



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 09:06 am BST

PDB ID : 3U88
Title : Crystal structure of human menin in complex with MLL1 and LEDGF
Authors : Huang, J.; Wan, B.; Lei, M.
Deposited on : 2011-10-16
Resolution : 3.00 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 : 2.11
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) : 2.11

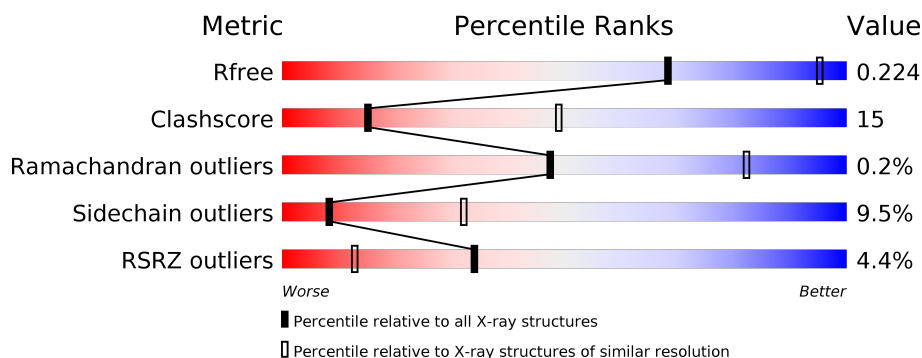
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	550	<div> <div>63%</div> <div>20%</div> <div>•</div> <div>13%</div> </div>
1	B	550	<div> <div>62%</div> <div>22%</div> <div>•</div> <div>12%</div> </div>
2	M	75	<div> <div>56%</div> <div>16%</div> <div>•</div> <div>25%</div> </div>
2	N	75	<div> <div>48%</div> <div>21%</div> <div>•</div> <div>27%</div> </div>
3	C	89	<div> <div>10%</div> <div>56%</div> <div>28%</div> <div>8%</div> <div>8%</div> </div>
3	D	89	<div> <div>43%</div> <div>55%</div> <div>19%</div> <div>•</div> <div>25%</div> </div>

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	GGB	A	613	-	-	X	-
5	GGB	C	109	-	-	X	-
6	0BR	A	612	-	-	X	-
8	SO4	M	154	-	-	X	-
8	SO4	N	154	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 9881 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 Menin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	477	Total	C	N	O	S	0	0	0
			3767	2414	643	696	14			
1	B	485	Total	C	N	O	S	0	0	0
			3811	2444	651	702	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP O00255
B	1	SER	-	expression tag	UNP O00255

- Molecule 2 is a protein called Histone-lysine N-methyltransferase 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	M	56	Total	C	N	O	0	0	0
			429	270	93	66			
2	N	55	Total	C	N	O	0	0	0
			420	265	92	63			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	5	SER	-	expression tag	UNP Q03164
M	6	ARG	-	expression tag	UNP Q03164
M	7	TRP	-	expression tag	UNP Q03164
M	8	ARG	-	expression tag	UNP Q03164
M	9	PHE	-	expression tag	UNP Q03164
M	10	PRO	-	expression tag	UNP Q03164
M	11	ALA	-	expression tag	UNP Q03164
M	12	ARG	-	expression tag	UNP Q03164
M	13	PRO	-	expression tag	UNP Q03164
M	14	GLY	-	expression tag	UNP Q03164

Continued on next page...

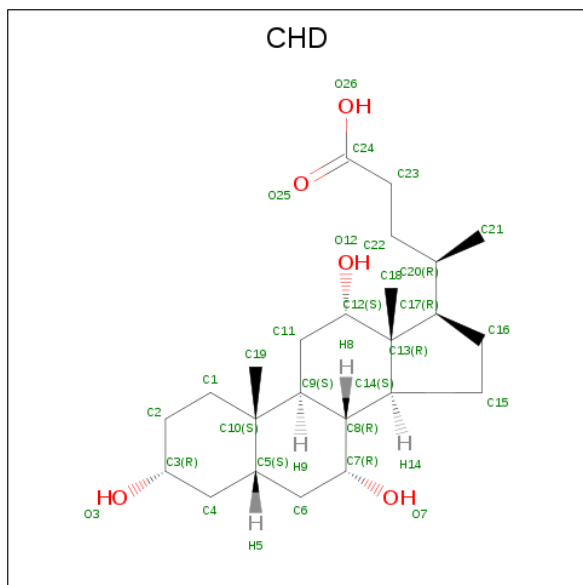
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
M	15	THR	-	expression tag	UNP Q03164
M	23	GLY	-	expression tag	UNP Q03164
M	24	ARG	-	expression tag	UNP Q03164
M	25	ARG	-	expression tag	UNP Q03164
M	26	GLY	-	expression tag	UNP Q03164
M	27	LEU	-	expression tag	UNP Q03164
M	28	GLY	-	expression tag	UNP Q03164
M	29	GLY	-	expression tag	UNP Q03164
M	30	ALA	-	expression tag	UNP Q03164
M	31	PRO	-	expression tag	UNP Q03164
M	32	ARG	-	expression tag	UNP Q03164
M	33	GLN	-	expression tag	UNP Q03164
M	34	ARG	-	expression tag	UNP Q03164
M	35	VAL	-	expression tag	UNP Q03164
N	5	SER	-	expression tag	UNP Q03164
N	6	ARG	-	expression tag	UNP Q03164
N	7	TRP	-	expression tag	UNP Q03164
N	8	ARG	-	expression tag	UNP Q03164
N	9	PHE	-	expression tag	UNP Q03164
N	10	PRO	-	expression tag	UNP Q03164
N	11	ALA	-	expression tag	UNP Q03164
N	12	ARG	-	expression tag	UNP Q03164
N	13	PRO	-	expression tag	UNP Q03164
N	14	GLY	-	expression tag	UNP Q03164
N	15	THR	-	expression tag	UNP Q03164
N	23	GLY	-	expression tag	UNP Q03164
N	24	ARG	-	expression tag	UNP Q03164
N	25	ARG	-	expression tag	UNP Q03164
N	26	GLY	-	expression tag	UNP Q03164
N	27	LEU	-	expression tag	UNP Q03164
N	28	GLY	-	expression tag	UNP Q03164
N	29	GLY	-	expression tag	UNP Q03164
N	30	ALA	-	expression tag	UNP Q03164
N	31	PRO	-	expression tag	UNP Q03164
N	32	ARG	-	expression tag	UNP Q03164
N	33	GLN	-	expression tag	UNP Q03164
N	34	ARG	-	expression tag	UNP Q03164
N	35	VAL	-	expression tag	UNP Q03164

- Molecule 3 is a protein called Lens epithelium-derived growth factor.

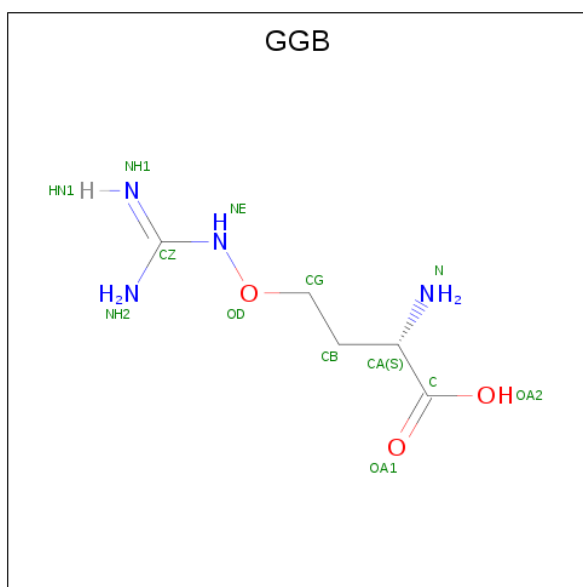
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	82	Total	C	N	O	S	18	0	0
			674	424	121	122	7			
3	D	67	Total	C	N	O	S	15	0	0
			544	343	97	98	6			

- Molecule 4 is CHOLIC ACID (three-letter code: CHD) (formula: $C_{24}H_{40}O_5$).



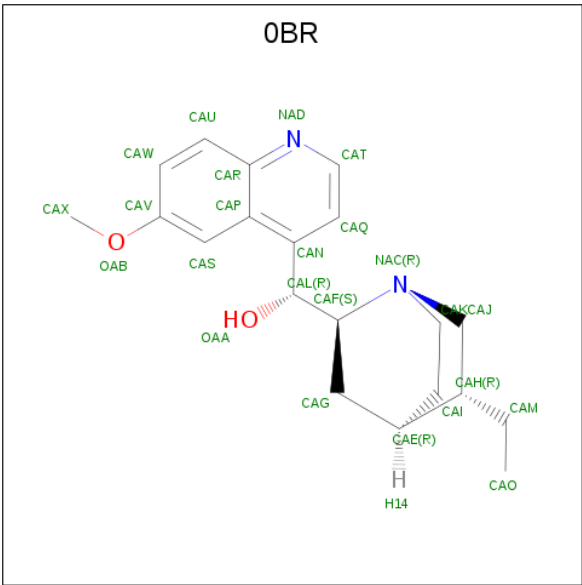
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			29	24	5		
4	B	1	Total	C	O	0	0
			29	24	5		

- Molecule 5 is L-CANAVANINE (three-letter code: GGB) (formula: $C_5H_{12}N_4O_3$).



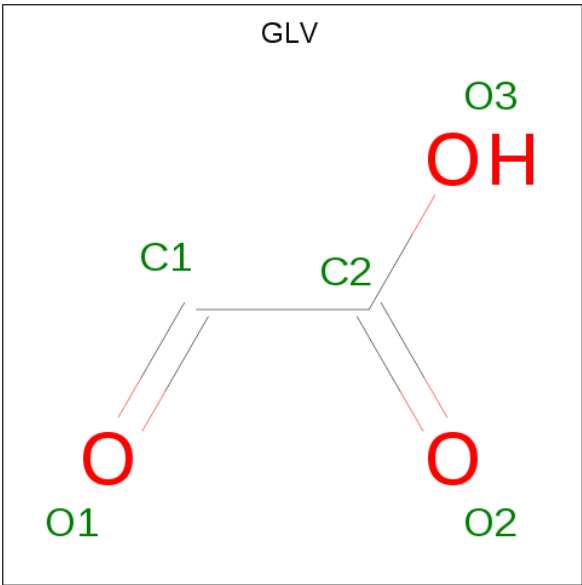
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			12	5	4	3		
5	A	1	Total	C	N	O	0	0
			12	5	4	3		
5	B	1	Total	C	N	O	0	0
			12	5	4	3		
5	C	1	Total	C	N	O	0	0
			12	5	4	3		
5	C	1	Total	C	N	O	0	0
			12	5	4	3		

- Molecule 6 is (4beta,8alpha,9R)-6'-methoxy-10,11-dihydrocinchonan-9-ol (three-letter code: 0BR) (formula: C₂₀H₂₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			24	20	2	2		
6	B	1	Total	C	N	O	0	0
			24	20	2	2		

- Molecule 7 is GLYOXYLIC ACID (three-letter code: GLV) (formula: C₂H₂O₃).



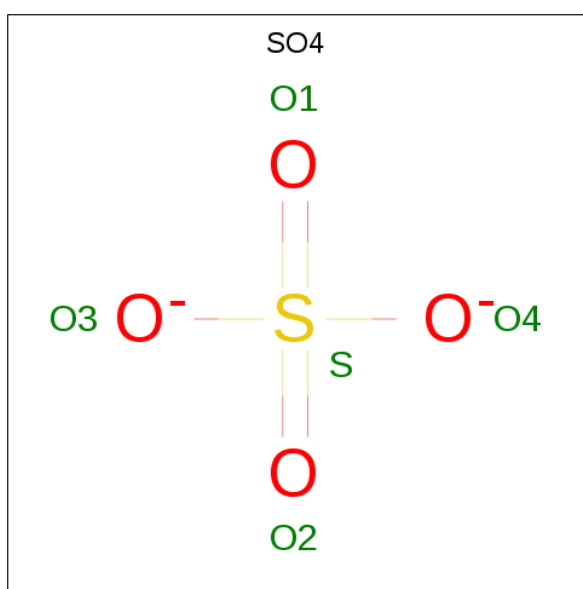
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			5	2	3		
7	A	1	Total	C	O	0	0
			5	2	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			5	2	3		
7	B	1	Total	C	O	0	0
			5	2	3		
7	C	1	Total	C	O	0	0
			5	2	3		
7	D	1	Total	C	O	0	0
			5	2	3		

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	O	S	0	0
			5	4	1		
8	A	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	B	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	N	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

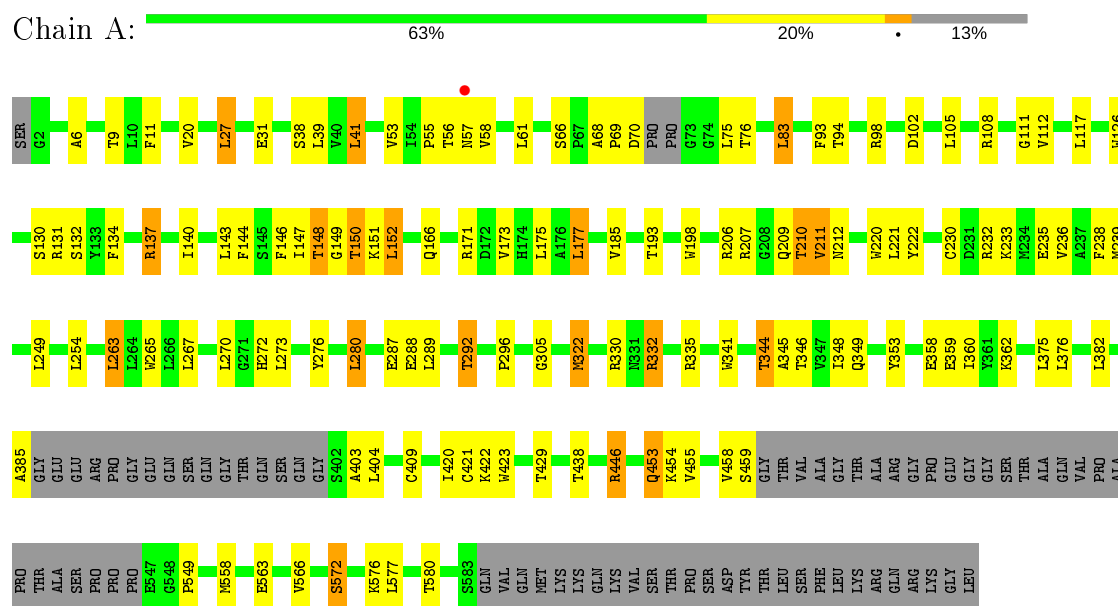
Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total	O	S	0	0
			5	4	1		

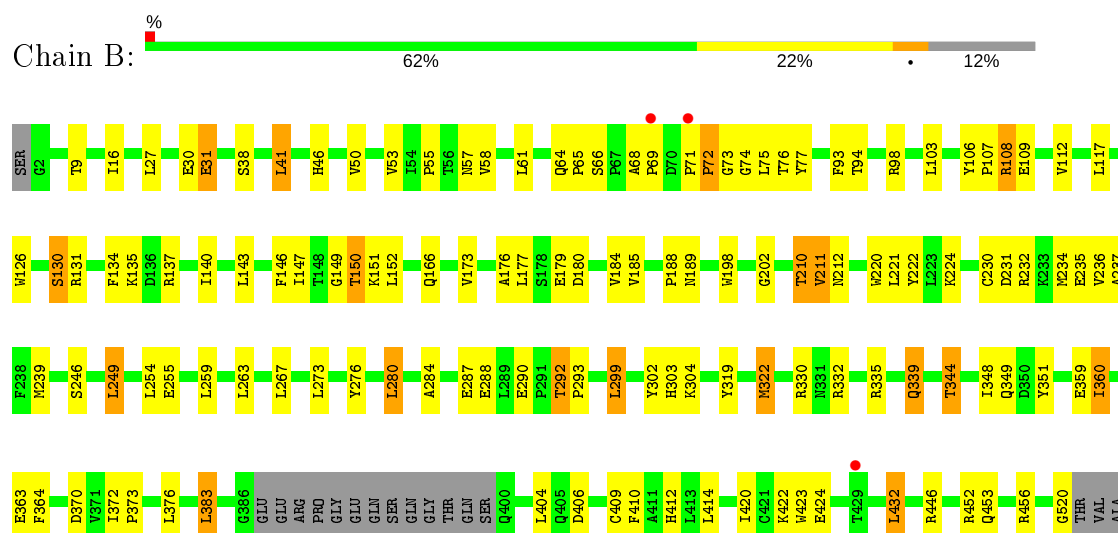
3 Residue-property plots

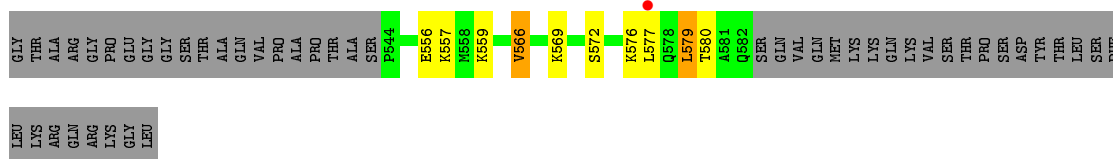
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Menin



• Molecule 1: Menin





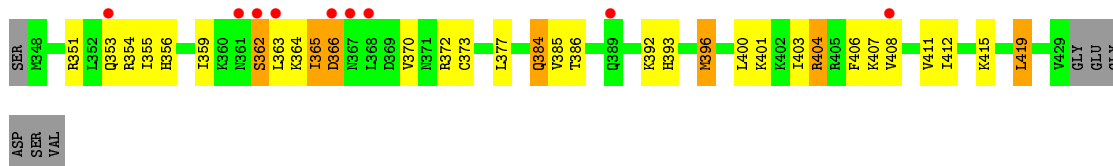
• Molecule 2: Histone-lysine N-methyltransferase 2A



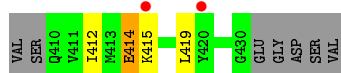
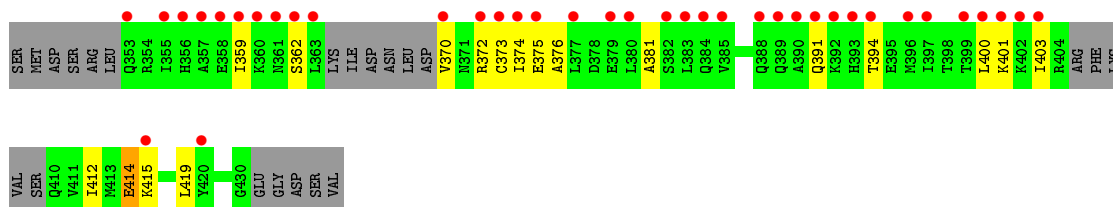
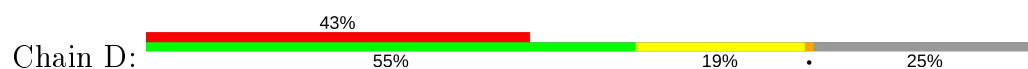
• Molecule 2: Histone-lysine N-methyltransferase 2A



• Molecule 3: Lens epithelium-derived growth factor



• Molecule 3: Lens epithelium-derived growth factor



4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	187.99Å 187.99Å 238.42Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.65 – 3.00 48.65 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.65-3.00) 99.8 (48.65-3.00)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.98 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.7 _650	Depositor
R, R_{free}	0.202 , 0.233 0.195 , 0.224	Depositor DCC
R_{free} test set	5048 reflections (10.07%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9881	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.35% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 0BR, CHD, SO4, GLV, GGB

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	0.38	0/3852	0.51	1/5228 (0.0%)
1	B	0.36	0/3902	0.51	0/5301
2	M	0.36	0/439	0.60	0/591
2	N	0.39	0/430	0.64	1/579 (0.2%)
3	C	0.26	0/679	0.42	0/905
3	D	0.24	0/546	0.43	0/725
All	All	0.36	0/9848	0.51	2/13329 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	111	GLY	N-CA-C	-5.29	99.88	113.10
1	A	385	ALA	N-CA-CB	-5.17	102.86	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3767	0	3736	104	0
1	B	3811	0	3780	108	0
2	M	429	0	443	12	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	N	420	0	437	16	0
3	C	674	0	715	26	0
3	D	544	0	576	17	0
4	A	29	0	39	1	0
4	B	29	0	39	0	0
5	A	24	0	21	9	0
5	B	12	0	11	2	0
5	C	24	0	22	13	0
6	A	24	0	26	20	0
6	B	24	0	26	7	0
7	A	15	0	3	1	0
7	B	5	0	1	0	0
7	C	5	0	1	0	0
7	D	5	0	1	0	0
8	A	10	0	0	0	0
8	B	10	0	0	0	0
8	M	10	0	0	3	0
8	N	10	0	0	2	0
All	All	9881	0	9877	295	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 15.

All (295) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:108:GGB:HCG1	5:C:109:GGB:OA1	1.44	1.15
6:A:612:0BR:H26	6:A:612:0BR:H16	1.30	1.11
6:A:612:0BR:OAA	6:A:612:0BR:H20	1.55	1.05
5:C:109:GGB:OD	5:C:109:GGB:N	1.86	1.02
1:A:38:SER:HA	1:A:239:MET:HE3	1.42	1.01
1:B:93:PHE:HB2	1:B:147:ILE:HD11	1.44	0.98
3:D:374:ILE:HD11	3:D:412:ILE:HG13	1.43	0.97
1:B:210:THR:HG23	1:B:212:ASN:H	1.30	0.96
3:D:400:LEU:HD23	3:D:403:ILE:HD11	1.50	0.93
1:B:38:SER:HA	1:B:239:MET:HE3	1.51	0.91
5:C:109:GGB:HCG1	5:C:109:GGB:HN21	1.32	0.91
1:A:210:THR:HG23	1:A:212:ASN:H	1.37	0.88
2:N:130:ARG:NH1	8:N:154:SO4:O3	2.07	0.87
3:C:362:SER:HB3	3:C:372:ARG:HD2	1.57	0.86
1:A:93:PHE:HB2	1:A:147:ILE:HD11	1.58	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:353:GLN:HG2	3:C:393:HIS:HE1	1.40	0.85
3:D:362:SER:HB3	3:D:372:ARG:HH11	1.40	0.85
3:C:353:GLN:HG2	3:C:393:HIS:CE1	2.11	0.85
5:C:109:GGB:CG	5:C:109:GGB:HN21	1.91	0.83
1:A:458:VAL:HG12	1:A:459:SER:H	1.44	0.82
1:A:185:VAL:HG12	1:A:193:THR:HG22	1.60	0.82
6:A:612:0BR:H12	6:B:612:0BR:OAB	1.81	0.80
5:C:108:GGB:HCG1	5:C:109:GGB:C	2.10	0.80
6:A:612:0BR:OAA	6:A:612:0BR:CAJ	2.31	0.78
2:N:126:LEU:O	2:N:130:ARG:HB2	1.84	0.75
1:A:131:ARG:O	6:A:612:0BR:H3	1.87	0.74
1:A:335:ARG:HG2	1:A:409:CYS:SG	2.28	0.73
6:A:612:0BR:H11	6:A:612:0BR:H4	1.68	0.73
1:B:287:GLU:OE2	1:B:292:THR:HG23	1.88	0.73
6:A:612:0BR:CAO	6:A:612:0BR:H16	2.13	0.73
1:A:66:SER:O	1:A:76:THR:HG22	1.89	0.72
1:A:38:SER:CA	1:A:239:MET:HE3	2.19	0.72
1:B:72:PRO:HB2	1:B:73:GLY:O	1.89	0.71
5:C:109:GGB:CG	5:C:109:GGB:NH2	2.51	0.70
1:A:455:VAL:HG22	1:A:549:PRO:HG2	1.73	0.69
3:C:363:LEU:O	5:C:109:GGB:NH2	2.25	0.69
1:A:144:PHE:O	1:A:148:THR:HB	1.92	0.69
6:A:612:0BR:H4	6:A:612:0BR:CAF	2.22	0.68
1:B:130:SER:O	6:B:612:0BR:OAA	2.11	0.68
3:D:362:SER:HB3	3:D:372:ARG:HD3	1.77	0.67
1:A:349:GLN:HB2	1:A:422:LYS:HB3	1.75	0.67
1:A:358:GLU:HG2	1:A:362:LYS:HE3	1.75	0.66
1:B:224:LYS:HD3	1:B:351:TYR:CE2	2.30	0.66
1:A:287:GLU:OE2	1:A:292:THR:HG23	1.96	0.66
1:A:198:TRP:CE3	6:A:612:0BR:H23	2.30	0.66
3:D:381:ALA:HB2	3:D:419:LEU:HD11	1.77	0.65
1:B:424:GLU:OE1	1:B:557:LYS:HE3	1.96	0.65
6:A:612:0BR:H26	6:A:612:0BR:CAI	2.15	0.65
1:B:332:ARG:HH12	2:N:27:LEU:HB2	1.62	0.65
1:B:249:LEU:HD12	1:B:249:LEU:H	1.62	0.64
1:B:173:VAL:O	1:B:232:ARG:NH2	2.31	0.64
1:B:30:GLU:H	1:B:30:GLU:CD	2.01	0.64
1:A:173:VAL:O	1:A:232:ARG:NH2	2.32	0.63
3:D:381:ALA:HB2	3:D:419:LEU:HD21	1.80	0.63
1:A:11:PHE:HB2	1:A:83:LEU:HD12	1.81	0.63
1:B:520:GLY:H	1:B:559:LYS:HE2	1.63	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:ASN:OD1	1:B:58:VAL:N	2.28	0.62
1:A:57:ASN:OD1	1:A:58:VAL:HG23	2.00	0.62
6:A:612:0BR:CAP	6:A:612:0BR:H13	2.24	0.62
1:B:410:PHE:CE2	1:B:414:LEU:HD11	2.35	0.62
1:B:72:PRO:N	1:B:73:GLY:HA2	2.14	0.61
6:A:612:0BR:CAS	6:A:612:0BR:CAG	2.79	0.61
1:A:359:GLU:HG3	2:M:12:ARG:NH2	2.15	0.61
1:A:232:ARG:O	1:A:236:VAL:HG23	2.01	0.61
1:A:198:TRP:HE1	7:A:615:GLV:H1	1.67	0.60
1:A:332:ARG:NH1	2:M:27:LEU:HD23	2.16	0.60
1:B:370:ASP:OD1	2:N:24:ARG:HD2	2.01	0.60
1:B:273:LEU:HB3	1:B:280:LEU:HD13	1.82	0.60
3:C:400:LEU:HD23	3:C:403:ILE:HD11	1.84	0.60
1:A:41:LEU:HD22	1:A:239:MET:HE2	1.84	0.60
1:B:332:ARG:NH1	2:N:27:LEU:HB2	2.17	0.60
3:D:401:LYS:HD3	3:D:401:LYS:O	2.02	0.59
6:A:612:0BR:CAP	6:A:612:0BR:CAG	2.78	0.59
5:C:109:GGB:NH2	5:C:109:GGB:HCG1	2.05	0.59
3:C:362:SER:HB3	3:C:372:ARG:CD	2.32	0.59
1:B:176:ALA:HB2	1:B:185:VAL:HG13	1.83	0.59
1:A:322:MET:HA	1:A:322:MET:HE3	1.86	0.58
1:B:339:GLN:HG3	1:B:412:HIS:CE1	2.38	0.58
1:A:273:LEU:HB3	1:A:280:LEU:HD13	1.84	0.58
3:C:370:VAL:HG13	3:C:412:ILE:HD11	1.85	0.58
1:A:280:LEU:HD23	1:A:305:GLY:HA2	1.86	0.58
1:A:453:GLN:HG3	1:A:566:VAL:CG2	2.34	0.58
1:A:376:LEU:HB3	1:A:446:ARG:HG2	1.85	0.58
1:A:267:LEU:HB3	1:A:273:LEU:CD1	2.34	0.57
1:B:420:ILE:O	1:B:423:TRP:HB3	2.04	0.57
1:A:335:ARG:NH1	1:A:403:ALA:HA	2.19	0.57
1:B:322:MET:HA	1:B:322:MET:HE3	1.87	0.57
1:A:171:ARG:HD2	5:A:614:GGB:OA2	2.05	0.57
1:B:149:GLY:O	1:B:150:THR:HG22	2.03	0.57
1:A:56:THR:OG1	2:M:110:PRO:HB3	2.04	0.57
1:B:572:SER:O	1:B:576:LYS:HG3	2.05	0.57
1:A:126:TRP:CD1	6:A:612:0BR:H7	2.40	0.56
1:A:151:LYS:HE2	5:A:613:GGB:HN1	1.70	0.56
1:A:572:SER:O	1:A:576:LYS:HG3	2.06	0.56
1:A:75:LEU:O	2:M:38:LEU:HD23	2.06	0.55
1:A:289:LEU:HD13	2:M:34:ARG:HH21	1.71	0.55
1:B:126:TRP:CH2	6:B:612:0BR:H18	2.42	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:SER:CA	1:B:239:MET:HE3	2.29	0.55
3:C:406:PHE:CE2	3:C:408:VAL:HB	2.42	0.55
6:A:612:0BR:CAS	6:A:612:0BR:CAF	2.82	0.55
1:B:130:SER:H	1:B:150:THR:HG23	1.69	0.55
1:B:41:LEU:CD2	1:B:239:MET:HE2	2.37	0.55
2:M:130:ARG:NH1	8:M:154:SO4:O3	2.40	0.55
1:A:6:ALA:O	1:A:9:THR:HG22	2.07	0.55
1:A:150:THR:O	1:A:150:THR:HG23	2.08	0.54
1:A:111:GLY:HA3	5:A:614:GGB:HN1A	1.72	0.54
1:A:403:ALA:HB1	1:A:409:CYS:SG	2.47	0.54
1:B:376:LEU:HB3	1:B:446:ARG:HG2	1.89	0.54
1:B:131:ARG:HA	6:B:612:0BR:OAA	2.07	0.54
1:A:112:VAL:C	5:A:614:GGB:HN21	2.11	0.54
1:B:53:VAL:O	1:B:55:PRO:HD3	2.08	0.54
1:A:53:VAL:O	1:A:55:PRO:HD3	2.08	0.53
6:A:612:0BR:H10	6:A:612:0BR:H20	1.68	0.53
1:B:41:LEU:HD22	1:B:239:MET:CE	2.39	0.53
1:B:273:LEU:HB3	1:B:280:LEU:CD1	2.39	0.53
5:C:108:GGB:N	5:C:108:GGB:OD	2.39	0.53
1:A:206:ARG:O	1:A:209:GLN:HB2	2.08	0.53
1:B:299:LEU:HD22	1:B:303:HIS:CD2	2.44	0.53
3:C:355:ILE:O	3:C:359:ILE:HG13	2.08	0.53
1:A:270:LEU:HB2	1:A:272:HIS:CD2	2.44	0.53
1:A:177:LEU:HD21	1:A:238:PHE:CD2	2.43	0.53
1:B:249:LEU:HD12	1:B:249:LEU:N	2.24	0.53
1:B:150:THR:HG23	1:B:150:THR:O	2.08	0.52
3:D:359:ILE:HG23	3:D:373:CYS:SG	2.50	0.52
1:B:432:LEU:HG	1:B:579:LEU:HD22	1.91	0.52
1:A:151:LYS:HE2	5:A:613:GGB:NH1	2.24	0.52
3:D:362:SER:CB	3:D:372:ARG:HD3	2.40	0.52
1:B:288:GLU:OE1	1:B:330:ARG:NH1	2.43	0.52
2:M:130:ARG:NH1	8:M:154:SO4:S	2.80	0.52
1:A:345:ALA:O	1:A:348:ILE:HG22	2.10	0.52
1:A:421:CYS:SG	1:A:558:MET:CE	2.98	0.52
1:B:211:VAL:HG22	1:B:222:TYR:CE2	2.45	0.51
3:C:411:VAL:O	3:C:415:LYS:HG3	2.11	0.51
1:A:39:LEU:HD21	1:A:147:ILE:HD12	1.92	0.51
5:C:108:GGB:CG	5:C:109:GGB:C	2.87	0.51
1:A:566:VAL:HG22	1:A:566:VAL:O	2.09	0.51
1:A:68:ALA:HB1	1:A:69:PRO:HD2	1.92	0.51
1:A:453:GLN:HA	1:A:566:VAL:HG21	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLY:O	1:A:150:THR:HG22	2.12	0.50
1:B:410:PHE:CE1	1:B:452:ARG:HG2	2.45	0.50
1:B:77:TYR:HB2	2:N:39:LEU:HD12	1.94	0.50
1:A:102:ASP:HB3	1:A:105:LEU:HG	1.92	0.50
1:B:180:ASP:HB2	1:B:220:TRP:CH2	2.47	0.50
3:C:377:LEU:HD22	3:C:419:LEU:HD23	1.93	0.50
1:B:146:PHE:O	1:B:150:THR:HA	2.12	0.50
1:A:288:GLU:OE1	1:A:330:ARG:NH1	2.46	0.49
1:B:349:GLN:HB2	1:B:422:LYS:HB3	1.93	0.49
1:B:75:LEU:O	2:N:38:LEU:HD23	2.13	0.49
1:A:453:GLN:HA	1:A:566:VAL:CG2	2.42	0.49
1:A:458:VAL:HG12	1:A:459:SER:N	2.22	0.49
1:B:103:LEU:HB2	3:D:414:GLU:HB3	1.93	0.49
3:D:391:GLN:O	3:D:394:THR:HG23	2.13	0.48
1:A:41:LEU:HD22	1:A:239:MET:CE	2.42	0.48
1:A:134:PHE:HD2	5:A:613:GGB:HN21	1.61	0.48
1:A:359:GLU:HG3	2:M:12:ARG:HH22	1.78	0.48
1:B:348:ILE:O	1:B:351:TYR:HB2	2.13	0.48
1:A:20:VAL:HG22	1:A:263:LEU:HD13	1.96	0.48
1:B:284:ALA:HB3	1:B:302:TYR:CE2	2.48	0.48
1:A:137:ARG:HH11	5:A:613:GGB:HN22	1.60	0.48
1:A:94:THR:HG23	1:A:98:ARG:CZ	2.44	0.48
1:B:335:ARG:HG3	1:B:409:CYS:SG	2.54	0.48
1:B:71:PRO:HA	1:B:72:PRO:C	2.33	0.48
1:B:232:ARG:O	1:B:236:VAL:HG23	2.14	0.48
1:B:179:GLU:HB3	1:B:319:TYR:CE1	2.49	0.48
1:A:220:TRP:CZ3	1:A:360:ILE:HB	2.49	0.48
1:B:410:PHE:CZ	1:B:452:ARG:HG2	2.49	0.48
1:A:211:VAL:HG22	1:A:222:TYR:CE2	2.49	0.47
1:A:31:GLU:HG3	1:A:166:GLN:HE21	1.79	0.47
1:A:438:THR:HG22	1:A:576:LYS:NZ	2.29	0.47
1:A:360:ILE:HD12	1:A:360:ILE:HA	1.74	0.47
1:B:383:LEU:HD23	1:B:383:LEU:HA	1.67	0.47
1:B:151:LYS:NZ	5:B:615:GGB:HN2	2.13	0.47
3:D:374:ILE:CD1	3:D:412:ILE:HG13	2.31	0.47
2:N:130:ARG:HD2	8:N:154:SO4:O3	2.15	0.47
1:B:237:ALA:HA	1:B:267:LEU:HD13	1.97	0.47
1:A:267:LEU:HB3	1:A:273:LEU:HD13	1.97	0.47
1:A:265:TRP:CH2	1:A:296:PRO:HD2	2.49	0.47
1:A:57:ASN:OD1	1:A:58:VAL:N	2.47	0.47
3:C:365:ILE:HG22	5:C:109:GGB:HCA	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:SER:N	1:B:150:THR:HG23	2.28	0.47
1:B:41:LEU:HD22	1:B:239:MET:HE2	1.97	0.47
1:B:58:VAL:HG12	1:B:61:LEU:H	1.80	0.47
3:C:362:SER:HB3	3:C:372:ARG:HB3	1.97	0.47
1:A:346:THR:O	1:A:349:GLN:HG2	2.15	0.47
1:B:188:PRO:O	1:B:189:ASN:HB2	2.15	0.47
2:M:130:ARG:NH1	8:M:154:SO4:O2	2.47	0.47
1:B:220:TRP:CE3	1:B:360:ILE:HB	2.50	0.46
1:B:72:PRO:CD	1:B:73:GLY:HA2	2.45	0.46
1:A:108:ARG:HD3	1:A:112:VAL:HG12	1.98	0.46
1:B:16:ILE:HG23	1:B:259:LEU:HD13	1.96	0.46
1:B:31:GLU:HG3	1:B:166:GLN:HE21	1.80	0.46
1:B:372:ILE:HB	1:B:373:PRO:HD3	1.96	0.46
1:B:140:ILE:O	1:B:152:LEU:HA	2.16	0.46
1:A:353:TYR:CD2	1:A:429:THR:HB	2.50	0.46
3:D:370:VAL:O	3:D:374:ILE:HG12	2.16	0.46
1:B:94:THR:HG23	1:B:98:ARG:HD2	1.97	0.46
3:D:373:CYS:O	3:D:376:ALA:HB3	2.15	0.46
1:B:330:ARG:HG2	2:N:26:GLY:HA3	1.98	0.46
1:A:210:THR:HG23	1:A:212:ASN:N	2.17	0.45
1:A:572:SER:OG	1:A:576:LYS:HE3	2.15	0.45
1:B:432:LEU:HG	1:B:579:LEU:CD2	2.46	0.45
1:A:576:LYS:O	1:A:580:THR:HG22	2.15	0.45
1:B:134:PHE:HD1	5:B:615:GGB:OA1	1.99	0.45
3:C:365:ILE:H	3:C:365:ILE:HG12	1.56	0.45
1:A:341:TRP:O	1:A:344:THR:HG22	2.16	0.45
1:B:230:CYS:HB3	1:B:235:GLU:HG3	1.99	0.45
1:B:55:PRO:HG2	1:B:61:LEU:HD23	1.98	0.45
3:D:415:LYS:O	3:D:419:LEU:HD23	2.17	0.45
3:C:385:VAL:HG12	3:C:386:THR:N	2.31	0.45
2:N:108:VAL:HB	2:N:109:GLY:O	2.16	0.45
1:B:94:THR:HG21	1:B:98:ARG:NH1	2.32	0.45
1:B:359:GLU:HG3	2:N:12:ARG:HH22	1.82	0.45
1:B:30:GLU:HG2	1:B:31:GLU:H	1.82	0.45
3:C:365:ILE:CG2	5:C:109:GGB:HCA	2.46	0.45
1:A:140:ILE:O	1:A:152:LEU:HA	2.17	0.44
1:B:41:LEU:HD23	1:B:239:MET:HE2	1.99	0.44
1:B:73:GLY:HA3	1:B:74:GLY:HA3	1.61	0.44
3:C:384:GLN:HB2	3:C:384:GLN:HE21	1.56	0.44
3:C:401:LYS:O	3:C:401:LYS:HG2	2.17	0.44
1:A:453:GLN:HG3	1:A:566:VAL:HG22	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:LYS:HE2	1:B:202:GLY:HA3	1.99	0.44
6:B:612:0BR:H26	6:B:612:0BR:H21	1.83	0.44
3:C:401:LYS:HG2	3:C:404:ARG:NH2	2.33	0.44
2:M:118:VAL:O	2:M:122:ILE:HG13	2.16	0.44
1:A:108:ARG:HB3	1:A:112:VAL:O	2.17	0.44
1:A:146:PHE:O	1:A:150:THR:HA	2.17	0.44
1:B:299:LEU:O	1:B:303:HIS:HD2	2.01	0.44
1:A:146:PHE:CD1	1:A:152:LEU:HD22	2.52	0.44
1:B:131:ARG:HA	1:B:131:ARG:HD3	1.75	0.44
1:A:131:ARG:HA	1:A:131:ARG:HD3	1.84	0.44
1:B:335:ARG:HD3	1:B:406:ASP:OD2	2.17	0.44
6:A:612:0BR:CAS	6:A:612:0BR:H12	2.47	0.44
1:A:134:PHE:O	1:A:137:ARG:HG2	2.18	0.43
6:A:612:0BR:H12	6:B:612:0BR:CAV	2.47	0.43
2:N:130:ARG:HG3	2:N:134:GLY:HA2	2.00	0.43
1:B:94:THR:CG2	1:B:98:ARG:HD2	2.49	0.43
1:B:360:ILE:HA	1:B:360:ILE:HD12	1.74	0.43
2:N:116:LEU:HD22	2:N:116:LEU:HA	1.62	0.43
1:A:55:PRO:HG2	1:A:61:LEU:HD23	2.01	0.43
3:D:374:ILE:HD11	3:D:412:ILE:CG1	2.32	0.43
2:M:12:ARG:HG2	2:M:13:PRO:O	2.19	0.43
1:A:236:VAL:O	1:A:239:MET:HG2	2.19	0.43
4:A:611:CHD:H111	4:A:611:CHD:H193	1.76	0.43
1:A:137:ARG:NH1	5:A:613:GGB:HN22	2.17	0.43
1:B:231:ASP:OD1	1:B:231:ASP:C	2.57	0.43
1:A:233:LYS:HD2	1:A:272:HIS:CE1	2.54	0.43
1:B:372:ILE:O	1:B:376:LEU:HG	2.19	0.43
1:A:198:TRP:CE3	6:A:612:0BR:CAM	3.00	0.42
1:B:453:GLN:HA	1:B:566:VAL:HG22	2.01	0.42
1:A:130:SER:OG	1:A:150:THR:CG2	2.68	0.42
1:A:41:LEU:CD2	1:A:239:MET:HE2	2.48	0.42
1:B:410:PHE:CZ	1:B:414:LEU:HD11	2.53	0.42
1:B:41:LEU:HD12	1:B:41:LEU:HA	1.73	0.42
1:B:134:PHE:HB2	1:B:137:ARG:HG3	2.02	0.42
1:B:359:GLU:HG3	2:N:12:ARG:NH2	2.34	0.42
3:C:365:ILE:HG23	5:C:109:GGB:CG	2.49	0.42
1:A:220:TRP:CE3	1:A:360:ILE:HB	2.54	0.42
3:C:356:HIS:NE2	3:C:396:MET:HA	2.34	0.42
1:A:126:TRP:CZ3	1:A:207:ARG:HD2	2.54	0.42
1:B:103:LEU:H	1:B:103:LEU:HD22	1.84	0.42
6:A:612:0BR:CAG	6:B:612:0BR:OAB	2.62	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:613:GGB:HN1A	5:A:613:GGB:HCG2	1.56	0.42
1:B:106:TYR:HA	1:B:107:PRO:HD2	1.85	0.42
1:B:135:LYS:HD2	1:B:198:TRP:NE1	2.35	0.42
1:A:344:THR:HG22	1:A:345:ALA:N	2.34	0.41
1:A:27:LEU:HA	1:A:27:LEU:HD12	1.79	0.41
1:B:348:ILE:HD12	1:B:351:TYR:CD1	2.55	0.41
1:B:41:LEU:HD22	1:B:239:MET:HE1	2.02	0.41
3:C:364:LYS:HG2	3:C:366:ASP:OD1	2.19	0.41
2:M:116:LEU:HD22	2:M:116:LEU:HA	1.57	0.41
1:B:292:THR:HA	1:B:293:PRO:HD3	1.90	0.41
1:B:220:TRP:CZ3	1:B:360:ILE:HB	2.55	0.41
1:B:68:ALA:HA	1:B:69:PRO:HD3	1.83	0.41
1:B:108:ARG:HG2	1:B:112:VAL:O	2.20	0.41
1:B:231:ASP:OD1	1:B:234:MET:HG3	2.21	0.41
1:B:64:GLN:HA	1:B:65:PRO:HD3	1.94	0.41
1:A:263:LEU:HA	1:A:263:LEU:HD12	1.89	0.41
3:D:412:ILE:N	3:D:412:ILE:HD12	2.35	0.41
1:A:273:LEU:HB3	1:A:280:LEU:CD1	2.49	0.41
3:C:363:LEU:HD11	3:C:373:CYS:SG	2.61	0.41
3:C:406:PHE:CZ	3:C:408:VAL:HB	2.55	0.41
1:B:16:ILE:HD11	1:B:255:GLU:HB2	2.03	0.41
1:A:31:GLU:HG3	1:A:166:GLN:NE2	2.36	0.41
1:B:46:HIS:O	1:B:50:VAL:HB	2.21	0.41
2:N:129:PHE:CD2	2:N:129:PHE:C	2.94	0.41
1:A:230:CYS:HB3	1:A:235:GLU:HG3	2.04	0.40
1:B:339:GLN:HG3	1:B:412:HIS:NE2	2.36	0.40
1:A:175:LEU:HG	1:A:177:LEU:HD13	2.03	0.40
3:C:351:ARG:O	3:C:355:ILE:HG13	2.21	0.40
3:C:362:SER:HB3	3:C:372:ARG:CG	2.52	0.40
1:A:420:ILE:O	1:A:423:TRP:HB3	2.21	0.40
1:B:299:LEU:HD23	1:B:299:LEU:HA	1.82	0.40
1:A:375:LEU:HD12	1:A:375:LEU:HA	1.89	0.40
1:B:363:GLU:OE1	2:N:15:THR:HG23	2.21	0.40
1:B:344:THR:CG2	1:B:364:PHE:CE2	3.05	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	469/550 (85%)	446 (95%)	23 (5%)	0	100	100
1	B	479/550 (87%)	449 (94%)	29 (6%)	1 (0%)	47	82
2	M	54/75 (72%)	48 (89%)	5 (9%)	1 (2%)	8	36
2	N	53/75 (71%)	50 (94%)	3 (6%)	0	100	100
3	C	80/89 (90%)	72 (90%)	8 (10%)	0	100	100
3	D	61/89 (68%)	57 (93%)	4 (7%)	0	100	100
All	All	1196/1428 (84%)	1122 (94%)	72 (6%)	2 (0%)	47	82

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	72	PRO
2	M	111	GLY

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	401/461 (87%)	369 (92%)	32 (8%)	12	40
1	B	405/461 (88%)	364 (90%)	41 (10%)	7	29
2	M	39/50 (78%)	34 (87%)	5 (13%)	4	19
2	N	38/50 (76%)	31 (82%)	7 (18%)	1	9
3	C	78/83 (94%)	68 (87%)	10 (13%)	4	19

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	D	62/83 (75%)	60 (97%)	2 (3%)	39 74
All	All	1023/1188 (86%)	926 (90%)	97 (10%)	8 32

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	LEU
1	A	41	LEU
1	A	70	ASP
1	A	83	LEU
1	A	117	LEU
1	A	132	SER
1	A	137	ARG
1	A	143	LEU
1	A	148	THR
1	A	150	THR
1	A	152	LEU
1	A	177	LEU
1	A	210	THR
1	A	211	VAL
1	A	221	LEU
1	A	249	LEU
1	A	254	LEU
1	A	263	LEU
1	A	276	TYR
1	A	280	LEU
1	A	292	THR
1	A	322	MET
1	A	332	ARG
1	A	344	THR
1	A	382	LEU
1	A	404	LEU
1	A	446	ARG
1	A	453	GLN
1	A	454	LYS
1	A	563	GLU
1	A	572	SER
1	A	577	LEU
1	B	9	THR
1	B	27	LEU
1	B	31	GLU
1	B	41	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	66	SER
1	B	76	THR
1	B	108	ARG
1	B	109	GLU
1	B	117	LEU
1	B	130	SER
1	B	143	LEU
1	B	150	THR
1	B	177	LEU
1	B	184	VAL
1	B	210	THR
1	B	211	VAL
1	B	221	LEU
1	B	246	SER
1	B	249	LEU
1	B	254	LEU
1	B	263	LEU
1	B	276	TYR
1	B	280	LEU
1	B	290	GLU
1	B	292	THR
1	B	299	LEU
1	B	304	LYS
1	B	322	MET
1	B	339	GLN
1	B	344	THR
1	B	360	ILE
1	B	383	LEU
1	B	404	LEU
1	B	432	LEU
1	B	456	ARG
1	B	556	GLU
1	B	566	VAL
1	B	569	LYS
1	B	577	LEU
1	B	579	LEU
1	B	580	THR
2	M	6	ARG
2	M	27	LEU
2	M	116	LEU
2	M	126	LEU
2	M	128	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	354	ARG
3	C	362	SER
3	C	365	ILE
3	C	366	ASP
3	C	384	GLN
3	C	392	LYS
3	C	396	MET
3	C	404	ARG
3	C	407	LYS
3	C	419	LEU
2	N	6	ARG
2	N	8	ARG
2	N	27	LEU
2	N	33	GLN
2	N	107	ARG
2	N	116	LEU
2	N	130	ARG
3	D	375	GLU
3	D	414	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	272	HIS
1	B	303	HIS
3	C	384	GLN
3	C	393	HIS
3	D	421	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

23 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
6	0BR	B	612	-	27,27,27	0.98	1 (3%)	39,39,39	1.43	8 (20%)
4	CHD	B	611	-	29,32,32	2.06	13 (44%)	48,51,51	1.90	12 (25%)
8	SO4	M	154	-	4,4,4	0.14	0	6,6,6	0.05	0
7	GLV	A	616	-	1,4,4	0.50	0	0,4,4	0.00	-
8	SO4	A	619	-	4,4,4	0.18	0	6,6,6	0.21	0
7	GLV	B	616	-	1,4,4	0.59	0	0,4,4	0.00	-
8	SO4	B	617	-	4,4,4	0.16	0	6,6,6	0.13	0
4	CHD	A	611	-	29,32,32	2.05	10 (34%)	48,51,51	2.11	18 (37%)
7	GLV	C	113	-	1,4,4	0.39	0	0,4,4	0.00	-
8	SO4	N	154	-	4,4,4	0.14	0	6,6,6	0.05	0
8	SO4	B	618	-	4,4,4	0.18	0	6,6,6	0.18	0
7	GLV	D	114	-	1,4,4	0.36	0	0,4,4	0.00	-
8	SO4	N	1	-	4,4,4	0.19	0	6,6,6	0.12	0
8	SO4	M	2	-	4,4,4	0.13	0	6,6,6	0.11	0
5	GGB	A	613	-	6,11,11	1.66	2 (33%)	4,13,13	3.19	3 (75%)
5	GGB	B	615	-	6,11,11	1.64	2 (33%)	4,13,13	3.16	3 (75%)
7	GLV	A	615	-	1,4,4	0.77	0	0,4,4	0.00	-
6	0BR	A	612	-	27,27,27	0.99	1 (3%)	39,39,39	1.43	8 (20%)
5	GGB	C	109	-	6,11,11	1.65	1 (16%)	4,13,13	3.02	3 (75%)
8	SO4	A	618	-	4,4,4	0.16	0	6,6,6	0.15	0
7	GLV	A	617	-	1,4,4	0.35	0	0,4,4	0.00	-
5	GGB	C	108	-	6,11,11	1.66	1 (16%)	4,13,13	3.02	3 (75%)
5	GGB	A	614	-	6,11,11	1.66	1 (16%)	4,13,13	3.24	3 (75%)

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	0BR	B	612	-	-	9/12/33/33	0/5/4/4
4	CHD	B	611	-	-	2/7/74/74	0/4/4/4
7	GLV	A	615	-	-	0/0/2/2	-
5	GGB	B	615	-	-	4/5/11/11	-
7	GLV	A	616	-	-	0/0/2/2	-
6	0BR	A	612	-	-	7/12/33/33	0/5/4/4
5	GGB	C	109	-	-	4/5/11/11	-
4	CHD	A	611	-	-	0/7/74/74	0/4/4/4
7	GLV	C	113	-	-	0/0/2/2	-
7	GLV	A	617	-	-	0/0/2/2	-
5	GGB	C	108	-	-	1/5/11/11	-
5	GGB	A	613	-	-	5/5/11/11	-
5	GGB	A	614	-	-	2/5/11/11	-
7	GLV	D	114	-	-	0/0/2/2	-
7	GLV	B	616	-	-	0/0/2/2	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	611	CHD	C10-C5	-4.03	1.48	1.55
4	A	611	CHD	C10-C5	-3.94	1.49	1.55
4	B	611	CHD	O12-C12	-3.91	1.37	1.43
4	A	611	CHD	O12-C12	-3.87	1.37	1.43
4	B	611	CHD	C13-C12	-3.66	1.48	1.54
4	A	611	CHD	C13-C12	-3.60	1.48	1.54
5	A	614	GGB	OD-NE	-3.32	1.33	1.40
4	A	611	CHD	C19-C10	-3.19	1.48	1.54
5	C	108	GGB	OD-NE	-3.17	1.33	1.40
5	C	109	GGB	OD-NE	-3.14	1.33	1.40
4	A	611	CHD	C6-C5	-3.13	1.48	1.53
4	B	611	CHD	C19-C10	-3.11	1.48	1.54
4	B	611	CHD	C6-C5	-2.99	1.49	1.53
5	B	615	GGB	OD-NE	-2.89	1.34	1.40
5	A	613	GGB	OD-NE	-2.87	1.34	1.40
4	B	611	CHD	C18-C13	-2.60	1.50	1.54
4	A	611	CHD	C18-C13	-2.52	1.50	1.54
4	A	611	CHD	C1-C10	-2.48	1.49	1.54
6	A	612	0BR	CAN-CAP	-2.44	1.39	1.43
6	B	612	0BR	CAN-CAP	-2.43	1.39	1.43
4	A	611	CHD	C13-C14	-2.43	1.51	1.55
4	B	611	CHD	C13-C14	-2.38	1.51	1.55
4	B	611	CHD	C16-C17	-2.38	1.49	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	611	CHD	C1-C10	-2.35	1.49	1.54
4	A	611	CHD	C16-C17	-2.33	1.49	1.54
4	B	611	CHD	C20-C17	-2.27	1.50	1.54
4	B	611	CHD	O7-C7	-2.22	1.38	1.43
4	B	611	CHD	C15-C14	-2.21	1.49	1.54
5	A	613	GGB	CZ-NE	2.16	1.39	1.34
4	A	611	CHD	O7-C7	-2.14	1.38	1.43
5	B	615	GGB	CZ-NE	2.12	1.39	1.34
4	B	611	CHD	C21-C20	-2.06	1.48	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	611	CHD	C18-C13-C17	-5.62	102.41	111.21
5	A	614	GGB	NH2-CZ-NH1	-4.96	105.00	120.26
5	A	613	GGB	NH2-CZ-NH1	-4.86	105.29	120.26
5	B	615	GGB	NH2-CZ-NH1	-4.85	105.32	120.26
4	A	611	CHD	C18-C13-C17	-4.79	103.72	111.21
4	B	611	CHD	C14-C8-C7	4.62	117.93	111.81
4	A	611	CHD	C17-C13-C12	4.50	121.77	117.67
4	B	611	CHD	C17-C13-C12	4.45	121.73	117.67
5	C	109	GGB	NH2-CZ-NH1	-4.42	106.64	120.26
5	C	108	GGB	NH2-CZ-NH1	-4.42	106.67	120.26
4	A	611	CHD	C14-C8-C7	4.18	117.35	111.81
4	A	611	CHD	C9-C10-C5	3.97	114.16	108.58
4	A	611	CHD	C19-C10-C9	-3.97	105.72	111.18
6	B	612	0BR	CAX-OAB-CAV	-3.71	109.47	117.51
6	A	612	0BR	CAX-OAB-CAV	-3.68	109.52	117.51
4	A	611	CHD	C18-C13-C14	3.57	116.80	111.21
4	B	611	CHD	C18-C13-C14	3.51	116.70	111.21
5	A	614	GGB	NE-CZ-NH1	3.48	126.66	120.59
4	A	611	CHD	C13-C14-C8	3.35	119.02	114.74
4	A	611	CHD	C21-C20-C22	-3.34	105.13	110.36
4	B	611	CHD	C13-C14-C8	3.19	118.81	114.74
5	B	615	GGB	NH2-CZ-NE	3.14	127.00	119.34
5	C	109	GGB	NH2-CZ-NE	3.07	126.83	119.34
5	C	108	GGB	NH2-CZ-NE	3.05	126.79	119.34
6	B	612	0BR	CAT-NAD-CAR	2.94	121.48	116.93
6	A	612	0BR	CAT-NAD-CAR	2.91	121.44	116.93
5	A	613	GGB	NE-CZ-NH1	2.90	125.66	120.59
4	A	611	CHD	C11-C12-C13	2.87	114.19	111.24
5	A	613	GGB	NH2-CZ-NE	2.84	126.27	119.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	611	CHD	C19-C10-C1	-2.84	103.69	108.26
6	A	612	0BR	CAS-CAP-CAN	-2.76	120.43	123.77
6	B	612	0BR	CAS-CAP-CAN	-2.76	120.43	123.77
4	B	611	CHD	C19-C10-C9	-2.71	107.45	111.18
5	C	108	GGB	NE-CZ-NH1	2.71	125.32	120.59
5	C	109	GGB	NE-CZ-NH1	2.67	125.25	120.59
4	A	611	CHD	C5-C6-C7	2.65	117.38	114.46
4	B	611	CHD	C19-C10-C1	-2.65	104.00	108.26
6	B	612	0BR	CAG-CAF-CAL	-2.60	110.97	113.90
6	A	612	0BR	CAG-CAF-CAL	-2.59	110.98	113.90
4	A	611	CHD	C1-C2-C3	2.57	113.76	110.47
4	A	611	CHD	C5-C4-C3	2.55	116.51	112.76
4	B	611	CHD	C15-C14-C8	-2.53	114.79	118.33
4	B	611	CHD	C1-C2-C3	2.45	113.61	110.47
6	B	612	0BR	CAQ-CAT-NAD	-2.43	120.82	124.58
6	A	612	0BR	CAQ-CAT-NAD	-2.41	120.84	124.58
6	A	612	0BR	CAK-NAC-CAJ	2.39	110.54	108.19
4	A	611	CHD	C1-C10-C5	2.36	111.26	107.77
4	A	611	CHD	C15-C14-C8	-2.36	115.04	118.33
6	A	612	0BR	CAP-CAR-NAD	-2.34	120.34	122.83
6	B	612	0BR	CAK-NAC-CAJ	2.33	110.49	108.19
6	B	612	0BR	CAP-CAR-NAD	-2.33	120.35	122.83
4	A	611	CHD	C9-C11-C12	2.32	117.36	114.30
5	B	615	GGB	NE-CZ-NH1	2.31	124.63	120.59
5	A	614	GGB	NH2-CZ-NE	2.31	124.98	119.34
6	A	612	0BR	CAH-CAJ-NAC	-2.25	109.28	112.23
4	B	611	CHD	C9-C10-C5	2.24	111.73	108.58
4	A	611	CHD	C14-C8-C9	-2.23	106.64	109.71
4	B	611	CHD	C6-C5-C10	-2.22	110.30	112.66
6	B	612	0BR	CAH-CAJ-NAC	-2.21	109.33	112.23
4	A	611	CHD	C22-C23-C24	-2.21	108.84	113.59
4	B	611	CHD	C5-C6-C7	2.05	116.72	114.46

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	612	0BR	CAE-CAH-CAM-CAO
6	B	612	0BR	CAJ-CAH-CAM-CAO
5	A	613	GGB	N-CA-CB-CG
5	A	613	GGB	C-CA-CB-CG
5	A	613	GGB	CA-CB-CG-OD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	A	613	GGB	CZ-NE-OD-CG
5	B	615	GGB	CA-CB-CG-OD
5	B	615	GGB	CZ-NE-OD-CG
6	A	612	0BR	CAG-CAF-CAL-CAN
6	A	612	0BR	CAG-CAF-CAL-OAA
6	A	612	0BR	NAC-CAF-CAL-OAA
6	A	612	0BR	CAE-CAH-CAM-CAO
6	A	612	0BR	CAJ-CAH-CAM-CAO
5	C	109	GGB	N-CA-CB-CG
5	C	109	GGB	CA-CB-CG-OD
5	C	109	GGB	CZ-NE-OD-CG
5	C	108	GGB	CB-CG-OD-NE
5	A	614	GGB	CA-CB-CG-OD
5	A	614	GGB	CZ-NE-OD-CG
6	A	612	0BR	CAF-CAL-CAN-CAQ
4	B	611	CHD	C21-C20-C22-C23
6	B	612	0BR	OAA-CAL-CAN-CAQ
6	B	612	0BR	CAF-CAL-CAN-CAP
6	B	612	0BR	OAA-CAL-CAN-CAP
6	B	612	0BR	CAF-CAL-CAN-CAQ
5	A	613	GGB	CB-CG-OD-NE
5	B	615	GGB	CB-CG-OD-NE
6	A	612	0BR	CAF-CAL-CAN-CAP
6	B	612	0BR	NAC-CAF-CAL-CAN
5	C	109	GGB	C-CA-CB-CG
6	B	612	0BR	CAG-CAF-CAL-OAA
6	B	612	0BR	NAC-CAF-CAL-OAA
5	B	615	GGB	C-CA-CB-CG
4	B	611	CHD	C17-C20-C22-C23

There are no ring outliers.

11 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	612	0BR	7	0
8	M	154	SO4	3	0
4	A	611	CHD	1	0
8	N	154	SO4	2	0
5	A	613	GGB	6	0
5	B	615	GGB	2	0
7	A	615	GLV	1	0
6	A	612	0BR	20	0

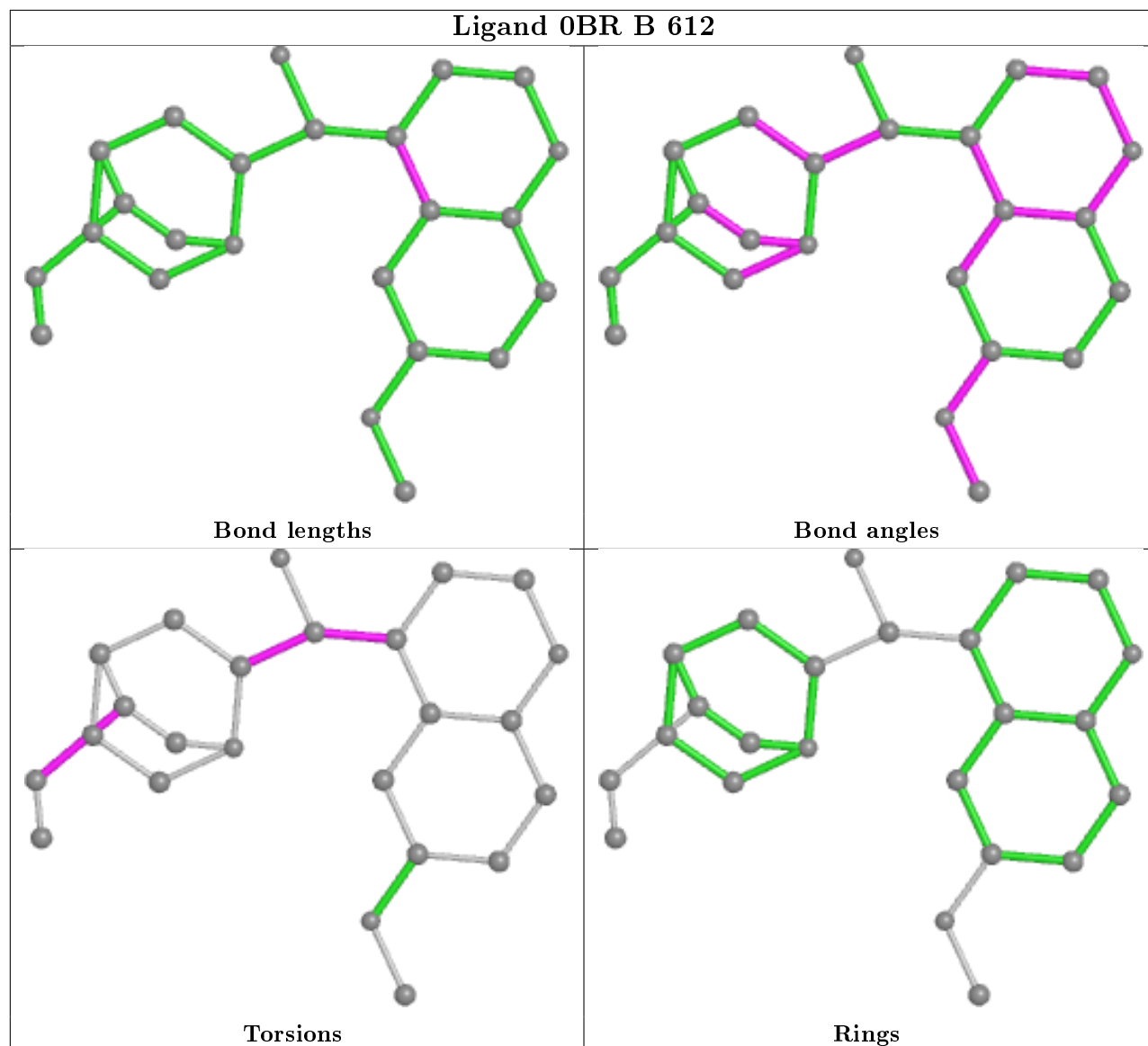
Continued on next page...

Continued from previous page...

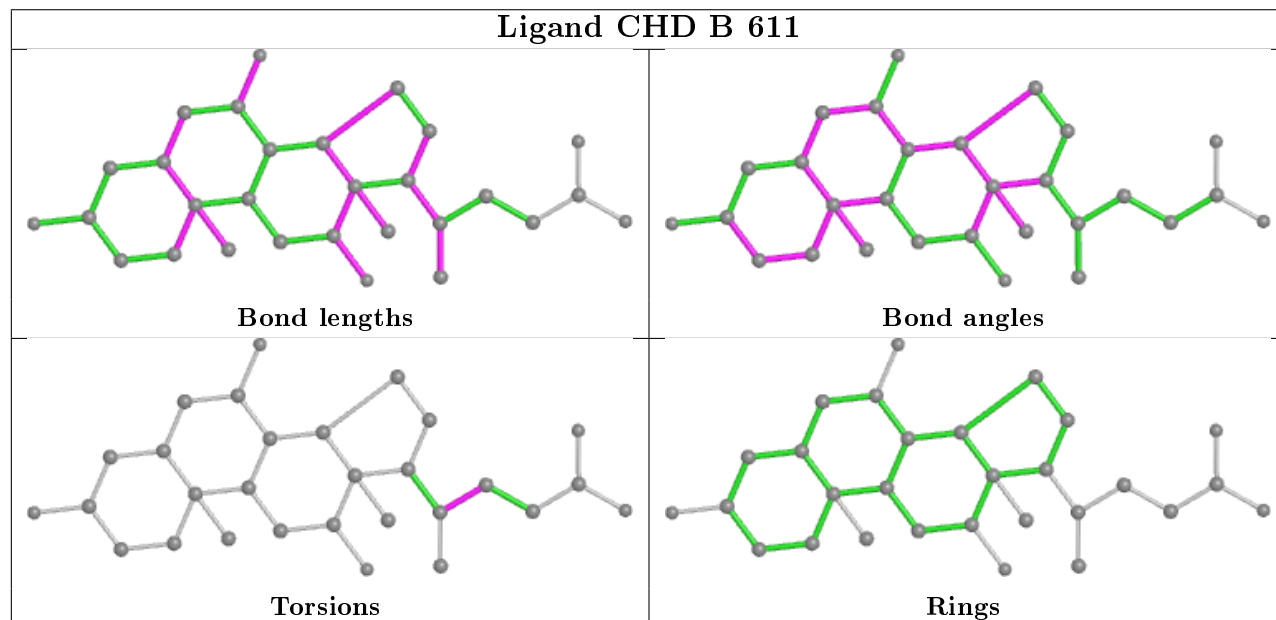
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	109	GGB	12	0
5	C	108	GGB	4	0
5	A	614	GGB	3	0

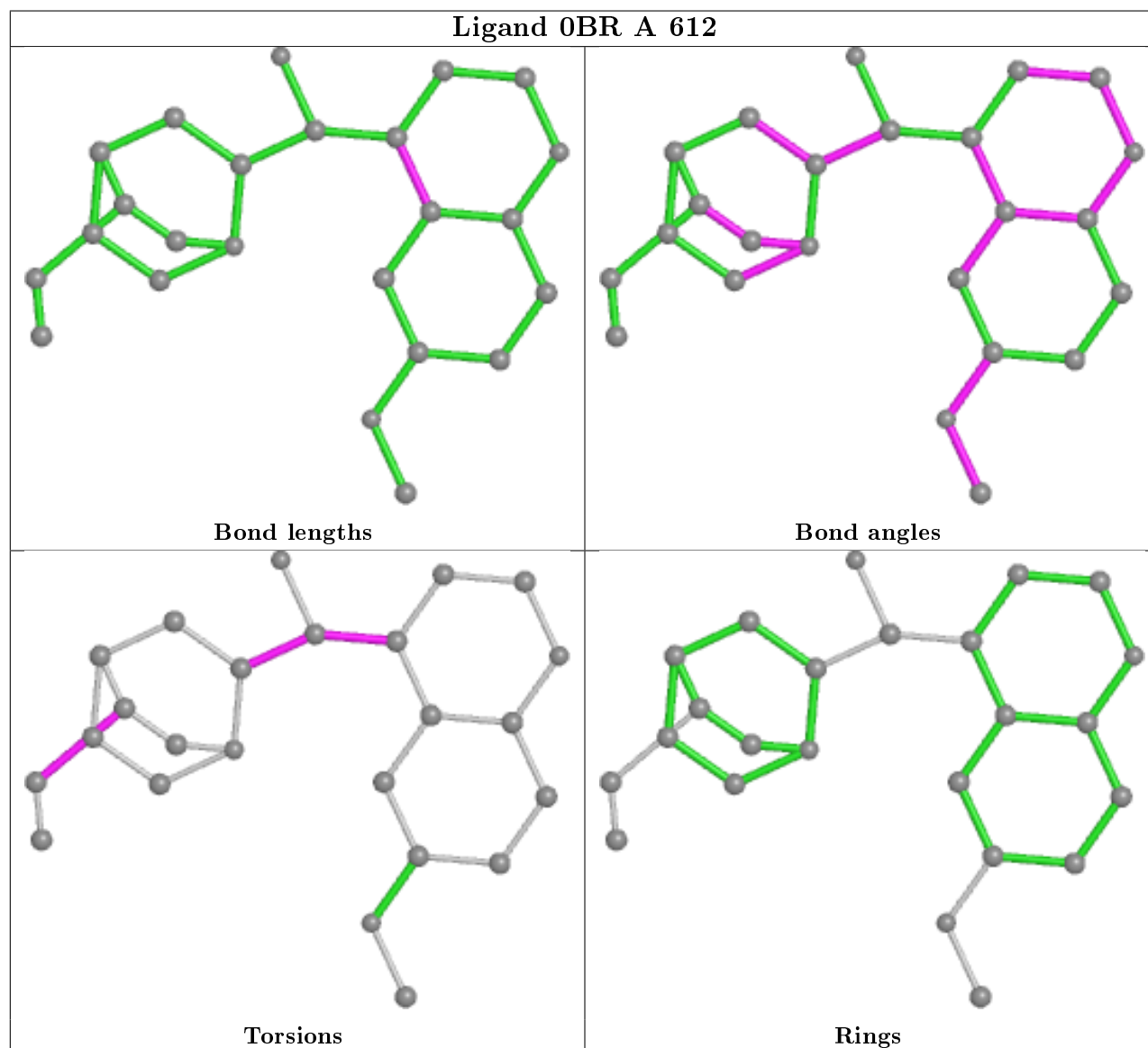
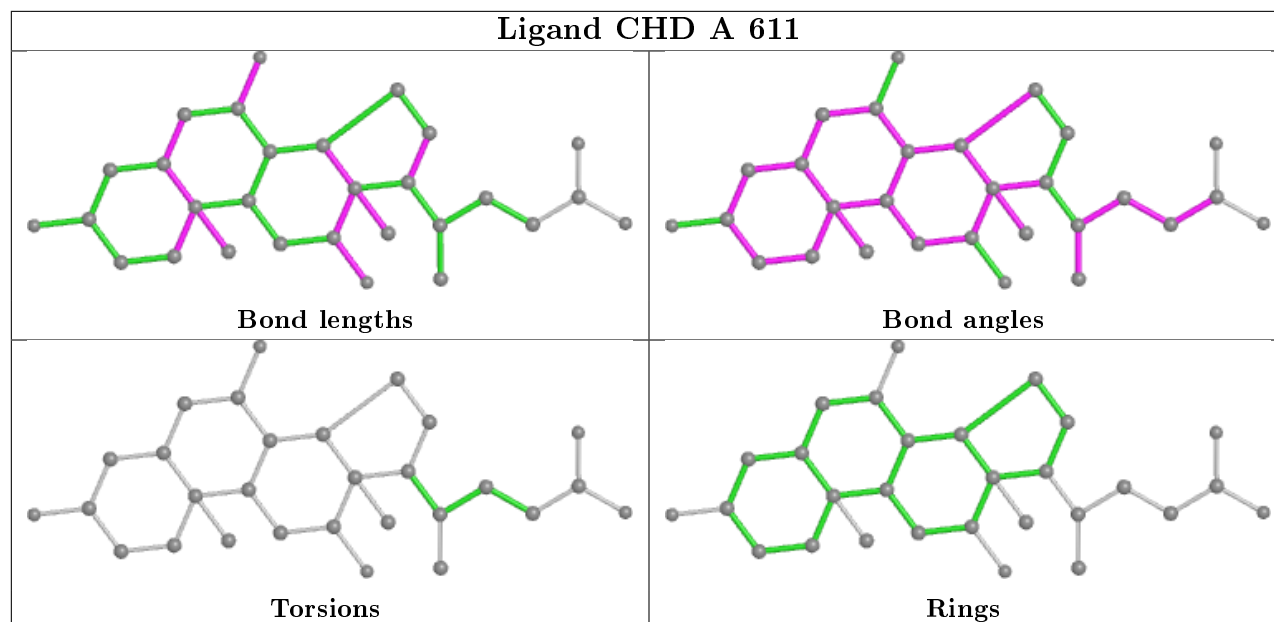
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 0BR B 612



Ligand CHD B 611





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	477/550 (86%)	-0.30	1 (0%) 95 87	44, 62, 94, 139	0
1	B	485/550 (88%)	-0.34	4 (0%) 86 65	49, 67, 102, 145	0
2	M	56/75 (74%)	-0.09	0 100 100	51, 80, 109, 123	0
2	N	55/75 (73%)	-0.04	2 (3%) 42 17	53, 87, 123, 136	0
3	C	82/89 (92%)	0.74	9 (10%) 5 2	85, 129, 154, 156	6 (7%)
3	D	67/89 (75%)	2.31	38 (56%) 0 0	99, 144, 165, 171	5 (7%)
All	All	1222/1428 (85%)	-0.08	54 (4%) 34 13	44, 69, 143, 171	11 (0%)

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	361	ASN	6.2
3	D	370	VAL	5.6
3	D	363	LEU	5.4
3	D	396	MET	5.1
3	D	373	CYS	4.9
3	D	355	ILE	4.6
3	C	363	LEU	4.4
3	D	399	THR	4.3
3	D	389	GLN	4.1
3	D	362	SER	4.0
3	D	392	LYS	3.8
3	D	359	ILE	3.8
3	D	356	HIS	3.5
3	D	372	ARG	3.5
3	D	385	VAL	3.5
3	D	377	LEU	3.5
3	D	397	ILE	3.5
3	D	360	LYS	3.4
3	D	394	THR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	361	ASN	3.3
3	D	403	ILE	3.2
3	D	420	TYR	3.2
3	D	380	LEU	3.2
3	C	366	ASP	3.2
3	D	375	GLU	3.2
3	C	408	VAL	3.0
1	B	429	THR	3.0
3	D	390	ALA	2.9
3	C	368	LEU	2.9
3	D	374	ILE	2.8
3	D	401	LYS	2.8
3	D	415	LYS	2.8
3	D	382	SER	2.8
3	D	358	GLU	2.8
3	D	400	LEU	2.8
3	D	391	GLN	2.8
3	D	393	HIS	2.8
3	D	384	GLN	2.8
3	C	367	ASN	2.7
3	D	388	GLN	2.7
3	D	402	LYS	2.6
3	D	383	LEU	2.6
3	D	357	ALA	2.5
2	N	132	VAL	2.4
1	A	57	ASN	2.4
3	D	379	GLU	2.3
3	C	362	SER	2.3
1	B	71	PRO	2.2
1	B	577	LEU	2.1
3	C	353	GLN	2.1
1	B	69	PRO	2.1
3	D	353	GLN	2.0
3	C	389	GLN	2.0
2	N	128	ARG	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

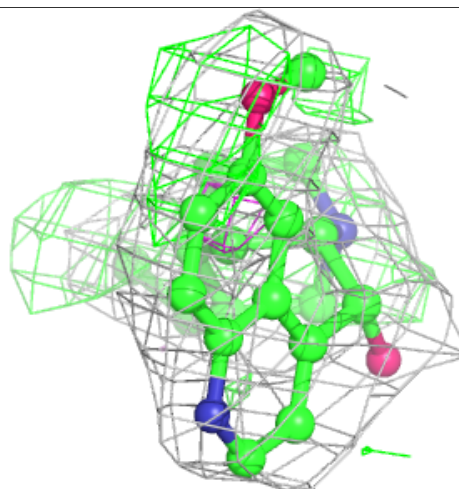
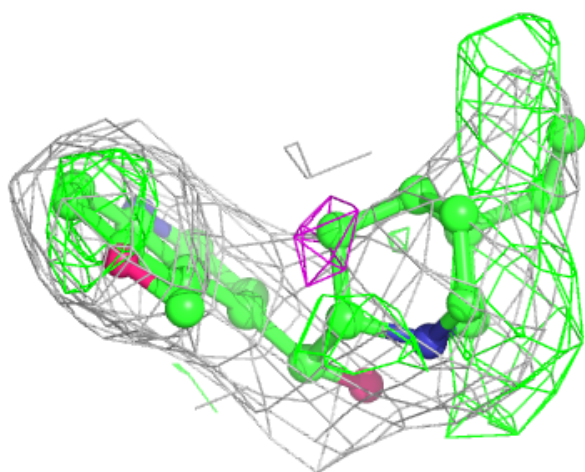
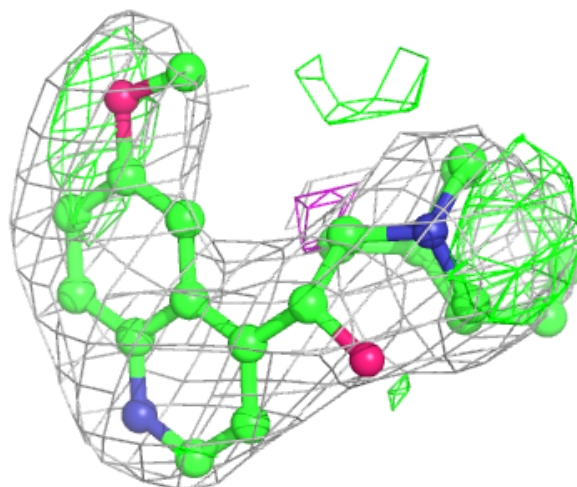
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GGB	C	109	12/12	0.69	0.40	115,126,131,132	0
7	GLV	D	114	5/5	0.80	0.31	109,110,110,111	0
7	GLV	A	616	5/5	0.81	0.34	61,74,76,88	2
7	GLV	B	616	5/5	0.85	0.28	64,65,76,78	1
5	GGB	B	615	12/12	0.86	0.33	76,84,106,107	6
8	SO4	N	154	5/5	0.87	0.18	119,120,135,137	0
5	GGB	A	613	12/12	0.87	0.30	67,87,98,100	4
5	GGB	C	108	12/12	0.87	0.33	113,120,132,133	0
8	SO4	B	617	5/5	0.88	0.18	114,115,124,136	0
7	GLV	C	113	5/5	0.88	0.16	88,94,100,101	0
5	GGB	A	614	12/12	0.88	0.25	78,93,108,108	5
7	GLV	A	615	5/5	0.90	0.26	57,64,71,76	1
6	0BR	A	612	24/24	0.91	0.31	54,61,67,70	7
6	0BR	B	612	24/24	0.91	0.28	53,61,67,72	0
8	SO4	M	154	5/5	0.93	0.12	107,122,128,136	0
8	SO4	B	618	5/5	0.93	0.11	93,95,98,114	0
8	SO4	A	618	5/5	0.94	0.14	84,100,102,114	0
7	GLV	A	617	5/5	0.94	0.17	72,73,85,88	1
4	CHD	A	611	29/29	0.94	0.29	55,64,72,74	5
8	SO4	A	619	5/5	0.94	0.13	80,88,103,113	0
8	SO4	N	1	5/5	0.95	0.11	89,95,105,115	0
4	CHD	B	611	29/29	0.95	0.27	52,62,75,77	6
8	SO4	M	2	5/5	0.96	0.14	87,88,103,105	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.

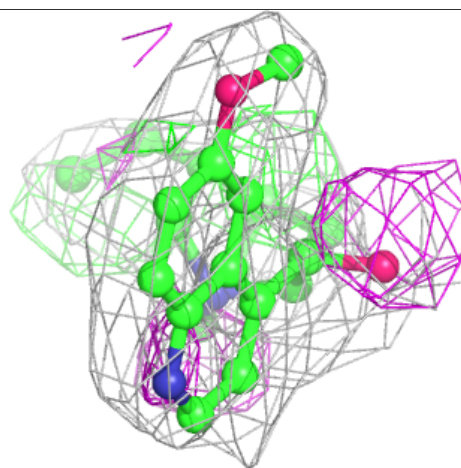
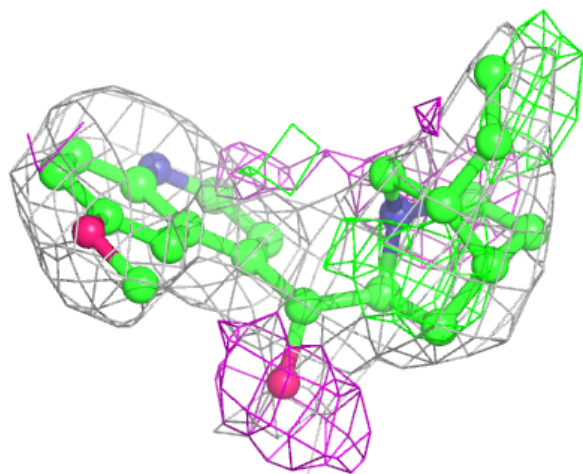
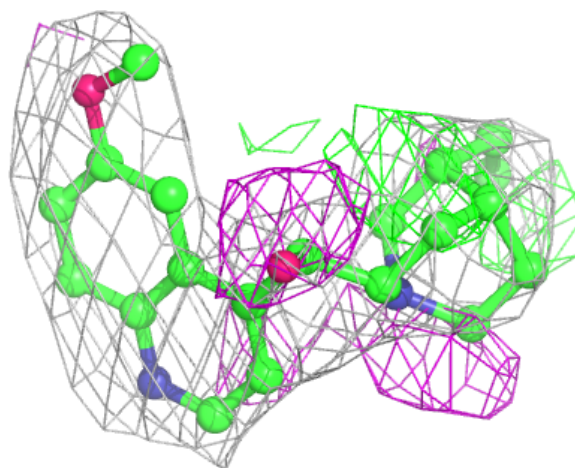
Electron density around 0BR A 612:

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



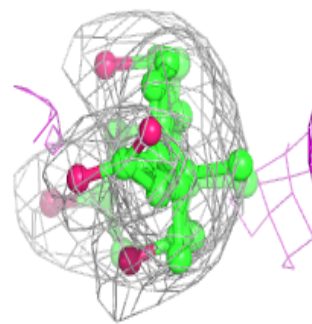
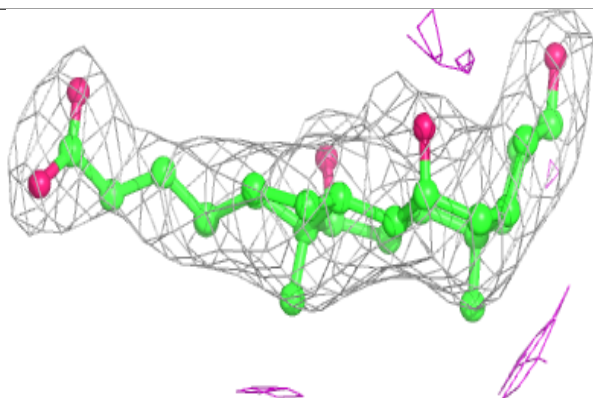
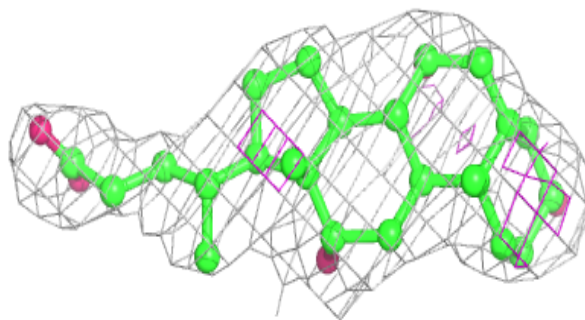
Electron density around 0BR B 612:

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

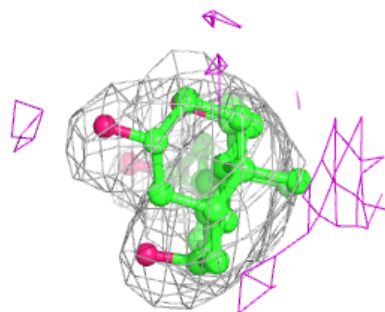
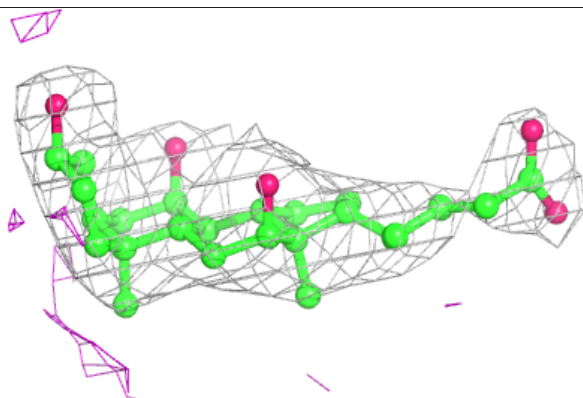
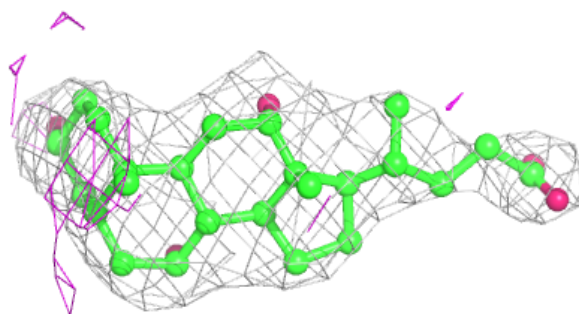


Electron density around CHD A 611:

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

**Electron density around CHD B 611:**

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



6.5 Other polymers

There are no such residues in this entry.