



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 11:12 AM UTC

PDB ID : 3DPM / pdb_00003dpm
Title : Structure of mature CPAF complexed with lactacystin
Authors : Chai, J.; Huang, Z.
Deposited on : 2008-07-09
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

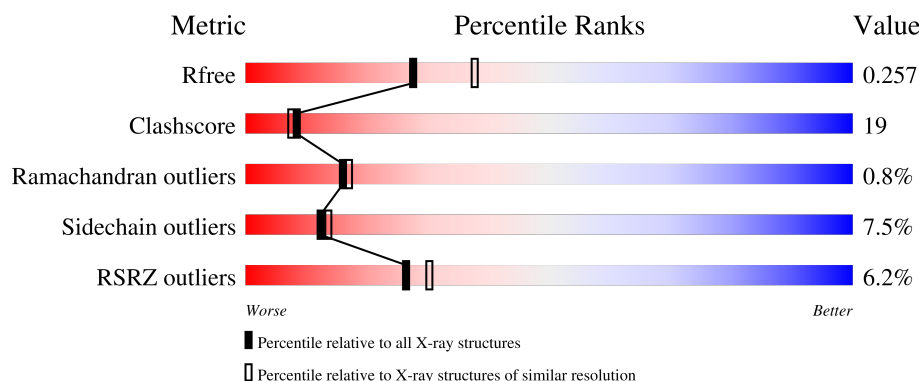
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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

Mol	Chain	Length	Quality of chain
1	A	583	
1	B	583	

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
2	LAS	A	800	-	-	X	-
2	LAS	B	800	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8559 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.

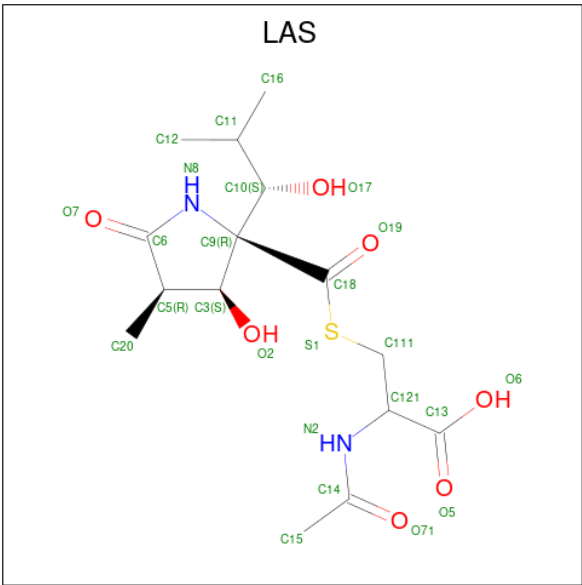
- Molecule 1 is a protein called Protein CT_858.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total	C	N	O	S	0	0	0
			4110	2630	689	778	13			
1	B	522	Total	C	N	O	S	0	0	0
			4110	2630	689	778	13			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	610	HIS	-	expression tag	UNP O84866
A	611	HIS	-	expression tag	UNP O84866
A	612	HIS	-	expression tag	UNP O84866
A	613	HIS	-	expression tag	UNP O84866
A	614	HIS	-	expression tag	UNP O84866
A	615	HIS	-	expression tag	UNP O84866
B	610	HIS	-	expression tag	UNP O84866
B	611	HIS	-	expression tag	UNP O84866
B	612	HIS	-	expression tag	UNP O84866
B	613	HIS	-	expression tag	UNP O84866
B	614	HIS	-	expression tag	UNP O84866
B	615	HIS	-	expression tag	UNP O84866

- Molecule 2 is N-acetyl-S-({(2R,3S,4R)-3-hydroxy-2-[(1S)-1-hydroxy-2-methylpropyl]-4-methyl-5-oxopyrrolidin-2-yl}carbonyl)cysteine (CCD ID: LAS) (formula: C₁₅H₂₄N₂O₇S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	10	1	4		
2	B	1	Total	C	N	O	0	0
			15	10	1	4		

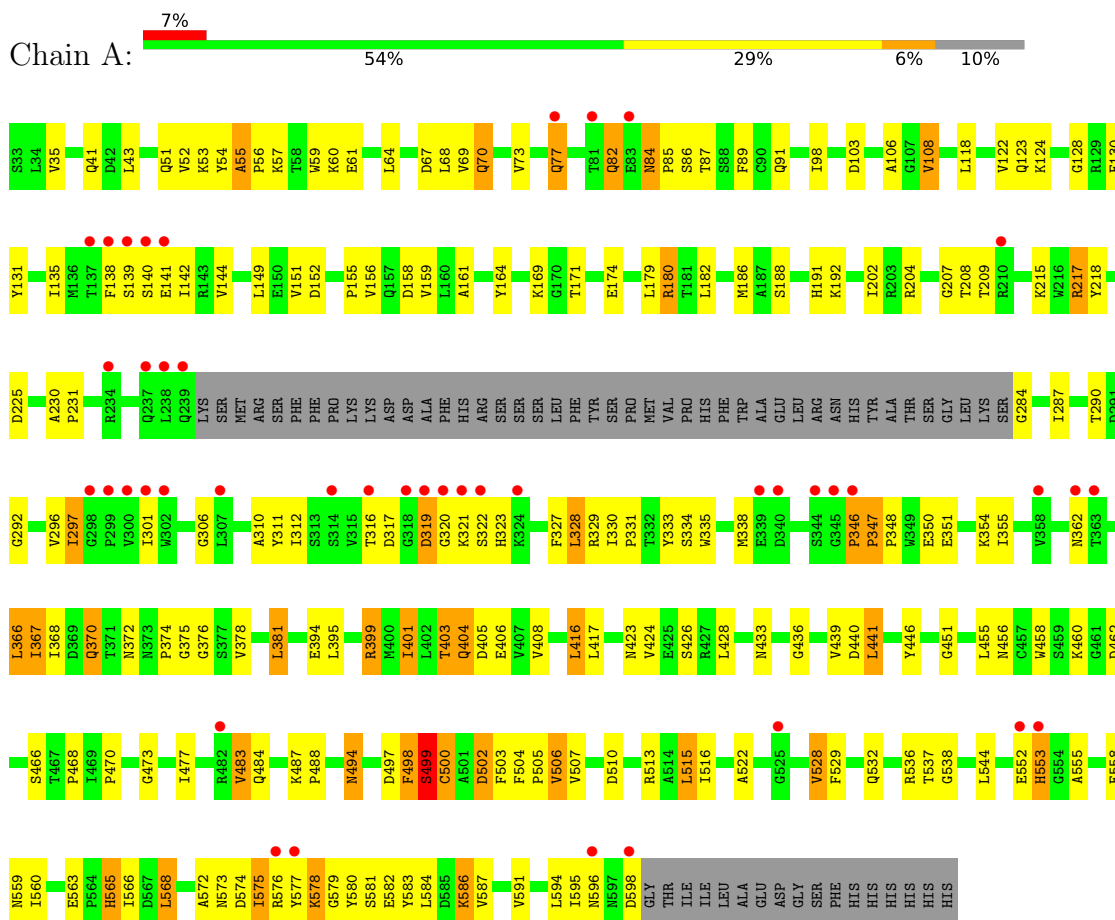
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	142	Total	O	0	0
			142	142		
3	B	167	Total	O	0	0
			167	167		

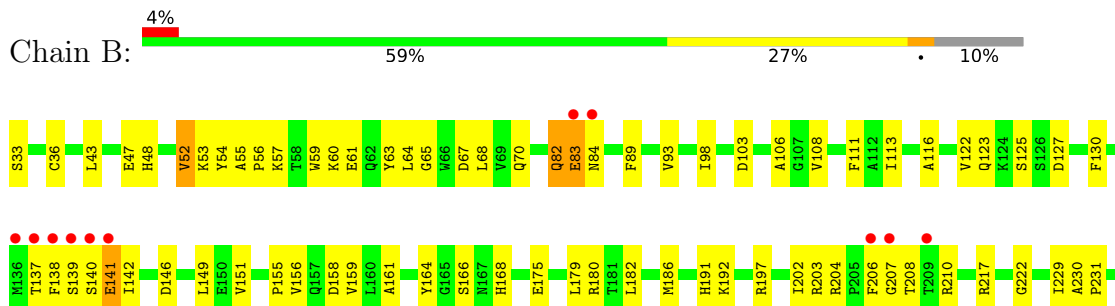
3 Residue-property plots

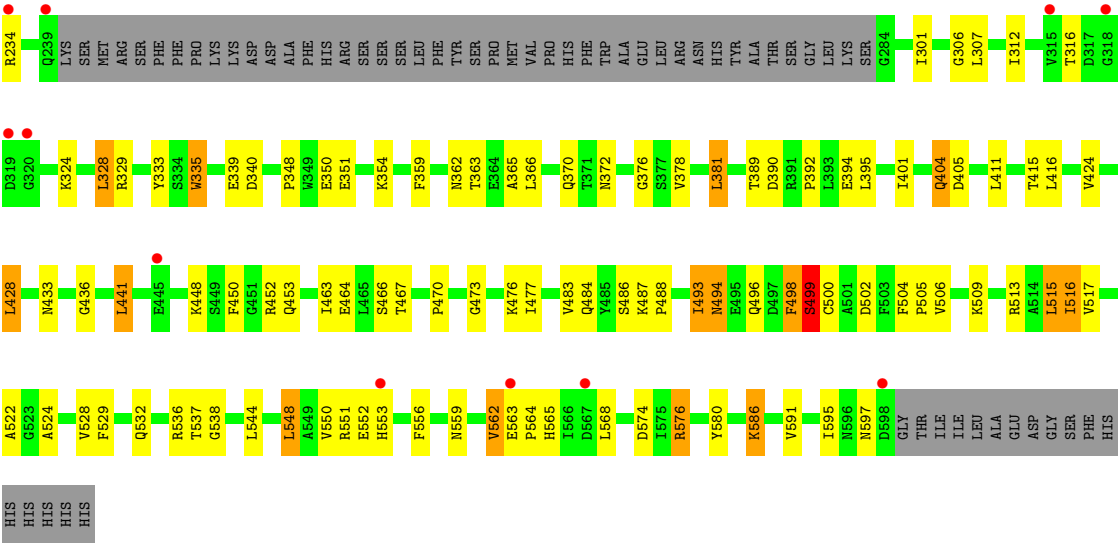
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Protein CT_858



• Molecule 1: Protein CT_858





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	63.64Å 112.07Å 164.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.35 20.00 – 2.35	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.35) 99.4 (20.00-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.259 0.228 , 0.257	Depositor DCC
R_{free} test set	1500 reflections (2.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.2	Xtriage
Anisotropy	0.512	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8559	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	0.48	2/4208 (0.0%)	0.97	25/5720 (0.4%)
1	B	0.50	2/4208 (0.0%)	0.97	11/5720 (0.2%)
All	All	0.49	4/8416 (0.0%)	0.97	36/11440 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	499	SER	C-N	8.56	1.45	1.33
1	B	498	PHE	C-N	8.38	1.45	1.33
1	B	499	SER	C-N	8.31	1.45	1.33
1	A	498	PHE	C-N	8.28	1.45	1.33

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	192	LYS	N-CA-C	-7.73	96.98	109.96
1	A	217	ARG	N-CA-C	-7.50	97.05	108.67
1	A	346	PRO	CA-C-N	7.36	124.96	119.66
1	A	346	PRO	C-N-CA	7.36	124.96	119.66
1	A	52	VAL	N-CA-C	7.32	117.85	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	ILE	N-CA-C	7.23	117.31	110.74
1	B	441	LEU	N-CA-C	-6.62	104.15	111.82
1	A	84	ASN	CA-C-N	6.57	126.54	119.78
1	A	84	ASN	C-N-CA	6.57	126.54	119.78
1	B	467	THR	N-CA-C	-6.42	101.22	110.08
1	A	207	GLY	N-CA-C	6.32	122.21	114.69
1	B	522	ALA	N-CA-C	6.22	118.86	111.71
1	A	483	VAL	N-CA-C	6.09	116.64	108.11
1	B	502	ASP	N-CA-C	-5.74	104.47	112.45
1	B	362	ASN	N-CA-C	5.72	119.93	111.87
1	A	502	ASP	N-CA-C	-5.63	104.63	112.45
1	A	537	THR	N-CA-C	-5.61	106.48	113.38
1	A	362	ASN	N-CA-C	5.59	119.64	112.26
1	A	565	HIS	N-CA-C	-5.56	105.13	111.14
1	A	403	THR	N-CA-C	-5.52	101.02	109.41
1	A	55	ALA	CA-C-N	-5.48	112.99	119.84
1	A	55	ALA	C-N-CA	-5.48	112.99	119.84
1	A	218	TYR	N-CA-C	5.44	117.83	109.07
1	B	52	VAL	CB-CA-C	-5.43	106.28	111.44
1	A	405	ASP	N-CA-C	-5.33	105.37	111.07
1	A	500	CYS	N-CA-C	5.32	119.25	112.34
1	A	522	ALA	N-CA-C	5.31	117.75	111.33
1	B	335	TRP	N-CA-C	5.29	117.74	111.33
1	B	65	GLY	N-CA-C	-5.25	107.00	115.08
1	A	399	ARG	N-CA-C	-5.18	100.72	108.96
1	A	192	LYS	N-CA-C	-5.15	100.91	109.46
1	A	498	PHE	CA-C-N	-5.15	111.70	121.54
1	A	498	PHE	C-N-CA	-5.15	111.70	121.54
1	B	463	ILE	N-CA-C	5.09	118.04	113.10
1	A	347	PRO	N-CA-C	5.06	115.99	110.58
1	B	553	HIS	N-CA-C	5.00	119.11	113.15

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	499	SER	Mainchain
1	B	499	SER	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4110	0	4047	166	0
1	B	4110	0	4047	154	0
2	A	15	0	16	10	0
2	B	15	0	16	10	0
3	A	142	0	0	3	0
3	B	167	0	0	2	0
All	All	8559	0	8126	312	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 19.

All (312) 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:A:553:HIS:CE1	1:A:555:ALA:HB3	1.73	1.21
1:A:553:HIS:CE1	1:A:555:ALA:CB	2.45	0.99
1:A:124:LYS:HE2	1:A:128:GLY:HA2	1.49	0.94
1:B:516:ILE:H	1:B:565:HIS:HD2	1.12	0.94
1:A:553:HIS:HE1	1:A:555:ALA:HB3	1.08	0.94
1:A:60:LYS:HZ2	1:A:559:ASN:HD21	1.18	0.90
1:A:82:GLN:HG3	1:A:89:PHE:CZ	2.09	0.87
1:B:359:PHE:O	1:B:363:THR:HG22	1.77	0.84
1:A:516:ILE:H	1:A:565:HIS:HD2	1.25	0.84
1:A:378:VAL:HG22	2:A:800:LAS:H16	1.63	0.79
1:B:576:ARG:HH11	1:B:576:ARG:HB3	1.47	0.79
1:A:186:MET:H	1:A:191:HIS:HD2	1.29	0.78
1:A:60:LYS:NZ	1:A:559:ASN:HD21	1.82	0.77
1:A:366:LEU:HD13	1:A:368:ILE:HD11	1.66	0.76
1:B:516:ILE:H	1:B:565:HIS:CD2	2.02	0.76
1:B:500:CYS:SG	2:B:800:LAS:C16	2.74	0.75
1:B:378:VAL:HG22	2:B:800:LAS:H16	1.70	0.74
1:A:587:VAL:O	1:A:591:VAL:HG23	1.87	0.73
1:B:515:LEU:HD12	1:B:517:VAL:HG23	1.71	0.73
1:B:365:ALA:HB2	1:B:595:ILE:HD11	1.72	0.72
1:A:59:TRP:HE1	1:A:559:ASN:HD22	1.37	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:LEU:HD23	1:A:169:LYS:HD2	1.71	0.72
1:B:378:VAL:CG2	2:B:800:LAS:H12	2.19	0.72
1:A:536:ARG:HA	1:B:404:GLN:HE22	1.55	0.71
1:B:591:VAL:O	1:B:595:ILE:HD13	1.91	0.70
1:B:186:MET:H	1:B:191:HIS:HD2	1.38	0.70
1:A:367:ILE:HD11	1:A:591:VAL:HG21	1.71	0.70
1:B:404:GLN:H	1:B:404:GLN:NE2	1.89	0.70
2:B:800:LAS:C18	2:B:800:LAS:H16B	2.21	0.70
1:A:462:ASP:HB2	1:B:234:ARG:HH21	1.55	0.69
1:A:404:GLN:HE22	1:B:536:ARG:HA	1.58	0.69
1:A:67:ASP:OD2	1:A:70:GLN:HB2	1.92	0.69
1:B:203:ARG:CZ	1:B:207:GLY:HA2	2.23	0.68
1:A:516:ILE:H	1:A:565:HIS:CD2	2.09	0.68
1:A:186:MET:H	1:A:191:HIS:CD2	2.12	0.68
1:A:498:PHE:O	1:A:499:SER:C	2.37	0.68
1:B:54:TYR:CZ	1:B:56:PRO:HG2	2.27	0.68
1:A:155:PRO:HG2	1:A:158:ASP:OD2	1.94	0.67
1:A:297:ILE:HD13	1:A:297:ILE:H	1.60	0.67
1:B:378:VAL:HG21	2:B:800:LAS:H12	1.77	0.67
1:B:378:VAL:CG2	2:B:800:LAS:H16	2.25	0.66
1:B:563:GLU:CD	1:B:563:GLU:H	2.04	0.66
1:A:433:ASN:HD22	1:A:436:GLY:H	1.43	0.66
1:A:503:PHE:O	1:A:506:VAL:HG12	1.96	0.66
1:B:493:ILE:HD13	1:B:517:VAL:O	1.96	0.66
1:A:378:VAL:CG2	2:A:800:LAS:H16	2.26	0.65
1:B:57:LYS:O	1:B:61:GLU:HG3	1.96	0.65
1:A:574:ASP:OD1	1:A:580:TYR:HA	1.97	0.65
1:A:433:ASN:ND2	1:A:436:GLY:H	1.94	0.64
1:A:161:ALA:HA	1:A:164:TYR:CD2	2.32	0.64
1:A:335:TRP:HB2	1:A:348:PRO:HG3	1.80	0.64
1:A:51:GLN:NE2	1:A:68:LEU:HD23	2.13	0.64
1:A:171:THR:OG1	1:A:174:GLU:HG3	1.98	0.63
1:B:576:ARG:HH11	1:B:576:ARG:CB	2.11	0.63
1:A:376:GLY:O	2:A:800:LAS:H16B	1.98	0.63
1:A:433:ASN:HA	1:A:439:VAL:HG23	1.81	0.63
1:B:82:GLN:O	1:B:83:GLU:HG3	1.98	0.63
1:B:328:LEU:C	1:B:328:LEU:HD13	2.24	0.62
1:A:367:ILE:HD11	1:A:591:VAL:CG2	2.29	0.62
1:B:83:GLU:O	1:B:84:ASN:C	2.42	0.62
1:B:433:ASN:HD22	1:B:436:GLY:H	1.45	0.62
1:B:186:MET:H	1:B:191:HIS:CD2	2.18	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ASP:HB2	1:B:234:ARG:NH2	2.14	0.61
1:A:316:THR:HG22	1:A:322:SER:OG	1.99	0.61
1:A:131:TYR:CE2	1:A:576:ARG:HG2	2.35	0.61
1:A:323:HIS:ND1	1:A:595:ILE:HG21	2.15	0.61
1:B:509:LYS:NZ	1:B:563:GLU:HG2	2.15	0.61
1:B:493:ILE:HD12	1:B:516:ILE:HG23	1.81	0.61
1:A:122:VAL:HG11	1:A:130:PHE:HB3	1.83	0.61
1:A:376:GLY:N	2:A:800:LAS:O19	2.35	0.60
1:A:124:LYS:CE	1:A:128:GLY:HA2	2.27	0.60
1:B:53:LYS:HB3	1:B:529:PHE:CZ	2.35	0.60
1:B:500:CYS:SG	2:B:800:LAS:H16	2.41	0.60
1:B:365:ALA:CB	1:B:595:ILE:HD11	2.32	0.60
1:A:404:GLN:CG	1:B:538:GLY:HA2	2.32	0.59
1:A:500:CYS:SG	2:A:800:LAS:C16	2.91	0.59
1:A:82:GLN:HG3	1:A:89:PHE:CE2	2.37	0.59
1:B:138:PHE:O	1:B:140:SER:N	2.35	0.59
1:A:568:LEU:HD11	1:A:586:LYS:HB3	1.84	0.59
1:A:529:PHE:CZ	1:A:544:LEU:HB2	2.38	0.59
1:B:335:TRP:HB2	1:B:348:PRO:HG3	1.85	0.58
1:B:515:LEU:HD12	1:B:517:VAL:CG2	2.33	0.58
1:A:54:TYR:CZ	1:A:56:PRO:HG2	2.37	0.58
1:A:563:GLU:CD	1:A:563:GLU:H	2.12	0.58
1:B:487:LYS:HB3	1:B:488:PRO:HD2	1.85	0.58
1:A:87:THR:O	1:A:91:GLN:HG3	2.04	0.58
1:B:500:CYS:SG	2:B:800:LAS:H16B	2.44	0.57
1:A:500:CYS:SG	2:A:800:LAS:H16A	2.44	0.57
1:B:376:GLY:N	2:B:800:LAS:O19	2.32	0.57
1:A:53:LYS:HB3	1:A:529:PHE:CZ	2.39	0.57
1:A:135:ILE:HD11	1:A:142:ILE:HG22	1.87	0.56
1:A:60:LYS:NZ	1:A:559:ASN:ND2	2.53	0.56
1:A:180:ARG:NH1	3:A:801:HOH:O	2.36	0.56
1:B:404:GLN:H	1:B:404:GLN:CD	2.13	0.56
1:B:470:PRO:HG2	1:B:473:GLY:HA2	1.87	0.56
1:B:506:VAL:HG23	1:B:562:VAL:CG2	2.36	0.56
1:B:155:PRO:HG2	1:B:158:ASP:OD2	2.06	0.56
1:A:306:GLY:HA3	1:A:351:GLU:OE2	2.06	0.56
1:B:141:GLU:O	1:B:204:ARG:NH2	2.38	0.56
1:B:493:ILE:HD11	1:B:564:PRO:HB3	1.86	0.56
1:A:287:ILE:HG22	1:A:374:PRO:HD3	1.88	0.55
1:B:401:ILE:HG13	1:B:464:GLU:O	2.06	0.55
1:A:536:ARG:HA	1:B:404:GLN:NE2	2.20	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:O	1:A:61:GLU:HG3	2.07	0.55
1:B:67:ASP:OD2	1:B:70:GLN:HB3	2.07	0.55
1:A:316:THR:HA	1:A:322:SER:HA	1.88	0.55
1:B:55:ALA:HB2	1:B:401:ILE:HD13	1.88	0.55
1:A:98:ILE:HG13	1:A:108:VAL:HG22	1.88	0.55
1:A:138:PHE:O	1:A:140:SER:N	2.40	0.55
2:A:800:LAS:H16A	2:A:800:LAS:C18	2.38	0.54
1:B:122:VAL:HG11	1:B:130:PHE:HB3	1.90	0.54
1:A:470:PRO:HG2	1:A:473:GLY:HA2	1.88	0.54
1:B:424:VAL:HG12	1:B:428:LEU:HD22	1.88	0.54
1:A:494:ASN:C	1:A:494:ASN:HD22	2.14	0.54
1:A:573:ASN:OD1	1:A:576:ARG:NH2	2.41	0.54
1:A:284:GLY:N	1:A:292:GLY:O	2.41	0.54
1:B:493:ILE:HD13	1:B:493:ILE:H	1.73	0.53
2:B:800:LAS:C16	2:B:800:LAS:C18	2.86	0.53
1:A:131:TYR:CD2	1:A:576:ARG:HG2	2.44	0.53
1:A:297:ILE:HG22	1:A:584:LEU:HD22	1.91	0.53
1:B:350:GLU:O	1:B:354:LYS:HG2	2.07	0.53
1:A:290:THR:O	1:A:329:ARG:HD3	2.08	0.53
1:B:98:ILE:HG13	1:B:108:VAL:CG2	2.39	0.53
1:A:487:LYS:HB3	1:A:488:PRO:HD2	1.91	0.53
1:A:404:GLN:HG3	1:B:538:GLY:HA2	1.90	0.52
1:B:576:ARG:CB	1:B:576:ARG:NH1	2.72	0.52
1:A:456:ASN:ND2	1:A:460:LYS:HE3	2.25	0.52
1:B:197:ARG:HG3	1:B:197:ARG:HH11	1.75	0.52
1:B:202:ILE:HD12	1:B:202:ILE:C	2.34	0.52
1:B:149:LEU:O	1:B:156:VAL:HG23	2.11	0.51
1:A:333:TYR:CE2	1:A:381:LEU:HD23	2.45	0.51
1:A:451:GLY:O	1:A:455:LEU:HG	2.10	0.51
1:A:538:GLY:HA2	1:B:404:GLN:CG	2.40	0.51
1:A:321:LYS:HD2	1:A:322:SER:N	2.26	0.51
1:B:161:ALA:HA	1:B:164:TYR:CE2	2.46	0.51
1:B:333:TYR:CE2	1:B:381:LEU:HD23	2.46	0.51
1:A:230:ALA:N	1:A:231:PRO:HD2	2.25	0.51
1:B:103:ASP:HB3	1:B:106:ALA:HB3	1.93	0.51
1:A:404:GLN:NE2	1:A:404:GLN:H	2.09	0.51
2:A:800:LAS:H11	3:A:907:HOH:O	2.11	0.51
1:A:494:ASN:C	1:A:494:ASN:ND2	2.69	0.50
1:A:122:VAL:CG1	1:A:130:PHE:HB3	2.41	0.50
1:B:528:VAL:HG12	1:B:529:PHE:N	2.26	0.50
1:B:56:PRO:O	1:B:60:LYS:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:N	1:A:142:ILE:HD12	2.27	0.50
1:B:55:ALA:CB	1:B:401:ILE:HD13	2.42	0.50
1:A:558:GLU:O	1:A:559:ASN:HB2	2.12	0.49
1:B:138:PHE:CD1	1:B:138:PHE:C	2.89	0.49
1:A:440:ASP:OD2	1:A:441:LEU:N	2.46	0.49
1:B:122:VAL:HG12	1:B:123:GLN:N	2.27	0.49
1:B:506:VAL:HG23	1:B:562:VAL:HG21	1.95	0.49
1:A:568:LEU:HD13	1:A:583:TYR:CD1	2.46	0.49
1:B:54:TYR:CE2	1:B:56:PRO:HG2	2.47	0.49
1:B:234:ARG:HD3	1:B:234:ARG:H	1.78	0.49
1:A:583:TYR:O	1:A:587:VAL:HG23	2.13	0.49
1:B:395:LEU:HD11	1:B:477:ILE:HG13	1.95	0.49
2:A:800:LAS:C16	2:A:800:LAS:C18	2.91	0.49
1:B:113:ILE:HG12	1:B:222:GLY:H	1.77	0.49
1:A:350:GLU:O	1:A:354:LYS:HG2	2.13	0.48
1:B:493:ILE:HD12	1:B:516:ILE:CG2	2.42	0.48
1:B:498:PHE:O	1:B:499:SER:C	2.54	0.48
1:A:404:GLN:NE2	1:B:536:ARG:HA	2.26	0.48
1:A:381:LEU:O	1:A:381:LEU:HD22	2.14	0.48
1:A:149:LEU:O	1:A:156:VAL:HG23	2.14	0.48
1:B:301:ILE:CD1	1:B:324:LYS:HD3	2.44	0.48
1:B:411:LEU:O	1:B:415:THR:HG23	2.13	0.48
1:B:161:ALA:HA	1:B:164:TYR:CD2	2.48	0.48
1:B:450:PHE:HA	3:B:1030:HOH:O	2.14	0.48
1:B:59:TRP:HE1	1:B:559:ASN:HD22	1.61	0.48
1:B:433:ASN:ND2	1:B:436:GLY:H	2.09	0.47
1:A:310:ALA:HA	1:A:327:PHE:O	2.14	0.47
1:B:206:PHE:HE1	1:B:208:THR:HG1	1.61	0.47
1:A:144:VAL:HG11	1:A:578:LYS:HD3	1.95	0.47
1:A:55:ALA:CB	1:A:401:ILE:HD13	2.44	0.47
1:A:297:ILE:H	1:A:297:ILE:CD1	2.26	0.47
1:A:515:LEU:HD12	1:A:594:LEU:HD11	1.97	0.47
1:B:595:ILE:HD12	1:B:595:ILE:N	2.29	0.47
1:B:60:LYS:HZ2	1:B:559:ASN:HD21	1.62	0.47
1:B:312:ILE:HD11	1:B:359:PHE:CD2	2.49	0.47
1:A:596:ASN:O	1:A:598:ASP:OD1	2.32	0.47
1:B:60:LYS:NZ	1:B:559:ASN:HD21	2.13	0.47
1:A:35:VAL:HG11	1:A:85:PRO:O	2.15	0.47
1:A:86:SER:HB2	1:A:225:ASP:OD2	2.15	0.47
1:A:77:GLN:OE1	1:A:77:GLN:HA	2.14	0.47
1:A:499:SER:O	1:A:502:ASP:HB2	2.16	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:HIS:CE1	1:A:555:ALA:H	2.33	0.47
1:B:203:ARG:NH2	1:B:207:GLY:HA2	2.30	0.47
1:B:137:THR:OG1	1:B:138:PHE:N	2.45	0.46
1:A:372:ASN:H	1:A:494:ASN:HD21	1.62	0.46
1:B:537:THR:O	1:B:537:THR:HG22	2.15	0.46
1:B:586:LYS:HD3	1:B:586:LYS:C	2.40	0.46
1:A:204:ARG:HG2	1:A:208:THR:O	2.16	0.46
1:B:448:LYS:HB3	1:B:452:ARG:HH12	1.80	0.46
1:A:586:LYS:O	1:A:586:LYS:HD3	2.15	0.46
1:B:82:GLN:HG3	1:B:89:PHE:CE2	2.51	0.46
1:B:116:ALA:HA	1:B:217:ARG:O	2.15	0.46
1:A:103:ASP:HB3	1:A:106:ALA:HB3	1.97	0.46
1:A:504:PHE:HB3	1:A:505:PRO:CD	2.45	0.46
1:B:504:PHE:HB3	1:B:505:PRO:CD	2.45	0.46
1:B:516:ILE:N	1:B:516:ILE:CD1	2.79	0.46
1:A:404:GLN:H	1:A:404:GLN:CD	2.24	0.46
1:A:458:TRP:O	1:B:229:ILE:HD13	2.16	0.46
1:A:296:VAL:HA	1:A:311:TYR:OH	2.16	0.46
1:B:151:VAL:HB	1:B:159:VAL:HG21	1.98	0.46
1:B:146:ASP:OD1	1:B:204:ARG:NH1	2.49	0.46
1:B:197:ARG:HG3	1:B:197:ARG:NH1	2.31	0.46
1:A:141:GLU:O	1:A:204:ARG:NH1	2.38	0.46
1:A:426:SER:OG	1:A:441:LEU:HA	2.16	0.46
1:B:448:LYS:HE2	1:B:452:ARG:HH22	1.80	0.46
1:A:215:LYS:O	1:A:217:ARG:NH1	2.49	0.45
1:A:301:ILE:HG12	1:A:312:ILE:O	2.16	0.45
1:A:395:LEU:HD21	1:A:477:ILE:HG12	1.98	0.45
1:A:328:LEU:HD13	1:A:328:LEU:C	2.40	0.45
1:B:202:ILE:HD12	1:B:202:ILE:O	2.16	0.45
1:B:504:PHE:HB3	1:B:505:PRO:HD3	1.98	0.45
1:A:123:GLN:CD	1:A:575:ILE:HD12	2.41	0.45
1:B:339:GLU:O	1:B:340:ASP:HB2	2.16	0.45
1:A:460:LYS:O	1:B:234:ARG:NH1	2.50	0.45
1:B:515:LEU:CD1	1:B:517:VAL:HG23	2.44	0.45
1:A:151:VAL:HB	1:A:159:VAL:HG21	1.98	0.45
1:A:319:ASP:C	1:A:321:LYS:H	2.24	0.45
1:A:553:HIS:CE1	1:A:555:ALA:HB2	2.47	0.45
1:B:499:SER:H	1:B:524:ALA:HB3	1.81	0.45
1:B:506:VAL:HG23	1:B:562:VAL:HG22	1.99	0.45
1:B:63:TYR:CD2	1:B:64:LEU:HD23	2.52	0.44
1:A:408:VAL:HG21	1:B:111:PHE:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:NZ	1:B:61:GLU:OE2	2.50	0.44
1:B:141:GLU:HG2	1:B:204:ARG:NH2	2.33	0.44
1:B:306:GLY:HA3	1:B:351:GLU:OE2	2.17	0.44
1:A:69:VAL:O	1:A:73:VAL:HG23	2.17	0.44
1:B:55:ALA:HA	1:B:401:ILE:CD1	2.47	0.44
1:B:140:SER:C	1:B:142:ILE:H	2.24	0.44
1:A:328:LEU:HD11	1:A:330:ILE:CD1	2.48	0.44
1:B:392:PRO:HB2	1:B:476:LYS:HD3	1.99	0.44
1:B:498:PHE:CD1	1:B:498:PHE:N	2.85	0.44
1:A:351:GLU:O	1:A:355:ILE:HG12	2.17	0.44
1:A:98:ILE:HG13	1:A:108:VAL:CG2	2.47	0.44
1:A:538:GLY:HA2	1:B:404:GLN:HG2	2.00	0.44
1:B:301:ILE:HD13	1:B:324:LYS:HD3	2.00	0.44
1:A:64:LEU:CD2	1:A:169:LYS:HD2	2.45	0.44
1:A:53:LYS:HE3	1:A:403:THR:HG23	2.00	0.44
1:A:82:GLN:HG2	3:A:841:HOH:O	2.17	0.44
1:A:144:VAL:HG11	1:A:578:LYS:CD	2.48	0.44
1:B:390:ASP:OD2	1:B:486:SER:CB	2.66	0.43
1:B:234:ARG:HD3	1:B:234:ARG:N	2.33	0.43
1:A:579:GLY:O	1:A:580:TYR:C	2.62	0.43
1:B:529:PHE:CZ	1:B:544:LEU:HB2	2.54	0.43
1:A:186:MET:HE2	1:A:188:SER:OG	2.18	0.43
1:B:140:SER:C	1:B:142:ILE:N	2.76	0.43
1:B:328:LEU:HD22	1:B:329:ARG:N	2.33	0.43
1:A:59:TRP:CH2	1:A:560:ILE:HD11	2.54	0.43
1:A:577:TYR:O	1:A:579:GLY:N	2.52	0.43
1:A:319:ASP:O	1:A:321:LYS:N	2.52	0.43
1:A:456:ASN:HD21	1:A:460:LYS:HE3	1.84	0.43
1:A:161:ALA:HA	1:A:164:TYR:CE2	2.54	0.42
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.91	0.42
1:B:33:SER:HB3	1:B:36:CYS:HB3	2.01	0.42
1:B:82:GLN:HB3	1:B:83:GLU:H	1.57	0.42
1:A:462:ASP:CG	1:A:466:SER:HA	2.45	0.42
1:A:577:TYR:N	1:A:577:TYR:CD2	2.86	0.42
1:B:47:GLU:HG3	1:B:68:LEU:HD11	2.01	0.42
1:A:394:GLU:HB2	1:A:552:GLU:OE2	2.19	0.42
1:A:399:ARG:HD2	1:A:468:PRO:HD3	2.00	0.42
1:B:548:LEU:HD13	1:B:556:PHE:CE2	2.55	0.42
1:A:209:THR:O	1:A:209:THR:HG23	2.20	0.42
1:A:566:ILE:N	1:A:566:ILE:HD12	2.35	0.42
1:B:89:PHE:O	1:B:93:VAL:HG23	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:125:SER:OG	1:B:127:ASP:OD2	2.34	0.42
1:B:301:ILE:HD11	1:B:312:ILE:HG21	2.01	0.42
1:A:123:GLN:NE2	1:A:575:ILE:HD12	2.34	0.42
1:B:48:HIS:O	1:B:52:VAL:HG23	2.18	0.42
1:A:572:ALA:O	1:A:576:ARG:HG3	2.20	0.42
1:B:168:HIS:HD2	3:B:928:HOH:O	2.03	0.42
1:A:297:ILE:HD13	1:A:297:ILE:N	2.30	0.42
1:B:381:LEU:HG	1:B:500:CYS:HB3	2.02	0.42
1:B:389:THR:O	1:B:484:GLN:HB3	2.19	0.42
1:A:59:TRP:HH2	1:A:560:ILE:HD11	1.85	0.41
1:A:399:ARG:CD	1:A:468:PRO:HD3	2.50	0.41
1:B:595:ILE:C	1:B:597:ASN:H	2.28	0.41
1:B:595:ILE:C	1:B:597:ASN:N	2.78	0.41
1:A:131:TYR:CZ	1:A:576:ARG:HD3	2.56	0.41
1:A:424:VAL:O	1:A:428:LEU:HD13	2.20	0.41
1:A:306:GLY:HA3	1:A:351:GLU:CD	2.45	0.41
1:A:370:GLN:O	1:A:497:ASP:OD1	2.39	0.41
1:B:208:THR:CG2	1:B:210:ARG:NE	2.83	0.41
1:B:595:ILE:N	1:B:595:ILE:CD1	2.84	0.41
1:B:180:ARG:HE	1:B:496:GLN:HE22	1.68	0.41
1:B:453:GLN:HE22	1:B:470:PRO:HD2	1.86	0.41
1:A:290:THR:HA	1:A:331:PRO:HB3	2.02	0.41
1:A:375:GLY:HA3	1:A:499:SER:HB3	2.03	0.41
1:A:573:ASN:HB2	1:A:582:GLU:OE2	2.20	0.41
1:B:574:ASP:CB	1:B:580:TYR:HA	2.51	0.41
1:A:416:LEU:HD22	1:A:416:LEU:O	2.21	0.41
1:B:55:ALA:HA	1:B:401:ILE:HD11	2.02	0.41
1:B:180:ARG:HA	1:B:180:ARG:HD3	1.76	0.41
1:B:230:ALA:HB3	1:B:231:PRO:CD	2.51	0.41
1:B:372:ASN:H	1:B:494:ASN:HD21	1.69	0.41
1:B:550:VAL:HG22	1:B:556:PHE:CD2	2.56	0.41
1:B:551:ARG:O	1:B:552:GLU:C	2.63	0.41
1:A:331:PRO:HG3	1:A:338:MET:HE3	2.03	0.41
1:B:424:VAL:HG12	1:B:428:LEU:CD2	2.50	0.41
1:B:494:ASN:ND2	1:B:494:ASN:C	2.79	0.41
1:A:346:PRO:HA	1:A:347:PRO:HD2	1.95	0.40
1:A:506:VAL:CG1	1:A:507:VAL:N	2.84	0.40
1:A:53:LYS:HE2	1:A:406:GLU:OE1	2.21	0.40
1:A:423:ASN:OD1	1:A:440:ASP:OD2	2.39	0.40
1:A:328:LEU:HD12	1:A:368:ILE:HD12	2.02	0.40
1:A:416:LEU:HD13	1:A:417:LEU:HG	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:528:VAL:HG13	2:A:800:LAS:H5	2.03	0.40
1:B:516:ILE:N	1:B:565:HIS:HD2	1.96	0.40
1:A:56:PRO:O	1:A:60:LYS:HG2	2.21	0.40
1:B:405:ASP:OD2	1:B:405:ASP:C	2.65	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	518/583 (89%)	488 (94%)	26 (5%)	4 (1%)	16	17
1	B	518/583 (89%)	489 (94%)	25 (5%)	4 (1%)	16	17
All	All	1036/1166 (89%)	977 (94%)	51 (5%)	8 (1%)	16	17

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	317	ASP
1	A	578	LYS
1	B	83	GLU
1	B	139	SER
1	A	139	SER
1	A	320	GLY
1	B	82	GLN
1	B	466	SER

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	452/506 (89%)	413 (91%)	39 (9%)	10	10
1	B	452/506 (89%)	423 (94%)	29 (6%)	16	18
All	All	904/1012 (89%)	836 (92%)	68 (8%)	12	13

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	43	LEU
1	A	70	GLN
1	A	77	GLN
1	A	82	GLN
1	A	84	ASN
1	A	108	VAL
1	A	152	ASP
1	A	179	LEU
1	A	180	ARG
1	A	182	LEU
1	A	202	ILE
1	A	297	ILE
1	A	319	ASP
1	A	328	LEU
1	A	334	SER
1	A	366	LEU
1	A	367	ILE
1	A	370	GLN
1	A	381	LEU
1	A	401	ILE
1	A	404	GLN
1	A	416	LEU
1	A	441	LEU
1	A	446	TYR
1	A	483	VAL
1	A	484	GLN
1	A	494	ASN
1	A	499	SER
1	A	506	VAL
1	A	510	ASP
1	A	513	ARG
1	A	515	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	528	VAL
1	A	532	GLN
1	A	553	HIS
1	A	568	LEU
1	A	581	SER
1	A	586	LYS
1	B	43	LEU
1	B	141	GLU
1	B	166	SER
1	B	175	GLU
1	B	179	LEU
1	B	182	LEU
1	B	307	LEU
1	B	316	THR
1	B	328	LEU
1	B	366	LEU
1	B	370	GLN
1	B	381	LEU
1	B	394	GLU
1	B	404	GLN
1	B	416	LEU
1	B	428	LEU
1	B	441	LEU
1	B	483	VAL
1	B	493	ILE
1	B	494	ASN
1	B	513	ARG
1	B	515	LEU
1	B	516	ILE
1	B	532	GLN
1	B	548	LEU
1	B	562	VAL
1	B	568	LEU
1	B	576	ARG
1	B	586	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	GLN
1	A	82	GLN
1	A	84	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	102	ASN
1	A	123	GLN
1	A	167	ASN
1	A	191	HIS
1	A	239	GLN
1	A	286	ASN
1	A	404	GLN
1	A	433	ASN
1	A	456	ASN
1	A	478	HIS
1	A	494	ASN
1	A	532	GLN
1	A	559	ASN
1	A	565	HIS
1	A	596	ASN
1	B	48	HIS
1	B	84	ASN
1	B	102	ASN
1	B	123	GLN
1	B	167	ASN
1	B	168	HIS
1	B	191	HIS
1	B	239	GLN
1	B	286	ASN
1	B	404	GLN
1	B	433	ASN
1	B	453	GLN
1	B	484	GLN
1	B	494	ASN
1	B	496	GLN
1	B	532	GLN
1	B	559	ASN
1	B	565	HIS

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
2	LAS	A	800	1	10,15,25	0.94	1 (10%)	13,23,37	4.01	5 (38%)
2	LAS	B	800	1	10,15,25	0.76	0	13,23,37	3.80	7 (53%)

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	LAS	A	800	1	-	4/6/32/48	0/1/1/1
2	LAS	B	800	1	-	1/6/32/48	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	800	LAS	C5-C6	2.39	1.54	1.52

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	LAS	C9-N8-C6	-11.34	107.05	114.58
2	B	800	LAS	C9-N8-C6	-9.32	108.39	114.58
2	B	800	LAS	C20-C5-C3	-6.70	109.64	116.53
2	A	800	LAS	C20-C5-C3	-6.00	110.36	116.53
2	B	800	LAS	O7-C6-C5	-4.49	122.60	126.17

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	LAS	O7-C6-C5	-4.08	122.93	126.17
2	A	800	LAS	O19-C18-C9	-3.38	119.03	124.25
2	B	800	LAS	C16-C11-C10	-3.03	104.08	111.83
2	B	800	LAS	C20-C5-C6	-2.59	106.82	112.40
2	A	800	LAS	C12-C11-C10	-2.27	106.03	111.83
2	B	800	LAS	C12-C11-C10	-2.21	106.18	111.83
2	B	800	LAS	O17-C10-C9	2.17	112.83	107.46

There are no chirality outliers.

All (5) torsion outliers are listed below:

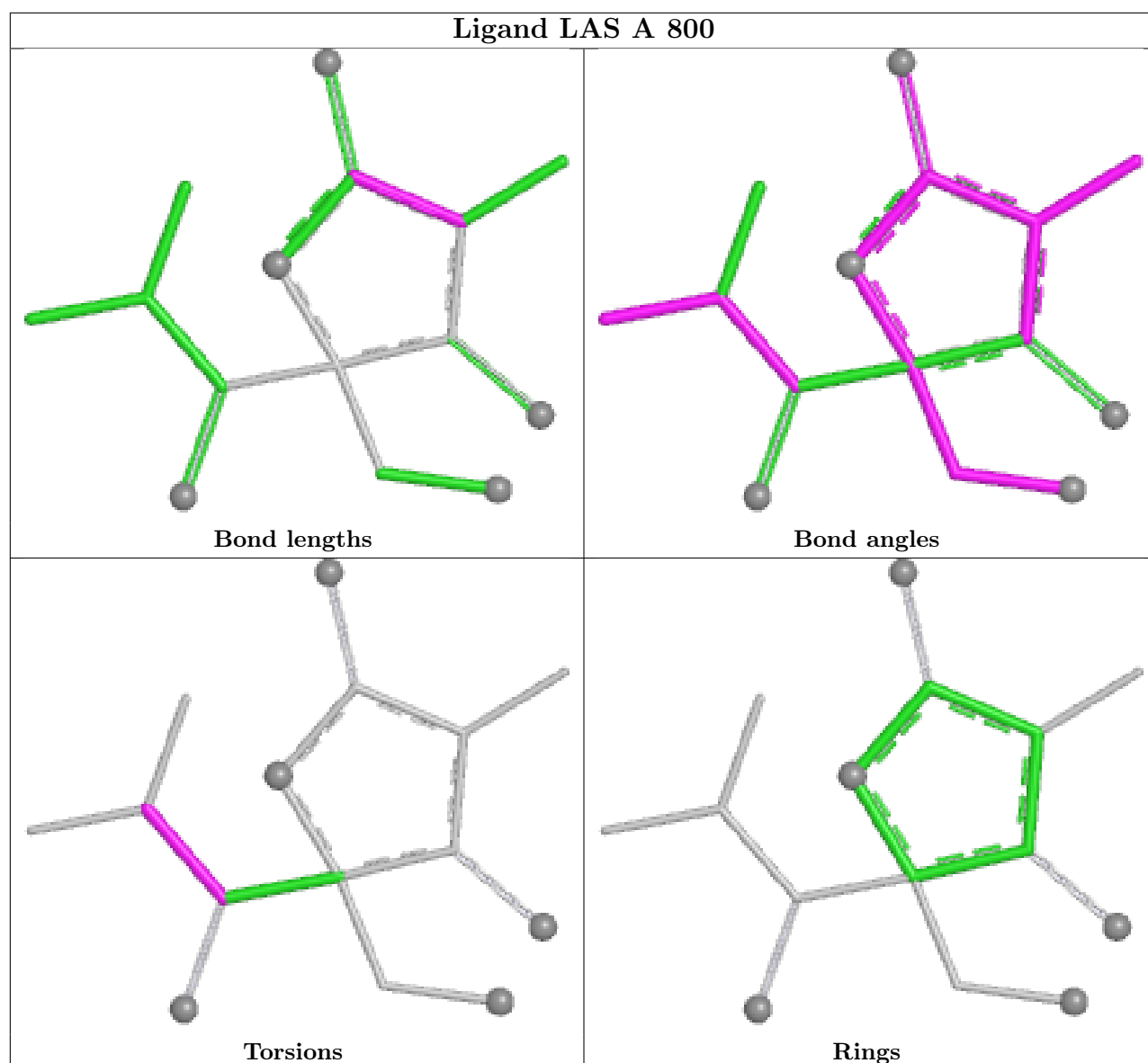
Mol	Chain	Res	Type	Atoms
2	A	800	LAS	C9-C10-C11-C16
2	A	800	LAS	O17-C10-C11-C16
2	A	800	LAS	O17-C10-C11-C12
2	A	800	LAS	C9-C10-C11-C12
2	B	800	LAS	O17-C10-C11-C16

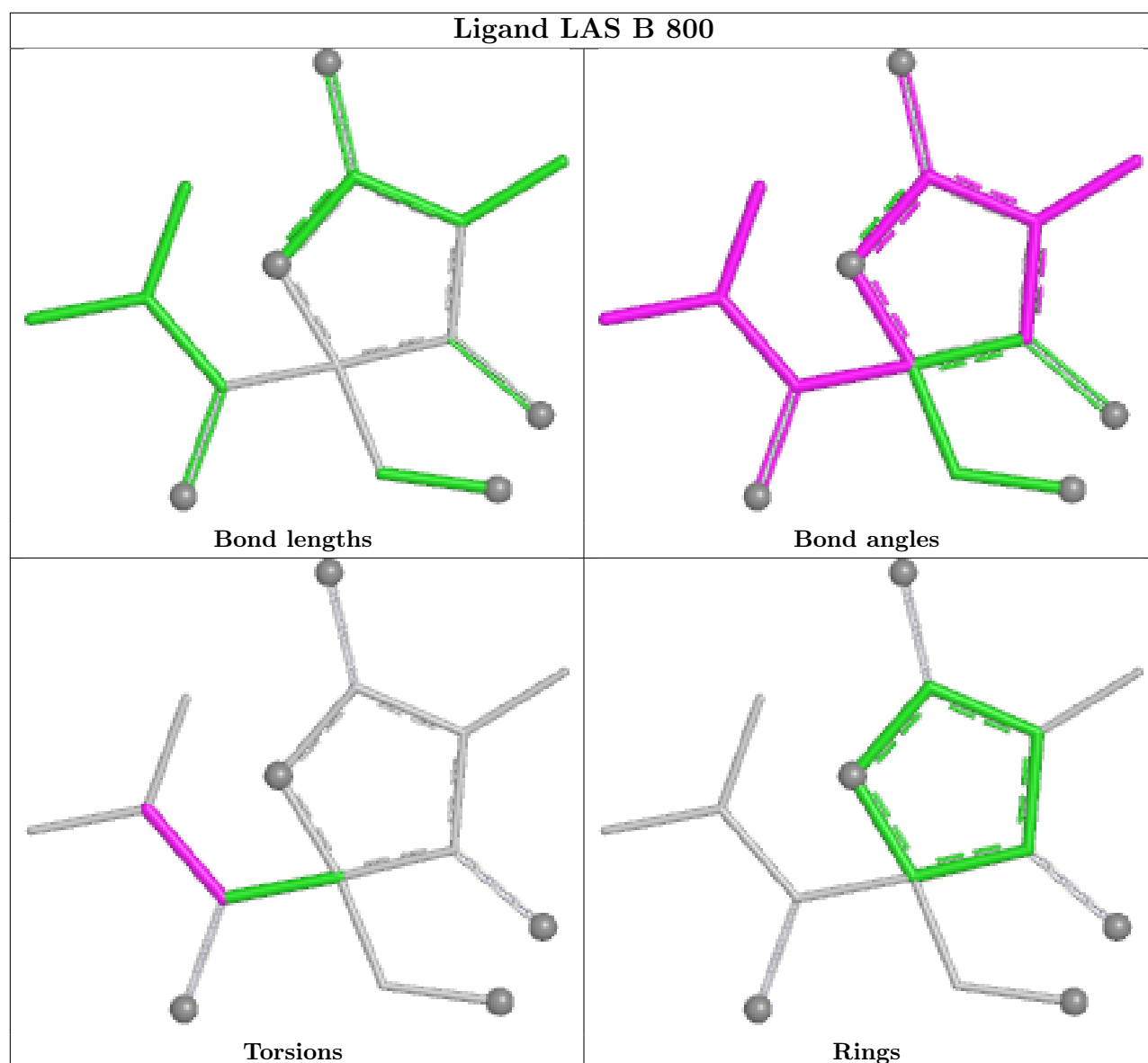
There are no ring outliers.

2 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	LAS	10	0
2	B	800	LAS	10	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

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	522/583 (89%)	0.42	43 (8%)	17 20	9, 25, 55, 82	0
1	B	522/583 (89%)	0.18	22 (4%)	40 46	8, 22, 44, 71	0
All	All	1044/1166 (89%)	0.30	65 (6%)	26 30	8, 23, 51, 82	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	138	PHE	6.3
1	A	339	GLU	5.3
1	B	239	GLN	4.8
1	A	139	SER	4.7
1	B	138	PHE	4.7
1	B	598	ASP	4.1
1	A	239	GLN	4.1
1	A	345	GLY	4.0
1	A	344	SER	3.8
1	B	139	SER	3.7
1	A	598	ASP	3.3
1	B	319	ASP	3.3
1	B	140	SER	3.3
1	B	141	GLU	3.2
1	B	206	PHE	3.2
1	A	322	SER	3.1
1	A	140	SER	3.1
1	A	321	LYS	3.1
1	A	141	GLU	3.1
1	A	301	ILE	3.0
1	A	234	ARG	3.0
1	A	577	TYR	3.0
1	A	307	LEU	3.0
1	B	136	MET	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	300	VAL	2.9
1	B	234	ARG	2.9
1	B	318	GLY	2.9
1	A	237	GLN	2.8
1	A	77	GLN	2.8
1	A	316	THR	2.7
1	B	83	GLU	2.7
1	A	318	GLY	2.7
1	B	563	GLU	2.6
1	B	320	GLY	2.6
1	A	553	HIS	2.6
1	B	553	HIS	2.5
1	A	363	THR	2.5
1	A	298	GLY	2.5
1	A	299	PRO	2.5
1	A	238	LEU	2.4
1	A	596	ASN	2.4
1	B	137	THR	2.4
1	A	482	ARG	2.4
1	A	320	GLY	2.4
1	B	315	VAL	2.4
1	A	83	GLU	2.4
1	A	314	SER	2.3
1	B	84	ASN	2.3
1	A	81	THR	2.3
1	A	358	VAL	2.3
1	A	210	ARG	2.2
1	A	340	ASP	2.2
1	B	207	GLY	2.2
1	A	576	ARG	2.1
1	A	552	GLU	2.1
1	B	567	ASP	2.1
1	A	302	TRP	2.1
1	A	525	GLY	2.1
1	A	137	THR	2.1
1	B	209	THR	2.1
1	B	445	GLU	2.1
1	A	346	PRO	2.1
1	A	324	LYS	2.0
1	A	319	ASP	2.0
1	A	362	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

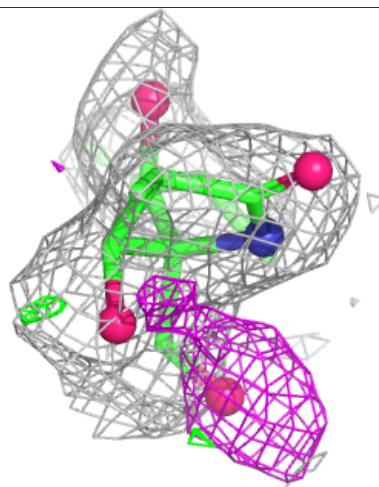
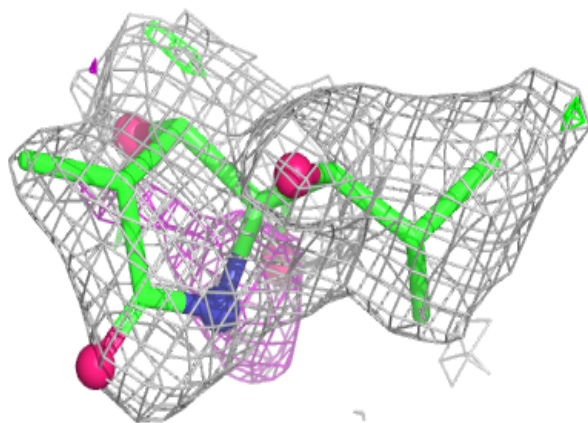
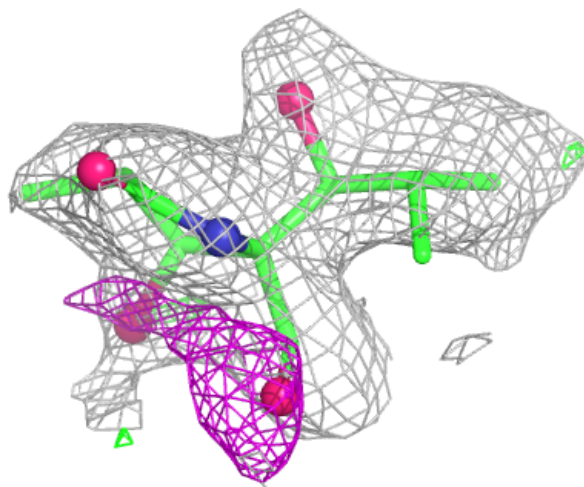
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	LAS	A	800	15/25	0.65	0.17	35,37,39,41	0
2	LAS	B	800	15/25	0.81	0.14	28,31,36,36	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.

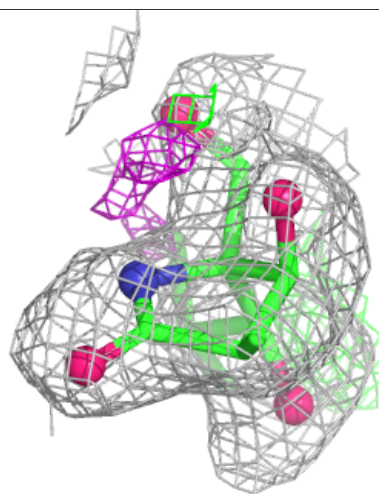
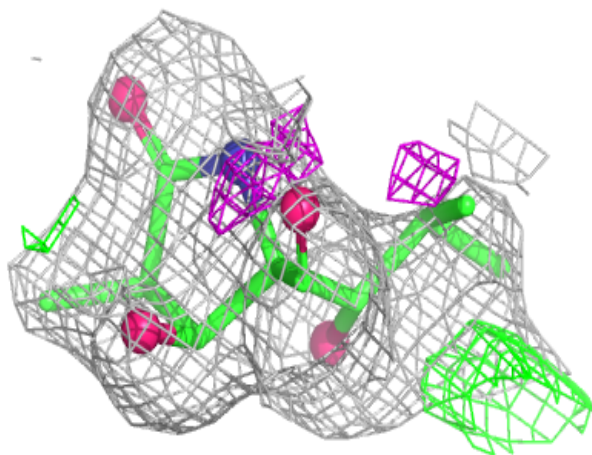
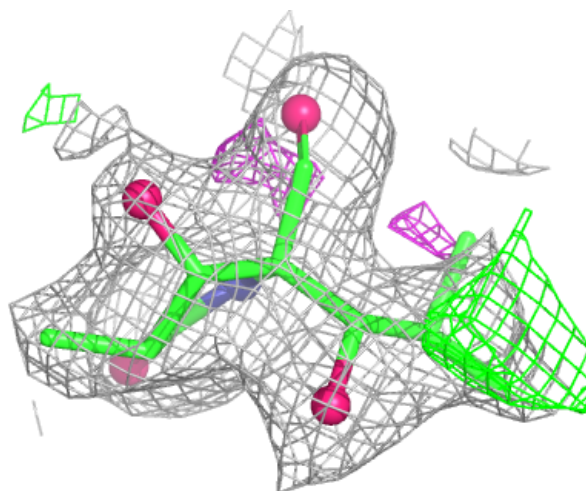
Electron density around LAS A 800:

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



Electron density around LAS B 800:

$2mF_o-DF_c$ (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.