Full wwPDB X-ray Structure Validation Report (i)

Jun 16, 2024 – 02:08 PM EDT

PDB ID	:	4Y95
Title	:	Crystal structure of the kinase domain of Bruton's tyrosine kinase with mutations in the activation loop
Authors	:	Wang, Q.; Rosen, C.E.; Kuriyan, J.
Deposited on	:	2015-02-16
Resolution	:	1.60 Å(reported)

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

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

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

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

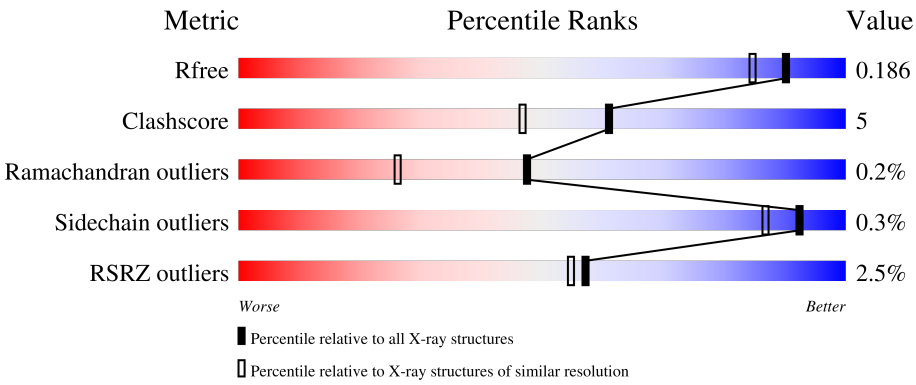
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.60 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	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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	266	2% 92% 8%
1	B	266	3% 93% 7%
1	C	266	2% 92% 8%
1	D	266	2% 93% 6%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18889 atoms, of which 8799 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 Non-specific protein-tyrosine kinase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	266	4358	1420	2151	354	411	22	0	11	0
1	B	266	4405	1429	2180	360	414	22	0	14	0
1	C	266	4360	1415	2154	354	414	23	0	12	0
1	D	265	4324	1405	2138	353	407	21	0	9	0

There are 40 discrepancies between the modelled and reference sequences:

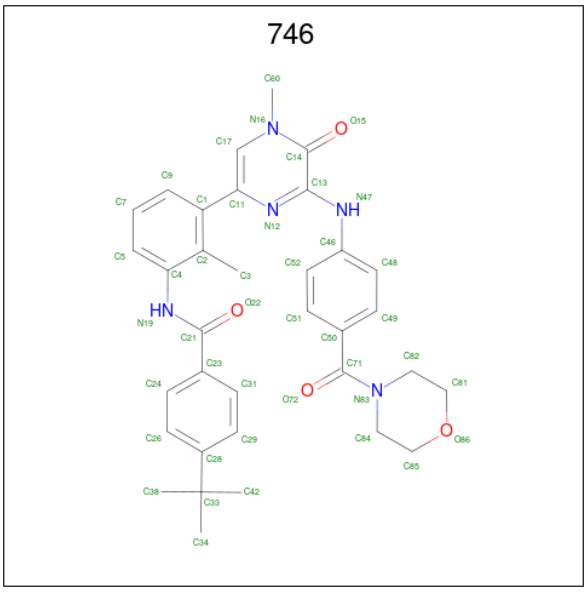
Chain	Residue	Modelled	Actual	Comment	Reference
A	394	ALA	-	expression tag	UNP Q3ZC95
A	542	MET	LEU	engineered mutation	UNP Q3ZC95
A	543	THR	SER	engineered mutation	UNP Q3ZC95
A	545	PHE	TYR	engineered mutation	UNP Q3ZC95
A	555	THR	VAL	engineered mutation	UNP Q3ZC95
A	557	THR	SER	engineered mutation	UNP Q3ZC95
A	562	LYS	ARG	engineered mutation	UNP Q3ZC95
A	564	ALA	SER	engineered mutation	UNP Q3ZC95
A	565	SER	PRO	engineered mutation	UNP Q3ZC95
A	617	PRO	TYR	engineered mutation	UNP Q3ZC95
B	394	ALA	-	expression tag	UNP Q3ZC95
B	542	MET	LEU	engineered mutation	UNP Q3ZC95
B	543	THR	SER	engineered mutation	UNP Q3ZC95
B	545	PHE	TYR	engineered mutation	UNP Q3ZC95
B	555	THR	VAL	engineered mutation	UNP Q3ZC95
B	557	THR	SER	engineered mutation	UNP Q3ZC95
B	562	LYS	ARG	engineered mutation	UNP Q3ZC95
B	564	ALA	SER	engineered mutation	UNP Q3ZC95
B	565	SER	PRO	engineered mutation	UNP Q3ZC95
B	617	PRO	TYR	engineered mutation	UNP Q3ZC95
C	394	ALA	-	expression tag	UNP Q3ZC95

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	542	MET	LEU	engineered mutation	UNP Q3ZC95
C	543	THR	SER	engineered mutation	UNP Q3ZC95
C	545	PHE	TYR	engineered mutation	UNP Q3ZC95
C	555	THR	VAL	engineered mutation	UNP Q3ZC95
C	557	THR	SER	engineered mutation	UNP Q3ZC95
C	562	LYS	ARG	engineered mutation	UNP Q3ZC95
C	564	ALA	SER	engineered mutation	UNP Q3ZC95
C	565	SER	PRO	engineered mutation	UNP Q3ZC95
C	617	PRO	TYR	engineered mutation	UNP Q3ZC95
D	394	ALA	-	expression tag	UNP Q3ZC95
D	542	MET	LEU	engineered mutation	UNP Q3ZC95
D	543	THR	SER	engineered mutation	UNP Q3ZC95
D	545	PHE	TYR	engineered mutation	UNP Q3ZC95
D	555	THR	VAL	engineered mutation	UNP Q3ZC95
D	557	THR	SER	engineered mutation	UNP Q3ZC95
D	562	LYS	ARG	engineered mutation	UNP Q3ZC95
D	564	ALA	SER	engineered mutation	UNP Q3ZC95
D	565	SER	PRO	engineered mutation	UNP Q3ZC95
D	617	PRO	TYR	engineered mutation	UNP Q3ZC95

- Molecule 2 is 4-tert-butyl-N-[2-methyl-3-(4-methyl-6-{[4-(morpholin-4-ylcarbonyl)phenyl]amino}-5-oxo-4,5-dihydropyrazin-2-yl)phenyl]benzamide (three-letter code: 746) (formula: $C_{34}H_{37}N_5O_4$).



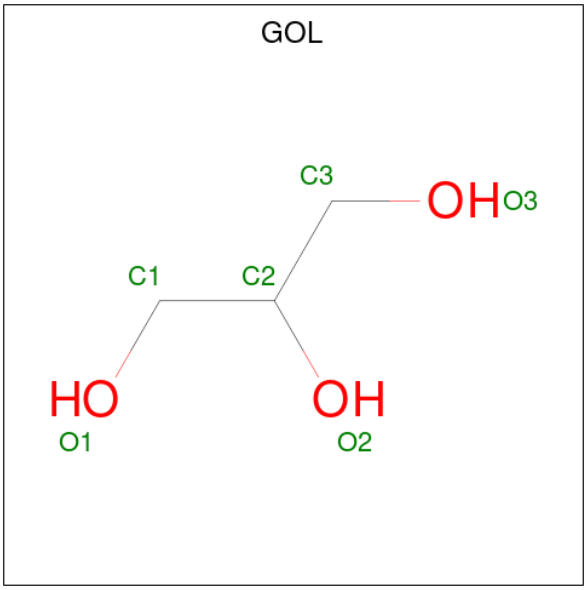
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	43	34	5	4	0	0

Continued on next page...

Continued from previous page...

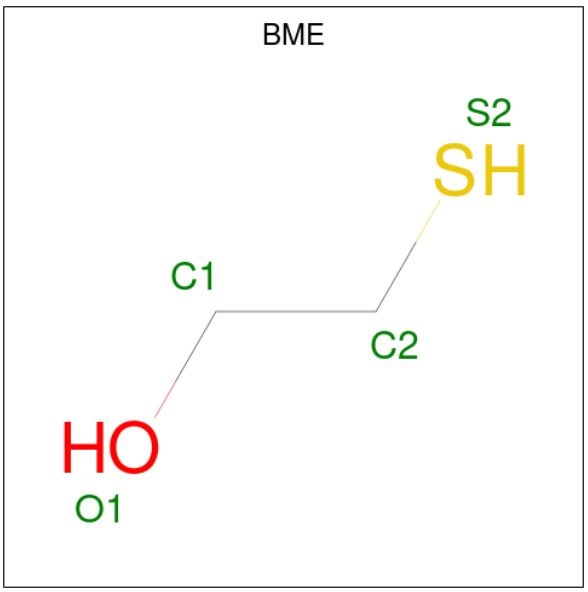
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	B	1	43	34	5	4	0	0
			Total	C	N	O		
2	C	1	43	34	5	4	0	0
			Total	C	N	O		
2	D	1	43	34	5	4	0	0

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



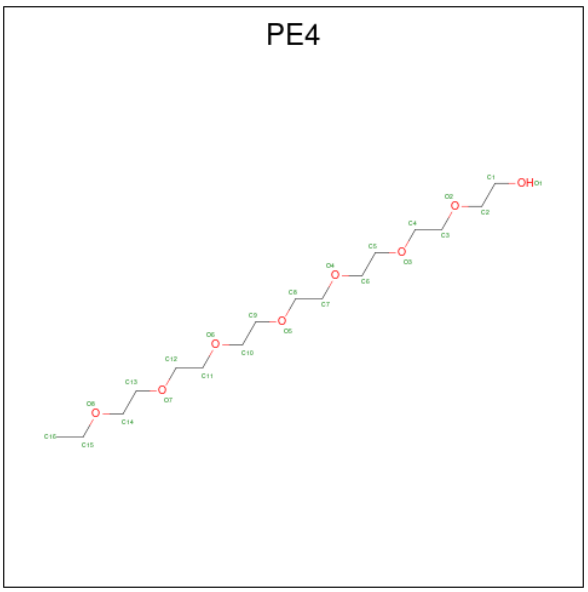
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
3	A	1	14	3	8	3	0	0
			Total	C	H	O		
3	B	1	14	3	8	3	0	0
			Total	C	H	O		
3	B	1	14	3	8	3	0	0
			Total	C	H	O		
3	C	1	28	6	16	6	0	1
			Total	C	H	O		
3	D	1	14	3	8	3	0	0
			Total	C	H	O		
3	D	1	14	3	8	3	0	0
			Total	C	H	O		
3	D	1	14	3	8	3	0	0
			Total	C	H	O		
3	D	1	14	3	8	3	0	0

- Molecule 4 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	O	S		
4	A	1	20	4	12	2	2	0	1
			Total	C	H	O	S		
4	B	1	20	4	12	2	2	0	1
			Total	C	H	O	S		
4	C	1	20	4	12	2	2	0	1

- Molecule 5 is 2-{2-[2-(2-{2-[2-(2-ETHOXY-ETHOXY)-ETHOXY]-ETHOXY}-ETHOXY)-ETHOXY]-ETHOXY}-ETHANOL (three-letter code: PE4) (formula: $C_{16}H_{34}O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
5	B	1	58	16	34	8	0	0
			Total	C	H	O		
5	C	1	58	16	34	8	0	0

- Molecule 6 is water.

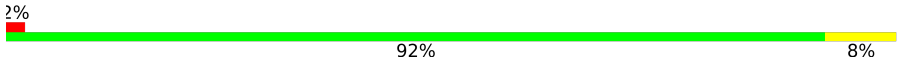
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	240	240	240	0	0
			Total	O		
6	B	237	237	237	0	0
			Total	O		
6	C	250	250	250	0	0
			Total	O		
6	D	241	241	241	0	0

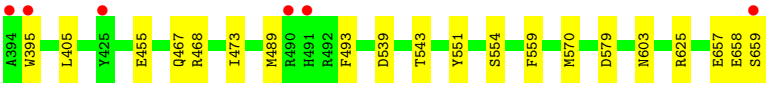
3 Residue-property plots (i)

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: Non-specific protein-tyrosine kinase

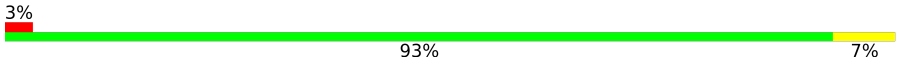
Chain A:

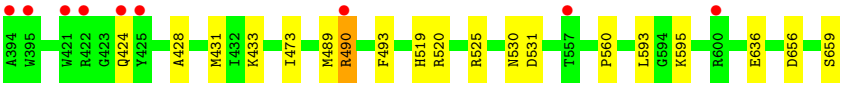




• Molecule 1: Non-specific protein-tyrosine kinase

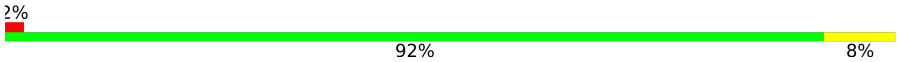
Chain B:

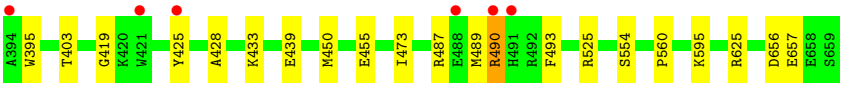




• Molecule 1: Non-specific protein-tyrosine kinase

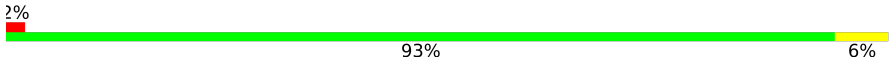
Chain C:

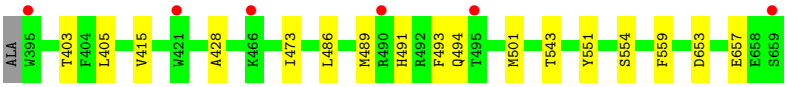




• Molecule 1: Non-specific protein-tyrosine kinase

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.93Å 79.07Å 79.18Å 90.73° 89.90° 89.99°	Depositor
Resolution (Å)	39.59 – 1.60 39.59 – 1.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (39.59-1.60) 93.9 (39.59-1.60)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.20 (at 1.60Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.155 , 0.184 0.156 , 0.186	Depositor DCC
R_{free} test set	2009 reflections (1.27%)	wwPDB-VP
Wilson B-factor (Å^2)	17.4	Xtriage
Anisotropy	0.227	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.42 , 41.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.045 for h,l,-k 0.045 for h,-l,k 0.468 for h,-k,-l 0.026 for -h,k,-l 0.026 for -h,-k,l 0.019 for -h,l,k 0.020 for -h,-l,-k	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	18889	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: BME, 746, PE4, GOL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.54	0/2291	0.70	1/3092 (0.0%)
1	B	0.48	0/2317	0.66	0/3125
1	C	0.52	1/2290 (0.0%)	0.65	0/3087
1	D	0.51	0/2263	0.69	0/3053
All	All	0.51	1/9161 (0.0%)	0.67	1/12357 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	439	GLU	CD-OE1	-6.18	1.18	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	579	ASP	CB-CG-OD2	-5.01	113.79	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	2207	2151	2172	13	0
1	B	2225	2180	2198	19	3

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2206	2154	2178	18	3
1	D	2186	2138	2149	15	0
2	A	43	0	37	4	0
2	B	43	0	37	6	0
2	C	43	0	37	5	0
2	D	43	0	37	4	0
3	A	6	8	8	1	0
3	B	12	16	16	0	0
3	C	12	16	16	0	0
3	D	24	32	32	1	0
4	A	8	12	12	1	0
4	B	8	12	12	0	0
4	C	8	12	12	0	0
5	B	24	34	34	7	0
5	C	24	34	34	6	0
6	A	240	0	0	6	1
6	B	237	0	0	4	2
6	C	250	0	0	3	3
6	D	241	0	0	3	2
All	All	10090	8799	9021	82	7

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 5.

All (82) 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:D:486:LEU:O	1:D:489:MET:O	1.86	0.92
1:B:433:LYS:HZ1	5:B:705:PE4:H101	1.39	0.87
1:B:433:LYS:HZ1	5:B:705:PE4:H81	1.44	0.83
1:D:491:HIS:ND1	6:D:801:HOH:O	2.10	0.82
1:C:625:ARG:HH22	1:C:657:GLU:HG3	1.55	0.71
1:B:433:LYS:NZ	5:B:705:PE4:H81	2.09	0.68
1:D:489:MET:HB2	1:D:493:PHE:CE2	2.29	0.67
1:B:473:ILE:HD12	1:B:473:ILE:N	2.11	0.65
1:B:433:LYS:NZ	5:B:705:PE4:H101	2.09	0.65
1:C:625:ARG:NH2	1:C:657:GLU:HG3	2.11	0.65
2:B:701:746:H3A	2:B:701:746:H17	1.79	0.65
1:C:473:ILE:N	1:C:473:ILE:HD12	2.12	0.64
1:B:433:LYS:HZ3	5:B:705:PE4:H132	1.65	0.61
2:B:701:746:H51	2:B:701:746:H84A	1.83	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1001:746:H3A	2:C:1001:746:H17	1.83	0.60
2:C:1001:746:H84A	2:C:1001:746:H51	1.84	0.60
2:B:701:746:H84A	2:B:701:746:C51	2.31	0.60
2:D:701:746:H3A	2:D:701:746:H17	1.82	0.59
2:A:701:746:H17	2:A:701:746:H3A	1.83	0.59
2:C:1001:746:H84A	2:C:1001:746:C51	2.32	0.59
2:A:701:746:O72	6:A:961:HOH:O	2.17	0.59
1:D:473:ILE:HD12	1:D:473:ILE:N	2.19	0.58
1:A:543:THR:HG22	1:A:551:TYR:OH	2.04	0.58
1:C:489:MET:HB2	1:C:493:PHE:CE2	2.39	0.58
1:D:543:THR:HG22	1:D:551:TYR:OH	2.05	0.56
1:A:489:MET:HB2	1:A:493:PHE:CE2	2.41	0.56
1:B:490:ARG:HG2	1:B:593:LEU:HB3	1.86	0.55
1:A:625:ARG:NH2	1:A:657:GLU:OE1	2.39	0.55
2:D:701:746:H84A	2:D:701:746:C51	2.38	0.54
2:A:701:746:C51	2:A:701:746:H84A	2.38	0.54
1:A:603:ASN:OD1	6:A:1031:HOH:O	2.18	0.53
1:C:455:GLU:OE2	6:C:1273:HOH:O	2.19	0.53
1:B:656:ASP:HB3	6:B:854:HOH:O	2.07	0.53
2:C:1001:746:H48	2:C:1001:746:N12	2.25	0.52
2:B:701:746:H48	2:B:701:746:N12	2.25	0.52
1:B:636:GLU:HG3	6:B:1006:HOH:O	2.10	0.51
6:A:1016:HOH:O	1:B:431:MET:HE1	2.10	0.50
1:C:433:LYS:NZ	5:C:1004:PE4:H81	2.27	0.50
1:A:570:MET:CE	6:A:1033:HOH:O	2.59	0.49
1:C:428:ALA:CB	2:C:1001:746:H60A	2.42	0.49
1:D:543:THR:HG23	6:D:897:HOH:O	2.13	0.49
1:A:543:THR:HG23	6:A:871:HOH:O	2.12	0.49
1:A:467:GLN:O	1:A:468:ARG:HD3	2.12	0.49
1:B:530:ASN:ND2	6:B:998:HOH:O	2.36	0.49
1:C:433:LYS:HZ3	5:C:1004:PE4:H132	1.78	0.48
1:C:433:LYS:HZ1	5:C:1004:PE4:H81	1.79	0.47
1:B:433:LYS:NZ	5:B:705:PE4:H151	2.30	0.47
1:B:531[B]:ASP:HB3	1:D:415[B]:VAL:HG11	1.97	0.47
2:A:701:746:H48	2:A:701:746:N12	2.30	0.47
1:A:539:ASP:OD1	4:A:703[B]:BME:O1	2.32	0.46
1:B:519:HIS:O	1:B:520:ARG:HB2	2.16	0.46
1:C:433:LYS:HZ3	5:C:1004:PE4:C13	2.28	0.46
1:D:403:THR:HG22	1:D:405:LEU:HD12	1.97	0.46
1:B:424[A]:GLN:HG2	1:D:403:THR:HG21	1.99	0.45
1:D:428:ALA:CB	2:D:701:746:H60A	2.46	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:493:PHE:CE1	1:D:501:MET:HE3	2.51	0.45
3:D:702:GOL:H2	6:D:982:HOH:O	2.16	0.45
1:B:428:ALA:CB	2:B:701:746:H60A	2.47	0.45
1:D:653:ASP:O	1:D:657:GLU:HG2	2.17	0.44
1:B:525:ARG:NH1	1:B:560:PRO:HB3	2.33	0.44
1:D:403:THR:HG22	1:D:405:LEU:CD1	2.48	0.44
1:B:489:MET:HB2	1:B:493:PHE:CE2	2.53	0.44
2:D:701:746:H48	2:D:701:746:N12	2.34	0.43
1:A:570:MET:HE1	6:A:1027:HOH:O	2.18	0.43
1:C:554:SER:HB3	6:C:1277:HOH:O	2.18	0.42
1:A:455:GLU:HB2	3:A:702:GOL:C3	2.48	0.42
1:C:525:ARG:NH1	1:C:560:PRO:HB3	2.35	0.42
1:C:395:TRP:CB	1:C:450[A]:MET:SD	3.08	0.42
1:A:554:SER:HA	1:A:559:PHE:CG	2.55	0.42
1:B:656:ASP:CB	6:B:854:HOH:O	2.64	0.42
1:C:425:TYR:N	1:C:425:TYR:CD1	2.87	0.42
1:A:658:GLU:O	1:A:659:SER:HB3	2.20	0.42
1:D:554:SER:HA	1:D:559:PHE:CG	2.55	0.42
1:C:433:LYS:NZ	5:C:1004:PE4:H151	2.35	0.42
1:C:625:ARG:HH22	1:C:657:GLU:CG	2.29	0.41
2:B:701:746:C17	2:B:701:746:C3	2.98	0.41
5:B:705:PE4:H132	5:B:705:PE4:H111	1.89	0.41
5:C:1004:PE4:H161	6:C:1130:HOH:O	2.21	0.41
1:D:493:PHE:CE1	1:D:501:MET:CE	3.03	0.41
1:C:487:ARG:O	1:C:490:ARG:HG3	2.21	0.40
1:C:403:THR:O	1:C:419:GLY:HA3	2.22	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:854:HOH:O	6:C:1161:HOH:O[1_645]	1.91	0.29
6:A:849:HOH:O	6:C:1159:HOH:O[1_556]	1.97	0.23
6:B:850:HOH:O	6:D:871:HOH:O[1_556]	1.98	0.22
1:B:659:SER:OG	1:C:595:LYS:NZ[1_645]	2.06	0.14
6:C:1164:HOH:O	6:D:856:HOH:O[1_465]	2.07	0.13
1:B:595:LYS:HZ1	1:C:656:ASP:O[1_545]	1.56	0.04
1:B:656:ASP:O	1:C:595:LYS:HZ1[1_645]	1.59	0.01

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	275/266 (103%)	268 (98%)	7 (2%)	0	100	100
1	B	278/266 (104%)	271 (98%)	6 (2%)	1 (0%)	34	15
1	C	276/266 (104%)	268 (97%)	7 (2%)	1 (0%)	34	15
1	D	272/266 (102%)	265 (97%)	7 (3%)	0	100	100
All	All	1101/1064 (104%)	1072 (97%)	27 (2%)	2 (0%)	47	26

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	490	ARG
1	C	490	ARG

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	244/238 (102%)	242 (99%)	2 (1%)	81	70
1	B	247/238 (104%)	247 (100%)	0	100	100
1	C	245/238 (103%)	245 (100%)	0	100	100
1	D	242/238 (102%)	241 (100%)	1 (0%)	91	84
All	All	978/952 (103%)	975 (100%)	3 (0%)	92	87

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	395	TRP
1	A	405	LEU
1	D	494	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	484	ASN
1	A	603	ASN
1	C	491	HIS

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)

21 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	746	C	1001	-	47,47,47	2.17	12 (25%)	61,68,68	1.41	11 (18%)
3	GOL	D	703	-	5,5,5	0.66	0	5,5,5	1.68	2 (40%)
3	GOL	C	1002[A]	-	5,5,5	0.30	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	PE4	B	705	-	23,23,23	0.72	0	22,22,22	1.55	6 (27%)
2	746	A	701	-	47,47,47	2.27	10 (21%)	61,68,68	1.34	10 (16%)
4	BME	C	1003[A]	-	3,3,3	0.29	0	1,2,2	0.09	0
3	GOL	D	704	-	5,5,5	0.37	0	5,5,5	0.37	0
3	GOL	D	702	-	5,5,5	0.50	0	5,5,5	0.58	0
3	GOL	B	702	-	5,5,5	0.34	0	5,5,5	0.15	0
4	BME	B	704[B]	-	3,3,3	0.24	0	1,2,2	0.42	0
4	BME	A	703[B]	-	3,3,3	0.24	0	1,2,2	0.39	0
3	GOL	A	702	-	5,5,5	0.37	0	5,5,5	1.01	1 (20%)
3	GOL	D	705	-	5,5,5	0.35	0	5,5,5	0.25	0
5	PE4	C	1004	-	23,23,23	0.57	0	22,22,22	0.66	0
2	746	D	701	-	47,47,47	2.22	10 (21%)	61,68,68	1.30	7 (11%)
4	BME	C	1003[B]	-	3,3,3	0.28	0	1,2,2	0.12	0
3	GOL	C	1002[B]	-	5,5,5	0.33	0	5,5,5	0.83	0
4	BME	B	704[A]	-	3,3,3	0.26	0	1,2,2	0.31	0
3	GOL	B	703	-	5,5,5	0.35	0	5,5,5	0.43	0
4	BME	A	703[A]	-	3,3,3	0.28	0	1,2,2	0.62	0
2	746	B	701	-	47,47,47	2.23	12 (25%)	61,68,68	1.39	11 (18%)

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	746	C	1001	-	-	3/29/38/38	0/5/5/5
3	GOL	D	703	-	-	2/4/4/4	-
3	GOL	C	1002[A]	-	-	0/4/4/4	-
5	PE4	B	705	-	-	8/21/21/21	-
2	746	A	701	-	-	3/29/38/38	0/5/5/5
4	BME	C	1003[A]	-	-	1/1/1/1	-
3	GOL	D	704	-	-	0/4/4/4	-
3	GOL	D	702	-	-	1/4/4/4	-
3	GOL	B	702	-	-	0/4/4/4	-
4	BME	B	704[B]	-	-	0/1/1/1	-
4	BME	A	703[B]	-	-	1/1/1/1	-
3	GOL	A	702	-	-	2/4/4/4	-
3	GOL	D	705	-	-	1/4/4/4	-
5	PE4	C	1004	-	-	9/21/21/21	-
2	746	D	701	-	-	3/29/38/38	0/5/5/5

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BME	C	1003[B]	-	-	0/1/1/1	-
3	GOL	C	1002[B]	-	-	2/4/4/4	-
4	BME	B	704[A]	-	-	0/1/1/1	-
3	GOL	B	703	-	-	2/4/4/4	-
4	BME	A	703[A]	-	-	0/1/1/1	-
2	746	B	701	-	-	3/29/38/38	0/5/5/5

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	746	C17-C11	10.58	1.49	1.36
2	D	701	746	C17-C11	10.32	1.49	1.36
2	B	701	746	C17-C11	9.78	1.48	1.36
2	C	1001	746	C17-C11	9.34	1.48	1.36
2	C	1001	746	C71-N83	5.38	1.46	1.34
2	A	701	746	C71-N83	5.37	1.46	1.34
2	D	701	746	C71-N83	5.37	1.46	1.34
2	C	1001	746	C13-N12	5.29	1.43	1.32
2	B	701	746	C13-N12	5.19	1.43	1.32
2	B	701	746	C71-N83	5.18	1.46	1.34
2	A	701	746	C13-N12	4.67	1.42	1.32
2	D	701	746	C13-N12	4.23	1.41	1.32
2	A	701	746	C17-N16	3.55	1.45	1.36
2	D	701	746	C17-N16	3.23	1.44	1.36
2	D	701	746	C14-N16	2.85	1.43	1.39
2	B	701	746	C50-C71	2.84	1.54	1.50
2	C	1001	746	C13-N47	2.83	1.42	1.36
2	A	701	746	C13-N47	2.80	1.42	1.36
2	B	701	746	C11-N12	2.78	1.44	1.38
2	A	701	746	C50-C71	2.75	1.54	1.50
2	C	1001	746	C50-C71	2.75	1.54	1.50
2	D	701	746	C13-N47	2.74	1.42	1.36
2	B	701	746	C17-N16	2.71	1.43	1.36
2	D	701	746	C50-C71	2.69	1.54	1.50
2	C	1001	746	C17-N16	2.64	1.43	1.36
2	C	1001	746	C21-N19	2.63	1.42	1.35
2	A	701	746	C21-N19	2.63	1.42	1.35
2	B	701	746	C13-N47	2.60	1.42	1.36
2	B	701	746	O72-C71	-2.59	1.17	1.22
2	D	701	746	C21-N19	2.57	1.42	1.35
2	B	701	746	C1-C2	-2.56	1.37	1.40
2	C	1001	746	O72-C71	-2.49	1.17	1.22

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	746	C21-N19	2.49	1.42	1.35
2	A	701	746	C14-N16	2.38	1.43	1.39
2	A	701	746	C1-C11	2.36	1.50	1.47
2	C	1001	746	C11-N12	2.33	1.43	1.38
2	A	701	746	C11-N12	2.32	1.43	1.38
2	B	701	746	C14-N16	2.31	1.42	1.39
2	D	701	746	C1-C11	2.24	1.50	1.47
2	C	1001	746	C1-C11	2.16	1.50	1.47
2	C	1001	746	C1-C2	-2.11	1.37	1.40
2	B	701	746	C1-C11	2.10	1.50	1.47
2	D	701	746	C1-C2	-2.10	1.37	1.40
2	C	1001	746	C14-N16	2.10	1.42	1.39

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	746	C81-C82-N83	4.03	118.42	109.84
2	A	701	746	C60-N16-C14	4.01	122.83	117.12
2	B	701	746	C81-C82-N83	3.86	118.05	109.84
2	C	1001	746	C85-C84-N83	3.41	117.11	109.84
2	B	701	746	C9-C1-C11	-3.41	113.96	119.37
2	D	701	746	O15-C14-C13	-3.34	118.60	122.23
5	B	705	PE4	C9-O5-C8	3.32	127.68	113.29
2	D	701	746	C9-C1-C11	-3.32	114.09	119.37
2	A	701	746	C9-C1-C11	-3.30	114.13	119.37
2	C	1001	746	C60-N16-C14	3.24	121.73	117.12
2	B	701	746	C60-N16-C14	3.07	121.49	117.12
2	D	701	746	C60-N16-C14	3.04	121.45	117.12
2	D	701	746	C85-C84-N83	3.02	116.27	109.84
2	C	1001	746	C2-C4-N19	-2.92	115.43	119.45
2	B	701	746	C85-C84-N83	2.91	116.03	109.84
5	B	705	PE4	O5-C9-C10	2.89	123.41	110.39
2	A	701	746	C2-C4-N19	-2.88	115.48	119.45
2	C	1001	746	C9-C1-C11	-2.82	114.89	119.37
2	B	701	746	C2-C4-N19	-2.81	115.58	119.45
2	A	701	746	C85-C84-N83	2.79	115.79	109.84
2	B	701	746	C52-C46-N47	-2.78	111.07	120.40
2	D	701	746	C2-C4-N19	-2.76	115.65	119.45
2	C	1001	746	C52-C46-N47	-2.69	111.35	120.40
2	C	1001	746	C48-C49-C50	-2.54	117.82	120.78
2	A	701	746	O15-C14-C13	-2.52	119.49	122.23
2	A	701	746	C4-N19-C21	-2.48	120.12	126.93

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	701	746	C48-C49-C50	-2.45	117.93	120.78
2	D	701	746	C4-N19-C21	-2.40	120.34	126.93
2	C	1001	746	C52-C46-C48	2.40	122.31	119.03
2	B	701	746	C50-C71-N83	2.32	121.66	118.72
5	B	705	PE4	O6-C10-C9	2.29	120.72	110.39
2	A	701	746	C51-C50-C49	2.27	121.82	118.59
5	B	705	PE4	C3-O2-C2	2.24	122.98	113.29
2	A	701	746	C52-C46-C48	2.23	122.09	119.03
2	A	701	746	C52-C46-N47	-2.22	112.93	120.40
2	C	1001	746	C50-C71-N83	2.22	121.54	118.72
2	B	701	746	O72-C71-N83	-2.21	118.68	122.34
3	D	703	GOL	C3-C2-C1	-2.17	103.25	111.70
5	B	705	PE4	C5-O3-C4	2.15	122.61	113.29
2	D	701	746	C52-C46-N47	-2.13	113.23	120.40
2	A	701	746	C9-C1-C2	2.10	122.23	120.72
3	D	703	GOL	O3-C3-C2	2.07	120.14	110.20
2	C	1001	746	C51-C50-C49	2.06	121.52	118.59
2	C	1001	746	C51-C52-C46	-2.03	117.95	120.30
5	B	705	PE4	O6-C11-C12	2.03	119.55	110.39
2	B	701	746	C4-N19-C21	-2.01	121.41	126.93
2	B	701	746	C52-C46-C48	2.00	121.77	119.03
3	A	702	GOL	O1-C1-C2	-2.00	100.60	110.20

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	GOL	O1-C1-C2-C3
3	D	703	GOL	C1-C2-C3-O3
3	D	703	GOL	O2-C2-C3-O3
5	B	705	PE4	C10-C9-O5-C8
5	C	1004	PE4	C13-C14-O8-C15
5	B	705	PE4	O4-C7-C8-O5
5	B	705	PE4	O6-C10-C9-O5
5	C	1004	PE4	O2-C3-C4-O3
5	B	705	PE4	O6-C11-C12-O7
5	C	1004	PE4	O4-C7-C8-O5
3	B	703	GOL	C1-C2-C3-O3
3	C	1002[B]	GOL	O1-C1-C2-C3
5	C	1004	PE4	O6-C11-C12-O7
3	A	702	GOL	O1-C1-C2-O2
3	B	703	GOL	O2-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	1002[B]	GOL	O1-C1-C2-O2
5	B	705	PE4	O1-C1-C2-O2
4	C	1003[A]	BME	O1-C1-C2-S2
5	C	1004	PE4	O6-C10-C9-O5
2	A	701	746	C2-C1-C11-C17
2	B	701	746	C2-C1-C11-C17
2	C	1001	746	C2-C1-C11-C17
2	D	701	746	C2-C1-C11-C17
3	D	702	GOL	O1-C1-C2-O2
5	C	1004	PE4	C6-C5-O3-C4
2	B	701	746	C5-C4-N19-C21
2	A	701	746	C5-C4-N19-C21
2	C	1001	746	C5-C4-N19-C21
2	D	701	746	C5-C4-N19-C21
5	B	705	PE4	C13-C14-O8-C15
5	B	705	PE4	O7-C13-C14-O8
5	C	1004	PE4	C11-C12-O7-C13
2	C	1001	746	C2-C4-N19-C21
2	D	701	746	C2-C4-N19-C21
2	A	701	746	C2-C4-N19-C21
5	B	705	PE4	C11-C12-O7-C13
2	B	701	746	C2-C4-N19-C21
5	C	1004	PE4	O7-C13-C14-O8
5	C	1004	PE4	C9-C10-O6-C11
4	A	703[B]	BME	O1-C1-C2-S2
3	D	705	GOL	O2-C2-C3-O3

There are no ring outliers.

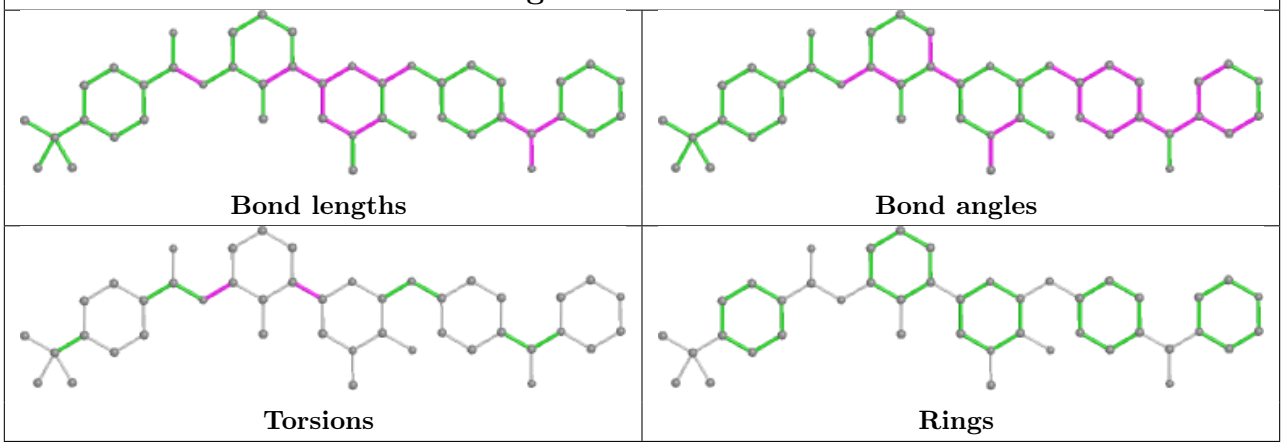
9 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	746	5	0
5	B	705	PE4	7	0
2	A	701	746	4	0
3	D	702	GOL	1	0
4	A	703[B]	BME	1	0
3	A	702	GOL	1	0
5	C	1004	PE4	6	0
2	D	701	746	4	0
2	B	701	746	6	0

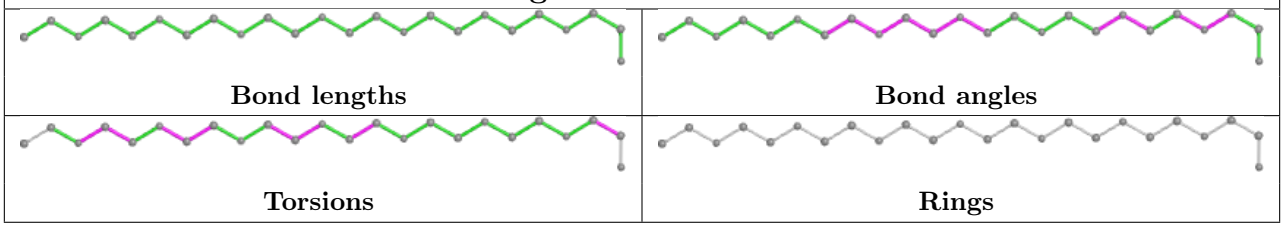
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

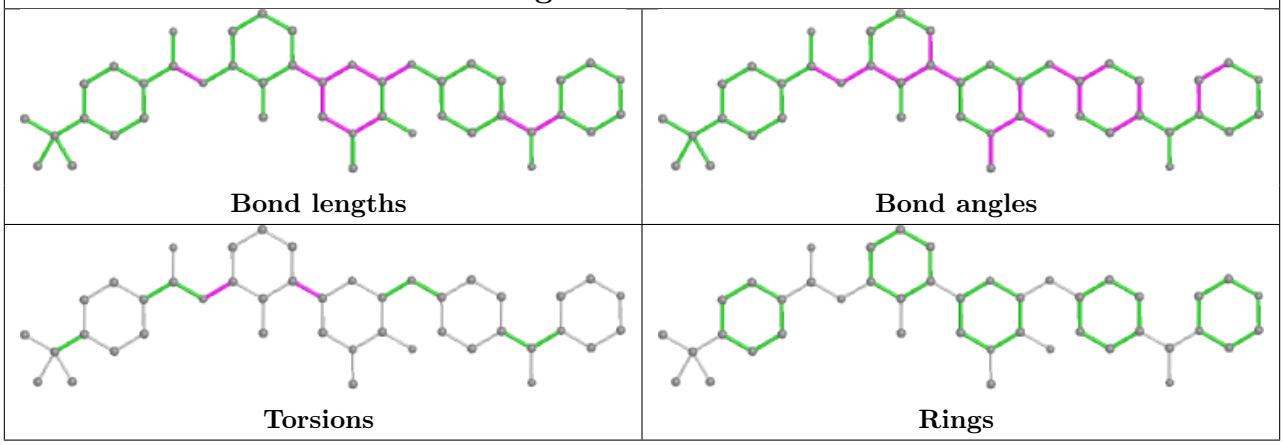
Ligand 746 C 1001



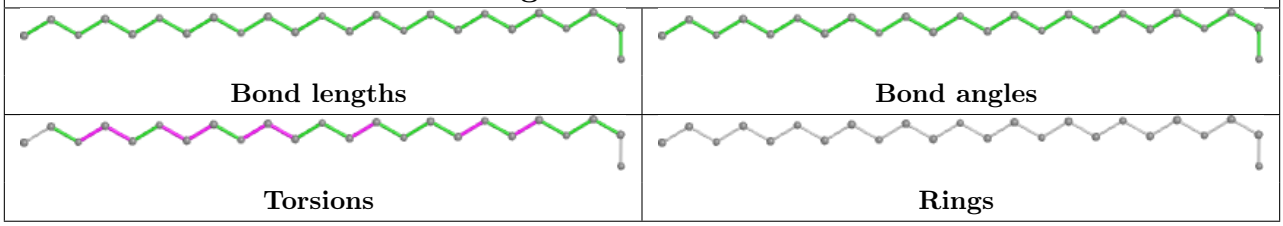
Ligand PE4 B 705



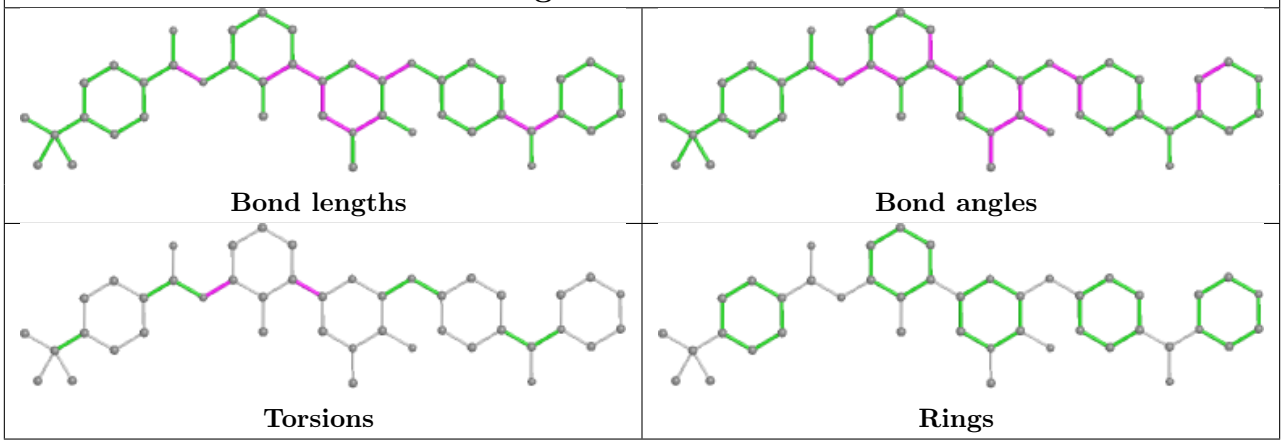
Ligand 746 A 701



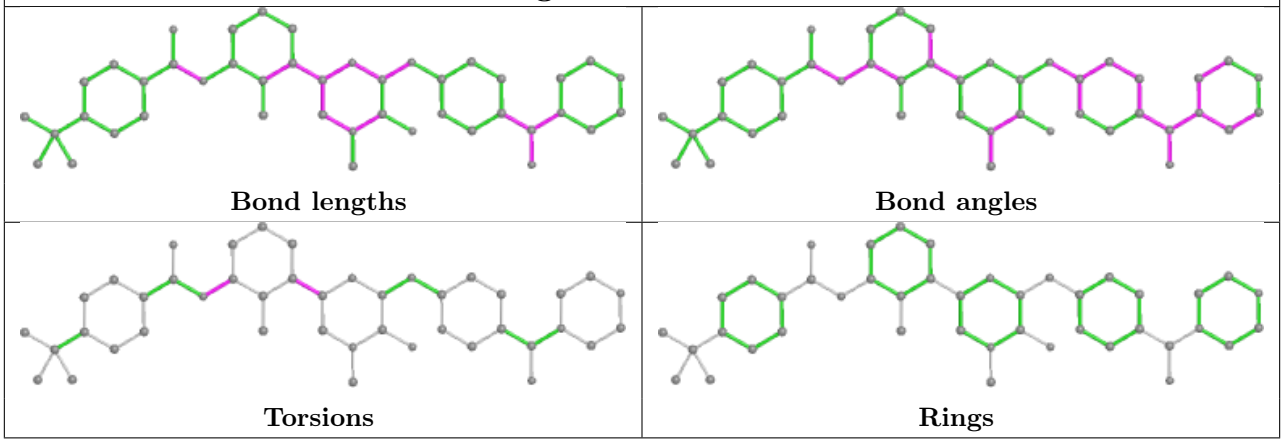
Ligand PE4 C 1004



Ligand 746 D 701



Ligand 746 B 701



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	266/266 (100%)	-0.11	6 (2%)	60	59	11, 19, 43, 77	0
1	B	266/266 (100%)	-0.09	9 (3%)	45	42	13, 20, 41, 71	0
1	C	266/266 (100%)	-0.11	6 (2%)	60	59	13, 20, 42, 68	0
1	D	265/266 (99%)	-0.09	6 (2%)	60	59	12, 19, 42, 65	0
All	All	1063/1064 (99%)	-0.10	27 (2%)	57	55	11, 20, 43, 77	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	395	TRP	8.8
1	D	659	SER	5.6
1	A	395	TRP	4.8
1	A	491	HIS	4.6
1	C	490	ARG	4.3
1	D	395	TRP	4.1
1	A	490	ARG	4.0
1	C	394	ALA	3.7
1	C	491	HIS	3.3
1	D	490	ARG	3.2
1	B	424[A]	GLN	3.1
1	D	466	LYS	3.0
1	B	425	TYR	2.9
1	C	425	TYR	2.9
1	B	421	TRP	2.8
1	C	421	TRP	2.6
1	A	394	ALA	2.4
1	B	394	ALA	2.4
1	A	659	SER	2.3
1	B	600	ARG	2.2
1	B	557[A]	THR	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	495	THR	2.2
1	C	488[A]	GLU	2.2
1	B	490	ARG	2.1
1	B	422	ARG	2.1
1	A	425	TYR	2.0
1	D	421	TRP	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
5	PE4	C	1004	24/24	0.74	0.17	30,48,73,73	0
5	PE4	B	705	24/24	0.81	0.13	30,50,64,68	0
4	BME	A	703[B]	4/4	0.84	0.19	23,28,31,35	10
3	GOL	D	702	6/6	0.84	0.16	25,33,45,54	0
4	BME	A	703[A]	4/4	0.84	0.19	22,27,32,38	10
4	BME	C	1003[A]	4/4	0.85	0.20	23,28,32,39	10
4	BME	C	1003[B]	4/4	0.85	0.20	15,27,37,45	10
4	BME	B	704[A]	4/4	0.90	0.22	26,31,33,39	10
4	BME	B	704[B]	4/4	0.90	0.22	25,30,42,51	10
3	GOL	D	703	6/6	0.91	0.13	17,40,58,58	0
3	GOL	B	702	6/6	0.92	0.10	26,36,45,50	0
3	GOL	A	702	6/6	0.93	0.10	15,26,52,52	0
3	GOL	B	703	6/6	0.93	0.12	19,26,35,40	0
2	746	A	701	43/43	0.94	0.10	11,16,39,49	0
3	GOL	D	704	6/6	0.95	0.12	20,29,47,57	0
3	GOL	D	705	6/6	0.95	0.13	24,38,49,56	0
2	746	D	701	43/43	0.95	0.09	12,16,41,49	0

Continued on next page...

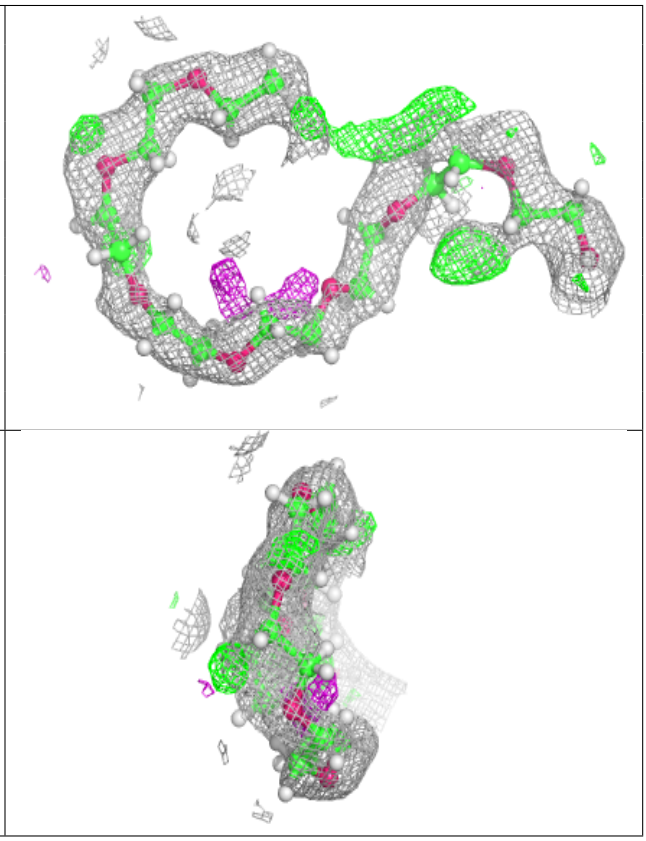
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	746	B	701	43/43	0.95	0.10	11,14,44,61	0
2	746	C	1001	43/43	0.95	0.10	11,14,42,61	0
3	GOL	C	1002[A]	6/6	0.96	0.10	17,22,35,43	14
3	GOL	C	1002[B]	6/6	0.96	0.10	17,23,31,31	14

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.

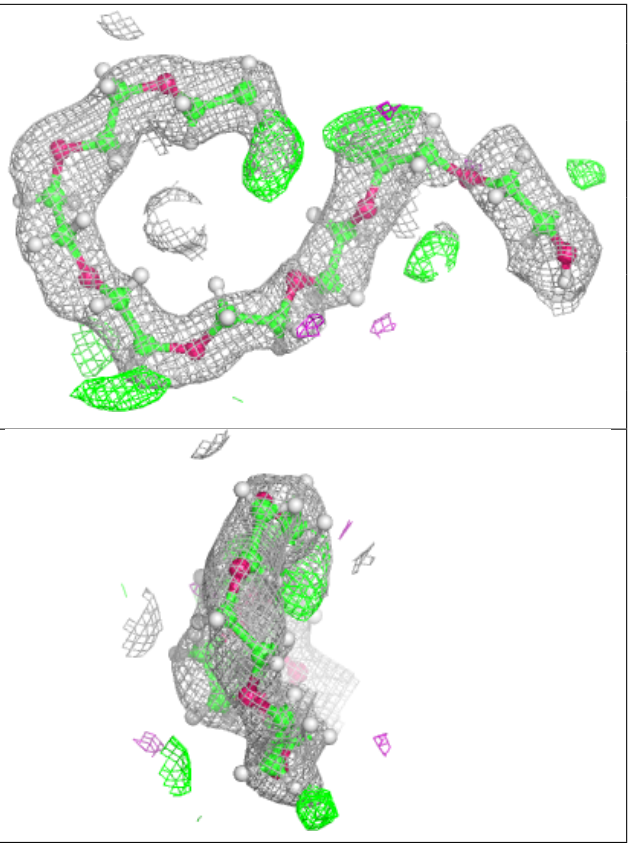
Electron density around PE4 C 1004:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



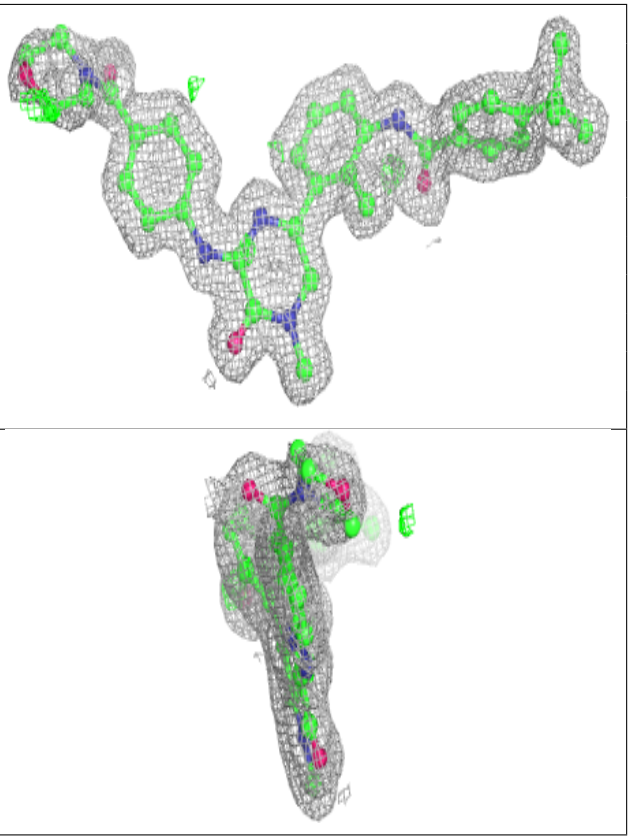
Electron density around PE4 B 705:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



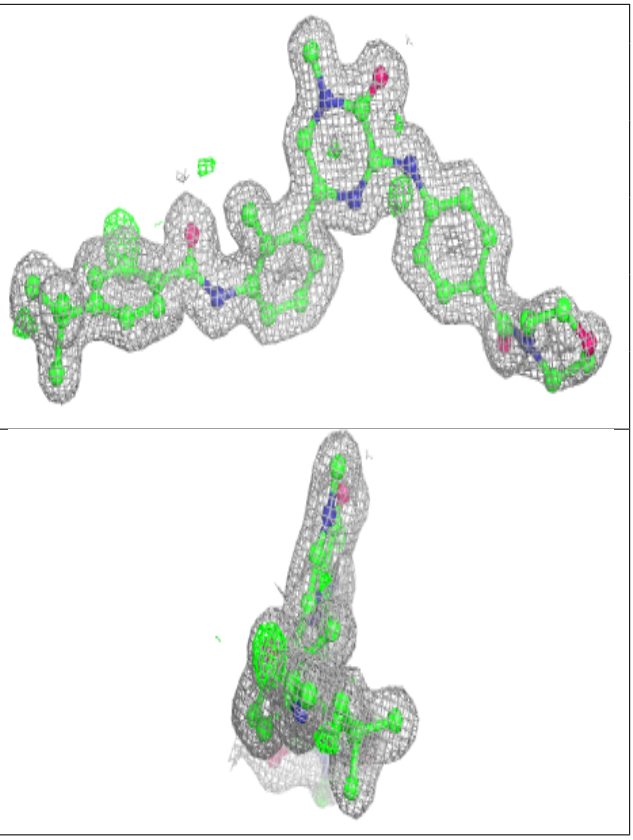
Electron density around 746 A 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



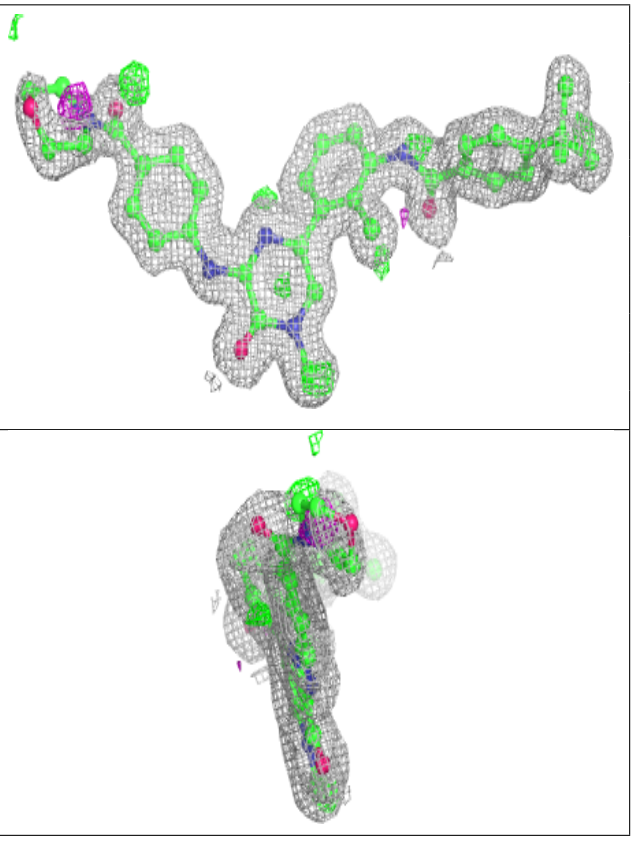
Electron density around 746 D 701:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



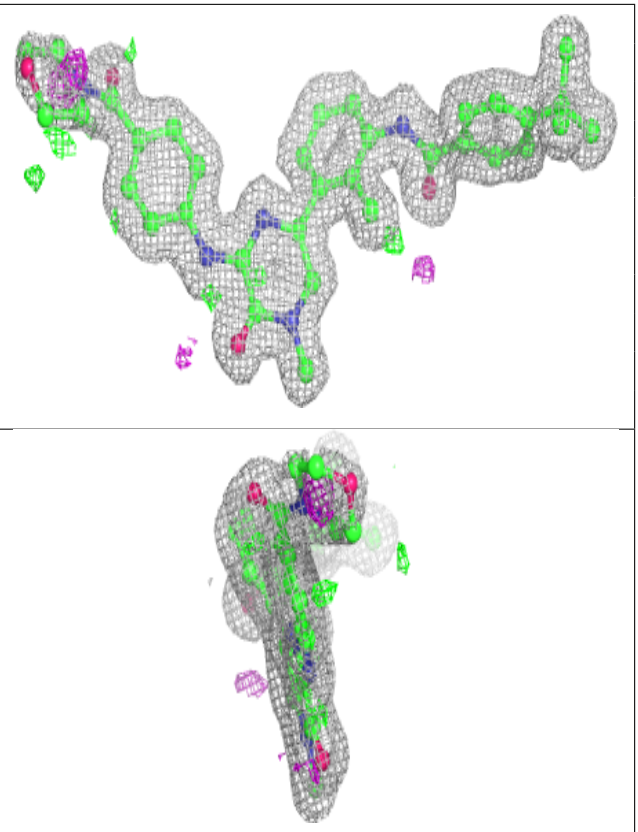
Electron density around 746 B 701:

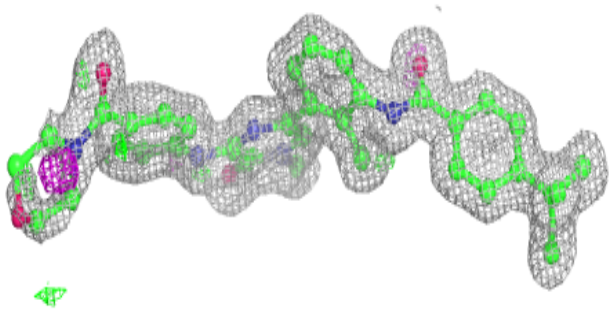
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 746 C 1001:

$2mF_o$-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.