Full wwPDB X-ray Structure Validation Report (i)

Oct 2, 2019 – 10:24 AM JST

PDB ID	:	6KUZ
Title	:	E.coli beta-galactosidase (E537Q) in complex with fluorescent probe KSL01
Deposited on	:	2019-09-03
Resolution	:	2.83 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

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

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

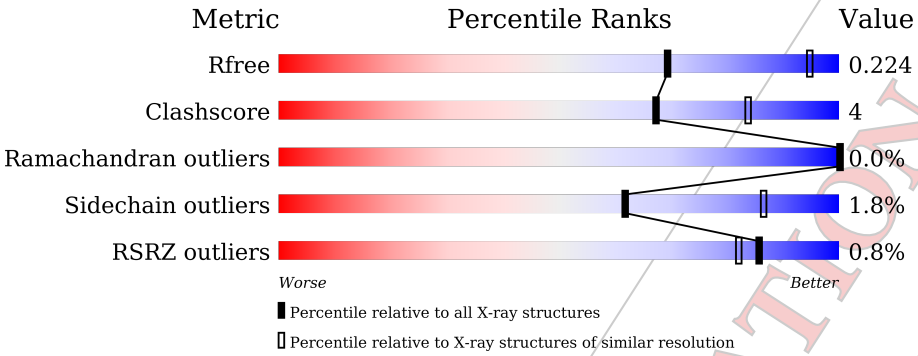
MolProbity	:	4.02b-467
Mogul	:	1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix)	:	1.13
EDS	:	2.5
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.5

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.83 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}	111664	3791 (2.88-2.80)
Clashscore	122126	4261 (2.88-2.80)
Ramachandran outliers	120053	4187 (2.88-2.80)
Sidechain outliers	120020	4190 (2.88-2.80)
RSRZ outliers	108989	3711 (2.88-2.80)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1024	89% 10%
1	B	1024	87% 12%
1	C	1024	90% 9%
1	D	1024	88% 12%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	DVL	A	1101	-	-	-	X
2	DVL	B	1101	-	-	-	X
2	DVL	C	1101	-	-	-	X
2	DVL	D	1101	-	-	-	X

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 33232 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.

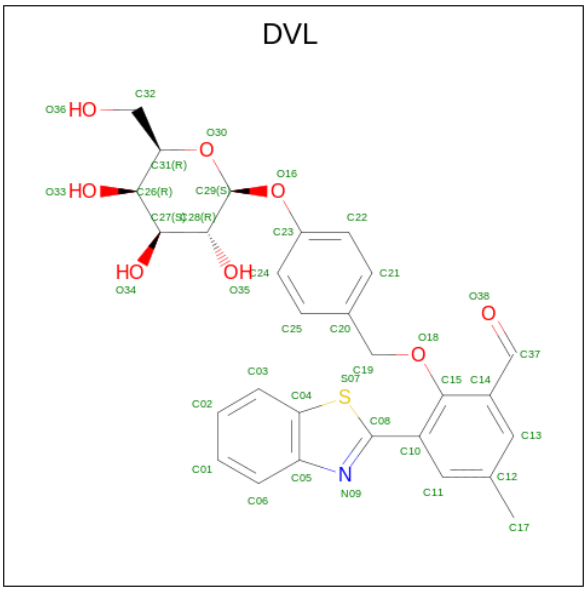
- Molecule 1 is a protein called Beta-galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1021	Total	C	N	O	S	0	3	0
			8164	5167	1446	1513	38			
1	B	1021	Total	C	N	O	S	0	3	0
			8156	5161	1450	1508	37			
1	C	1021	Total	C	N	O	S	0	0	0
			8066	5113	1429	1487	37			
1	D	1020	Total	C	N	O	S	0	0	0
			8071	5115	1432	1487	37			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	537	GLN	GLU	engineered mutation	UNP P00722
B	537	GLN	GLU	engineered mutation	UNP P00722
C	537	GLN	GLU	engineered mutation	UNP P00722
D	537	GLN	GLU	engineered mutation	UNP P00722

- Molecule 2 is 3-(1,3-benzothiazol-2-yl)-2-[[4-[(2 {S},3 {R},4 {S},5 {R},6 {R})-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxyphenyl]methoxy]-5-methyl-benzaldehyde (three-letter code: DVL) (formula: $C_{28}H_{27}NO_8S$) (labeled as "Ligand of Interest" by author).

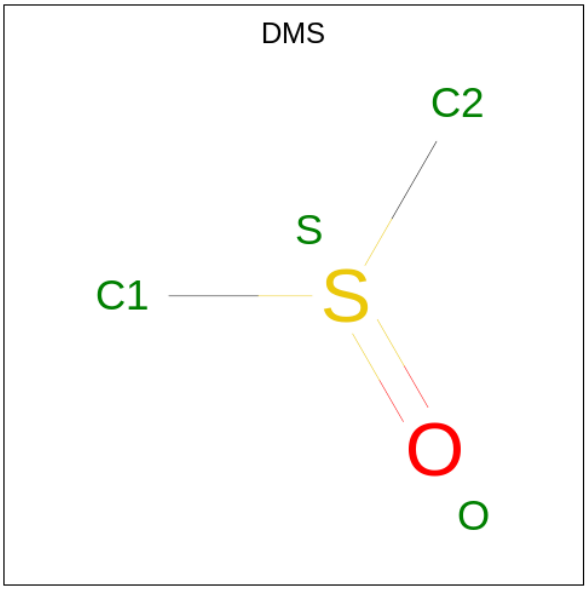


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			38	28	1	8	1		
2	B	1	Total	C	N	O	S	0	0
			38	28	1	8	1		
2	C	1	Total	C	N	O	S	0	0
			38	28	1	8	1		
2	D	1	Total	C	N	O	S	0	0
			38	28	1	8	1		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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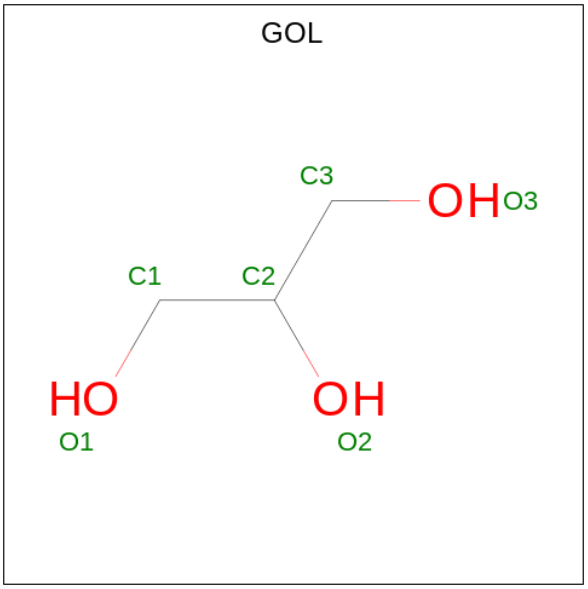
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	B	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4 2 1 1	0	0
4	C	1	Total C O S 4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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total Mg 2 2	0	0
5	A	2	Total Mg 2 2	0	0
5	D	2	Total Mg 2 2	0	0
5	C	2	Total Mg 2 2	0	0

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



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

- Molecule 7 is water.

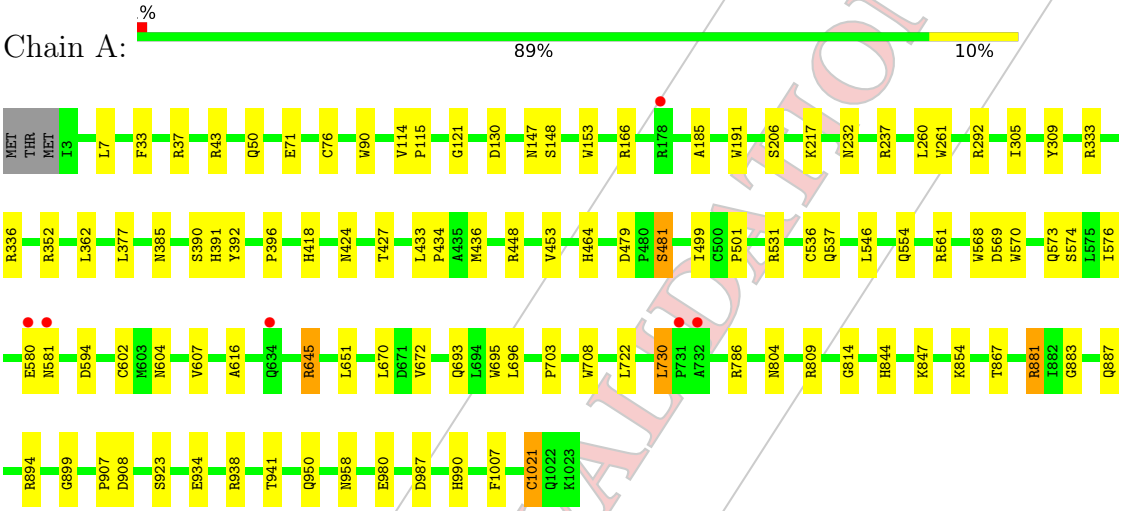
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	132	Total O 132 132	0	0
7	B	121	Total O 121 121	0	0
7	C	91	Total O 91 91	0	0
7	D	113	Total O 113 113	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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 geometryand 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.

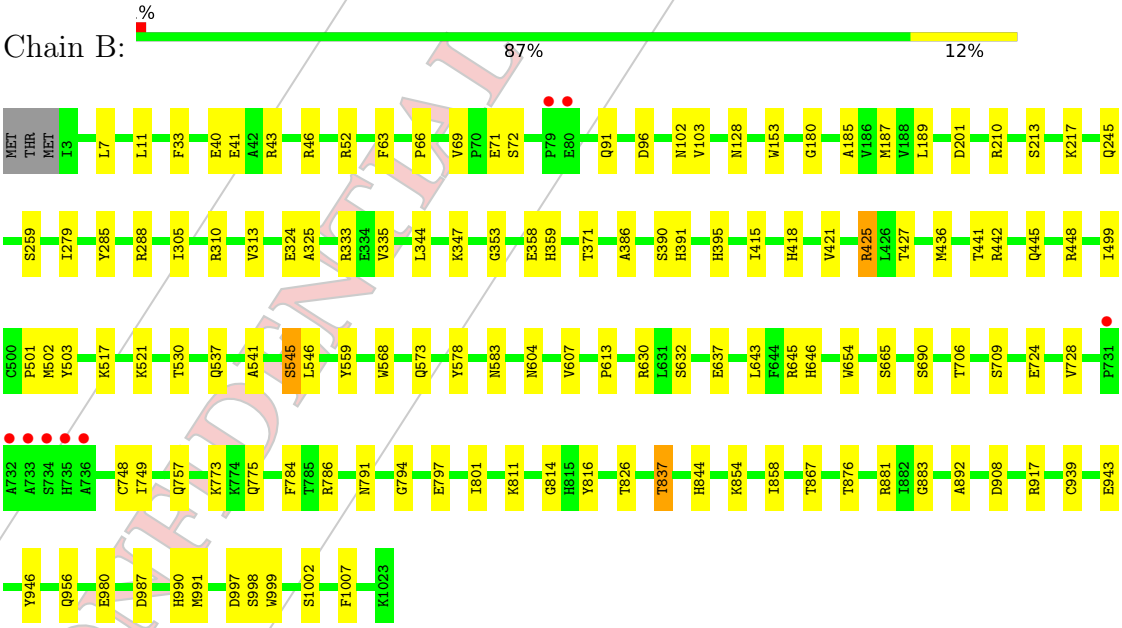
• Molecule 1: Beta-galactosidase

Chain A:



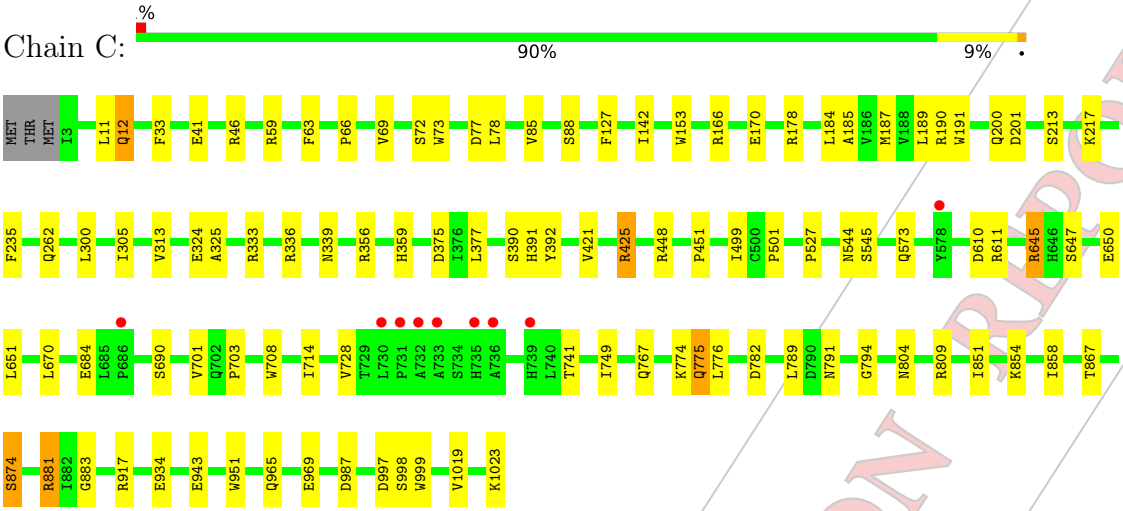
• Molecule 1: Beta-galactosidase

Chain B:



• Molecule 1: Beta-galactosidase

Chain C:



• Molecule 1: Beta-galactosidase

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	248.17Å 85.51Å 243.05Å 90.00° 94.09° 90.00°	Depositor
Resolution (Å)	29.50 – 2.83 29.48 – 2.83	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.50-2.83) 97.0 (29.48-2.83)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 2.85Å)	Xtriage
Refinement program	REFMAC 7.0.076	Depositor
R, R_{free}	0.182 , 0.224 0.185 , 0.224	Depositor DCC
R_{free} test set	5871 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	41.3	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 36.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	33232	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.47% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DVL, MG, DMS, NA, GOL

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	0.62	0/8406	0.72	0/11475
1	B	0.62	0/8396	0.72	0/11459
1	C	0.62	0/8307	0.71	0/11349
1	D	0.62	0/8312	0.72	0/11357
All	All	0.62	0/33421	0.72	0/45640

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	8164	0	7732	59	0
1	B	8156	0	7731	77	0
1	C	8066	0	7609	60	0
1	D	8071	0	7619	71	0
2	A	38	0	0	2	0
2	B	38	0	0	5	0
2	C	38	0	0	2	0
2	D	38	0	0	2	0
3	A	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	52	0	78	1	0
4	B	32	0	48	0	0
4	C	20	0	30	0	0
4	D	36	0	54	1	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
5	C	2	0	0	0	0
5	D	2	0	0	0	0
6	D	6	0	8	0	0
7	A	132	0	0	3	0
7	B	121	0	0	3	0
7	C	91	0	0	1	0
7	D	113	0	0	1	0
All	All	33232	0	30909	266	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 4.

All (266) 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:773:LYS:HE2	1:B:775:GLN:HE22	1.44	0.82
1:B:305:ILE:HD11	1:B:645:ARG:HB3	1.66	0.77
1:A:427:THR:HA	1:A:436:MET:HE1	1.68	0.75
1:B:427:THR:HA	1:B:436:MET:HE1	1.69	0.74
1:B:545:SER:HB2	1:B:791:ASN:HD21	1.53	0.73
1:A:568:TRP:HE1	1:A:604:ASN:HD22	1.35	0.72
1:C:881:ARG:NH2	1:C:934:GLU:OE1	2.24	0.71
1:D:427:THR:HA	1:D:436:MET:HE1	1.72	0.71
1:D:656:VAL:HG21	1:D:685:LEU:HD23	1.72	0.70
1:A:786:ARG:HB2	1:A:934:GLU:HG3	1.73	0.70
1:A:479:ASP:OD1	1:A:481:SER:HB3	1.92	0.70
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.74	0.68
1:A:418:HIS:HE2	2:A:1101:DVL:C13	2.05	0.68
1:B:530:THR:HG22	7:B:1271:HOH:O	1.94	0.67
1:B:630:ARG:NH1	1:B:637:GLU:OE1	2.28	0.66
1:D:568:TRP:HE1	1:D:604:ASN:HD22	1.42	0.66
1:A:934:GLU:OE2	1:A:958:ASN:ND2	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:545:SER:HB2	1:C:791:ASN:HD21	1.61	0.65
1:B:939:CYS:HA	1:B:956:GLN:HG3	1.80	0.64
1:B:749:ILE:HD13	1:B:858:ILE:HD12	1.78	0.64
1:A:362:LEU:HG	1:A:576:ILE:HD12	1.79	0.64
1:B:285:TYR:HB3	1:B:288:ARG:HG3	1.79	0.64
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.80	0.63
1:B:333:ARG:HG3	1:B:333:ARG:HH11	1.64	0.63
1:A:887:GLN:NE2	1:A:980:GLU:O	2.33	0.62
1:B:7:LEU:N	1:B:71:GLU:OE2	2.27	0.62
1:B:537:GLN:NE2	2:B:1101:DVL:O34	2.33	0.62
1:C:1023:LYS:HE2	1:C:1023:LYS:HA	1.82	0.62
1:C:377:LEU:HD22	1:C:708:TRP:HA	1.81	0.61
1:A:377:LEU:HD22	1:A:708:TRP:HA	1.82	0.61
1:C:421:VAL:O	1:C:425:ARG:NH1	2.27	0.61
1:B:153:TRP:HB2	1:B:185:ALA:HB3	1.82	0.61
1:A:580:GLU:HG2	1:A:581:ASN:OD1	2.00	0.60
1:C:153:TRP:HB2	1:C:185:ALA:HB3	1.84	0.60
1:C:881:ARG:NH1	1:C:987:ASP:OD2	2.35	0.59
1:C:544:ASN:HB3	1:C:789:LEU:HD22	1.85	0.59
1:C:41:GLU:OE1	1:C:46:ARG:NH1	2.36	0.58
1:B:568:TRP:HE1	1:B:604:ASN:HD22	1.49	0.58
1:D:745:MET:HE2	1:D:761:GLN:CG	2.34	0.58
1:A:333:ARG:HG3	1:A:333:ARG:HH11	1.68	0.57
1:B:421:VAL:O	1:B:425:ARG:NH1	2.29	0.57
1:C:767:GLN:OE1	1:C:774:LYS:HB3	2.04	0.57
1:A:352:ARG:HB2	1:A:385:ASN:HB2	1.86	0.57
1:B:502:MET:O	1:B:517:LYS:HE3	2.03	0.57
1:A:33:PHE:CD2	1:A:217:LYS:HE3	2.39	0.57
1:A:166:ARG:HG3	1:A:392:TYR:HB2	1.85	0.57
1:C:59:ARG:HD3	1:C:77:ASP:OD2	2.06	0.56
1:D:153:TRP:HB2	1:D:185:ALA:HB3	1.86	0.56
1:B:245:GLN:HG2	1:B:288:ARG:HD3	1.86	0.56
1:D:352:ARG:HB2	1:D:385:ASN:HB2	1.87	0.56
1:D:907:PRO:HG2	1:D:990:HIS:O	2.06	0.56
1:C:33:PHE:CD2	1:C:217:LYS:HE3	2.40	0.56
1:B:41:GLU:OE2	1:B:46:ARG:NH1	2.38	0.56
1:B:607:VAL:HG12	1:B:613:PRO:HA	1.86	0.56
1:B:646:HIS:HB3	7:B:1307:HOH:O	2.06	0.56
1:B:826:THR:HB	1:B:837:THR:HG23	1.88	0.55
1:C:775:GLN:HE21	1:C:775:GLN:HA	1.70	0.55
2:A:1101:DVL:O33	2:A:1101:DVL:O36	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:786:ARG:CB	1:B:881:ARG:HH21	2.20	0.55
1:D:35:SER:OG	1:D:37:ARG:NH1	2.39	0.55
1:B:33:PHE:CD2	1:B:217:LYS:HE3	2.42	0.55
1:D:651:LEU:HD21	1:D:667:GLU:HB3	1.88	0.55
1:C:190:ARG:HD3	1:C:191:TRP:CE2	2.42	0.55
1:D:881:ARG:NH2	1:D:934:GLU:OE1	2.33	0.55
1:A:907:PRO:HG2	1:A:990:HIS:O	2.07	0.54
1:C:190:ARG:HD3	1:C:191:TRP:CZ2	2.42	0.54
1:C:85:VAL:O	1:C:88:SER:HB3	2.07	0.54
1:B:201:ASP:HB3	2:B:1101:DVL:C32	2.38	0.54
1:D:128:ASN:ND2	1:D:180:GLY:HA2	2.22	0.54
1:A:7:LEU:N	1:A:71:GLU:OE2	2.39	0.54
1:D:883:GLY:HA3	1:D:987:ASP:HA	1.90	0.53
2:C:1101:DVL:C19	2:C:1101:DVL:C37	2.86	0.53
1:D:448:ARG:HD3	7:D:1263:HOH:O	2.06	0.53
1:B:279:ILE:HD12	1:B:285:TYR:CE2	2.43	0.53
1:D:262:GLN:HE22	1:D:299:LYS:HD2	1.73	0.53
1:A:580:GLU:HB3	1:D:799:THR:HG22	1.89	0.53
1:D:59:ARG:HB2	1:D:124:SER:OG	2.08	0.53
1:A:424:ASN:ND2	1:A:464:HIS:O	2.36	0.53
1:C:201:ASP:HB3	2:C:1101:DVL:C32	2.39	0.52
1:A:333:ARG:NH2	1:A:453:VAL:O	2.42	0.52
1:B:503:TYR:HH	2:B:1101:DVL:C27	2.23	0.52
1:C:749:ILE:HD13	1:C:858:ILE:HD12	1.91	0.52
1:A:153:TRP:HB2	1:A:185:ALA:HB3	1.91	0.52
1:C:63:PHE:CD2	1:C:69:VAL:HG22	2.45	0.52
1:D:33:PHE:CD2	1:D:217:LYS:HE3	2.44	0.52
1:A:166:ARG:HG3	1:A:392:TYR:CB	2.39	0.51
1:B:210:ARG:NH1	1:B:395:HIS:N	2.59	0.51
1:A:424:ASN:HD21	1:A:464:HIS:C	2.12	0.51
1:B:448:ARG:HG2	1:B:448:ARG:O	2.09	0.51
1:B:773:LYS:HE2	1:B:775:GLN:NE2	2.21	0.51
1:B:854:LYS:HA	1:B:867:THR:O	2.10	0.51
1:D:741:THR:HG23	1:D:748:CYS:HB2	1.92	0.51
1:D:571:VAL:HG23	1:D:607:VAL:HG23	1.91	0.51
1:A:114:VAL:HG13	1:A:115:PRO:HD2	1.92	0.51
1:C:794:GLY:HA2	1:C:998:SER:O	2.10	0.51
1:D:147:ASN:HB3	1:D:206:SER:HA	1.93	0.50
1:B:797:GLU:O	1:B:801:ILE:HD13	2.11	0.50
1:C:187:MET:HE3	1:C:189:LEU:HD11	1.93	0.50
1:A:804:ASN:O	1:A:809:ARG:NH1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:128:ASN:HD21	1:D:180:GLY:HA2	1.76	0.50
1:C:333:ARG:HE	1:C:451:PRO:HA	1.76	0.50
1:B:784:PHE:HA	1:B:881:ARG:O	2.12	0.50
1:D:427:THR:HG21	1:D:462:SER:HB3	1.94	0.50
1:D:418:HIS:HE2	2:D:1101:DVL:C13	2.26	0.49
1:C:883:GLY:HA3	1:C:987:ASP:HA	1.94	0.49
1:A:883:GLY:HA3	1:A:987:ASP:HA	1.93	0.49
1:D:217:LYS:NZ	1:D:324:GLU:OE1	2.46	0.49
1:A:43:ARG:HD2	1:A:261:TRP:CD2	2.48	0.49
1:D:658:LEU:HD23	1:D:694:LEU:HD13	1.94	0.49
1:A:847:LYS:NZ	1:B:724:GLU:O	2.46	0.49
4:A:1115:DMS:H12	7:A:1275:HOH:O	2.13	0.49
1:B:210:ARG:NH1	1:B:358:GLU:OE1	2.46	0.49
1:A:693:GLN:NE2	1:A:695:TRP:HE1	2.10	0.48
1:B:442[B]:ARG:NH1	7:B:1206:HOH:O	2.45	0.48
1:B:63:PHE:CD2	1:B:69:VAL:HG22	2.49	0.48
1:C:333:ARG:HH21	1:C:333:ARG:HG3	1.78	0.48
1:D:166:ARG:HG3	1:D:392:TYR:HB2	1.95	0.48
1:B:499:ILE:HG22	1:B:501:PRO:HD3	1.94	0.48
1:B:892:ALA:HB3	1:B:946:TYR:CE1	2.48	0.48
1:C:333:ARG:HG3	1:C:333:ARG:NH2	2.29	0.48
1:D:745:MET:CE	1:D:761:GLN:CG	2.91	0.48
1:D:745:MET:HE2	1:D:761:GLN:HG3	1.95	0.48
1:B:541:ALA:HA	1:B:545:SER:OG	2.13	0.48
1:D:262:GLN:O	1:D:262:GLN:HG3	2.14	0.48
1:B:333:ARG:NH1	1:B:333:ARG:HG3	2.25	0.47
1:A:499:ILE:HG22	1:A:501:PRO:HD3	1.96	0.47
1:C:854:LYS:HA	1:C:867:THR:O	2.14	0.47
1:A:147:ASN:HA	1:A:148:SER:HA	1.64	0.47
1:A:574:SER:HB3	7:A:1304:HOH:O	2.15	0.47
1:A:899:GLY:HA3	1:A:941:THR:HG22	1.97	0.47
1:B:917:ARG:NH2	1:B:943:GLU:OE1	2.48	0.47
1:C:142:ILE:HG23	1:C:170:GLU:HG2	1.96	0.47
1:C:645:ARG:NH2	1:C:650:GLU:OE1	2.48	0.47
1:D:59:ARG:HD3	1:D:77:ASP:OD1	2.16	0.46
1:A:147:ASN:HB3	1:A:206:SER:HA	1.98	0.46
1:D:313:VAL:O	1:D:325:ALA:HA	2.16	0.46
1:C:305:ILE:HD11	1:C:645:ARG:HB3	1.96	0.46
2:B:1101:DVL:C28	2:B:1101:DVL:C24	2.91	0.46
1:D:952:ARG:HB2	1:D:1019:VAL:HG23	1.98	0.46
1:D:991:MET:HG2	1:D:992:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:HG22	1:B:344:LEU:HD12	1.98	0.46
1:C:651:LEU:HD23	1:C:703:PRO:HG3	1.96	0.46
1:A:651:LEU:HG	1:A:703:PRO:HG3	1.96	0.46
1:B:40:GLU:OE2	1:B:43:ARG:NE	2.38	0.46
1:D:471:LEU:O	1:D:475:ILE:HG13	2.16	0.46
1:D:665:SER:OG	1:D:666:GLY:N	2.49	0.45
1:B:102:ASN:HA	1:B:201:ASP:OD1	2.15	0.45
1:B:390:SER:HA	1:B:391:HIS:HA	1.72	0.45
1:B:441:THR:O	1:B:445:GLN:HG3	2.16	0.45
1:B:43:ARG:O	1:B:310:ARG:HD2	2.16	0.45
1:C:804:ASN:O	1:C:809:ARG:NH1	2.50	0.45
1:D:568:TRP:CD2	1:D:569:ASP:HB3	2.52	0.45
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.98	0.45
2:D:1101:DVL:C37	2:D:1101:DVL:C19	2.94	0.45
1:D:749:ILE:O	1:D:755:ARG:HA	2.16	0.45
1:A:396:PRO:HG3	7:A:1210:HOH:O	2.17	0.45
1:D:479:ASP:OD2	1:D:482:ARG:NH1	2.49	0.45
1:D:745:MET:CE	1:D:761:GLN:CD	2.85	0.45
1:B:883:GLY:HA3	1:B:987:ASP:HA	1.99	0.44
1:C:917:ARG:NH2	1:C:943:GLU:OE1	2.50	0.44
1:B:908:ASP:HB3	1:B:1007:PHE:CD2	2.53	0.44
1:D:336:ARG:HD3	1:D:338:GLU:OE2	2.18	0.44
1:C:313:VAL:O	1:C:325:ALA:HA	2.17	0.44
1:C:670:LEU:HA	1:C:670:LEU:HD23	1.87	0.44
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.53	0.44
1:A:37:ARG:NH1	1:A:50:GLN:HG2	2.32	0.44
2:B:1101:DVL:C37	2:B:1101:DVL:C19	2.96	0.44
1:C:235:PHE:HB3	1:C:300:LEU:HD11	2.00	0.44
1:A:854:LYS:HA	1:A:867:THR:O	2.18	0.44
1:B:814:GLY:HA3	1:B:844:HIS:CG	2.53	0.44
1:C:12:GLN:HB3	1:C:12:GLN:HE21	1.65	0.44
1:A:568:TRP:CD2	1:A:569:ASP:HB3	2.52	0.44
1:D:354:VAL:HB	1:D:384:PHE:CE1	2.52	0.44
1:A:390:SER:HA	1:A:391:HIS:HA	1.82	0.44
1:C:527:PRO:HB3	1:D:339:ASN:O	2.18	0.44
1:D:573:GLN:HB2	1:D:602:CYS:O	2.17	0.44
1:B:545:SER:HB2	1:B:791:ASN:ND2	2.29	0.43
1:B:347:LYS:HB3	1:B:643:LEU:HD22	2.00	0.43
1:B:728:VAL:HG12	1:B:728:VAL:O	2.18	0.43
1:B:359:HIS:CD2	1:B:573:GLN:HA	2.53	0.43
1:D:854:LYS:HA	1:D:867:THR:O	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:PHE:CE1	1:C:184:LEU:HG	2.53	0.43
1:D:706:THR:OG1	1:D:709:SER:HB3	2.17	0.43
1:B:421:VAL:O	1:B:425:ARG:HD2	2.17	0.43
1:B:990:HIS:HD2	1:B:991:MET:O	2.01	0.43
1:D:424:ASN:HD21	1:D:464:HIS:C	2.21	0.43
1:B:786:ARG:HA	1:B:881:ARG:HH21	1.83	0.43
1:B:427:THR:HA	1:B:436:MET:CE	2.46	0.43
1:C:200:GLN:HG2	1:C:391:HIS:HB2	2.01	0.43
1:C:166:ARG:HG3	1:C:392:TYR:HB2	2.01	0.43
1:C:356:ARG:NH1	1:C:375:ASP:OD2	2.50	0.43
1:D:499:ILE:HG22	1:D:501:PRO:HD3	2.01	0.43
1:B:187:MET:HE3	1:B:189:LEU:HD21	2.00	0.42
1:D:305:ILE:HD11	1:D:645:ARG:HB3	2.01	0.42
1:B:313:VAL:O	1:B:325:ALA:HA	2.20	0.42
1:B:578:TYR:HA	1:B:583:ASN:O	2.18	0.42
1:A:670:LEU:HD23	1:A:670:LEU:HA	1.85	0.42
1:D:433:LEU:HB3	1:D:434:PRO:HD3	2.02	0.42
1:D:414:ASN:O	1:D:439:ARG:HD3	2.18	0.42
1:C:610:ASP:O	1:C:611:ARG:HB2	2.19	0.42
1:C:701:VAL:HG22	1:C:714:ILE:HG12	2.02	0.42
1:D:457:SER:HA	1:D:485:GLN:O	2.20	0.42
1:D:691:ALA:HA	1:D:725:ASN:HB2	2.01	0.42
1:A:114:VAL:CG1	1:A:191:TRP:HB2	2.50	0.42
1:B:103:VAL:HG22	1:B:418:HIS:CE1	2.55	0.42
1:D:200:GLN:HG2	1:D:391:HIS:HB2	2.01	0.42
1:C:339:ASN:O	1:D:527:PRO:HB3	2.19	0.42
1:A:90:TRP:CZ3	1:A:121:GLY:HA3	2.55	0.42
1:A:232:ASN:ND2	1:A:237:ARG:HB2	2.35	0.42
1:B:279:ILE:HD12	1:B:285:TYR:CD2	2.55	0.42
1:D:424:ASN:ND2	1:D:464:HIS:O	2.47	0.42
1:A:433:LEU:HB3	1:A:434:PRO:HD3	2.02	0.42
1:A:950:GLN:HB3	1:A:1021:CYS:HB3	2.02	0.42
1:B:545:SER:OG	1:B:546:LEU:N	2.52	0.42
1:B:654:TRP:CZ2	1:B:665:SER:O	2.73	0.42
1:D:896:ASN:HB3	1:D:945:ASN:HB2	2.02	0.42
1:D:619:GLU:HA	1:D:912:ALA:HB2	2.02	0.42
1:A:696:LEU:HB2	1:A:722:LEU:HD11	2.02	0.42
1:A:730:LEU:H	1:A:730:LEU:HD23	1.85	0.42
1:C:951:TRP:HA	1:C:1019:VAL:O	2.19	0.42
1:C:390:SER:HA	1:C:391:HIS:HA	1.75	0.42
1:B:794:GLY:HA2	1:B:998:SER:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:965:GLN:O	1:C:969:GLU:HG2	2.20	0.41
1:A:881:ARG:HD3	1:A:987:ASP:OD1	2.20	0.41
1:A:573:GLN:HB2	1:A:602:CYS:O	2.21	0.41
1:B:997:ASP:HB2	1:B:999:TRP:CE2	2.55	0.41
1:C:881:ARG:HD3	1:C:987:ASP:OD1	2.21	0.41
1:A:814:GLY:HA3	1:A:844:HIS:CG	2.55	0.41
1:B:217:LYS:NZ	1:B:324:GLU:OE1	2.53	0.41
1:B:128:ASN:HA	1:B:180:GLY:O	2.21	0.41
1:C:874:SER:HB3	1:D:724:GLU:HB2	2.03	0.41
1:C:775:GLN:O	1:C:776:LEU:HD23	2.21	0.41
1:C:851:ILE:HD11	1:D:726:LEU:HB3	2.02	0.41
1:C:997:ASP:HB2	1:C:999:TRP:CE2	2.55	0.41
1:D:138:GLN:HE22	1:D:140:ARG:HE	1.69	0.41
1:D:499:ILE:O	1:D:533:LEU:HA	2.21	0.41
1:D:621:LYS:HE2	1:D:717:TRP:HZ3	1.86	0.41
1:A:531:ARG:O	1:A:561:ARG:NH1	2.48	0.41
1:B:521:LYS:HD3	1:B:559:TYR:CE1	2.55	0.41
1:B:706:THR:OG1	1:B:709:SER:N	2.54	0.41
1:C:12:GLN:NE2	7:C:1206:HOH:O	2.48	0.41
1:D:568:TRP:CG	1:D:569:ASP:HB3	2.56	0.41
1:A:908:ASP:HB3	1:A:1007:PHE:CD2	2.56	0.41
1:A:536:CYS:O	1:A:537:GLN:HG3	2.20	0.41
1:B:415:ILE:HD13	1:B:436:MET:HG2	2.03	0.41
1:B:811:LYS:HG2	1:B:816:TYR:CD2	2.56	0.41
1:C:359:HIS:CD2	1:C:573:GLN:HA	2.56	0.41
1:A:570:TRP:O	1:A:607:VAL:HG22	2.20	0.41
1:C:11:LEU:HD13	1:C:66:PRO:HB2	2.02	0.41
1:C:217:LYS:NZ	1:C:324:GLU:OE1	2.54	0.41
1:D:289:VAL:HG23	4:D:1108:DMS:H23	2.02	0.41
1:A:568:TRP:HA	1:A:569:ASP:HA	1.89	0.41
1:A:546:LEU:HD22	1:A:616:ALA:HB1	2.03	0.41
1:C:73:TRP:HB2	1:C:78:LEU:HD21	2.03	0.41
1:B:748:CYS:SG	1:B:757:GLN:HG3	2.61	0.40
1:D:787:ALA:HA	1:D:788:PRO:HD3	1.96	0.40
1:A:260:LEU:HD11	1:A:309:TYR:HB3	2.02	0.40
1:A:333:ARG:NH1	1:A:333:ARG:HG3	2.35	0.40
1:D:696:LEU:HB2	1:D:722:LEU:HD11	2.02	0.40
1:D:337:ILE:HA	1:D:341:LEU:O	2.21	0.40
1:B:11:LEU:HD13	1:B:66:PRO:HB2	2.03	0.40
1:B:353:GLY:HA2	1:B:386:ALA:O	2.22	0.40
1:B:91:GLN:HG3	1:B:96:ASP:OD1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1011:ALA:HB3	1:D:1014:TYR:CZ	2.57	0.40
1:D:645:ARG:NH2	1:D:650:GLU:OE2	2.53	0.40
1:C:728:VAL:HG12	1:D:851:ILE:HD11	2.03	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	1022/1024 (100%)	983 (96%)	39 (4%)	0	100	100
1	B	1022/1024 (100%)	983 (96%)	39 (4%)	0	100	100
1	C	1019/1024 (100%)	974 (96%)	44 (4%)	1 (0%)	53	82
1	D	1018/1024 (99%)	978 (96%)	40 (4%)	0	100	100
All	All	4081/4096 (100%)	3918 (96%)	162 (4%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	684	GLU

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	863/876 (98%)	847 (98%)	16 (2%)	60	85
1	B	859/876 (98%)	846 (98%)	13 (2%)	67	89
1	C	842/876 (96%)	826 (98%)	16 (2%)	60	85
1	D	844/876 (96%)	828 (98%)	16 (2%)	60	85
All	All	3408/3504 (97%)	3347 (98%)	61 (2%)	62	86

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	CYS
1	A	130	ASP
1	A	292	ARG
1	A	336	ARG
1	A	448	ARG
1	A	481	SER
1	A	554	GLN
1	A	594	ASP
1	A	645	ARG
1	A	672	VAL
1	A	730	LEU
1	A	881	ARG
1	A	894	ARG
1	A	923	SER
1	A	938	ARG
1	A	1021	CYS
1	B	52	ARG
1	B	72	SER
1	B	213	SER
1	B	259	SER
1	B	371	THR
1	B	425	ARG
1	B	545	SER
1	B	632	SER
1	B	690	SER
1	B	837	THR
1	B	876	THR
1	B	980	GLU
1	B	1002	SER
1	C	12	GLN
1	C	72	SER
1	C	178	ARG
1	C	213	SER

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Mol	Chain	Res	Type
1	C	262	GLN
1	C	336	ARG
1	C	425	ARG
1	C	448	ARG
1	C	645	ARG
1	C	647	SER
1	C	690	SER
1	C	741	THR
1	C	775	GLN
1	C	782	ASP
1	C	874	SER
1	C	881	ARG
1	D	40	GLU
1	D	72	SER
1	D	138	GLN
1	D	333	ARG
1	D	394	ASN
1	D	448	ARG
1	D	519	SER
1	D	581	ASN
1	D	618	THR
1	D	645	ARG
1	D	647	SER
1	D	665	SER
1	D	690	SER
1	D	745	MET
1	D	859	ASP
1	D	923	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	693	GLN
1	A	761	GLN
1	B	221	GLN
1	B	653	HIS
1	B	775	GLN
1	B	791	ASN
1	B	1022	GLN
1	C	12	GLN
1	C	445	GLN
1	C	775	GLN

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Mol	Chain	Res	Type
1	C	903	GLN
1	C	1017	GLN
1	D	128	ASN
1	D	262	GLN
1	D	424	ASN
1	D	757	GLN
1	D	896	ASN
1	D	1017	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 60 ligands modelled in this entry, 20 are monoatomic - leaving 40 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	$\#\|Z\| > 2$
2	DVL	A	1101	3	40,42,42	1.11	2 (5%)	52,60,60	1.73	13 (25%)
4	DMS	A	1105	3	3,3,3	0.41	0	3,3,3	0.15	0
4	DMS	A	1106	-	3,3,3	0.38	0	3,3,3	0.17	0
4	DMS	A	1107	-	3,3,3	0.43	0	3,3,3	0.10	0
4	DMS	A	1108	-	3,3,3	0.36	0	3,3,3	0.14	0
4	DMS	A	1109	-	3,3,3	0.39	0	3,3,3	0.25	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	DMS	A	1110	-	3,3,3	0.25	0	3,3,3	0.30	0
4	DMS	A	1111	-	3,3,3	0.40	0	3,3,3	0.24	0
4	DMS	A	1112	-	3,3,3	0.29	0	3,3,3	0.17	0
4	DMS	A	1113	-	3,3,3	0.37	0	3,3,3	0.05	0
4	DMS	A	1114	-	3,3,3	0.30	0	3,3,3	0.24	0
4	DMS	A	1115	-	3,3,3	0.35	0	3,3,3	0.37	0
4	DMS	A	1116	-	3,3,3	0.36	0	3,3,3	0.21	0
4	DMS	A	1117	-	3,3,3	0.38	0	3,3,3	0.11	0
2	DVL	B	1101	5	40,42,42	1.22	3 (7%)	52,60,60	1.90	14 (26%)
4	DMS	B	1105	-	3,3,3	0.41	0	3,3,3	0.12	0
4	DMS	B	1106	-	3,3,3	0.53	0	3,3,3	0.27	0
4	DMS	B	1107	-	3,3,3	0.38	0	3,3,3	0.20	0
4	DMS	B	1108	-	3,3,3	0.45	0	3,3,3	0.39	0
4	DMS	B	1109	-	3,3,3	0.36	0	3,3,3	0.05	0
4	DMS	B	1110	-	3,3,3	0.38	0	3,3,3	0.12	0
4	DMS	B	1111	-	3,3,3	0.40	0	3,3,3	0.06	0
4	DMS	B	1112	-	3,3,3	0.40	0	3,3,3	0.07	0
2	DVL	C	1101	3,5	40,42,42	1.25	3 (7%)	52,60,60	2.18	18 (34%)
4	DMS	C	1105	-	3,3,3	0.42	0	3,3,3	0.05	0
4	DMS	C	1106	-	3,3,3	0.45	0	3,3,3	0.14	0
4	DMS	C	1107	-	3,3,3	0.28	0	3,3,3	0.24	0
4	DMS	C	1108	-	3,3,3	0.34	0	3,3,3	0.08	0
4	DMS	C	1109	-	3,3,3	0.34	0	3,3,3	0.13	0
2	DVL	D	1101	3	40,42,42	1.14	1 (2%)	52,60,60	1.82	12 (23%)
4	DMS	D	1105	-	3,3,3	0.42	0	3,3,3	0.14	0
4	DMS	D	1106	-	3,3,3	0.37	0	3,3,3	0.24	0
4	DMS	D	1107	-	3,3,3	0.34	0	3,3,3	0.06	0
4	DMS	D	1108	-	3,3,3	0.34	0	3,3,3	0.22	0
4	DMS	D	1109	-	3,3,3	0.45	0	3,3,3	0.10	0
4	DMS	D	1110	-	3,3,3	0.38	0	3,3,3	0.12	0
4	DMS	D	1111	-	3,3,3	0.36	0	3,3,3	0.18	0
4	DMS	D	1112	-	3,3,3	0.38	0	3,3,3	0.15	0
4	DMS	D	1113	-	3,3,3	0.19	0	3,3,3	0.18	0
6	GOL	D	1114	-	5,5,5	0.13	0	5,5,5	0.35	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	DVL	A	1101	3	-	7/15/37/37	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	DVL	B	1101	5	-	8/15/37/37	0/5/5/5
2	DVL	C	1101	3,5	-	9/15/37/37	0/5/5/5
2	DVL	D	1101	3	-	7/15/37/37	0/5/5/5
6	GOL	D	1114	-	-	0/4/4/4	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	DVL	C14-C37	-4.57	1.36	1.47
2	D	1101	DVL	C14-C37	-4.53	1.36	1.47
2	C	1101	DVL	C14-C37	-4.48	1.36	1.47
2	A	1101	DVL	C14-C37	-4.25	1.37	1.47
2	C	1101	DVL	O16-C29	3.05	1.45	1.41
2	A	1101	DVL	C02-C03	2.27	1.41	1.36
2	B	1101	DVL	C02-C03	2.18	1.41	1.36
2	C	1101	DVL	C02-C03	2.11	1.41	1.36
2	B	1101	DVL	O16-C29	2.04	1.44	1.41

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1101	DVL	O16-C29-C28	6.25	116.26	107.17
2	D	1101	DVL	C28-C27-C26	5.15	119.86	110.82
2	C	1101	DVL	O18-C19-C20	5.01	123.99	109.16
2	C	1101	DVL	C23-O16-C29	4.90	124.98	117.80
2	B	1101	DVL	O18-C19-C20	4.43	122.26	109.16
2	A	1101	DVL	O18-C19-C20	4.41	122.21	109.16
2	C	1101	DVL	O30-C31-C32	4.20	116.90	106.43
2	C	1101	DVL	C08-N09-C05	4.04	111.79	103.78
2	B	1101	DVL	C28-C27-C26	4.00	117.84	110.82
2	B	1101	DVL	C08-N09-C05	3.96	111.62	103.78
2	A	1101	DVL	C08-N09-C05	3.75	111.21	103.78
2	C	1101	DVL	C13-C14-C37	-3.74	111.52	119.02
2	A	1101	DVL	C28-C27-C26	3.71	117.34	110.82
2	B	1101	DVL	O18-C15-C14	3.67	124.16	119.09
2	D	1101	DVL	C08-N09-C05	3.66	111.03	103.78
2	D	1101	DVL	O30-C31-C32	3.63	115.48	106.43
2	B	1101	DVL	C29-C28-C27	3.62	117.53	109.98
2	D	1101	DVL	O18-C19-C20	3.59	119.78	109.16
2	D	1101	DVL	C13-C14-C37	-3.58	111.85	119.02
2	B	1101	DVL	O16-C29-C28	3.52	112.29	107.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1101	DVL	O30-C31-C32	3.46	115.06	106.43
2	D	1101	DVL	O16-C29-C28	3.40	112.11	107.17
2	A	1101	DVL	O30-C31-C32	3.26	114.56	106.43
2	A	1101	DVL	C19-O18-C15	3.19	123.50	113.96
2	A	1101	DVL	O16-C29-C28	3.17	111.77	107.17
2	B	1101	DVL	C19-O18-C15	3.12	123.28	113.96
2	C	1101	DVL	C15-C14-C37	3.07	128.50	120.38
2	C	1101	DVL	O30-C31-C26	-2.96	104.29	109.68
2	B	1101	DVL	C04-C05-N09	2.95	114.90	108.04
2	D	1101	DVL	C15-C14-C37	2.89	128.03	120.38
2	D	1101	DVL	C04-C05-N09	2.88	114.74	108.04
2	C	1101	DVL	O18-C15-C14	2.87	123.05	119.09
2	A	1101	DVL	C32-C31-C26	-2.81	106.41	113.00
2	C	1101	DVL	C04-C05-N09	2.80	114.55	108.04
2	D	1101	DVL	O34-C27-C26	-2.79	103.86	110.34
2	A	1101	DVL	C04-C05-N09	2.79	114.53	108.04
2	D	1101	DVL	O18-C15-C14	2.77	122.90	119.09
2	B	1101	DVL	C05-C04-S07	-2.74	108.51	112.00
2	C	1101	DVL	C29-C28-C27	2.69	115.60	109.98
2	C	1101	DVL	C19-C20-C21	2.62	126.85	120.66
2	B	1101	DVL	C13-C14-C37	-2.62	113.78	119.02
2	C	1101	DVL	O30-C29-O16	2.57	114.61	108.37
2	C	1101	DVL	C05-C04-S07	-2.53	108.77	112.00
2	A	1101	DVL	O30-C29-O16	2.46	114.33	108.37
2	A	1101	DVL	C23-O16-C29	2.42	121.34	117.80
2	B	1101	DVL	O34-C27-C28	-2.38	104.83	110.34
2	A	1101	DVL	C29-C28-C27	2.37	114.94	109.98
2	B	1101	DVL	C15-C14-C37	2.36	126.62	120.38
2	D	1101	DVL	C05-C04-S07	-2.33	109.03	112.00
2	D	1101	DVL	C29-C28-C27	2.19	114.56	109.98
2	A	1101	DVL	C05-C04-S07	-2.14	109.27	112.00
2	C	1101	DVL	C28-C27-C26	2.14	114.58	110.82
2	B	1101	DVL	C19-C20-C25	-2.08	115.73	120.66
2	C	1101	DVL	C11-C12-C13	2.06	120.58	118.09
2	A	1101	DVL	C19-C20-C21	2.05	125.50	120.66
2	C	1101	DVL	C19-C20-C25	-2.05	115.82	120.66
2	C	1101	DVL	O35-C28-C27	-2.03	105.64	110.34

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1101	DVL	N09-C08-C10-C11
2	C	1101	DVL	C15-C14-C37-O38
2	C	1101	DVL	C28-C29-O16-C23
2	B	1101	DVL	N09-C08-C10-C11
2	B	1101	DVL	S07-C08-C10-C11
2	B	1101	DVL	C15-C14-C37-O38
2	B	1101	DVL	C28-C29-O16-C23
2	D	1101	DVL	N09-C08-C10-C11
2	D	1101	DVL	C15-C14-C37-O38
2	D	1101	DVL	C28-C29-O16-C23
2	A	1101	DVL	S07-C08-C10-C11
2	A	1101	DVL	C15-C14-C37-O38
2	A	1101	DVL	C28-C29-O16-C23
2	A	1101	DVL	C20-C19-O18-C15
2	C	1101	DVL	C13-C14-C37-O38
2	B	1101	DVL	C13-C14-C37-O38
2	D	1101	DVL	C13-C14-C37-O38
2	A	1101	DVL	C13-C14-C37-O38
2	C	1101	DVL	C14-C15-O18-C19
2	B	1101	DVL	C14-C15-O18-C19
2	C	1101	DVL	C10-C15-O18-C19
2	D	1101	DVL	C14-C15-O18-C19
2	B	1101	DVL	C10-C15-O18-C19
2	C	1101	DVL	O30-C31-C32-O36
2	C	1101	DVL	C26-C31-C32-O36
2	D	1101	DVL	C10-C15-O18-C19
2	A	1101	DVL	C14-C15-O18-C19
2	B	1101	DVL	C20-C19-O18-C15
2	D	1101	DVL	C20-C19-O18-C15
2	A	1101	DVL	C10-C15-O18-C19
2	C	1101	DVL	C20-C19-O18-C15

There are no ring outliers.

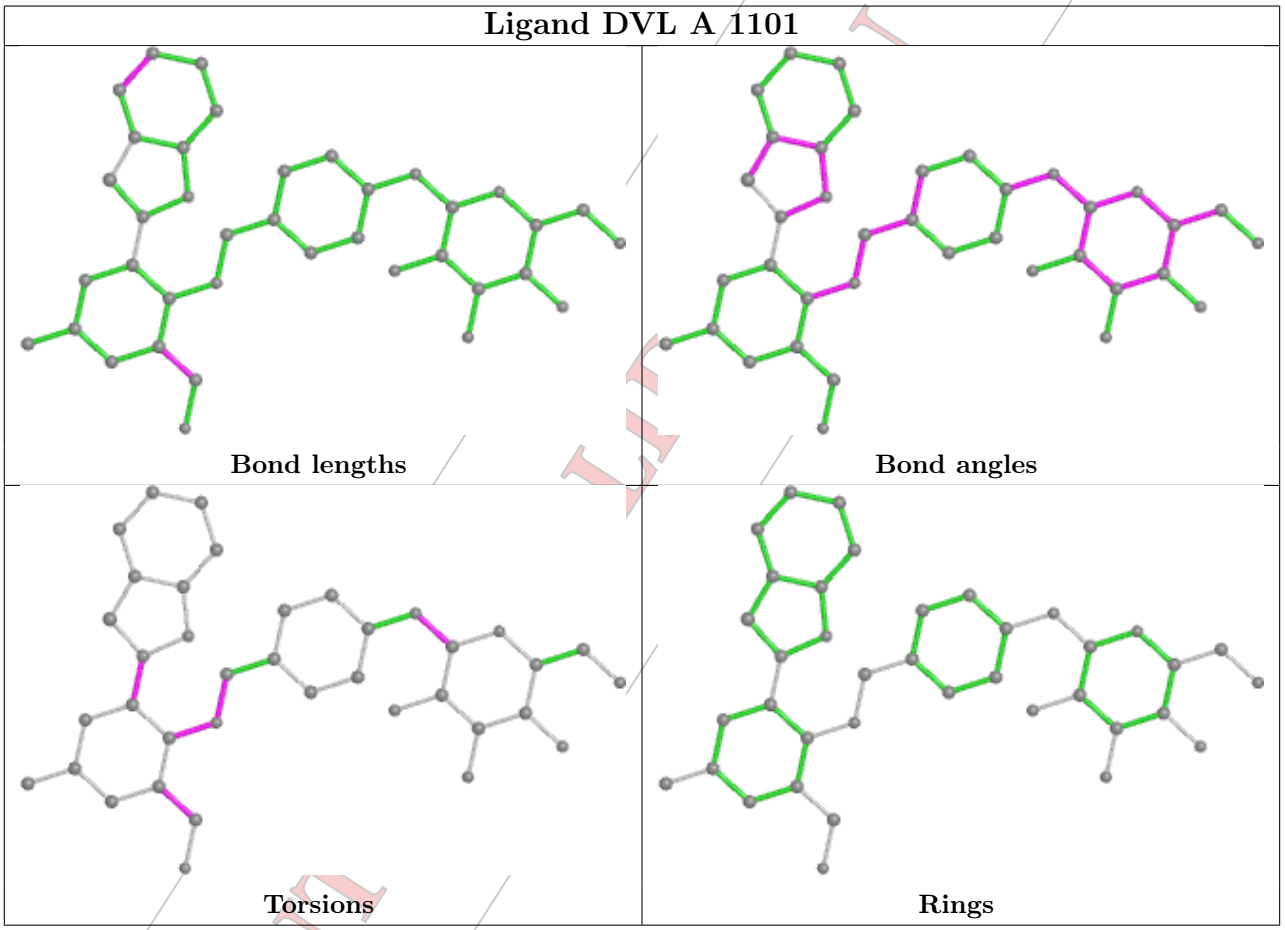
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1101	DVL	2	0
2	B	1101	DVL	5	0
2	C	1101	DVL	2	0
2	D	1101	DVL	2	0

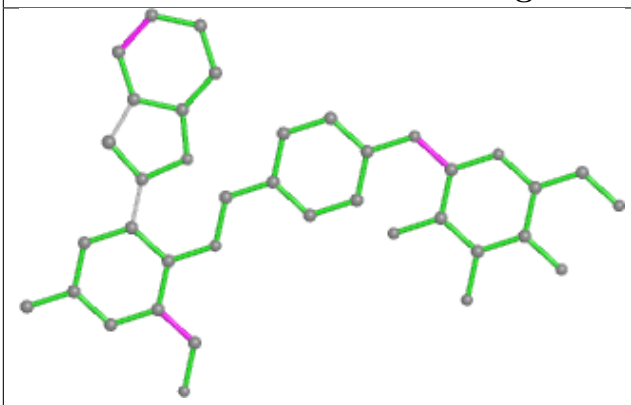
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

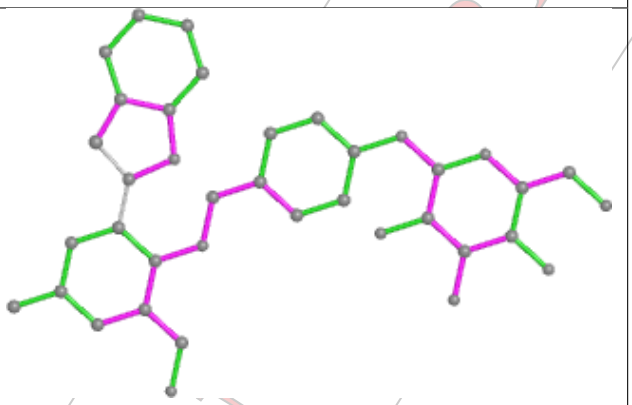
Ligand DVL A 1101



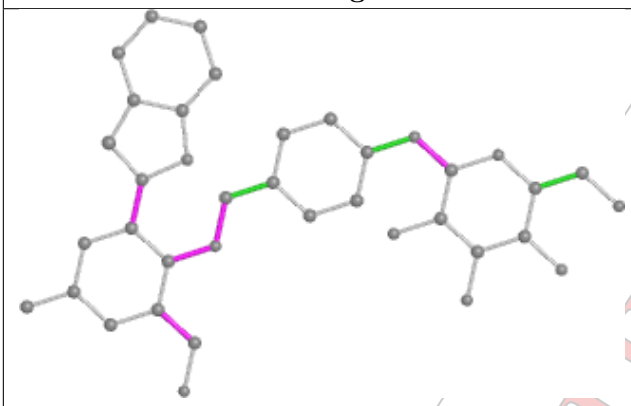
Ligand DVL B 1101



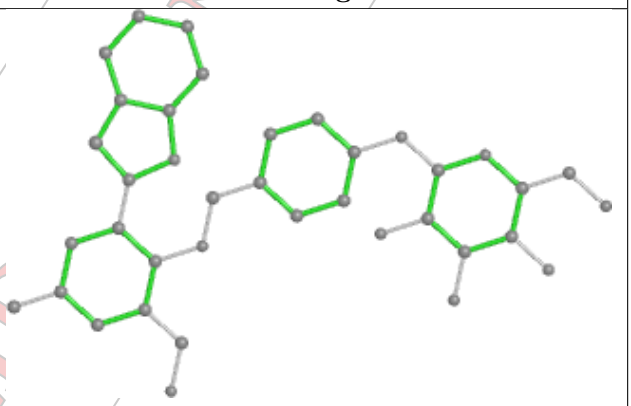
Bond lengths



Bond angles

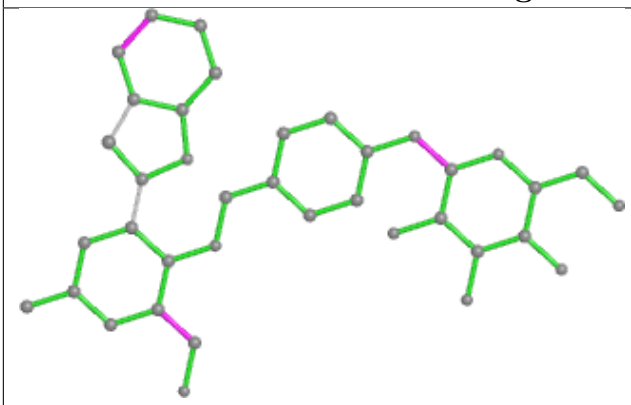


Torsions

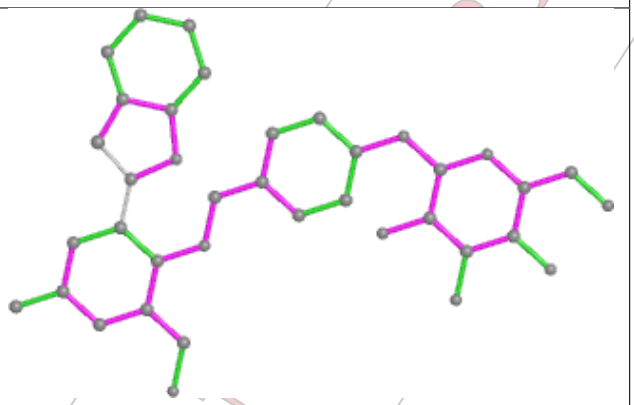


Rings

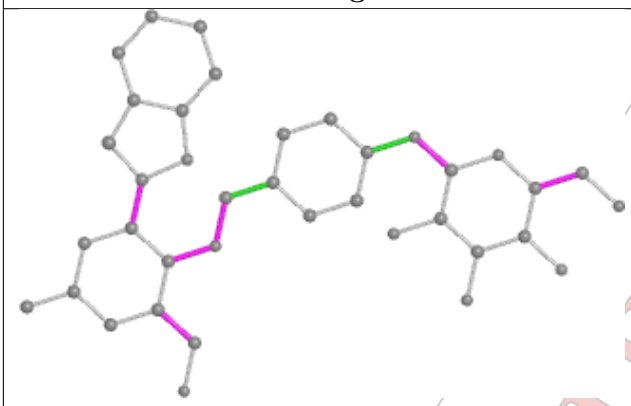
Ligand DVL C 1101



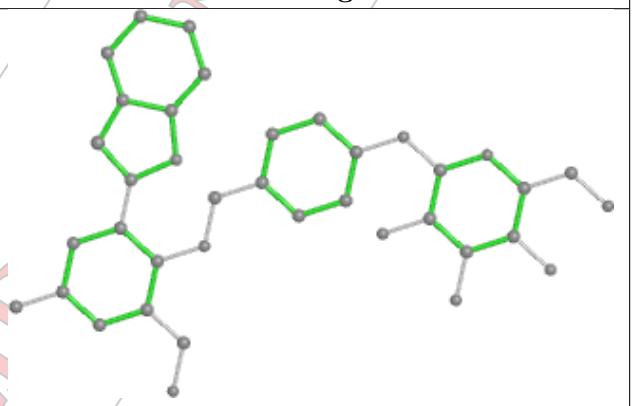
Bond lengths



Bond angles

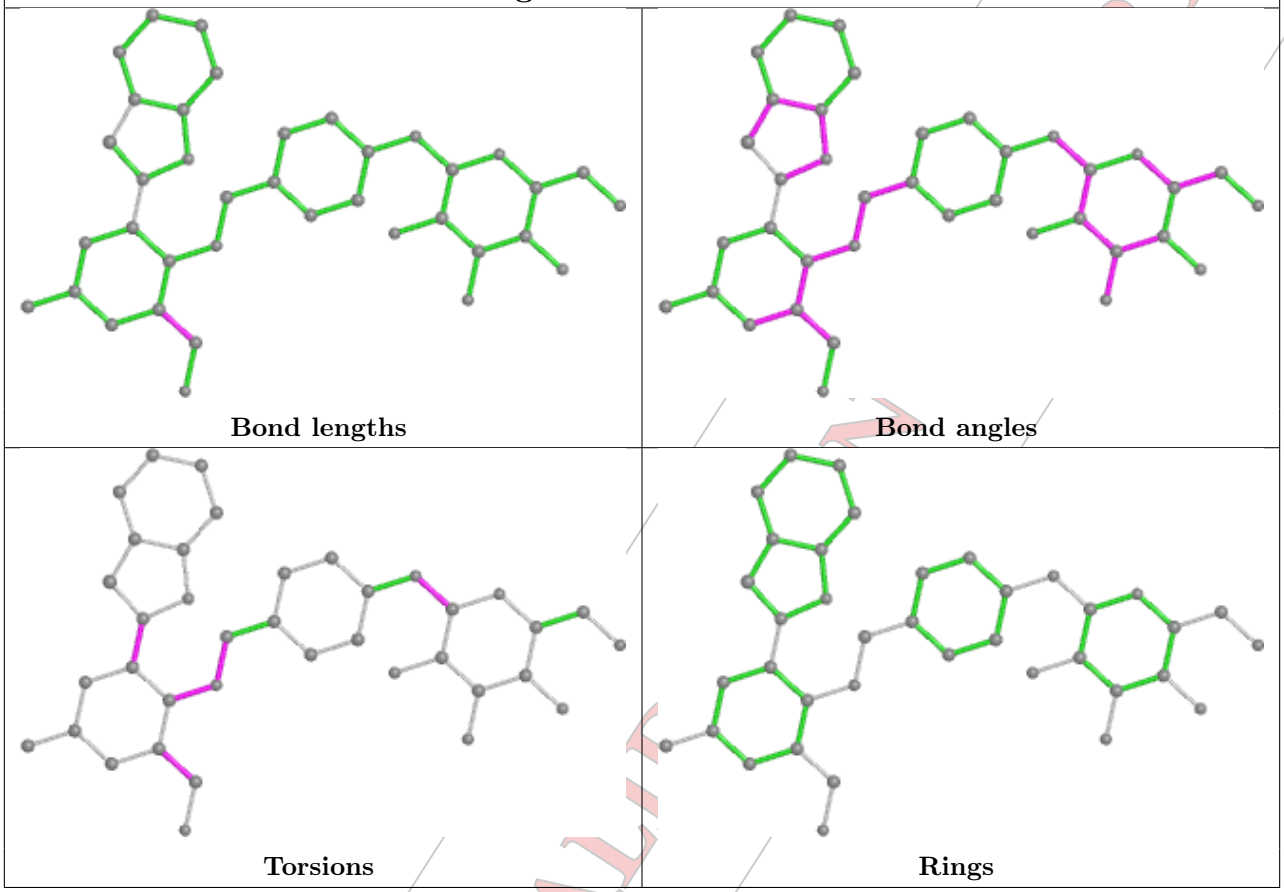


Torsions



Rings

Ligand DVL D 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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1021/1024 (99%)	-0.41	6 (0%)	89	86	23, 35, 56, 84	0
1	B	1021/1024 (99%)	-0.37	8 (0%)	86	82	24, 36, 58, 106	0
1	C	1021/1024 (99%)	-0.32	9 (0%)	84	80	25, 40, 65, 115	0
1	D	1020/1024 (99%)	-0.36	10 (0%)	82	78	24, 37, 61, 112	0
All	All	4083/4096 (99%)	-0.37	33 (0%)	86	82	23, 37, 61, 115	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	733	ALA	6.3
1	D	732	ALA	4.9
1	C	732	ALA	4.3
1	A	732	ALA	3.7
1	C	731	PRO	3.7
1	D	731	PRO	3.7
1	B	733	ALA	3.7
1	B	735	HIS	3.5
1	B	734	SER	3.4
1	A	731	PRO	3.1
1	B	731	PRO	2.9
1	C	735	HIS	2.7
1	C	733	ALA	2.7
1	D	735	HIS	2.6
1	D	581	ASN	2.6
1	C	739	HIS	2.5
1	C	686	PRO	2.4
1	A	580	GLU	2.4
1	A	634	GLN	2.4
1	B	732	ALA	2.3
1	A	581	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	578	TYR	2.2
1	D	734	SER	2.2
1	D	752	GLY	2.2
1	B	80	GLU	2.1
1	C	730	LEU	2.1
1	C	736	ALA	2.1
1	A	178	ARG	2.1
1	B	79	PRO	2.1
1	D	753	ASN	2.1
1	C	578	TYR	2.1
1	B	736	ALA	2.1
1	D	736	ALA	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 carbohydrates in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	DVL	B	1101	38/38	0.68	0.53	69,117,181,184	0
2	DVL	A	1101	38/38	0.68	0.47	56,95,149,156	0
2	DVL	D	1101	38/38	0.69	0.47	82,122,165,168	0
4	DMS	B	1108	4/4	0.74	0.38	62,63,67,76	0
2	DVL	C	1101	38/38	0.76	0.45	67,124,184,192	0
4	DMS	D	1111	4/4	0.81	0.32	58,66,69,70	0
4	DMS	A	1111	4/4	0.83	0.31	82,84,97,101	0
3	NA	B	1104	1/1	0.84	0.24	46,46,46,46	0
4	DMS	A	1117	4/4	0.84	0.28	84,85,92,95	0
4	DMS	B	1107	4/4	0.85	0.32	79,81,85,89	0
4	DMS	B	1111	4/4	0.87	0.35	79,91,92,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMS	B	1110	4/4	0.89	0.55	82,91,94,96	0
4	DMS	A	1107	4/4	0.89	0.28	69,78,81,82	0
4	DMS	D	1108	4/4	0.90	0.44	61,65,67,72	0
4	DMS	D	1112	4/4	0.91	0.31	57,64,68,72	0
3	NA	A	1103	1/1	0.91	0.14	35,35,35,35	0
4	DMS	A	1110	4/4	0.91	0.34	82,84,88,93	0
4	DMS	D	1107	4/4	0.91	0.31	67,77,80,83	0
3	NA	A	1104	1/1	0.92	0.12	60,60,60,60	0
4	DMS	A	1109	4/4	0.92	0.20	60,61,62,65	0
4	DMS	D	1110	4/4	0.92	0.37	65,71,77,78	0
6	GOL	D	1114	6/6	0.92	0.41	54,59,62,62	0
4	DMS	A	1108	4/4	0.92	0.29	73,77,81,85	0
4	DMS	D	1113	4/4	0.93	0.23	66,73,79,82	0
4	DMS	A	1105	4/4	0.93	0.23	62,68,73,74	0
4	DMS	A	1114	4/4	0.93	0.35	63,65,70,71	0
4	DMS	A	1106	4/4	0.94	0.24	63,65,70,70	0
5	MG	A	1119	1/1	0.94	0.08	31,31,31,31	0
4	DMS	D	1109	4/4	0.94	0.27	61,63,67,73	0
3	NA	C	1104	1/1	0.94	0.06	41,41,41,41	0
4	DMS	A	1112	4/4	0.94	0.30	66,69,70,73	0
4	DMS	B	1106	4/4	0.94	0.25	58,58,59,66	0
3	NA	C	1103	1/1	0.94	0.29	28,28,28,28	0
4	DMS	C	1106	4/4	0.94	0.30	66,78,80,85	0
4	DMS	D	1105	4/4	0.94	0.38	67,78,79,81	0
4	DMS	C	1108	4/4	0.95	0.27	64,64,71,72	0
4	DMS	A	1115	4/4	0.95	0.17	47,51,52,56	0
3	NA	D	1103	1/1	0.95	0.22	34,34,34,34	0
3	NA	D	1104	1/1	0.95	0.12	50,50,50,50	0
4	DMS	C	1107	4/4	0.95	0.24	67,70,71,74	0
4	DMS	B	1112	4/4	0.95	0.21	65,65,71,73	0
3	NA	B	1103	1/1	0.95	0.17	30,30,30,30	0
4	DMS	D	1106	4/4	0.95	0.24	53,59,59,63	0
5	MG	D	1116	1/1	0.95	0.17	42,42,42,42	0
4	DMS	A	1113	4/4	0.96	0.27	55,57,67,70	0
4	DMS	B	1105	4/4	0.96	0.15	55,60,60,63	0
5	MG	C	1111	1/1	0.96	0.06	42,42,42,42	0
4	DMS	A	1116	4/4	0.96	0.27	51,56,57,57	0
5	MG	B	1113	1/1	0.97	0.12	37,37,37,37	0
3	NA	D	1102	1/1	0.97	0.19	34,34,34,34	0
5	MG	A	1118	1/1	0.97	0.15	36,36,36,36	0
4	DMS	C	1109	4/4	0.97	0.12	50,56,57,60	0
5	MG	C	1110	1/1	0.98	0.12	40,40,40,40	0

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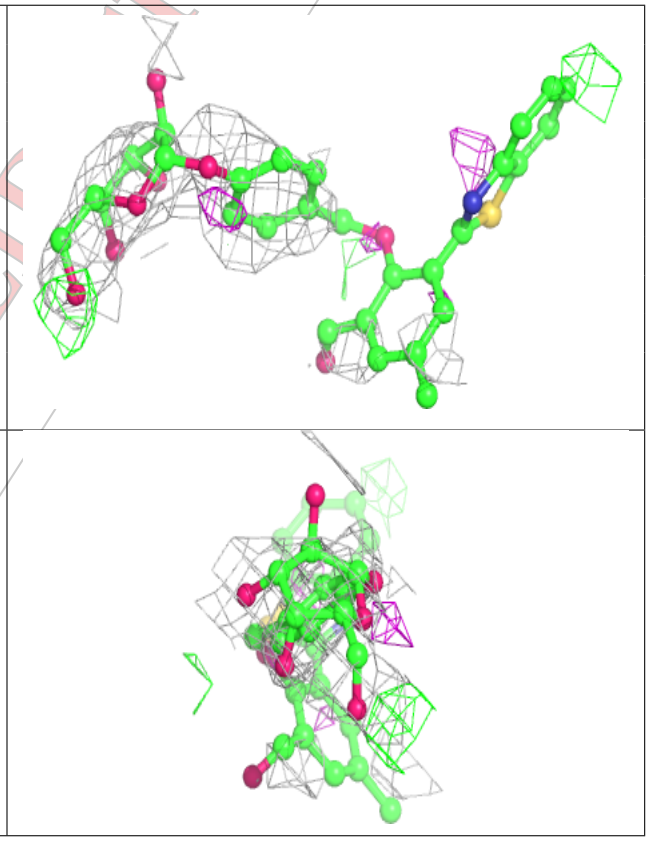
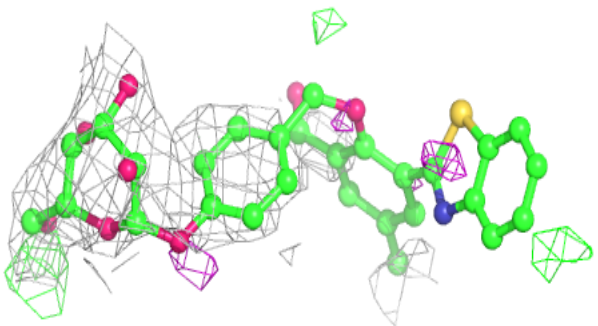
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMS	B	1109	4/4	0.98	0.26	63,71,73,76	0
3	NA	A	1102	1/1	0.98	0.26	44,44,44,44	0
3	NA	C	1102	1/1	0.98	0.12	37,37,37,37	0
5	MG	B	1114	1/1	0.98	0.06	40,40,40,40	0
3	NA	B	1102	1/1	0.98	0.08	44,44,44,44	0
4	DMS	C	1105	4/4	0.98	0.40	61,69,71,71	0
5	MG	D	1115	1/1	0.98	0.14	43,43,43,43	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 DVL B 1101:

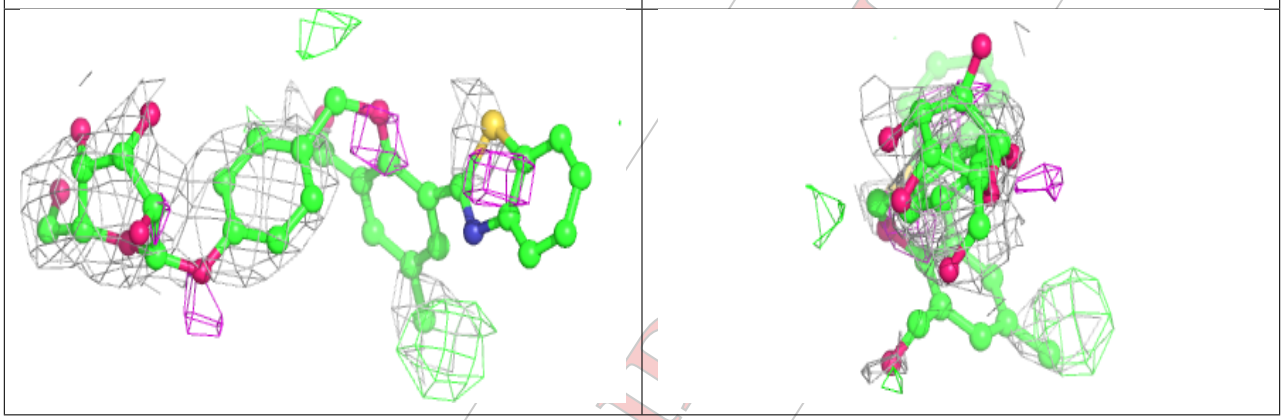
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





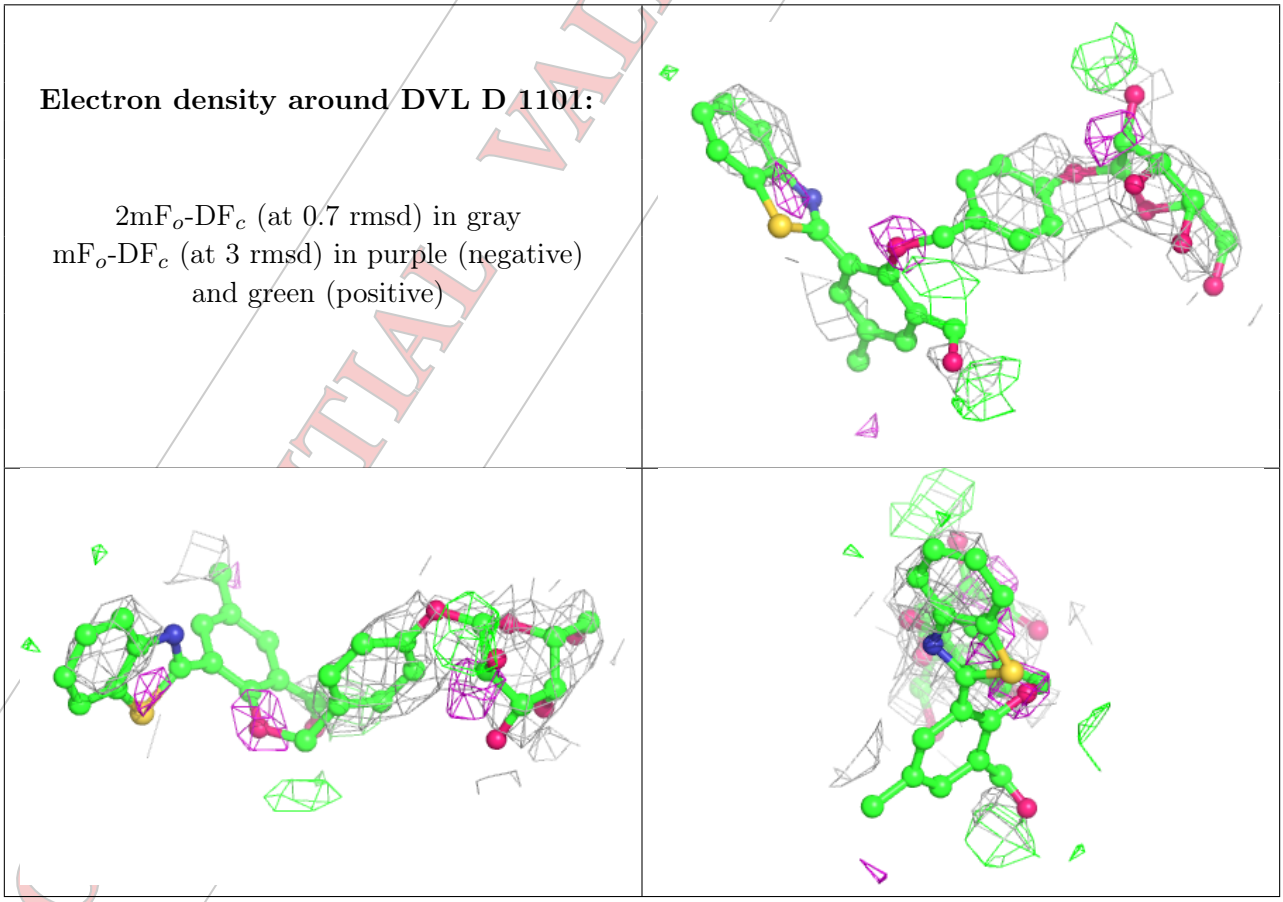
Electron density around DVL A 1101:

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



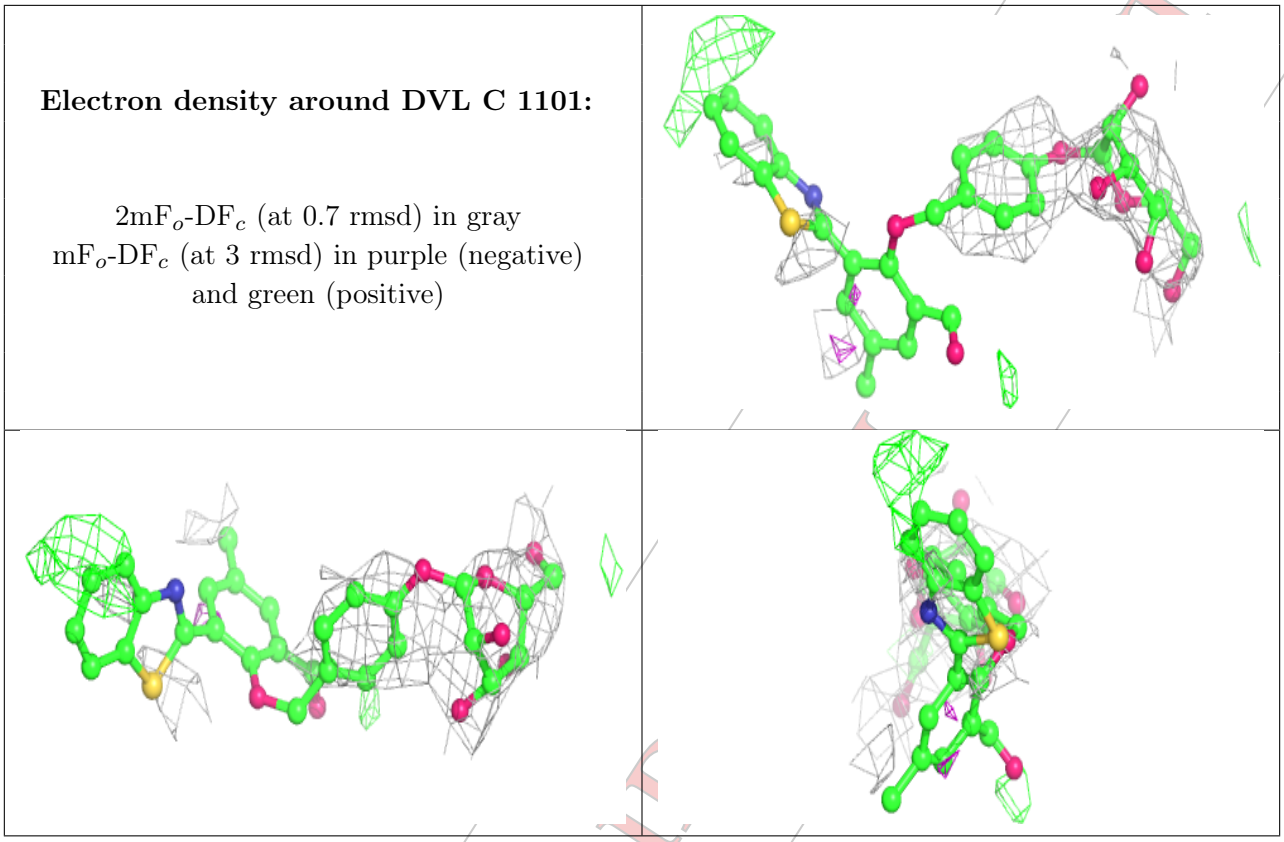
Electron density around DVL D 1101:

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



Electron density around DVL C 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.