



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:37 PM UTC

PDB ID : 3FG4 / pdb_00003fg4
Title : Crystal structure of Delta413-417:GS I805A LOX
Authors : Neau, D.B.; Newcomer, M.E.
Deposited on : 2008-12-04
Resolution : 2.31 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

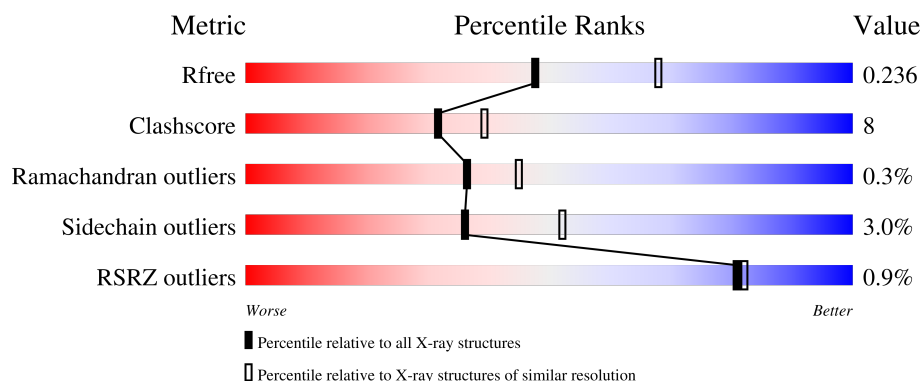
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.31 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7754 (2.34-2.30)
Clashscore	190562	8383 (2.34-2.30)
Ramachandran outliers	187476	8303 (2.34-2.30)
Sidechain outliers	187428	8303 (2.34-2.30)
RSRZ outliers	180081	7760 (2.34-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	696	% 80% 16% ..
1	B	696	% 84% 12% ..
1	C	696	% 82% 14% ..
1	D	696	% 80% 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
5	ACY	A	2201[B]	-	-	X	-
5	ACY	C	2203	-	-	X	-
5	ACY	D	2202	-	-	X	-
5	ACY	D	2203	-	-	X	-
6	GOL	A	1068[A]	-	-	X	-
6	GOL	A	2303	-	-	X	-
6	GOL	A	2305	-	-	X	-
6	GOL	D	2304	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 23613 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 Allene oxide synthase-lipoxygenase protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	682	Total	C	N	O	S	0	12	0
			5487	3504	928	1042	13			
1	B	676	Total	C	N	O	S	0	8	0
			5362	3425	903	1021	13			
1	C	681	Total	C	N	O	S	0	15	0
			5471	3492	923	1043	13			
1	D	678	Total	C	N	O	S	0	16	0
			5453	3487	913	1040	13			

There are 56 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	368	MET	-	expression tag	UNP O16025
A	369	HIS	-	expression tag	UNP O16025
A	370	HIS	-	expression tag	UNP O16025
A	371	HIS	-	expression tag	UNP O16025
A	372	HIS	-	expression tag	UNP O16025
A	373	HIS	-	expression tag	UNP O16025
A	?	-	TRP	deletion	UNP O16025
A	?	-	PHE	deletion	UNP O16025
A	?	-	HIS	deletion	UNP O16025
A	413	GLY	ASN	engineered mutation	UNP O16025
A	414	SER	ASP	engineered mutation	UNP O16025
A	782	ILE	VAL	SEE REMARK 999	UNP O16025
A	805	ALA	ILE	engineered mutation	UNP O16025
A	963	ILE	VAL	SEE REMARK 999	UNP O16025
B	368	MET	-	expression tag	UNP O16025
B	369	HIS	-	expression tag	UNP O16025
B	370	HIS	-	expression tag	UNP O16025
B	371	HIS	-	expression tag	UNP O16025
B	372	HIS	-	expression tag	UNP O16025
B	373	HIS	-	expression tag	UNP O16025
B	?	-	TRP	deletion	UNP O16025

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	PHE	deletion	UNP O16025
B	?	-	HIS	deletion	UNP O16025
B	413	GLY	ASN	engineered mutation	UNP O16025
B	414	SER	ASP	engineered mutation	UNP O16025
B	782	ILE	VAL	SEE REMARK 999	UNP O16025
B	805	ALA	ILE	engineered mutation	UNP O16025
B	963	ILE	VAL	SEE REMARK 999	UNP O16025
C	368	MET	-	expression tag	UNP O16025
C	369	HIS	-	expression tag	UNP O16025
C	370	HIS	-	expression tag	UNP O16025
C	371	HIS	-	expression tag	UNP O16025
C	372	HIS	-	expression tag	UNP O16025
C	373	HIS	-	expression tag	UNP O16025
C	?	-	TRP	deletion	UNP O16025
C	?	-	PHE	deletion	UNP O16025
C	?	-	HIS	deletion	UNP O16025
C	413	GLY	ASN	engineered mutation	UNP O16025
C	414	SER	ASP	engineered mutation	UNP O16025
C	782	ILE	VAL	SEE REMARK 999	UNP O16025
C	805	ALA	ILE	engineered mutation	UNP O16025
C	963	ILE	VAL	SEE REMARK 999	UNP O16025
D	368	MET	-	expression tag	UNP O16025
D	369	HIS	-	expression tag	UNP O16025
D	370	HIS	-	expression tag	UNP O16025
D	371	HIS	-	expression tag	UNP O16025
D	372	HIS	-	expression tag	UNP O16025
D	373	HIS	-	expression tag	UNP O16025
D	?	-	TRP	deletion	UNP O16025
D	?	-	PHE	deletion	UNP O16025
D	?	-	HIS	deletion	UNP O16025
D	413	GLY	ASN	engineered mutation	UNP O16025
D	414	SER	ASP	engineered mutation	UNP O16025
D	782	ILE	VAL	SEE REMARK 999	UNP O16025
D	805	ALA	ILE	engineered mutation	UNP O16025
D	963	ILE	VAL	SEE REMARK 999	UNP O16025

- Molecule 2 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0

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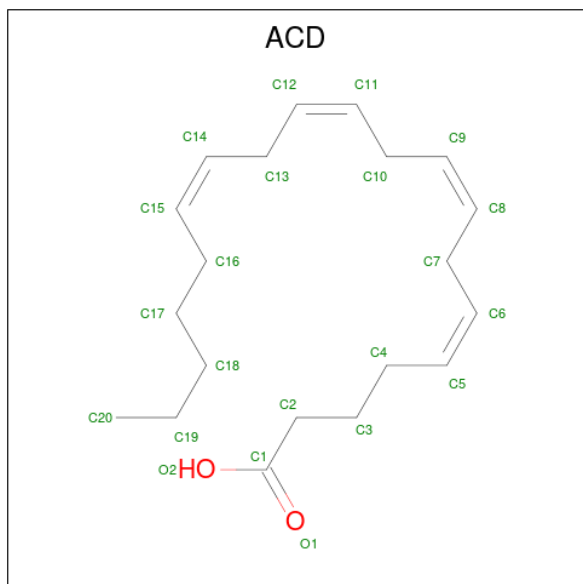
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total	Fe	0	0
			1	1		
2	D	1	Total	Fe	0	0
			1	1		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Ca	0	0
			3	3		
3	B	1	Total	Ca	0	0
			1	1		
3	C	3	Total	Ca	0	0
			3	3		
3	D	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ARACHIDONIC ACID (CCD ID: ACD) (formula: C₂₀H₃₂O₂).



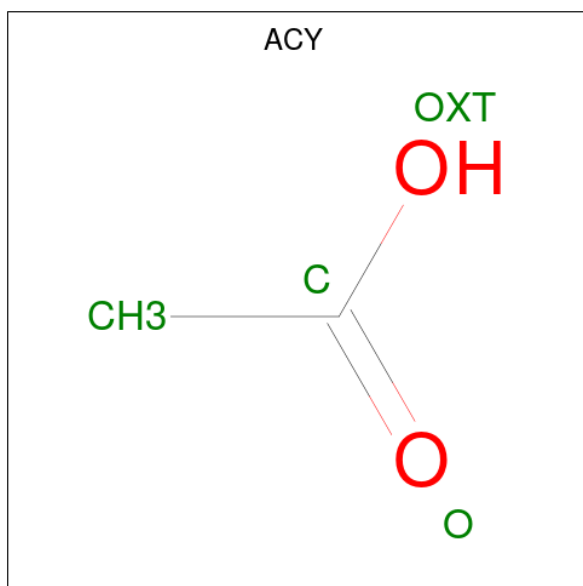
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	C	0	0
			9	9		
4	B	1	Total	C	0	0
			8	8		
4	C	1	Total	C	0	0
			9	9		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total C 8 8	0	0

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



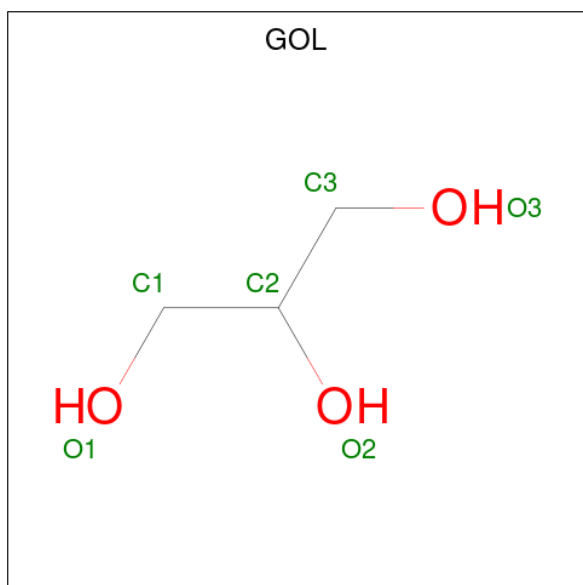
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 8 4 4	0	1
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	C	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		
5	D	1	Total	C	O	0	0
			4	2	2		

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 6 3 3	0	0
6	A	1	Total C O 12 6 6	0	1
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0
6	C	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
6	D	1	Total C O 6 3 3	0	0

- Molecule 7 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total 1	Cl 1	0	0
7	C	1	Total 1	Cl 1	0	0
7	D	1	Total 1	Cl 1	0	0

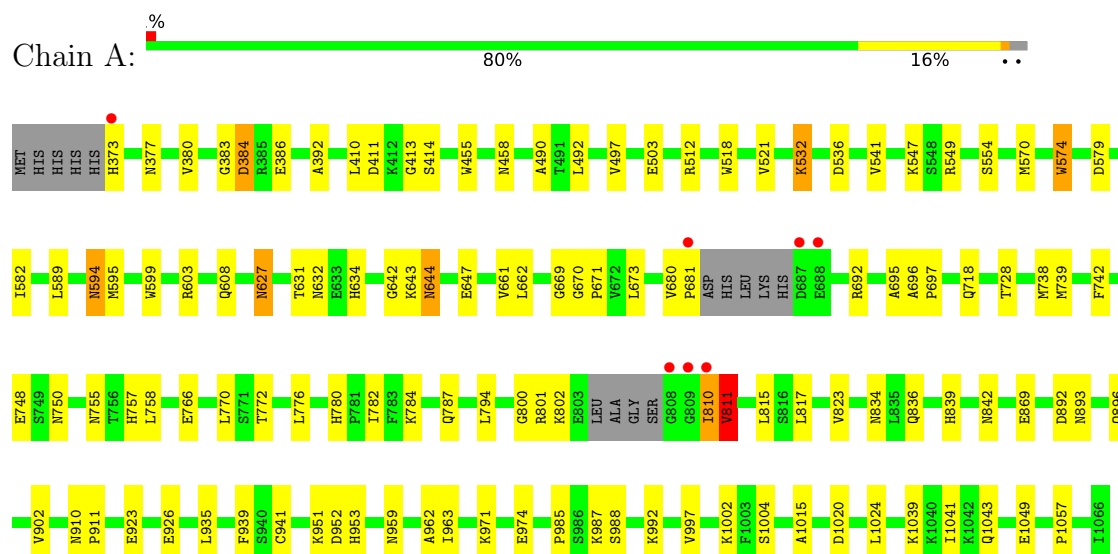
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	504	Total 504	O 504	0	0
8	B	311	Total 311	O 311	0	0
8	C	443	Total 443	O 443	0	0
8	D	324	Total 324	O 324	0	0

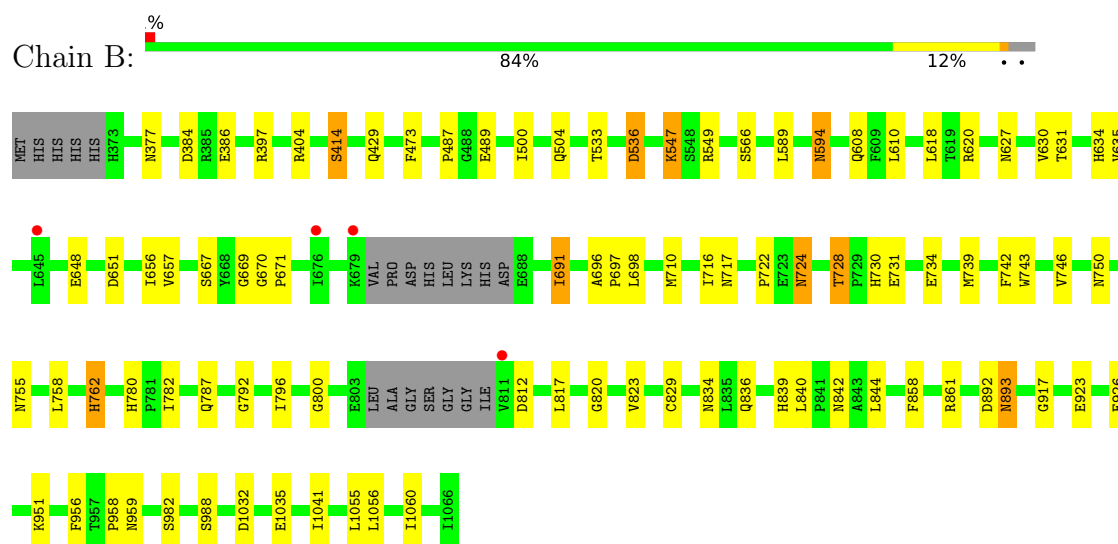
3 Residue-property plots [i](#)

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.

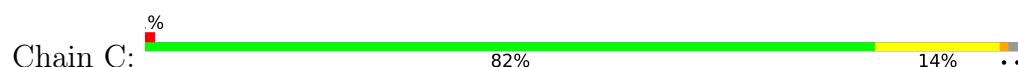
- Molecule 1: Allene oxide synthase-lipoxygenase protein



- Molecule 1: Allene oxide synthase-lipoxygenase protein



- Molecule 1: Allene oxide synthase-lipoxygenase protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	104.36Å 170.38Å 104.90Å 90.00° 95.51° 90.00°	Depositor
Resolution (Å)	30.03 – 2.31 30.03 – 2.31	Depositor EDS
% Data completeness (in resolution range)	99.2 (30.03-2.31) 99.2 (30.03-2.31)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.25 (at 2.31Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.168 , 0.239 0.167 , 0.236	Depositor DCC
R_{free} test set	7906 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	26.2	Xtriage
Anisotropy	0.243	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.068 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	23613	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, CL, GOL, ACD, ACY, FE2

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	1.19	7/5668 (0.1%)	1.13	18/7709 (0.2%)
1	B	1.02	2/5533 (0.0%)	1.06	13/7542 (0.2%)
1	C	1.12	6/5661 (0.1%)	1.09	11/7706 (0.1%)
1	D	1.03	1/5638 (0.0%)	1.09	23/7673 (0.3%)
All	All	1.09	16/22500 (0.1%)	1.09	65/30630 (0.2%)

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	1
1	B	0	1
1	C	0	2
1	D	0	1
All	All	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	414	SER	C-N	22.23	1.62	1.33
1	B	414	SER	C-N	20.50	1.59	1.33
1	C	414	SER	C-N	15.91	1.57	1.33
1	A	414	SER	C-N	7.61	1.42	1.33
1	A	541	VAL	CA-CB	6.84	1.62	1.54
1	C	676	ILE	CA-CB	6.24	1.61	1.54
1	A	823	VAL	CA-CB	5.55	1.61	1.54
1	C	582	ILE	CA-CB	5.46	1.62	1.54
1	A	902	VAL	CA-CB	5.38	1.61	1.54
1	C	796	ILE	CA-CB	5.23	1.61	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	787	GLN	C-O	-5.22	1.19	1.24
1	C	407	TYR	CA-CB	5.13	1.59	1.53
1	A	521	VAL	C-O	-5.04	1.18	1.24
1	B	762	HIS	CA-C	5.01	1.59	1.52
1	C	991	ALA	CA-CB	5.01	1.61	1.53
1	A	739	MET	CA-C	5.01	1.59	1.52

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	SER	O-C-N	-8.93	111.67	122.65
1	A	414	SER	CA-C-N	7.95	135.21	123.12
1	A	414	SER	C-N-CA	7.95	135.21	123.12
1	D	384	ASP	N-CA-C	7.58	122.28	112.89
1	D	793	VAL	CB-CA-C	-7.51	102.00	112.14
1	D	635	VAL	N-CA-C	7.04	119.96	113.20
1	A	574	TRP	N-CA-C	-6.76	98.91	109.25
1	B	917	GLY	CA-C-N	-6.66	117.79	122.59
1	B	917	GLY	C-N-CA	-6.66	117.79	122.59
1	C	851	ASP	CB-CA-C	6.66	116.76	110.17
1	B	840	LEU	CA-C-N	-6.55	111.78	119.05
1	B	840	LEU	C-N-CA	-6.55	111.78	119.05
1	D	917	GLY	CA-C-N	-6.53	117.89	122.59
1	D	917	GLY	C-N-CA	-6.53	117.89	122.59
1	A	492	LEU	N-CA-C	-6.42	101.75	110.36
1	D	794	LEU	N-CA-C	-6.25	104.55	111.36
1	A	987	LYS	N-CA-C	6.15	117.99	111.28
1	C	787	GLN	CA-C-N	-6.14	113.36	119.56
1	C	787	GLN	C-N-CA	-6.14	113.36	119.56
1	B	698	LEU	N-CA-C	-6.11	99.94	109.72
1	C	928	LEU	N-CA-C	-5.99	104.83	111.36
1	C	744	LEU	N-CA-C	-5.87	104.96	111.36
1	C	501	VAL	CB-CA-C	5.85	120.30	112.22
1	C	414	SER	CA-C-N	-5.72	114.25	123.23
1	C	414	SER	C-N-CA	-5.72	114.25	123.23
1	D	414	SER	O-C-N	-5.70	116.01	122.68
1	D	764	THR	N-CA-C	5.70	117.57	111.36
1	B	787	GLN	CA-C-N	-5.68	113.96	119.87
1	B	787	GLN	C-N-CA	-5.68	113.96	119.87
1	C	949	SER	N-CA-C	-5.68	106.33	113.20
1	A	718	GLN	N-CA-C	5.61	118.32	111.82
1	C	1060	ILE	N-CA-C	5.59	113.08	107.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	635	VAL	CB-CA-C	-5.58	105.18	110.70
1	D	966	HIS	CA-C-N	-5.54	114.68	120.38
1	D	966	HIS	C-N-CA	-5.54	114.68	120.38
1	D	497	VAL	CA-C-N	-5.53	114.08	119.78
1	D	497	VAL	C-N-CA	-5.53	114.08	119.78
1	A	414	SER	O-C-N	-5.40	116.89	122.94
1	A	570	MET	N-CA-C	5.39	117.85	111.33
1	D	577	TYR	N-CA-C	-5.38	105.50	111.36
1	A	810	ILE	CA-C-N	5.30	131.24	121.70
1	A	810	ILE	C-N-CA	5.30	131.24	121.70
1	D	544	THR	N-CA-C	-5.29	103.50	110.43
1	A	497	VAL	CA-C-N	-5.26	114.36	119.78
1	A	497	VAL	C-N-CA	-5.26	114.36	119.78
1	A	669	GLY	N-CA-C	-5.25	108.39	115.21
1	A	974	GLU	CA-CB-CG	5.24	124.58	114.10
1	A	728	THR	CA-C-N	-5.22	114.44	119.87
1	A	728	THR	C-N-CA	-5.22	114.44	119.87
1	D	670	GLY	N-CA-C	5.20	122.95	112.34
1	B	724	ASN	CA-C-N	5.20	125.17	120.03
1	B	724	ASN	C-N-CA	5.20	125.17	120.03
1	D	573	ASN	CA-C-N	-5.16	115.33	122.30
1	D	573	ASN	C-N-CA	-5.16	115.33	122.30
1	D	718	GLN	N-CA-C	5.14	116.97	111.36
1	B	710	MET	CA-C-N	-5.12	114.53	119.90
1	B	710	MET	C-N-CA	-5.12	114.53	119.90
1	A	941	CYS	N-CA-C	5.10	116.52	111.07
1	D	412	LYS	N-CA-C	-5.09	99.95	110.80
1	C	769	ALA	N-CA-C	-5.09	105.64	111.14
1	D	401	ALA	N-CA-C	5.06	117.45	111.33
1	B	1041	ILE	N-CA-C	-5.05	105.62	110.72
1	D	760	ARG	N-CA-C	5.05	119.31	113.20
1	A	811	VAL	N-CA-C	5.04	125.11	111.00
1	D	905	ASN	N-CA-C	5.00	119.53	113.38

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	410	LEU	Peptide
1	B	414	SER	Mainchain
1	C	414	SER	Mainchain
1	C	589	LEU	Peptide

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Mol	Chain	Res	Type	Group
1	D	414	SER	Mainchain

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	5487	0	5213	109	0
1	B	5362	0	4994	60	0
1	C	5471	0	5155	88	0
1	D	5453	0	5138	89	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	3	0	0	0	0
3	B	1	0	0	0	0
3	C	3	0	0	0	0
3	D	1	0	0	0	0
4	A	9	0	15	1	0
4	B	8	0	13	1	0
4	C	9	0	15	5	0
4	D	8	0	13	1	0
5	A	32	0	24	6	0
5	B	16	0	12	0	0
5	C	24	0	18	3	0
5	D	16	0	12	7	0
6	A	54	0	72	20	0
6	B	18	0	24	2	0
6	C	30	0	40	3	0
6	D	18	0	24	6	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	504	0	0	12	0
8	B	311	0	0	3	0
8	C	443	0	0	9	0
8	D	324	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	23613	0	20782	347	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (347) 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)
1:C:758:LEU:HD11	4:C:2001:ACD:H161	1.44	0.99
1:B:893[A]:ASN:H	1:B:893[A]:ASN:ND2	1.51	0.98
1:D:608:GLN:HB2	5:D:2203:ACY:H3	1.46	0.98
1:A:532:LYS:HG2	1:A:536:ASP:OD2	1.64	0.97
6:A:1068[A]:GOL:H12	1:B:1032:ASP:OD1	1.64	0.96
1:C:608:GLN:HE22	1:C:959:ASN:HD21	1.03	0.95
1:A:532:LYS:O	1:A:802:LYS:HE2	1.70	0.92
1:C:631:THR:H	1:C:634:HIS:HD2	1.16	0.91
1:B:631:THR:H	1:B:634:HIS:HD2	1.15	0.90
1:A:755:ASN:ND2	6:A:2303:GOL:H31	1.86	0.90
1:A:834:ASN:HD22	1:A:836:GLN:H	1.18	0.90
1:A:755:ASN:HD21	6:A:2303:GOL:H31	1.36	0.89
1:A:631:THR:H	1:A:634:HIS:HD2	1.22	0.87
1:C:834:ASN:HD22	1:C:836:GLN:H	1.24	0.85
1:D:666:LYS:HZ3	1:D:670:GLY:HA2	1.40	0.85
1:A:608:GLN:HE22	1:A:959:ASN:HD21	1.25	0.85
1:D:599:TRP:HE1	5:D:2202:ACY:H3	1.42	0.83
1:D:608:GLN:HE22	1:D:959:ASN:HD21	1.26	0.83
1:D:893[A]:ASN:ND2	1:D:893[A]:ASN:H	1.72	0.83
1:A:532:LYS:CD	1:A:532:LYS:H	1.92	0.82
1:C:386[B]:GLU:OE1	1:C:549:ARG:NH2	2.13	0.82
1:C:780:HIS:HD2	1:C:782:ILE:H	1.26	0.81
1:C:627:ASN:HD22	1:C:627:ASN:H	1.28	0.81
1:D:666:LYS:NZ	1:D:670:GLY:HA2	1.96	0.81
1:C:372:HIS:N	8:C:1516:HOH:O	2.11	0.81
1:A:755:ASN:HD21	6:A:2303:GOL:C3	1.94	0.80
1:B:834:ASN:HD22	1:B:836:GLN:H	1.29	0.80
1:B:893[A]:ASN:H	1:B:893[A]:ASN:HD22	0.82	0.79
1:A:780:HIS:HD2	1:A:782:ILE:H	1.29	0.78
1:B:780:HIS:HD2	1:B:782:ILE:H	1.31	0.78
1:A:547[B]:LYS:HD2	1:A:547[B]:LYS:O	1.83	0.78
1:C:758:LEU:CD1	4:C:2001:ACD:H161	2.13	0.77
1:A:532:LYS:HE3	1:A:536:ASP:HB3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1033:LYS:NZ	8:D:1080:HOH:O	2.15	0.77
1:A:532:LYS:HG2	1:A:536:ASP:CG	2.10	0.76
1:A:627:ASN:HD22	1:A:627:ASN:H	1.33	0.76
1:B:728:THR:CG2	1:B:730:HIS:H	1.99	0.76
1:A:802:LYS:HD2	1:A:802:LYS:N	2.00	0.76
1:C:503:GLU:OE2	8:C:1521:HOH:O	2.03	0.76
1:B:728:THR:HG22	1:B:730:HIS:H	1.50	0.76
1:A:951:LYS:NZ	8:A:1151:HOH:O	2.18	0.76
1:B:631:THR:H	1:B:634:HIS:CD2	2.03	0.75
1:C:547:LYS:HD2	1:C:791:TYR:OH	1.87	0.75
1:D:893[A]:ASN:H	1:D:893[A]:ASN:HD22	1.33	0.74
1:A:532:LYS:NZ	1:A:536:ASP:HB3	2.03	0.74
1:C:631:THR:H	1:C:634:HIS:CD2	2.04	0.73
1:A:755:ASN:ND2	6:A:2303:GOL:C3	2.51	0.73
1:A:532:LYS:CE	1:A:536:ASP:HB3	2.19	0.73
1:B:608:GLN:HE22	1:B:959:ASN:HD21	1.37	0.72
1:D:1007[B]:GLU:OE1	8:D:1087:HOH:O	2.08	0.72
1:D:608:GLN:CB	5:D:2203:ACY:H3	2.20	0.72
1:C:384[B]:ASP:OD1	8:C:1455:HOH:O	2.07	0.71
1:D:631:THR:H	1:D:634:HIS:HD2	1.36	0.70
1:A:839:HIS:HD2	1:A:842:ASN:H	1.40	0.70
1:A:383:GLY:HA2	6:A:2305:GOL:H31	1.73	0.70
1:D:834:ASN:HD22	1:D:836:GLN:H	1.38	0.70
1:B:839:HIS:HD2	1:B:842:ASN:H	1.39	0.70
1:D:603:ARG:HD3	1:D:603:ARG:C	2.17	0.70
1:D:589:LEU:HB3	1:D:951:LYS:HG3	1.73	0.70
1:C:411:ASP:OD1	6:D:2303:GOL:H31	1.92	0.69
1:A:532:LYS:H	1:A:532:LYS:HD3	1.56	0.69
1:D:644:ASN:HD21	1:D:647:GLU:HG3	1.58	0.69
1:D:627:ASN:H	1:D:627:ASN:HD22	1.39	0.68
1:A:413:GLY:O	6:A:1068[A]:GOL:H11	1.93	0.68
1:D:644:ASN:ND2	1:D:647:GLU:HG3	2.09	0.67
1:B:397:ARG:HD2	1:B:404:ARG:HD2	1.77	0.67
1:C:1020[B]:ASP:OD1	8:C:1246:HOH:O	2.13	0.67
1:C:386[A]:GLU:OE2	1:C:549:ARG:NH2	2.19	0.67
1:D:839:HIS:HD2	1:D:842:ASN:H	1.43	0.66
1:B:533:THR:O	1:B:536:ASP:HB2	1.96	0.65
6:A:1068[B]:GOL:O1	6:A:1068[B]:GOL:O3	2.04	0.65
1:B:820:GLY:O	1:B:823:VAL:HG12	1.97	0.64
1:B:631:THR:N	1:B:634:HIS:HD2	1.93	0.64
1:C:413:GLY:O	6:D:2303:GOL:H11	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:834:ASN:ND2	1:C:836:GLN:H	1.93	0.64
1:A:631:THR:H	1:A:634:HIS:CD2	2.11	0.64
1:C:589:LEU:HB3	1:C:951:LYS:HG3	1.79	0.64
1:A:547[B]:LYS:HD3	1:A:1004[B]:SER:HB2	1.81	0.63
1:D:547:LYS:HD2	1:D:547:LYS:O	1.98	0.63
1:D:631:THR:H	1:D:634:HIS:CD2	2.15	0.63
1:B:839:HIS:HE1	8:B:1121:HOH:O	1.82	0.62
1:A:644[A]:ASN:ND2	1:A:647:GLU:H	1.98	0.62
1:A:384:ASP:H	6:A:2305:GOL:H31	1.64	0.62
1:B:386[B]:GLU:OE1	1:B:549:ARG:NH2	2.30	0.62
1:A:377:ASN:ND2	8:A:237:HOH:O	2.31	0.61
6:A:1068[A]:GOL:O3	6:A:1068[A]:GOL:O1	2.13	0.61
1:A:384:ASP:H	6:A:2305:GOL:C3	2.14	0.61
1:D:386[A]:GLU:CD	1:D:549:ARG:HH22	2.07	0.61
1:C:594:ASN:C	1:C:594:ASN:HD22	2.07	0.61
1:D:739:MET:CE	1:D:983:THR:HG21	2.31	0.61
1:C:739:MET:HE3	1:C:742:PHE:HB2	1.81	0.61
1:C:800:GLY:HA3	4:C:2001:ACD:H172	1.83	0.60
1:A:392:ALA:O	6:A:1068[B]:GOL:H11	2.02	0.60
1:C:753:GLN:HG2	8:C:1097:HOH:O	2.01	0.60
1:C:644[A]:ASN:ND2	1:C:647:GLU:H	1.98	0.60
1:C:997:VAL:HG23	5:C:2203:ACY:H1	1.82	0.60
1:B:1056:LEU:O	1:B:1060:ILE:HG13	2.01	0.60
1:D:739:MET:HE1	1:D:983:THR:HG21	1.84	0.60
1:D:780:HIS:HD2	1:D:782:ILE:H	1.49	0.59
1:A:750:ASN:ND2	1:A:815:LEU:HG	2.17	0.59
1:C:497:VAL:CG1	1:C:501:VAL:HG22	2.32	0.58
1:A:503:GLU:OE2	8:A:288:HOH:O	2.17	0.58
1:A:780:HIS:CD2	1:A:782:ILE:H	2.18	0.58
1:A:953:HIS:CE1	5:A:2201[B]:ACY:H3	2.38	0.58
1:D:599:TRP:NE1	5:D:2202:ACY:H3	2.15	0.58
1:D:644:ASN:C	1:D:644:ASN:HD22	2.11	0.58
1:D:839:HIS:HE1	8:D:194:HOH:O	1.87	0.58
1:A:662:LEU:O	1:A:673:LEU:HD23	2.03	0.58
1:A:532:LYS:HD3	1:A:532:LYS:N	2.19	0.58
1:C:780:HIS:CD2	1:C:782:ILE:H	2.14	0.58
1:D:579:ASP:CG	6:D:2304:GOL:H2	2.29	0.58
1:D:708:HIS:ND1	8:D:1241:HOH:O	2.32	0.57
1:A:810:ILE:HA	1:A:811:VAL:C	2.30	0.57
1:D:659:PHE:HB2	1:D:697:PRO:HD2	1.87	0.57
1:D:749:SER:O	1:D:753[A]:GLN:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:ALA:O	1:C:503:GLU:HG3	2.05	0.57
1:D:386[A]:GLU:OE2	1:D:549:ARG:NH2	2.38	0.57
1:A:801:ARG:HD3	8:A:1084:HOH:O	2.05	0.57
1:A:748:GLU:OE1	5:A:2201[A]:ACY:OXT	2.24	0.56
1:A:386:GLU:CD	1:A:549:ARG:HH22	2.13	0.55
1:C:997:VAL:HG23	5:C:2203:ACY:CH3	2.36	0.55
1:C:644[A]:ASN:HD22	1:C:647:GLU:H	1.54	0.55
1:A:839:HIS:CD2	1:A:842:ASN:H	2.20	0.55
1:C:594:ASN:HD22	1:C:595:MET:N	2.05	0.55
1:B:834:ASN:ND2	1:B:836:GLN:H	2.03	0.55
1:C:839:HIS:HD2	1:C:842:ASN:H	1.52	0.55
1:A:772:THR:HG23	1:A:776:LEU:HD12	1.89	0.55
1:D:738:MET:HG3	1:D:742:PHE:CE1	2.41	0.55
1:D:644:ASN:ND2	1:D:647:GLU:H	2.04	0.54
1:A:532:LYS:HZ1	1:A:536:ASP:HB3	1.69	0.54
1:D:554:SER:HB3	1:D:1002[A]:LYS:HD2	1.89	0.54
1:D:573:ASN:O	6:D:2304:GOL:O2	2.25	0.54
1:D:988:SER:HA	5:D:2204:ACY:H2	1.88	0.54
1:B:800:GLY:HA3	4:B:2001:ACD:H181	1.89	0.54
1:D:554:SER:HB3	1:D:1002[A]:LYS:CD	2.38	0.54
1:A:532:LYS:CG	1:A:536:ASP:OD2	2.49	0.54
1:B:728:THR:HG22	1:B:730:HIS:N	2.19	0.53
1:A:780:HIS:HE1	1:A:892:ASP:OD2	1.91	0.53
1:D:594:ASN:ND2	1:D:952:ASP:HB3	2.23	0.53
1:D:733:ASN:HB3	1:D:736:ASP:OD2	2.09	0.53
1:A:839:HIS:HE1	8:A:63:HOH:O	1.91	0.53
1:C:377:ASN:ND2	8:C:1204:HOH:O	2.41	0.53
1:A:458:ASN:OD1	6:A:2305:GOL:H2	2.09	0.53
1:D:579:ASP:OD2	6:D:2304:GOL:H2	2.07	0.53
1:B:670:GLY:N	1:B:671:PRO:CD	2.71	0.53
6:A:1068[A]:GOL:O3	1:B:1035:GLU:OE2	2.22	0.53
1:C:758:LEU:HD11	4:C:2001:ACD:C16	2.29	0.52
1:B:589:LEU:HB3	1:B:951:LYS:CG	2.40	0.52
1:C:608:GLN:NE2	1:C:959:ASN:HD21	1.88	0.52
1:D:598:ARG:NH1	1:D:1049[B]:GLU:OE1	2.39	0.52
1:B:780:HIS:CD2	1:B:782:ILE:H	2.19	0.52
1:B:829:CYS:O	6:B:2304:GOL:O1	2.26	0.52
1:C:834:ASN:HD22	1:C:836:GLN:N	1.99	0.52
1:D:473:PHE:CE2	1:D:487:PRO:HD3	2.45	0.52
1:B:594:ASN:HD22	1:B:594:ASN:C	2.18	0.52
1:C:659:PHE:HB2	1:C:697:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:997:VAL:CG2	5:C:2203:ACY:H1	2.38	0.52
1:D:780:HIS:HE1	1:D:892:ASP:OD2	1.93	0.52
1:A:411:ASP:HA	8:A:1108:HOH:O	2.09	0.52
1:D:641:ARG:HB2	1:D:648:GLU:OE1	2.10	0.52
1:D:630:VAL:HG22	1:D:726:ILE:HD12	1.92	0.52
1:C:477:ARG:HG3	1:C:477:ARG:HH11	1.75	0.51
1:B:547:LYS:HD2	1:B:547:LYS:O	2.10	0.51
1:D:815:LEU:HD12	1:D:962:ALA:HB1	1.92	0.51
1:D:1023:ALA:O	1:D:1027:ILE:HG13	2.10	0.51
1:D:800:GLY:HA3	4:D:2001:ACD:H162	1.93	0.51
1:A:953:HIS:CE1	5:A:2201[B]:ACY:CH3	2.94	0.51
1:C:497:VAL:HG13	1:C:501:VAL:HG22	1.92	0.51
1:C:780:HIS:HD2	1:C:782:ILE:N	2.03	0.51
1:C:938:THR:HA	1:C:942:GLN:HB3	1.92	0.51
1:A:532:LYS:HE3	1:A:536:ASP:CB	2.37	0.50
1:C:549:ARG:NH1	1:D:1005[B]:GLU:HG2	2.26	0.50
1:D:750:ASN:HD21	1:D:817:LEU:H	1.57	0.50
1:D:739:MET:HE1	1:D:983:THR:CG2	2.40	0.50
1:C:627:ASN:H	1:C:627:ASN:ND2	2.02	0.50
1:D:497:VAL:HG13	1:D:501:VAL:HB	1.93	0.50
1:C:695:ALA:C	1:C:697:PRO:HD3	2.37	0.50
1:C:1020[A]:ASP:OD1	1:C:1023:ALA:N	2.39	0.50
1:A:627:ASN:H	1:A:627:ASN:ND2	2.05	0.50
1:A:413:GLY:O	6:A:1068[A]:GOL:C1	2.59	0.50
1:B:780:HIS:HE1	1:B:892:ASP:OD2	1.95	0.50
1:C:547:LYS:HE3	1:C:791:TYR:HE2	1.77	0.50
1:D:578:ASP:OD1	5:D:2202:ACY:H2	2.11	0.50
1:D:750:ASN:ND2	1:D:815:LEU:HG	2.27	0.50
1:D:844:LEU:HD13	1:D:861:ARG:HG3	1.93	0.50
1:A:579:ASP:O	1:A:582:ILE:HG22	2.12	0.49
1:A:594:ASN:C	1:A:594:ASN:HD22	2.20	0.49
1:C:529:ILE:HB	1:C:794:LEU:HD22	1.94	0.49
1:C:636:ASN:HD21	6:C:2301:GOL:C1	2.26	0.49
1:C:892:ASP:O	1:C:896:GLN:HG2	2.13	0.49
1:A:554:SER:HB3	1:A:1002:LYS:HD3	1.94	0.49
1:A:963:ILE:O	1:A:985:PRO:HD3	2.12	0.49
1:B:839:HIS:CD2	1:B:842:ASN:H	2.26	0.49
1:C:589:LEU:O	1:C:951:LYS:HE2	2.12	0.49
1:A:1049:GLU:OE2	8:A:1363:HOH:O	2.20	0.49
1:C:497:VAL:HG11	1:C:501:VAL:HG22	1.94	0.49
1:C:547:LYS:CD	1:C:791:TYR:OH	2.57	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ASN:HB3	1:A:911:PRO:HD2	1.95	0.48
1:A:413:GLY:O	6:A:1068[A]:GOL:H2	2.13	0.48
1:C:631:THR:N	1:C:634:HIS:HD2	1.97	0.48
1:D:840:LEU:HB3	1:D:841:PRO:HD3	1.95	0.48
1:B:489:GLU:N	1:B:489:GLU:OE1	2.46	0.48
1:A:935:LEU:HD11	1:A:939:PHE:CE1	2.49	0.48
1:B:610:LEU:HD22	1:B:858:PHE:CG	2.48	0.48
1:C:636:ASN:HD21	6:C:2301:GOL:H11	1.78	0.48
1:A:766:GLU:HG3	1:A:794:LEU:HD23	1.96	0.48
1:A:1039:LYS:O	1:A:1043:GLN:HG3	2.13	0.48
1:B:750:ASN:HD21	1:B:817:LEU:H	1.62	0.48
1:C:676:ILE:HD12	1:C:676:ILE:C	2.39	0.48
1:D:662:LEU:O	1:D:673:LEU:HD23	2.14	0.47
1:C:797:ASP:HA	4:C:2001:ACD:H171	1.96	0.47
1:A:490:ALA:HB2	1:A:784:LYS:HE3	1.96	0.47
1:A:518:TRP:CE3	1:A:770:LEU:HD23	2.50	0.47
1:C:662:LEU:O	1:C:673:LEU:HD23	2.15	0.47
1:A:661:VAL:HG21	6:A:2303:GOL:H2	1.96	0.47
1:B:504:GLN:NE2	8:B:1192:HOH:O	2.48	0.47
1:C:594:ASN:C	1:C:594:ASN:ND2	2.73	0.47
1:D:547:LYS:HD3	1:D:1004:SER:HB2	1.96	0.47
1:D:839:HIS:CD2	1:D:842:ASN:H	2.28	0.47
1:D:619:THR:HG22	1:D:620:ARG:O	2.15	0.47
1:B:739:MET:HE3	1:B:742:PHE:HB2	1.98	0.46
1:A:780:HIS:HD2	1:A:782:ILE:N	2.07	0.46
1:C:1020[A]:ASP:O	1:C:1024:LEU:HG	2.14	0.46
1:A:670:GLY:N	1:A:671:PRO:CD	2.78	0.46
1:A:892:ASP:O	1:A:896:GLN:HG2	2.15	0.46
1:B:844:LEU:HD13	1:B:861:ARG:HG3	1.97	0.46
1:D:764:THR:HB	1:D:907:TRP:CZ2	2.51	0.46
1:D:884:LYS:HA	1:D:884:LYS:HD3	1.80	0.46
1:A:490:ALA:HB2	1:A:784:LYS:CE	2.46	0.46
1:C:765:THR:HB	1:C:939:PHE:CE2	2.51	0.46
1:D:847:ARG:NH1	8:D:1208:HOH:O	2.38	0.46
1:C:1008:ARG:HG3	1:C:1008:ARG:NH1	2.30	0.45
1:C:851:ASP:HA	1:C:852:PRO:HD3	1.81	0.45
1:D:385:ARG:NH1	8:D:1356:HOH:O	2.23	0.45
1:A:386:GLU:OE2	1:A:549:ARG:NH2	2.43	0.45
1:C:702:TYR:HB2	1:C:712:ILE:HD13	1.99	0.45
1:D:780:HIS:CD2	1:D:782:ILE:H	2.31	0.45
1:A:644[A]:ASN:HD22	1:A:647:GLU:H	1.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:696:ALA:N	1:B:697:PRO:CD	2.79	0.45
1:D:473:PHE:HE2	1:D:487:PRO:HD3	1.80	0.45
1:B:834:ASN:ND2	1:B:836:GLN:HB2	2.32	0.45
1:D:507:LYS:O	1:D:511[B]:GLN:HG3	2.15	0.45
1:B:834:ASN:HD22	1:B:836:GLN:HB2	1.81	0.45
1:A:784:LYS:HE3	8:A:1101:HOH:O	2.16	0.45
1:A:800:GLY:HA3	4:A:2001:ACD:H172	1.99	0.45
1:A:1015:ALA:HB2	6:A:2305:GOL:H11	1.99	0.45
1:B:755:ASN:HD21	6:B:2304:GOL:H11	1.82	0.45
1:D:851:ASP:HA	1:D:852:PRO:HD3	1.88	0.45
1:A:757:HIS:HE1	8:A:315:HOH:O	1.91	0.45
1:A:738:MET:HG3	1:A:742:PHE:CE1	2.52	0.44
1:D:594:ASN:C	1:D:594:ASN:HD22	2.25	0.44
1:D:750:ASN:ND2	1:D:817:LEU:H	2.15	0.44
1:D:938:THR:HA	1:D:942:GLN:HB3	1.99	0.44
1:B:377:ASN:ND2	8:B:1114:HOH:O	2.51	0.44
1:B:750:ASN:HD22	1:B:817:LEU:HB2	1.81	0.44
1:C:380:VAL:HG11	1:C:455:TRP:CZ2	2.52	0.44
1:C:1008:ARG:HG3	1:C:1008:ARG:HH11	1.81	0.44
1:D:395:THR:HA	1:D:408:LEU:O	2.17	0.44
1:A:910:ASN:HB3	1:A:911:PRO:CD	2.47	0.44
1:A:997:VAL:HG23	5:A:2203:ACY:H1	1.99	0.44
1:D:509:LEU:HD23	1:D:509:LEU:HA	1.83	0.44
1:D:644:ASN:HD22	1:D:647:GLU:H	1.64	0.44
1:A:644[A]:ASN:HD21	1:A:647:GLU:HG3	1.82	0.44
1:A:594:ASN:ND2	1:A:952:ASP:HB3	2.32	0.44
1:B:656:ILE:HG12	1:B:657:VAL:N	2.33	0.44
1:A:643:LYS:HB3	1:A:647:GLU:HB2	1.99	0.44
1:A:695:ALA:C	1:A:697:PRO:HD3	2.42	0.44
1:B:728:THR:HG23	1:B:730:HIS:H	1.78	0.44
1:B:627:ASN:H	1:B:627:ASN:HD22	1.66	0.44
1:B:696:ALA:N	1:B:697:PRO:HD3	2.33	0.44
1:D:373:HIS:HA	1:D:430:GLY:O	2.18	0.43
1:D:575:ASP:OD1	6:D:2304:GOL:O1	2.35	0.43
1:A:642:GLY:N	6:A:2301:GOL:O3	2.49	0.43
1:C:636:ASN:ND2	6:C:2301:GOL:H11	2.33	0.43
1:C:1045:ASN:HB3	1:C:1051:PRO:HB3	1.99	0.43
1:A:696:ALA:N	1:A:697:PRO:HD3	2.34	0.43
1:A:532:LYS:O	1:A:802:LYS:CE	2.53	0.43
1:C:630:VAL:HG22	1:C:726:ILE:HD13	1.99	0.43
1:C:910:ASN:HB3	1:C:911:PRO:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:834:ASN:ND2	1:A:836:GLN:H	2.00	0.43
1:B:743:TRP:O	1:B:746:VAL:HG12	2.18	0.43
1:C:498:PRO:HB2	1:C:501:VAL:CG1	2.49	0.43
1:A:599:TRP:HB2	1:A:959:ASN:HD22	1.83	0.43
1:C:738:MET:HG3	1:C:742:PHE:CE1	2.54	0.43
1:C:750:ASN:HD21	1:C:817:LEU:H	1.67	0.43
1:C:839:HIS:HE1	8:C:1262:HOH:O	2.01	0.43
1:D:733:ASN:O	1:D:736:ASP:HB2	2.19	0.43
1:A:680:VAL:HA	1:A:681:PRO:HD3	1.85	0.43
1:D:739:MET:HE2	1:D:983:THR:HG21	2.01	0.42
1:A:750:ASN:HD21	1:A:817:LEU:H	1.67	0.42
1:C:528:ASN:HB2	1:C:766:GLU:OE2	2.20	0.42
1:D:632[B]:ASN:OD1	1:D:645:LEU:HB3	2.19	0.42
1:A:532:LYS:HE2	8:A:1461:HOH:O	2.19	0.42
1:C:780:HIS:HE1	1:C:892:ASP:OD2	2.02	0.42
1:A:815:LEU:HD12	1:A:815:LEU:HA	1.88	0.42
1:A:748:GLU:OE1	5:A:2201[B]:ACY:H2	2.20	0.42
1:B:792:GLY:O	1:B:796:ILE:HG22	2.20	0.42
1:C:830:PHE:HA	1:C:833:VAL:HG13	2.00	0.42
1:C:839:HIS:CD2	1:C:842:ASN:H	2.35	0.42
1:C:1042:LYS:NZ	1:C:1058[B]:GLU:OE1	2.50	0.42
1:A:632:ASN:HB2	8:A:103:HOH:O	2.18	0.42
1:A:1041:ILE:HG13	6:A:2306:GOL:H32	2.02	0.42
1:D:666:LYS:NZ	1:D:670:GLY:CA	2.75	0.42
1:C:619:THR:HG22	1:C:847:ARG:HG2	2.02	0.42
1:D:432:ASP:OD1	1:D:466:THR:OG1	2.35	0.42
1:A:518:TRP:CZ3	1:A:770:LEU:HD23	2.55	0.41
1:A:589:LEU:HB3	1:A:951:LYS:HG3	2.02	0.41
1:A:815:LEU:HD12	1:A:962:ALA:HB1	2.01	0.41
1:A:988:SER:O	1:A:992:LYS:HG3	2.20	0.41
1:B:669:GLY:HA3	1:B:691:ILE:HG13	2.02	0.41
1:B:716:ILE:HG22	1:B:717:ASN:ND2	2.35	0.41
1:A:893:ASN:H	1:A:893:ASN:ND2	2.18	0.41
1:B:1055:LEU:HD23	1:B:1055:LEU:HA	1.84	0.41
1:C:608:GLN:HE22	1:C:959:ASN:ND2	1.88	0.41
1:A:608:GLN:HB3	5:A:2201[B]:ACY:H1	2.02	0.41
1:A:1020:ASP:O	1:A:1024:LEU:HG	2.20	0.41
1:B:648:GLU:OE2	1:B:648:GLU:HA	2.21	0.41
1:C:766:GLU:HG3	1:C:794:LEU:HD23	2.03	0.41
1:A:594:ASN:HD22	1:A:595:MET:N	2.18	0.41
1:B:728:THR:O	1:B:731:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ILE:HG21	1:C:462:ILE:HD12	2.02	0.41
1:C:454:ASP:HB2	1:C:539:ARG:NH1	2.36	0.41
1:A:373:HIS:N	8:A:256:HOH:O	2.52	0.41
1:A:692:ARG:HD3	1:A:963:ILE:HG12	2.01	0.41
1:B:618:LEU:HD12	1:B:657:VAL:HG13	2.03	0.41
1:B:717:ASN:HB2	1:B:724:ASN:HD21	1.85	0.41
1:D:444:ASP:OD1	1:D:444:ASP:C	2.62	0.41
1:A:512:ARG:NH1	1:A:776:LEU:O	2.51	0.41
1:B:473:PHE:HE2	1:B:487:PRO:HD3	1.86	0.41
1:D:753[B]:GLN:NE2	1:D:757:HIS:HD1	2.19	0.40
1:C:757:HIS:HE1	8:C:1099:HOH:O	1.99	0.40
1:A:380:VAL:HG11	1:A:455:TRP:CZ2	2.57	0.40
1:C:512:ARG:HD2	1:C:773:TRP:O	2.22	0.40
1:D:753[B]:GLN:HE22	1:D:757:HIS:HD1	1.70	0.40
1:A:696:ALA:N	1:A:697:PRO:CD	2.85	0.40
1:B:951:LYS:HD2	1:B:951:LYS:C	2.46	0.40
1:B:956:PHE:CE2	1:B:958:PRO:HD2	2.56	0.40
1:C:547:LYS:HG2	8:C:1538:HOH:O	2.21	0.40
1:D:599:TRP:HE1	5:D:2202:ACY:CH3	2.25	0.40
1:D:627:ASN:H	1:D:627:ASN:ND2	2.14	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	688/696 (99%)	660 (96%)	27 (4%)	1 (0%)	48 59
1	B	678/696 (97%)	651 (96%)	24 (4%)	3 (0%)	30 37
1	C	690/696 (99%)	660 (96%)	27 (4%)	3 (0%)	30 37
1	D	688/696 (99%)	662 (96%)	25 (4%)	1 (0%)	48 59
All	All	2744/2784 (99%)	2633 (96%)	103 (4%)	8 (0%)	36 45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	811	VAL
1	B	812	ASP
1	C	810	ILE
1	D	412	LYS
1	B	762	HIS
1	C	762	HIS
1	C	808	GLY
1	B	722	PRO

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	579/601 (96%)	564 (97%)	15 (3%)	40	57
1	B	552/601 (92%)	530 (96%)	22 (4%)	28	41
1	C	574/601 (96%)	558 (97%)	16 (3%)	38	55
1	D	568/601 (94%)	550 (97%)	18 (3%)	34	50
All	All	2273/2404 (95%)	2202 (97%)	71 (3%)	36	51

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	384	ASP
1	A	532	LYS
1	A	574	TRP
1	A	594	ASN
1	A	603	ARG
1	A	627	ASN
1	A	644[A]	ASN
1	A	644[B]	ASN
1	A	758	LEU
1	A	869	GLU
1	A	923	GLU
1	A	926[A]	GLU

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Mol	Chain	Res	Type
1	A	926[B]	GLU
1	A	971	LYS
1	A	1057	PRO
1	B	384	ASP
1	B	429	GLN
1	B	500	ILE
1	B	536	ASP
1	B	547	LYS
1	B	566	SER
1	B	594	ASN
1	B	620	ARG
1	B	630	VAL
1	B	635	VAL
1	B	651	ASP
1	B	667	SER
1	B	691	ILE
1	B	728	THR
1	B	734	GLU
1	B	758	LEU
1	B	893[A]	ASN
1	B	893[B]	ASN
1	B	923	GLU
1	B	926	GLU
1	B	982	SER
1	B	988	SER
1	C	497	VAL
1	C	501	VAL
1	C	503	GLU
1	C	514	LEU
1	C	521	VAL
1	C	594	ASN
1	C	627	ASN
1	C	644[A]	ASN
1	C	644[B]	ASN
1	C	676	ILE
1	C	833	VAL
1	C	895	ILE
1	C	899	ILE
1	C	926	GLU
1	C	988	SER
1	C	1019	GLU
1	D	384	ASP

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Mol	Chain	Res	Type
1	D	411	ASP
1	D	428	VAL
1	D	497	VAL
1	D	547	LYS
1	D	594	ASN
1	D	627	ASN
1	D	644	ASN
1	D	651	ASP
1	D	676	ILE
1	D	746	VAL
1	D	758	LEU
1	D	793	VAL
1	D	812	ASP
1	D	893[A]	ASN
1	D	893[B]	ASN
1	D	1043	GLN
1	D	1057	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	GLN
1	A	467	GLN
1	A	594	ASN
1	A	627	ASN
1	A	634	HIS
1	A	715	GLN
1	A	730	HIS
1	A	750	ASN
1	A	780	HIS
1	A	834	ASN
1	A	839	HIS
1	A	842	ASN
1	A	947	ASN
1	A	959	ASN
1	B	377	ASN
1	B	458	ASN
1	B	504	GLN
1	B	594	ASN
1	B	608	GLN
1	B	614	ASN
1	B	627	ASN

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Mol	Chain	Res	Type
1	B	634	HIS
1	B	636	ASN
1	B	708	HIS
1	B	730	HIS
1	B	750	ASN
1	B	780	HIS
1	B	834	ASN
1	B	839	HIS
1	B	842	ASN
1	B	905	ASN
1	B	947	ASN
1	B	1043	GLN
1	C	377	ASN
1	C	429	GLN
1	C	458	ASN
1	C	467	GLN
1	C	495	ASN
1	C	552	GLN
1	C	594	ASN
1	C	627	ASN
1	C	634	HIS
1	C	730	HIS
1	C	750	ASN
1	C	753	GLN
1	C	780	HIS
1	C	834	ASN
1	C	839	HIS
1	C	842	ASN
1	C	947	ASN
1	C	950	GLN
1	C	959	ASN
1	C	1043	GLN
1	D	467	GLN
1	D	495	ASN
1	D	504	GLN
1	D	517	GLN
1	D	594	ASN
1	D	627	ASN
1	D	634	HIS
1	D	644	ASN
1	D	730	HIS
1	D	750	ASN

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Mol	Chain	Res	Type
1	D	780	HIS
1	D	834	ASN
1	D	839	HIS
1	D	842	ASN
1	D	947	ASN
1	D	950	GLN
1	D	959	ASN
1	D	1043	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 62 ligands modelled in this entry, 16 are monoatomic - leaving 46 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	$\# Z > 2$
5	ACY	D	2203	-	3,3,3	1.05	0	3,3,3	0.76	0
6	GOL	A	2304	-	5,5,5	0.48	0	5,5,5	1.07	0
6	GOL	C	2304	-	5,5,5	0.45	0	5,5,5	1.03	0
5	ACY	A	2207	-	3,3,3	0.89	0	3,3,3	0.90	0
5	ACY	C	2204	-	3,3,3	0.85	0	3,3,3	0.77	0
6	GOL	A	2306	-	5,5,5	0.56	0	5,5,5	1.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	C	2302	-	5,5,5	0.56	0	5,5,5	0.85	0
6	GOL	B	2303	-	5,5,5	0.33	0	5,5,5	0.37	0
6	GOL	A	1068[A]	-	5,5,5	0.31	0	5,5,5	1.19	0
4	ACD	C	2001	-	8,8,21	0.34	0	7,7,21	0.74	0
5	ACY	A	2201[A]	-	3,3,3	1.10	0	3,3,3	0.60	0
5	ACY	A	2205	-	3,3,3	1.15	0	3,3,3	0.63	0
5	ACY	D	2202	-	3,3,3	1.00	0	3,3,3	0.51	0
4	ACD	A	2001	-	8,8,21	0.50	0	7,7,21	1.10	0
5	ACY	C	2203	-	3,3,3	0.68	0	3,3,3	2.31	2 (66%)
5	ACY	A	2206	-	3,3,3	0.75	0	3,3,3	1.18	0
4	ACD	D	2001	-	7,7,21	0.46	0	6,6,21	0.64	0
6	GOL	D	2303	-	5,5,5	0.54	0	5,5,5	0.52	0
6	GOL	A	2301	-	5,5,5	0.36	0	5,5,5	0.33	0
5	ACY	D	2201	-	3,3,3	0.67	0	3,3,3	1.24	0
6	GOL	B	2301	-	5,5,5	0.51	0	5,5,5	0.60	0
5	ACY	B	2202	-	3,3,3	0.99	0	3,3,3	0.36	0
6	GOL	D	1067	-	5,5,5	0.53	0	5,5,5	0.52	0
5	ACY	A	2202	-	3,3,3	0.74	0	3,3,3	1.38	0
5	ACY	B	2201	-	3,3,3	0.78	0	3,3,3	1.30	0
5	ACY	C	2201	-	3,3,3	1.21	0	3,3,3	0.91	0
4	ACD	B	2001	-	7,7,21	0.56	0	6,6,21	0.73	0
6	GOL	A	2303	-	5,5,5	0.61	0	5,5,5	1.40	1 (20%)
5	ACY	B	2204	-	3,3,3	0.85	0	3,3,3	0.93	0
5	ACY	A	2204	-	3,3,3	0.68	0	3,3,3	1.45	0
5	ACY	C	2205	-	3,3,3	0.97	0	3,3,3	0.53	0
6	GOL	B	2304	-	5,5,5	0.45	0	5,5,5	0.76	0
6	GOL	A	1068[B]	-	5,5,5	0.51	0	5,5,5	0.79	0
5	ACY	C	2206	-	3,3,3	0.81	0	3,3,3	1.10	0
6	GOL	C	2301	-	5,5,5	0.62	0	5,5,5	0.91	0
5	ACY	B	2203	-	3,3,3	0.80	0	3,3,3	1.08	0
5	ACY	A	2201[B]	-	3,3,3	0.76	0	3,3,3	0.98	0
6	GOL	D	2304	-	5,5,5	0.51	0	5,5,5	0.84	0
6	GOL	A	2302	-	5,5,5	0.38	0	5,5,5	0.65	0
6	GOL	A	2305	-	5,5,5	0.51	0	5,5,5	1.24	0
6	GOL	A	2307	-	5,5,5	0.60	0	5,5,5	0.85	0
6	GOL	C	2305	-	5,5,5	0.23	0	5,5,5	0.90	0
5	ACY	A	2203	-	3,3,3	0.51	0	3,3,3	2.18	1 (33%)
5	ACY	D	2204	-	3,3,3	0.91	0	3,3,3	0.70	0
5	ACY	C	2202	-	3,3,3	0.87	0	3,3,3	0.78	0
6	GOL	C	2306	-	5,5,5	0.38	0	5,5,5	0.83	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
6	GOL	A	2304	-	-	2/4/4/4	-
6	GOL	C	2304	-	-	2/4/4/4	-
6	GOL	A	2306	-	-	0/4/4/4	-
6	GOL	C	2302	-	-	1/4/4/4	-
6	GOL	B	2303	-	-	4/4/4/4	-
6	GOL	A	1068[A]	-	-	2/4/4/4	-
4	ACD	C	2001	-	-	4/6/6/19	-
4	ACD	A	2001	-	-	4/6/6/19	-
4	ACD	D	2001	-	-	3/5/5/19	-
6	GOL	D	2303	-	-	4/4/4/4	-
6	GOL	A	2301	-	-	1/4/4/4	-
6	GOL	B	2301	-	-	2/4/4/4	-
6	GOL	D	1067	-	-	0/4/4/4	-
4	ACD	B	2001	-	-	3/5/5/19	-
6	GOL	A	2303	-	-	2/4/4/4	-
6	GOL	B	2304	-	-	4/4/4/4	-
6	GOL	A	1068[B]	-	-	4/4/4/4	-
6	GOL	C	2301	-	-	0/4/4/4	-
6	GOL	D	2304	-	-	0/4/4/4	-
6	GOL	A	2302	-	-	1/4/4/4	-
6	GOL	A	2305	-	-	2/4/4/4	-
6	GOL	A	2307	-	-	2/4/4/4	-
6	GOL	C	2305	-	-	2/4/4/4	-
6	GOL	C	2306	-	-	0/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2203	ACY	O-C-CH3	-3.06	109.96	122.53
5	A	2203	ACY	O-C-CH3	-2.97	110.36	122.53
6	A	2303	GOL	O2-C2-C1	2.38	119.04	109.18
5	C	2203	ACY	OXT-C-O	2.37	130.83	122.03

There are no chirality outliers.

All (49) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2304	GOL	O1-C1-C2-C3
6	A	2307	GOL	O1-C1-C2-C3
6	A	1068[A]	GOL	O1-C1-C2-O2
6	A	1068[A]	GOL	O1-C1-C2-C3
6	A	1068[B]	GOL	O1-C1-C2-C3
6	B	2301	GOL	C1-C2-C3-O3
6	B	2303	GOL	O1-C1-C2-C3
6	B	2303	GOL	C1-C2-C3-O3
6	B	2304	GOL	C1-C2-C3-O3
6	C	2305	GOL	C1-C2-C3-O3
6	C	2305	GOL	O2-C2-C3-O3
6	D	2303	GOL	O1-C1-C2-C3
6	D	2303	GOL	C1-C2-C3-O3
6	B	2303	GOL	O1-C1-C2-O2
6	B	2304	GOL	O1-C1-C2-O2
6	A	2302	GOL	C1-C2-C3-O3
6	A	2303	GOL	O1-C1-C2-C3
6	A	2305	GOL	O1-C1-C2-C3
6	A	1068[B]	GOL	C1-C2-C3-O3
6	B	2304	GOL	O1-C1-C2-C3
6	C	2304	GOL	O1-C1-C2-C3
4	C	2001	ACD	C16-C17-C18-C19
6	A	2303	GOL	O1-C1-C2-O2
6	A	2304	GOL	O1-C1-C2-O2
6	A	2305	GOL	O1-C1-C2-O2
6	A	2307	GOL	O1-C1-C2-O2
6	A	1068[B]	GOL	O1-C1-C2-O2
6	B	2304	GOL	O2-C2-C3-O3
6	D	2303	GOL	O1-C1-C2-O2
6	D	2303	GOL	O2-C2-C3-O3
4	A	2001	ACD	C15-C16-C17-C18
4	C	2001	ACD	C15-C16-C17-C18
4	A	2001	ACD	C12-C13-C14-C15
4	B	2001	ACD	C15-C16-C17-C18
6	B	2301	GOL	O2-C2-C3-O3
6	B	2303	GOL	O2-C2-C3-O3
4	D	2001	ACD	C15-C16-C17-C18
6	C	2302	GOL	C1-C2-C3-O3
4	D	2001	ACD	C16-C17-C18-C19
4	D	2001	ACD	C17-C18-C19-C20
6	C	2304	GOL	O1-C1-C2-O2
6	A	1068[B]	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	C	2001	ACD	C12-C13-C14-C15
6	A	2301	GOL	O2-C2-C3-O3
4	A	2001	ACD	C17-C18-C19-C20
4	B	2001	ACD	C14-C15-C16-C17
4	C	2001	ACD	C17-C18-C19-C20
4	A	2001	ACD	C14-C15-C16-C17
4	B	2001	ACD	C17-C18-C19-C20

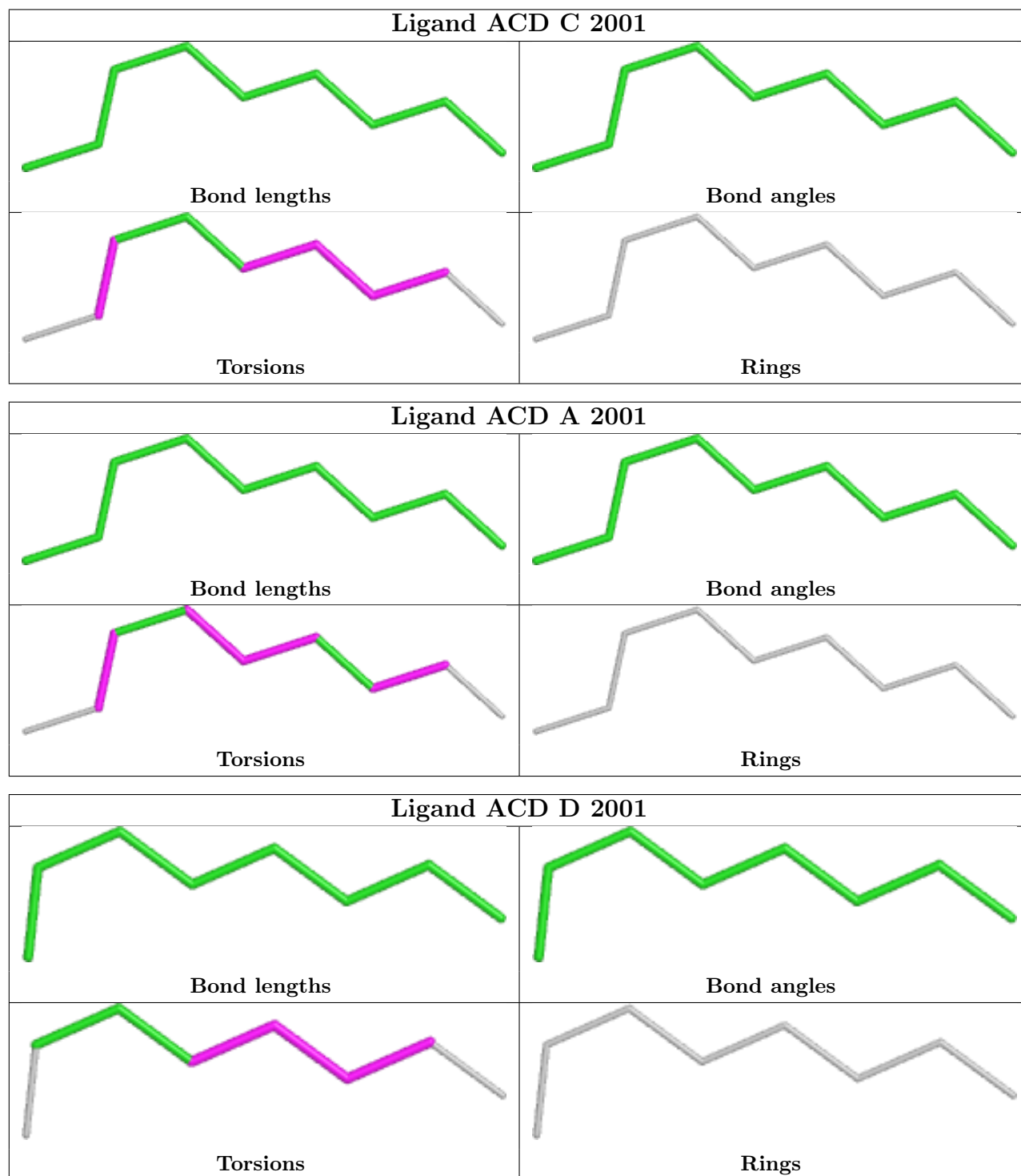
There are no ring outliers.

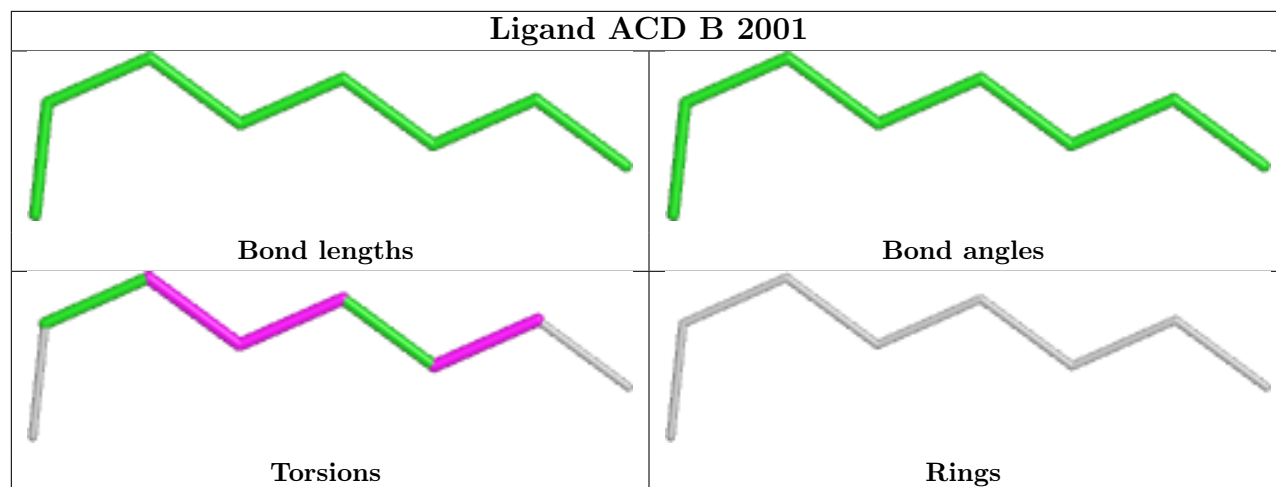
21 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	2203	ACY	2	0
6	A	2306	GOL	1	0
6	A	1068[A]	GOL	6	0
4	C	2001	ACD	5	0
5	A	2201[A]	ACY	1	0
5	D	2202	ACY	4	0
4	A	2001	ACD	1	0
5	C	2203	ACY	3	0
4	D	2001	ACD	1	0
6	D	2303	GOL	2	0
6	A	2301	GOL	1	0
4	B	2001	ACD	1	0
6	A	2303	GOL	5	0
6	B	2304	GOL	2	0
6	A	1068[B]	GOL	2	0
6	C	2301	GOL	3	0
5	A	2201[B]	ACY	4	0
6	D	2304	GOL	4	0
6	A	2305	GOL	5	0
5	A	2203	ACY	1	0
5	D	2204	ACY	1	0

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

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	414:SER	C	418:PHE	N	1.62

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	682/696 (97%)	-0.71	7 (1%) 79 81	8, 21, 36, 72	13 (1%)
1	B	676/696 (97%)	-0.41	4 (0%) 85 86	11, 30, 58, 81	10 (1%)
1	C	681/696 (97%)	-0.68	8 (1%) 76 78	9, 23, 40, 95	17 (2%)
1	D	678/696 (97%)	-0.49	6 (0%) 81 82	10, 28, 51, 92	16 (2%)
All	All	2717/2784 (97%)	-0.57	25 (0%) 81 82	8, 25, 50, 95	56 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	810	ILE	3.5
1	C	680	VAL	3.3
1	C	807	SER	3.1
1	C	808	GLY	3.1
1	A	681	PRO	3.1
1	B	676	ILE	3.0
1	D	808	GLY	2.9
1	A	687	ASP	2.9
1	A	808	GLY	2.8
1	C	803	GLU	2.7
1	A	810	ILE	2.6
1	B	679	LYS	2.6
1	D	810	ILE	2.5
1	C	811	VAL	2.5
1	C	488	GLY	2.3
1	D	804	LEU	2.3
1	C	809	GLY	2.3
1	B	811	VAL	2.3
1	A	688	GLU	2.3
1	B	645	LEU	2.2
1	D	678	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	809	GLY	2.2
1	D	373	HIS	2.1
1	A	373	HIS	2.0
1	D	411	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	2307	6/6	0.70	0.25	44,57,62,63	0
5	ACY	A	2205	4/4	0.76	0.19	39,40,46,47	0
5	ACY	A	2207	4/4	0.79	0.14	44,48,51,67	0
5	ACY	A	2206	4/4	0.79	0.15	33,35,36,52	0
6	GOL	D	2303	6/6	0.79	0.15	39,42,45,63	0
6	GOL	C	2305	6/6	0.80	0.17	45,51,56,60	0
4	ACD	B	2001	8/22	0.81	0.17	38,41,54,57	0
6	GOL	B	2303	6/6	0.81	0.16	44,51,55,94	0
4	ACD	A	2001	9/22	0.82	0.19	31,43,51,53	0
6	GOL	C	2306	6/6	0.82	0.16	26,46,51,58	0
5	ACY	D	2202	4/4	0.82	0.12	50,50,53,67	0
5	ACY	C	2205	4/4	0.83	0.17	42,42,50,56	0
4	ACD	C	2001	9/22	0.84	0.16	38,45,49,54	0
4	ACD	D	2001	8/22	0.85	0.16	28,38,46,53	0
5	ACY	D	2201	4/4	0.85	0.13	37,43,44,52	0
5	ACY	A	2204	4/4	0.86	0.13	34,43,46,53	0
5	ACY	C	2206	4/4	0.86	0.16	44,45,53,55	0
5	ACY	B	2202	4/4	0.86	0.17	46,50,54,62	0
5	ACY	C	2204	4/4	0.87	0.12	34,44,45,46	0

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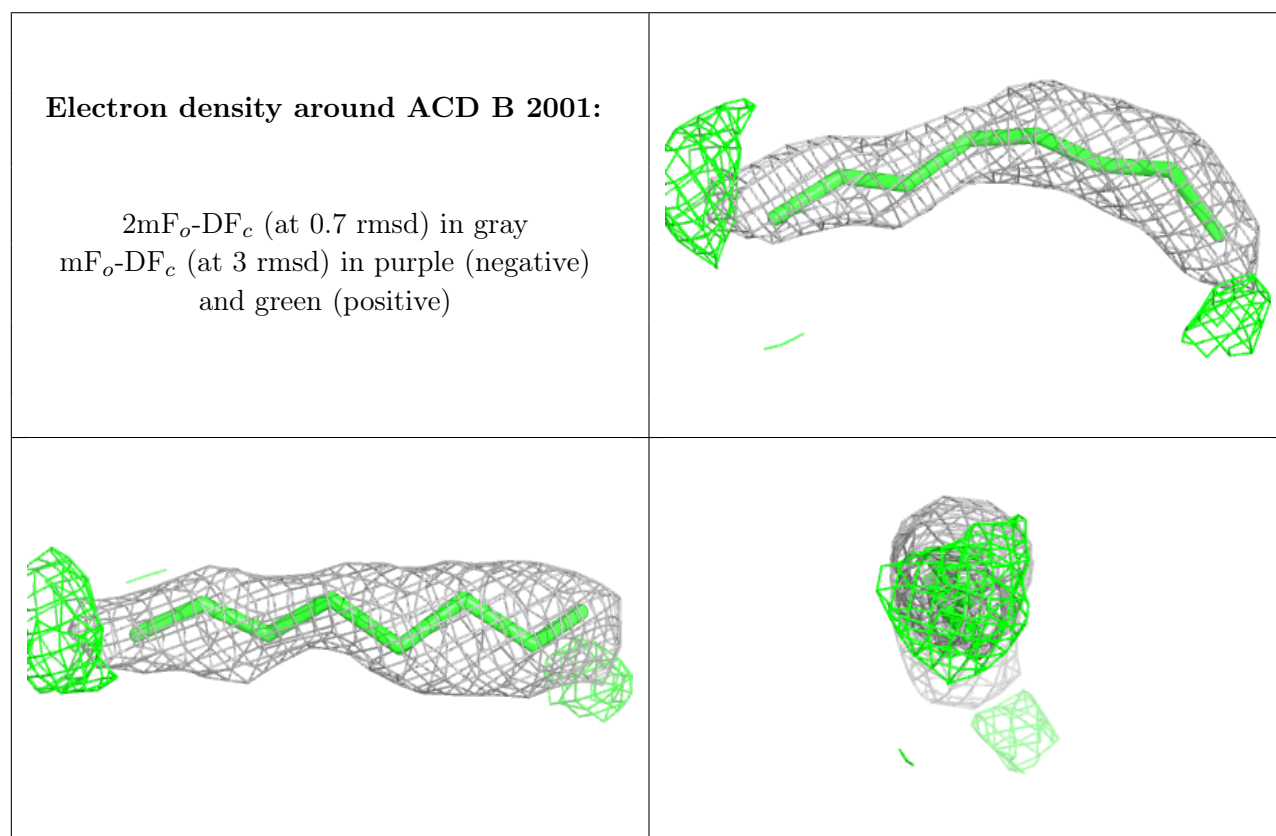
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACY	A	2203	4/4	0.87	0.13	29,32,48,52	0
6	GOL	A	2304	6/6	0.87	0.15	25,38,48,49	0
5	ACY	C	2202	4/4	0.87	0.13	38,38,44,46	0
6	GOL	D	2304	6/6	0.87	0.12	32,45,50,55	0
5	ACY	A	2202	4/4	0.88	0.16	39,44,44,46	0
6	GOL	C	2301	6/6	0.89	0.12	32,40,55,56	0
6	GOL	C	2304	6/6	0.89	0.13	22,36,53,62	0
5	ACY	C	2203	4/4	0.89	0.13	35,39,40,45	0
6	GOL	A	2305	6/6	0.89	0.16	30,38,46,51	0
5	ACY	B	2204	4/4	0.89	0.15	39,41,51,56	0
5	ACY	B	2201	4/4	0.89	0.09	28,32,36,38	0
6	GOL	A	1068[B]	6/6	0.90	0.20	20,27,33,33	6
6	GOL	A	2306	6/6	0.90	0.13	40,44,50,50	0
5	ACY	B	2203	4/4	0.90	0.13	36,40,44,48	0
6	GOL	A	1068[A]	6/6	0.90	0.20	7,13,20,21	6
6	GOL	A	2303	6/6	0.91	0.10	27,30,41,44	0
5	ACY	D	2204	4/4	0.91	0.12	38,39,46,51	0
6	GOL	B	2304	6/6	0.92	0.10	35,46,54,59	0
6	GOL	A	2301	6/6	0.94	0.07	26,31,39,40	0
6	GOL	B	2301	6/6	0.95	0.07	32,35,35,44	0
5	ACY	C	2201	4/4	0.96	0.11	23,26,26,30	0
6	GOL	D	1067	6/6	0.96	0.07	30,32,35,35	0
5	ACY	D	2203	4/4	0.96	0.08	26,33,33,36	0
6	GOL	A	2302	6/6	0.97	0.06	23,28,33,38	0
6	GOL	C	2302	6/6	0.97	0.05	26,30,33,33	0
2	FE2	B	1500	1/1	0.98	0.03	29,29,29,29	0
7	CL	B	2401	1/1	0.98	0.04	29,29,29,29	0
3	CA	A	1067	1/1	0.99	0.02	18,18,18,18	0
3	CA	C	1501	1/1	0.99	0.03	25,25,25,25	0
3	CA	C	1502	1/1	0.99	0.04	19,19,19,19	0
2	FE2	A	1500	1/1	0.99	0.02	20,20,20,20	0
2	FE2	C	1500	1/1	0.99	0.02	19,19,19,19	0
2	FE2	D	1500	1/1	0.99	0.02	25,25,25,25	0
3	CA	A	1501	1/1	0.99	0.03	22,22,22,22	0
5	ACY	A	2201[A]	4/4	0.99	0.04	7,7,8,10	4
5	ACY	A	2201[B]	4/4	0.99	0.04	6,9,11,14	4
7	CL	A	2401	1/1	0.99	0.03	28,28,28,28	0
3	CA	A	1502	1/1	0.99	0.04	21,21,21,21	0
7	CL	C	2401	1/1	0.99	0.04	23,23,23,23	0
7	CL	D	2401	1/1	0.99	0.03	26,26,26,26	0
3	CA	D	1501	1/1	1.00	0.02	25,25,25,25	0
3	CA	B	1501	1/1	1.00	0.03	23,23,23,23	0

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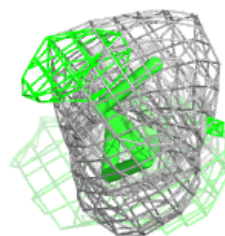
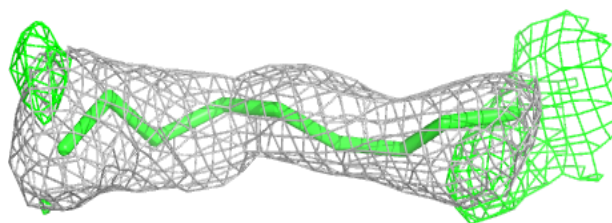
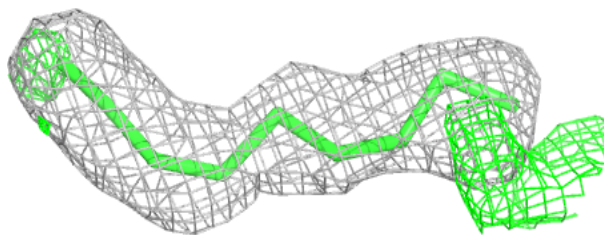
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	C	1067	1/1	1.00	0.01	20,20,20,20	0

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.

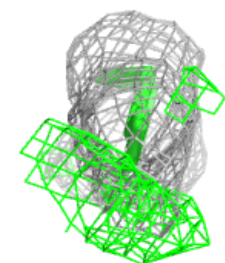
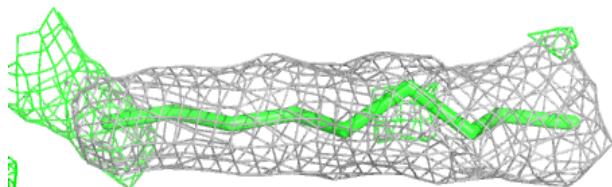
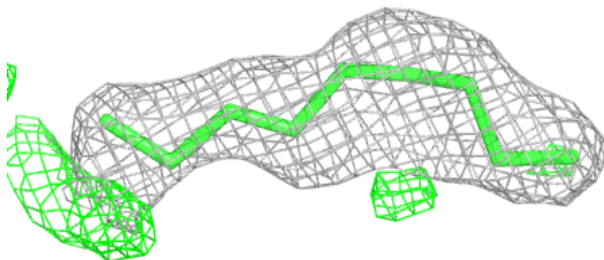


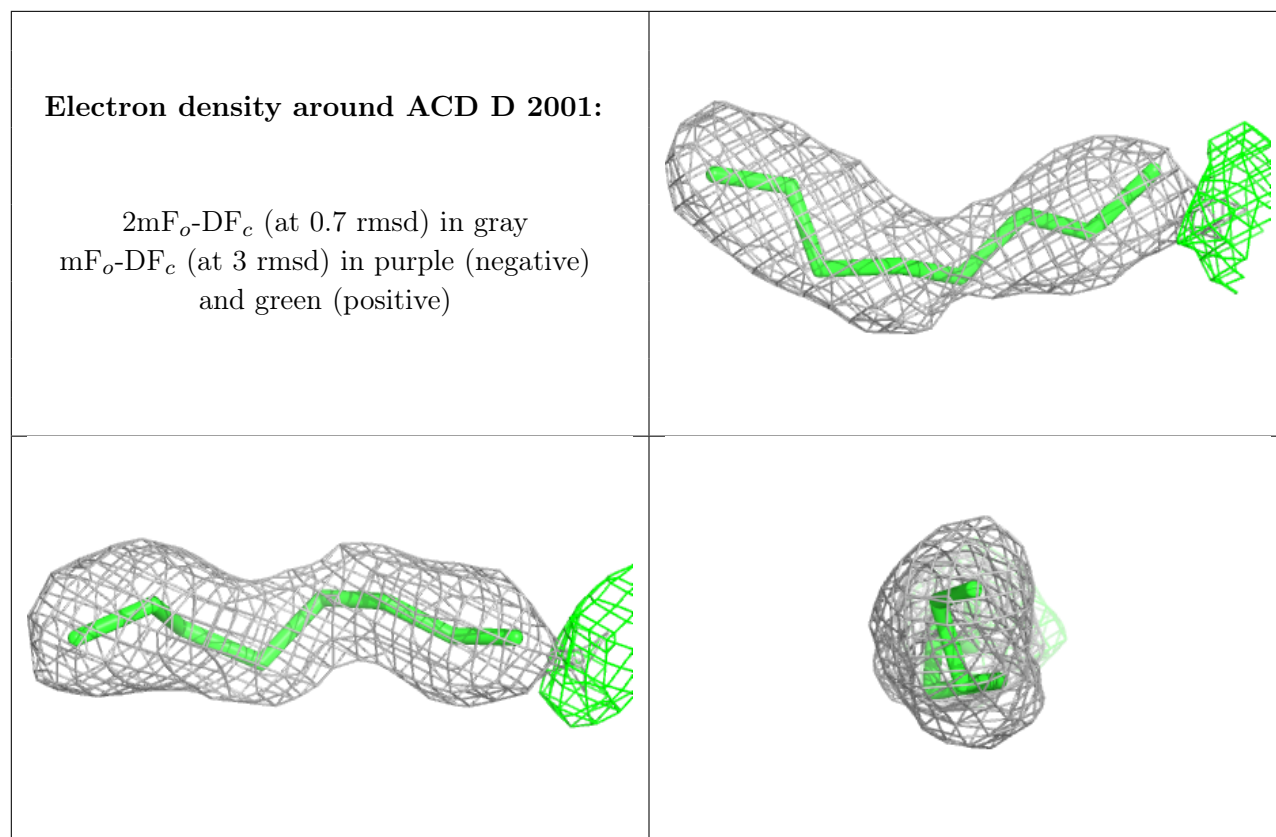
Electron density around ACD A 2001:

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

**Electron density around ACD C 2001:**

$2mF_o-DF_c$ (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.