	CNC	O3-C2P-C1P	2.16	111.22	106.92
3	A	501	CNC	C12-C11-C10	-2.15	121.00	124.64
3	A	501	CNC	C30-C31-C32	2.13	119.82	112.59

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	501	CNC	N24
3	A	501	CNC	C3

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Mol	Chain	Res	Type	Atom
3	B	501	CNC	N24
3	B	501	CNC	C3

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	505	GOL	O1-C1-C2-C3
5	A	506	GOL	O1-C1-C2-C3
5	A	507	GOL	C1-C2-C3-O3
5	B	502	GOL	O1-C1-C2-C3
3	A	501	CNC	C3R-C4R-C5R-O8R
5	A	505	GOL	O1-C1-C2-O2
3	A	501	CNC	O6R-C4R-C5R-O8R
5	A	504	GOL	C1-C2-C3-O3
5	A	506	GOL	C1-C2-C3-O3
5	A	508	GOL	C1-C2-C3-O3
5	A	506	GOL	O1-C1-C2-O2
5	A	506	GOL	O2-C2-C3-O3
5	A	507	GOL	O2-C2-C3-O3
5	B	502	GOL	O1-C1-C2-O2
3	A	501	CNC	C2-C3-C30-C31
5	A	504	GOL	O2-C2-C3-O3
5	A	508	GOL	O1-C1-C2-O2
3	A	501	CNC	C2P-O3-P-O2
3	A	501	CNC	C13-C48-C49-C50
5	A	508	GOL	O1-C1-C2-C3

There are no ring outliers.

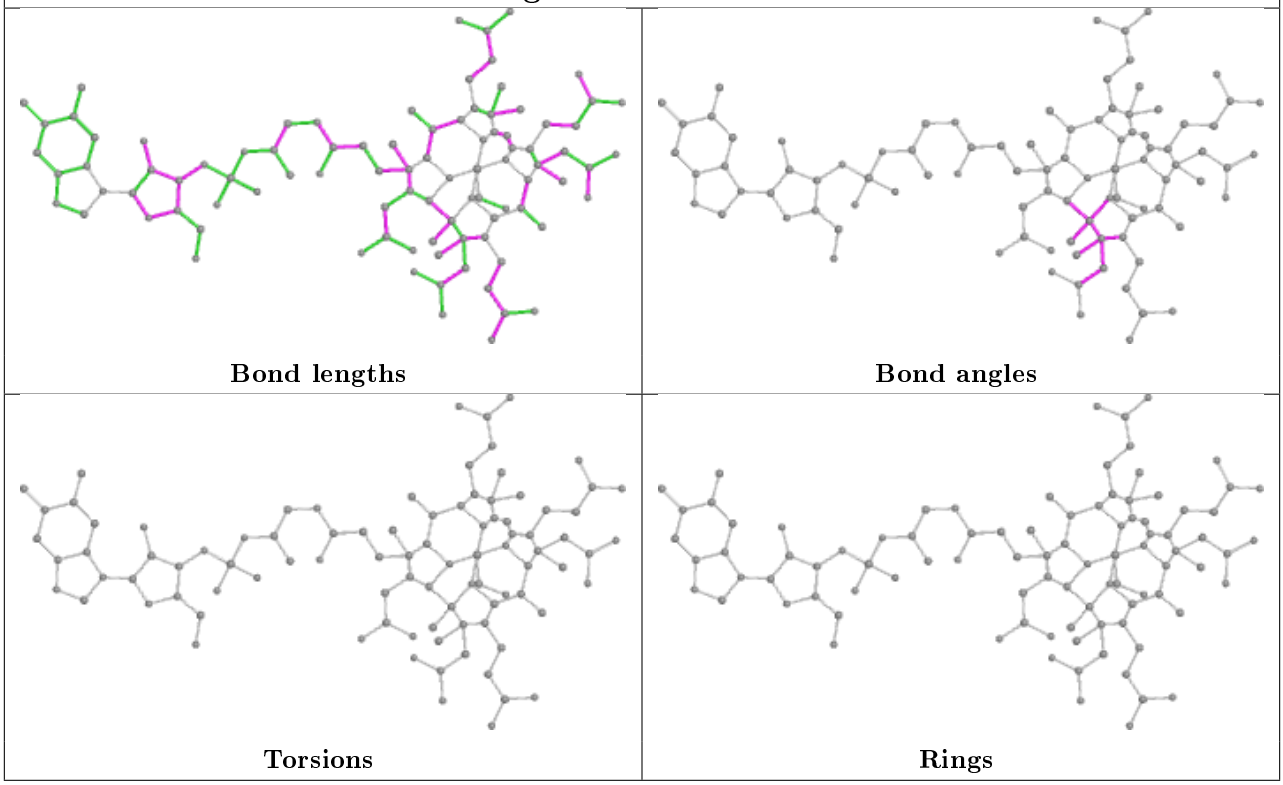
5 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	CNC	8	0
5	A	505	GOL	2	0
3	A	501	CNC	11	0
5	A	507	GOL	1	0
5	A	504	GOL	1	0

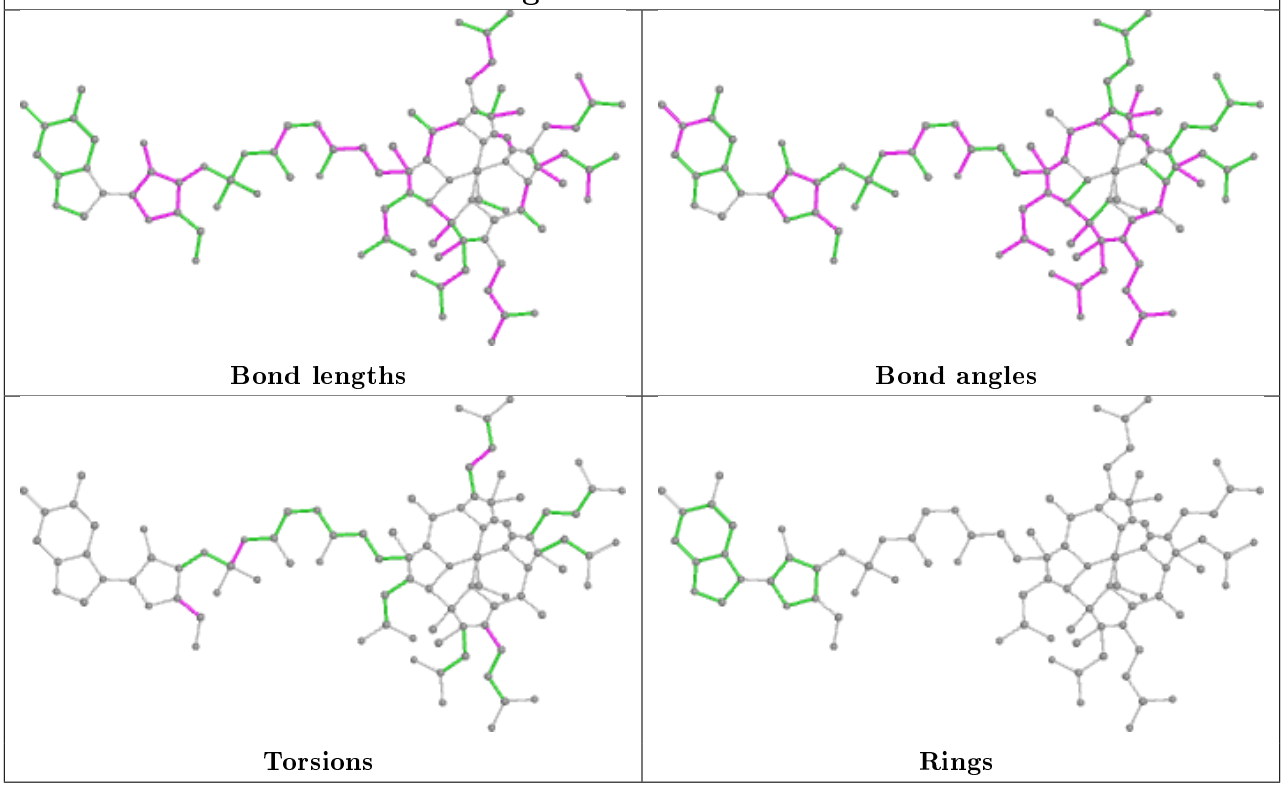
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand CNC B 501



Ligand CNC A 501



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	400/409 (97%)	-0.14	17 (4%)	35	41	31, 47, 83, 103	0
1	B	399/409 (97%)	-0.11	13 (3%)	46	53	31, 51, 87, 106	0
2	C	78/119 (65%)	1.87	31 (39%)	0	0	47, 98, 144, 159	0
2	D	79/119 (66%)	1.56	22 (27%)	0	0	44, 93, 143, 153	0
All	All	956/1056 (90%)	0.18	83 (8%)	10	13	31, 52, 113, 159	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	130	LEU	11.7
2	C	89	CYS	8.6
2	C	54	CYS	8.4
2	D	130	LEU	7.1
2	D	57	THR	7.1
2	D	141	LEU	6.9
2	D	171	GLU	6.7
1	A	306	PRO	6.6
1	A	78	CYS	6.6
2	D	63	THR	6.6
2	D	89	CYS	6.6
2	D	70	LEU	6.4
1	A	305	ILE	6.2
2	D	74	CYS	6.2
2	C	131	ALA	6.2
1	A	304	THR	6.1
1	B	80	GLY	6.0
1	B	170	GLN	5.8
2	C	88	GLU	5.6
2	D	88	GLU	5.4
2	C	61	CYS	5.3

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Mol	Chain	Res	Type	RSRZ
2	C	169	THR	5.1
1	A	80	GLY	5.1
1	B	168	PHE	5.1
2	C	56	PRO	5.1
2	D	170	ASN	5.0
1	A	302	ALA	4.9
2	D	140	THR	4.8
2	C	57	THR	4.7
1	B	79	GLN	4.7
2	C	59	PHE	4.6
2	D	61	CYS	4.6
2	C	70	LEU	4.6
2	C	55	PRO	4.5
2	C	141	LEU	4.4
1	B	242	GLY	4.4
1	A	79	GLN	4.3
1	B	78	CYS	4.2
2	D	142	SER	4.2
1	A	303	GLU	3.9
1	B	304	THR	3.9
1	B	167	PRO	3.7
2	D	143	ASP	3.7
2	C	53	SER	3.7
2	D	62	ARG	3.6
2	D	64	SER	3.5
2	C	143	ASP	3.5
2	C	87	GLU	3.5
2	C	168	GLY	3.5
1	B	305	ILE	3.5
1	B	129	LYS	3.4
2	C	165	LEU	3.4
1	B	303	GLU	3.4
2	C	74	CYS	3.3
2	C	170	ASN	3.3
2	D	59	PHE	3.2
1	B	81	LYS	3.0
1	A	168	PHE	3.0
2	D	53	SER	3.0
1	A	68	GLY	3.0
1	B	241	ARG	2.9
2	D	56	PRO	2.9
2	C	66	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	140	THR	2.7
2	C	62	ARG	2.7
2	D	87	GLU	2.7
2	C	133	LEU	2.7
2	D	54	CYS	2.6
2	C	67	CYS	2.6
2	C	63	THR	2.6
2	D	84	SER	2.5
2	C	60	GLN	2.4
1	A	230	LEU	2.4
1	A	141	LEU	2.3
1	A	241	ARG	2.3
1	A	127	ASP	2.3
1	A	144	LEU	2.2
2	C	166	GLY	2.2
2	C	58	LYS	2.2
2	C	73	ARG	2.2
1	A	244	GLU	2.0
2	C	167	CYS	2.0
1	A	183	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
5	GOL	A	508	6/6	0.71	0.25	92,97,97,97	0
5	GOL	A	504	6/6	0.73	0.25	87,88,89,90	0
5	GOL	A	505	6/6	0.74	0.20	88,90,96,100	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	GOL	B	502	6/6	0.80	0.18	82,86,87,88	0
5	GOL	A	506	6/6	0.82	0.21	72,88,92,94	0
5	GOL	A	507	6/6	0.89	0.20	67,74,83,92	0
4	CA	C	202	1/1	0.92	0.04	77,77,77,77	0
4	CA	D	202	1/1	0.95	0.04	80,80,80,80	0
4	CA	A	503	1/1	0.96	0.08	60,60,60,60	0
3	CNC	A	501	93/93	0.96	0.20	21,35,67,74	15
4	CA	A	502	1/1	0.96	0.06	63,63,63,63	0
3	CNC	B	501	93/93	0.97	0.17	25,34,56,75	20
4	CA	D	201	1/1	0.99	0.05	42,42,42,42	0
4	CA	C	201	1/1	0.99	0.08	45,45,45,45	0

6.5 Other polymers (i)

There are no such residues in this entry.