Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 08:34 PM EDT

PDB ID	:	4FWG
Title	:	Crystal structure of the Lon-like protease MtaLonC in complex with lactacystin
Authors	:	Chang, C.I.; Kuo, C.I.; Huang, K.F.
Deposited on	:	2012-07-01
Resolution	:	1.99 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:

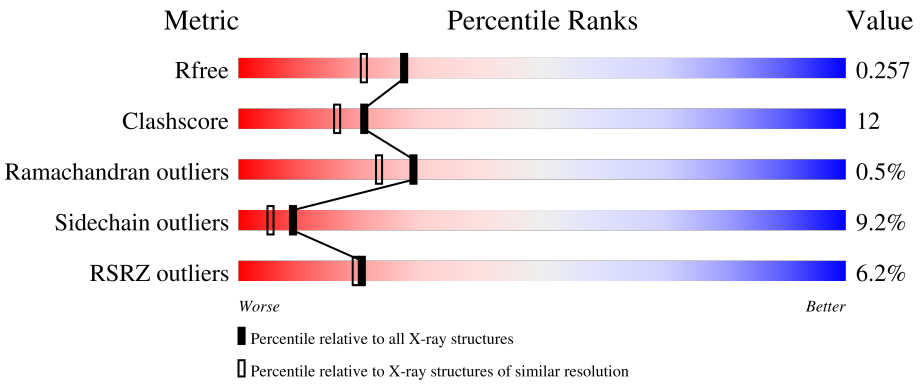
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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

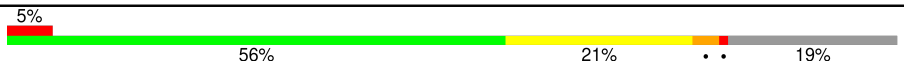
The reported resolution of this entry is 1.99 Å.

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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	732	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5178 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.

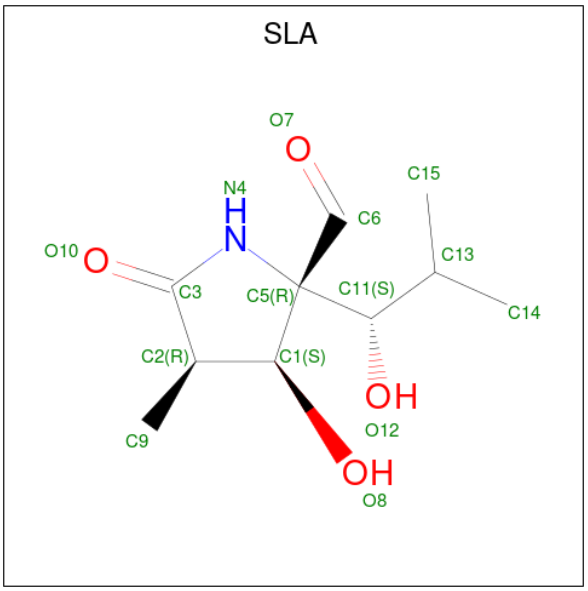
- Molecule 1 is a protein called TTC1975 peptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	594	4575	2902	813	849	2	9	0	2	0

There are 18 discrepancies between the modelled and reference sequences:

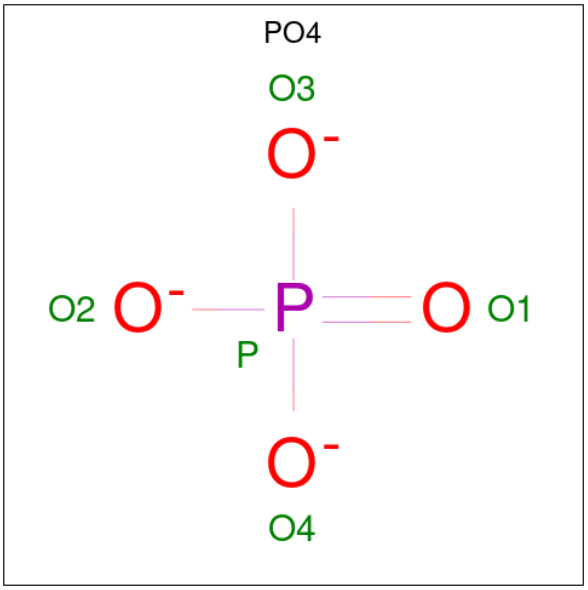
Chain	Residue	Modelled	Actual	Comment	Reference
A	91	MSE	LEU	engineered mutation	UNP C9DRU9
A	188	MSE	LEU	engineered mutation	UNP C9DRU9
A	359	MSE	ILE	engineered mutation	UNP C9DRU9
A	390	MSE	LEU	engineered mutation	UNP C9DRU9
A	557	MSE	TYR	engineered mutation	UNP C9DRU9
A	720	LYS	-	expression tag	UNP C9DRU9
A	721	LEU	-	expression tag	UNP C9DRU9
A	722	ALA	-	expression tag	UNP C9DRU9
A	723	ALA	-	expression tag	UNP C9DRU9
A	724	ALA	-	expression tag	UNP C9DRU9
A	725	LEU	-	expression tag	UNP C9DRU9
A	726	GLU	-	expression tag	UNP C9DRU9
A	727	HIS	-	expression tag	UNP C9DRU9
A	728	HIS	-	expression tag	UNP C9DRU9
A	729	HIS	-	expression tag	UNP C9DRU9
A	730	HIS	-	expression tag	UNP C9DRU9
A	731	HIS	-	expression tag	UNP C9DRU9
A	732	HIS	-	expression tag	UNP C9DRU9

- Molecule 2 is Omuralide, open form (three-letter code: SLA) (formula: $C_{10}H_{17}NO_4$).



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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	P		
3	A	1	5	4	1	0	0

- Molecule 4 is water.

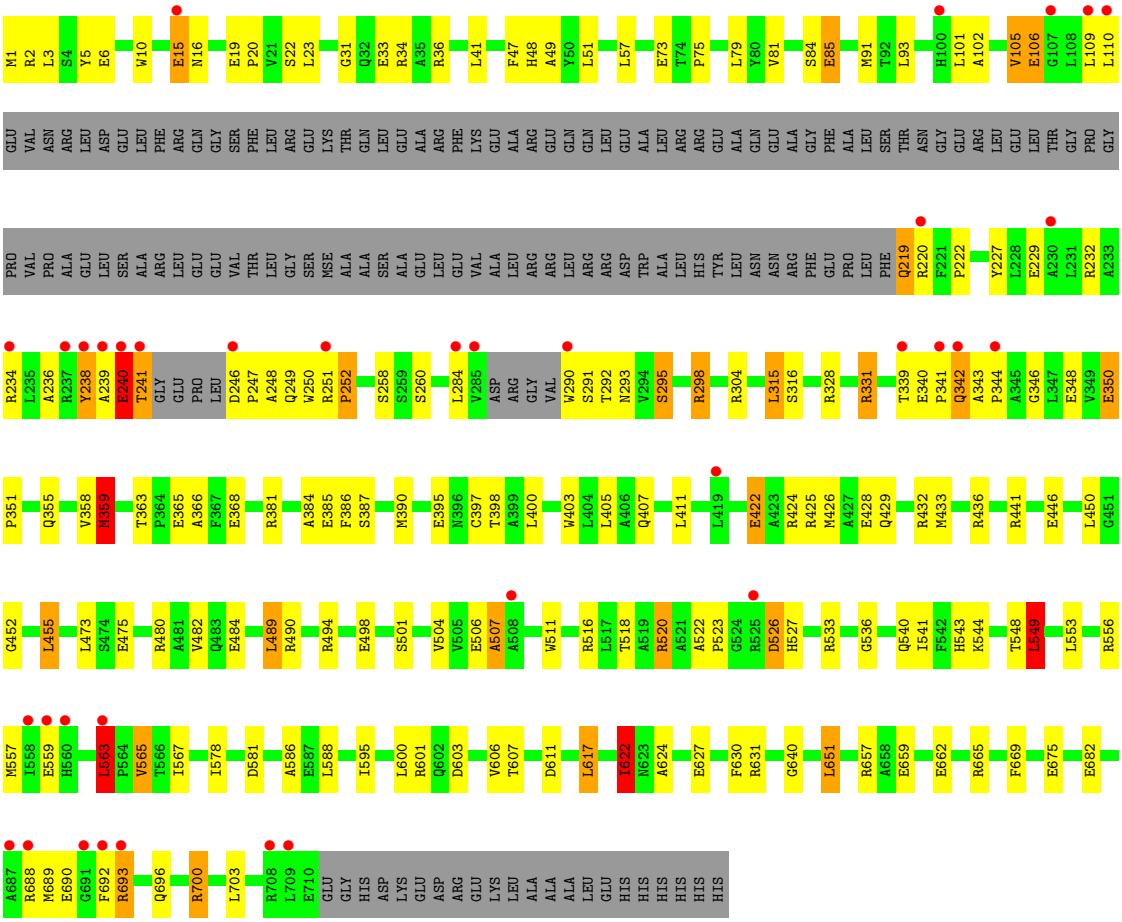
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	583	583	583	0	0

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: TTC1975 peptidase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 6	Depositor
Cell constants a, b, c, α, β, γ	115.99Å 115.99Å 135.05Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.99 19.87 – 1.99	Depositor EDS
% Data completeness (in resolution range)	99.3 (20.00-1.99) 99.6 (19.87-1.99)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.17 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.230 , 0.259 0.219 , 0.257	Depositor DCC
R_{free} test set	3485 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 52.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.54$, $< L^2 > = 0.39$	Xtriage
Estimated twinning fraction	0.011 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.748 for H, K, L 0.252 for K, H, -L	Depositor
Outliers	1 of 70161 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5178	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.55% 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: PO4, SLA

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	1.50	44/4662 (0.9%)	1.35	41/6319 (0.6%)

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	475	GLU	CD-OE2	9.06	1.35	1.25
1	A	665	ARG	N-CA	6.98	1.60	1.46
1	A	5	TYR	CE1-CZ	6.90	1.47	1.38
1	A	662	GLU	N-CA	6.89	1.60	1.46
1	A	385	GLU	C-O	6.76	1.36	1.23
1	A	511	TRP	CD2-CE2	6.72	1.49	1.41
1	A	511	TRP	CG-CD2	6.54	1.54	1.43
1	A	473	LEU	N-CA	6.40	1.59	1.46
1	A	316	SER	CA-CB	-6.37	1.43	1.52
1	A	669	PHE	CB-CG	6.34	1.62	1.51
1	A	548	THR	N-CA	6.30	1.58	1.46
1	A	428	GLU	N-CA	6.26	1.58	1.46
1	A	675	GLU	CD-OE2	6.23	1.32	1.25
1	A	627	GLU	CB-CG	6.08	1.63	1.52
1	A	424	ARG	CZ-NH1	6.00	1.40	1.33
1	A	6	GLU	CD-OE1	5.94	1.32	1.25
1	A	543	HIS	C-O	5.90	1.34	1.23
1	A	482	VAL	C-O	5.77	1.34	1.23
1	A	541	ILE	N-CA	5.75	1.57	1.46
1	A	359	MSE	CG-SE	-5.67	1.76	1.95
1	A	657	ARG	C-O	5.66	1.34	1.23
1	A	403	TRP	CD2-CE2	5.63	1.48	1.41
1	A	640	GLY	N-CA	5.62	1.54	1.46
1	A	520	ARG	CZ-NH1	5.58	1.40	1.33
1	A	386	PHE	CA-CB	-5.57	1.41	1.53
1	A	363	THR	N-CA	5.57	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	387	SER	CB-OG	5.51	1.49	1.42
1	A	540	GLN	C-O	5.51	1.33	1.23
1	A	400	LEU	N-CA	5.41	1.57	1.46
1	A	651	LEU	N-CA	5.36	1.57	1.46
1	A	511	TRP	CZ3-CH2	5.34	1.48	1.40
1	A	10	TRP	NE1-CE2	-5.32	1.30	1.37
1	A	397	CYS	N-CA	5.32	1.56	1.46
1	A	586	ALA	N-CA	5.31	1.56	1.46
1	A	47	PHE	CG-CD1	5.30	1.46	1.38
1	A	541	ILE	C-O	5.30	1.33	1.23
1	A	31	GLY	CA-C	5.29	1.60	1.51
1	A	627	GLU	CA-CB	5.21	1.65	1.53
1	A	624	ALA	C-O	5.19	1.33	1.23
1	A	10	TRP	CD2-CE2	5.18	1.47	1.41
1	A	290	TRP	CD2-CE2	5.16	1.47	1.41
1	A	250	TRP	CD2-CE2	5.08	1.47	1.41
1	A	446	GLU	CD-OE1	5.05	1.31	1.25
1	A	452	GLY	N-CA	5.02	1.53	1.46

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	432	ARG	NE-CZ-NH2	-18.26	111.17	120.30
1	A	631	ARG	NE-CZ-NH2	-13.25	113.68	120.30
1	A	432	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	A	622	ILE	CG1-CB-CG2	-10.42	88.48	111.40
1	A	549	LEU	CB-CG-CD2	-9.81	94.32	111.00
1	A	516	ARG	NE-CZ-NH2	-9.40	115.60	120.30
1	A	331	ARG	NE-CZ-NH1	9.16	124.88	120.30
1	A	381	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	390	MSE	CG-SE-CE	7.53	115.46	98.90
1	A	611	ASP	CB-CG-OD1	7.43	124.99	118.30
1	A	424	ARG	NE-CZ-NH2	-7.15	116.73	120.30
1	A	611	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	A	544	LYS	CD-CE-NZ	-6.85	95.95	111.70
1	A	34	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	A	631	ARG	CG-CD-NE	-6.58	97.98	111.80
1	A	425	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	A	520	ARG	CG-CD-NE	6.41	125.27	111.80
1	A	432	ARG	CG-CD-NE	-6.41	98.33	111.80
1	A	549	LEU	CA-CB-CG	6.41	130.03	115.30
1	A	520	ARG	NE-CZ-NH2	-6.33	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	331	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	A	520	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	304	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	441	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	41	LEU	CB-CG-CD2	-5.79	101.15	111.00
1	A	359	MSE	CG-SE-CE	5.74	111.52	98.90
1	A	516	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	A	581	ASP	CB-CG-OD1	5.53	123.28	118.30
1	A	455	LEU	CA-CB-CG	5.51	127.98	115.30
1	A	328	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	450	LEU	CB-CG-CD1	-5.47	101.71	111.00
1	A	473	LEU	CB-CG-CD1	-5.46	101.73	111.00
1	A	422	GLU	OE1-CD-OE2	-5.30	116.94	123.30
1	A	549	LEU	CB-CG-CD1	-5.28	102.03	111.00
1	A	384	ALA	N-CA-CB	-5.28	102.71	110.10
1	A	581	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	A	563	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	489	LEU	CB-CG-CD1	5.20	119.84	111.00
1	A	617	LEU	CA-CB-CG	5.17	127.19	115.30
1	A	501	SER	N-CA-C	-5.12	97.16	111.00
1	A	565	VAL	CB-CA-C	-5.12	101.67	111.40

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	4575	0	4601	113	0
2	A	15	0	16	1	0
3	A	5	0	0	0	0
4	A	583	0	0	15	0
All	All	5178	0	4617	113	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 12.

All (113) 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:692:PHE:H	1:A:693:ARG:HB3	1.16	1.09
1:A:2:ARG:HD3	4:A:1238:HOH:O	1.53	1.06
1:A:692:PHE:H	1:A:693:ARG:CB	1.77	0.97
1:A:106:GLU:HG2	1:A:251:ARG:NH1	1.85	0.91
1:A:48:HIS:HD2	1:A:358:VAL:H	1.22	0.87
1:A:692:PHE:N	1:A:693:ARG:HB3	1.89	0.87
1:A:692:PHE:N	1:A:693:ARG:CB	2.45	0.80
1:A:422:GLU:O	1:A:426:MSE:HG3	1.87	0.75
1:A:102:ALA:O	1:A:105:VAL:HG12	1.87	0.74
1:A:365:GLU:O	1:A:368:GLU:HG2	1.87	0.74
1:A:219:GLN:HE21	1:A:219:GLN:N	1.86	0.72
1:A:3:LEU:HD11	1:A:651:LEU:CD2	2.19	0.72
1:A:693:ARG:CG	1:A:693:ARG:HH11	2.05	0.69
1:A:346:GLY:HA3	4:A:1365:HOH:O	1.91	0.69
1:A:526:ASP:HB2	1:A:563:LEU:HB2	1.75	0.68
1:A:48:HIS:CD2	1:A:358:VAL:H	2.10	0.68
1:A:567:ILE:HD11	1:A:595:ILE:HD11	1.76	0.67
1:A:15:GLU:OE1	1:A:15:GLU:HA	1.93	0.66
1:A:549:LEU:HD21	1:A:588:LEU:HB2	1.76	0.66
1:A:51:LEU:HD11	1:A:359:MSE:HE2	1.78	0.65
1:A:3:LEU:HD11	1:A:651:LEU:HD21	1.80	0.64
1:A:506:GLU:O	1:A:507:ALA:CB	2.46	0.63
1:A:106:GLU:CG	1:A:251:ARG:NH1	2.60	0.63
1:A:506:GLU:O	1:A:507:ALA:HB2	1.98	0.62
1:A:480:ARG:O	1:A:484:GLU:HG3	2.00	0.62
1:A:249:GLN:CG	1:A:249:GLN:O	2.49	0.61
1:A:298:ARG:HG2	4:A:1034:HOH:O	2.01	0.61
1:A:33:GLU:OE1	1:A:36:ARG:NE	2.34	0.60
1:A:692:PHE:CA	1:A:693:ARG:HB2	2.32	0.59
1:A:411:LEU:CD1	1:A:455:LEU:HD23	2.33	0.59
1:A:315:LEU:HD13	1:A:366:ALA:CB	2.33	0.58
1:A:105:VAL:HG11	1:A:252:PRO:HD3	1.86	0.58
1:A:693:ARG:NH1	1:A:693:ARG:HG2	2.19	0.57
1:A:293:ASN:OD1	1:A:295:SER:HB3	2.04	0.57
1:A:342:GLN:NE2	1:A:342:GLN:H	2.03	0.57
1:A:49:ALA:HB3	1:A:359:MSE:CE	2.36	0.55
1:A:693:ARG:HH11	1:A:693:ARG:HG2	1.72	0.55
1:A:51:LEU:CD1	1:A:359:MSE:HE2	2.38	0.54
1:A:85:GLU:HG3	1:A:249:GLN:NE2	2.23	0.54
1:A:411:LEU:HD13	1:A:455:LEU:HD23	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:LEU:N	1:A:79:LEU:HD23	2.23	0.53
1:A:298:ARG:CG	4:A:1034:HOH:O	2.55	0.53
1:A:490:ARG:NH1	4:A:1249:HOH:O	2.41	0.53
1:A:692:PHE:CA	1:A:693:ARG:CB	2.88	0.52
1:A:249:GLN:HB2	1:A:293:ASN:HB2	1.90	0.52
1:A:81:VAL:HG11	1:A:91:MSE:HE1	1.92	0.51
1:A:234:ARG:HH12	1:A:238:TYR:HB2	1.76	0.51
1:A:106:GLU:CG	1:A:251:ARG:HH12	2.24	0.50
1:A:693:ARG:CG	1:A:693:ARG:NH1	2.67	0.50
1:A:692:PHE:N	1:A:693:ARG:HB2	2.24	0.50
1:A:85:GLU:HG3	1:A:249:GLN:HE21	1.77	0.50
1:A:105:VAL:HG21	1:A:227:TYR:OH	2.12	0.49
1:A:350:GLU:HG3	1:A:351:PRO:HD2	1.95	0.49
1:A:553:LEU:HD22	1:A:557:MSE:CE	2.43	0.48
1:A:84[B]:SER:OG	1:A:85:GLU:N	2.46	0.48
1:A:340:GLU:HB3	1:A:342:GLN:HE22	1.79	0.48
1:A:504:VAL:HB	2:A:801:SLA:H2	1.94	0.48
1:A:490:ARG:HD2	4:A:1412:HOH:O	2.12	0.48
1:A:659:GLU:HG3	4:A:928:HOH:O	2.13	0.48
1:A:57:LEU:HA	1:A:436:ARG:HA	1.96	0.47
1:A:81:VAL:HG11	1:A:91:MSE:CE	2.45	0.47
1:A:682:GLU:OE2	1:A:689:MSE:HG2	2.15	0.47
1:A:15:GLU:OE1	1:A:15:GLU:CA	2.63	0.46
1:A:506:GLU:HG2	4:A:1265:HOH:O	2.15	0.46
1:A:284:LEU:HG	1:A:291:SER:HB3	1.98	0.46
1:A:630:PHE:CE2	1:A:659:GLU:HG2	2.50	0.46
1:A:688:ARG:NH2	4:A:1450:HOH:O	2.49	0.46
1:A:49:ALA:HB3	1:A:359:MSE:HE3	1.98	0.45
1:A:567:ILE:CD1	1:A:595:ILE:HD11	2.45	0.45
1:A:601:ARG:HB3	1:A:603:ASP:OD1	2.15	0.45
1:A:622:ILE:HG23	1:A:622:ILE:HD12	1.01	0.45
1:A:700:ARG:HB3	4:A:1404:HOH:O	2.16	0.45
1:A:298:ARG:CD	4:A:1034:HOH:O	2.64	0.45
1:A:236:ALA:O	1:A:240:GLU:HB2	2.16	0.45
1:A:249:GLN:O	1:A:249:GLN:HG3	2.17	0.45
1:A:498:GLU:HG2	1:A:518:THR:HG22	1.98	0.45
1:A:109:LEU:HA	1:A:110:LEU:HA	1.80	0.44
1:A:343:ALA:HA	1:A:344:PRO:HD2	1.79	0.44
1:A:494:ARG:HA	1:A:600:LEU:O	2.16	0.44
1:A:359:MSE:HE2	1:A:359:MSE:HB3	1.89	0.44
1:A:219:GLN:HG2	1:A:220:ARG:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:606:VAL:HG12	1:A:607:THR:N	2.32	0.44
1:A:22:SER:HA	1:A:405:LEU:HD11	2.00	0.44
1:A:526:ASP:OD1	1:A:563:LEU:HD12	2.17	0.44
1:A:578:ILE:HD13	1:A:578:ILE:HG21	1.69	0.44
1:A:340:GLU:HB3	1:A:342:GLN:NE2	2.33	0.44
1:A:411:LEU:HD12	1:A:455:LEU:HD23	2.00	0.43
1:A:75:PRO:HD2	1:A:258:SER:OG	2.19	0.43
1:A:315:LEU:HD13	1:A:366:ALA:HB1	2.00	0.43
1:A:102:ALA:C	1:A:105:VAL:HG12	2.38	0.43
1:A:522:ALA:HB1	1:A:523:PRO:HD2	2.00	0.43
1:A:246:ASP:C	1:A:248:ALA:H	2.22	0.43
1:A:246:ASP:HA	1:A:247:PRO:HA	1.91	0.42
1:A:51:LEU:HD11	1:A:359:MSE:CE	2.47	0.42
1:A:19:GLU:HA	1:A:20:PRO:HD3	1.88	0.42
1:A:33:GLU:CD	1:A:36:ARG:HH21	2.21	0.42
1:A:340:GLU:HA	1:A:341:PRO:HD2	1.89	0.42
1:A:219:GLN:CG	1:A:220:ARG:H	2.33	0.42
1:A:239:ALA:C	1:A:241:THR:N	2.73	0.42
1:A:350:GLU:HG3	1:A:351:PRO:CD	2.50	0.42
1:A:219:GLN:O	1:A:222:PRO:HD3	2.21	0.41
1:A:559:GLU:HG2	4:A:971:HOH:O	2.20	0.41
1:A:23:LEU:HD22	1:A:398:THR:HG23	2.01	0.41
1:A:520:ARG:HD3	1:A:520:ARG:HA	1.78	0.41
1:A:49:ALA:HB3	1:A:359:MSE:HE1	2.02	0.41
1:A:229:GLU:HA	1:A:232:ARG:HG2	2.02	0.41
1:A:342:GLN:H	1:A:342:GLN:HE21	1.68	0.41
1:A:578:ILE:HG22	4:A:1461:HOH:O	2.20	0.41
1:A:239:ALA:O	1:A:241:THR:N	2.53	0.41
1:A:239:ALA:C	1:A:241:THR:H	2.24	0.40
1:A:536:GLY:HA2	4:A:1454:HOH:O	2.21	0.40
1:A:688:ARG:HA	1:A:688:ARG:HD2	1.89	0.40
1:A:407:GLN:NE2	4:A:966:HOH:O	2.51	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	588/732 (80%)	560 (95%)	25 (4%)	3 (0%)	29 23

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	GLU
1	A	507	ALA
1	A	526	ASP

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	467/568 (82%)	423 (91%)	44 (9%)	8 5

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	15	GLU
1	A	16	ASN
1	A	73	GLU
1	A	85	GLU
1	A	93	LEU
1	A	101	LEU
1	A	105	VAL
1	A	106	GLU
1	A	219	GLN
1	A	238	TYR
1	A	240	GLU
1	A	241	THR
1	A	252	PRO

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Mol	Chain	Res	Type
1	A	260	SER
1	A	292	THR
1	A	295	SER
1	A	298	ARG
1	A	315	LEU
1	A	331	ARG
1	A	339	THR
1	A	342	GLN
1	A	348	GLU
1	A	350	GLU
1	A	355	GLN
1	A	359	MSE
1	A	395	GLU
1	A	429	GLN
1	A	433	MSE
1	A	489	LEU
1	A	527[A]	HIS
1	A	527[B]	HIS
1	A	533	ARG
1	A	549	LEU
1	A	556	ARG
1	A	563	LEU
1	A	565	VAL
1	A	617	LEU
1	A	622	ILE
1	A	690	GLU
1	A	693	ARG
1	A	696	GLN
1	A	700	ARG
1	A	703	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	97	GLN
1	A	249	GLN
1	A	342	GLN
1	A	429	GLN
1	A	597	ASN
1	A	668	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	SLA	A	801	1	10,15,15	2.60	4 (40%)	13,23,23	4.49	3 (23%)
3	PO4	A	802	-	4,4,4	1.38	1 (25%)	6,6,6	1.90	2 (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	SLA	A	801	1	-	0/6/32/32	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	SLA	C3-N4	-5.47	1.28	1.34
2	A	801	SLA	O10-C3	4.20	1.31	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	SLA	O7-C6	2.81	1.29	1.20
3	A	802	PO4	P-O2	-2.32	1.47	1.54
2	A	801	SLA	C2-C3	-2.29	1.50	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	SLA	O10-C3-C2	-13.60	115.36	126.17
2	A	801	SLA	C5-N4-C3	-7.53	109.58	114.58
3	A	802	PO4	O3-P-O2	2.99	117.20	107.91
2	A	801	SLA	O12-C11-C13	-2.90	103.68	109.90
3	A	802	PO4	O4-P-O1	-2.42	102.40	110.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	SLA	1	0

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	585/732 (79%)	0.32	36 (6%) 20 19	15, 28, 75, 100	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	285	VAL	6.6
1	A	342	GLN	5.6
1	A	109	LEU	4.8
1	A	560	HIS	4.8
1	A	110	LEU	4.6
1	A	692	PHE	4.5
1	A	239	ALA	4.4
1	A	237	ARG	4.4
1	A	693	ARG	4.3
1	A	508	ALA	4.3
1	A	525	ARG	4.0
1	A	341	PRO	3.6
1	A	241	THR	3.5
1	A	558	ILE	3.4
1	A	284	LEU	3.4
1	A	240	GLU	3.4
1	A	691	GLY	3.3
1	A	708	ARG	3.2
1	A	419	LEU	3.1
1	A	290	TRP	2.9
1	A	339	THR	2.7
1	A	688	ARG	2.7
1	A	234	ARG	2.7
1	A	107	GLY	2.6
1	A	687	ALA	2.6
1	A	709	LEU	2.5
1	A	559	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	246	ASP	2.5
1	A	15	GLU	2.4
1	A	100	HIS	2.3
1	A	238	TYR	2.3
1	A	230	ALA	2.3
1	A	563	LEU	2.2
1	A	344	PRO	2.1
1	A	251	ARG	2.1
1	A	220	ARG	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	SLA	A	801	15/15	0.95	0.08	19,24,26,27	0
3	PO4	A	802	5/5	0.99	0.06	19,23,25,31	0

6.5 Other polymers (i)

There are no such residues in this entry.