Full wwPDB X-ray Structure Validation Report (i)

Oct 22, 2023 – 04:23 PM EDT

PDB ID	:	3DPM
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 (i) 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 (i)) were used in the production of this report:

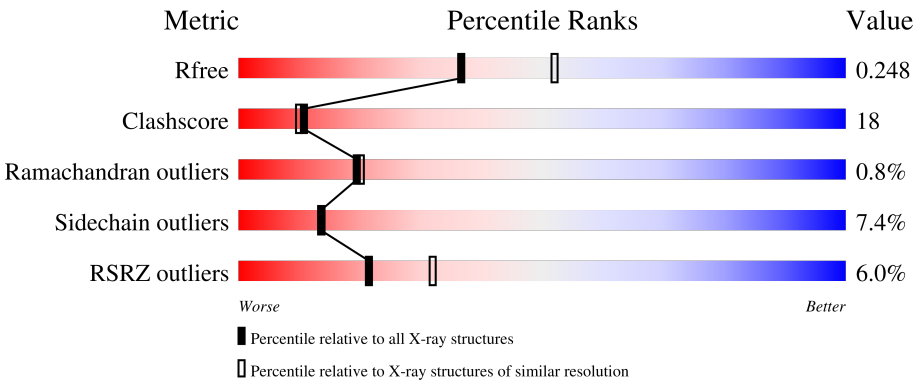
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.35 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}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (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 <=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	7% 55% 30% • 10%
1	B	583	4% 62% 25% • 10%

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 (i)

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.

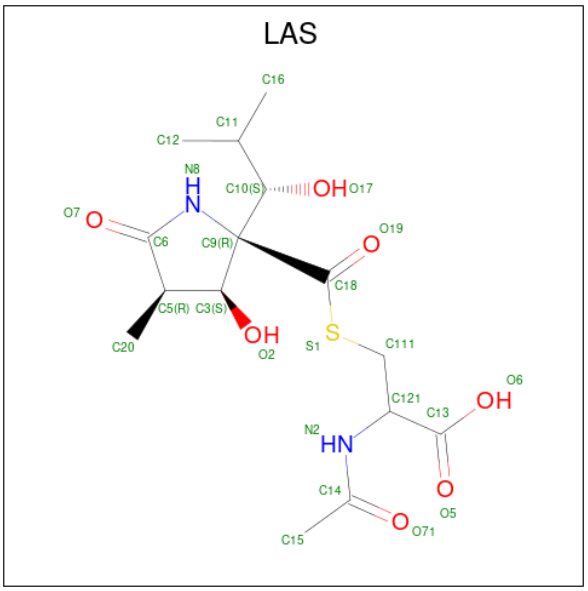
- Molecule 1 is a protein called Protein CT_858.

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

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 (three-letter code: LAS) (formula: $C_{15}H_{24}N_2O_7S$).



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

- Molecule 3 is water.

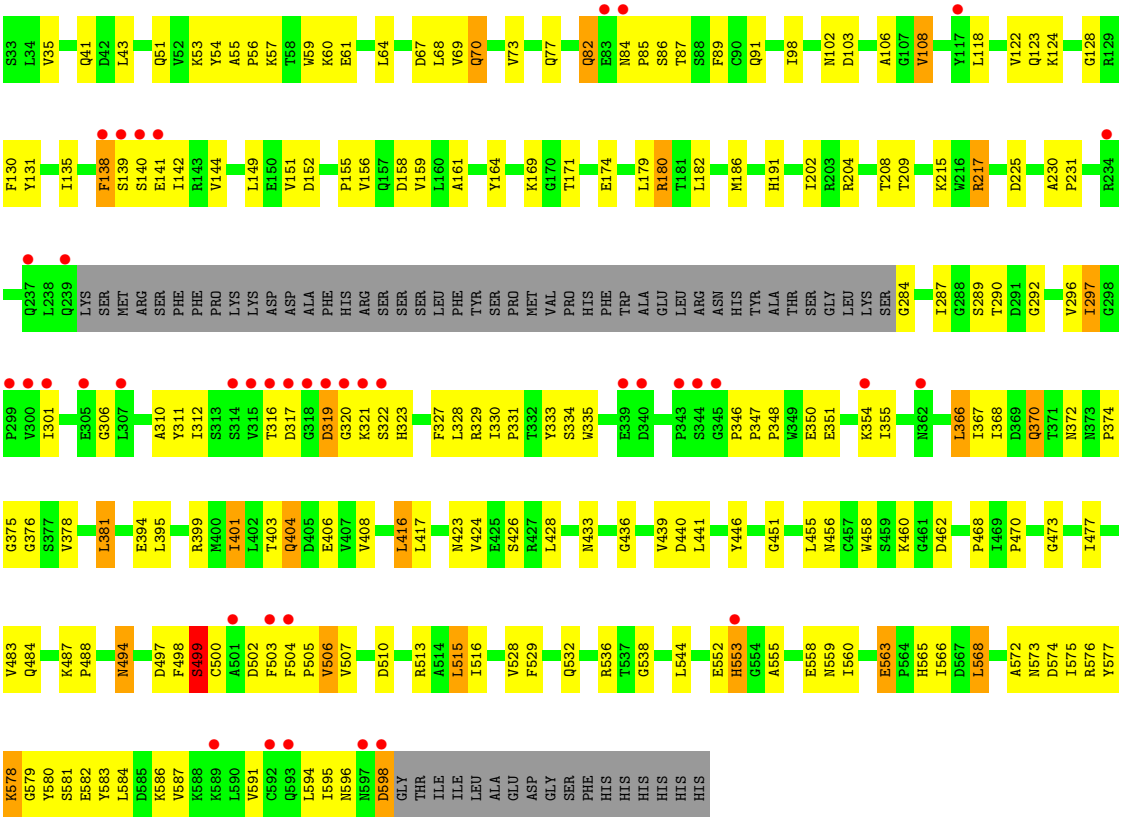
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	142	142	142	0	0
			Total	O		
3	B	167	167	167	0	0

3 Residue-property plots (i)

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

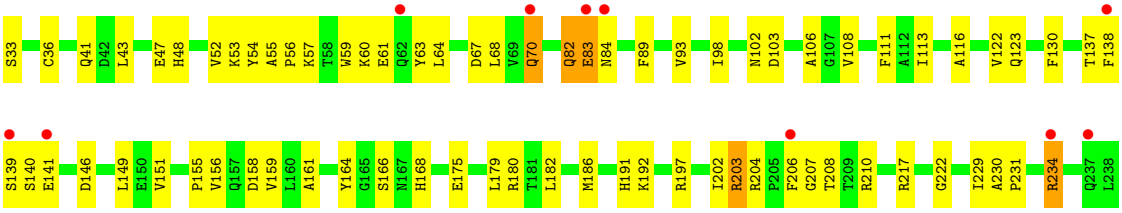
• Molecule 1: Protein CT_858

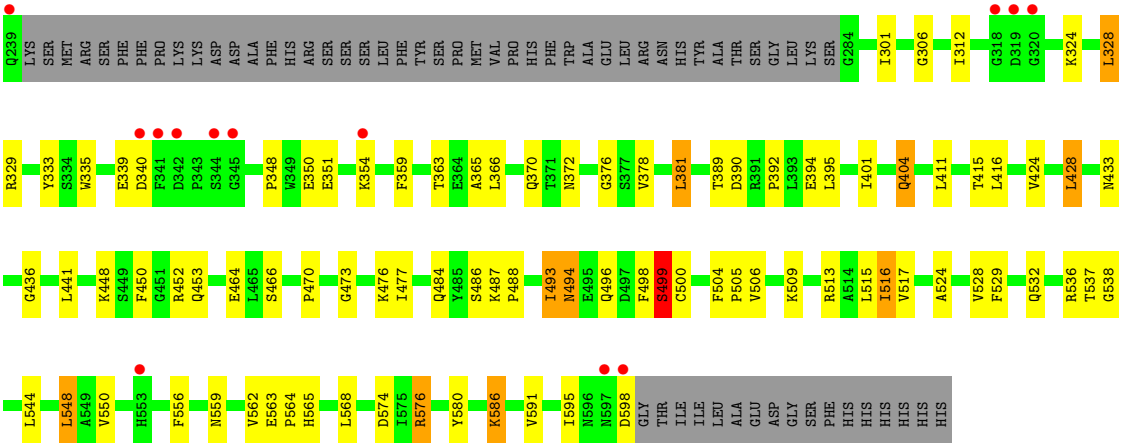
Chain A:



• Molecule 1: Protein CT_858

Chain B:




Q239 LYS SER MET ARG SER PHE PHE PRO LYS LYS ASP ASP ALA PHE HIS ARG SER SER SER LEU PHE TYR SER PRO MET VAL PRO HIS PHE TRP ALA GLU LEU ARG ASN HIS TYR ALA THR SER GLY LEU LYS SER G284 I301 G306 I312 G318 D319 G320 K324 L328
R329 Y333 S334 W335 E339 D340 F341 D342 P343 S344 G345 P348 W349 E350 E351 K354 F359 T363 E364 A365 L366 Q370 T371 N372 G376 S377 V378 L381 T389 D390 R391 P392 L393 E394 L395 I401 Q404 L411 T415 L416 V424 L428 N433
G436 L441 K448 S449 F450 G451 R452 Q453 E464 L465 S466 P470 G473 K476 I477 Q484 Y485 S486 K487 P488 I493 N494 E495 Q496 D497 F498 S499 C500 F504 P505 V506 K509 R513 A514 L515 I516 V517 A524 V528 F529 Q532 R536 T537 G538
L544 L548 A549 V550 H553 F556 N559 V562 E563 P564 H565 L568 D574 I575 R576 Y580 K586 V591 I595 N596 M597 D598 GLY THR ILE ILE LEU ALA GLU ASP GLY SER PHE HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

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 33.11 – 2.33	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.35) 98.1 (33.11-2.33)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.44 (at 2.34Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.259 0.223 , 0.248	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)	0.38 , 41.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[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 (i)

5.1 Standard geometry (i)

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	0.40	0/4208	0.64	1/5720 (0.0%)
1	B	0.41	0/4208	0.66	1/5720 (0.0%)
All	All	0.41	0/8416	0.65	2/11440 (0.0%)

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

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	192	LYS	N-CA-C	-5.19	96.98	111.00
1	A	217	ARG	N-CA-C	-5.17	97.05	111.00

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 (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	4110	0	4047	163	0
1	B	4110	0	4047	145	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	300	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 18.

All (300) 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: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:60:LYS:HZ2	1:A:559:ASN:HD21	1.32	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

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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: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: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:A:498:PHE:O	1:A:499:SER:C	2.37	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:A:367:ILE:HD11	1:A:591:VAL:CG2	2.29	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:563:GLU:CD	1:B:563:GLU:H	2.04	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:B:328:LEU:C	1:B:328:LEU:HD13	2.24	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:83:GLU:O	1:B:84:ASN:C	2.42	0.57
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:563:GLU:CD	1:A:563:GLU:H	2.12	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: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:B:404:GLN:H	1:B:404:GLN:CD	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:494:ASN:C	1:A:494:ASN:HD22	2.14	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: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:202:ILE:HD12	1:B:202:ILE:C	2.34	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:494:ASN:C	1:A:494:ASN:ND2	2.69	0.46
1:B:537:THR:O	1:B:537:THR:HG22	2.15	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: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: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: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: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:138:PHE:CD1	1:B:138:PHE:C	2.89	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:498:PHE:O	1:B:499:SER:C	2.54	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:284:GLY:N	1:A:289:SER:HG	2.16	0.43
1:B:529:PHE:CZ	1:B:544:LEU:HB2	2.54	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: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
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:60:LYS:HZ3	1:A:559:ASN:ND2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ARG:CD	1:A:468:PRO:HD3	2.50	0.41
1:B:586:LYS:HD3	1:B:586:LYS:C	2.40	0.41
1:A:131:TYR:CZ	1:A:576:ARG:HD3	2.56	0.41
1:A:404:GLN:H	1:A:404:GLN:CD	2.24	0.41
1:A:424:VAL:O	1:A:428:LEU:HD13	2.20	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:328:LEU:HD13	1:A:328:LEU:C	2.40	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:A:123:GLN:CD	1:A:575:ILE:HD12	2.41	0.41
1:B:424:VAL:HG12	1:B:428:LEU:CD2	2.50	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:319:ASP:C	1:A:321:LYS:H	2.24	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
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

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%)	19	20
1	B	518/583 (89%)	489 (94%)	25 (5%)	4 (1%)	19	20
All	All	1036/1166 (89%)	977 (94%)	51 (5%)	8 (1%)	19	20

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%)	415 (92%)	37 (8%)	11	11
1	B	452/506 (89%)	422 (93%)	30 (7%)	16	17
All	All	904/1012 (89%)	837 (93%)	67 (7%)	13	14

All (67) 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	82	GLN
1	A	84	ASN
1	A	102	ASN
1	A	108	VAL
1	A	138	PHE
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	334	SER
1	A	366	LEU
1	A	370	GLN
1	A	381	LEU
1	A	401	ILE
1	A	404	GLN
1	A	416	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
1	A	532	GLN
1	A	553	HIS
1	A	563	GLU
1	A	568	LEU
1	A	581	SER
1	A	598	ASP
1	B	41	GLN
1	B	43	LEU
1	B	70	GLN
1	B	102	ASN
1	B	166	SER
1	B	175	GLU

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Mol	Chain	Res	Type
1	B	179	LEU
1	B	182	LEU
1	B	203	ARG
1	B	234	ARG
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	493	ILE
1	B	494	ASN
1	B	499	SER
1	B	513	ARG
1	B	516	ILE
1	B	532	GLN
1	B	548	LEU
1	B	568	LEU
1	B	576	ARG
1	B	586	LYS
1	B	598	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	51	GLN
1	A	82	GLN
1	A	84	ASN
1	A	102	ASN
1	A	123	GLN
1	A	167	ASN
1	A	168	HIS
1	A	191	HIS
1	A	239	GLN
1	A	286	ASN
1	A	404	GLN
1	A	433	ASN
1	A	453	GLN

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Mol	Chain	Res	Type
1	A	456	ASN
1	A	494	ASN
1	A	496	GLN
1	A	532	GLN
1	A	559	ASN
1	A	565	HIS
1	A	596	ASN
1	B	48	HIS
1	B	62	GLN
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	494	ASN
1	B	496	GLN
1	B	532	GLN
1	B	559	ASN
1	B	565	HIS
1	B	596	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	B	800	1	10,15,25	0.75	0	12,23,37	3.81	7 (58%)
2	LAS	A	800	1	10,15,25	0.93	1 (10%)	12,23,37	3.89	4 (33%)

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	B	800	1	-	1/6/32/48	0/1/1/1
2	LAS	A	800	1	-	4/6/32/48	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 (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	800	LAS	C9-N8-C6	-10.81	107.05	114.58
2	B	800	LAS	C9-N8-C6	-8.89	108.39	114.58
2	B	800	LAS	C20-C5-C3	-6.55	109.64	116.54
2	A	800	LAS	C20-C5-C3	-5.87	110.36	116.54
2	B	800	LAS	O7-C6-C5	-4.49	122.60	126.17
2	A	800	LAS	O7-C6-C5	-4.08	122.93	126.17
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

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
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

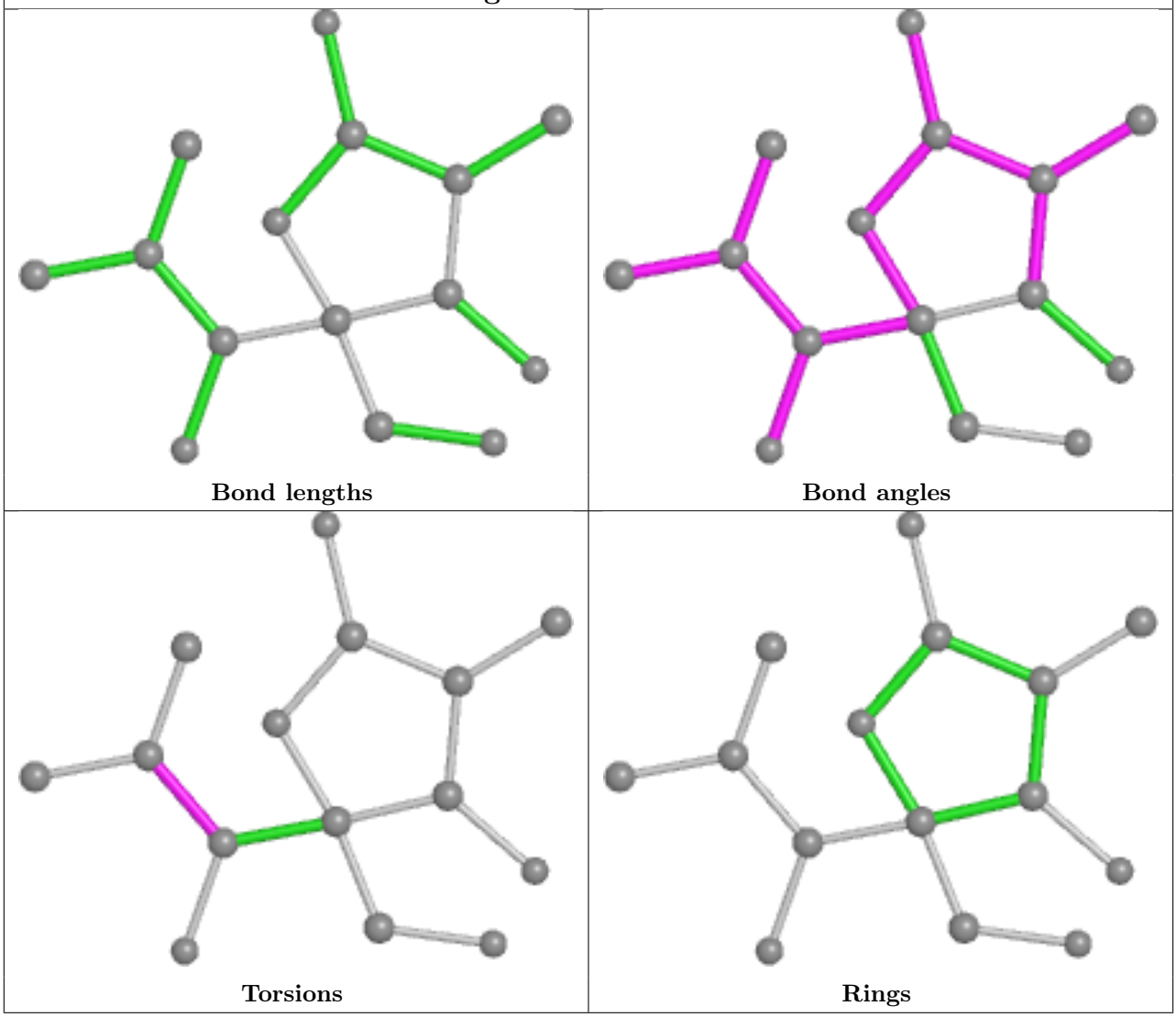
There are no ring outliers.

2 monomers are involved in 20 short contacts:

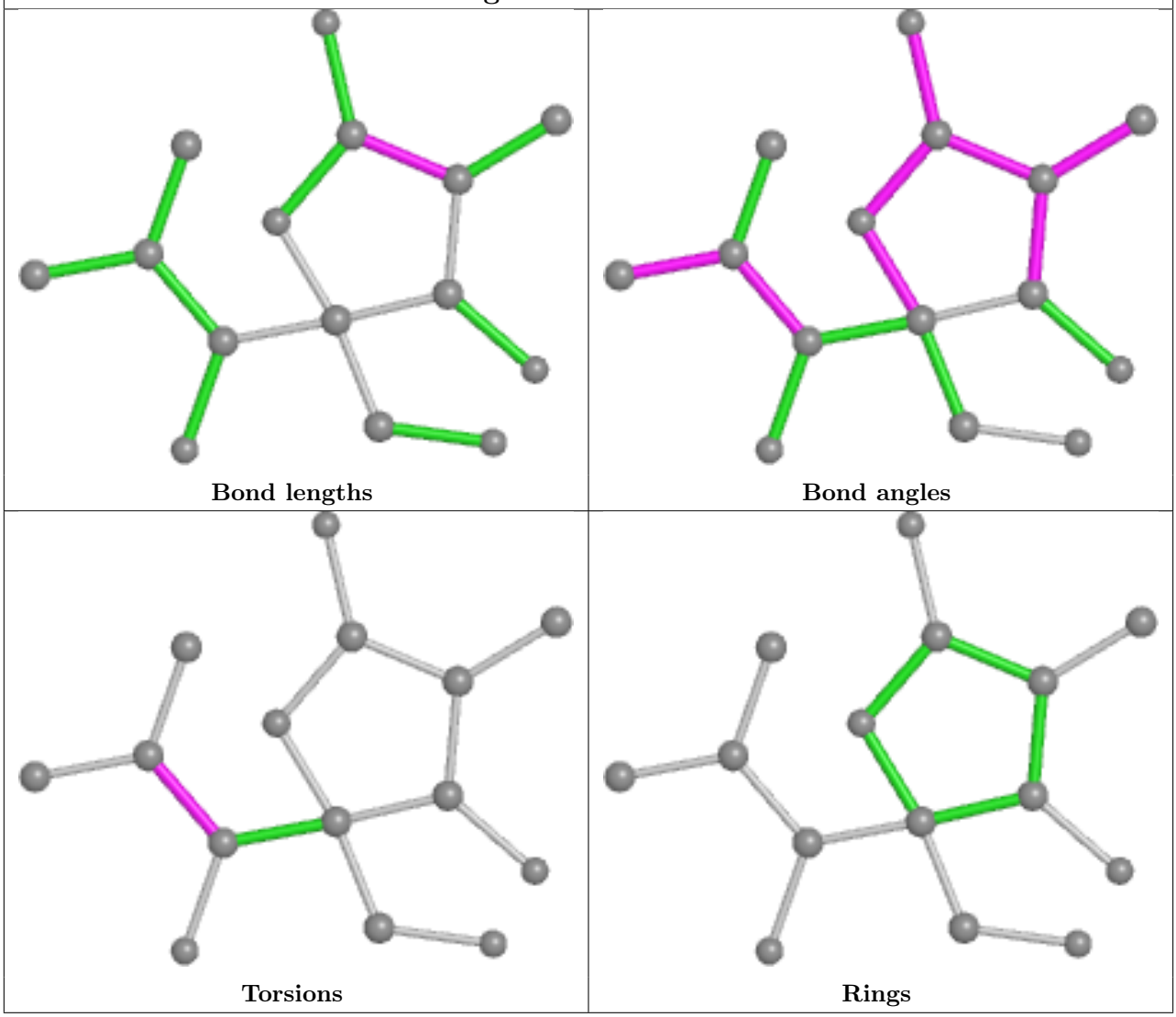
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	800	LAS	10	0
2	A	800	LAS	10	0

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 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 LAS B 800



Ligand LAS A 800



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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.39	40 (7%)	13	20	9, 25, 55, 82	0
1	B	522/583 (89%)	0.17	23 (4%)	34	46	8, 22, 44, 71	0
All	All	1044/1166 (89%)	0.28	63 (6%)	21	32	8, 23, 51, 82	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	138	PHE	8.9
1	A	344	SER	7.4
1	A	239	GLN	7.3
1	B	239	GLN	6.6
1	A	139	SER	6.5
1	A	598	ASP	6.3
1	B	318	GLY	6.2
1	A	339	GLU	5.5
1	A	300	VAL	5.2
1	A	138	PHE	5.1
1	B	598	ASP	5.1
1	A	345	GLY	5.0
1	B	139	SER	4.9
1	B	319	ASP	4.3
1	A	318	GLY	4.3
1	A	314	SER	4.3
1	A	316	THR	4.2
1	B	553	HIS	4.2
1	A	234	ARG	4.1
1	A	321	LYS	3.9
1	A	320	GLY	3.8
1	A	343	PRO	3.5
1	A	317	ASP	3.5
1	A	592	CYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	501	ALA	3.3
1	A	322	SER	3.3
1	A	553	HIS	3.0
1	A	315	VAL	3.0
1	B	83	GLU	2.9
1	A	597	ASN	2.8
1	B	597	ASN	2.8
1	A	305	GLU	2.8
1	B	340	ASP	2.7
1	A	319	ASP	2.6
1	A	83	GLU	2.6
1	A	237	GLN	2.6
1	A	503	PHE	2.6
1	B	62	GLN	2.6
1	A	307	LEU	2.6
1	B	354	LYS	2.6
1	B	70	GLN	2.5
1	B	237	GLN	2.5
1	A	340	ASP	2.5
1	B	341	PHE	2.4
1	A	141	GLU	2.4
1	B	345	GLY	2.4
1	A	504	PHE	2.4
1	A	84	ASN	2.4
1	B	344	SER	2.4
1	B	342	ASP	2.3
1	B	320	GLY	2.3
1	A	354	LYS	2.3
1	A	140	SER	2.3
1	A	593	GLN	2.3
1	B	234	ARG	2.2
1	A	117	TYR	2.2
1	A	362	ASN	2.2
1	B	84	ASN	2.2
1	B	141	GLU	2.2
1	A	589	LYS	2.1
1	A	301	ILE	2.1
1	A	299	PRO	2.0
1	B	206	PHE	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

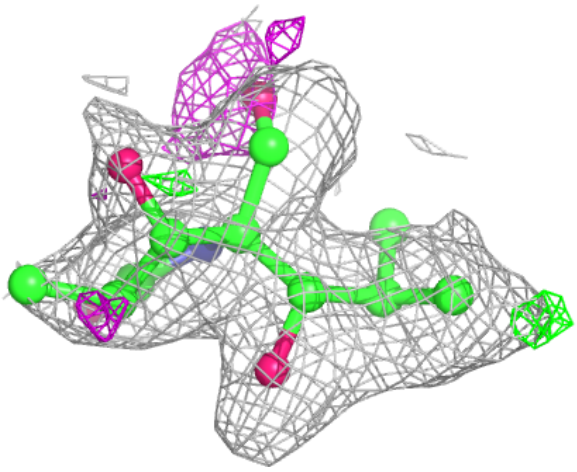
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

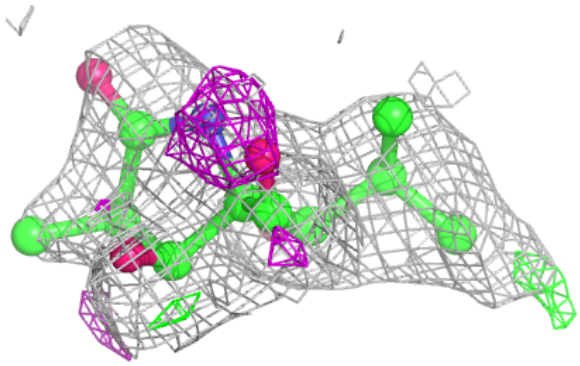
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	LAS	A	800	15/25	0.79	0.23	35,37,39,41	0
2	LAS	B	800	15/25	0.89	0.20	28,31,36,36	0

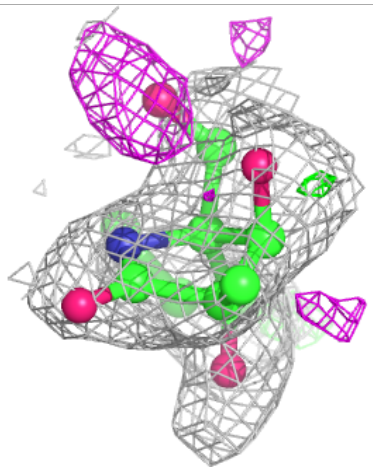
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

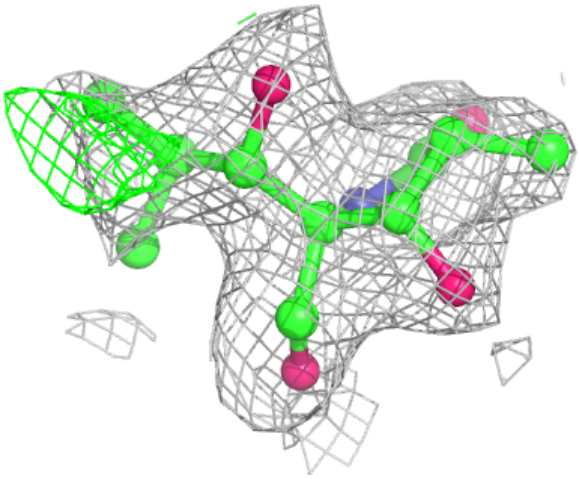


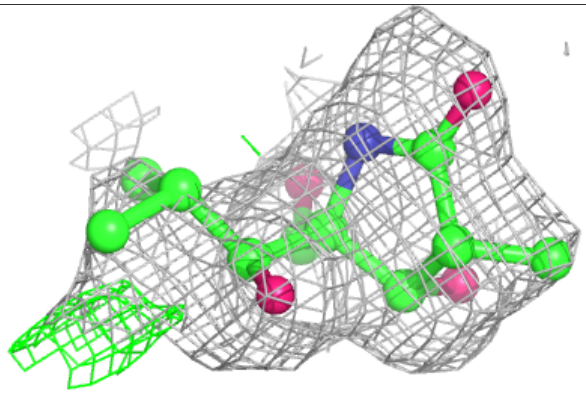




Electron density around LAS B 800:

$2mF_o$-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.