Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 09:19 PM EDT

PDB ID	:	4Q4E
Title	:	Crystal structure of E.coli aminopeptidase N in complex with actinonin
Authors	:	Reddi, R.; Ganji, R.J.; Addlagatta, A.
Deposited on	:	2014-04-14
Resolution	:	1.90 Å(reported)

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

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

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

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

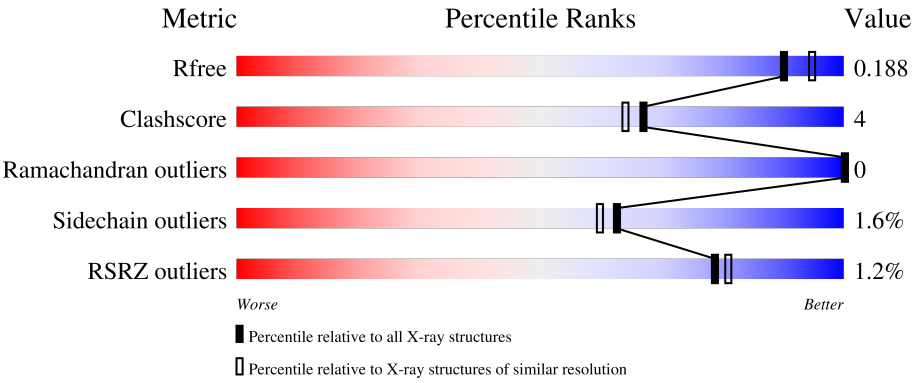
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 1.90 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	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

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	891	% 89% 7%

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
4	GOL	A	905	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	906	-	X	-	-
4	GOL	A	907	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8113 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 Aminopeptidase N.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	866	7028	4452	1212	1336	28	0	14	0

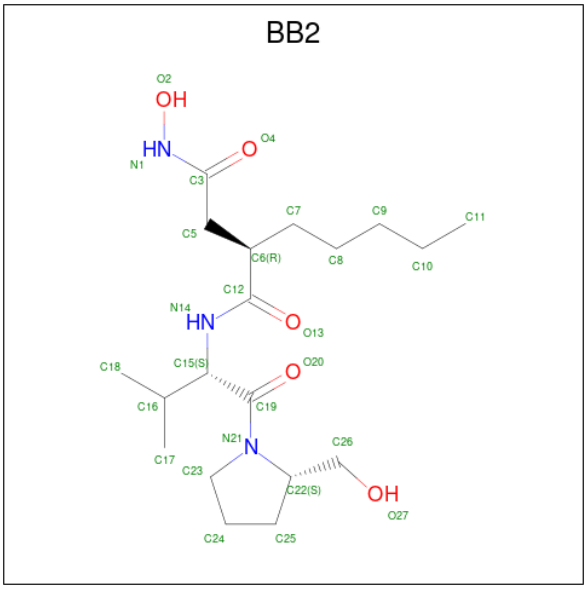
There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP P04825
A	-19	GLY	-	expression tag	UNP P04825
A	-18	SER	-	expression tag	UNP P04825
A	-17	SER	-	expression tag	UNP P04825
A	-16	HIS	-	expression tag	UNP P04825
A	-15	HIS	-	expression tag	UNP P04825
A	-14	HIS	-	expression tag	UNP P04825
A	-13	HIS	-	expression tag	UNP P04825
A	-12	HIS	-	expression tag	UNP P04825
A	-11	HIS	-	expression tag	UNP P04825
A	-10	SER	-	expression tag	UNP P04825
A	-9	SER	-	expression tag	UNP P04825
A	-8	GLY	-	expression tag	UNP P04825
A	-7	GLU	-	expression tag	UNP P04825
A	-6	ASN	-	expression tag	UNP P04825
A	-5	LEU	-	expression tag	UNP P04825
A	-4	TYR	-	expression tag	UNP P04825
A	-3	PHE	-	expression tag	UNP P04825
A	-2	GLN	-	expression tag	UNP P04825
A	-1	GLY	-	expression tag	UNP P04825
A	0	HIS	-	expression tag	UNP P04825

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

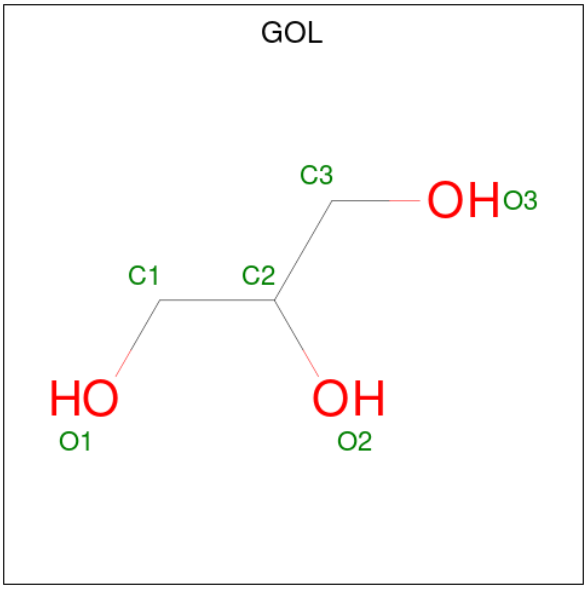
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0

- Molecule 3 is ACTINONIN (three-letter code: BB2) (formula: $C_{19}H_{35}N_3O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	27	19	3	5	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0

- Molecule 5 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Na 1 1	0	0

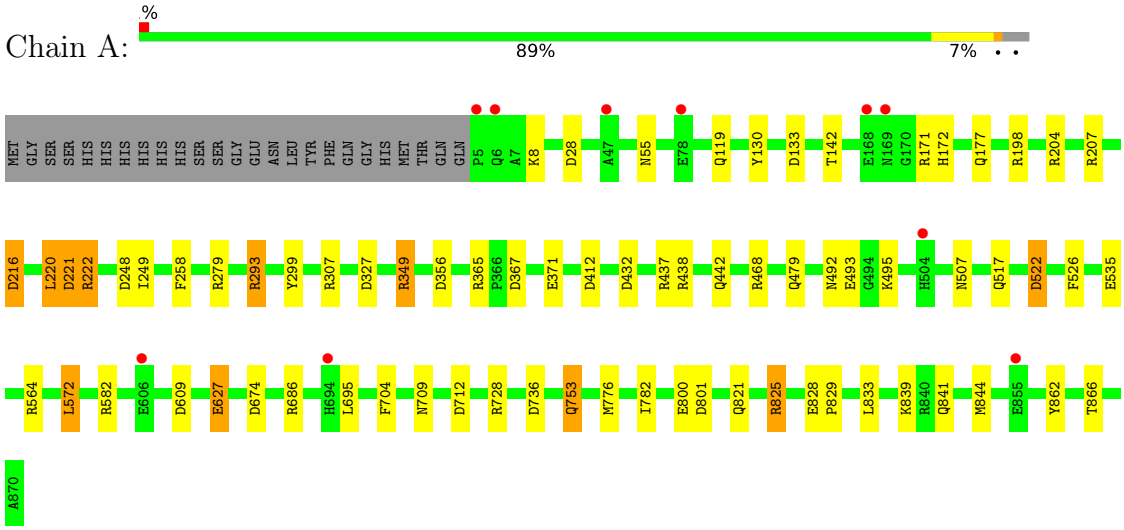
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1008	Total O 1008 1008	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: Aminopeptidase N



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	120.45Å 120.45Å 170.75Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	16.10 – 1.90 16.10 – 1.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (16.10-1.90) 97.2 (16.10-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.83 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.147 , 0.181 0.158 , 0.188	Depositor DCC
R_{free} test set	5498 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	20.2	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 58.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.015 for -h,-k,l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8113	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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: ZN, GOL, NA, BB2

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	1.10	5/7217 (0.1%)	1.12	48/9799 (0.5%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	TYR	CZ-OH	5.62	1.47	1.37
1	A	207	ARG	CD-NE	-5.24	1.37	1.46
1	A	627[A]	GLU	CD-OE2	-5.11	1.20	1.25
1	A	627[B]	GLU	CD-OE2	-5.11	1.20	1.25
1	A	371	GLU	CD-OE1	-5.03	1.20	1.25

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	207	ARG	NE-CZ-NH2	-16.62	111.99	120.30
1	A	293	ARG	NE-CZ-NH1	16.46	128.53	120.30
1	A	293	ARG	NE-CZ-NH2	-14.94	112.83	120.30
1	A	248	ASP	CB-CG-OD1	-11.62	107.84	118.30
1	A	207	ARG	NE-CZ-NH1	10.39	125.50	120.30
1	A	349[A]	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	A	349[B]	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	A	367	ASP	CB-CG-OD1	9.17	126.55	118.30
1	A	204	ARG	NE-CZ-NH1	9.13	124.86	120.30
1	A	736	ASP	CB-CG-OD1	8.52	125.97	118.30
1	A	365	ARG	NE-CZ-NH1	7.97	124.28	120.30
1	A	825	ARG	NE-CZ-NH2	-7.69	116.45	120.30
1	A	522[A]	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	522[B]	ASP	CB-CG-OD1	7.30	124.87	118.30
1	A	307	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	307	ARG	NE-CZ-NH1	7.18	123.89	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	432	ASP	CB-CG-OD1	7.09	124.68	118.30
1	A	438	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	221	ASP	CB-CG-OD1	7.07	124.67	118.30
1	A	365	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	A	564	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	198	ARG	NE-CZ-NH1	-6.39	117.11	120.30
1	A	844	MET	CG-SD-CE	-6.31	90.11	100.20
1	A	609	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	293	ARG	CD-NE-CZ	6.15	132.21	123.60
1	A	736	ASP	CB-CG-OD2	-6.14	112.77	118.30
1	A	825	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	686	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	A	349[A]	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	349[B]	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	801	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	728	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	130	TYR	CB-CG-CD2	5.64	124.38	121.00
1	A	627[A]	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	A	627[B]	GLU	OE1-CD-OE2	-5.58	116.60	123.30
1	A	438	ARG	NE-CZ-NH2	-5.47	117.57	120.30
1	A	204	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	582	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	28	ASP	CB-CG-OD1	5.40	123.16	118.30
1	A	130	TYR	CB-CG-CD1	-5.39	117.77	121.00
1	A	222	ARG	NE-CZ-NH1	5.39	122.99	120.30
1	A	728	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	A	609	ASP	CB-CG-OD2	-5.27	113.55	118.30
1	A	437	ARG	NE-CZ-NH1	5.27	122.94	120.30
1	A	299	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	A	572	LEU	CB-CG-CD1	5.24	119.90	111.00
1	A	207	ARG	CG-CD-NE	-5.22	100.84	111.80
1	A	412	ASP	CB-CG-OD1	5.13	122.92	118.30

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	7028	0	6875	51	0
2	A	1	0	0	0	0
3	A	27	0	34	0	0
4	A	48	0	63	13	0
5	A	1	0	0	0	0
6	A	1008	0	0	23	0
All	All	8113	0	6972	55	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 4.

All (55) 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:216[A]:ASP:OD2	4:A:907:GOL:H12	1.27	1.33
1:A:216[A]:ASP:OD2	4:A:907:GOL:C1	1.89	1.19
1:A:171[B]:ARG:HG3	1:A:171[B]:ARG:HH11	1.09	1.16
1:A:627[B]:GLU:HG3	6:A:1513:HOH:O	1.55	1.07
1:A:171[B]:ARG:NH1	6:A:1664:HOH:O	1.92	1.01
1:A:627[B]:GLU:HG2	6:A:1095:HOH:O	1.65	0.96
1:A:171[B]:ARG:HG3	1:A:171[B]:ARG:NH1	1.79	0.94
1:A:119[B]:GLN:HE22	1:A:821:GLN:HE22	1.22	0.86
1:A:249:ILE:CG2	6:A:1483:HOH:O	2.21	0.86
1:A:216[A]:ASP:CG	4:A:907:GOL:H12	1.96	0.84
1:A:535:GLU:OE1	4:A:906:GOL:H12	1.81	0.81
1:A:249:ILE:HG22	6:A:1483:HOH:O	1.78	0.78
1:A:142[A]:THR:HG22	1:A:177:GLN:HG3	1.69	0.74
1:A:8:LYS:HD2	6:A:1850:HOH:O	1.87	0.73
1:A:862:TYR:O	1:A:866:THR:HG23	1.90	0.72
1:A:171[A]:ARG:NH1	6:A:1336:HOH:O	2.11	0.71
1:A:442:GLN:HE22	1:A:479:GLN:H	1.37	0.71
1:A:349[B]:ARG:NH2	6:A:1982:HOH:O	2.23	0.69
1:A:171[B]:ARG:NH1	1:A:171[B]:ARG:CG	2.56	0.66
1:A:216[A]:ASP:OD2	4:A:907:GOL:H11	1.89	0.66
1:A:249:ILE:HG23	6:A:1483:HOH:O	1.91	0.65
1:A:55:ASN:HD22	1:A:133:ASP:H	1.45	0.65
1:A:507:ASN:HD21	4:A:905:GOL:H12	1.64	0.62
4:A:905:GOL:C1	6:A:1593:HOH:O	2.49	0.59
1:A:776:MET:O	1:A:782:ILE:HD11	2.05	0.56
4:A:905:GOL:H11	6:A:1593:HOH:O	2.05	0.56
1:A:507:ASN:HD21	4:A:905:GOL:C1	2.18	0.56
1:A:468:ARG:NH2	6:A:1967:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:GLN:HE21	1:A:753:GLN:HA	1.72	0.55
1:A:119[A]:GLN:CD	6:A:1977:HOH:O	2.45	0.54
1:A:119[A]:GLN:NE2	1:A:258:PHE:CZ	2.76	0.54
4:A:905:GOL:H12	6:A:1593:HOH:O	2.09	0.52
1:A:119[B]:GLN:HE22	1:A:821:GLN:NE2	2.01	0.52
1:A:627[B]:GLU:CG	6:A:1095:HOH:O	2.39	0.51
1:A:709:ASN:ND2	1:A:712:ASP:H	2.09	0.51
1:A:171[B]:ARG:HH11	1:A:171[B]:ARG:CG	1.96	0.50
1:A:220:LEU:HB2	6:A:1404:HOH:O	2.11	0.49
1:A:800:GLU:HG2	6:A:1956:HOH:O	2.11	0.49
1:A:222:ARG:HG2	1:A:279:ARG:HB2	1.95	0.47
1:A:825:ARG:HD3	6:A:1781:HOH:O	2.13	0.47
4:A:905:GOL:H2	6:A:1329:HOH:O	2.15	0.45
1:A:828:GLU:HB3	1:A:829:PRO:HD3	1.98	0.45
1:A:442:GLN:NE2	1:A:479:GLN:H	2.11	0.43
1:A:171[B]:ARG:HD3	6:A:1336:HOH:O	2.18	0.43
1:A:119[B]:GLN:NE2	1:A:821:GLN:HE22	2.03	0.43
1:A:829:PRO:HG3	4:A:904:GOL:H2	2.00	0.42
1:A:825:ARG:NH1	6:A:1347:HOH:O	2.52	0.42
1:A:119[A]:GLN:NE2	6:A:1155:HOH:O	2.52	0.41
1:A:492:ASN:HB3	1:A:526:PHE:CE2	2.55	0.41
1:A:704:PHE:CZ	4:A:910:GOL:H12	2.56	0.41
1:A:833:LEU:O	1:A:841:GLN:HG2	2.20	0.41
1:A:221:ASP:OD2	1:A:279:ARG:NH1	2.52	0.41
1:A:493:GLU:HB2	1:A:495:LYS:HD3	2.04	0.40
1:A:171[B]:ARG:CD	6:A:1336:HOH:O	2.69	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	878/891 (98%)	866 (99%)	12 (1%)	0	100 100

There are no Ramachandran outliers to report.

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	755/763 (99%)	741 (98%)	14 (2%)	57 53

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	172	HIS
1	A	216[A]	ASP
1	A	216[B]	ASP
1	A	220	LEU
1	A	293	ARG
1	A	327	ASP
1	A	356	ASP
1	A	517[A]	GLN
1	A	517[B]	GLN
1	A	572	LEU
1	A	674	ASP
1	A	695	LEU
1	A	753	GLN
1	A	839	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	65	HIS
1	A	219	ASN
1	A	430	ASN

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Mol	Chain	Res	Type
1	A	442	GLN
1	A	549	GLN
1	A	623	ASN
1	A	665	GLN
1	A	682	ASN
1	A	709	ASN
1	A	753	GLN
1	A	821	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)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 for Mogul analysis.

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	$\#\|Z\| > 2$
4	GOL	A	910	-	5,5,5	0.66	0	5,5,5	2.02	2 (40%)
4	GOL	A	903	-	5,5,5	0.90	0	5,5,5	1.42	1 (20%)
4	GOL	A	906	-	5,5,5	1.53	2 (40%)	5,5,5	2.30	2 (40%)
4	GOL	A	908	-	5,5,5	0.33	0	5,5,5	0.60	0
3	BB2	A	902	2	27,27,27	0.69	1 (3%)	34,35,35	1.58	4 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	A	907	-	5,5,5	0.74	0	5,5,5	1.43	1 (20%)
4	GOL	A	904	-	5,5,5	1.16	1 (20%)	5,5,5	1.31	0
4	GOL	A	909	-	5,5,5	0.41	0	5,5,5	0.61	0
4	GOL	A	905	-	5,5,5	1.24	0	5,5,5	1.26	1 (20%)

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
4	GOL	A	910	-	-	2/4/4/4	-
4	GOL	A	903	-	-	2/4/4/4	-
4	GOL	A	906	-	-	2/4/4/4	-
4	GOL	A	908	-	-	2/4/4/4	-
3	BB2	A	902	2	-	3/33/43/43	0/1/1/1
4	GOL	A	907	-	-	2/4/4/4	-
4	GOL	A	904	-	-	2/4/4/4	-
4	GOL	A	909	-	-	3/4/4/4	-
4	GOL	A	905	-	-	2/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	906	GOL	O3-C3	-2.44	1.32	1.42
4	A	906	GOL	C3-C2	-2.31	1.42	1.51
3	A	902	BB2	O20-C19	2.07	1.26	1.22
4	A	904	GOL	O3-C3	2.00	1.50	1.42

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	BB2	O4-C3-N1	-5.26	116.82	123.27
3	A	902	BB2	C5-C3-N1	4.95	122.64	115.14
4	A	906	GOL	C3-C2-C1	-3.99	96.20	111.70
4	A	910	GOL	O2-C2-C1	3.26	123.49	109.12
4	A	906	GOL	O3-C3-C2	-3.18	94.95	110.20
3	A	902	BB2	O2-N1-C3	-2.64	115.89	119.79
3	A	902	BB2	O20-C19-C15	-2.45	115.21	119.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	907	GOL	O1-C1-C2	-2.42	98.61	110.20
4	A	910	GOL	C3-C2-C1	-2.34	102.59	111.70
4	A	905	GOL	O1-C1-C2	-2.27	99.30	110.20
4	A	903	GOL	C3-C2-C1	-2.03	103.81	111.70

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	903	GOL	C1-C2-C3-O3
4	A	906	GOL	O1-C1-C2-O2
4	A	907	GOL	O1-C1-C2-C3
4	A	908	GOL	O1-C1-C2-C3
4	A	909	GOL	C1-C2-C3-O3
4	A	910	GOL	C1-C2-C3-O3
4	A	910	GOL	O2-C2-C3-O3
4	A	904	GOL	C1-C2-C3-O3
4	A	905	GOL	C1-C2-C3-O3
4	A	906	GOL	O1-C1-C2-C3
4	A	904	GOL	O2-C2-C3-O3
4	A	907	GOL	O1-C1-C2-O2
4	A	909	GOL	O2-C2-C3-O3
3	A	902	BB2	C11-C10-C9-C8
4	A	903	GOL	O2-C2-C3-O3
4	A	905	GOL	O2-C2-C3-O3
4	A	908	GOL	O1-C1-C2-O2
3	A	902	BB2	N21-C22-C26-O27
4	A	909	GOL	O1-C1-C2-C3
3	A	902	BB2	C7-C8-C9-C10

There are no ring outliers.

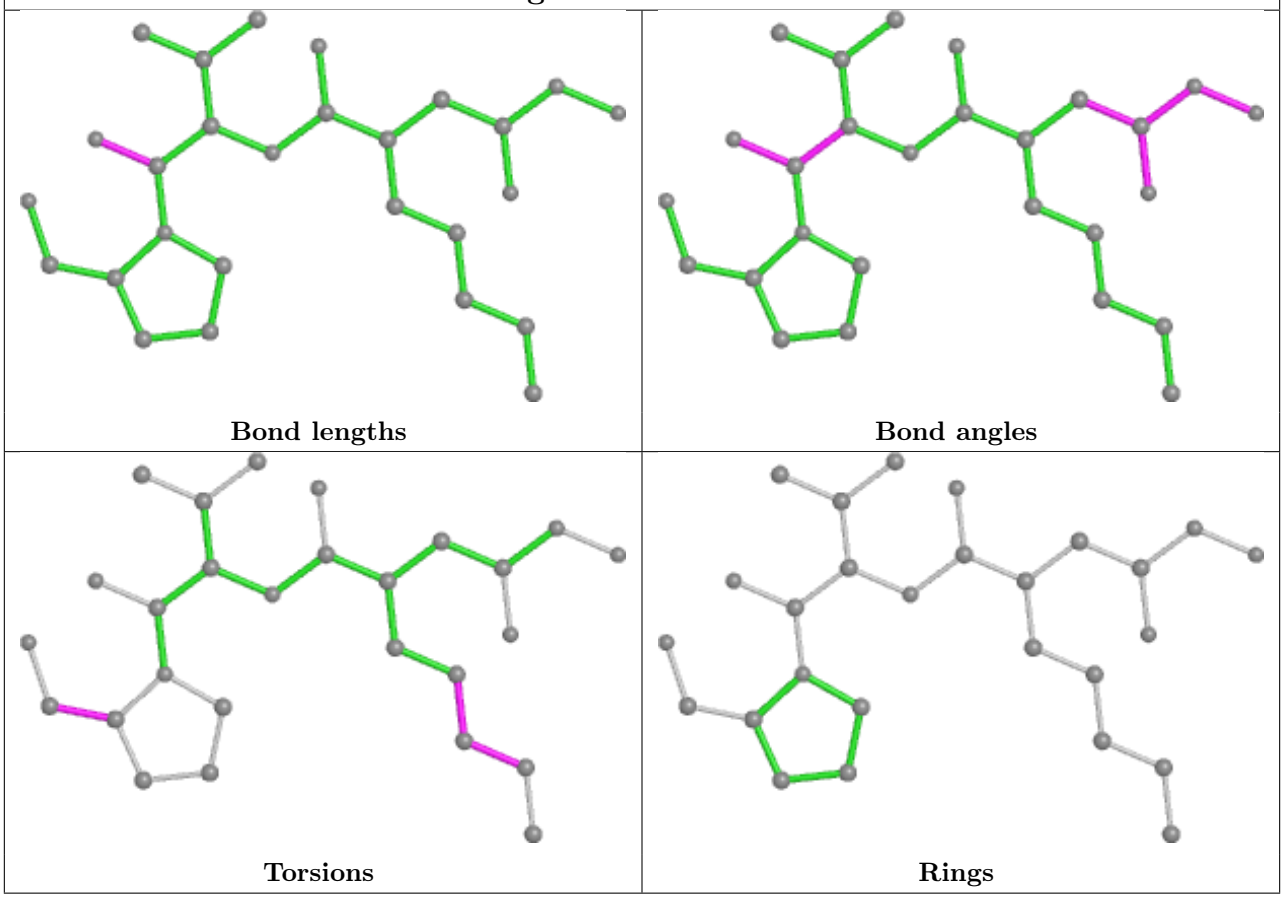
5 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	910	GOL	1	0
4	A	906	GOL	1	0
4	A	907	GOL	4	0
4	A	904	GOL	1	0
4	A	905	GOL	6	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 BB2 A 902



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	866/891 (97%)	-0.55	10 (1%)	79	81	11, 18, 31, 53	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	504	HIS	3.2
1	A	6	GLN	2.5
1	A	606	GLU	2.4
1	A	78	GLU	2.3
1	A	168	GLU	2.2
1	A	694	HIS	2.2
1	A	47	ALA	2.2
1	A	855	GLU	2.1
1	A	5	PRO	2.1
1	A	169	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

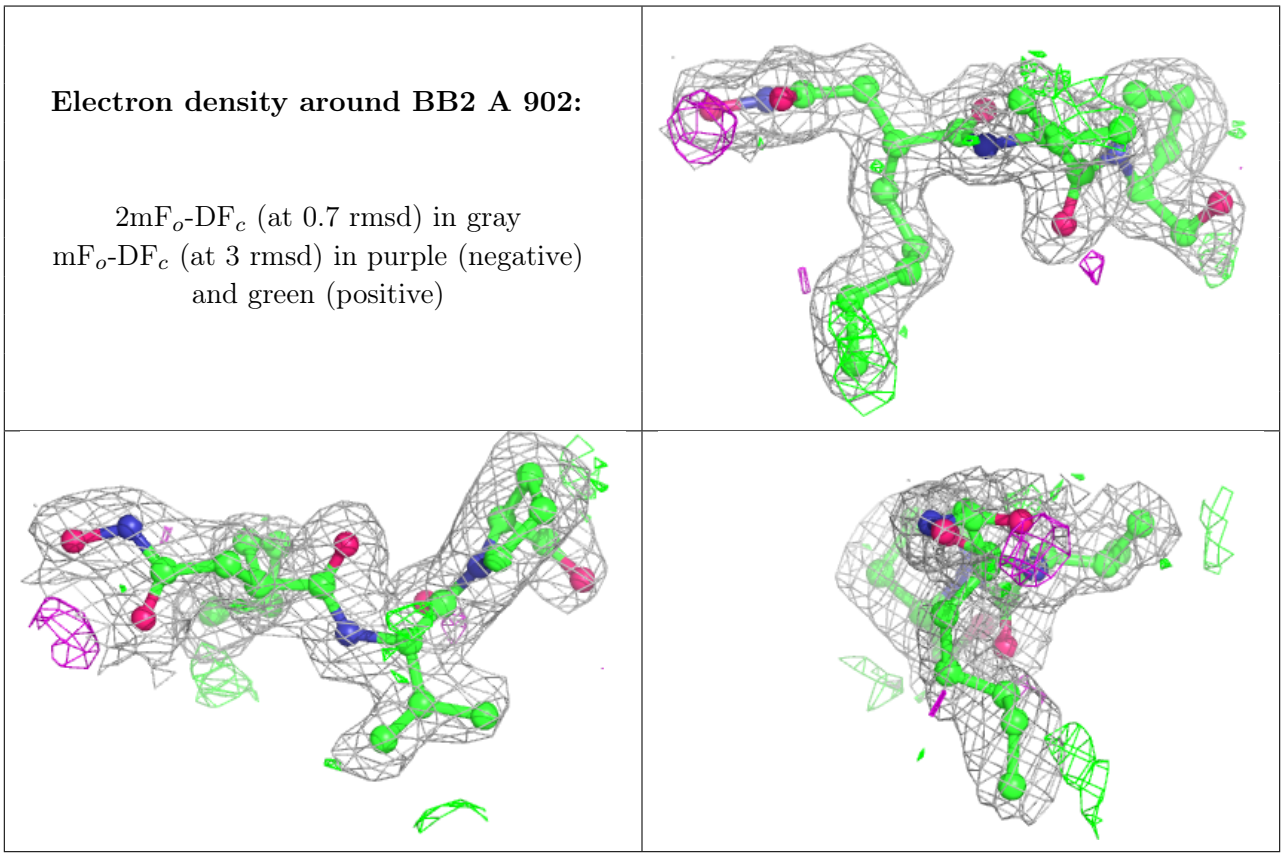
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
4	GOL	A	904	6/6	0.75	0.20	41,51,55,55	0
4	GOL	A	908	6/6	0.82	0.23	51,60,64,66	0
4	GOL	A	909	6/6	0.86	0.20	54,59,63,76	0
4	GOL	A	910	6/6	0.87	0.21	37,44,47,52	0
4	GOL	A	905	6/6	0.90	0.18	28,37,45,48	0
4	GOL	A	906	6/6	0.92	0.22	22,40,50,52	0
3	BB2	A	902	27/27	0.93	0.12	12,27,38,47	0
4	GOL	A	903	6/6	0.95	0.18	29,37,51,56	0
4	GOL	A	907	6/6	0.96	0.10	21,25,32,34	2
5	NA	A	911	1/1	0.99	0.09	26,26,26,26	0
2	ZN	A	901	1/1	1.00	0.02	13,13,13,13	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 BB2 A 902:

$2mF_o$-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.