



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 03:20 PM BST

PDB ID : 6VKO
Title : Crystal Structure of human PARP-1 CAT domain bound to inhibitor UKTT15
Authors : Langelier, M.F.; Pascal, J.M.
Deposited on : 2020-01-21
Resolution : 2.80 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 : 2.13.1
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) : 2.13.1

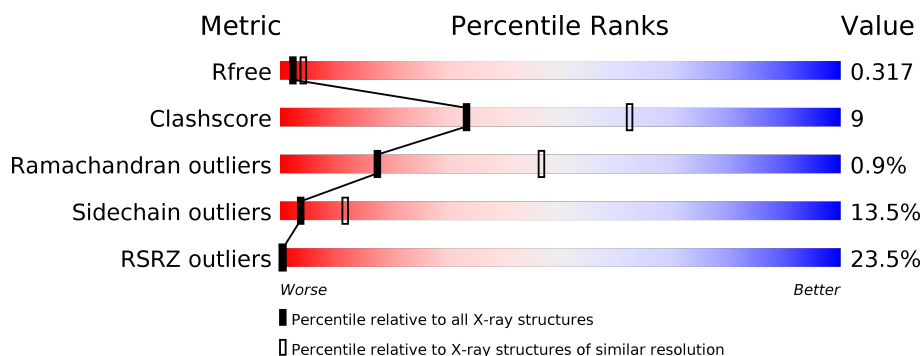
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	372	<div> <div>27%</div> <div>66% 23% • 9%</div> </div>
1	B	372	<div> <div>25%</div> <div>66% 23% • 9%</div> </div>
1	C	372	<div> <div>17%</div> <div>64% 24% • 9%</div> </div>
1	D	372	<div> <div>17%</div> <div>65% 24% • 9%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10970 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 Poly [ADP-ribose] polymerase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	340	Total	C	N	O	S	0	1	0
			2686	1713	455	507	11			
1	B	340	Total	C	N	O	S	0	1	0
			2683	1712	454	506	11			
1	C	340	Total	C	N	O	S	0	1	0
			2683	1712	454	506	11			
1	D	340	Total	C	N	O	S	0	1	0
			2683	1712	454	506	11			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	640	MET	-	initiating methionine	UNP P09874
A	641	GLY	-	expression tag	UNP P09874
A	642	SER	-	expression tag	UNP P09874
A	643	SER	-	expression tag	UNP P09874
A	644	HIS	-	expression tag	UNP P09874
A	645	HIS	-	expression tag	UNP P09874
A	646	HIS	-	expression tag	UNP P09874
A	647	HIS	-	expression tag	UNP P09874
A	648	HIS	-	expression tag	UNP P09874
A	649	HIS	-	expression tag	UNP P09874
A	650	SER	-	expression tag	UNP P09874
A	651	SER	-	expression tag	UNP P09874
A	652	GLY	-	expression tag	UNP P09874
A	653	LEU	-	expression tag	UNP P09874
A	654	VAL	-	expression tag	UNP P09874
A	655	PRO	-	expression tag	UNP P09874
A	656	ARG	-	expression tag	UNP P09874
A	657	GLY	-	expression tag	UNP P09874
A	658	SER	-	expression tag	UNP P09874
A	659	HIS	-	expression tag	UNP P09874
A	660	MET	-	expression tag	UNP P09874

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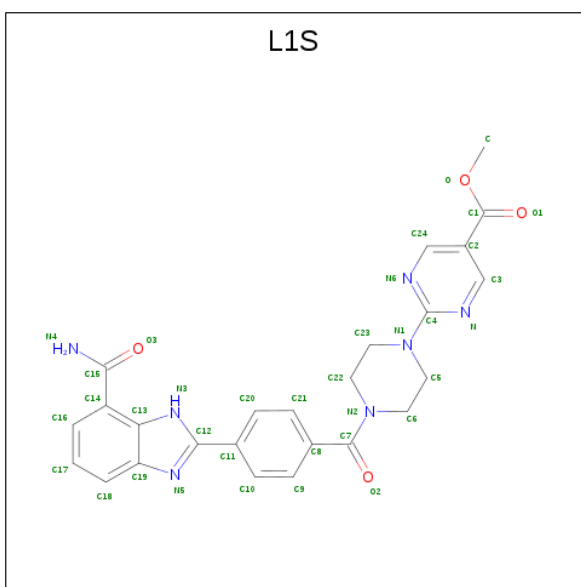
Chain	Residue	Modelled	Actual	Comment	Reference
A	762	ALA	VAL	variant	UNP P09874
B	640	MET	-	initiating methionine	UNP P09874
B	641	GLY	-	expression tag	UNP P09874
B	642	SER	-	expression tag	UNP P09874
B	643	SER	-	expression tag	UNP P09874
B	644	HIS	-	expression tag	UNP P09874
B	645	HIS	-	expression tag	UNP P09874
B	646	HIS	-	expression tag	UNP P09874
B	647	HIS	-	expression tag	UNP P09874
B	648	HIS	-	expression tag	UNP P09874
B	649	HIS	-	expression tag	UNP P09874
B	650	SER	-	expression tag	UNP P09874
B	651	SER	-	expression tag	UNP P09874
B	652	GLY	-	expression tag	UNP P09874
B	653	LEU	-	expression tag	UNP P09874
B	654	VAL	-	expression tag	UNP P09874
B	655	PRO	-	expression tag	UNP P09874
B	656	ARG	-	expression tag	UNP P09874
B	657	GLY	-	expression tag	UNP P09874
B	658	SER	-	expression tag	UNP P09874
B	659	HIS	-	expression tag	UNP P09874
B	660	MET	-	expression tag	UNP P09874
B	762	ALA	VAL	variant	UNP P09874
C	640	MET	-	initiating methionine	UNP P09874
C	641	GLY	-	expression tag	UNP P09874
C	642	SER	-	expression tag	UNP P09874
C	643	SER	-	expression tag	UNP P09874
C	644	HIS	-	expression tag	UNP P09874
C	645	HIS	-	expression tag	UNP P09874
C	646	HIS	-	expression tag	UNP P09874
C	647	HIS	-	expression tag	UNP P09874
C	648	HIS	-	expression tag	UNP P09874
C	649	HIS	-	expression tag	UNP P09874
C	650	SER	-	expression tag	UNP P09874
C	651	SER	-	expression tag	UNP P09874
C	652	GLY	-	expression tag	UNP P09874
C	653	LEU	-	expression tag	UNP P09874
C	654	VAL	-	expression tag	UNP P09874
C	655	PRO	-	expression tag	UNP P09874
C	656	ARG	-	expression tag	UNP P09874
C	657	GLY	-	expression tag	UNP P09874
C	658	SER	-	expression tag	UNP P09874

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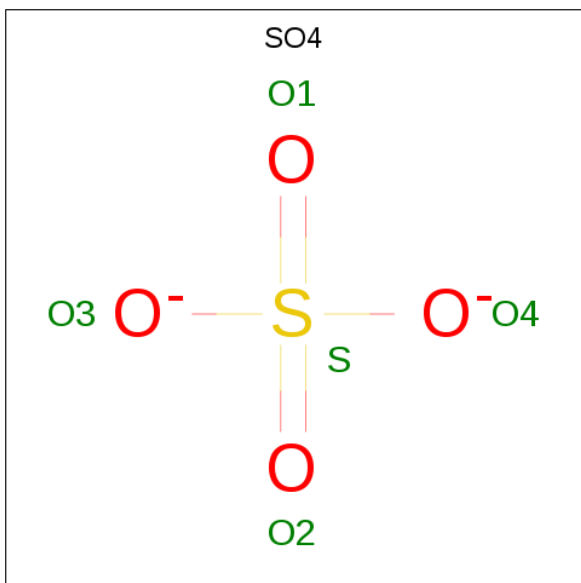
Chain	Residue	Modelled	Actual	Comment	Reference
C	659	HIS	-	expression tag	UNP P09874
C	660	MET	-	expression tag	UNP P09874
C	762	ALA	VAL	variant	UNP P09874
D	640	MET	-	initiating methionine	UNP P09874
D	641	GLY	-	expression tag	UNP P09874
D	642	SER	-	expression tag	UNP P09874
D	643	SER	-	expression tag	UNP P09874
D	644	HIS	-	expression tag	UNP P09874
D	645	HIS	-	expression tag	UNP P09874
D	646	HIS	-	expression tag	UNP P09874
D	647	HIS	-	expression tag	UNP P09874
D	648	HIS	-	expression tag	UNP P09874
D	649	HIS	-	expression tag	UNP P09874
D	650	SER	-	expression tag	UNP P09874
D	651	SER	-	expression tag	UNP P09874
D	652	GLY	-	expression tag	UNP P09874
D	653	LEU	-	expression tag	UNP P09874
D	654	VAL	-	expression tag	UNP P09874
D	655	PRO	-	expression tag	UNP P09874
D	656	ARG	-	expression tag	UNP P09874
D	657	GLY	-	expression tag	UNP P09874
D	658	SER	-	expression tag	UNP P09874
D	659	HIS	-	expression tag	UNP P09874
D	660	MET	-	expression tag	UNP P09874
D	762	ALA	VAL	variant	UNP P09874

- Molecule 2 is methyl 2-{4-[4-(7-carbamoyl-1H-benzimidazol-2-yl)benzene-1-carbonyl]piperazin-1-yl}pyrimidine-5-carboxylate (three-letter code: L1S) (formula: C₂₅H₂₃N₇O₄) (labeled as "Ligand of Interest" by author).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			36	25	7	4		
2	B	1	Total	C	N	O	0	0
			36	25	7	4		
2	C	1	Total	C	N	O	0	0
			36	25	7	4		
2	D	1	Total	C	N	O	0	0
			36	25	7	4		

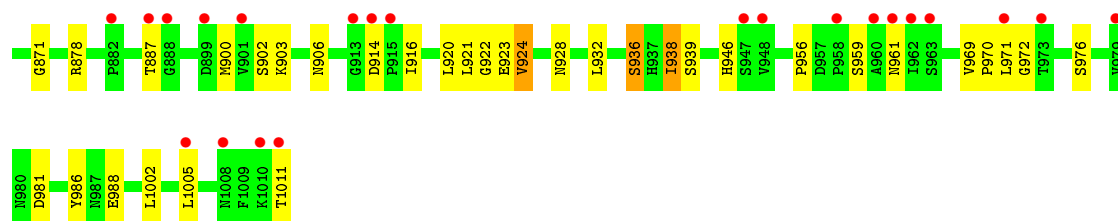
- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



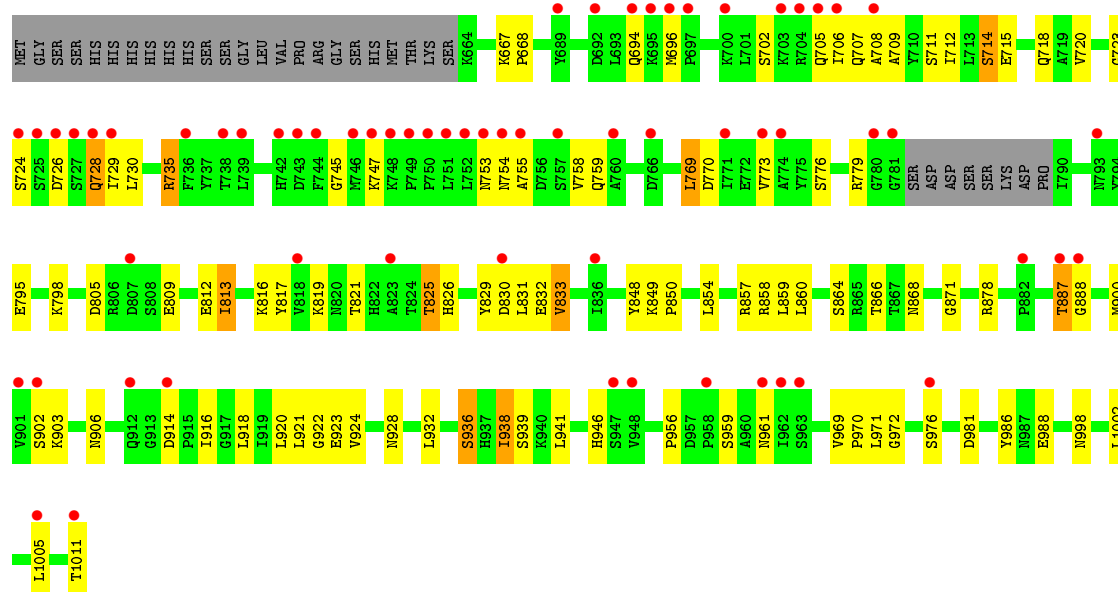
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

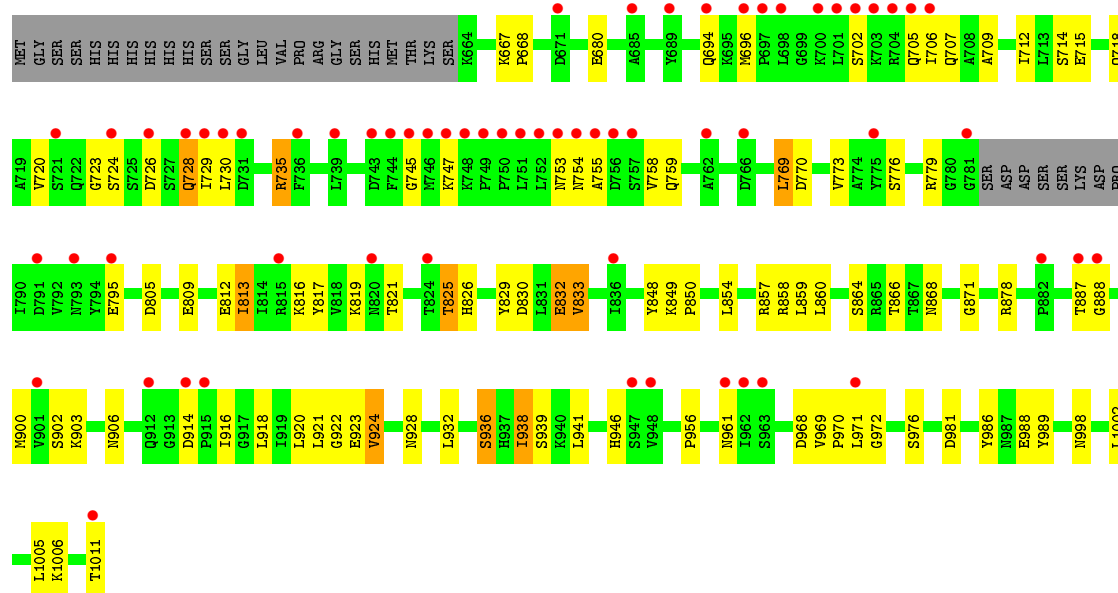
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	6	Total O 6 6	0	0
4	B	8	Total O 8 8	0	0
4	C	7	Total O 7 7	0	0
4	D	10	Total O 10 10	0	0



- Molecule 1: Poly [ADP-ribose] polymerase 1



- Molecule 1: Poly [ADP-ribose] polymerase 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	139.70Å 129.75Å 102.72Å 90.00° 111.36° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 47.83 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-2.80) 95.0 (47.83-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.284 , 0.312 0.290 , 0.317	Depositor DCC
R_{free} test set	2028 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.294	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 78.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	10970	wwPDB-VP
Average B, all atoms (Å ²)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 61.30 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3371e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, L1S

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	0.70	0/2736	0.84	0/3692
1	B	0.70	0/2736	0.84	0/3692
1	C	0.71	0/2736	0.84	0/3692
1	D	0.70	0/2736	0.84	0/3692
All	All	0.70	0/10944	0.84	0/14768

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	920	LEU	Peptide
1	B	920	LEU	Peptide
1	C	887	THR	Peptide
1	C	920	LEU	Peptide
1	D	920	LEU	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	2686	0	2730	46	0
1	B	2683	0	2731	40	0
1	C	2683	0	2731	50	0
1	D	2683	0	2731	51	0
2	A	36	0	0	0	0
2	B	36	0	0	0	0
2	C	36	0	0	3	0
2	D	36	0	0	4	0
3	A	15	0	0	1	0
3	B	15	0	0	1	0
3	C	15	0	0	2	0
3	D	15	0	0	2	0
4	A	6	0	0	0	1
4	B	8	0	0	0	0
4	C	7	0	0	0	0
4	D	10	0	0	0	0
All	All	10970	0	10923	187	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 9.

All (187) 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:B:858:ARG:NH2	3:B:1103:SO4:O4	1.90	1.05
1:C:858:ARG:NH2	3:C:1103:SO4:O3	1.93	1.01
1:B:813:ILE:O	1:B:813:ILE:HD12	1.83	0.79
1:C:813:ILE:HD12	1:C:813:ILE:O	1.83	0.78
1:A:813:ILE:O	1:A:813:ILE:HD12	1.83	0.77
1:D:813:ILE:O	1:D:813:ILE:HD12	1.83	0.77
1:D:859:LEU:HA	1:D:922:GLY:O	1.89	0.72
1:B:859:LEU:HA	1:B:922:GLY:O	1.89	0.72
1:A:859:LEU:HA	1:A:922:GLY:O	1.89	0.72
1:C:712:ILE:HD12	1:C:735:ARG:HD2	1.71	0.72
1:C:859:LEU:HA	1:C:922:GLY:O	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ILE:HD12	1:A:735:ARG:HD2	1.74	0.69
1:A:859:LEU:HG	1:A:921:LEU:HD22	1.77	0.67
1:B:859:LEU:HG	1:B:921:LEU:HD22	1.77	0.66
1:C:859:LEU:HG	1:C:921:LEU:HD22	1.78	0.66
1:B:712:ILE:HD12	1:B:735:ARG:HD2	1.77	0.65
1:C:829:TYR:OH	1:C:906:ASN:OD1	2.14	0.65
1:D:859:LEU:HG	1:D:921:LEU:HD22	1.77	0.65
1:D:712:ILE:HD12	1:D:735:ARG:HD2	1.78	0.64
1:D:755:ALA:HA	1:D:758:VAL:HG12	1.81	0.62
1:B:755:ALA:HA	1:B:758:VAL:HG12	1.82	0.62
1:C:755:ALA:HA	1:C:758:VAL:HG12	1.82	0.61
1:B:829:TYR:OH	1:B:906:ASN:OD1	2.14	0.61
1:A:829:TYR:OH	1:A:906:ASN:OD1	2.14	0.61
1:D:829:TYR:OH	1:D:906:ASN:OD1	2.14	0.61
1:A:755:ALA:HA	1:A:758:VAL:HG12	1.82	0.60
1:D:961[A]:ASN:ND2	1:D:970:PRO:HA	2.18	0.59
1:C:961[A]:ASN:ND2	1:C:970:PRO:HA	2.18	0.58
1:C:928:ASN:H	1:C:946:HIS:HD2	1.51	0.58
1:D:928:ASN:H	1:D:946:HIS:HD2	1.50	0.58
1:C:849:LYS:NZ	3:C:1104:SO4:O4	2.32	0.58
1:B:961[A]:ASN:ND2	1:B:970:PRO:HA	2.19	0.57
1:B:928:ASN:H	1:B:946:HIS:HD2	1.51	0.57
1:A:928:ASN:H	1:A:946:HIS:HD2	1.52	0.57
1:B:770:ASP:OD1	1:B:878:ARG:NH2	2.36	0.57
1:A:706:ILE:HG21	1:A:769:LEU:HG	1.87	0.57
1:D:759:GLN:HG3	2:D:1101:LIS:C3	2.35	0.57
1:B:813:ILE:HD11	1:B:969:VAL:HG11	1.87	0.56
1:C:825:THR:HB	1:C:986:TYR:OH	2.05	0.56
1:D:770:ASP:OD1	1:D:878:ARG:NH2	2.37	0.56
1:D:825:THR:HB	1:D:986:TYR:OH	2.06	0.56
1:B:706:ILE:HG21	1:B:769:LEU:HG	1.87	0.55
1:B:825:THR:HB	1:B:986:TYR:OH	2.06	0.55
1:D:706:ILE:HG21	1:D:769:LEU:HG	1.87	0.55
1:D:813:ILE:HD11	1:D:969:VAL:HG11	1.89	0.55
1:A:825:THR:HB	1:A:986:TYR:OH	2.07	0.54
1:B:956:PRO:HB3	1:B:972:GLY:O	2.07	0.54
1:C:706:ILE:HG21	1:C:769:LEU:HG	1.90	0.54
1:C:813:ILE:HD11	1:C:969:VAL:HG11	1.89	0.54
1:D:813:ILE:HA	1:D:816:LYS:HD2	1.90	0.54
1:D:956:PRO:HB3	1:D:972:GLY:O	2.08	0.53
1:B:932:LEU:HD13	1:B:936:SER:OG	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:956:PRO:HB3	1:A:972:GLY:O	2.09	0.53
1:C:770:ASP:OD1	1:C:878:ARG:NH2	2.36	0.53
1:D:726:ASP:HA	1:D:729:ILE:HB	1.90	0.53
1:A:932:LEU:HD13	1:A:936:SER:OG	2.09	0.53
1:C:726:ASP:HA	1:C:729:ILE:HB	1.90	0.53
1:C:956:PRO:HB3	1:C:972:GLY:O	2.08	0.53
1:D:705:GLN:O	1:D:709:ALA:N	2.42	0.53
1:B:726:ASP:HA	1:B:729:ILE:HB	1.90	0.52
1:C:888:GLY:HA3	2:C:1101:L1S:C4	2.38	0.52
1:A:813:ILE:HD11	1:A:969:VAL:HG11	1.90	0.52
1:A:726:ASP:HA	1:A:729:ILE:HB	1.90	0.52
1:C:932:LEU:HD13	1:C:936:SER:OG	2.09	0.52
1:D:770:ASP:HB3	1:D:868:ASN:HA	1.92	0.52
1:C:705:GLN:O	1:C:709:ALA:N	2.42	0.52
1:A:705:GLN:O	1:A:709:ALA:N	2.42	0.51
1:C:770:ASP:HB3	1:C:868:ASN:HA	1.93	0.51
1:A:770:ASP:OD1	1:A:878:ARG:NH2	2.36	0.51
1:A:773:VAL:HG11	1:A:871:GLY:HA2	1.93	0.51
1:B:705:GLN:O	1:B:709:ALA:N	2.42	0.51
1:D:932:LEU:HD13	1:D:936:SER:OG	2.10	0.51
1:B:773:VAL:HG11	1:B:871:GLY:HA2	1.93	0.50
1:D:773:VAL:HG11	1:D:871:GLY:HA2	1.93	0.50
1:D:759:GLN:HG2	2:D:1101:L1S:C4	2.41	0.50
1:A:715:GLU:HA	1:A:718:GLN:HB2	1.94	0.50
1:B:715:GLU:HA	1:B:718:GLN:HB2	1.94	0.50
1:C:759:GLN:HG2	2:C:1101:L1S:C4	2.42	0.49
1:D:715:GLU:HA	1:D:718:GLN:HB2	1.94	0.49
1:A:849:LYS:N	1:A:850:PRO:CD	2.75	0.49
1:D:849:LYS:N	1:D:850:PRO:CD	2.75	0.49
1:B:770:ASP:HB3	1:B:868:ASN:HA	1.94	0.49
1:D:826:HIS:ND1	1:D:902:SER:HB3	2.28	0.49
1:C:849:LYS:N	1:C:850:PRO:CD	2.75	0.49
1:C:773:VAL:HG11	1:C:871:GLY:HA2	1.93	0.49
1:C:854:LEU:O	1:C:857:ARG:HD3	2.12	0.49
1:A:770:ASP:HB3	1:A:868:ASN:HA	1.94	0.49
1:B:813:ILE:CD1	1:B:969:VAL:HG11	2.43	0.48
1:B:849:LYS:N	1:B:850:PRO:CD	2.76	0.48
1:C:715:GLU:HA	1:C:718:GLN:HB2	1.95	0.48
1:B:854:LEU:O	1:B:857:ARG:HD3	2.13	0.48
1:D:854:LEU:O	1:D:857:ARG:HD3	2.13	0.48
1:D:712:ILE:HD12	1:D:735:ARG:CD	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961[A]:ASN:OD1	1:A:970:PRO:HA	2.14	0.48
1:A:809:GLU:O	1:A:812:GLU:N	2.47	0.48
1:A:854:LEU:O	1:A:857:ARG:HD3	2.13	0.48
1:D:728:GLN:HE21	1:D:728:GLN:N	2.12	0.48
1:B:728:GLN:HE21	1:B:728:GLN:N	2.12	0.48
1:B:809:GLU:O	1:B:812:GLU:N	2.47	0.48
1:C:809:GLU:O	1:C:812:GLU:N	2.47	0.48
1:B:858:ARG:HB3	1:B:860:LEU:HG	1.95	0.47
1:A:728:GLN:N	1:A:728:GLN:HE21	2.12	0.47
1:D:858:ARG:HB3	1:D:860:LEU:HG	1.97	0.47
1:A:833:VAL:HA	1:A:1005:LEU:HD23	1.96	0.47
1:B:712:ILE:HD12	1:B:735:ARG:CD	2.43	0.47
1:D:888:GLY:HA3	2:D:1101:L1S:C4	2.44	0.47
1:B:938:ILE:O	1:B:938:ILE:HG22	2.15	0.47
1:D:809:GLU:O	1:D:812:GLU:N	2.47	0.47
1:C:858:ARG:HB3	1:C:860:LEU:HG	1.95	0.47
1:C:928:ASN:N	1:C:946:HIS:HD2	2.13	0.47
1:A:813:ILE:CD1	1:A:969:VAL:HG11	2.45	0.47
1:C:728:GLN:N	1:C:728:GLN:HE21	2.12	0.47
1:B:928:ASN:N	1:B:946:HIS:HD2	2.12	0.47
1:C:712:ILE:HD12	1:C:735:ARG:CD	2.42	0.47
1:C:833:VAL:HA	1:C:1005:LEU:HD23	1.96	0.46
1:B:833:VAL:HA	1:B:1005:LEU:HD23	1.97	0.46
1:D:833:VAL:HA	1:D:1005:LEU:HD23	1.97	0.46
1:A:928:ASN:N	1:A:946:HIS:HD2	2.13	0.46
1:A:849:LYS:NZ	3:A:1104:SO4:O4	2.47	0.45
1:A:826:HIS:ND1	1:A:902:SER:HB3	2.30	0.45
1:B:981:ASP:O	1:B:981:ASP:OD1	2.34	0.45
1:B:826:HIS:ND1	1:B:902:SER:HB3	2.31	0.45
1:D:813:ILE:CD1	1:D:969:VAL:HG11	2.46	0.45
1:A:981:ASP:OD1	1:A:981:ASP:O	2.35	0.45
1:C:813:ILE:CD1	1:C:969:VAL:HG11	2.46	0.45
1:D:928:ASN:N	1:D:946:HIS:HD2	2.12	0.45
1:D:728:GLN:H	1:D:728:GLN:HE21	1.65	0.45
1:D:981:ASP:OD1	1:D:981:ASP:O	2.34	0.45
1:A:858:ARG:HB3	1:A:860:LEU:HG	1.97	0.45
1:A:938:ILE:HG22	1:A:938:ILE:O	2.16	0.45
1:C:728:GLN:HE21	1:C:728:GLN:H	1.65	0.45
1:D:938:ILE:HG22	1:D:938:ILE:O	2.17	0.45
1:A:728:GLN:H	1:A:728:GLN:HE21	1.65	0.44
1:C:813:ILE:HA	1:C:816:LYS:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:826:HIS:ND1	1:C:902:SER:HB3	2.32	0.44
1:D:848:TYR:OH	1:D:923:GLU:HG2	2.18	0.44
1:C:848:TYR:OH	1:C:923:GLU:HG2	2.18	0.44
1:B:728:GLN:HE21	1:B:728:GLN:H	1.65	0.44
1:B:848:TYR:OH	1:B:923:GLU:HG2	2.18	0.44
1:A:712:ILE:HD12	1:A:735:ARG:CD	2.44	0.44
1:A:813:ILE:HA	1:A:816:LYS:HD2	2.00	0.44
1:C:938:ILE:O	1:C:938:ILE:HG22	2.17	0.43
1:D:667:LYS:N	1:D:668:PRO:HD2	2.33	0.43
1:B:1002:LEU:C	1:B:1002:LEU:HD23	2.39	0.43
1:C:981:ASP:OD1	1:C:981:ASP:O	2.35	0.43
1:C:831:LEU:HA	1:C:831:LEU:HD12	1.89	0.43
1:D:849:LYS:NZ	3:D:1104:SO4:O2	2.51	0.43
1:A:848:TYR:OH	1:A:923:GLU:HG2	2.18	0.43
1:A:903:LYS:HE2	1:A:988:GLU:HG2	2.01	0.43
1:C:708:ALA:O	1:C:711:SER:OG	2.28	0.43
1:A:1002:LEU:HD23	1:A:1002:LEU:C	2.39	0.43
1:C:903:LYS:HE2	1:C:988:GLU:HG2	2.01	0.43
1:D:1002:LEU:HD23	1:D:1002:LEU:C	2.39	0.43
1:C:1002:LEU:C	1:C:1002:LEU:HD23	2.38	0.43
1:C:918:LEU:HD22	1:C:1002:LEU:HD21	2.02	0.42
1:B:903:LYS:HE2	1:B:988:GLU:HG2	2.02	0.42
1:C:970:PRO:HG2	1:C:970:PRO:O	2.20	0.42
1:A:821:THR:HG22	1:A:972:GLY:O	2.20	0.42
1:A:941:LEU:HD12	1:A:941:LEU:HA	1.96	0.41
1:C:938:ILE:HG21	1:C:941:LEU:HD13	2.02	0.41
1:D:903:LYS:HE2	1:D:988:GLU:HG2	2.02	0.41
1:D:858:ARG:NH2	3:D:1103:SO4:O1	2.36	0.41
1:A:667:LYS:N	1:A:668:PRO:HD2	2.36	0.41
1:A:892:GLY:HA2	1:A:937:HIS:CD2	2.55	0.41
1:B:813:ILE:HA	1:B:816:LYS:HD2	2.01	0.41
1:C:821:THR:HG22	1:C:972:GLY:O	2.20	0.41
1:C:848:TYR:CG	1:C:998:ASN:HB2	2.55	0.41
1:D:848:TYR:CG	1:D:998:ASN:HB2	2.56	0.41
1:C:759:GLN:HG3	2:C:1101:L1S:C3	2.51	0.41
1:D:858:ARG:HG2	1:D:968:ASP:HB2	2.01	0.41
1:D:821:THR:HG22	1:D:972:GLY:O	2.21	0.41
1:B:860:LEU:HD12	1:B:924:VAL:HG13	2.03	0.41
1:D:755:ALA:HB1	2:D:1101:L1S:C	2.50	0.41
1:D:989:TYR:N	1:D:989:TYR:CD1	2.89	0.41
1:A:848:TYR:CG	1:A:998:ASN:HB2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:667:LYS:N	1:C:668:PRO:HD2	2.35	0.41
1:A:938:ILE:HG21	1:A:941:LEU:HD13	2.03	0.41
1:C:714:SER:OG	1:C:715:GLU:N	2.54	0.41
1:D:860:LEU:HD12	1:D:924:VAL:HG13	2.03	0.41
1:D:832:GLU:HB2	1:D:1006:LYS:HB3	2.03	0.41
1:A:970:PRO:O	1:A:970:PRO:HG2	2.22	0.40
1:B:667:LYS:N	1:B:668:PRO:HD2	2.37	0.40
1:A:714:SER:OG	1:A:715:GLU:N	2.54	0.40
1:A:860:LEU:HD12	1:A:924:VAL:HG13	2.03	0.40
1:D:918:LEU:HD22	1:D:1002:LEU:HD21	2.04	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)
4:A:1204:HOH:O	4:A:1204:HOH:O[2_657]	1.35	0.85

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	337/372 (91%)	307 (91%)	27 (8%)	3 (1%)	17	46
1	B	337/372 (91%)	309 (92%)	25 (7%)	3 (1%)	17	46
1	C	337/372 (91%)	306 (91%)	28 (8%)	3 (1%)	17	46
1	D	337/372 (91%)	307 (91%)	27 (8%)	3 (1%)	17	46
All	All	1348/1488 (91%)	1229 (91%)	107 (8%)	12 (1%)	17	46

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	723	GLY
1	A	745	GLY
1	B	723	GLY
1	B	745	GLY
1	C	723	GLY
1	C	745	GLY
1	D	723	GLY
1	D	745	GLY
1	A	938	ILE
1	B	938	ILE
1	C	938	ILE
1	D	938	ILE

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	298/326 (91%)	258 (87%)	40 (13%)	4	12
1	B	298/326 (91%)	256 (86%)	42 (14%)	3	10
1	C	298/326 (91%)	259 (87%)	39 (13%)	4	12
1	D	298/326 (91%)	259 (87%)	39 (13%)	4	12
All	All	1192/1304 (91%)	1032 (87%)	160 (13%)	4	12

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	694	GLN
1	A	696	MET
1	A	702	SER
1	A	707	GLN
1	A	714	SER
1	A	720	VAL
1	A	724	SER
1	A	728	GLN
1	A	730	LEU
1	A	735	ARG

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Mol	Chain	Res	Type
1	A	747	LYS
1	A	753	ASN
1	A	754	ASN
1	A	759	GLN
1	A	769	LEU
1	A	776	SER
1	A	779	ARG
1	A	795	GLU
1	A	798	LYS
1	A	805	ASP
1	A	809	GLU
1	A	813	ILE
1	A	817	TYR
1	A	819	LYS
1	A	825	THR
1	A	830	ASP
1	A	833	VAL
1	A	864	SER
1	A	866	THR
1	A	887	THR
1	A	900	MET
1	A	914	ASP
1	A	924	VAL
1	A	936	SER
1	A	939	SER
1	A	941	LEU
1	A	959	SER
1	A	971	LEU
1	A	976	SER
1	A	1011	THR
1	B	664	LYS
1	B	694	GLN
1	B	696	MET
1	B	702	SER
1	B	707	GLN
1	B	714	SER
1	B	720	VAL
1	B	724	SER
1	B	728	GLN
1	B	730	LEU
1	B	735	ARG
1	B	747	LYS

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Mol	Chain	Res	Type
1	B	753	ASN
1	B	754	ASN
1	B	759	GLN
1	B	769	LEU
1	B	776	SER
1	B	779	ARG
1	B	795	GLU
1	B	798	LYS
1	B	805	ASP
1	B	809	GLU
1	B	813	ILE
1	B	817	TYR
1	B	819	LYS
1	B	825	THR
1	B	830	ASP
1	B	832	GLU
1	B	833	VAL
1	B	864	SER
1	B	866	THR
1	B	887	THR
1	B	900	MET
1	B	914	ASP
1	B	916	ILE
1	B	924	VAL
1	B	936	SER
1	B	939	SER
1	B	959	SER
1	B	971	LEU
1	B	976	SER
1	B	1011	THR
1	C	694	GLN
1	C	696	MET
1	C	702	SER
1	C	707	GLN
1	C	714	SER
1	C	720	VAL
1	C	724	SER
1	C	728	GLN
1	C	730	LEU
1	C	735	ARG
1	C	747	LYS
1	C	753	ASN

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Mol	Chain	Res	Type
1	C	754	ASN
1	C	769	LEU
1	C	776	SER
1	C	779	ARG
1	C	795	GLU
1	C	798	LYS
1	C	805	ASP
1	C	813	ILE
1	C	817	TYR
1	C	819	LYS
1	C	825	THR
1	C	830	ASP
1	C	832	GLU
1	C	833	VAL
1	C	864	SER
1	C	866	THR
1	C	887	THR
1	C	900	MET
1	C	914	ASP
1	C	916	ILE
1	C	924	VAL
1	C	936	SER
1	C	939	SER
1	C	959	SER
1	C	971	LEU
1	C	976	SER
1	C	1011	THR
1	D	680	GLU
1	D	694	GLN
1	D	696	MET
1	D	702	SER
1	D	707	GLN
1	D	714	SER
1	D	720	VAL
1	D	724	SER
1	D	728	GLN
1	D	730	LEU
1	D	735	ARG
1	D	747	LYS
1	D	753	ASN
1	D	754	ASN
1	D	769	LEU

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Mol	Chain	Res	Type
1	D	776	SER
1	D	779	ARG
1	D	795	GLU
1	D	805	ASP
1	D	813	ILE
1	D	817	TYR
1	D	819	LYS
1	D	825	THR
1	D	830	ASP
1	D	832	GLU
1	D	833	VAL
1	D	864	SER
1	D	866	THR
1	D	887	THR
1	D	900	MET
1	D	914	ASP
1	D	916	ILE
1	D	924	VAL
1	D	936	SER
1	D	939	SER
1	D	941	LEU
1	D	971	LEU
1	D	976	SER
1	D	1011	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	694	GLN
1	A	722	GLN
1	A	728	GLN
1	A	753	ASN
1	A	754	ASN
1	A	820	ASN
1	A	846	GLN
1	A	937	HIS
1	A	946	HIS
1	B	722	GLN
1	B	728	GLN
1	B	753	ASN
1	B	754	ASN
1	B	820	ASN

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Mol	Chain	Res	Type
1	B	846	GLN
1	B	937	HIS
1	B	946	HIS
1	C	694	GLN
1	C	722	GLN
1	C	728	GLN
1	C	753	ASN
1	C	754	ASN
1	C	820	ASN
1	C	846	GLN
1	C	937	HIS
1	C	946	HIS
1	D	694	GLN
1	D	722	GLN
1	D	728	GLN
1	D	753	ASN
1	D	754	ASN
1	D	820	ASN
1	D	846	GLN
1	D	937	HIS
1	D	946	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

16 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	$\# Z > 2$
3	SO4	B	1104	-	4,4,4	0.38	0	6,6,6	0.09	0
3	SO4	A	1104	-	4,4,4	0.38	0	6,6,6	0.06	0
3	SO4	D	1104	-	4,4,4	0.38	0	6,6,6	0.09	0
3	SO4	D	1103	-	4,4,4	0.38	0	6,6,6	0.12	0
3	SO4	C	1103	-	4,4,4	0.39	0	6,6,6	0.07	0
3	SO4	C	1104	-	4,4,4	0.37	0	6,6,6	0.06	0
3	SO4	A	1103	-	4,4,4	0.38	0	6,6,6	0.06	0
3	SO4	B	1102	-	4,4,4	0.40	0	6,6,6	0.09	0
3	SO4	A	1102	-	4,4,4	0.39	0	6,6,6	0.09	0
3	SO4	D	1102	-	4,4,4	0.36	0	6,6,6	0.11	0
2	L1S	B	1101	-	39,40,40	0.59	1 (2%)	49,57,57	0.51	0
2	L1S	C	1101	-	39,40,40	0.57	0	49,57,57	0.58	0
2	L1S	A	1101	-	39,40,40	0.62	1 (2%)	49,57,57	0.50	0
3	SO4	C	1102	-	4,4,4	0.36	0	6,6,6	0.13	0
2	L1S	D	1101	-	39,40,40	0.60	0	49,57,57	0.51	0
3	SO4	B	1103	-	4,4,4	0.35	0	6,6,6	0.12	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
2	L1S	B	1101	-	-	8/26/36/36	0/5/5/5
2	L1S	C	1101	-	-	4/26/36/36	0/5/5/5
2	L1S	A	1101	-	-	8/26/36/36	0/5/5/5
2	L1S	D	1101	-	-	6/26/36/36	0/5/5/5

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	L1S	C12-N3	-2.17	1.33	1.35
2	B	1101	L1S	C12-N3	-2.03	1.33	1.35

There are no bond angle outliers.

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1101	L1S	C2-C1-O-C
2	A	1101	L1S	C2-C1-O-C
2	B	1101	L1S	O1-C1-O-C
2	A	1101	L1S	O1-C1-O-C
2	D	1101	L1S	C2-C1-O-C
2	D	1101	L1S	O1-C1-O-C
2	B	1101	L1S	N6-C4-N1-C5
2	A	1101	L1S	N6-C4-N1-C5
2	B	1101	L1S	N-C4-N1-C5
2	B	1101	L1S	C10-C11-C12-N3
2	C	1101	L1S	C10-C11-C12-N3
2	A	1101	L1S	C10-C11-C12-N3
2	A	1101	L1S	N-C4-N1-C5
2	B	1101	L1S	C10-C11-C12-N5
2	B	1101	L1S	C20-C11-C12-N3
2	B	1101	L1S	C20-C11-C12-N5
2	C	1101	L1S	C10-C11-C12-N5
2	C	1101	L1S	C20-C11-C12-N3
2	C	1101	L1S	C20-C11-C12-N5
2	A	1101	L1S	C10-C11-C12-N5
2	A	1101	L1S	C20-C11-C12-N3
2	A	1101	L1S	C20-C11-C12-N5
2	D	1101	L1S	C10-C11-C12-N3
2	D	1101	L1S	C10-C11-C12-N5
2	D	1101	L1S	C20-C11-C12-N5
2	D	1101	L1S	C20-C11-C12-N3

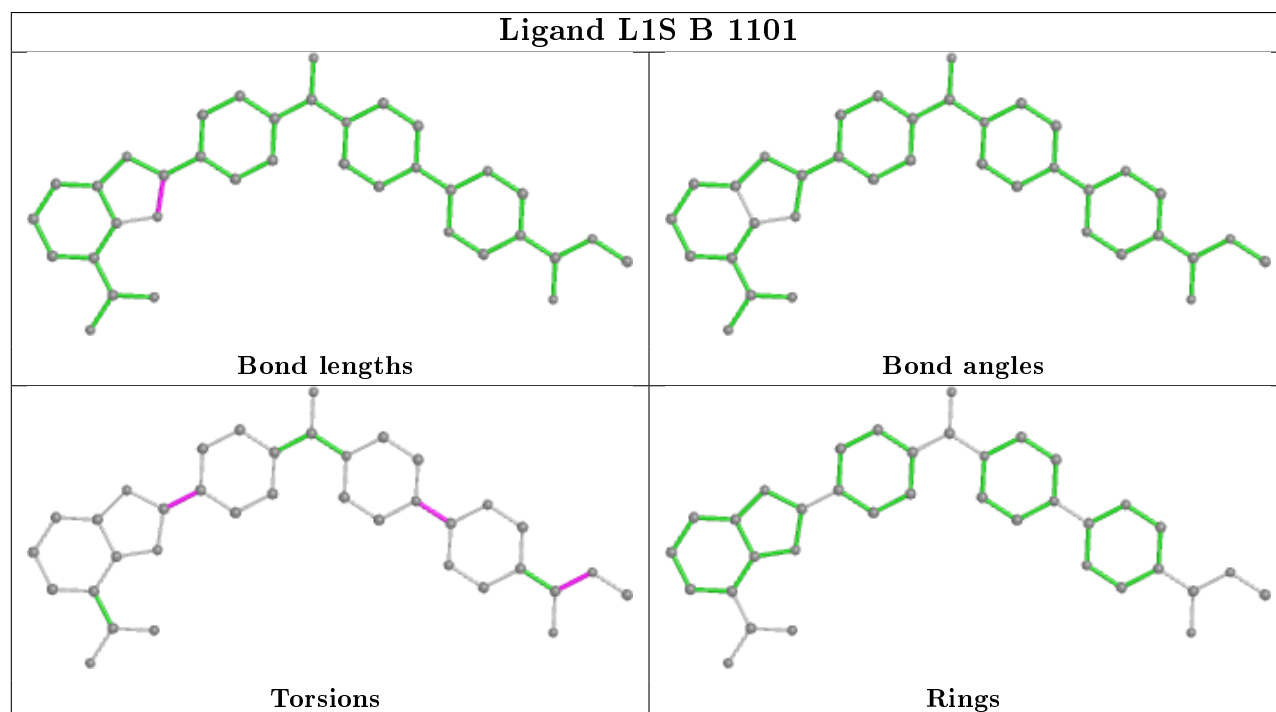
There are no ring outliers.

8 monomers are involved in 13 short contacts:

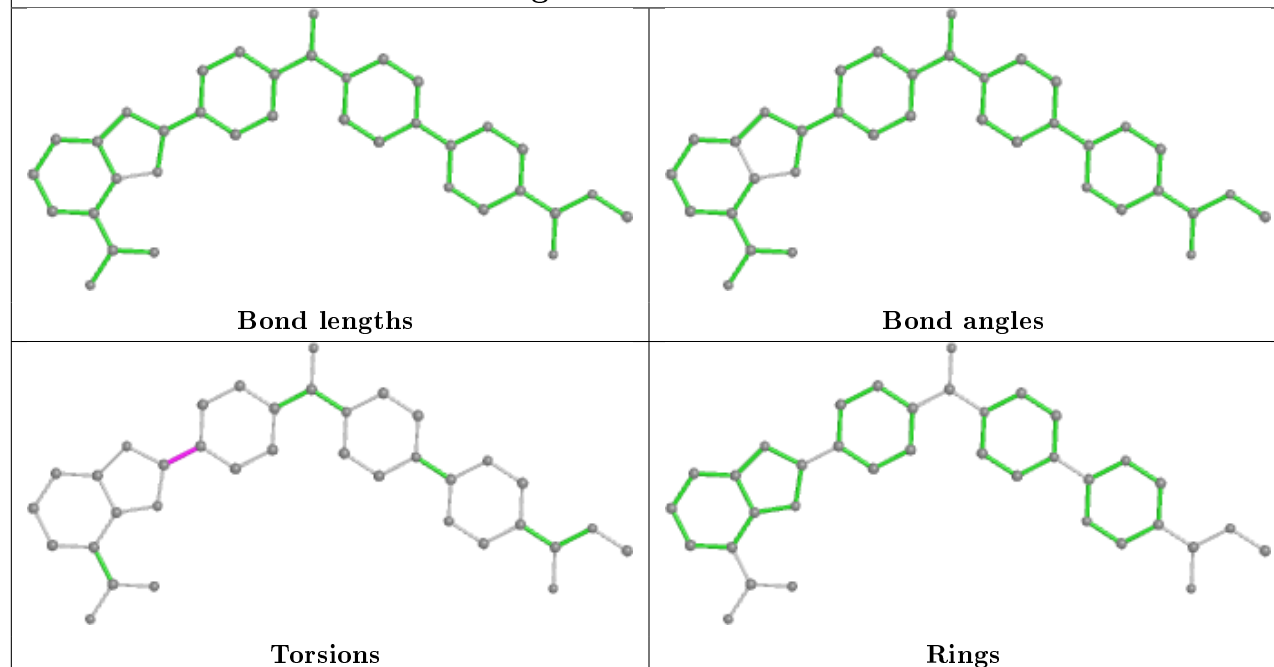
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1104	SO4	1	0
3	D	1104	SO4	1	0
3	D	1103	SO4	1	0
3	C	1103	SO4	1	0
3	C	1104	SO4	1	0
2	C	1101	L1S	3	0
2	D	1101	L1S	4	0
3	B	1103	SO4	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

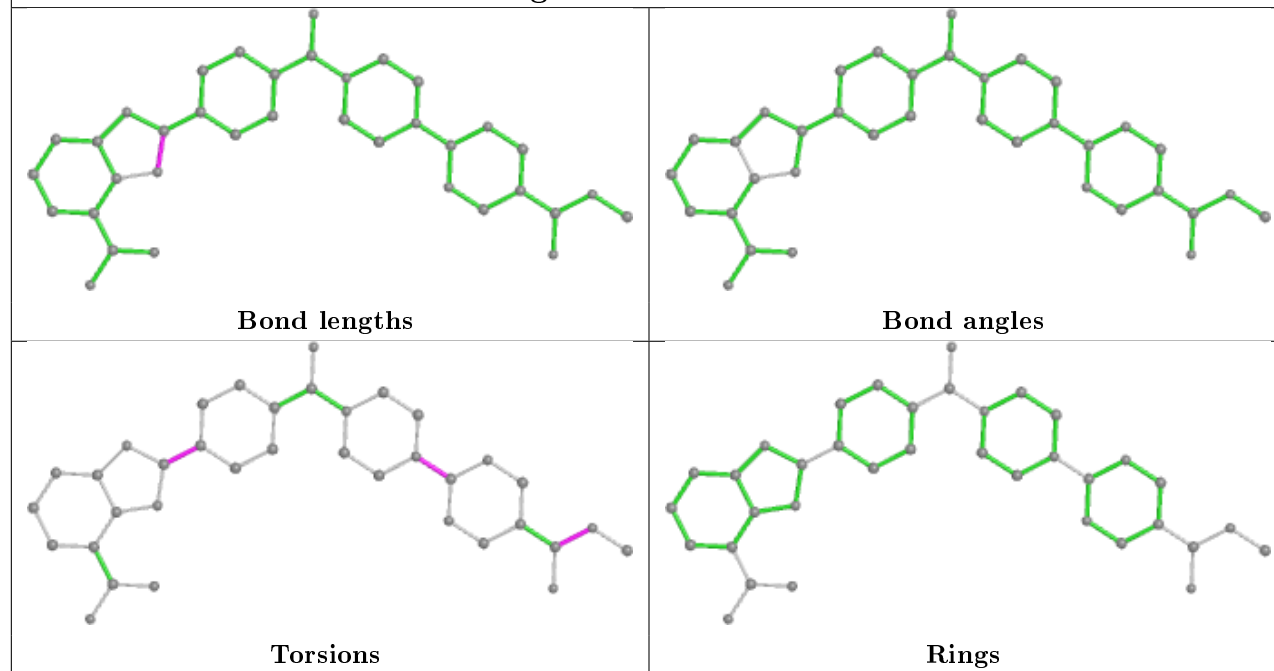
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

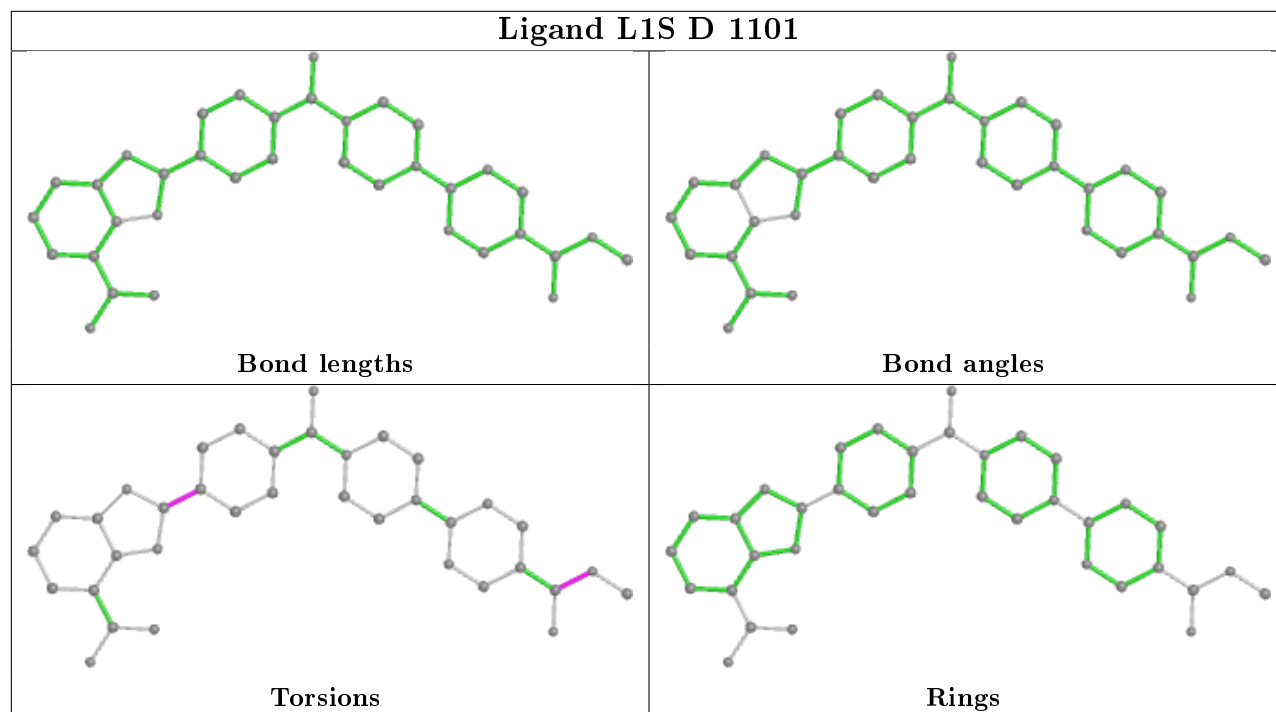


Ligand L1S C 1101



Ligand L1S A 1101





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	340/372 (91%)	1.67	101 (29%) 0 0	52, 97, 161, 180	0
1	B	340/372 (91%)	1.60	92 (27%) 0 0	53, 92, 154, 203	0
1	C	340/372 (91%)	1.32	64 (18%) 1 1	46, 86, 157, 193	0
1	D	340/372 (91%)	1.33	63 (18%) 1 1	49, 91, 160, 194	0
All	All	1360/1488 (91%)	1.48	320 (23%) 0 0	46, 92, 159, 203	0

All (320) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	751	LEU	12.3
1	B	705	GLN	11.6
1	A	753	ASN	11.6
1	D	705	GLN	11.5
1	D	781	GLY	10.8
1	B	753	ASN	10.3
1	D	751	LEU	10.2
1	D	753	ASN	10.0
1	C	705	GLN	9.9
1	A	705	GLN	9.7
1	D	747	LYS	9.4
1	C	753	ASN	8.8
1	A	751	LEU	8.6
1	C	752	LEU	8.2
1	B	706	ILE	8.1
1	A	752	LEU	8.1
1	A	697	PRO	8.1
1	A	888	GLY	7.5
1	C	781	GLY	7.2
1	D	888	GLY	7.0
1	D	752	LEU	7.0

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Mol	Chain	Res	Type	RSRZ
1	C	726	ASP	6.8
1	D	755	ALA	6.8
1	A	729	ILE	6.8
1	B	747	LYS	6.6
1	B	746	MET	6.5
1	C	729	ILE	6.4
1	A	750	PRO	6.4
1	C	747	LYS	6.3
1	A	887	THR	6.1
1	C	888	GLY	6.1
1	D	754	ASN	5.9
1	B	726	ASP	5.7
1	D	703	LYS	5.5
1	A	696	MET	5.5
1	B	888	GLY	5.5
1	C	744	PHE	5.5
1	C	696	MET	5.5
1	B	692	ASP	5.4
1	A	747	LYS	5.4
1	B	749	PRO	5.4
1	A	721	SER	5.3
1	B	691	ILE	5.1
1	A	746	MET	5.1
1	B	948	VAL	5.0
1	C	750	PRO	5.0
1	D	696	MET	5.0
1	C	697	PRO	4.9
1	B	914	ASP	4.9
1	B	750	PRO	4.9
1	A	774	ALA	4.9
1	B	752	LEU	4.9
1	C	948	VAL	4.8
1	B	697	PRO	4.8
1	C	706	ILE	4.8
1	B	781	GLY	4.7
1	D	706	ILE	4.7
1	B	1011	THR	4.7
1	B	689	TYR	4.7
1	A	737	TYR	4.6
1	B	729	ILE	4.6
1	C	774	ALA	4.6
1	A	744	PHE	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	1011	THR	4.6
1	D	729	ILE	4.5
1	A	948	VAL	4.5
1	A	706	ILE	4.5
1	A	781	GLY	4.5
1	D	728	GLN	4.4
1	B	696	MET	4.4
1	A	689	TYR	4.4
1	B	687	VAL	4.4
1	B	688	GLU	4.3
1	B	887	THR	4.3
1	B	947	SER	4.3
1	A	692	ASP	4.3
1	D	704	ARG	4.3
1	B	670	GLN	4.3
1	C	887	THR	4.2
1	A	687	VAL	4.2
1	C	728	GLN	4.2
1	B	766	ASP	4.2
1	B	736	PHE	4.2
1	A	912	GLN	4.2
1	D	1011	THR	4.1
1	A	766	ASP	4.1
1	B	743	ASP	4.1
1	B	836	ILE	4.1
1	A	1008	ASN	4.1
1	B	744	PHE	4.0
1	B	754	ASN	4.0
1	C	780	GLY	4.0
1	C	725	SER	4.0
1	B	760	ALA	3.9
1	B	761	LYS	3.9
1	B	757	SER	3.9
1	A	680	GLU	3.9
1	A	882	PRO	3.9
1	D	750	PRO	3.8
1	A	754	ASN	3.8
1	B	1010	LYS	3.8
1	A	757	SER	3.8
1	A	700	LYS	3.8
1	D	748	LYS	3.8
1	C	793	ASN	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	748	LYS	3.8
1	B	739	LEU	3.7
1	A	743	ASP	3.7
1	D	746	MET	3.7
1	B	700	LYS	3.7
1	A	836	ILE	3.7
1	D	766	ASP	3.7
1	A	728	GLN	3.7
1	B	741	PRO	3.6
1	C	914	ASP	3.6
1	D	689	TYR	3.6
1	B	779	ARG	3.6
1	A	693	LEU	3.6
1	B	818	VAL	3.6
1	B	755	ALA	3.6
1	B	703	LYS	3.6
1	B	774	ALA	3.6
1	A	818	VAL	3.6
1	B	751	LEU	3.5
1	C	1011	THR	3.5
1	C	961[A]	ASN	3.5
1	A	703	LYS	3.5
1	A	691	ILE	3.5
1	B	704	ARG	3.5
1	A	962	ILE	3.4
1	D	962	ILE	3.4
1	C	727	SER	3.4
1	A	861	TRP	3.4
1	A	913	GLY	3.4
1	A	914	ASP	3.4
1	A	815	ARG	3.4
1	D	915	PRO	3.4
1	A	736	PHE	3.4
1	A	779	ARG	3.4
1	A	749	PRO	3.4
1	D	749	PRO	3.3
1	D	757	SER	3.3
1	A	791	ASP	3.3
1	C	755	ALA	3.3
1	A	1009	PHE	3.3
1	B	728	GLN	3.3
1	B	899	ASP	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	730	LEU	3.3
1	C	963	SER	3.2
1	D	721	SER	3.2
1	C	962	ILE	3.2
1	A	899	ASP	3.2
1	D	914	ASP	3.2
1	D	756	ASP	3.2
1	B	756	ASP	3.2
1	A	830	ASP	3.2
1	A	961[A]	ASN	3.1
1	D	743	ASP	3.1
1	D	700	LYS	3.1
1	A	704	ARG	3.1
1	A	773	VAL	3.1
1	A	665	LEU	3.1
1	C	754	ASN	3.1
1	A	958	PRO	3.1
1	C	704	ARG	3.0
1	A	726	ASP	3.0
1	B	882	PRO	3.0
1	C	746	MET	3.0
1	D	948	VAL	3.0
1	B	961[A]	ASN	3.0
1	B	714	SER	3.0
1	D	744	PHE	3.0
1	C	748	LYS	3.0
1	A	742	HIS	3.0
1	A	868	ASN	2.9
1	C	700	LYS	2.9
1	A	807	ASP	2.9
1	B	780	GLY	2.9
1	C	947	SER	2.9
1	D	961[A]	ASN	2.9
1	B	962	ILE	2.9
1	A	963	SER	2.9
1	B	815	ARG	2.9
1	D	815	ARG	2.9
1	D	887	THR	2.9
1	D	697	PRO	2.9
1	B	737	TYR	2.8
1	B	823	ALA	2.8
1	D	963	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	703	LYS	2.8
1	A	708	ALA	2.8
1	A	671	ASP	2.8
1	A	765	LEU	2.8
1	B	693	LEU	2.8
1	C	695	LYS	2.8
1	C	760	ALA	2.7
1	A	771	ILE	2.7
1	C	902	SER	2.7
1	B	708	ALA	2.7
1	D	702	SER	2.7
1	A	817	TYR	2.7
1	C	708	ALA	2.7
1	C	823	ALA	2.7
1	A	764	MET	2.7
1	B	868	ASN	2.7
1	C	976	SER	2.7
1	D	775	TYR	2.7
1	A	772	GLU	2.7
1	D	795	GLU	2.6
1	D	901	VAL	2.6
1	D	730	LEU	2.6
1	A	898	ALA	2.6
1	C	882	PRO	2.6
1	D	736	PHE	2.6
1	D	882	PRO	2.6
1	B	695	LYS	2.6
1	B	765	LEU	2.6
1	A	804	VAL	2.6
1	D	971	LEU	2.6
1	A	915	PRO	2.6
1	D	698	LEU	2.5
1	A	947	SER	2.5
1	D	791	ASP	2.5
1	B	830	ASP	2.5
1	A	960	ALA	2.5
1	B	973	THR	2.5
1	C	807	ASP	2.5
1	D	726	ASP	2.5
1	C	724	SER	2.5
1	C	757	SER	2.5
1	A	901	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	958	PRO	2.4
1	A	775	TYR	2.4
1	D	793	ASN	2.4
1	C	739	LEU	2.4
1	B	775	TYR	2.4
1	B	683	LYS	2.4
1	D	671	ASP	2.4
1	C	736	PHE	2.4
1	A	865	ARG	2.4
1	A	674	LYS	2.4
1	A	701	LEU	2.4
1	C	773	VAL	2.4
1	A	793	ASN	2.4
1	B	845	CYS	2.4
1	B	901	VAL	2.4
1	B	718	GLN	2.4
1	B	960	ALA	2.4
1	A	760	ALA	2.3
1	B	748	LYS	2.3
1	B	865	ARG	2.3
1	A	971	LEU	2.3
1	B	971	LEU	2.3
1	D	820	ASN	2.3
1	C	1005	LEU	2.3
1	C	738	THR	2.3
1	B	773	VAL	2.3
1	C	901	VAL	2.3
1	A	832	GLU	2.3
1	B	915	PRO	2.3
1	C	692	ASP	2.3
1	D	701	LEU	2.3
1	C	689	TYR	2.3
1	A	755	ALA	2.3
1	A	780	GLY	2.3
1	A	767	ASN	2.3
1	B	694	GLN	2.3
1	A	902	SER	2.2
1	A	698	LEU	2.2
1	B	764	MET	2.2
1	B	804	VAL	2.2
1	A	761	LYS	2.2
1	A	1010	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	724	SER	2.2
1	A	1005	LEU	2.2
1	B	861	TRP	2.2
1	D	739	LEU	2.2
1	B	724	SER	2.2
1	B	1005	LEU	2.2
1	B	686	MET	2.2
1	C	749	PRO	2.2
1	A	702	SER	2.2
1	D	824	THR	2.2
1	A	686	MET	2.2
1	B	1008	ASN	2.2
1	B	958	PRO	2.2
1	A	667	LYS	2.2
1	C	694	GLN	2.2
1	C	912	GLN	2.1
1	B	742	HIS	2.1
1	C	830	ASP	2.1
1	D	685	ALA	2.1
1	D	694	GLN	2.1
1	D	912	GLN	2.1
1	B	795	GLU	2.1
1	C	742	HIS	2.1
1	A	710	TYR	2.1
1	D	731	ASP	2.1
1	A	714	SER	2.1
1	A	688	GLU	2.1
1	B	762	ALA	2.1
1	B	979	VAL	2.1
1	B	738	THR	2.1
1	C	836	ILE	2.1
1	B	913	GLY	2.1
1	A	732	LEU	2.1
1	B	721	SER	2.1
1	A	805	ASP	2.1
1	C	743	ASP	2.1
1	C	771	ILE	2.1
1	D	947	SER	2.1
1	A	718	GLN	2.0
1	D	762	ALA	2.0
1	D	836	ILE	2.0
1	B	963	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	719	ALA	2.0
1	C	766	ASP	2.0
1	D	745	GLY	2.0
1	C	818	VAL	2.0
1	A	820	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

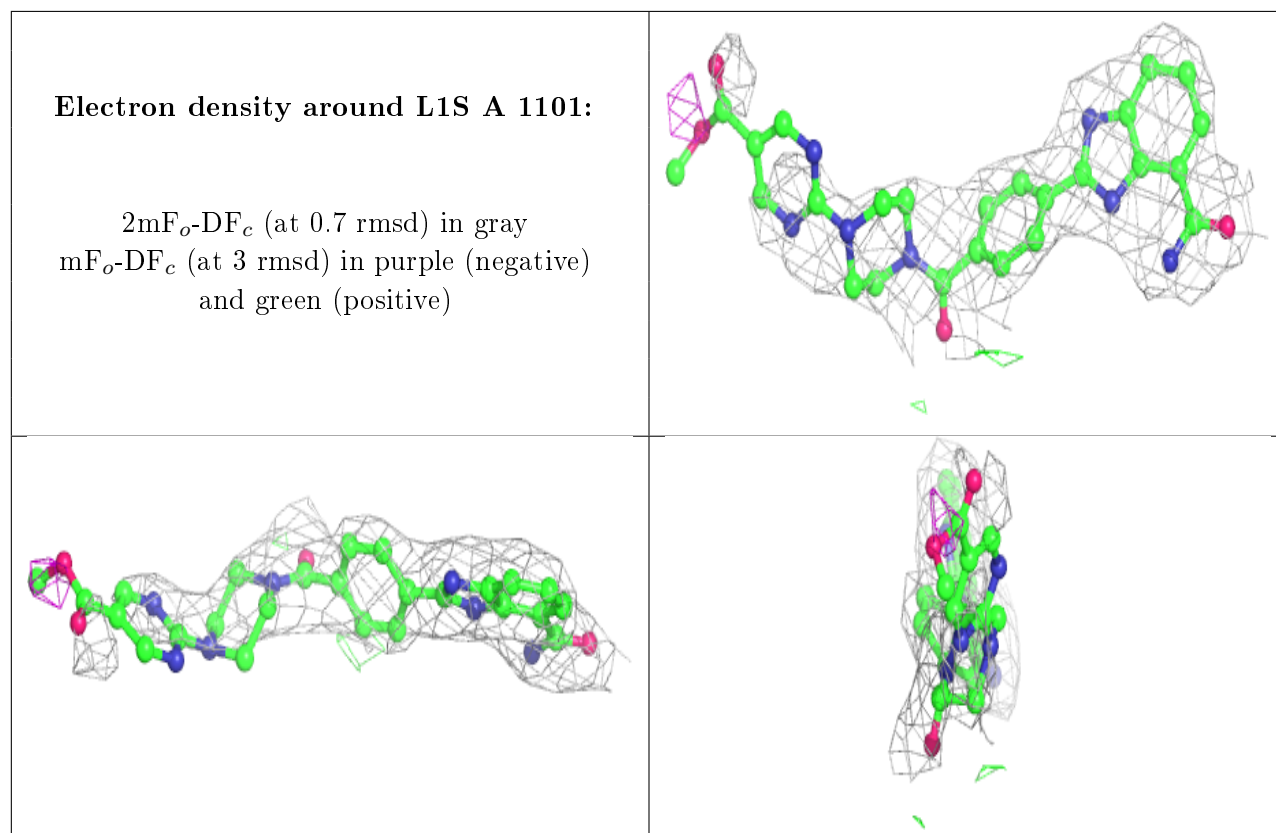
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	SO4	B	1104	5/5	0.86	0.21	87,91,95,99	0
2	L1S	A	1101	36/36	0.86	0.39	50,80,145,156	0
2	L1S	B	1101	36/36	0.87	0.37	65,80,141,153	0
3	SO4	A	1104	5/5	0.89	0.20	91,95,99,103	0
2	L1S	D	1101	36/36	0.89	0.35	54,72,122,130	0
3	SO4	B	1102	5/5	0.90	0.22	91,94,96,100	0
3	SO4	D	1103	5/5	0.91	0.21	78,79,81,92	0
2	L1S	C	1101	36/36	0.91	0.32	46,72,131,134	0
3	SO4	B	1103	5/5	0.91	0.20	73,82,88,88	0
3	SO4	D	1102	5/5	0.92	0.21	82,85,88,90	0
3	SO4	D	1104	5/5	0.92	0.20	91,93,95,96	0
3	SO4	A	1102	5/5	0.92	0.23	90,94,99,101	0
3	SO4	C	1104	5/5	0.93	0.16	79,86,87,88	0
3	SO4	C	1102	5/5	0.93	0.21	78,79,82,83	0
3	SO4	C	1103	5/5	0.94	0.18	77,81,84,88	0
3	SO4	A	1103	5/5	0.95	0.15	87,92,97,100	0

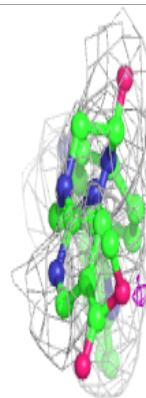
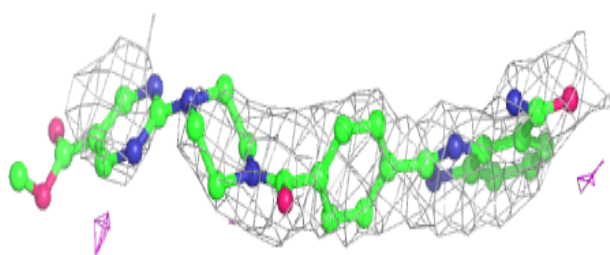
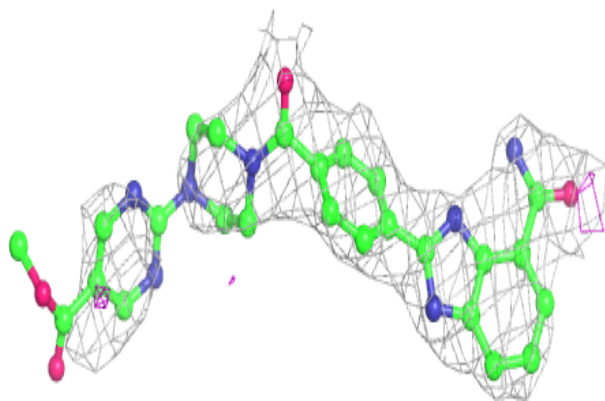
The following is a graphical depiction of the model fit to experimental electron density of all

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.

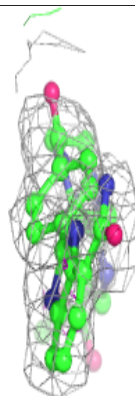
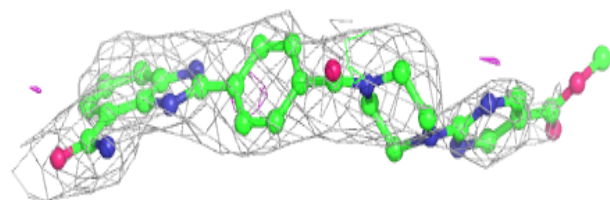
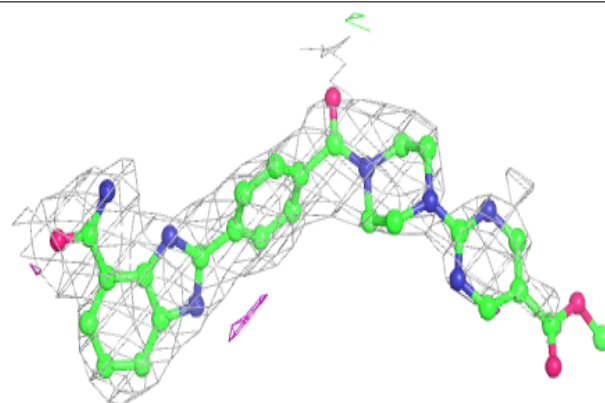


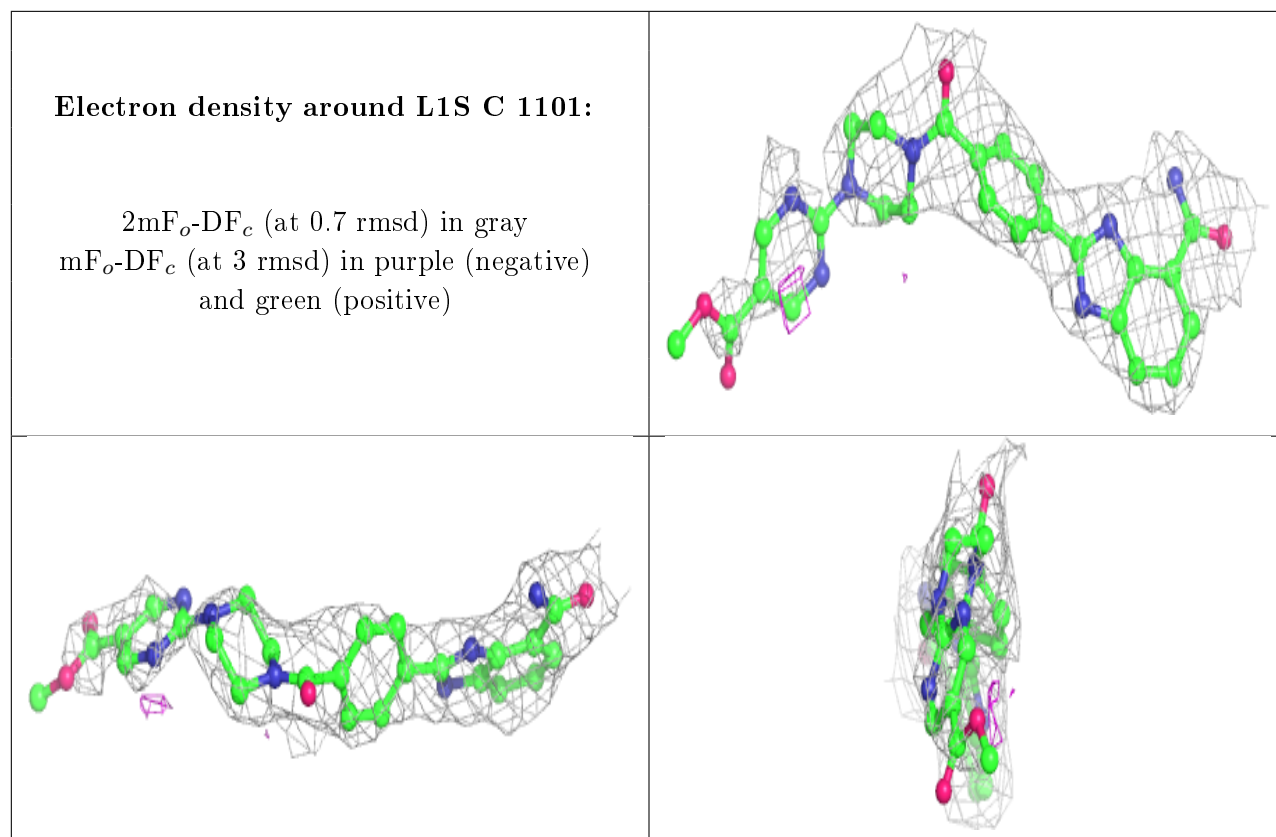
Electron density around LIS B 1101:

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

**Electron density around LIS D 1101:**

$2mF_o-DF_c$ (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.