Full wwPDB X-ray Structure Validation Report (i)

Jun 18, 2024 – 08:26 PM EDT

PDB ID	:	4FWD
Title	:	Crystal structure of the Lon-like protease MtaLonC in complex with bortezomib
Authors	:	Chang, C.I.; Kuo, C.I.; Huang, K.F.
Deposited on	:	2012-06-30
Resolution	:	2.03 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:

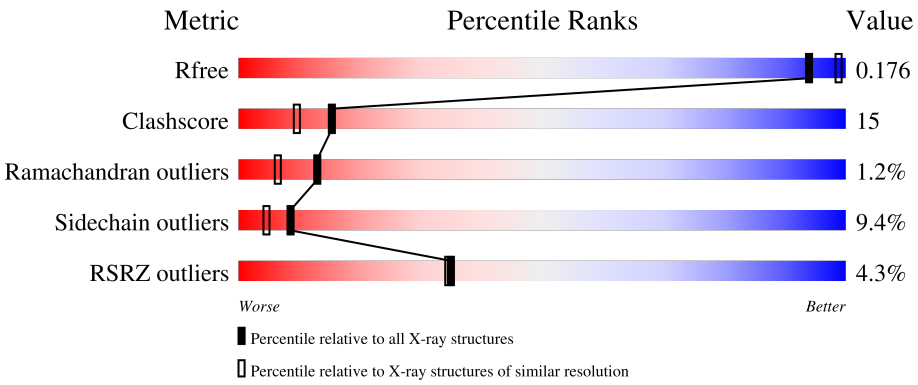
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 2.03 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	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

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	3% 54% 20% 5% • 20%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4942 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.

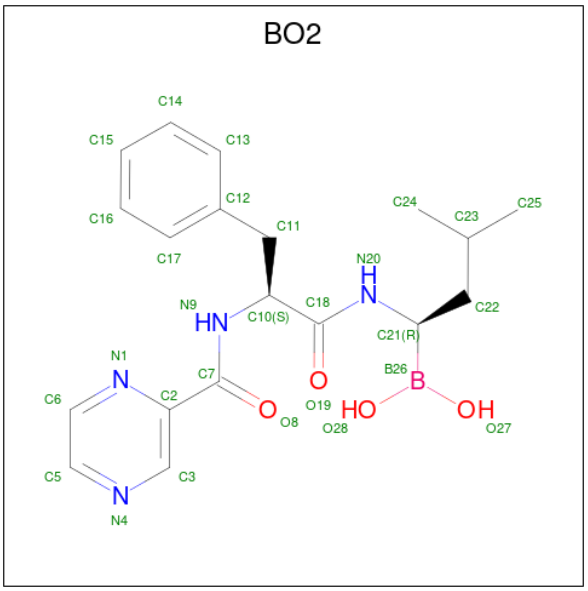
- Molecule 1 is a protein called TTC1975 peptidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	587	4514	2865	799	842	8	0	2	0

There are 13 discrepancies between the modelled and reference sequences:

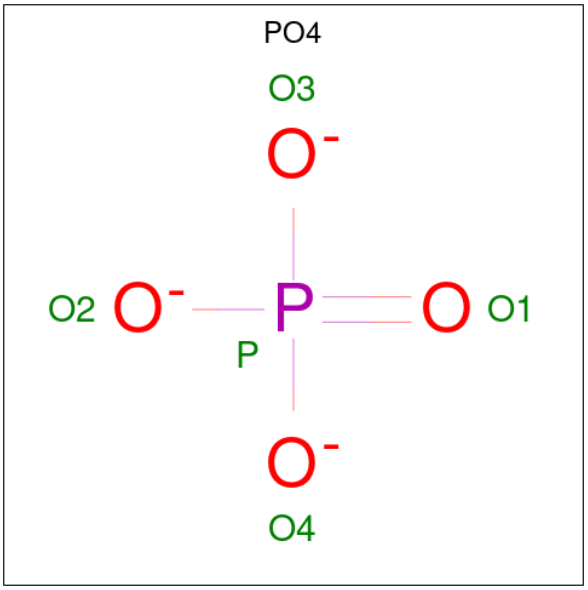
Chain	Residue	Modelled	Actual	Comment	Reference
A	720	LYS	-	expression tag	UNP C9DRU9
A	721	LEU	-	expression tag	UNP C9DRU9
A	722	ALA	-	expression tag	UNP C9DRU9
A	723	ALA	-	expression tag	UNP C9DRU9
A	724	ALA	-	expression tag	UNP C9DRU9
A	725	LEU	-	expression tag	UNP C9DRU9
A	726	GLU	-	expression tag	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 N-[(1R)-1-(DIHYDROXYBORYL)-3-METHYLBUTYL]-N-(PYRAZIN-2-YLCARBONYL)-L-PHENYLALANINAMIDE (three-letter code: BO2) (formula: $C_{19}H_{25}BN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	B	C	N	O		
2	A	1	28	1	19	4	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.

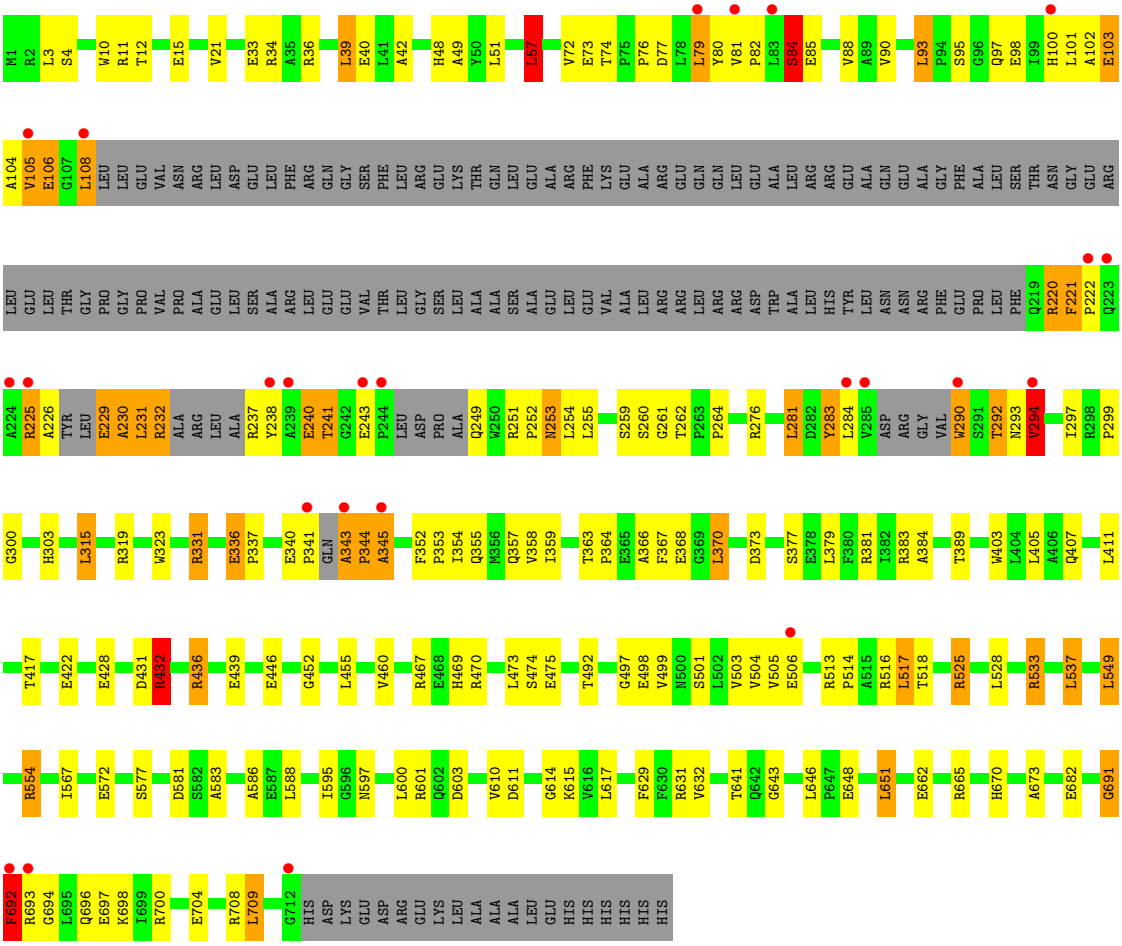
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	395	395	395	0	0

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	115.92Å 115.92Å 135.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.03 47.08 – 2.02	Depositor EDS
% Data completeness (in resolution range)	97.1 (30.00-2.03) 97.0 (47.08-2.02)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.46 (at 2.01Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.170 , 0.195 0.151 , 0.176	Depositor DCC
R_{free} test set	3328 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 31.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.407 for h,-h-k,-l	Xtriage
Reported twinning fraction	0.582 for H, K, L 0.418 for K, H, -L	Depositor
Outliers	0 of 65525 reflections	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	4942	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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, BO2

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	1.45	27/4608 (0.6%)	1.42	44/6256 (0.7%)

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	4

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	651	LEU	N-CA	7.25	1.60	1.46
1	A	452	GLY	N-CA	6.58	1.55	1.46
1	A	432	ARG	CD-NE	-6.38	1.35	1.46
1	A	469	HIS	C-O	6.35	1.35	1.23
1	A	691	GLY	N-CA	6.34	1.55	1.46
1	A	446	GLU	CD-OE1	6.32	1.32	1.25
1	A	10	TRP	CD2-CE2	6.13	1.48	1.41
1	A	33	GLU	CD-OE1	6.09	1.32	1.25
1	A	601	ARG	CZ-NH2	6.05	1.41	1.33
1	A	473	LEU	N-CA	5.98	1.58	1.46
1	A	572	GLU	CD-OE1	-5.90	1.19	1.25
1	A	497	GLY	N-CA	5.85	1.54	1.46
1	A	474	SER	CB-OG	5.84	1.49	1.42
1	A	475	GLU	CD-OE1	5.76	1.31	1.25
1	A	614	GLY	N-CA	5.75	1.54	1.46
1	A	323	TRP	CD2-CE2	5.64	1.48	1.41
1	A	641	THR	CB-CG2	5.62	1.70	1.52
1	A	682	GLU	N-CA	5.60	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	290	TRP	CD2-CE2	5.54	1.48	1.41
1	A	572	GLU	CD-OE2	-5.50	1.19	1.25
1	A	422	GLU	CD-OE1	-5.43	1.19	1.25
1	A	470	ARG	CD-NE	5.40	1.55	1.46
1	A	4	SER	CA-CB	5.38	1.61	1.52
1	A	367	PHE	CG-CD2	5.19	1.46	1.38
1	A	460	VAL	CB-CG1	5.11	1.63	1.52
1	A	384	ALA	CA-CB	5.09	1.63	1.52
1	A	549	LEU	C-O	5.02	1.32	1.23

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	432	ARG	NE-CZ-NH2	-18.43	111.09	120.30
1	A	554	ARG	NE-CZ-NH2	-14.68	112.96	120.30
1	A	436	ARG	NE-CZ-NH1	-10.74	114.93	120.30
1	A	373	ASP	CB-CG-OD2	-10.30	109.03	118.30
1	A	432	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	A	373	ASP	CB-CG-OD1	9.45	126.80	118.30
1	A	554	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	A	549	LEU	CB-CG-CD2	-9.19	95.38	111.00
1	A	572	GLU	C-N-CA	-9.07	99.03	121.70
1	A	631	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	581	ASP	CB-CG-OD1	7.76	125.28	118.30
1	A	381	ARG	NE-CZ-NH1	-7.48	116.56	120.30
1	A	383	ARG	NE-CZ-NH2	7.39	124.00	120.30
1	A	516	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	A	57	LEU	CA-CB-CG	7.25	131.99	115.30
1	A	517	LEU	CB-CG-CD2	7.25	123.33	111.00
1	A	665	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	A	692	PHE	N-CA-C	7.10	130.18	111.00
1	A	572	GLU	O-C-N	-7.09	111.35	122.70
1	A	600	LEU	CB-CG-CD1	-6.95	99.19	111.00
1	A	319	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	A	665	ARG	CG-CD-NE	-6.76	97.59	111.80
1	A	432	ARG	CG-CD-NE	-6.67	97.80	111.80
1	A	370	LEU	CA-CB-CG	-6.61	100.09	115.30
1	A	537	LEU	CB-CG-CD1	-6.61	99.77	111.00
1	A	611	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	276	ARG	NE-CZ-NH1	6.55	123.57	120.30
1	A	513	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	A	319	ARG	NE-CZ-NH2	-6.27	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	698	LYS	CD-CE-NZ	-6.15	97.56	111.70
1	A	431[A]	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	431[B]	ASP	CB-CG-OD1	5.99	123.69	118.30
1	A	603	ASP	CB-CG-OD1	5.89	123.60	118.30
1	A	629	PHE	CB-CG-CD1	-5.80	116.74	120.80
1	A	11	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	A	588	LEU	CB-CG-CD2	-5.47	101.70	111.00
1	A	281	LEU	CB-CG-CD1	-5.39	101.83	111.00
1	A	467	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	549	LEU	CB-CA-C	-5.29	100.16	110.20
1	A	34	ARG	NE-CZ-NH1	-5.24	117.68	120.30
1	A	39	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	230	ALA	N-CA-C	-5.22	96.92	111.00
1	A	439	GLU	CA-CB-CG	-5.16	102.05	113.40
1	A	709	LEU	CB-CG-CD1	5.09	119.65	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	231	LEU	Peptide
1	A	343	ALA	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	4514	0	4531	136	0
2	A	28	0	25	5	0
3	A	5	0	0	0	0
4	A	395	0	0	11	0
All	All	4942	0	4556	136	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (136) 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:229:GLU:CB	1:A:230:ALA:HA	1.78	1.13
1:A:229:GLU:HB2	1:A:230:ALA:CA	1.75	1.12
1:A:492:THR:HG22	4:A:1083:HOH:O	1.51	1.09
1:A:503:VAL:HG12	2:A:801:BO2:C24	1.82	1.09
1:A:692:PHE:HZ	1:A:696:GLN:HB3	1.20	1.06
1:A:229:GLU:HB2	1:A:230:ALA:HA	1.07	1.04
1:A:220:ARG:HH11	1:A:220:ARG:HG3	1.25	1.01
1:A:82:PRO:HG3	1:A:294:VAL:HG21	1.47	0.95
1:A:101:LEU:HB2	1:A:221:PHE:CE2	2.02	0.94
1:A:253:ASN:HD22	1:A:254:LEU:N	1.67	0.93
1:A:503:VAL:HG12	2:A:801:BO2:H241	1.56	0.88
1:A:692:PHE:CZ	1:A:696:GLN:HB3	2.10	0.86
1:A:300:GLY:H	1:A:303:HIS:HD2	1.22	0.85
1:A:525:ARG:HD2	1:A:525:ARG:H	1.42	0.83
1:A:82:PRO:HG3	1:A:294:VAL:CG2	2.12	0.80
1:A:72:VAL:O	1:A:261:GLY:HA3	1.81	0.79
1:A:103:GLU:HA	1:A:106:GLU:HB2	1.65	0.79
1:A:232:ARG:HA	4:A:1231:HOH:O	1.81	0.78
1:A:101:LEU:HA	1:A:104:ALA:HB3	1.64	0.78
1:A:352:PHE:HB2	1:A:353:PRO:HD2	1.64	0.77
1:A:503:VAL:HG12	2:A:801:BO2:H243	1.67	0.77
1:A:81:VAL:HG12	1:A:252:PRO:HB3	1.70	0.73
1:A:221:PHE:H	1:A:222:PRO:CD	2.02	0.72
1:A:103:GLU:HA	1:A:106:GLU:CB	2.18	0.72
1:A:221:PHE:N	1:A:222:PRO:CD	2.51	0.72
1:A:106:GLU:HA	1:A:106:GLU:OE1	1.89	0.71
1:A:525:ARG:HD2	1:A:525:ARG:N	2.05	0.71
1:A:253:ASN:HD22	1:A:253:ASN:C	1.89	0.70
1:A:93:LEU:HB2	4:A:1238:HOH:O	1.92	0.68
1:A:82:PRO:CG	1:A:294:VAL:HG21	2.22	0.68
1:A:48:HIS:HD2	1:A:358:VAL:H	1.43	0.67
1:A:549:LEU:HD21	1:A:610:VAL:HG21	1.79	0.64
1:A:48:HIS:CD2	1:A:358:VAL:H	2.15	0.64
1:A:505:VAL:HG11	4:A:1208:HOH:O	1.96	0.64
1:A:262:THR:HG23	1:A:262:THR:O	1.97	0.63
1:A:237:ARG:HA	1:A:240:GLU:HB3	1.80	0.63
1:A:341:PRO:O	1:A:343:ALA:HB3	1.97	0.63
1:A:693:ARG:HA	1:A:697:GLU:OE1	2.00	0.62
1:A:692:PHE:HD2	1:A:694:GLY:H	1.48	0.62
1:A:77:ASP:OD2	1:A:95:SER:HA	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:VAL:HG22	1:A:264:PRO:HB3	1.83	0.61
1:A:220:ARG:HG3	1:A:220:ARG:NH1	2.03	0.60
1:A:253:ASN:C	1:A:253:ASN:ND2	2.55	0.60
1:A:76:PRO:HB3	1:A:93:LEU:O	2.02	0.59
1:A:615:LYS:HE3	4:A:915:HOH:O	2.02	0.59
1:A:221:PHE:H	1:A:222:PRO:HD3	1.68	0.58
1:A:79:LEU:HD21	1:A:93:LEU:HD22	1.86	0.58
1:A:255:LEU:HD22	1:A:299:PRO:HB3	1.87	0.57
1:A:389:THR:OG1	1:A:432:ARG:HD3	2.05	0.57
1:A:241:THR:HG22	1:A:243:GLU:HB2	1.86	0.57
1:A:221:PHE:N	1:A:222:PRO:HD3	2.20	0.56
1:A:300:GLY:H	1:A:303:HIS:CD2	2.13	0.56
1:A:101:LEU:HB2	1:A:221:PHE:HE2	1.66	0.55
1:A:74:THR:OG1	1:A:260:SER:HA	2.06	0.55
1:A:21:VAL:HG12	1:A:405:LEU:HD11	1.89	0.54
1:A:101:LEU:HB2	1:A:221:PHE:CD2	2.43	0.53
1:A:229:GLU:CB	1:A:230:ALA:CA	2.52	0.53
1:A:237:ARG:HA	1:A:240:GLU:CB	2.40	0.52
1:A:567:ILE:HD11	1:A:595:ILE:HD11	1.92	0.52
1:A:108:LEU:HD11	4:A:1178:HOH:O	2.08	0.52
1:A:583:ALA:HB2	2:A:801:BO2:H23	1.90	0.52
1:A:281:LEU:CD1	1:A:337:PRO:HB2	2.40	0.52
1:A:105:VAL:HG11	1:A:252:PRO:HD2	1.92	0.51
1:A:262:THR:O	1:A:262:THR:CG2	2.59	0.51
1:A:72:VAL:CG2	1:A:264:PRO:HB3	2.40	0.51
1:A:238:TYR:HD2	1:A:243:GLU:O	1.93	0.51
1:A:290:TRP:N	1:A:290:TRP:CD1	2.79	0.50
1:A:260:SER:HB2	1:A:262:THR:HG22	1.94	0.49
1:A:220:ARG:O	1:A:221:PHE:CB	2.60	0.49
1:A:220:ARG:O	1:A:221:PHE:HB2	2.13	0.49
1:A:82:PRO:HD3	1:A:294:VAL:HG11	1.94	0.49
1:A:498:GLU:HG2	1:A:518:THR:HG22	1.95	0.49
1:A:221:PHE:H	1:A:222:PRO:HD2	1.78	0.48
1:A:103:GLU:HA	1:A:106:GLU:HB3	1.93	0.48
1:A:249:GLN:CG	1:A:249:GLN:O	2.60	0.48
1:A:343:ALA:N	1:A:344:PRO:HA	2.29	0.48
1:A:403:TRP:O	1:A:407:GLN:HG2	2.13	0.48
1:A:533:ARG:NH2	4:A:1031:HOH:O	2.41	0.48
1:A:709:LEU:HD23	1:A:709:LEU:HA	1.71	0.48
1:A:101:LEU:O	1:A:105:VAL:HB	2.13	0.47
1:A:42:ALA:O	1:A:357:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:VAL:CG1	1:A:294:VAL:HG13	2.45	0.47
1:A:100:HIS:HB3	1:A:221:PHE:HZ	1.80	0.47
1:A:97:GLN:CG	1:A:97:GLN:O	2.63	0.47
1:A:363:THR:HB	1:A:364:PRO:HD2	1.96	0.47
1:A:525:ARG:N	1:A:525:ARG:CD	2.72	0.47
1:A:549:LEU:HA	1:A:549:LEU:HD23	1.67	0.47
1:A:90:VAL:HG11	1:A:352:PHE:CD1	2.50	0.47
1:A:283:TYR:N	1:A:283:TYR:CD2	2.82	0.46
1:A:220:ARG:HH11	1:A:220:ARG:CG	2.10	0.46
1:A:370:LEU:HD23	1:A:370:LEU:HA	1.38	0.46
1:A:554:ARG:HG2	4:A:1215:HOH:O	2.15	0.46
1:A:292:THR:CG2	1:A:293:ASN:N	2.79	0.46
1:A:428:GLU:OE2	4:A:1152:HOH:O	2.21	0.46
1:A:549:LEU:HD21	1:A:610:VAL:CG2	2.44	0.46
1:A:692:PHE:CZ	1:A:697:GLU:N	2.84	0.45
1:A:281:LEU:HD23	1:A:292:THR:HG21	1.97	0.45
1:A:411:LEU:HD13	1:A:455:LEU:HD23	1.98	0.45
1:A:225:ARG:CG	1:A:226:ALA:N	2.78	0.45
1:A:549:LEU:CD2	1:A:610:VAL:HG21	2.45	0.45
1:A:81:VAL:HG12	1:A:252:PRO:CB	2.42	0.45
1:A:229:GLU:HB3	1:A:230:ALA:HA	1.84	0.44
1:A:648:GLU:HA	1:A:673:ALA:HB1	1.99	0.44
1:A:57:LEU:HA	1:A:436:ARG:HA	1.99	0.44
1:A:79:LEU:N	1:A:79:LEU:HD23	2.32	0.44
1:A:88:VAL:HG12	1:A:294:VAL:HG13	1.99	0.44
1:A:344:PRO:HD2	1:A:345:ALA:H	1.83	0.44
1:A:225:ARG:HG2	1:A:226:ALA:N	2.32	0.43
1:A:315:LEU:HD13	1:A:366:ALA:CB	2.48	0.43
1:A:504:VAL:CG2	2:A:801:BO2:H112	2.47	0.43
1:A:643:GLY:HA3	1:A:670:HIS:O	2.17	0.43
1:A:354:ILE:HD13	1:A:354:ILE:HA	1.89	0.43
1:A:340:GLU:HA	1:A:341:PRO:HD2	1.85	0.43
1:A:514:PRO:CG	1:A:632:VAL:HG21	2.49	0.42
1:A:108:LEU:CD1	4:A:1178:HOH:O	2.66	0.42
1:A:220:ARG:NH1	1:A:220:ARG:CG	2.75	0.42
1:A:692:PHE:HE1	1:A:700:ARG:HH22	1.60	0.42
1:A:106:GLU:C	1:A:108:LEU:N	2.73	0.42
1:A:108:LEU:C	1:A:108:LEU:HD12	2.39	0.42
1:A:336:GLU:HA	1:A:337:PRO:HD3	1.94	0.42
1:A:79:LEU:HA	1:A:253:ASN:O	2.20	0.42
1:A:84:SER:OG	1:A:85:GLU:N	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ALA:O	1:A:359:ILE:HA	2.20	0.41
1:A:100:HIS:O	1:A:102:ALA:N	2.53	0.41
1:A:36:ARG:HD2	1:A:40:GLU:OE1	2.21	0.41
1:A:528:LEU:HD12	1:A:528:LEU:HA	1.75	0.41
1:A:331:ARG:HD2	1:A:379:LEU:HD21	2.03	0.41
1:A:12:THR:HB	1:A:417:THR:CG2	2.51	0.41
1:A:344:PRO:CD	1:A:345:ALA:H	2.34	0.41
1:A:704:GLU:HG3	1:A:708:ARG:HH11	1.86	0.41
1:A:80:TYR:CE1	1:A:297:ILE:HG21	2.55	0.40
1:A:499:VAL:HG11	1:A:586:ALA:HB1	2.03	0.40
1:A:237:ARG:N	4:A:1234:HOH:O	2.53	0.40
1:A:405:LEU:HD23	1:A:405:LEU:HA	1.95	0.40
1:A:3:LEU:HD11	1:A:651:LEU:CD2	2.52	0.40
1:A:537:LEU:O	1:A:577:SER:HA	2.22	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	575/732 (79%)	545 (95%)	23 (4%)	7 (1%)	13 6

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	221	PHE
1	A	225	ARG
1	A	344	PRO
1	A	692	PHE
1	A	294	VAL
1	A	84	SER
1	A	345	ALA

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	461/578 (80%)	418 (91%)	43 (9%)	9 5

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	GLU
1	A	39	LEU
1	A	51	LEU
1	A	57	LEU
1	A	73	GLU
1	A	79	LEU
1	A	84	SER
1	A	93	LEU
1	A	98	GLU
1	A	103	GLU
1	A	105	VAL
1	A	106	GLU
1	A	108	LEU
1	A	220	ARG
1	A	229	GLU
1	A	231	LEU
1	A	232	ARG
1	A	240	GLU
1	A	241	THR
1	A	251	ARG
1	A	253	ASN
1	A	259	SER
1	A	283	TYR
1	A	284	LEU
1	A	292	THR
1	A	294	VAL
1	A	315	LEU
1	A	331	ARG
1	A	336	GLU
1	A	355	GLN

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Mol	Chain	Res	Type
1	A	368	GLU
1	A	377	SER
1	A	432	ARG
1	A	501	SER
1	A	506	GLU
1	A	517	LEU
1	A	525	ARG
1	A	533	ARG
1	A	597	ASN
1	A	617	LEU
1	A	646	LEU
1	A	662	GLU
1	A	692	PHE

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

Mol	Chain	Res	Type
1	A	48	HIS
1	A	253	ASN
1	A	303	HIS
1	A	527	HIS
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)

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	BO2	A	801	1	25,29,29	1.86	4 (16%)	33,38,38	2.20	9 (27%)
3	PO4	A	802	-	4,4,4	1.28	0	6,6,6	2.24	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	BO2	A	801	1	-	8/23/28/28	0/2/2/2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	BO2	C11-C12	-6.20	1.36	1.51
2	A	801	BO2	C2-C7	-4.87	1.37	1.50
2	A	801	BO2	C11-C10	-2.87	1.47	1.54
2	A	801	BO2	C5-N4	2.21	1.40	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	BO2	C7-C2-N1	5.80	124.20	117.42
2	A	801	BO2	C6-N1-C2	4.75	123.06	116.93
2	A	801	BO2	C21-C22-C23	4.69	121.30	115.32
3	A	802	PO4	O3-P-O2	3.73	119.53	107.91
2	A	801	BO2	C3-C2-C7	-3.60	115.11	119.71
2	A	801	BO2	C2-C3-N4	-3.09	117.92	121.97
2	A	801	BO2	C5-C6-N1	-2.83	118.20	122.19
3	A	802	PO4	O4-P-O2	-2.70	99.53	107.91
2	A	801	BO2	C6-C5-N4	-2.67	118.64	121.96
2	A	801	BO2	C5-N4-C3	2.63	121.46	116.85
2	A	801	BO2	C12-C11-C10	-2.30	107.23	113.36

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	BO2	B26-C21-C22-C23
2	A	801	BO2	C21-C22-C23-C24
2	A	801	BO2	C21-C22-C23-C25
2	A	801	BO2	N1-C2-C7-N9
2	A	801	BO2	C3-C2-C7-O8
2	A	801	BO2	C3-C2-C7-N9
2	A	801	BO2	N1-C2-C7-O8
2	A	801	BO2	N20-C21-C22-C23

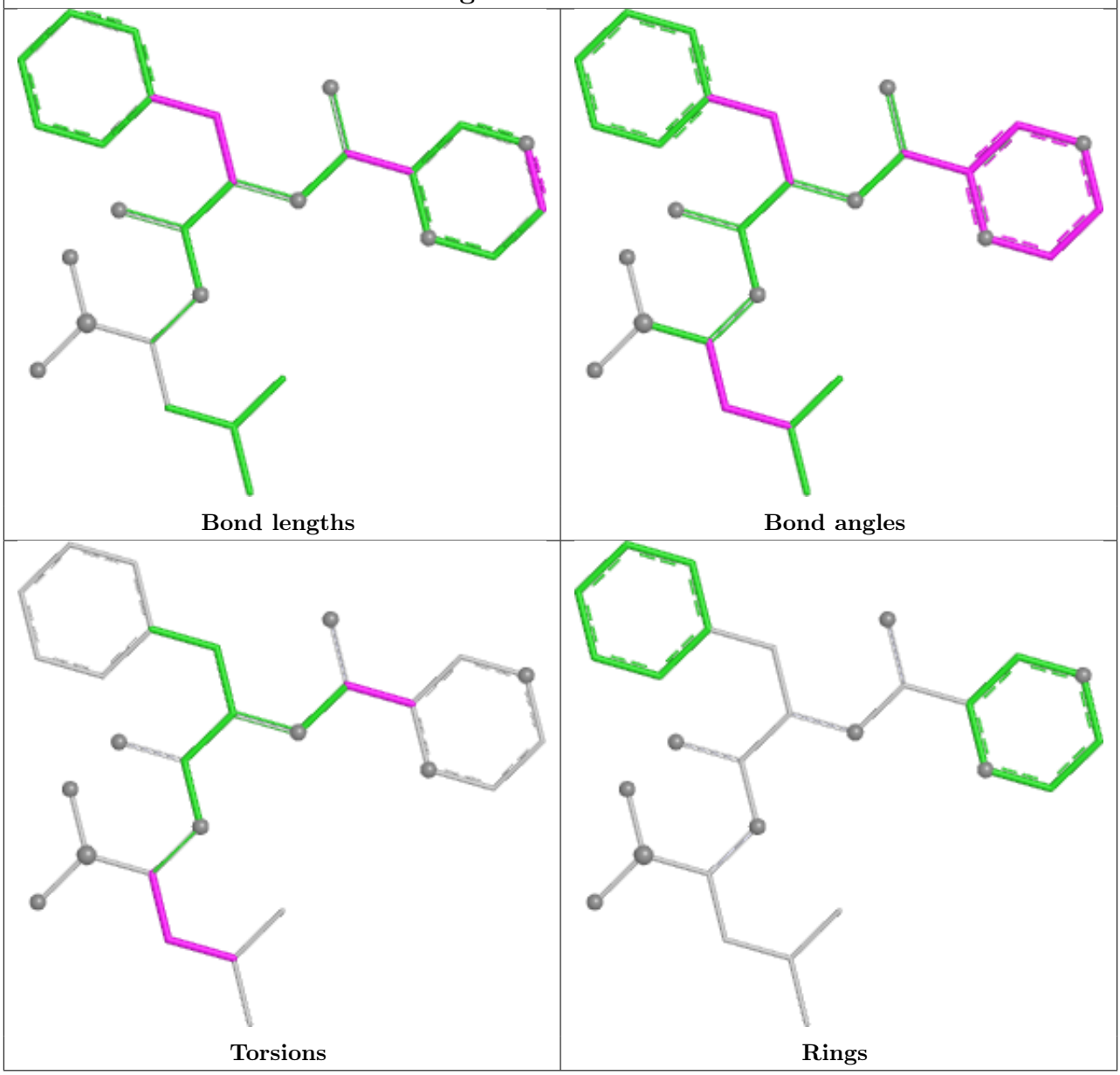
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	BO2	5	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 BO2 A 801



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	587/732 (80%)	-0.07	25 (4%) 35 34	20, 32, 85, 112	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	LEU	7.6
1	A	290	TRP	6.0
1	A	223	GLN	5.6
1	A	285	VAL	4.0
1	A	224	ALA	4.0
1	A	692	PHE	3.8
1	A	105	VAL	3.6
1	A	81	VAL	3.5
1	A	222	PRO	3.4
1	A	244	PRO	3.2
1	A	341	PRO	3.2
1	A	243	GLU	3.1
1	A	712	GLY	3.0
1	A	345	ALA	3.0
1	A	238	TYR	2.9
1	A	79	LEU	2.9
1	A	343	ALA	2.8
1	A	239	ALA	2.7
1	A	294	VAL	2.7
1	A	100	HIS	2.6
1	A	225	ARG	2.4
1	A	83	LEU	2.3
1	A	506	GLU	2.3
1	A	108	LEU	2.2
1	A	693	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)

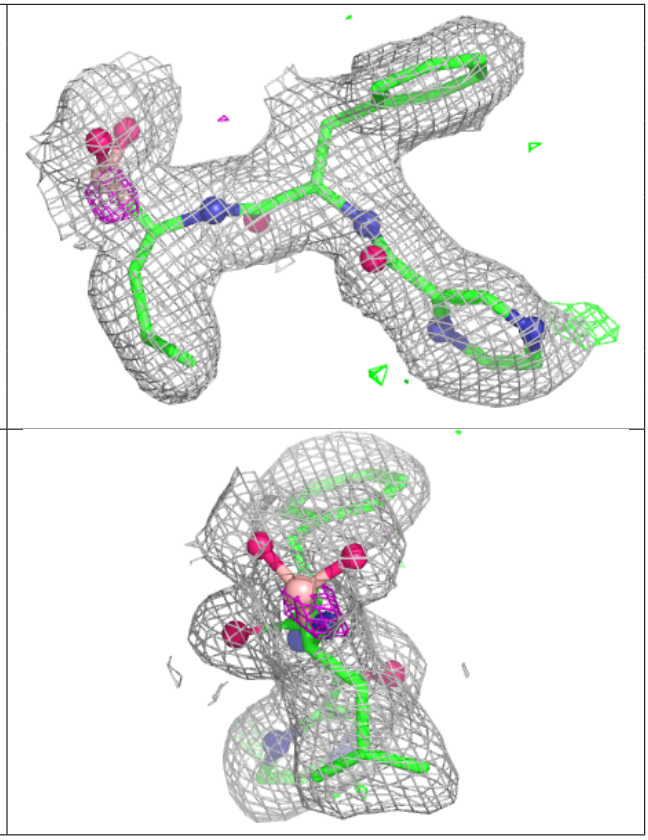
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	BO2	A	801	28/28	0.92	0.12	27,44,82,97	0
3	PO4	A	802	5/5	0.99	0.12	29,29,31,38	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 BO2 A 801:

$2mF_o$-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.