



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 11, 2022 – 02:07 PM EST

PDB ID : 7KY0
Title : Inactive conformation of EGFR (T790M/V948R) kinase in complex with BI-4020
Authors : Beyett, T.S.; Eck, M.J.
Deposited on : 2020-12-06
Resolution : 3.10 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 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	:	2.25
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)	:	2.25

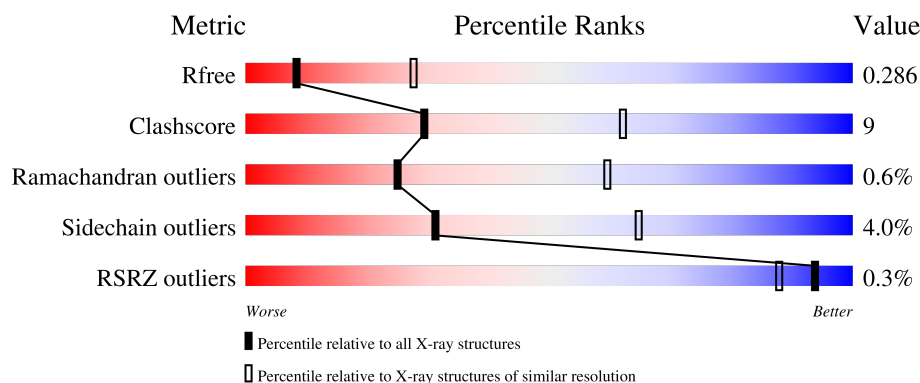
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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 $\leq 5\%$. 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	331	<div> <div></div> <div>69%</div> <div>17%</div> <div>•</div> <div>13%</div> </div>
1	B	331	<div> <div></div> <div>64%</div> <div>21%</div> <div>•</div> <div>14%</div> </div>
1	C	331	<div> <div>%</div> <div>65%</div> <div>20%</div> <div>••</div> <div>13%</div> </div>
1	D	331	<div> <div></div> <div>72%</div> <div>17%</div> <div>•</div> <div>11%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9491 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.

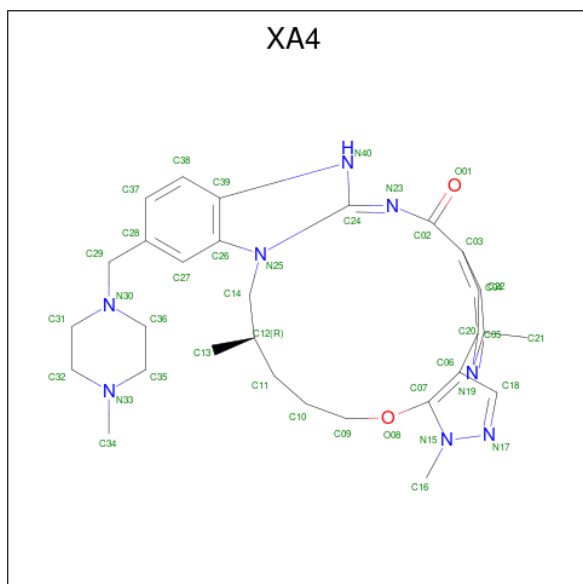
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	294	Total	C	N	O	S	0	0	0
			2372	1524	404	425	19			
1	A	288	Total	C	N	O	S	0	0	0
			2320	1492	392	418	18			
1	B	285	Total	C	N	O	S	0	0	0
			2301	1481	390	412	18			
1	C	289	Total	C	N	O	S	0	0	0
			2338	1503	398	418	19			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	694	THR	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	694	THR	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	SER	-	expression tag	UNP P00533
C	694	THR	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is (20R)-10,15,20-trimethyl-2-[(4-methylpiperazin-1-yl)methyl]-18,19,20,21-tetrahydro-15H,17H-12,8-(metheno)pyrazolo[3',4':2,3][1,5,10,12]oxatriazacycloheptadecino[1,2,11-a]benzimidazol-7(6H)-one (three-letter code: XA4) (formula: C₃₀H₃₈N₈O₂) (labeled as "Ligand of Interest" by depositor).



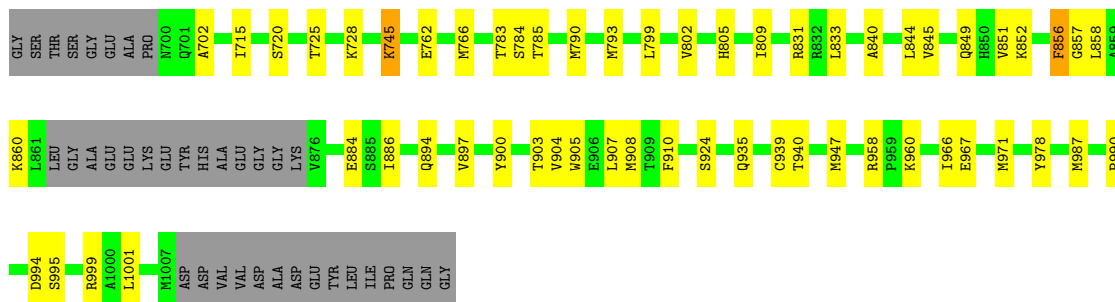
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	N	O	0	0
			40	30	8	2		
2	A	1	Total	C	N	O	0	0
			40	30	8	2		
2	B	1	Total	C	N	O	0	0
			40	30	8	2		
2	C	1	Total	C	N	O	0	0
			40	30	8	2		

3 Residue-property plots

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.

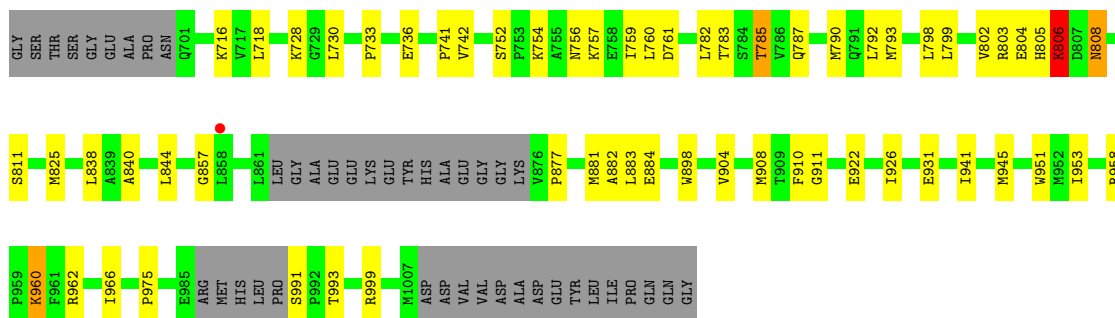
- Molecule 1: Epidermal growth factor receptor

Chain D: 



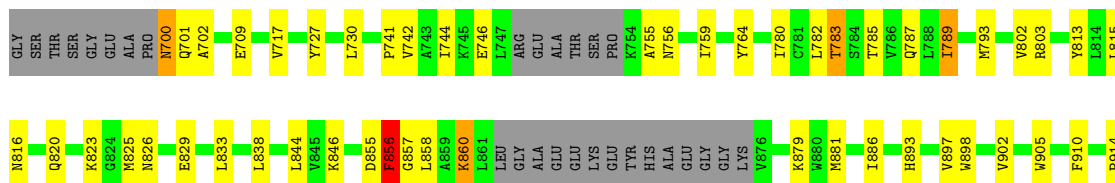
- Molecule 1: Epidermal growth factor receptor

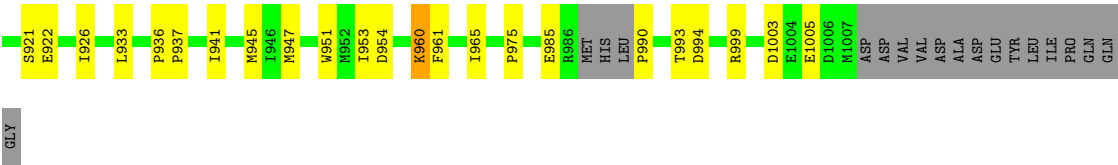
Chain A: 



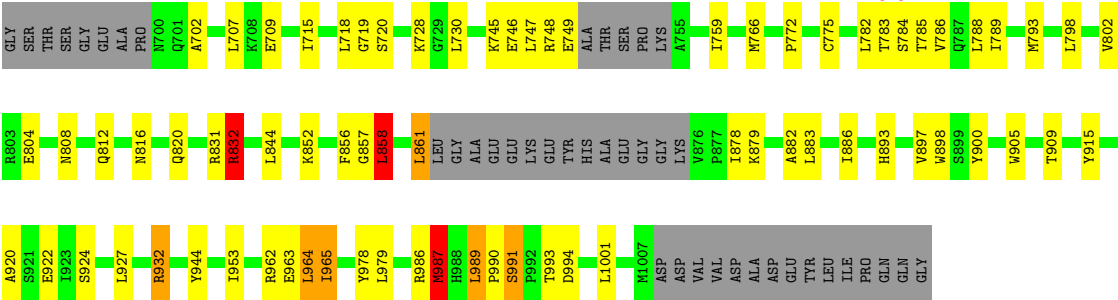
- Molecule 1: Epidermal growth factor receptor

Chain B: 





● Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.22Å 100.73Å 86.79Å 90.00° 101.07° 90.00°	Depositor
Resolution (Å)	68.92 – 3.10 68.91 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (68.92-3.10) 97.1 (68.91-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 3.13Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.238 , 0.292 0.238 , 0.286	Depositor DCC
R_{free} test set	1049 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.421	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9491	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.82% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: XA4

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	0.50	0/2369	0.71	0/3201
1	B	0.52	1/2349 (0.0%)	0.69	2/3171 (0.1%)
1	C	0.77	2/2388 (0.1%)	0.78	6/3226 (0.2%)
1	D	0.52	0/2424	0.70	0/3277
All	All	0.59	3/9530 (0.0%)	0.72	8/12875 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	944	TYR	CE1-CZ	-6.19	1.30	1.38
1	C	944	TYR	CE2-CZ	-5.23	1.31	1.38
1	B	954	ASP	CB-CG	5.04	1.62	1.51

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	954	ASP	CB-CG-OD1	7.78	125.31	118.30
1	C	987	MET	N-CA-C	-6.08	94.59	111.00
1	C	989	LEU	CA-CB-CG	5.90	128.87	115.30
1	C	858	LEU	CA-CB-CG	5.68	128.36	115.30
1	B	856	PHE	CB-CA-C	5.62	121.65	110.40
1	C	932	ARG	NE-CZ-NH1	-5.31	117.65	120.30
1	C	965	ILE	CG1-CB-CG2	-5.18	100.00	111.40
1	C	964	LEU	CB-CA-C	-5.05	100.61	110.20

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	2320	0	2367	37	0
1	B	2301	0	2350	48	0
1	C	2338	0	2383	69	0
1	D	2372	0	2421	33	0
2	A	40	0	0	0	0
2	B	40	0	0	0	0
2	C	40	0	0	2	0
2	D	40	0	0	0	0
All	All	9491	0	9521	180	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 9.

All (180) 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:C:989:LEU:HG	1:C:990:PRO:CD	1.37	1.55
1:C:989:LEU:CG	1:C:990:PRO:HD2	1.54	1.37
1:C:989:LEU:HG	1:C:990:PRO:HD3	1.35	1.05
1:C:989:LEU:CG	1:C:990:PRO:CD	2.21	1.00
1:C:927:LEU:HD22	1:C:932:ARG:NH1	1.85	0.90
1:C:989:LEU:HG	1:C:990:PRO:HD2	0.89	0.88
1:C:927:LEU:CD2	1:C:932:ARG:NH1	2.37	0.88
1:C:989:LEU:CB	1:C:990:PRO:HD2	2.03	0.87
1:B:756:ASN:HB3	1:B:782:LEU:HD13	1.56	0.86
1:C:986:ARG:NE	1:C:986:ARG:O	2.08	0.86
1:B:756:ASN:HB3	1:B:782:LEU:CD1	2.06	0.85
1:D:990:PRO:HB2	1:D:994:ASP:HB2	1.64	0.80
1:C:989:LEU:CB	1:C:990:PRO:CD	2.54	0.79
1:C:858:LEU:HD22	1:C:858:LEU:H	1.48	0.77
1:C:812:GLN:HG2	1:C:989:LEU:HD13	1.73	0.70
1:C:900:TYR:CE2	1:C:964:LEU:HD13	2.27	0.69
1:C:709:GLU:OE2	1:C:783:THR:HG21	1.93	0.68
1:B:829:GLU:OE2	1:B:960:LYS:NZ	2.26	0.68
1:C:927:LEU:CD2	1:C:932:ARG:HH11	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:709:GLU:CG	1:C:783:THR:HG21	2.25	0.66
1:B:823:LYS:HA	1:B:965:ILE:HD11	1.77	0.66
1:C:927:LEU:HD23	1:C:932:ARG:NH1	2.11	0.66
1:A:793:MET:HG3	1:A:844:LEU:HD13	1.79	0.64
1:B:700:ASN:C	1:B:702:ALA:H	2.02	0.64
1:B:993:THR:HA	1:C:702:ALA:O	1.98	0.63
1:C:709:GLU:HG3	1:C:783:THR:HG21	1.81	0.63
1:C:812:GLN:CG	1:C:989:LEU:HD13	2.28	0.63
1:B:780:ILE:CD1	1:B:782:LEU:HD21	2.28	0.62
1:C:720:SER:HB2	1:C:748:ARG:HH12	1.64	0.61
1:C:989:LEU:CG	1:C:990:PRO:HD3	2.10	0.61
1:C:759:ILE:HG23	1:C:858:LEU:HD11	1.81	0.61
1:C:745:LYS:HD2	1:C:788:LEU:HD12	1.82	0.61
1:C:766:MET:SD	1:C:857:GLY:HA2	2.41	0.60
1:A:802:VAL:HG12	1:A:910:PHE:HA	1.83	0.60
1:B:780:ILE:HG12	1:B:782:LEU:HD23	1.82	0.60
1:C:927:LEU:HD23	1:C:932:ARG:HH11	1.66	0.59
1:C:858:LEU:H	1:C:858:LEU:CD2	2.17	0.58
1:A:898:TRP:CE3	1:A:951:TRP:HA	2.40	0.57
1:C:989:LEU:CD2	1:C:990:PRO:HD2	2.31	0.57
1:B:941:ILE:O	1:B:945:MET:HG3	2.05	0.57
1:C:927:LEU:HD22	1:C:932:ARG:HH12	1.69	0.57
1:A:798:LEU:O	1:A:802:VAL:HG23	2.04	0.57
1:D:935:GLN:NE2	1:D:939:CYS:O	2.37	0.56
1:A:783:THR:HG21	1:A:787:GLN:HE21	1.71	0.56
1:C:786:VAL:HG12	1:C:786:VAL:O	2.04	0.56
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.70	0.56
1:D:720:SER:HA	1:D:725:THR:HA	1.88	0.55
1:B:756:ASN:CB	1:B:782:LEU:HD13	2.33	0.55
1:B:881:MET:HE2	1:B:886:ILE:HG12	1.88	0.55
1:A:756:ASN:HB3	1:A:782:LEU:HD13	1.89	0.54
1:D:802:VAL:HG12	1:D:910:PHE:HA	1.87	0.54
1:C:793:MET:HG3	1:C:844:LEU:HD13	1.89	0.54
1:C:886:ILE:HG21	1:C:924:SER:HB3	1.88	0.54
1:A:960:LYS:HZ2	1:A:960:LYS:HB3	1.73	0.54
1:D:966:ILE:HD13	1:B:803:ARG:HD3	1.90	0.54
1:D:831:ARG:O	1:D:833:LEU:HG	2.07	0.54
1:A:926:ILE:HB	1:A:931:GLU:OE2	2.08	0.54
1:A:966:ILE:HD11	1:C:719:GLY:HA2	1.90	0.54
1:D:715:ILE:HG12	1:D:728:LYS:O	2.08	0.54
1:C:709:GLU:OE2	1:C:783:THR:CG2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:967:GLU:HG2	1:D:971:MET:HE2	1.91	0.53
1:A:825:MET:SD	1:A:838:LEU:HD22	2.48	0.53
1:C:882:ALA:HA	1:C:898:TRP:CD2	2.44	0.53
1:B:825:MET:SD	1:B:838:LEU:HD22	2.49	0.52
1:B:990:PRO:HB2	1:B:994:ASP:HB2	1.91	0.52
1:C:804:GLU:HG3	2:C:1101:XA4:C34	2.39	0.52
1:B:922:GLU:O	1:B:926:ILE:HG23	2.10	0.52
1:B:905:TRP:CD1	1:B:947:MET:HE1	2.45	0.52
1:C:927:LEU:CD2	1:C:932:ARG:HH12	2.18	0.52
1:C:991:SER:HB2	1:C:994:ASP:H	1.75	0.52
1:B:702:ALA:O	1:C:993:THR:HA	2.10	0.51
1:B:700:ASN:C	1:B:702:ALA:N	2.64	0.51
1:C:709:GLU:CD	1:C:783:THR:HG21	2.31	0.50
1:C:715:ILE:HD13	1:C:730:LEU:HG	1.93	0.50
1:A:759:ILE:C	1:A:761:ASP:H	2.15	0.50
1:A:960:LYS:HB3	1:A:960:LYS:NZ	2.26	0.50
1:B:717:VAL:HG22	1:B:727:TYR:CE2	2.46	0.50
1:D:849:GLN:NE2	1:D:990:PRO:HG3	2.27	0.50
1:A:799:LEU:HD13	1:A:840:ALA:HB3	1.94	0.50
1:B:879:LYS:HD3	1:B:914:PRO:O	2.12	0.50
1:C:905:TRP:O	1:C:909:THR:OG1	2.26	0.49
1:A:785:THR:O	1:A:787:GLN:HG2	2.11	0.49
1:D:802:VAL:CG1	1:D:910:PHE:HA	2.42	0.49
1:A:960:LYS:HZ2	1:A:962:ARG:HH12	1.61	0.49
1:B:780:ILE:HD11	1:B:782:LEU:HD21	1.93	0.49
1:C:715:ILE:HG12	1:C:728:LYS:O	2.13	0.49
1:C:816:ASN:O	1:C:820:GLN:HG3	2.13	0.49
1:A:802:VAL:CG1	1:A:910:PHE:HA	2.43	0.49
1:A:904:VAL:O	1:A:908:MET:HG2	2.11	0.49
1:B:780:ILE:CD1	1:B:782:LEU:CD2	2.90	0.49
1:B:793:MET:HG3	1:B:844:LEU:HD13	1.94	0.48
1:B:893:HIS:O	1:B:897:VAL:HG23	2.13	0.48
1:C:766:MET:HE1	1:C:858:LEU:HD13	1.95	0.48
1:C:991:SER:OG	1:C:994:ASP:OD2	2.31	0.48
1:A:811:SER:OG	1:A:975:PRO:HB2	2.14	0.48
1:A:941:ILE:O	1:A:945:MET:HG3	2.14	0.47
1:B:780:ILE:HD11	1:B:782:LEU:CD2	2.44	0.47
1:D:905:TRP:CD1	1:D:947:MET:HE1	2.50	0.47
1:B:813:TYR:OH	1:B:990:PRO:HD3	2.15	0.47
1:D:799:LEU:HD13	1:D:840:ALA:HB3	1.97	0.47
1:B:898:TRP:O	1:B:902:VAL:HG23	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:831:ARG:O	1:C:832:ARG:HB2	2.13	0.47
1:B:742:VAL:HG12	1:C:1001:LEU:HD21	1.96	0.47
1:C:893:HIS:O	1:C:897:VAL:HG23	2.14	0.46
1:A:884:GLU:OE1	1:A:958:ARG:NH2	2.41	0.46
1:C:766:MET:CE	1:C:858:LEU:HD13	2.44	0.46
1:B:709:GLU:OE2	1:B:783:THR:HG21	2.16	0.46
1:C:978:TYR:O	1:C:979:LEU:HD23	2.15	0.46
1:D:995:SER:O	1:D:999:ARG:HG3	2.16	0.46
1:D:805:HIS:O	1:D:809:ILE:HG13	2.16	0.46
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.81	0.45
1:A:811:SER:CB	1:A:975:PRO:HB2	2.47	0.45
1:B:815:LEU:HD12	1:B:975:PRO:HB3	1.97	0.45
1:D:783:THR:OG1	1:D:785:THR:O	2.30	0.45
1:C:856:PHE:CG	1:C:856:PHE:O	2.69	0.45
1:A:733:PRO:HB2	1:A:736:GLU:CG	2.46	0.45
1:A:803:ARG:HG2	1:A:911:GLY:HA3	1.99	0.45
1:C:775:CYS:SG	1:C:844:LEU:HD12	2.57	0.45
1:C:879:LYS:HB3	1:C:915:TYR:HD2	1.82	0.45
1:C:798:LEU:O	1:C:802:VAL:HG23	2.16	0.45
1:A:884:GLU:OE2	1:A:958:ARG:NH1	2.49	0.44
1:B:826:ASN:HB2	1:B:961:PHE:HB3	1.98	0.44
1:A:922:GLU:O	1:A:926:ILE:HG23	2.18	0.44
1:B:881:MET:HE2	1:B:886:ILE:CG1	2.47	0.44
1:C:858:LEU:HG	1:C:861:LEU:HB3	1.99	0.44
1:D:900:TYR:O	1:D:904:VAL:HG23	2.17	0.44
1:D:903:THR:O	1:D:907:LEU:HG	2.18	0.44
1:B:816:ASN:O	1:B:820:GLN:HG3	2.17	0.44
1:B:802:VAL:HG12	1:B:910:PHE:HA	1.99	0.44
1:C:882:ALA:HB2	1:C:898:TRP:CB	2.48	0.44
1:D:745:LYS:HB2	1:D:790:MET:CE	2.48	0.43
1:B:744:ILE:HG12	1:B:789:ILE:HG13	2.00	0.43
1:C:747:LEU:C	1:C:749:GLU:H	2.21	0.43
1:A:883:LEU:HD23	1:A:953:ILE:HG13	2.01	0.43
1:D:833:LEU:HD13	1:D:856:PHE:CZ	2.52	0.43
1:B:780:ILE:HD13	1:B:782:LEU:HD21	1.99	0.43
1:D:845:VAL:HG22	1:D:851:VAL:HG12	2.00	0.43
1:C:715:ILE:HD11	1:C:728:LYS:HG2	2.00	0.43
1:D:884:GLU:OE2	1:D:958:ARG:NH1	2.50	0.43
1:D:940:THR:OG1	1:D:978:TYR:O	2.20	0.43
1:C:844:LEU:HD11	2:C:1101:XA4:C20	2.49	0.43
1:A:733:PRO:HB2	1:A:736:GLU:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:HIS:O	1:A:806:LYS:C	2.57	0.42
1:D:793:MET:HG3	1:D:844:LEU:HD13	2.00	0.42
1:D:1001:LEU:HD21	1:A:742:VAL:HG12	2.01	0.42
1:B:746:GLU:HG3	1:B:787:GLN:HG2	2.01	0.42
1:C:965:ILE:HG21	1:C:965:ILE:HD13	1.64	0.42
1:C:987:MET:H	1:C:987:MET:HG3	1.55	0.42
1:A:730:LEU:HD23	1:A:741:PRO:HA	2.02	0.42
1:C:883:LEU:HD23	1:C:953:ILE:HG13	2.01	0.42
1:A:811:SER:HB2	1:A:975:PRO:HB2	2.01	0.42
1:A:960:LYS:NZ	1:A:962:ARG:HH12	2.18	0.42
1:B:846:LYS:NZ	1:B:1005:GLU:OE2	2.41	0.42
1:B:860:LYS:HA	1:B:860:LYS:HD3	1.51	0.42
1:A:882:ALA:HA	1:A:898:TRP:CD2	2.55	0.42
1:A:877:PRO:O	1:A:881:MET:HG3	2.19	0.42
1:B:833:LEU:HD13	1:B:856:PHE:CZ	2.54	0.42
1:C:772:PRO:O	1:C:852:LYS:HE3	2.20	0.42
1:D:702:ALA:O	1:A:993:THR:HA	2.19	0.41
1:D:762:GLU:O	1:D:766:MET:HG3	2.20	0.41
1:C:782:LEU:HA	1:C:782:LEU:HD23	1.84	0.41
1:B:730:LEU:HD23	1:B:741:PRO:HA	2.02	0.41
1:D:886:ILE:HG21	1:D:924:SER:HB3	2.01	0.41
1:B:700:ASN:HD22	1:B:700:ASN:HA	1.57	0.41
1:C:707:LEU:HD12	1:C:789:ILE:HD13	2.01	0.41
1:D:715:ILE:HD11	1:D:728:LYS:HG2	2.03	0.41
1:B:701:GLN:HG3	1:B:764:TYR:CE1	2.55	0.41
1:D:793:MET:HE3	1:D:852:LYS:HD3	2.03	0.41
1:C:746:GLU:CG	1:C:785:THR:HB	2.50	0.41
1:C:878:ILE:HB	1:C:920:ALA:HB1	2.03	0.41
1:D:894:GLN:O	1:D:897:VAL:HB	2.21	0.41
1:A:718:LEU:HD23	1:A:718:LEU:HA	1.92	0.40
1:A:728:LYS:HD2	1:A:792:LEU:HD21	2.02	0.40
1:C:718:LEU:HD11	1:C:728:LYS:HB2	2.03	0.40
1:B:999:ARG:HA	1:B:1003:ASP:HB3	2.03	0.40
1:B:755:ALA:O	1:B:759:ILE:HG13	2.22	0.40
1:D:715:ILE:HD11	1:D:728:LYS:HE2	2.04	0.40
1:B:933:LEU:HB2	1:B:951:TRP:CH2	2.57	0.40
1:D:904:VAL:O	1:D:908:MET:HG2	2.22	0.40
1:B:936:PRO:HA	1:B:937:PRO:HD3	1.96	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	282/331 (85%)	268 (95%)	11 (4%)	3 (1%)	14	46
1	B	277/331 (84%)	268 (97%)	7 (2%)	2 (1%)	22	57
1	C	283/331 (86%)	271 (96%)	11 (4%)	1 (0%)	34	69
1	D	290/331 (88%)	285 (98%)	4 (1%)	1 (0%)	41	73
All	All	1132/1324 (86%)	1092 (96%)	33 (3%)	7 (1%)	25	59

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	808	ASN
1	C	832	ARG
1	A	806	LYS
1	B	857	GLY
1	A	857	GLY
1	B	855	ASP
1	D	857	GLY

5.3.2 Protein sidechains

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	257/290 (89%)	244 (95%)	13 (5%)	24	56
1	B	255/290 (88%)	244 (96%)	11 (4%)	29	62
1	C	259/290 (89%)	249 (96%)	10 (4%)	32	65

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	263/290 (91%)	256 (97%)	7 (3%)	44 74
All	All	1034/1160 (89%)	993 (96%)	41 (4%)	31 65

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	745	LYS
1	D	784	SER
1	D	856	PHE
1	D	858	LEU
1	D	860	LYS
1	D	960	LYS
1	D	987	MET
1	A	716	LYS
1	A	752	SER
1	A	754	LYS
1	A	757	LYS
1	A	760	LEU
1	A	785	THR
1	A	790	MET
1	A	804	GLU
1	A	806	LYS
1	A	808	ASN
1	A	960	LYS
1	A	991	SER
1	A	999	ARG
1	B	700	ASN
1	B	783	THR
1	B	785	THR
1	B	789	ILE
1	B	856	PHE
1	B	858	LEU
1	B	860	LYS
1	B	921	SER
1	B	953	ILE
1	B	960	LYS
1	B	985	GLU
1	C	784	SER
1	C	808	ASN
1	C	832	ARG
1	C	858	LEU
1	C	861	LEU

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Mol	Chain	Res	Type
1	C	922	GLU
1	C	962	ARG
1	C	963	GLU
1	C	987	MET
1	C	991	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	808	ASN
1	A	826	ASN
1	B	700	ASN
1	B	849	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](#)

4 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	XA4	B	1101	-	36,45,45	1.41	4 (11%)	45,65,65	2.24	15 (33%)
2	XA4	C	1101	-	36,45,45	1.94	7 (19%)	45,65,65	3.93	15 (33%)
2	XA4	A	1101	-	36,45,45	1.60	6 (16%)	45,65,65	4.11	17 (37%)
2	XA4	D	1101	-	36,45,45	1.34	3 (8%)	45,65,65	2.15	14 (31%)

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	XA4	B	1101	-	-	11/17/37/37	0/5/6/6
2	XA4	C	1101	-	-	8/17/37/37	0/5/6/6
2	XA4	A	1101	-	-	10/17/37/37	0/5/6/6
2	XA4	D	1101	-	-	7/17/37/37	0/5/6/6

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	XA4	O08-C07	6.40	1.42	1.34
2	B	1101	XA4	O08-C07	4.84	1.40	1.34
2	D	1101	XA4	O08-C07	4.83	1.40	1.34
2	C	1101	XA4	C04-C05	4.73	1.47	1.39
2	A	1101	XA4	O08-C07	4.21	1.39	1.34
2	C	1101	XA4	C16-N15	4.12	1.55	1.47
2	A	1101	XA4	C14-N25	-4.12	1.44	1.48
2	A	1101	XA4	C04-C05	3.62	1.45	1.39
2	C	1101	XA4	C32-N33	3.28	1.53	1.46
2	D	1101	XA4	C03-C02	-2.70	1.45	1.49
2	B	1101	XA4	C14-N25	-2.64	1.45	1.48
2	D	1101	XA4	C38-C37	2.55	1.42	1.36
2	B	1101	XA4	C03-C02	-2.50	1.46	1.49
2	B	1101	XA4	C38-C37	2.45	1.41	1.36
2	C	1101	XA4	C27-C28	2.44	1.43	1.37
2	A	1101	XA4	C32-N33	2.43	1.51	1.46
2	A	1101	XA4	C27-C28	2.17	1.42	1.37
2	C	1101	XA4	C38-C37	2.13	1.41	1.36
2	A	1101	XA4	C04-C03	2.03	1.42	1.39
2	C	1101	XA4	O01-C02	2.03	1.27	1.23

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	XA4	C03-C02-N23	21.50	147.86	114.89
2	C	1101	XA4	C03-C02-N23	20.59	146.46	114.89
2	A	1101	XA4	O01-C02-N23	-9.47	103.42	124.71
2	C	1101	XA4	O01-C02-N23	-8.84	104.84	124.71
2	B	1101	XA4	C03-C02-N23	7.96	127.11	114.89
2	D	1101	XA4	C03-C02-N23	6.53	124.91	114.89
2	A	1101	XA4	O01-C02-C03	-5.93	108.41	120.60
2	C	1101	XA4	O01-C02-C03	-5.78	108.70	120.60
2	A	1101	XA4	C04-C03-C02	5.65	127.74	119.92
2	B	1101	XA4	C22-C03-C02	5.28	127.22	119.92
2	D	1101	XA4	C22-C03-C02	5.14	127.02	119.92
2	B	1101	XA4	O01-C02-N23	-4.98	113.53	124.71
2	C	1101	XA4	C04-C03-C02	4.78	126.53	119.92
2	D	1101	XA4	O01-C02-N23	-4.46	114.69	124.71
2	A	1101	XA4	C39-N40-C24	4.17	113.82	104.28
2	C	1101	XA4	C39-N40-C24	3.95	113.31	104.28
2	A	1101	XA4	C05-N19-C20	3.88	122.46	118.45
2	C	1101	XA4	C31-C32-N33	-3.78	106.53	110.80
2	C	1101	XA4	C05-N19-C20	3.76	122.33	118.45
2	D	1101	XA4	C04-C05-N19	-3.61	118.06	122.35
2	B	1101	XA4	C03-C04-C05	3.47	122.86	119.40
2	D	1101	XA4	C18-N17-N15	3.43	107.80	104.23
2	C	1101	XA4	C32-C31-N30	3.39	117.60	110.64
2	A	1101	XA4	C22-C03-C02	-3.32	115.31	119.92
2	B	1101	XA4	C04-C05-N19	-3.25	118.49	122.35
2	A	1101	XA4	C34-N33-C35	-3.20	105.88	110.66
2	D	1101	XA4	C34-N33-C35	-3.15	105.94	110.66
2	B	1101	XA4	C18-N17-N15	3.07	107.43	104.23
2	D	1101	XA4	C04-C03-C02	-3.07	115.67	119.92
2	D	1101	XA4	C34-N33-C32	-3.00	106.18	110.66
2	A	1101	XA4	C35-N33-C32	2.96	113.67	109.52
2	D	1101	XA4	C03-C04-C05	2.96	122.35	119.40
2	C	1101	XA4	C22-C03-C02	-2.90	115.90	119.92
2	D	1101	XA4	C05-N19-C20	2.88	121.43	118.45
2	B	1101	XA4	C04-C03-C02	-2.78	116.07	119.92
2	A	1101	XA4	C32-C31-N30	2.69	116.16	110.64
2	A	1101	XA4	C04-C05-N19	-2.68	119.16	122.35
2	B	1101	XA4	C37-C38-C39	-2.66	117.49	120.84
2	C	1101	XA4	C37-C38-C39	-2.66	117.50	120.84
2	C	1101	XA4	C18-N17-N15	2.59	106.93	104.23
2	C	1101	XA4	C04-C05-N19	-2.57	119.29	122.35
2	B	1101	XA4	C34-N33-C32	-2.57	106.81	110.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1101	XA4	C06-C05-N19	2.50	122.22	116.45
2	B	1101	XA4	C04-C03-C22	-2.49	116.64	119.63
2	C	1101	XA4	C29-N30-C36	-2.46	105.59	111.06
2	B	1101	XA4	C34-N33-C35	-2.43	107.03	110.66
2	C	1101	XA4	C03-C22-C20	2.38	122.88	119.75
2	A	1101	XA4	C03-C22-C20	2.38	122.87	119.75
2	A	1101	XA4	C37-C38-C39	-2.35	117.89	120.84
2	A	1101	XA4	C04-C03-C22	-2.34	116.82	119.63
2	D	1101	XA4	C37-C38-C39	-2.34	117.90	120.84
2	A	1101	XA4	C31-C32-N33	2.33	113.44	110.80
2	C	1101	XA4	C28-C29-N30	-2.23	108.80	113.12
2	B	1101	XA4	C04-C05-C06	-2.21	119.29	122.25
2	A	1101	XA4	C18-N17-N15	2.18	106.50	104.23
2	D	1101	XA4	C31-C32-N33	-2.17	108.35	110.80
2	D	1101	XA4	C06-C05-N19	2.15	121.41	116.45
2	B	1101	XA4	C39-N40-C24	2.14	109.17	104.28
2	D	1101	XA4	C04-C03-C22	-2.10	117.11	119.63
2	A	1101	XA4	C34-N33-C32	-2.09	107.53	110.66
2	B	1101	XA4	C05-N19-C20	2.01	120.52	118.45

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1101	XA4	C13-C12-C14-N25
2	D	1101	XA4	C11-C12-C14-N25
2	D	1101	XA4	C09-C10-C11-C12
2	D	1101	XA4	C10-C09-O08-C07
2	A	1101	XA4	C13-C12-C14-N25
2	A	1101	XA4	C11-C12-C14-N25
2	A	1101	XA4	C03-C02-N23-C24
2	A	1101	XA4	O01-C02-N23-C24
2	C	1101	XA4	C13-C12-C14-N25
2	C	1101	XA4	C03-C02-N23-C24
2	C	1101	XA4	O01-C02-N23-C24
2	C	1101	XA4	C10-C09-O08-C07
2	C	1101	XA4	C28-C29-N30-C36
2	A	1101	XA4	C28-C29-N30-C31
2	A	1101	XA4	C28-C29-N30-C36
2	C	1101	XA4	C28-C29-N30-C31
2	B	1101	XA4	C28-C29-N30-C36
2	B	1101	XA4	O08-C09-C10-C11

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Mol	Chain	Res	Type	Atoms
2	A	1101	XA4	O08-C09-C10-C11
2	B	1101	XA4	N23-C02-C03-C22
2	D	1101	XA4	O08-C09-C10-C11
2	C	1101	XA4	C11-C12-C14-N25
2	B	1101	XA4	C10-C11-C12-C13
2	B	1101	XA4	C28-C29-N30-C31
2	B	1101	XA4	O01-C02-C03-C22
2	D	1101	XA4	C10-C11-C12-C14
2	A	1101	XA4	C10-C11-C12-C14
2	D	1101	XA4	C10-C11-C12-C13
2	A	1101	XA4	C10-C11-C12-C13
2	B	1101	XA4	N23-C02-C03-C04
2	B	1101	XA4	C10-C11-C12-C14
2	B	1101	XA4	C10-C09-O08-C07
2	B	1101	XA4	O01-C02-C03-C04
2	C	1101	XA4	C09-C10-C11-C12
2	A	1101	XA4	C09-C10-C11-C12
2	B	1101	XA4	C09-C10-C11-C12

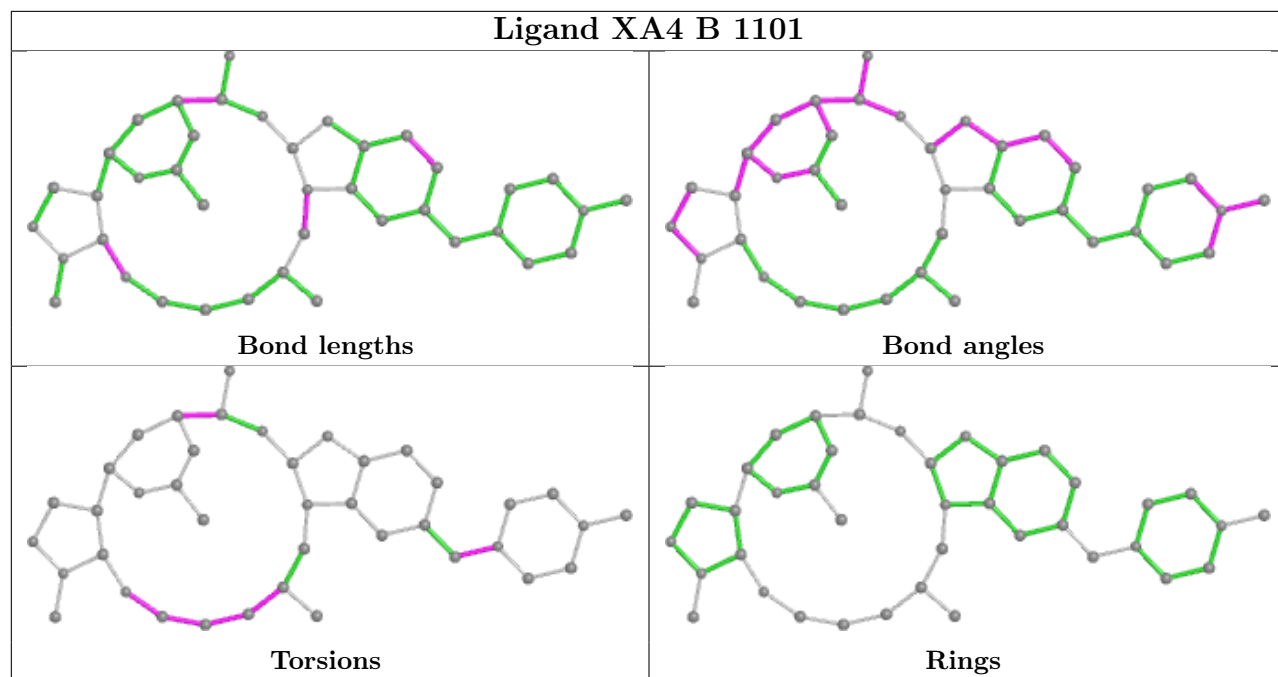
There are no ring outliers.

1 monomer is involved in 2 short contacts:

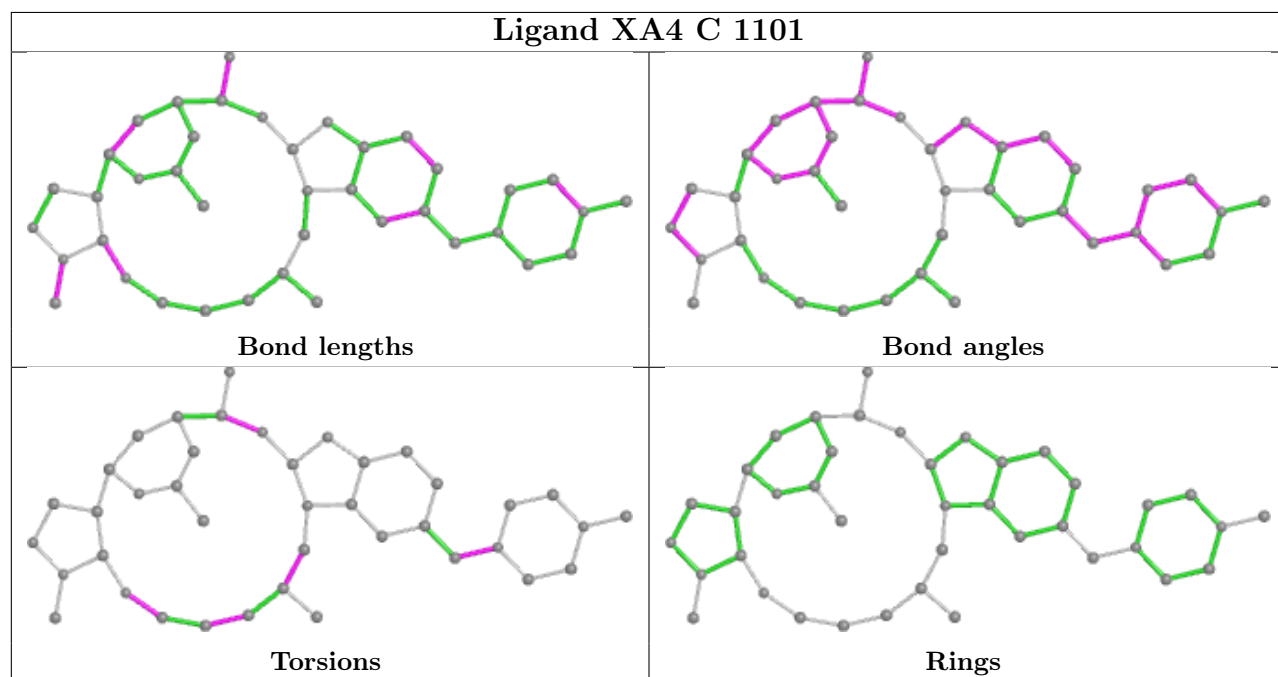
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1101	XA4	2	0

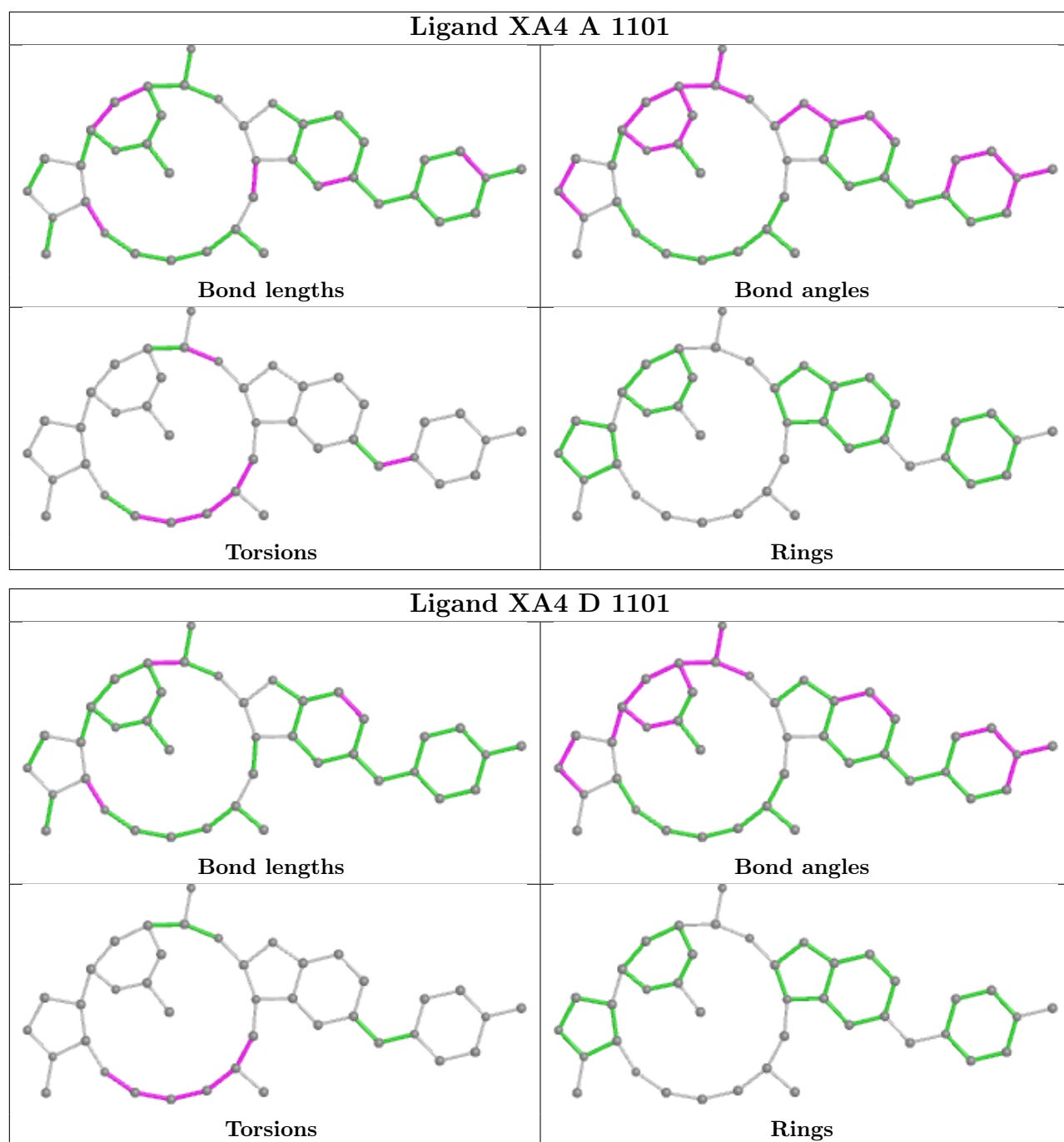
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 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 XA4 B 1101



Ligand XA4 C 1101





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	288/331 (87%)	-0.22	1 (0%) 94 88	22, 40, 65, 86	0
1	B	285/331 (86%)	0.02	0 100 100	32, 55, 78, 101	0
1	C	289/331 (87%)	-0.12	2 (0%) 87 75	26, 46, 79, 97	0
1	D	294/331 (88%)	-0.23	0 100 100	18, 35, 64, 81	0
All	All	1156/1324 (87%)	-0.14	3 (0%) 94 88	18, 44, 73, 101	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	784	SER	3.1
1	C	783	THR	2.5
1	A	858	LEU	2.3

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](#)

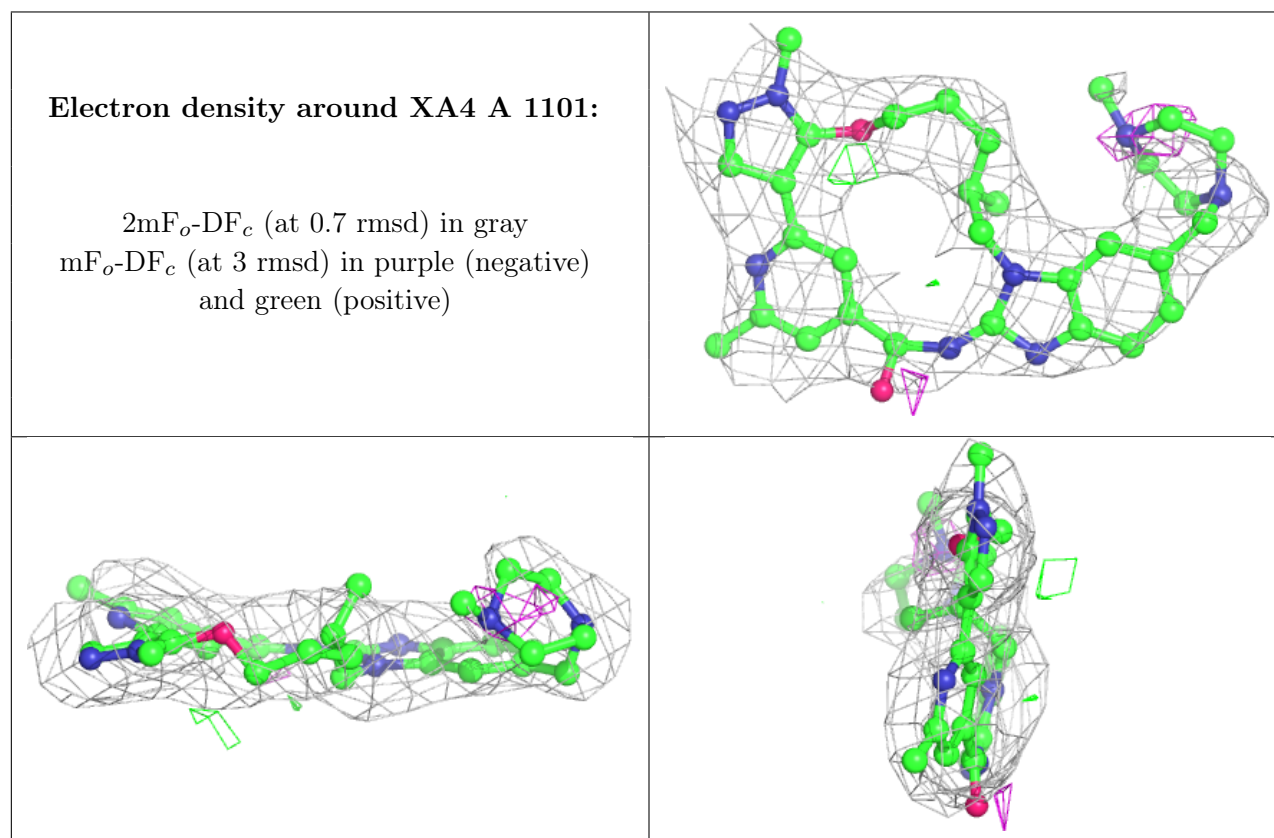
There are no monosaccharides in this entry.

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.

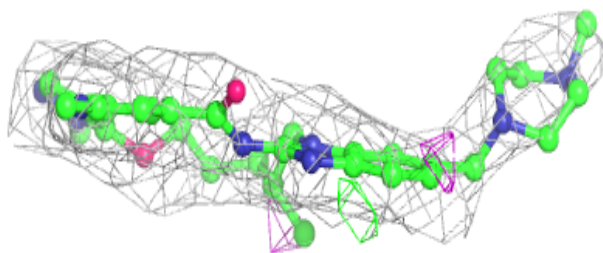
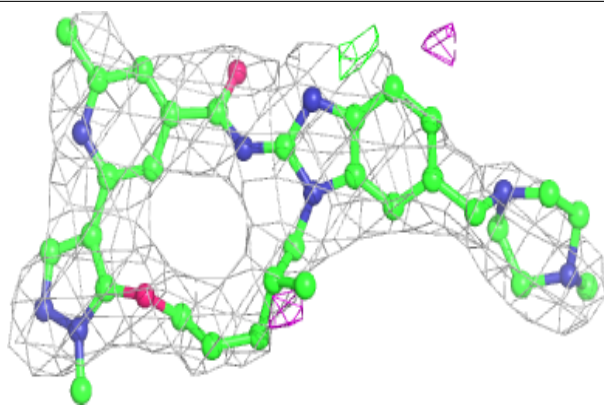
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	XA4	A	1101	40/40	0.88	0.25	23,32,43,45	0
2	XA4	B	1101	40/40	0.89	0.26	29,39,52,59	0
2	XA4	C	1101	40/40	0.90	0.24	32,42,51,57	0
2	XA4	D	1101	40/40	0.92	0.26	25,31,47,48	0

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.

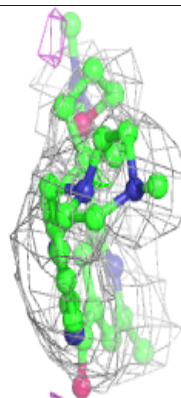
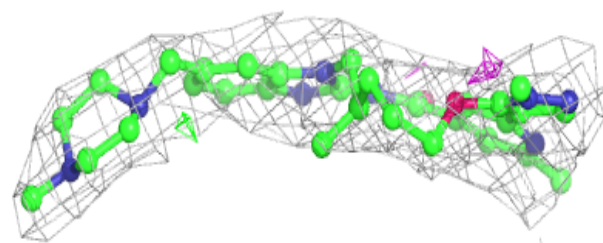
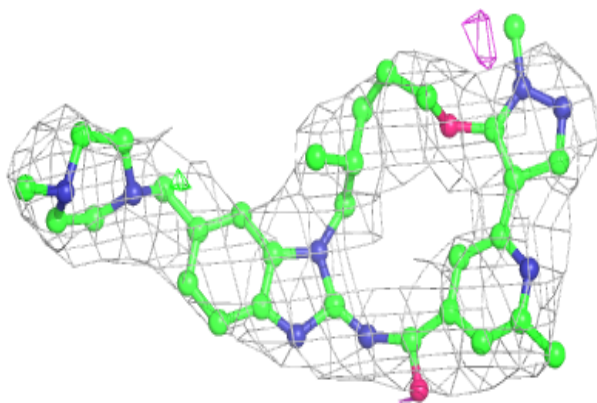


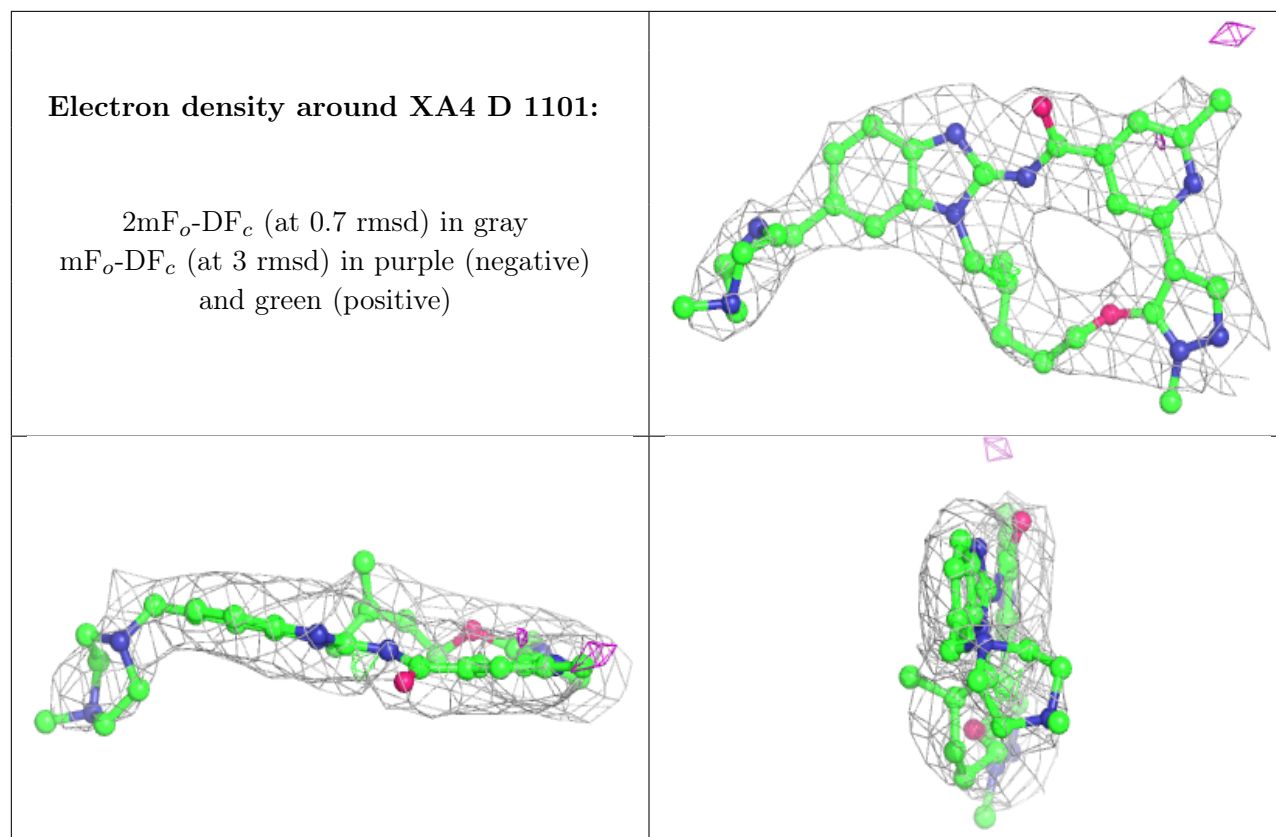
Electron density around XA4 B 1101:

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

**Electron density around XA4 C 1101:**

$2mF_o-DF_c$ (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.