Full wwPDB X-ray Structure Validation Report (i)

Sep 11, 2023 – 04:50 pm BST

PDB ID	:	8PYI
Title	:	Human IGF1R with inhibitor 6
Authors	:	Dreyer, M.K.; Wang, J.; Elkins, J.M.
Deposited on	:	2023-07-25
Resolution	:	3.06 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:

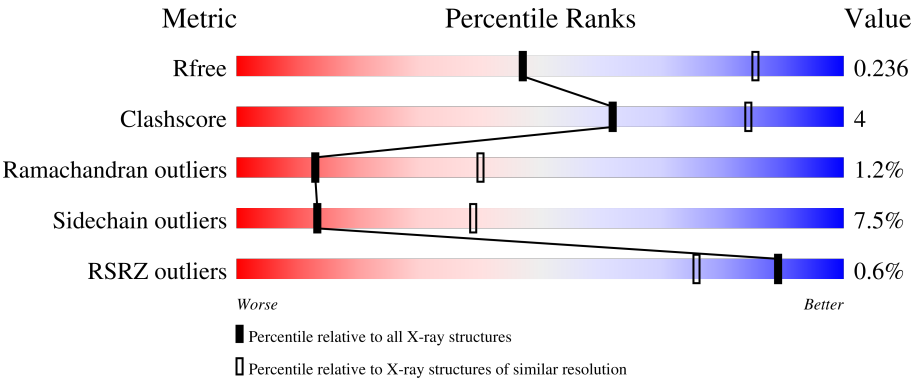
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.06 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	1754 (3.10-3.02)
Clashscore	141614	1864 (3.10-3.02)
Ramachandran outliers	138981	1794 (3.10-3.02)
Sidechain outliers	138945	1793 (3.10-3.02)
RSRZ outliers	127900	1713 (3.10-3.02)

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	AAA	321	73% 15% • 10%
1	BBB	321	75% 12% •• 11%
1	CCC	321	76% 12% • 11%
1	DDD	321	74% 13% • 11%
1	EEE	321	75% 12% • 11%

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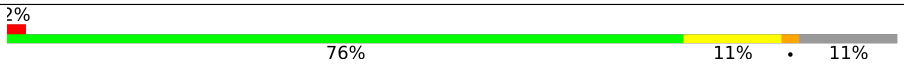
Mol	Chain	Length	Quality of chain
1	FFF	321	
1	GGG	321	
1	HHH	321	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18860 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 Insulin-like growth factor 1 receptor beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	288	Total	C	N	O	S	0	0	0
			2311	1471	384	434	22			
1	BBB	287	Total	C	N	O	S	0	0	0
			2306	1468	383	433	22			
1	CCC	286	Total	C	N	O	S	0	0	0
			2296	1461	379	434	22			
1	DDD	287	Total	C	N	O	S	0	0	0
			2307	1467	383	435	22			
1	EEE	285	Total	C	N	O	S	0	0	0
			2292	1459	378	433	22			
1	FFF	287	Total	C	N	O	S	0	0	0
			2307	1468	384	433	22			
1	GGG	284	Total	C	N	O	S	0	0	0
			2285	1454	377	432	22			
1	HHH	285	Total	C	N	O	S	0	0	0
			2294	1460	381	431	22			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	973	MET	-	initiating methionine	UNP P08069
AAA	1287	ALA	-	expression tag	UNP P08069
AAA	1288	GLU	-	expression tag	UNP P08069
AAA	1289	ASN	-	expression tag	UNP P08069
AAA	1290	LEU	-	expression tag	UNP P08069
AAA	1291	TYR	-	expression tag	UNP P08069
AAA	1292	PHE	-	expression tag	UNP P08069
AAA	1293	GLN	-	expression tag	UNP P08069
BBB	973	MET	-	initiating methionine	UNP P08069
BBB	1287	ALA	-	expression tag	UNP P08069
BBB	1288	GLU	-	expression tag	UNP P08069
BBB	1289	ASN	-	expression tag	UNP P08069
BBB	1290	LEU	-	expression tag	UNP P08069

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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	1291	TYR	-	expression tag	UNP P08069
BBB	1292	PHE	-	expression tag	UNP P08069
BBB	1293	GLN	-	expression tag	UNP P08069
CCC	973	MET	-	initiating methionine	UNP P08069
CCC	1287	ALA	-	expression tag	UNP P08069
CCC	1288	GLU	-	expression tag	UNP P08069
CCC	1289	ASN	-	expression tag	UNP P08069
CCC	1290	LEU	-	expression tag	UNP P08069
CCC	1291	TYR	-	expression tag	UNP P08069
CCC	1292	PHE	-	expression tag	UNP P08069
CCC	1293	GLN	-	expression tag	UNP P08069
DDD	973	MET	-	initiating methionine	UNP P08069
DDD	1287	ALA	-	expression tag	UNP P08069
DDD	1288	GLU	-	expression tag	UNP P08069
DDD	1289	ASN	-	expression tag	UNP P08069
DDD	1290	LEU	-	expression tag	UNP P08069
DDD	1291	TYR	-	expression tag	UNP P08069
DDD	1292	PHE	-	expression tag	UNP P08069
DDD	1293	GLN	-	expression tag	UNP P08069
EEE	973	MET	-	initiating methionine	UNP P08069
EEE	1287	ALA	-	expression tag	UNP P08069
EEE	1288	GLU	-	expression tag	UNP P08069
EEE	1289	ASN	-	expression tag	UNP P08069
EEE	1290	LEU	-	expression tag	UNP P08069
EEE	1291	TYR	-	expression tag	UNP P08069
EEE	1292	PHE	-	expression tag	UNP P08069
EEE	1293	GLN	-	expression tag	UNP P08069
FFF	973	MET	-	initiating methionine	UNP P08069
FFF	1287	ALA	-	expression tag	UNP P08069
FFF	1288	GLU	-	expression tag	UNP P08069
FFF	1289	ASN	-	expression tag	UNP P08069
FFF	1290	LEU	-	expression tag	UNP P08069
FFF	1291	TYR	-	expression tag	UNP P08069
FFF	1292	PHE	-	expression tag	UNP P08069
FFF	1293	GLN	-	expression tag	UNP P08069
GGG	973	MET	-	initiating methionine	UNP P08069
GGG	1287	ALA	-	expression tag	UNP P08069
GGG	1288	GLU	-	expression tag	UNP P08069
GGG	1289	ASN	-	expression tag	UNP P08069
GGG	1290	LEU	-	expression tag	UNP P08069
GGG	1291	TYR	-	expression tag	UNP P08069
GGG	1292	PHE	-	expression tag	UNP P08069

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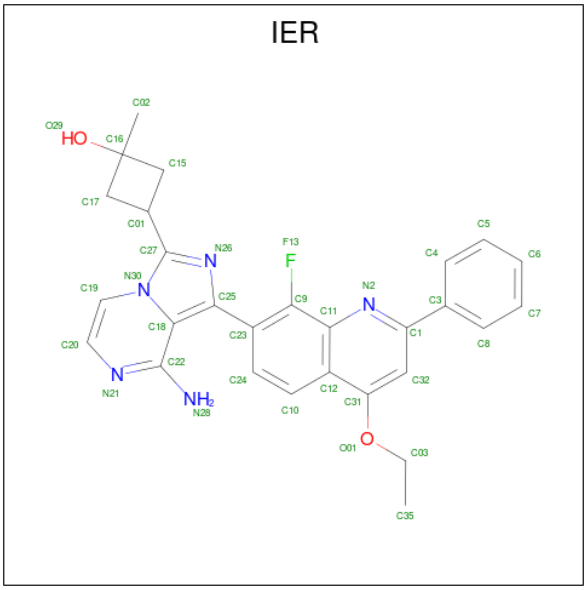
Chain	Residue	Modelled	Actual	Comment	Reference
GGG	1293	GLN	-	expression tag	UNP P08069
HHH	973	MET	-	initiating methionine	UNP P08069
HHH	1287	ALA	-	expression tag	UNP P08069
HHH	1288	GLU	-	expression tag	UNP P08069
HHH	1289	ASN	-	expression tag	UNP P08069
HHH	1290	LEU	-	expression tag	UNP P08069
HHH	1291	TYR	-	expression tag	UNP P08069
HHH	1292	PHE	-	expression tag	UNP P08069
HHH	1293	GLN	-	expression tag	UNP P08069

- Molecule 2 is 3-[8-azanyl-1-(4-ethoxy-8-fluoranyl-2-phenyl-quinolin-7-yl)imidazo[1,5-a]pyrazin-3-yl]-1-methyl-cyclobutan-1-ol (three-letter code: IER) (formula: $C_{28}H_{26}FN_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	AAA	1	Total	C	F	N	O	0	0
			36	28	1	5	2		
2	BBB	1	Total	C	F	N	O	0	0
			36	28	1	5	2		
2	CCC	1	Total	C	F	N	O	0	0
			36	28	1	5	2		
2	DDD	1	Total	C	F	N	O	0	0
			36	28	1	5	2		
2	EEE	1	Total	C	F	N	O	0	0
			36	28	1	5	2		
2	FFF	1	Total	C	F	N	O	0	0
			36	28	1	5	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	GGG	1	Total	C	F	N	O	0	0
			36	28	1	5	2		
2	HHH	1	Total	C	F	N	O	0	0
			36	28	1	5	2		

- Molecule 3 is water.

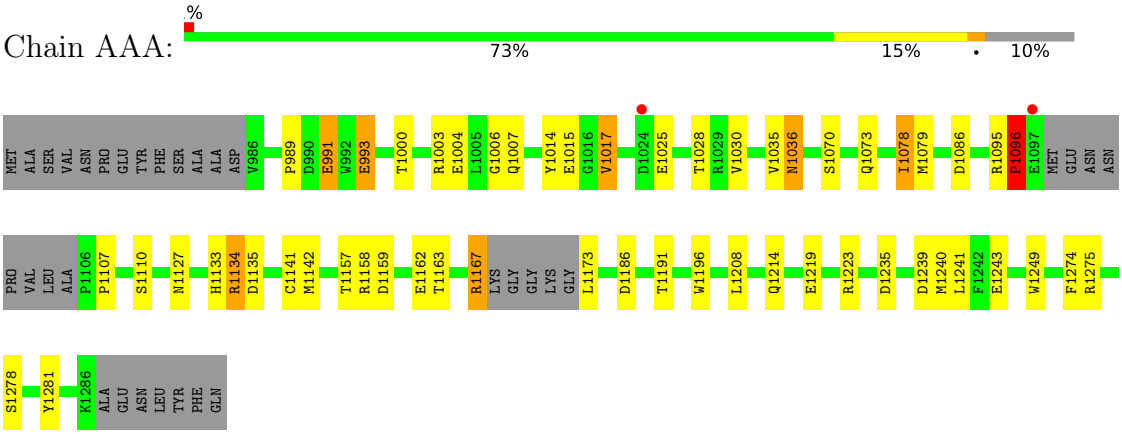
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	19	Total	O	0	0
			19	19		
3	BBB	27	Total	O	0	0
			27	27		
3	CCC	24	Total	O	0	0
			24	24		
3	DDD	27	Total	O	0	0
			27	27		
3	EEE	19	Total	O	0	0
			19	19		
3	FFF	21	Total	O	0	0
			21	21		
3	GGG	24	Total	O	0	0
			24	24		
3	HHH	13	Total	O	0	0
			13	13		

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.

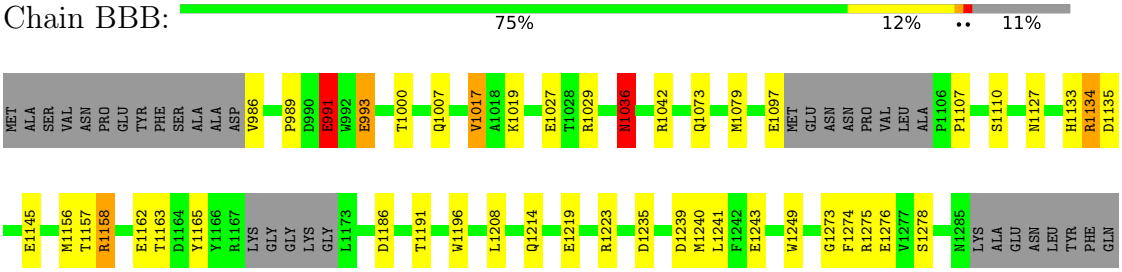
• Molecule 1: Insulin-like growth factor 1 receptor beta chain

Chain AAA:



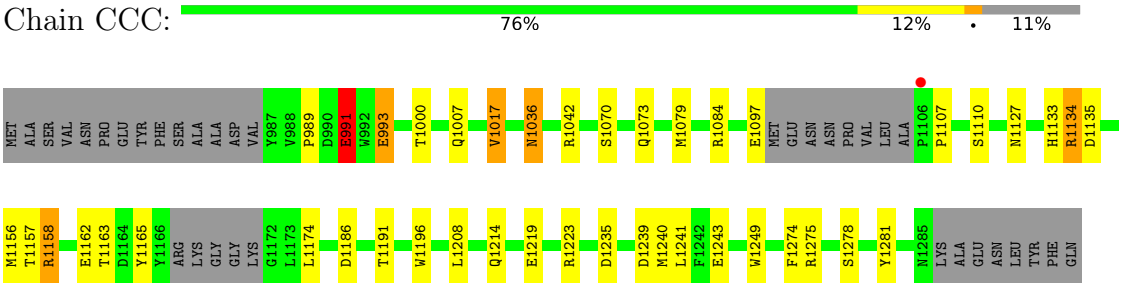
• Molecule 1: Insulin-like growth factor 1 receptor beta chain

Chain BBB:



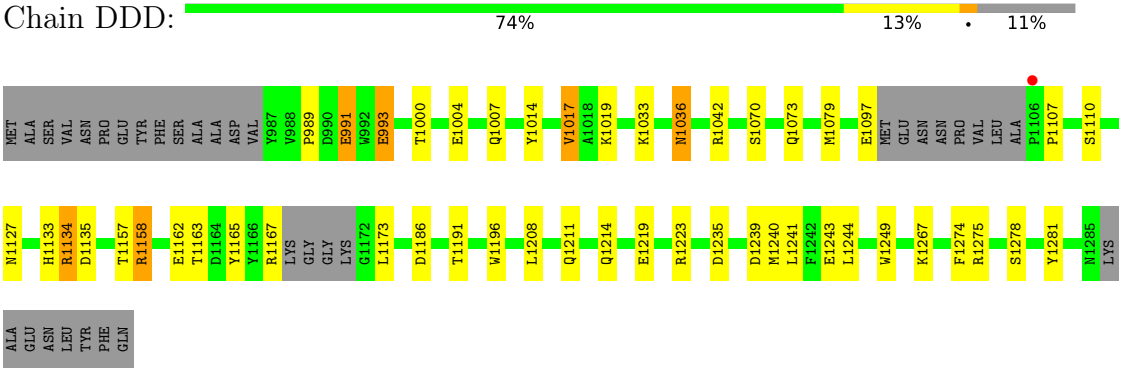
• Molecule 1: Insulin-like growth factor 1 receptor beta chain

Chain CCC:



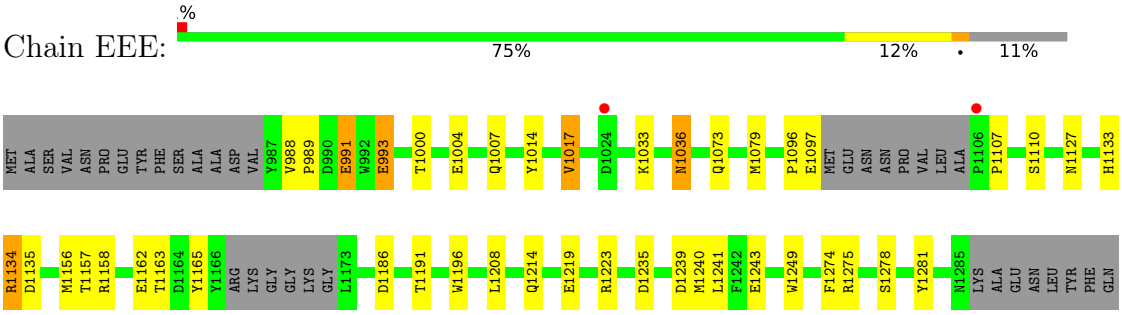
• Molecule 1: Insulin-like growth factor 1 receptor beta chain

Chain DDD:



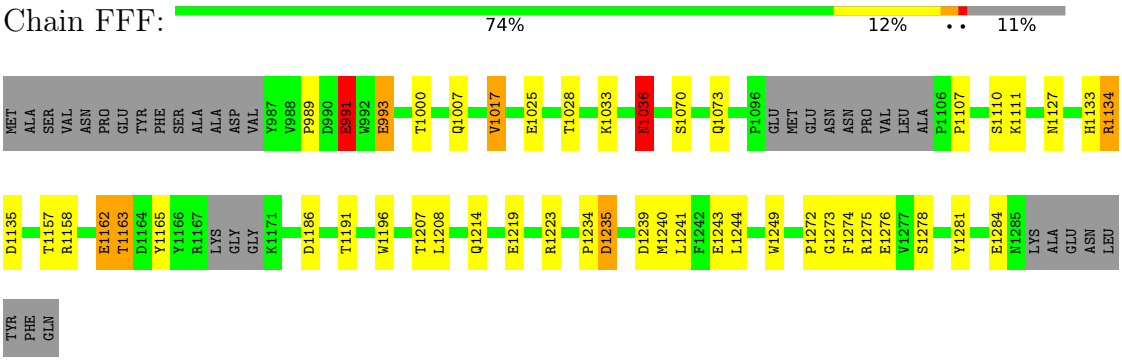
• Molecule 1: Insulin-like growth factor 1 receptor beta chain

Chain EEE:



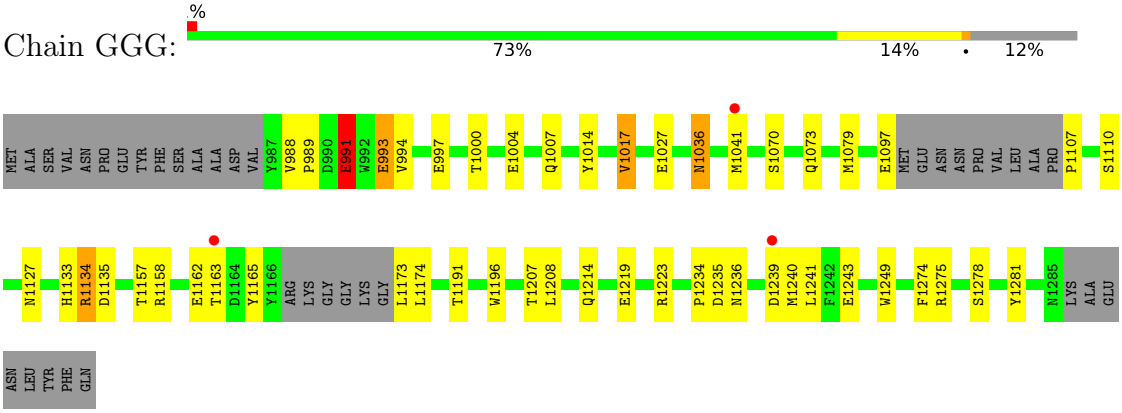
• Molecule 1: Insulin-like growth factor 1 receptor beta chain

Chain FFF:



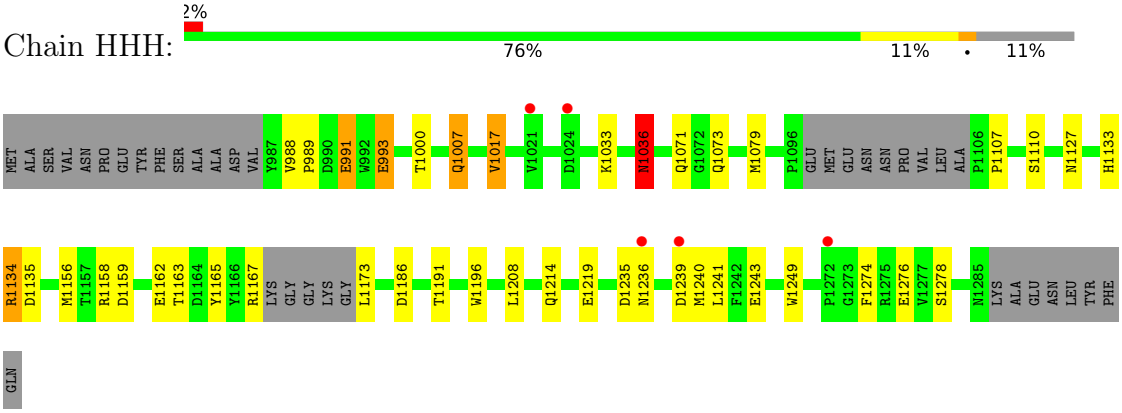
• Molecule 1: Insulin-like growth factor 1 receptor beta chain

Chain GGG:



• Molecule 1: Insulin-like growth factor 1 receptor beta chain

Chain HHH:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	128.59Å 103.95Å 191.82Å 90.00° 100.17° 90.00°	Depositor
Resolution (Å)	63.47 – 3.06 63.47 – 3.06	Depositor EDS
% Data completeness (in resolution range)	99.6 (63.47-3.06) 99.6 (63.47-3.06)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.38 (at 3.07Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.235 0.195 , 0.236	Depositor DCC
R_{free} test set	2372 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	52.3	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 65.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	18860	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IER

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	AAA	0.66	0/2360	0.82	3/3183 (0.1%)
1	BBB	0.67	0/2355	0.79	1/3177 (0.0%)
1	CCC	0.66	0/2345	0.79	1/3163 (0.0%)
1	DDD	0.65	0/2356	0.78	2/3177 (0.1%)
1	EEE	0.66	0/2341	0.79	3/3158 (0.1%)
1	FFF	0.66	0/2356	0.82	3/3176 (0.1%)
1	GGG	0.66	0/2333	0.79	0/3146
1	HHH	0.65	0/2343	0.78	0/3160
All	All	0.66	0/18789	0.80	13/25340 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	EEE	0	1

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	FFF	1158	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	EEE	1158	ARG	NE-CZ-NH1	7.53	124.06	120.30
1	FFF	1158	ARG	CG-CD-NE	-7.48	96.10	111.80
1	AAA	1158	ARG	CG-CD-NE	-7.35	96.36	111.80
1	EEE	1158	ARG	CG-CD-NE	-7.23	96.61	111.80
1	AAA	1158	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	FFF	1158	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	EEE	1158	ARG	NE-CZ-NH2	-6.33	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	1158	ARG	NE-CZ-NH1	-6.18	117.21	120.30
1	CCC	1158	ARG	NE-CZ-NH1	-5.83	117.39	120.30
1	AAA	1158	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	DDD	1158	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	DDD	1158	ARG	NE-CZ-NH2	5.08	122.84	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	EEE	1096	PRO	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	AAA	2311	0	2263	26	0
1	BBB	2306	0	2264	22	3
1	CCC	2296	0	2249	21	1
1	DDD	2307	0	2262	25	0
1	EEE	2292	0	2246	19	0
1	FFF	2307	0	2269	25	3
1	GGG	2285	0	2239	23	5
1	HHH	2294	0	2253	20	5
2	AAA	36	0	0	0	0
2	BBB	36	0	0	0	0
2	CCC	36	0	0	0	0
2	DDD	36	0	0	1	0
2	EEE	36	0	0	1	0
2	FFF	36	0	0	1	0
2	GGG	36	0	0	0	0
2	HHH	36	0	0	1	0
3	AAA	19	0	0	0	0
3	BBB	27	0	0	3	0
3	CCC	24	0	0	2	0
3	DDD	27	0	0	3	1
3	EEE	19	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	FFF	21	0	0	1	0
3	GGG	24	0	0	1	0
3	HHH	13	0	0	3	0
All	All	18860	0	18045	163	10

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 (163) 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:CCC:1127:ASN:HB3	3:CCC:3114:HOH:O	1.07	1.22
1:DDD:1211:GLN:HG3	3:HHH:3110:HOH:O	1.85	0.77
1:AAA:1141:CYS:O	1:AAA:1142:MET:HE2	1.89	0.72
1:AAA:1086:ASP:HA	1:AAA:1142:MET:HE2	1.70	0.72
1:AAA:1006:GLY:HA2	1:BBB:986:VAL:HB	1.72	0.71
1:GGG:994:VAL:O	3:GGG:3101:HOH:O	2.08	0.71
1:GGG:1036:ASN:HD22	1:GGG:1036:ASN:N	1.94	0.66
1:EEE:1036:ASN:N	1:EEE:1036:ASN:HD22	1.94	0.66
1:AAA:1036:ASN:N	1:AAA:1036:ASN:HD22	1.94	0.66
1:FFF:1036:ASN:HD22	1:FFF:1036:ASN:N	1.94	0.65
1:HHH:1036:ASN:HD22	1:HHH:1036:ASN:N	1.95	0.65
1:DDD:1275:ARG:HG3	3:DDD:3112:HOH:O	1.96	0.65
1:FFF:1284:GLU:OE2	3:FFF:3101:HOH:O	2.15	0.65
1:CCC:1036:ASN:HD22	1:CCC:1036:ASN:N	1.94	0.65
1:DDD:1036:ASN:HD22	1:DDD:1036:ASN:N	1.94	0.64
1:BBB:1156:MET:HG2	1:CCC:1165:TYR:CZ	2.34	0.63
1:AAA:1030:VAL:HG11	1:AAA:1078:ILE:HD12	1.80	0.62
1:BBB:1107:PRO:HD3	1:BBB:1208:LEU:HD21	1.81	0.62
1:AAA:1003:ARG:NH1	1:AAA:1015:GLU:OE1	2.32	0.62
1:BBB:1036:ASN:HD22	1:BBB:1036:ASN:N	1.96	0.62
1:AAA:1223:ARG:NH2	1:BBB:1186:ASP:OD1	2.32	0.62
1:BBB:1223:ARG:NH2	1:CCC:1186:ASP:OD1	2.34	0.61
1:CCC:1107:PRO:HD3	1:CCC:1208:LEU:HD21	1.83	0.60
1:BBB:1042:ARG:NE	3:BBB:3103:HOH:O	2.33	0.60
1:DDD:1042:ARG:HD3	3:DDD:3114:HOH:O	2.02	0.59
1:EEE:1107:PRO:HD3	1:EEE:1208:LEU:HD21	1.83	0.59
1:CCC:1042:ARG:NE	3:CCC:3102:HOH:O	2.35	0.58
1:GGG:1000:THR:HB	1:GGG:1017:VAL:HG12	1.86	0.58
1:DDD:1036:ASN:HD22	1:DDD:1036:ASN:H	1.52	0.57
1:HHH:1071:GLN:OE1	3:HHH:3101:HOH:O	2.18	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:GGG:1133:HIS:O	1:GGG:1134:ARG:HB2	2.05	0.57
1:AAA:1036:ASN:HD22	1:AAA:1036:ASN:H	1.52	0.57
1:DDD:1133:HIS:O	1:DDD:1134:ARG:HB2	2.05	0.56
1:GGG:1107:PRO:HD3	1:GGG:1208:LEU:HD21	1.86	0.56
1:HHH:1133:HIS:O	1:HHH:1134:ARG:HB2	2.05	0.56
1:BBB:1133:HIS:O	1:BBB:1134:ARG:HB2	2.05	0.56
1:CCC:1133:HIS:O	1:CCC:1134:ARG:HB2	2.04	0.56
1:FFF:1000:THR:HB	1:FFF:1017:VAL:HG12	1.87	0.56
1:EEE:1036:ASN:HD22	1:EEE:1036:ASN:H	1.53	0.56
1:FFF:1036:ASN:HD22	1:FFF:1036:ASN:H	1.54	0.56
1:AAA:1133:HIS:O	1:AAA:1134:ARG:HB2	2.06	0.56
1:CCC:1036:ASN:HD22	1:CCC:1036:ASN:H	1.52	0.56
1:HHH:1071:GLN:HG3	3:HHH:3101:HOH:O	2.04	0.56
1:EEE:1133:HIS:O	1:EEE:1134:ARG:HB2	2.06	0.55
1:AAA:1107:PRO:HD3	1:AAA:1208:LEU:HD21	1.89	0.55
1:AAA:1000:THR:HB	1:AAA:1017:VAL:HG12	1.88	0.55
1:AAA:1030:VAL:HG11	1:AAA:1078:ILE:CD1	2.37	0.55
1:FFF:1133:HIS:O	1:FFF:1134:ARG:HB2	2.06	0.54
1:GGG:1036:ASN:HD22	1:GGG:1036:ASN:H	1.53	0.54
1:HHH:1107:PRO:HD3	1:HHH:1208:LEU:HD21	1.88	0.54
1:AAA:1186:ASP:OD1	1:FFF:1223:ARG:NH2	2.40	0.53
1:EEE:1000:THR:HB	1:EEE:1017:VAL:HG12	1.91	0.53
1:CCC:1223:ARG:NH2	1:FFF:1186:ASP:OD1	2.41	0.53
1:BBB:1000:THR:HB	1:BBB:1017:VAL:HG12	1.91	0.53
1:HHH:1036:ASN:HD22	1:HHH:1036:ASN:H	1.56	0.53
1:HHH:1000:THR:HB	1:HHH:1017:VAL:HG12	1.90	0.52
1:FFF:1107:PRO:HD3	1:FFF:1208:LEU:HD21	1.91	0.52
1:EEE:1186:ASP:OD1	1:GGG:1223:ARG:NH2	2.43	0.52
1:DDD:1000:THR:HB	1:DDD:1017:VAL:HG12	1.91	0.52
1:GGG:1041:MET:HB3	1:HHH:1007:GLN:HE22	1.76	0.51
1:DDD:993:GLU:OE1	1:DDD:1070:SER:OG	2.23	0.50
1:DDD:1107:PRO:HD3	1:DDD:1208:LEU:HD21	1.94	0.50
1:CCC:1000:THR:HB	1:CCC:1017:VAL:HG12	1.93	0.49
1:EEE:1165:TYR:HB3	1:GGG:1173:LEU:HG	1.95	0.49
1:CCC:1156:MET:HG2	1:FFF:1165:TYR:CZ	2.49	0.48
1:DDD:1033:LYS:NZ	2:DDD:3000:IER:N2	2.62	0.48
1:FFF:1273:GLY:O	1:FFF:1276:GLU:HG3	2.14	0.48
1:BBB:1274:PHE:O	1:BBB:1278:SER:HB3	2.14	0.47
1:BBB:1029:ARG:HG2	3:BBB:3111:HOH:O	2.14	0.47
1:GGG:991:GLU:H	1:GGG:991:GLU:HG3	1.57	0.47
1:BBB:1036:ASN:HD22	1:BBB:1036:ASN:H	1.59	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EEE:989:PRO:HB3	1:EEE:993:GLU:HG3	1.97	0.46
1:CCC:993:GLU:OE1	1:CCC:1070:SER:OG	2.24	0.46
1:FFF:1274:PHE:O	1:FFF:1278:SER:HB3	2.16	0.46
1:DDD:989:PRO:HB3	1:DDD:993:GLU:HG3	1.97	0.46
1:BBB:1145:GLU:HB2	3:BBB:3124:HOH:O	2.16	0.45
1:AAA:1159:ASP:OD2	1:AAA:1167:ARG:HD3	2.17	0.45
1:CCC:1274:PHE:O	1:CCC:1278:SER:HB3	2.16	0.45
1:DDD:1186:ASP:OD1	1:EEE:1223:ARG:NH2	2.49	0.45
1:FFF:1033:LYS:NZ	2:FFF:3000:IER:N2	2.65	0.45
1:HHH:1033:LYS:NZ	2:HHH:3000:IER:N2	2.65	0.45
1:GGG:989:PRO:HB3	1:GGG:993:GLU:HG3	1.99	0.45
1:HHH:1274:PHE:O	1:HHH:1278:SER:HB3	2.15	0.45
1:CCC:1127:ASN:ND2	1:CCC:1191:THR:HB	2.32	0.45
1:EEE:1274:PHE:O	1:EEE:1278:SER:HB3	2.17	0.45
1:DDD:1274:PHE:O	1:DDD:1278:SER:HB3	2.17	0.44
1:AAA:989:PRO:HB3	1:AAA:993:GLU:HG3	1.98	0.44
1:AAA:1274:PHE:O	1:AAA:1278:SER:HB3	2.17	0.44
1:GGG:993:GLU:OE1	1:GGG:1070:SER:OG	2.24	0.44
1:AAA:993:GLU:OE2	1:AAA:1070:SER:OG	2.25	0.44
1:BBB:1127:ASN:ND2	1:BBB:1191:THR:HB	2.33	0.44
1:GGG:1274:PHE:O	1:GGG:1278:SER:HB3	2.17	0.44
1:BBB:989:PRO:HB3	1:BBB:993:GLU:HG3	1.99	0.44
1:BBB:991:GLU:H	1:BBB:991:GLU:HG3	1.57	0.44
1:CCC:989:PRO:HB3	1:CCC:993:GLU:HG3	2.00	0.44
1:DDD:1267:LYS:HD2	3:DDD:3113:HOH:O	2.17	0.43
1:EEE:1196:TRP:CE3	1:EEE:1249:TRP:HA	2.53	0.43
1:FFF:1196:TRP:CE3	1:FFF:1249:TRP:HA	2.54	0.43
1:GGG:1127:ASN:ND2	1:GGG:1191:THR:HB	2.33	0.43
1:CCC:1036:ASN:N	1:CCC:1036:ASN:ND2	2.65	0.43
1:FFF:1162:GLU:O	1:FFF:1163:THR:OG1	2.35	0.43
1:CCC:1196:TRP:CE3	1:CCC:1249:TRP:HA	2.54	0.43
1:EEE:1033:LYS:NZ	2:EEE:3000:IER:N2	2.66	0.43
1:DDD:1036:ASN:N	1:DDD:1036:ASN:ND2	2.65	0.43
1:FFF:1244:LEU:HD12	1:FFF:1244:LEU:HA	1.91	0.43
1:HHH:1196:TRP:CE3	1:HHH:1249:TRP:HA	2.53	0.43
1:CCC:1135:ASP:HB2	1:CCC:1157:THR:CG2	2.48	0.43
1:DDD:1127:ASN:ND2	1:DDD:1191:THR:HB	2.34	0.43
1:HHH:989:PRO:HB3	1:HHH:993:GLU:HG3	2.00	0.43
1:CCC:1135:ASP:HB2	1:CCC:1157:THR:HG23	2.01	0.43
1:FFF:1127:ASN:ND2	1:FFF:1191:THR:HB	2.34	0.43
1:FFF:989:PRO:HB3	1:FFF:993:GLU:HG3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:1135:ASP:HB2	1:BBB:1157:THR:CG2	2.49	0.43
1:EEE:1036:ASN:N	1:EEE:1036:ASN:ND2	2.65	0.42
1:GGG:1196:TRP:CE3	1:GGG:1249:TRP:HA	2.54	0.42
1:HHH:1127:ASN:ND2	1:HHH:1191:THR:HB	2.34	0.42
1:AAA:1127:ASN:ND2	1:AAA:1191:THR:HB	2.34	0.42
1:BBB:1196:TRP:CE3	1:BBB:1249:TRP:HA	2.54	0.42
1:DDD:1196:TRP:CE3	1:DDD:1249:TRP:HA	2.54	0.42
1:GGG:1004:GLU:HG2	1:GGG:1014:TYR:CE1	2.54	0.42
1:DDD:1004:GLU:HG2	1:DDD:1014:TYR:CE1	2.54	0.42
1:GGG:1165:TYR:HB3	1:HHH:1173:LEU:HG	2.00	0.42
1:DDD:1223:ARG:NH2	1:HHH:1186:ASP:OD1	2.48	0.42
1:HHH:1036:ASN:N	1:HHH:1036:ASN:ND2	2.66	0.42
1:AAA:1196:TRP:CE3	1:AAA:1249:TRP:HA	2.55	0.42
1:BBB:1135:ASP:HB2	1:BBB:1157:THR:HG23	2.02	0.42
1:DDD:1135:ASP:OD2	1:HHH:1165:TYR:OH	2.26	0.42
1:FFF:991:GLU:H	1:FFF:991:GLU:HG3	1.55	0.42
1:GGG:1135:ASP:HB2	1:GGG:1157:THR:CG2	2.50	0.42
1:GGG:1207:THR:HG22	1:GGG:1234:PRO:HB3	2.02	0.42
1:EEE:1127:ASN:ND2	1:EEE:1191:THR:HB	2.35	0.41
1:GGG:1036:ASN:N	1:GGG:1036:ASN:ND2	2.65	0.41
1:GGG:1275:ARG:HA	1:GGG:1281:TYR:CD2	2.55	0.41
1:FFF:1025:GLU:OE2	1:FFF:1028:THR:HG23	2.20	0.41
1:DDD:1165:TYR:CZ	1:EEE:1156:MET:HG2	2.54	0.41
1:AAA:1095:ARG:O	1:AAA:1096:PRO:C	2.58	0.41
1:CCC:1275:ARG:HA	1:CCC:1281:TYR:CD2	2.55	0.41
1:AAA:1173:LEU:HG	1:BBB:1165:TYR:HB3	2.03	0.41
1:DDD:1135:ASP:HB2	1:DDD:1157:THR:CG2	2.51	0.41
1:DDD:1275:ARG:HA	1:DDD:1281:TYR:CD2	2.56	0.41
1:AAA:1036:ASN:N	1:AAA:1036:ASN:ND2	2.66	0.41
1:EEE:1135:ASP:HB2	1:EEE:1157:THR:HG23	2.03	0.41
1:HHH:1159:ASP:CG	1:HHH:1167:ARG:HH12	2.24	0.41
1:AAA:1025:GLU:OE2	1:AAA:1028:THR:HG23	2.21	0.41
1:DDD:1244:LEU:HD12	1:DDD:1244:LEU:HA	1.92	0.41
1:EEE:1275:ARG:HA	1:EEE:1281:TYR:CD2	2.56	0.41
1:FFF:1036:ASN:N	1:FFF:1036:ASN:ND2	2.65	0.41
1:FFF:1135:ASP:HB2	1:FFF:1157:THR:CG2	2.51	0.41
1:AAA:1004:GLU:HG2	1:AAA:1014:TYR:CE1	2.55	0.40
1:AAA:1135:ASP:HB2	1:AAA:1157:THR:HG23	2.03	0.40
1:EEE:1135:ASP:HB2	1:EEE:1157:THR:CG2	2.51	0.40
1:AAA:1275:ARG:HA	1:AAA:1281:TYR:CD2	2.55	0.40
1:FFF:1135:ASP:HB2	1:FFF:1157:THR:HG23	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:991:GLU:H	1:CCC:991:GLU:HG3	1.56	0.40
1:FFF:993:GLU:OE1	1:FFF:1070:SER:OG	2.24	0.40
1:FFF:1207:THR:HG22	1:FFF:1234:PRO:HB3	2.03	0.40
1:GGG:1165:TYR:OH	1:HHH:1135:ASP:OD2	2.27	0.40
1:EEE:1004:GLU:HG2	1:EEE:1014:TYR:CE1	2.55	0.40
1:BBB:1036:ASN:N	1:BBB:1036:ASN:ND2	2.67	0.40
1:BBB:1273:GLY:O	1:BBB:1276:GLU:HG3	2.22	0.40
1:DDD:1135:ASP:HB2	1:DDD:1157:THR:HG23	2.03	0.40
1:FFF:1275:ARG:HA	1:FFF:1281:TYR:CD2	2.57	0.40
1:GGG:1165:TYR:CZ	1:HHH:1156:MET:HG2	2.56	0.40

All (10) 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)
1:GGG:1236:ASN:OD1	1:HHH:1276:GLU:O[3_455]	1.35	0.85
1:GGG:1236:ASN:CG	1:HHH:1276:GLU:O[3_455]	1.62	0.58
1:BBB:1275:ARG:NH1	1:FFF:1272:PRO:CB[1_565]	1.76	0.44
1:GGG:1236:ASN:CB	1:HHH:1276:GLU:O[3_455]	1.77	0.43
1:GGG:1027:GLU:OE2	1:GGG:1027:GLU:OE2[2_656]	1.82	0.38
1:FFF:1235:ASP:O	1:HHH:1236:ASN:ND2[3_445]	2.01	0.19
1:GGG:1236:ASN:CA	1:HHH:1276:GLU:O[3_455]	2.13	0.07
1:BBB:1275:ARG:CZ	1:FFF:1272:PRO:CB[1_565]	2.14	0.06
1:BBB:1027:GLU:O	1:CCC:1084:ARG:NH2[4_555]	2.15	0.05
3:DDD:3120:HOH:O	3:DDD:3120:HOH:O[2_656]	2.16	0.04

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	AAA	282/321 (88%)	267 (95%)	11 (4%)	4 (1%)	11 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	BBB	281/321 (88%)	269 (96%)	8 (3%)	4 (1%)	11	36
1	CCC	280/321 (87%)	266 (95%)	11 (4%)	3 (1%)	14	42
1	DDD	281/321 (88%)	268 (95%)	10 (4%)	3 (1%)	14	42
1	EEE	279/321 (87%)	266 (95%)	10 (4%)	3 (1%)	14	42
1	FFF	281/321 (88%)	268 (95%)	9 (3%)	4 (1%)	11	36
1	GGG	278/321 (87%)	266 (96%)	9 (3%)	3 (1%)	14	42
1	HHH	279/321 (87%)	267 (96%)	8 (3%)	4 (1%)	11	36
All	All	2241/2568 (87%)	2137 (95%)	76 (3%)	28 (1%)	13	40

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	AAA	1096	PRO
1	AAA	1162	GLU
1	AAA	1163	THR
1	BBB	1162	GLU
1	BBB	1163	THR
1	CCC	1162	GLU
1	CCC	1163	THR
1	DDD	1162	GLU
1	DDD	1163	THR
1	EEE	1162	GLU
1	EEE	1163	THR
1	FFF	1162	GLU
1	FFF	1163	THR
1	GGG	1162	GLU
1	GGG	1163	THR
1	HHH	1162	GLU
1	HHH	1163	THR
1	AAA	991	GLU
1	BBB	991	GLU
1	CCC	991	GLU
1	EEE	991	GLU
1	FFF	991	GLU
1	GGG	991	GLU
1	HHH	991	GLU
1	BBB	1036	ASN
1	DDD	991	GLU
1	FFF	1036	ASN
1	HHH	1036	ASN

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	AAA	252/280 (90%)	232 (92%)	20 (8%)	12	36
1	BBB	253/280 (90%)	234 (92%)	19 (8%)	13	39
1	CCC	252/280 (90%)	233 (92%)	19 (8%)	13	39
1	DDD	253/280 (90%)	232 (92%)	21 (8%)	11	35
1	EEE	252/280 (90%)	234 (93%)	18 (7%)	14	41
1	FFF	253/280 (90%)	237 (94%)	16 (6%)	18	45
1	GGG	251/280 (90%)	230 (92%)	21 (8%)	11	34
1	HHH	252/280 (90%)	234 (93%)	18 (7%)	14	41
All	All	2018/2240 (90%)	1866 (92%)	152 (8%)	13	39

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	991	GLU
1	AAA	993	GLU
1	AAA	1007	GLN
1	AAA	1017	VAL
1	AAA	1035	VAL
1	AAA	1036	ASN
1	AAA	1073	GLN
1	AAA	1078	ILE
1	AAA	1079	MET
1	AAA	1096	PRO
1	AAA	1110	SER
1	AAA	1134	ARG
1	AAA	1167	ARG
1	AAA	1214	GLN
1	AAA	1219	GLU
1	AAA	1235	ASP
1	AAA	1239	ASP
1	AAA	1240	MET
1	AAA	1241	LEU

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Mol	Chain	Res	Type
1	AAA	1243	GLU
1	BBB	991	GLU
1	BBB	993	GLU
1	BBB	1007	GLN
1	BBB	1017	VAL
1	BBB	1019	LYS
1	BBB	1036	ASN
1	BBB	1073	GLN
1	BBB	1079	MET
1	BBB	1097	GLU
1	BBB	1110	SER
1	BBB	1134	ARG
1	BBB	1158	ARG
1	BBB	1214	GLN
1	BBB	1219	GLU
1	BBB	1235	ASP
1	BBB	1239	ASP
1	BBB	1240	MET
1	BBB	1241	LEU
1	BBB	1243	GLU
1	CCC	991	GLU
1	CCC	993	GLU
1	CCC	1007	GLN
1	CCC	1017	VAL
1	CCC	1036	ASN
1	CCC	1073	GLN
1	CCC	1079	MET
1	CCC	1097	GLU
1	CCC	1110	SER
1	CCC	1134	ARG
1	CCC	1158	ARG
1	CCC	1174	LEU
1	CCC	1214	GLN
1	CCC	1219	GLU
1	CCC	1235	ASP
1	CCC	1239	ASP
1	CCC	1240	MET
1	CCC	1241	LEU
1	CCC	1243	GLU
1	DDD	991	GLU
1	DDD	993	GLU
1	DDD	1007	GLN

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Mol	Chain	Res	Type
1	DDD	1017	VAL
1	DDD	1019	LYS
1	DDD	1036	ASN
1	DDD	1073	GLN
1	DDD	1079	MET
1	DDD	1097	GLU
1	DDD	1110	SER
1	DDD	1134	ARG
1	DDD	1158	ARG
1	DDD	1167	ARG
1	DDD	1173	LEU
1	DDD	1214	GLN
1	DDD	1219	GLU
1	DDD	1235	ASP
1	DDD	1239	ASP
1	DDD	1240	MET
1	DDD	1241	LEU
1	DDD	1243	GLU
1	EEE	988	VAL
1	EEE	991	GLU
1	EEE	993	GLU
1	EEE	1007	GLN
1	EEE	1017	VAL
1	EEE	1036	ASN
1	EEE	1073	GLN
1	EEE	1079	MET
1	EEE	1097	GLU
1	EEE	1110	SER
1	EEE	1134	ARG
1	EEE	1214	GLN
1	EEE	1219	GLU
1	EEE	1235	ASP
1	EEE	1239	ASP
1	EEE	1240	MET
1	EEE	1241	LEU
1	EEE	1243	GLU
1	FFF	991	GLU
1	FFF	993	GLU
1	FFF	1007	GLN
1	FFF	1017	VAL
1	FFF	1036	ASN
1	FFF	1073	GLN

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Mol	Chain	Res	Type
1	FFF	1110	SER
1	FFF	1111	LYS
1	FFF	1134	ARG
1	FFF	1214	GLN
1	FFF	1219	GLU
1	FFF	1235	ASP
1	FFF	1239	ASP
1	FFF	1240	MET
1	FFF	1241	LEU
1	FFF	1243	GLU
1	GGG	988	VAL
1	GGG	991	GLU
1	GGG	993	GLU
1	GGG	997	GLU
1	GGG	1007	GLN
1	GGG	1017	VAL
1	GGG	1036	ASN
1	GGG	1073	GLN
1	GGG	1079	MET
1	GGG	1097	GLU
1	GGG	1110	SER
1	GGG	1134	ARG
1	GGG	1158	ARG
1	GGG	1174	LEU
1	GGG	1214	GLN
1	GGG	1219	GLU
1	GGG	1235	ASP
1	GGG	1239	ASP
1	GGG	1240	MET
1	GGG	1241	LEU
1	GGG	1243	GLU
1	HHH	988	VAL
1	HHH	991	GLU
1	HHH	993	GLU
1	HHH	1007	GLN
1	HHH	1017	VAL
1	HHH	1036	ASN
1	HHH	1073	GLN
1	HHH	1079	MET
1	HHH	1110	SER
1	HHH	1134	ARG
1	HHH	1158	ARG

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Mol	Chain	Res	Type
1	HHH	1214	GLN
1	HHH	1219	GLU
1	HHH	1235	ASP
1	HHH	1239	ASP
1	HHH	1240	MET
1	HHH	1241	LEU
1	HHH	1243	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

8 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	IER	CCC	3000	-	36,41,41	1.77	3 (8%)	42,62,62	2.05	13 (30%)
2	IER	BBB	3000	-	36,41,41	1.95	3 (8%)	42,62,62	1.70	10 (23%)
2	IER	AAA	3000	-	36,41,41	1.87	6 (16%)	42,62,62	1.67	5 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	IER	EEE	3000	-	36,41,41	2.12	2 (5%)	42,62,62	1.69	11 (26%)
2	IER	GGG	3000	-	36,41,41	1.72	3 (8%)	42,62,62	1.99	10 (23%)
2	IER	HHH	3000	-	36,41,41	1.76	5 (13%)	42,62,62	1.57	9 (21%)
2	IER	FFF	3000	-	36,41,41	2.13	6 (16%)	42,62,62	1.68	9 (21%)
2	IER	DDD	3000	-	36,41,41	1.79	3 (8%)	42,62,62	1.62	6 (14%)

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	IER	CCC	3000	-	-	6/10/25/25	0/6/6/6
2	IER	BBB	3000	-	-	6/10/25/25	0/6/6/6
2	IER	AAA	3000	-	-	6/10/25/25	0/6/6/6
2	IER	EEE	3000	-	-	6/10/25/25	0/6/6/6
2	IER	GGG	3000	-	-	4/10/25/25	0/6/6/6
2	IER	HHH	3000	-	-	5/10/25/25	0/6/6/6
2	IER	FFF	3000	-	-	6/10/25/25	0/6/6/6
2	IER	DDD	3000	-	-	5/10/25/25	0/6/6/6

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	EEE	3000	IER	C23-C25	-9.75	1.37	1.49
2	FFF	3000	IER	C23-C25	-8.47	1.38	1.49
2	BBB	3000	IER	C23-C25	-8.45	1.38	1.49
2	DDD	3000	IER	C23-C25	-7.60	1.39	1.49
2	CCC	3000	IER	C23-C25	-6.98	1.40	1.49
2	HHH	3000	IER	C23-C25	-6.91	1.40	1.49
2	GGG	3000	IER	C23-C25	-6.63	1.41	1.49
2	EEE	3000	IER	C3-C1	-6.62	1.38	1.48
2	FFF	3000	IER	C3-C1	-6.28	1.39	1.48
2	AAA	3000	IER	C23-C25	-6.17	1.41	1.49
2	AAA	3000	IER	C3-C1	-6.00	1.39	1.48
2	BBB	3000	IER	C3-C1	-5.85	1.39	1.48
2	CCC	3000	IER	C3-C1	-5.58	1.40	1.48
2	GGG	3000	IER	C3-C1	-5.44	1.40	1.48
2	DDD	3000	IER	C3-C1	-5.07	1.40	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	HHH	3000	IER	C3-C1	-4.89	1.41	1.48
2	GGG	3000	IER	C27-C01	3.23	1.55	1.50
2	HHH	3000	IER	C27-C01	3.15	1.55	1.50
2	AAA	3000	IER	C27-C01	2.85	1.54	1.50
2	CCC	3000	IER	C27-N26	-2.76	1.30	1.34
2	FFF	3000	IER	C17-C01	-2.73	1.52	1.55
2	FFF	3000	IER	C10-C12	-2.55	1.37	1.42
2	AAA	3000	IER	C10-C24	2.43	1.41	1.36
2	FFF	3000	IER	C27-N26	-2.38	1.31	1.34
2	BBB	3000	IER	O29-C16	-2.30	1.41	1.44
2	FFF	3000	IER	C23-C9	-2.29	1.35	1.39
2	DDD	3000	IER	C27-C01	2.27	1.54	1.50
2	AAA	3000	IER	O29-C16	-2.22	1.41	1.44
2	HHH	3000	IER	O29-C16	-2.17	1.41	1.44
2	AAA	3000	IER	C10-C12	-2.09	1.38	1.42
2	HHH	3000	IER	C1-N2	2.07	1.36	1.33

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	GGG	3000	IER	C1-N2-C11	8.30	124.63	118.26
2	CCC	3000	IER	C1-N2-C11	6.38	123.15	118.26
2	AAA	3000	IER	C1-N2-C11	5.70	122.63	118.26
2	DDD	3000	IER	C1-N2-C11	5.53	122.50	118.26
2	BBB	3000	IER	C1-N2-C11	4.99	122.09	118.26
2	DDD	3000	IER	C32-C1-N2	-4.49	118.13	122.23
2	AAA	3000	IER	F13-C9-C23	-4.28	114.04	119.95
2	HHH	3000	IER	C1-N2-C11	4.22	121.50	118.26
2	FFF	3000	IER	C1-N2-C11	4.17	121.46	118.26
2	CCC	3000	IER	C03-O01-C31	-4.11	113.69	118.01
2	FFF	3000	IER	C3-C1-N2	3.81	122.37	117.09
2	AAA	3000	IER	C03-O01-C31	-3.59	114.25	118.01
2	GGG	3000	IER	O29-C16-C02	3.54	115.60	107.97
2	EEE	3000	IER	C24-C23-C9	3.53	120.42	115.77
2	BBB	3000	IER	C32-C1-N2	-3.47	119.06	122.23
2	EEE	3000	IER	C32-C1-C3	-3.46	117.25	121.85
2	GGG	3000	IER	C17-C01-C27	-3.46	106.85	119.20
2	HHH	3000	IER	C20-N21-C22	3.39	122.57	117.61
2	FFF	3000	IER	C15-C01-C27	-3.38	107.15	119.20
2	CCC	3000	IER	C18-C22-N21	3.35	123.58	117.88
2	CCC	3000	IER	C5-C4-C3	3.26	124.66	120.56
2	BBB	3000	IER	C24-C23-C25	-3.14	116.25	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	3000	IER	C3-C1-N2	3.10	121.38	117.09
2	CCC	3000	IER	F13-C9-C23	-3.09	115.68	119.95
2	HHH	3000	IER	C3-C1-N2	3.06	121.33	117.09
2	BBB	3000	IER	O29-C16-C02	3.06	114.57	107.97
2	CCC	3000	IER	O29-C16-C02	3.03	114.51	107.97
2	FFF	3000	IER	C32-C1-N2	-2.98	119.51	122.23
2	EEE	3000	IER	C20-N21-C22	2.96	121.94	117.61
2	EEE	3000	IER	O29-C16-C02	2.89	114.19	107.97
2	EEE	3000	IER	C24-C23-C25	-2.84	116.62	120.14
2	EEE	3000	IER	C03-O01-C31	-2.82	115.05	118.01
2	CCC	3000	IER	C17-C01-C27	-2.81	109.18	119.20
2	FFF	3000	IER	C32-C1-C3	-2.81	118.12	121.85
2	HHH	3000	IER	C32-C1-C3	-2.70	118.26	121.85
2	HHH	3000	IER	C17-C01-C15	-2.65	85.97	88.08
2	GGG	3000	IER	C20-N21-C22	2.64	121.48	117.61
2	CCC	3000	IER	C7-C8-C3	-2.64	117.25	120.56
2	HHH	3000	IER	C24-C23-C9	2.63	119.23	115.77
2	CCC	3000	IER	C6-C5-C4	-2.60	116.23	120.19
2	BBB	3000	IER	C5-C4-C3	2.56	123.78	120.56
2	CCC	3000	IER	O01-C03-C35	-2.55	99.48	108.21
2	EEE	3000	IER	C1-N2-C11	2.55	120.22	118.26
2	GGG	3000	IER	F13-C9-C23	-2.54	116.44	119.95
2	GGG	3000	IER	C32-C1-N2	-2.53	119.92	122.23
2	HHH	3000	IER	C24-C23-C25	-2.53	117.00	120.14
2	GGG	3000	IER	C12-C11-N2	-2.53	117.56	122.78
2	DDD	3000	IER	C20-N21-C22	2.51	121.29	117.61
2	BBB	3000	IER	C15-C01-C27	-2.44	110.49	119.20
2	HHH	3000	IER	C4-C3-C1	-2.41	117.47	121.28
2	AAA	3000	IER	C12-C11-N2	-2.41	117.82	122.78
2	CCC	3000	IER	C6-C7-C8	2.40	123.84	120.19
2	EEE	3000	IER	C17-C01-C27	-2.40	110.64	119.20
2	GGG	3000	IER	F13-C9-C11	2.38	123.15	118.12
2	FFF	3000	IER	C20-N21-C22	2.33	121.03	117.61
2	BBB	3000	IER	C24-C23-C9	2.31	118.81	115.77
2	DDD	3000	IER	C5-C4-C3	2.23	123.36	120.56
2	BBB	3000	IER	C18-C22-N28	-2.23	118.73	123.84
2	HHH	3000	IER	C32-C1-N2	-2.22	120.20	122.23
2	FFF	3000	IER	C24-C23-C9	2.21	118.67	115.77
2	BBB	3000	IER	C20-N21-C22	2.18	120.81	117.61
2	EEE	3000	IER	C31-C12-C11	2.16	122.17	117.19
2	CCC	3000	IER	O29-C16-C17	-2.15	108.64	115.81
2	BBB	3000	IER	C18-C22-N21	2.14	121.53	117.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	EEE	3000	IER	C10-C12-C31	-2.14	117.66	122.58
2	AAA	3000	IER	C20-N21-C22	2.13	120.72	117.61
2	FFF	3000	IER	O01-C31-C12	2.12	120.93	115.01
2	FFF	3000	IER	C24-C23-C25	-2.09	117.55	120.14
2	GGG	3000	IER	C19-C20-N21	-2.09	119.63	122.49
2	CCC	3000	IER	C12-C11-N2	-2.07	118.51	122.78
2	EEE	3000	IER	C15-C01-C27	-2.07	111.83	119.20
2	GGG	3000	IER	C18-C22-N21	2.06	121.39	117.88
2	DDD	3000	IER	C15-C01-C27	-2.05	111.87	119.20

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	AAA	3000	IER	C9-C23-C25-C18
2	AAA	3000	IER	C24-C23-C25-N26
2	BBB	3000	IER	C9-C23-C25-C18
2	BBB	3000	IER	C24-C23-C25-N26
2	CCC	3000	IER	C9-C23-C25-C18
2	CCC	3000	IER	C24-C23-C25-N26
2	DDD	3000	IER	C9-C23-C25-C18
2	DDD	3000	IER	C24-C23-C25-N26
2	EEE	3000	IER	C24-C23-C25-N26
2	FFF	3000	IER	C9-C23-C25-C18
2	FFF	3000	IER	C24-C23-C25-N26
2	GGG	3000	IER	C24-C23-C25-N26
2	HHH	3000	IER	C9-C23-C25-C18
2	HHH	3000	IER	C24-C23-C25-N26
2	EEE	3000	IER	N2-C1-C3-C4
2	EEE	3000	IER	C32-C1-C3-C4
2	EEE	3000	IER	C32-C1-C3-C8
2	EEE	3000	IER	N2-C1-C3-C8
2	FFF	3000	IER	C32-C1-C3-C4
2	FFF	3000	IER	N2-C1-C3-C4
2	CCC	3000	IER	C32-C1-C3-C4
2	BBB	3000	IER	C32-C1-C3-C4
2	BBB	3000	IER	N2-C1-C3-C4
2	FFF	3000	IER	N2-C1-C3-C8
2	CCC	3000	IER	N2-C1-C3-C4
2	CCC	3000	IER	C32-C1-C3-C8
2	FFF	3000	IER	C32-C1-C3-C8
2	BBB	3000	IER	N2-C1-C3-C8

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Mol	Chain	Res	Type	Atoms
2	BBB	3000	IER	C32-C1-C3-C8
2	CCC	3000	IER	N2-C1-C3-C8
2	AAA	3000	IER	N2-C1-C3-C8
2	HHH	3000	IER	C32-C31-O01-C03
2	AAA	3000	IER	N2-C1-C3-C4
2	AAA	3000	IER	C32-C1-C3-C8
2	DDD	3000	IER	C32-C1-C3-C4
2	AAA	3000	IER	C32-C1-C3-C4
2	HHH	3000	IER	C12-C31-O01-C03
2	DDD	3000	IER	N2-C1-C3-C4
2	EEE	3000	IER	C9-C23-C25-C18
2	GGG	3000	IER	C9-C23-C25-C18
2	HHH	3000	IER	C32-C1-C3-C4
2	DDD	3000	IER	C32-C1-C3-C8
2	GGG	3000	IER	C32-C1-C3-C4
2	GGG	3000	IER	N2-C1-C3-C4

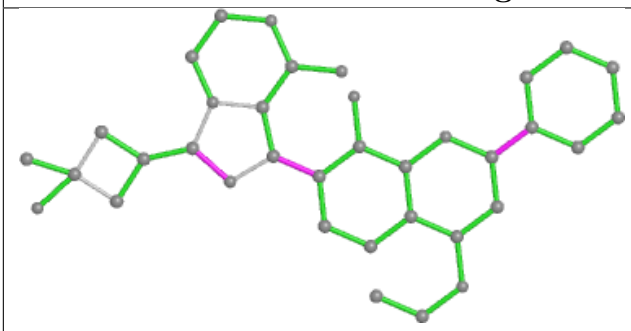
There are no ring outliers.

4 monomers are involved in 4 short contacts:

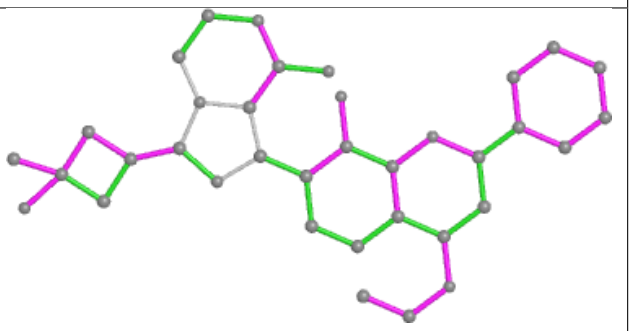
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	EEE	3000	IER	1	0
2	HHH	3000	IER	1	0
2	FFF	3000	IER	1	0
2	DDD	3000	IER	1	0

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.

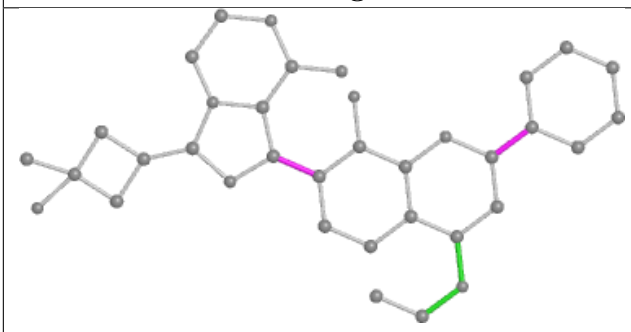
Ligand IER CCC 3000



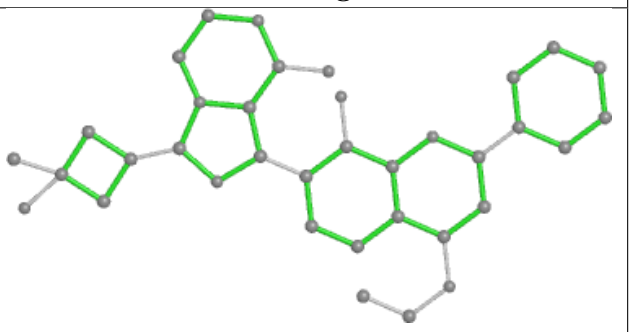
Bond lengths



Bond angles

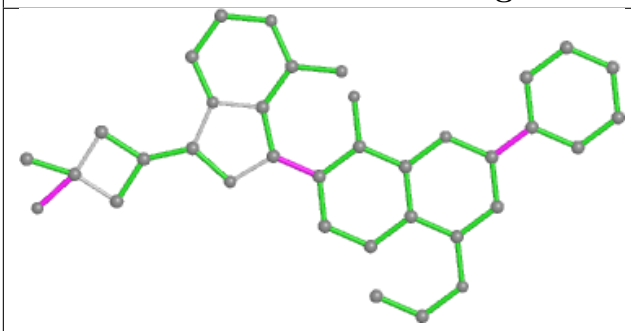


Torsions

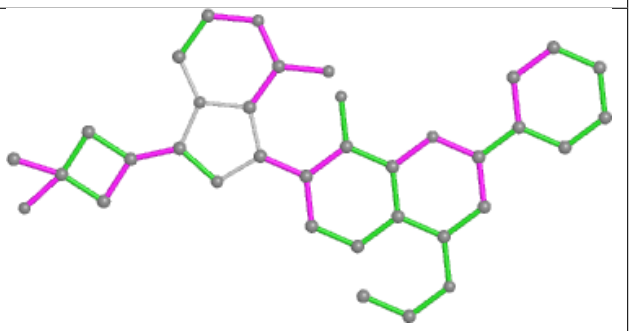


Rings

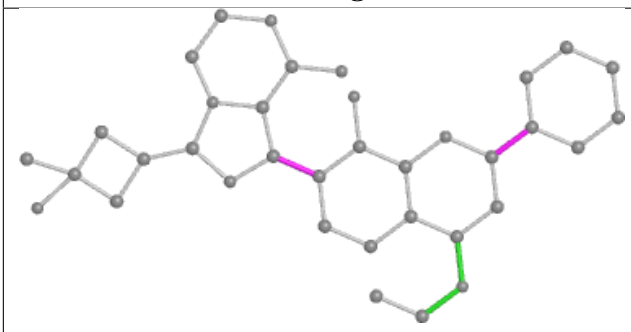
Ligand IER BBB 3000



Bond lengths



Bond angles



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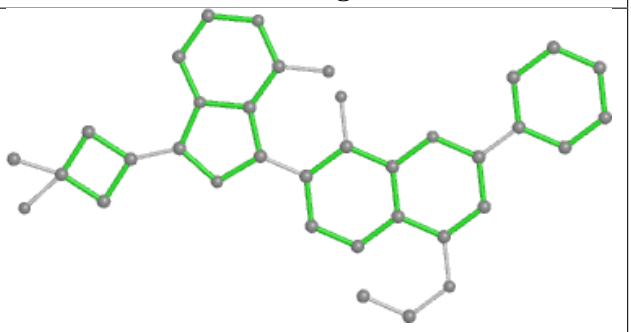
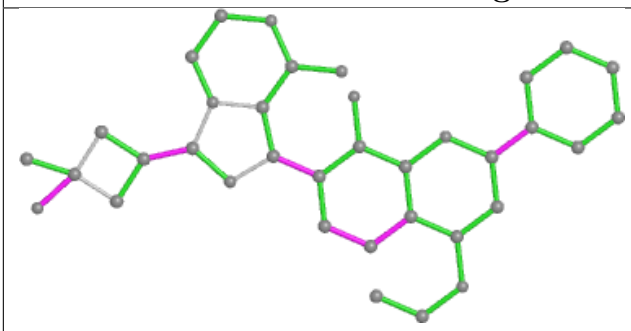
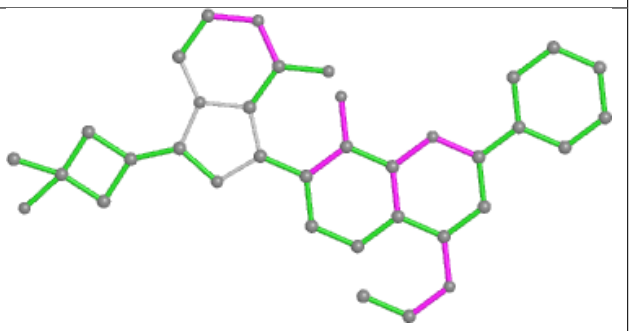


Rings

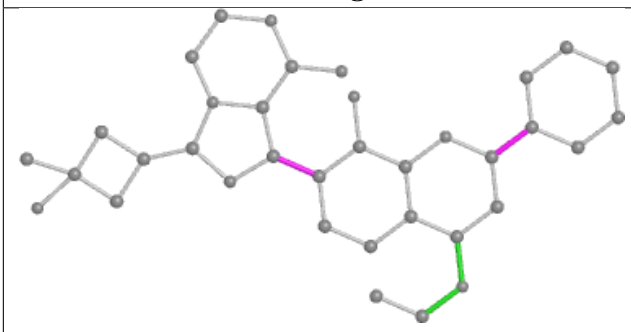
Ligand IER AAA 3000



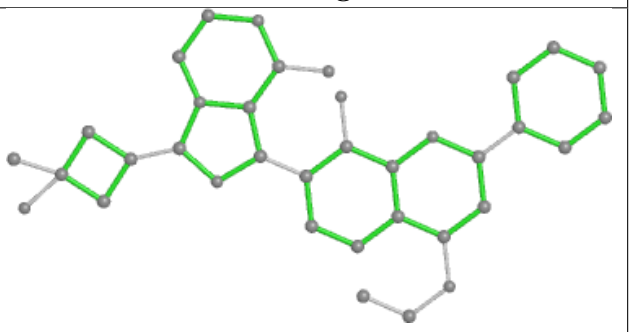
Bond lengths



Bond angles

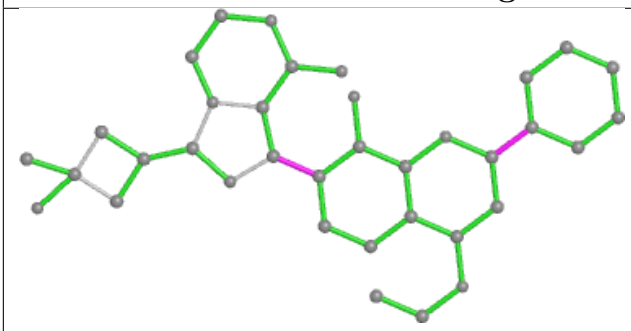


Torsions

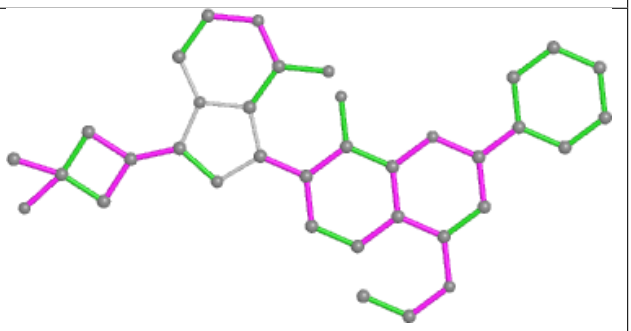


Rings

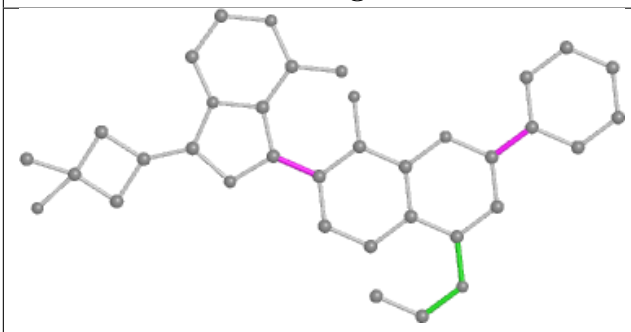
Ligand IER EEE 3000



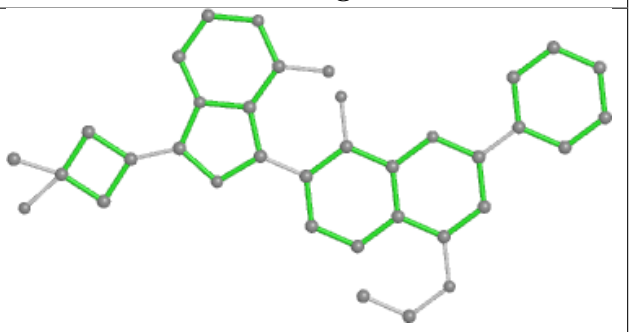
Bond lengths



Bond angles

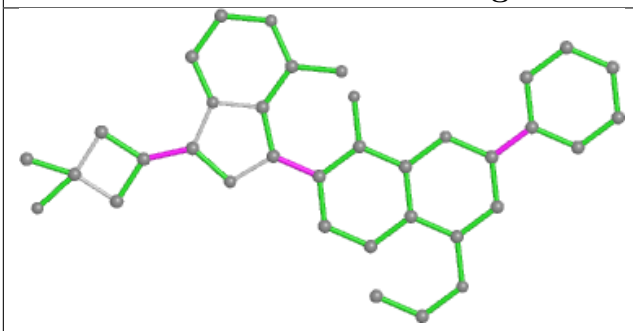


Torsions

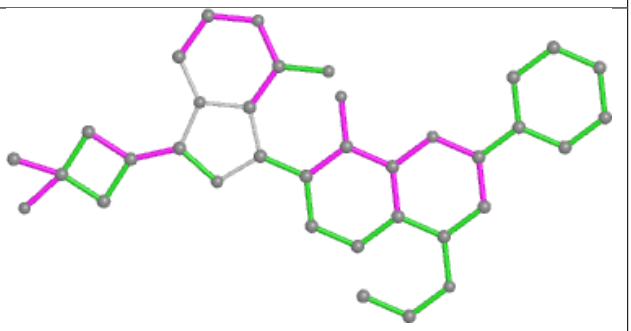


Rings

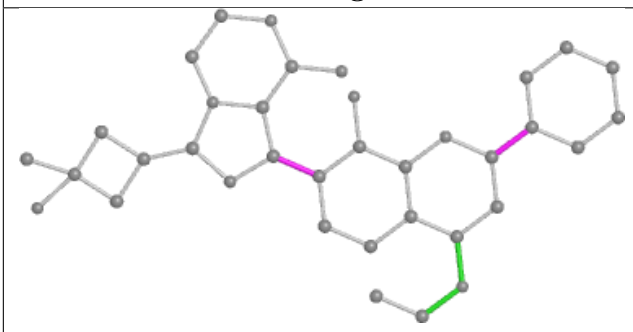
Ligand IER GGG 3000



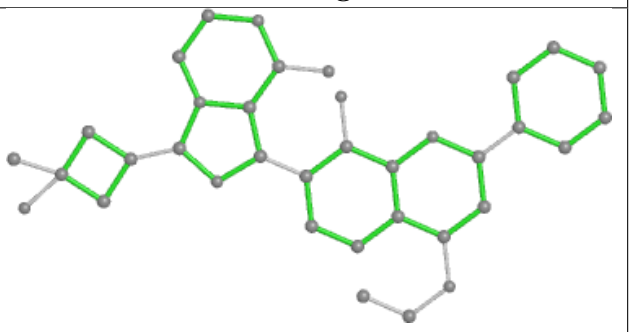
Bond lengths



Bond angles

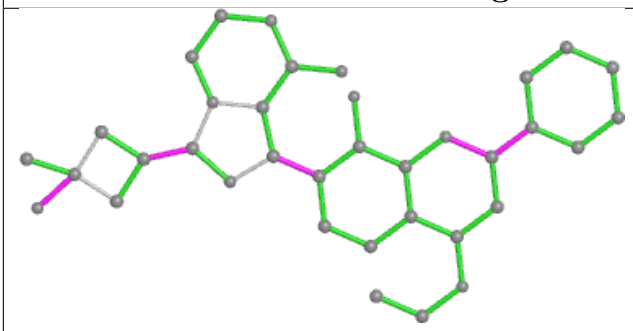


Torsions

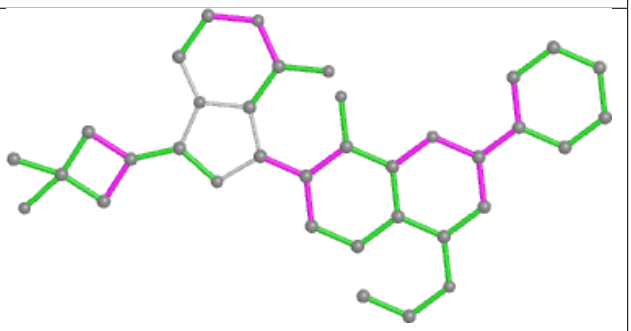


Rings

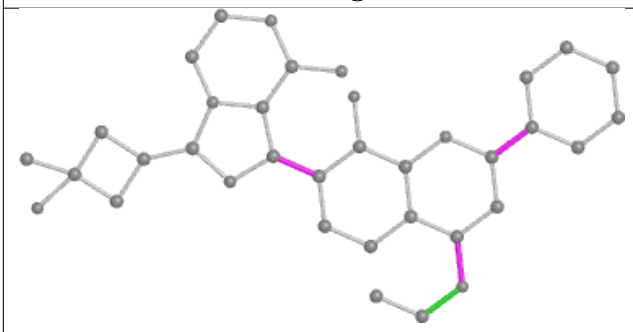
Ligand IER HHH 3000



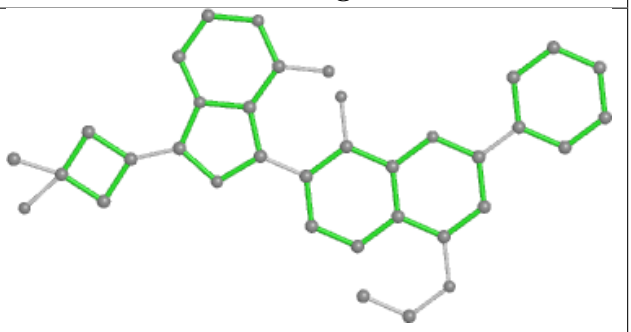
Bond lengths



Bond angles

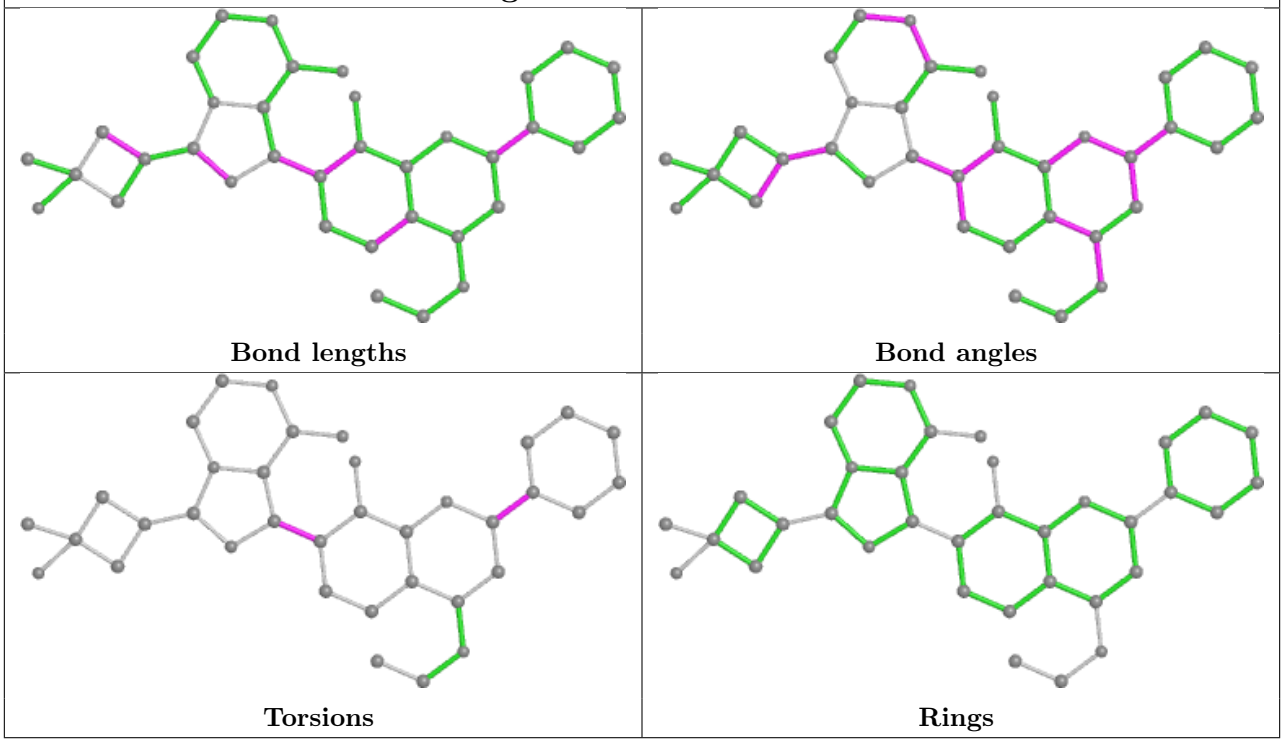


Torsions

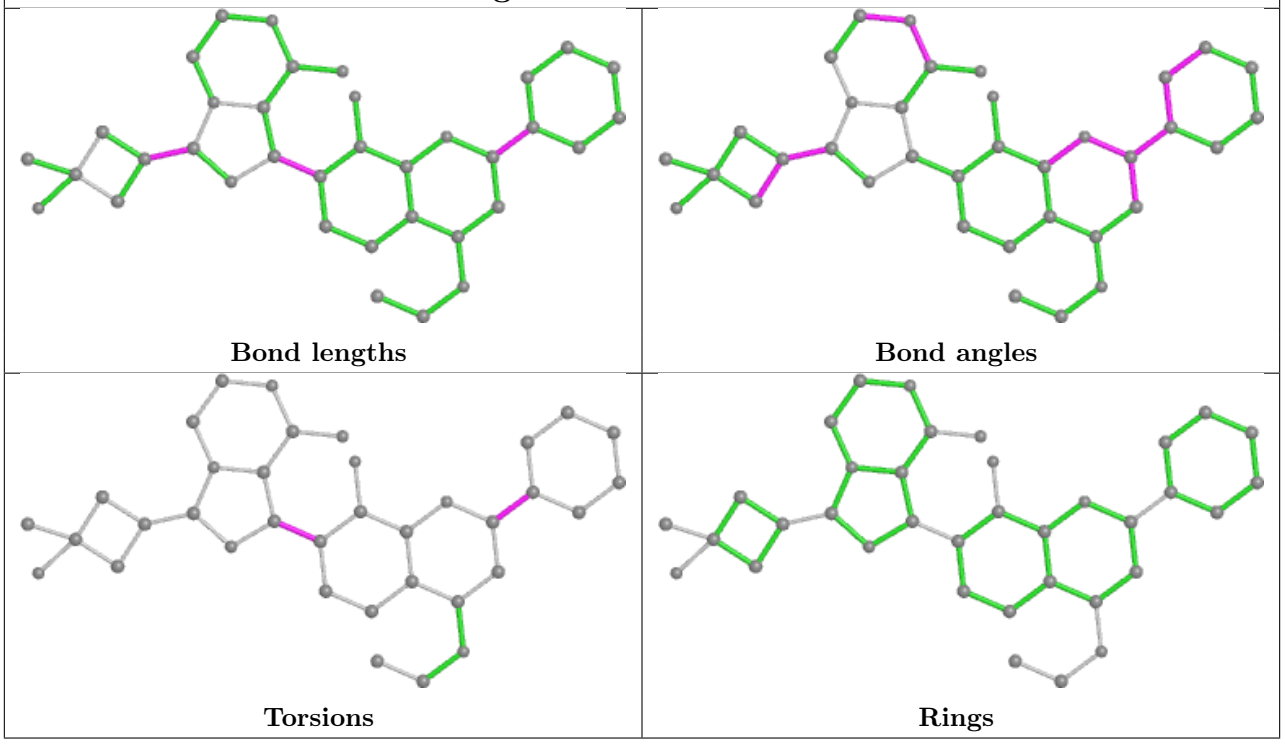


Rings

Ligand IER FFF 3000



Ligand IER DDD 3000



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	AAA	288/321 (89%)	-0.25	2 (0%) 87 72	29, 52, 91, 128	0
1	BBB	287/321 (89%)	-0.37	0 100 100	27, 44, 85, 134	0
1	CCC	286/321 (89%)	-0.28	1 (0%) 94 85	28, 50, 86, 143	0
1	DDD	287/321 (89%)	-0.26	1 (0%) 94 85	28, 52, 96, 171	0
1	EEE	285/321 (88%)	-0.18	2 (0%) 87 72	28, 56, 96, 131	0
1	FFF	287/321 (89%)	-0.26	0 100 100	26, 52, 89, 161	0
1	GGG	284/321 (88%)	-0.05	3 (1%) 80 60	32, 60, 105, 137	0
1	HHH	285/321 (88%)	0.03	5 (1%) 68 45	34, 68, 124, 162	0
All	All	2289/2568 (89%)	-0.20	14 (0%) 89 76	26, 54, 101, 171	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	DDD	1106	PRO	6.0
1	EEE	1106	PRO	5.3
1	HHH	1024	ASP	3.6
1	EEE	1024	ASP	3.5
1	CCC	1106	PRO	3.3
1	HHH	1236	ASN	3.0
1	GGG	1041	MET	2.9
1	HHH	1239	ASP	2.8
1	HHH	1272	PRO	2.5
1	AAA	1097	GLU	2.3
1	GGG	1239	ASP	2.2
1	AAA	1024	ASP	2.2
1	HHH	1021	VAL	2.0
1	GGG	1163	THR	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)

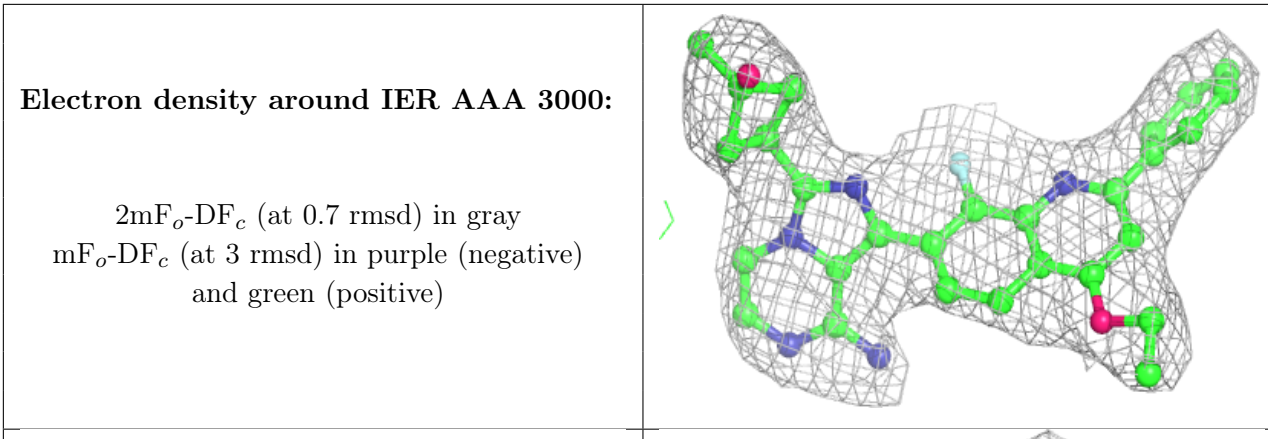
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	IER	AAA	3000	36/36	0.97	0.20	33,39,49,52	0
2	IER	CCC	3000	36/36	0.97	0.18	33,35,39,44	0
2	IER	DDD	3000	36/36	0.97	0.17	29,39,48,57	0
2	IER	GGG	3000	36/36	0.97	0.23	34,45,59,62	0
2	IER	HHH	3000	36/36	0.97	0.21	38,45,57,60	0
2	IER	FFF	3000	36/36	0.98	0.20	30,36,42,44	0
2	IER	BBB	3000	36/36	0.98	0.17	27,31,37,42	0
2	IER	EEE	3000	36/36	0.98	0.20	34,39,50,53	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.

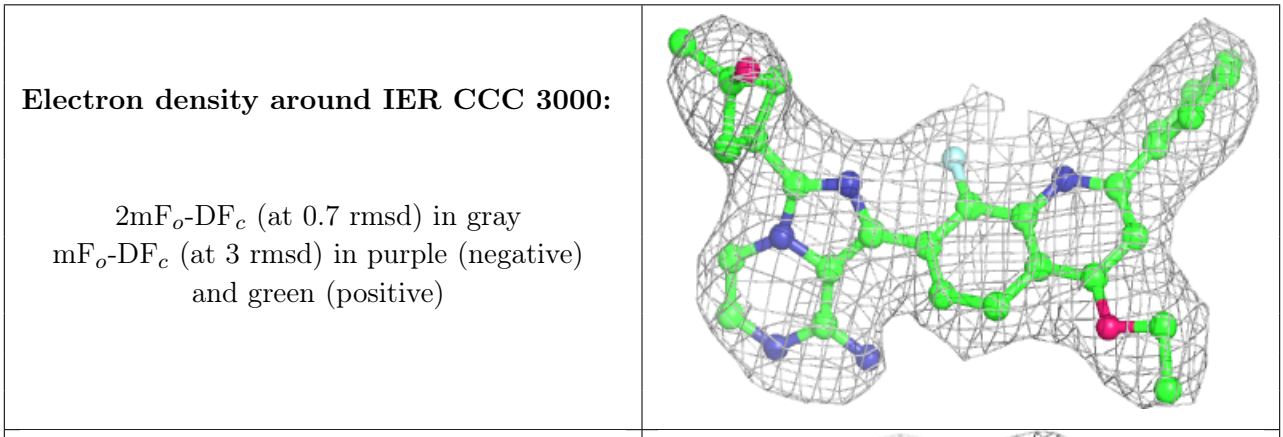
Electron density around IER AAA 3000:

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



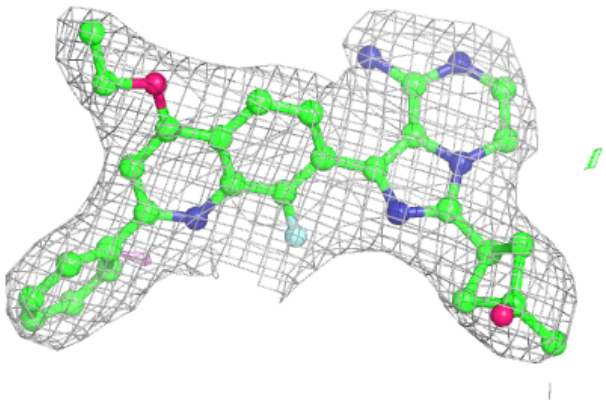
Electron density around IER CCC 3000:

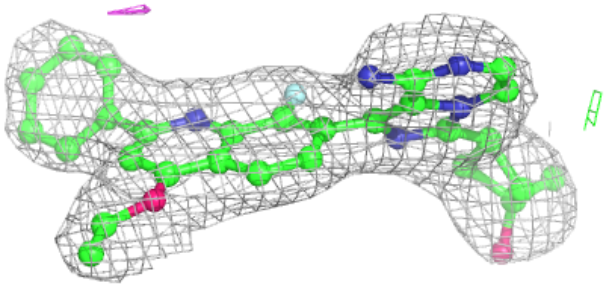
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

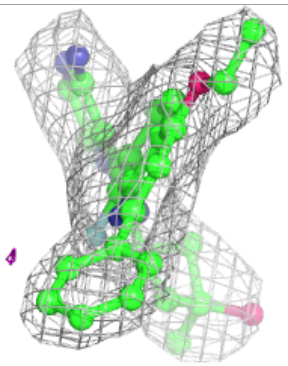


Electron density around IER DDD 3000:

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

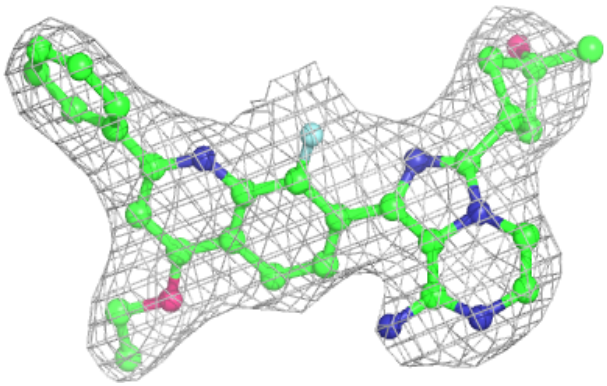


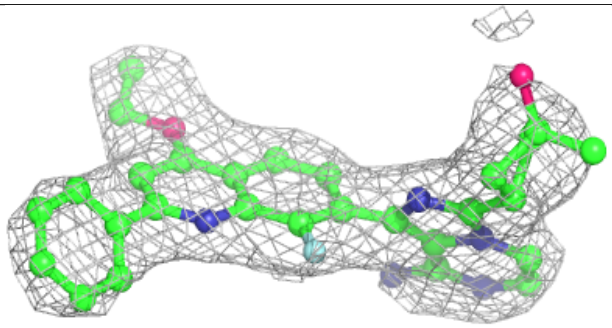


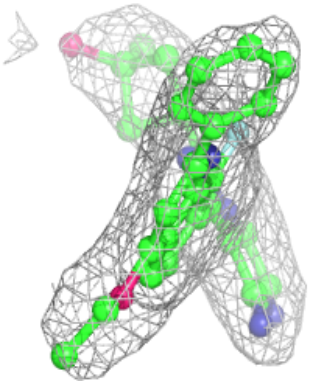


Electron density around IER GGG 3000:

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

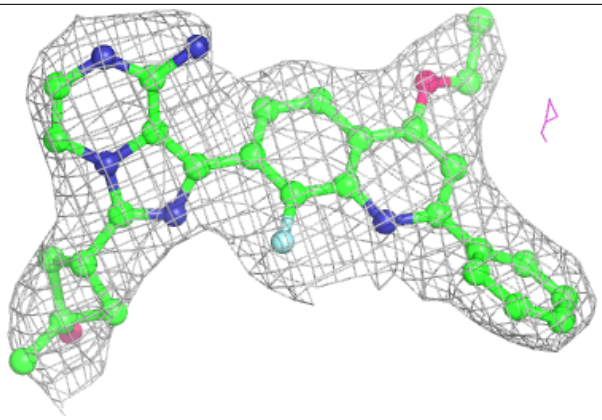


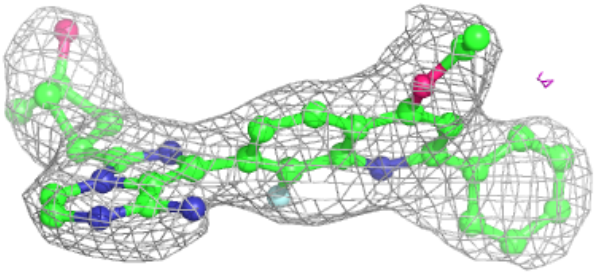


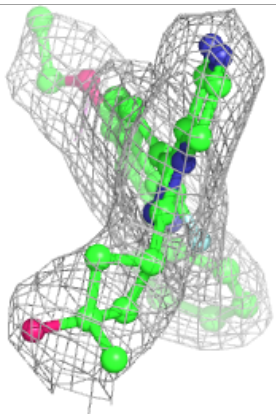


Electron density around IER HHH 3000:

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

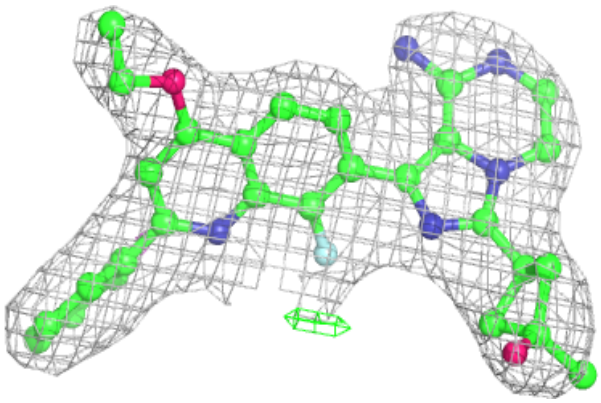


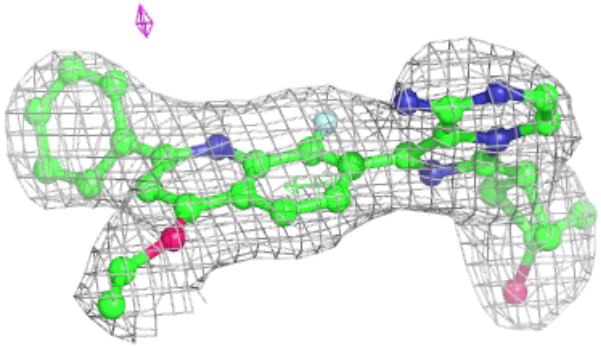




Electron density around IER FFF 3000:

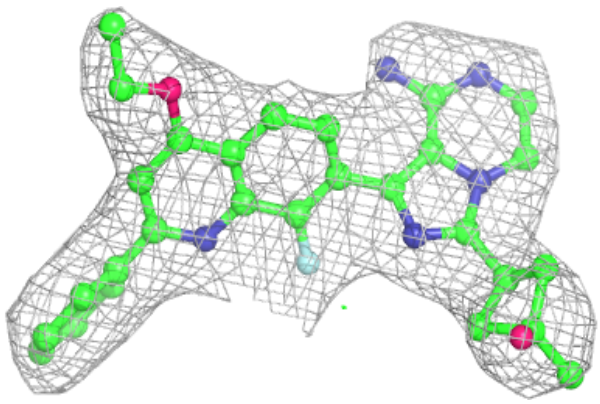
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

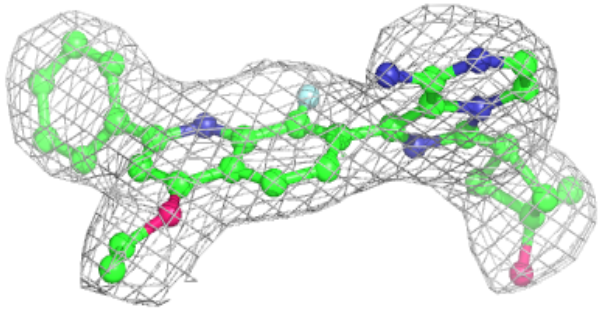


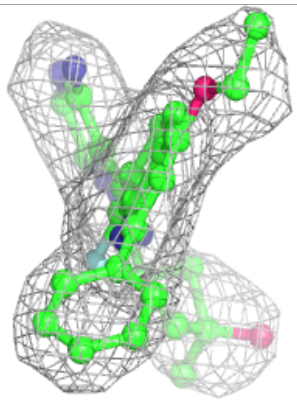


Electron density around IER BBB 3000:

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

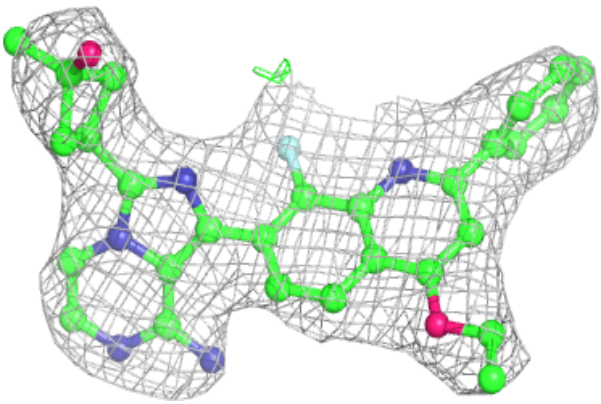


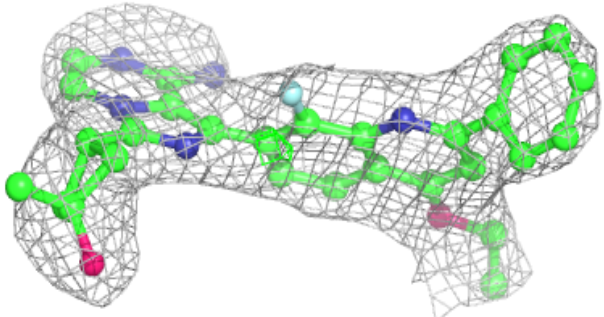


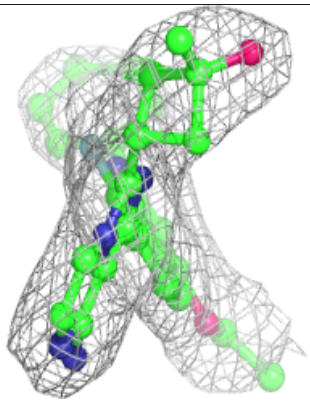


Electron density around IER EEE 3000:

$2mF_o$-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.