Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 08:16 PM EDT

PDB ID	:	4FW9
Title	:	Crystal structure of the Lon-like protease MtaLonC
Authors	:	Chang, C.I.; Ihara, K.; Kuo, C.I.; Huang, K.F.; Wakatsuki, S.
Deposited on	:	2012-06-30
Resolution	:	2.00 Å(reported)

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

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

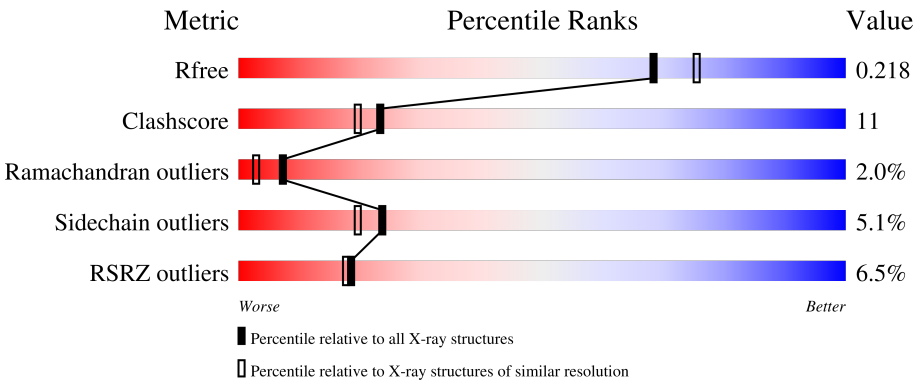
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

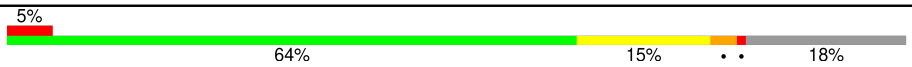
The reported resolution of this entry is 2.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	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 3 unique types of molecules in this entry. The entry contains 5043 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.

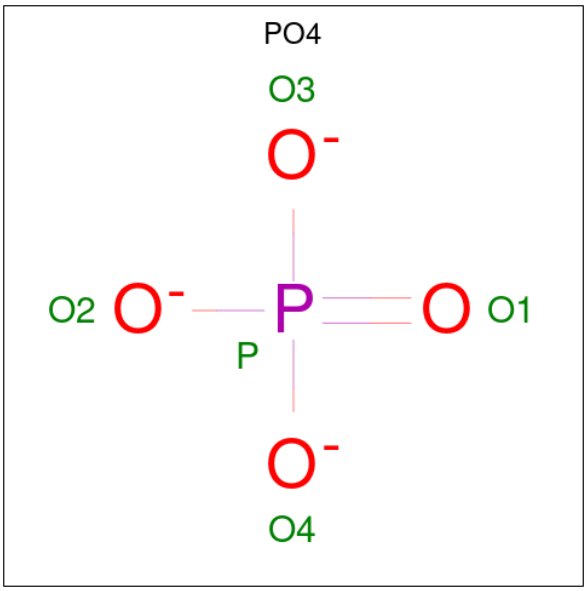
- Molecule 1 is a protein called TTC1975 peptidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	603	4633	2939	822	862	2	8	0	1	0

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	91	MSE	LEU	ENGINEERED MUTATION	UNP C9DRU9
A	359	MSE	ILE	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 PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 3 is water.

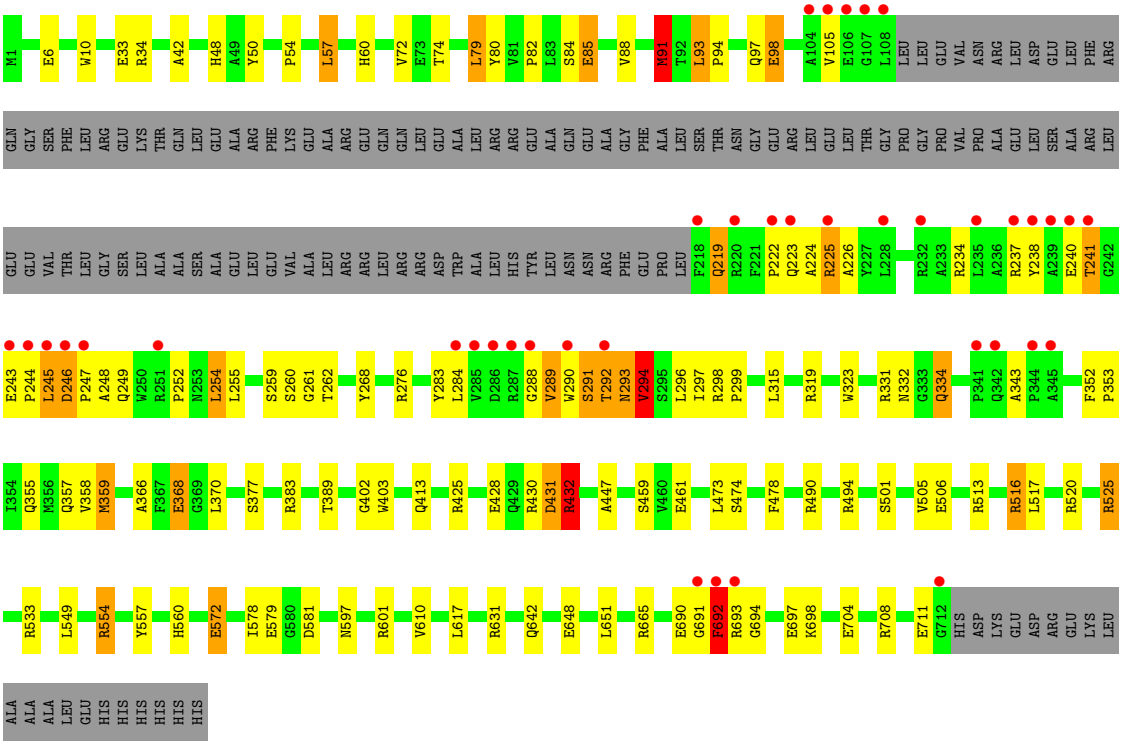
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	405	405	405	0	0

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	115.68Å 115.68Å 136.78Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.00 – 2.00 136.78 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (50.00-2.00) 99.9 (136.78-2.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.66 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.183 , 0.218 0.183 , 0.218	Depositor DCC
R_{free} test set	3533 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	29.0	Xtriage
Anisotropy	0.409	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 39.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.087 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5043	wwPDB-VP
Average B, all atoms (Å^2)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% 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

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	1.37	26/4726 (0.6%)	1.37	41/6413 (0.6%)

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	3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	359	MSE	CB-CG	9.52	1.80	1.52
1	A	432	ARG	CD-NE	-9.15	1.30	1.46
1	A	10	TRP	CD2-CE2	8.68	1.51	1.41
1	A	579	GLU	CD-OE2	-7.73	1.17	1.25
1	A	431	ASP	CG-OD1	7.39	1.42	1.25
1	A	474	SER	CB-OG	6.90	1.51	1.42
1	A	6	GLU	CD-OE1	6.87	1.33	1.25
1	A	572	GLU	CG-CD	6.70	1.61	1.51
1	A	268	TYR	CE1-CZ	6.21	1.46	1.38
1	A	473	LEU	N-CA	6.14	1.58	1.46
1	A	478	PHE	CG-CD1	6.05	1.47	1.38
1	A	323	TRP	CD2-CE2	5.87	1.48	1.41
1	A	403	TRP	CD2-CE2	5.71	1.48	1.41
1	A	290	TRP	CD2-CE2	5.60	1.48	1.41
1	A	557	TYR	CE1-CZ	5.52	1.45	1.38
1	A	6	GLU	CG-CD	5.39	1.60	1.51
1	A	402	GLY	N-CA	5.39	1.54	1.46
1	A	428	GLU	CD-OE2	5.26	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	461	GLU	CG-CD	5.25	1.59	1.51
1	A	33	GLU	CD-OE2	5.23	1.31	1.25
1	A	60	HIS	CG-CD2	5.18	1.44	1.35
1	A	501	SER	CB-OG	-5.17	1.35	1.42
1	A	572	GLU	CB-CG	5.12	1.61	1.52
1	A	50	TYR	CG-CD2	5.12	1.45	1.39
1	A	579	GLU	CG-CD	5.08	1.59	1.51
1	A	334	GLN	CD-OE1	5.01	1.34	1.24

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	-28.09	106.25	120.30
1	A	432	ARG	NE-CZ-NH1	20.91	130.76	120.30
1	A	554	ARG	NE-CZ-NH1	16.57	128.59	120.30
1	A	431	ASP	CB-CG-OD2	-14.90	104.89	118.30
1	A	554	ARG	NE-CZ-NH2	-13.93	113.33	120.30
1	A	431	ASP	CB-CG-OD1	12.86	129.87	118.30
1	A	359	MSE	CB-CG-SE	-10.09	82.43	112.70
1	A	631	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	A	572	GLU	C-N-CA	-8.84	99.61	121.70
1	A	572	GLU	OE1-CD-OE2	-8.77	112.77	123.30
1	A	319	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	A	34	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	A	665	ARG	CG-CD-NE	-7.85	95.31	111.80
1	A	383	ARG	NE-CZ-NH2	7.64	124.12	120.30
1	A	431	ASP	N-CA-CB	-7.41	97.26	110.60
1	A	579	GLU	OE1-CD-OE2	-7.29	114.55	123.30
1	A	319	ARG	NE-CZ-NH2	-6.93	116.83	120.30
1	A	425	ARG	NE-CZ-NH2	-6.89	116.86	120.30
1	A	631	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	581	ASP	CB-CG-OD1	6.58	124.23	118.30
1	A	516	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	A	432	ARG	CG-CD-NE	-6.41	98.34	111.80
1	A	432	ARG	CD-NE-CZ	6.28	132.40	123.60
1	A	490	ARG	NE-CZ-NH1	-6.26	117.17	120.30
1	A	331	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	57	LEU	CB-CG-CD2	-6.20	100.46	111.00
1	A	642	GLN	CA-CB-CG	-5.90	100.43	113.40
1	A	432	ARG	CB-CG-CD	-5.48	97.35	111.60
1	A	383	ARG	NE-CZ-NH1	-5.39	117.60	120.30
1	A	513	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	554	ARG	CB-CG-CD	-5.36	97.66	111.60
1	A	91	MSE	CG-SE-CE	5.36	110.69	98.90
1	A	516	ARG	CG-CD-NE	-5.29	100.69	111.80
1	A	91	MSE	N-CA-CB	-5.21	101.23	110.60
1	A	425	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	276	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	572	GLU	O-C-N	-5.09	114.56	122.70
1	A	6	GLU	CG-CD-OE1	5.04	128.38	118.30
1	A	359	MSE	CB-CA-C	5.02	120.45	110.40
1	A	601	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	A	430	ARG	NE-CZ-NH1	-5.00	117.80	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	246	ASP	Peptide
1	A	691	GLY	Peptide
1	A	692	PHE	Peptide

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	4633	0	4647	105	0
2	A	5	0	0	0	0
3	A	405	0	0	13	0
All	All	5043	0	4647	105	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 11.

All (105) 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:359:MSE:CB	1:A:359:MSE:CG	1.81	1.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:MSE:CB	1:A:359:MSE:SE	2.51	1.09
1:A:413:GLN:HG3	3:A:1291:HOH:O	1.66	0.96
1:A:692:PHE:HD2	1:A:692:PHE:O	1.51	0.93
1:A:225:ARG:HG3	1:A:226:ALA:N	1.87	0.90
1:A:359:MSE:SE	1:A:359:MSE:HB3	2.26	0.84
1:A:245:LEU:CB	1:A:246:ASP:HA	2.07	0.84
1:A:254:LEU:HD23	3:A:1085:HOH:O	1.82	0.79
1:A:525:ARG:HD2	1:A:525:ARG:H	1.47	0.79
1:A:246:ASP:C	1:A:248:ALA:HA	2.04	0.78
1:A:284:LEU:H	1:A:291:SER:HB2	1.49	0.77
1:A:249:GLN:HB2	1:A:293:ASN:CB	2.17	0.74
1:A:247:PRO:N	1:A:248:ALA:HA	2.04	0.73
1:A:711:GLU:HG3	1:A:711:GLU:O	1.88	0.72
1:A:82:PRO:HD3	1:A:294:VAL:HG21	1.71	0.71
1:A:692:PHE:O	1:A:692:PHE:CD2	2.40	0.71
1:A:74:THR:OG1	1:A:260:SER:HA	1.92	0.70
1:A:505:VAL:CG2	3:A:1094:HOH:O	2.39	0.69
1:A:284:LEU:O	1:A:291:SER:HB3	1.93	0.69
1:A:549:LEU:CD2	1:A:610:VAL:HG21	2.25	0.67
1:A:249:GLN:CG	1:A:249:GLN:O	2.42	0.67
1:A:54:PRO:HD2	1:A:57:LEU:HD11	1.76	0.66
1:A:88:VAL:CG1	1:A:294:VAL:HG13	2.25	0.66
1:A:79:LEU:HD11	1:A:91:MSE:HE3	1.77	0.66
1:A:249:GLN:HB2	1:A:293:ASN:HB2	1.77	0.66
1:A:315:LEU:HD13	1:A:366:ALA:CB	2.27	0.64
1:A:225:ARG:HG3	1:A:226:ALA:H	1.62	0.64
1:A:79:LEU:HD21	1:A:93:LEU:HD22	1.79	0.64
1:A:48:HIS:HD2	1:A:358:VAL:H	1.45	0.64
1:A:245:LEU:CB	1:A:246:ASP:CA	2.76	0.64
1:A:246:ASP:O	1:A:248:ALA:HA	1.96	0.64
1:A:72:VAL:O	1:A:261:GLY:HA3	1.98	0.63
1:A:97:GLN:O	1:A:97:GLN:HG3	1.99	0.63
1:A:284:LEU:N	1:A:291:SER:HB2	2.12	0.63
1:A:692:PHE:HA	1:A:694:GLY:H	1.63	0.63
1:A:332:ASN:HB2	1:A:334:GLN:HG3	1.79	0.63
1:A:48:HIS:CD2	1:A:358:VAL:H	2.16	0.63
1:A:516:ARG:CZ	3:A:1133:HOH:O	2.46	0.62
1:A:494:ARG:NE	3:A:1288:HOH:O	2.33	0.62
1:A:238:TYR:HD1	1:A:243:GLU:O	1.82	0.61
1:A:85:GLU:HG3	1:A:249:GLN:NE2	2.15	0.61
1:A:288:GLY:O	1:A:289:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:693:ARG:HA	1:A:697:GLU:OE1	2.01	0.60
1:A:240:GLU:HG2	1:A:240:GLU:O	2.02	0.59
1:A:94:PRO:HD3	1:A:223:GLN:NE2	2.16	0.59
1:A:255:LEU:HD22	1:A:299:PRO:HB3	1.85	0.58
1:A:692:PHE:HA	1:A:694:GLY:N	2.18	0.58
1:A:525:ARG:HD2	1:A:525:ARG:N	2.18	0.58
1:A:105:VAL:HG21	1:A:252:PRO:HD3	1.86	0.57
1:A:572:GLU:HA	1:A:572:GLU:OE1	2.05	0.57
1:A:389:THR:OG1	1:A:432:ARG:CD	2.53	0.56
1:A:249:GLN:O	1:A:249:GLN:HG3	2.05	0.56
1:A:549:LEU:HD21	1:A:610:VAL:CG2	2.36	0.56
1:A:80:TYR:CE1	1:A:297:ILE:HG21	2.41	0.56
1:A:549:LEU:CD2	1:A:610:VAL:CG2	2.84	0.55
1:A:249:GLN:HB2	1:A:293:ASN:HB3	1.88	0.55
1:A:241:THR:HB	1:A:243:GLU:HB2	1.89	0.54
1:A:315:LEU:HD13	1:A:366:ALA:HB2	1.89	0.54
1:A:82:PRO:CD	1:A:294:VAL:HG21	2.36	0.54
1:A:234:ARG:HH22	1:A:243:GLU:HB3	1.73	0.54
1:A:554:ARG:NH2	3:A:1218:HOH:O	2.40	0.54
1:A:560:HIS:HE1	3:A:1031:HOH:O	1.91	0.52
1:A:389:THR:OG1	1:A:432:ARG:HD3	2.10	0.52
1:A:88:VAL:HG11	1:A:294:VAL:HG13	1.93	0.50
1:A:549:LEU:HD21	1:A:610:VAL:HG21	1.93	0.50
1:A:98:GLU:HG2	1:A:254:LEU:HD12	1.92	0.50
1:A:79:LEU:HD11	1:A:91:MSE:CE	2.42	0.50
1:A:88:VAL:HG12	1:A:294:VAL:HG13	1.94	0.50
1:A:704:GLU:HG3	1:A:708:ARG:HH11	1.76	0.50
1:A:389:THR:OG1	1:A:432:ARG:HD2	2.11	0.50
1:A:447:ALA:O	1:A:459:SER:HB2	2.14	0.48
1:A:560:HIS:CE1	3:A:1031:HOH:O	2.66	0.48
1:A:289:VAL:CG1	1:A:289:VAL:O	2.62	0.48
1:A:82:PRO:HD3	1:A:294:VAL:HG11	1.96	0.47
1:A:247:PRO:N	1:A:248:ALA:CA	2.75	0.47
1:A:225:ARG:CZ	1:A:225:ARG:HB2	2.44	0.47
1:A:572:GLU:HG3	3:A:1133:HOH:O	2.14	0.47
1:A:240:GLU:O	1:A:240:GLU:CG	2.63	0.46
1:A:247:PRO:HD2	1:A:249:GLN:HB3	1.96	0.46
1:A:517:LEU:C	1:A:517:LEU:HD23	2.35	0.46
1:A:289:VAL:O	1:A:289:VAL:HG12	2.15	0.46
1:A:98:GLU:HG2	1:A:254:LEU:CD1	2.46	0.46
1:A:284:LEU:N	1:A:291:SER:CB	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:PHE:HB3	3:A:1022:HOH:O	2.16	0.45
1:A:94:PRO:O	1:A:97:GLN:HB3	2.17	0.45
1:A:520:ARG:HD3	3:A:1135:HOH:O	2.17	0.44
1:A:292:THR:OG1	1:A:293:ASN:N	2.48	0.44
1:A:42:ALA:O	1:A:357:GLN:NE2	2.50	0.44
1:A:284:LEU:HG	1:A:296:LEU:HD11	1.99	0.44
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.82	0.44
1:A:254:LEU:CD2	3:A:1085:HOH:O	2.50	0.44
1:A:283:TYR:CE1	1:A:343:ALA:HB2	2.53	0.44
1:A:237:ARG:HA	1:A:240:GLU:HB3	1.99	0.43
1:A:80:TYR:CE1	1:A:297:ILE:CG2	3.01	0.43
1:A:648:GLU:O	1:A:651:LEU:HG	2.19	0.42
1:A:352:PHE:HB2	1:A:353:PRO:CD	2.50	0.42
1:A:711:GLU:O	1:A:711:GLU:CG	2.58	0.42
1:A:283:TYR:HA	1:A:291:SER:HB2	2.01	0.41
1:A:368:GLU:OE1	1:A:368:GLU:HA	2.03	0.41
1:A:82:PRO:CG	1:A:294:VAL:HG21	2.50	0.41
1:A:283:TYR:HD1	1:A:291:SER:OG	2.03	0.41
1:A:698:LYS:HE3	3:A:1231:HOH:O	2.19	0.41
1:A:85:GLU:CG	1:A:249:GLN:NE2	2.83	0.41
1:A:219:GLN:OE1	1:A:219:GLN:HA	2.20	0.41
1:A:238:TYR:CD2	1:A:238:TYR:C	2.92	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	600/732 (82%)	568 (95%)	20 (3%)	12 (2%)	7 3

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	244	PRO
1	A	245	LEU
1	A	291	SER
1	A	293	ASN
1	A	219	GLN
1	A	289	VAL
1	A	224	ALA
1	A	241	THR
1	A	292	THR
1	A	84	SER
1	A	222	PRO
1	A	294	VAL

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	471/571 (82%)	447 (95%)	24 (5%)	24 19

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	LEU
1	A	85	GLU
1	A	91	MSE
1	A	93	LEU
1	A	98	GLU
1	A	225	ARG
1	A	254	LEU
1	A	259	SER
1	A	262	THR
1	A	294	VAL
1	A	298	ARG
1	A	355	GLN
1	A	368	GLU
1	A	377	SER
1	A	431	ASP

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Mol	Chain	Res	Type
1	A	432	ARG
1	A	506	GLU
1	A	525	ARG
1	A	533	ARG
1	A	578	ILE
1	A	597	ASN
1	A	617	LEU
1	A	690	GLU
1	A	692	PHE

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	223	GLN
1	A	249	GLN
1	A	332	ASN
1	A	334	GLN
1	A	462	GLN
1	A	597	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)

1 ligand is 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	PO4	A	801	-	4,4,4	1.13	0	6,6,6	1.93	3 (50%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	PO4	O3-P-O2	2.81	116.65	107.91
2	A	801	PO4	O4-P-O1	-2.35	102.63	110.95
2	A	801	PO4	O4-P-O3	-2.09	101.40	107.91

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	596/732 (81%)	-0.31	39 (6%) 18 18	18, 31, 95, 144	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	TRP	10.1
1	A	245	LEU	8.5
1	A	108	LEU	6.1
1	A	692	PHE	5.3
1	A	286	ASP	5.0
1	A	218	PHE	4.9
1	A	288	GLY	4.6
1	A	712	GLY	4.5
1	A	284	LEU	4.5
1	A	244	PRO	4.2
1	A	237	ARG	3.9
1	A	344	PRO	3.8
1	A	247	PRO	3.8
1	A	287	ARG	3.7
1	A	223	GLN	3.6
1	A	239	ALA	3.6
1	A	292	THR	3.5
1	A	107	GLY	3.5
1	A	235	LEU	3.5
1	A	222	PRO	3.4
1	A	285	VAL	3.3
1	A	693	ARG	3.3
1	A	241	THR	3.2
1	A	105	VAL	3.0
1	A	342	GLN	2.8
1	A	225	ARG	2.8
1	A	220	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	228	LEU	2.8
1	A	246	ASP	2.6
1	A	341	PRO	2.6
1	A	691	GLY	2.5
1	A	106	GLU	2.4
1	A	240	GLU	2.4
1	A	232	ARG	2.4
1	A	251	ARG	2.2
1	A	345	ALA	2.2
1	A	104	ALA	2.1
1	A	238	TYR	2.1
1	A	243	GLU	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	PO4	A	801	5/5	0.99	0.06	24,30,33,33	0

6.5 Other polymers (i)

There are no such residues in this entry.