Full wwPDB X-ray Structure Validation Report ⓘ

Aug 28, 2026 – 01:50 am BST

PDB ID	:	7B74 / pdb_00007b74
Title	:	Chimeric Streptavidin With A Dimerization Domain For Artificial Transfer Hydrogenation
Authors	:	Igareta, N.V.; Ward, T.R.
Deposited on	:	2020-12-09
Resolution	:	1.85 Å(reported)

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

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

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

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

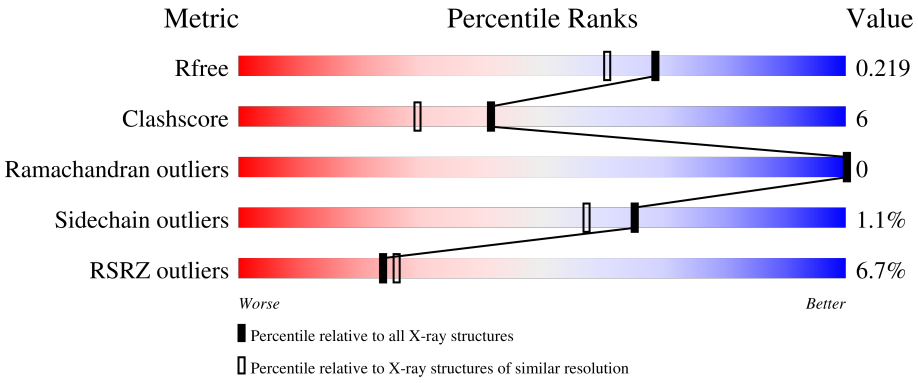
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 1.85 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}	180053	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	194	4% 59% 37%
1	BBB	194	6% 56% 8% 36%
1	CCC	194	4% 53% 9% 37%
1	DDD	194	4% 56% 7% 37%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 7478 atoms, of which 3467 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 Streptavidin,Superoxide dismutase [Cu-Zn],Streptavidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	122	Total	C	H	N	O	37	0	0
			1764	568	855	158	183			
1	BBB	125	Total	C	H	N	O	38	2	0
			1811	582	879	161	189			
1	CCC	123	Total	C	H	N	O	39	3	0
			1784	573	866	159	186			
1	DDD	122	Total	C	H	N	O	38	2	0
			1782	573	867	158	184			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	1	MET	-	initiating methionine	UNP P22629
AAA	2	ALA	-	expression tag	UNP P22629
AAA	3	SER	-	expression tag	UNP P22629
AAA	4	MET	-	expression tag	UNP P22629
AAA	5	THR	-	expression tag	UNP P22629
AAA	6	GLY	-	expression tag	UNP P22629
AAA	7	GLY	-	expression tag	UNP P22629
AAA	8	GLN	-	expression tag	UNP P22629
AAA	9	GLN	-	expression tag	UNP P22629
AAA	10	MET	-	expression tag	UNP P22629
AAA	11	GLY	-	expression tag	UNP P22629
AAA	12	ARG	-	expression tag	UNP P22629
AAA	13	ASP	-	expression tag	UNP P22629
AAA	14	GLN	-	expression tag	UNP P22629
AAA	146	ALA	SER	engineered mutation	UNP P22629
BBB	1	MET	-	initiating methionine	UNP P22629
BBB	2	ALA	-	expression tag	UNP P22629
BBB	3	SER	-	expression tag	UNP P22629
BBB	4	MET	-	expression tag	UNP P22629
BBB	5	THR	-	expression tag	UNP P22629
BBB	6	GLY	-	expression tag	UNP P22629

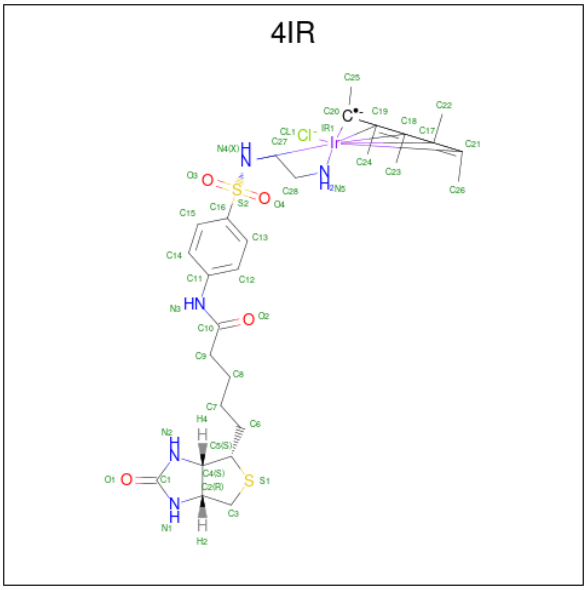
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Chain	Residue	Modelled	Actual	Comment	Reference
BBB	7	GLY	-	expression tag	UNP P22629
BBB	8	GLN	-	expression tag	UNP P22629
BBB	9	GLN	-	expression tag	UNP P22629
BBB	10	MET	-	expression tag	UNP P22629
BBB	11	GLY	-	expression tag	UNP P22629
BBB	12	ARG	-	expression tag	UNP P22629
BBB	13	ASP	-	expression tag	UNP P22629
BBB	14	GLN	-	expression tag	UNP P22629
BBB	146	ALA	SER	engineered mutation	UNP P22629
CCC	1	MET	-	initiating methionine	UNP P22629
CCC	2	ALA	-	expression tag	UNP P22629
CCC	3	SER	-	expression tag	UNP P22629
CCC	4	MET	-	expression tag	UNP P22629
CCC	5	THR	-	expression tag	UNP P22629
CCC	6	GLY	-	expression tag	UNP P22629
CCC	7	GLY	-	expression tag	UNP P22629
CCC	8	GLN	-	expression tag	UNP P22629
CCC	9	GLN	-	expression tag	UNP P22629
CCC	10	MET	-	expression tag	UNP P22629
CCC	11	GLY	-	expression tag	UNP P22629
CCC	12	ARG	-	expression tag	UNP P22629
CCC	13	ASP	-	expression tag	UNP P22629
CCC	14	GLN	-	expression tag	UNP P22629
CCC	146	ALA	SER	engineered mutation	UNP P22629
DDD	1	MET	-	initiating methionine	UNP P22629
DDD	2	ALA	-	expression tag	UNP P22629
DDD	3	SER	-	expression tag	UNP P22629
DDD	4	MET	-	expression tag	UNP P22629
DDD	5	THR	-	expression tag	UNP P22629
DDD	6	GLY	-	expression tag	UNP P22629
DDD	7	GLY	-	expression tag	UNP P22629
DDD	8	GLN	-	expression tag	UNP P22629
DDD	9	GLN	-	expression tag	UNP P22629
DDD	10	MET	-	expression tag	UNP P22629
DDD	11	GLY	-	expression tag	UNP P22629
DDD	12	ARG	-	expression tag	UNP P22629
DDD	13	ASP	-	expression tag	UNP P22629
DDD	14	GLN	-	expression tag	UNP P22629
DDD	146	ALA	SER	engineered mutation	UNP P22629

- Molecule 2 is {N-(4-{(S)-[2-(amino-kappaN)ethyl]sulfamoyl-kappaN}phenyl)-5-[(3aS,4S,6aR)-2-oxohexahydro-1H-thieno[3,4-d]imidazol-4-yl]pentanamide}chlorido[(1,2,3,4,5-eta)-pentamethylcyclopentadienyl]iridium(2+) (CCD ID: 4IR) (formula: $C_{28}H_{42}ClIrN_5O_4S_2$) (labeled

as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	AAA	1	Total	C	Ir	N	O	S	0	0
			40	28	1	5	4	2		
2	BBB	1	Total	C	Ir	N	O	S	0	0
			40	28	1	5	4	2		
2	CCC	1	Total	C	Ir	N	O	S	0	0
			40	28	1	5	4	2		
2	DDD	1	Total	C	Ir	N	O	S	0	0
			40	28	1	5	4	2		

- Molecule 3 is water.

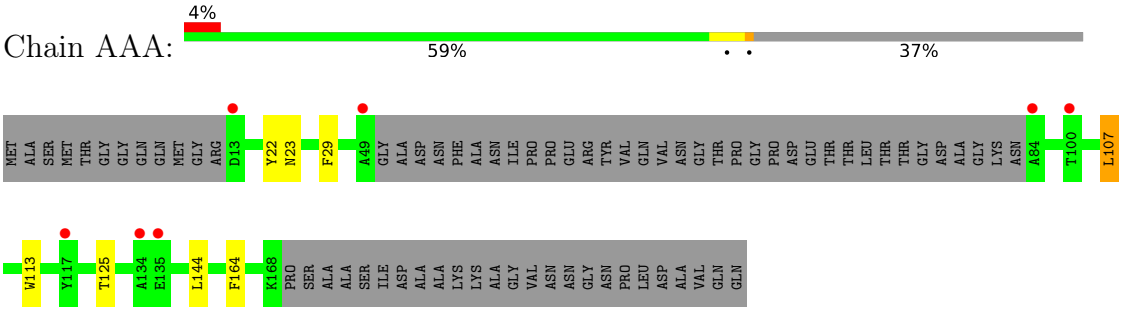
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	AAA	38	Total	O	0	0
			38	38		
3	BBB	47	Total	O	0	0
			47	47		
3	CCC	50	Total	O	0	0
			50	50		
3	DDD	42	Total	O	0	0
			42	42		

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.

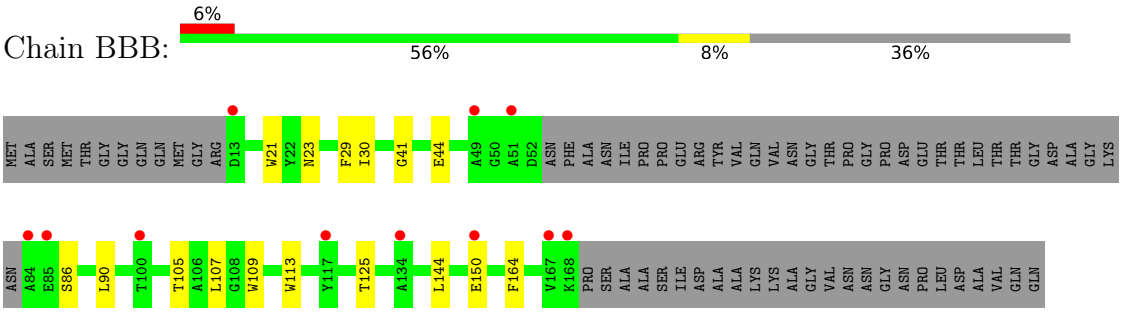
• Molecule 1: Streptavidin,Superoxide dismutase [Cu-Zn],Streptavidin

Chain AAA:



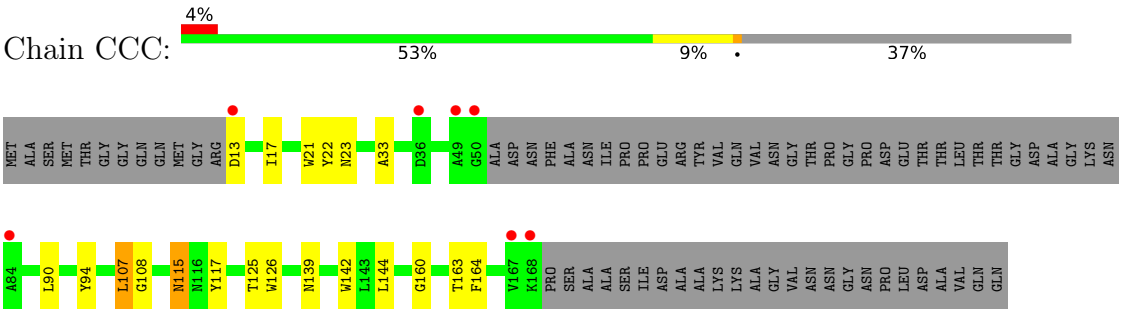
• Molecule 1: Streptavidin,Superoxide dismutase [Cu-Zn],Streptavidin

Chain BBB:



• Molecule 1: Streptavidin,Superoxide dismutase [Cu-Zn],Streptavidin

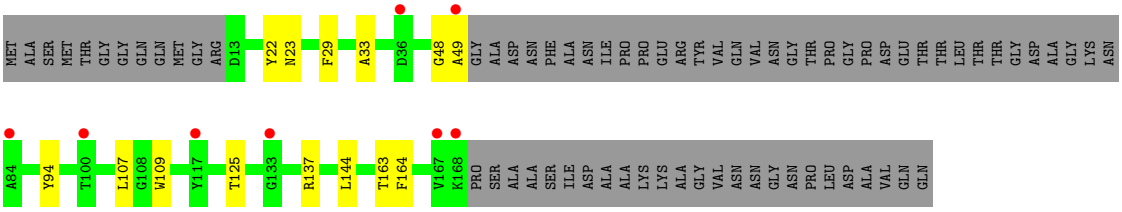
Chain CCC:



• Molecule 1: Streptavidin,Superoxide dismutase [Cu-Zn],Streptavidin

Chain DDD:




MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG D13 Y22 N23 F29 A33 D36 G48 A49 GLY ALA ASP ASN PHE ALA ASN ILE PRO PRO GLU ARG TYR VAL GLN VAL ASN GLY THR PRO GLY PRO ASP GLU THR THR LEU THR THR GLY ASP ALA GLY LYS ASN
A84 Y94 T100 L107 G108 W109 Y117 T125 G133 R137 L144 T163 F164 V167 K168 PRO SER ALA ALA SER ILE ASP ALA ALA LYS LYS ALA GLY VAL ASN ASN GLY ASN PRO LEU ASP ALA VAL GLN GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	57.28Å 57.31Å 88.03Å 90.00° 94.62° 90.00°	Depositor
Resolution (Å)	47.98 – 1.85 47.98 – 1.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (47.98-1.85) 98.3 (47.98-1.85)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.56 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC 5.8.0267	Depositor
R, R_{free}	0.191 , 0.218 0.194 , 0.219	Depositor DCC
R_{free} test set	2503 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	19.7	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.43 , 33.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7478	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 6.10% 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: 4IR

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	1.04	0/930	1.33	1/1271 (0.1%)
1	BBB	1.10	1/962 (0.1%)	1.31	2/1315 (0.2%)
1	CCC	1.09	0/947	1.29	0/1294
1	DDD	1.04	0/945	1.30	1/1292 (0.1%)
All	All	1.07	1/3784 (0.0%)	1.31	4/5172 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	105	THR	C-O	5.01	1.29	1.24

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	DDD	29	PHE	CA-CB-CG	6.12	119.92	113.80
1	AAA	29	PHE	CB-CA-C	6.07	119.85	110.14
1	BBB	29	PHE	CB-CA-C	5.32	118.99	110.16
1	BBB	29	PHE	CA-CB-CG	5.16	118.96	113.80

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	AAA	909	855	851	9	0
1	BBB	932	879	873	11	0
1	CCC	918	866	851	15	0
1	DDD	915	867	861	10	0
2	AAA	40	0	24	1	0
2	BBB	40	0	24	3	0
2	CCC	40	0	24	2	0
2	DDD	40	0	24	0	0
3	AAA	38	0	0	0	0
3	BBB	47	0	0	0	0
3	CCC	50	0	0	0	0
3	DDD	42	0	0	0	0
All	All	4011	3467	3532	47	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 6.

All (47) 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:BBB:144:LEU:C	1:BBB:144:LEU:HD23	2.27	0.60
2:BBB:201:4IR:O2	2:BBB:201:4IR:C14	2.49	0.56
1:AAA:107:LEU:C	1:AAA:107:LEU:HD12	2.32	0.54
1:CCC:144:LEU:C	1:CCC:144:LEU:HD23	2.35	0.52
2:CCC:201:4IR:O2	2:CCC:201:4IR:C12	2.56	0.52
1:AAA:125:THR:HB	1:CCC:125:THR:HB	1.92	0.51
1:AAA:144:LEU:C	1:AAA:144:LEU:HD23	2.37	0.50
2:BBB:201:4IR:O2	2:BBB:201:4IR:H14	2.11	0.49
1:CCC:115:ASN:ND2	1:CCC:117:TYR:H	2.11	0.49
1:AAA:23:ASN:HB3	1:AAA:164:PHE:CE1	2.47	0.49
1:BBB:23:ASN:HB3	1:BBB:164:PHE:CE1	2.48	0.48
1:BBB:107[B]:LEU:HD11	1:BBB:109:TRP:HZ3	1.78	0.48
1:DDD:23:ASN:HB3	1:DDD:164:PHE:CE1	2.48	0.48
1:CCC:90:LEU:HD12	1:CCC:90:LEU:C	2.39	0.48
1:DDD:22:TYR:O	1:DDD:164:PHE:HA	2.15	0.46
1:DDD:144:LEU:HD23	1:DDD:144:LEU:C	2.41	0.46
1:CCC:33:ALA:HB1	1:CCC:94:TYR:CE1	2.50	0.46
1:BBB:125:THR:HB	1:DDD:125:THR:HB	1.98	0.45
2:CCC:201:4IR:O2	2:CCC:201:4IR:H12	2.15	0.45
1:CCC:115:ASN:HD22	1:CCC:117:TYR:H	1.64	0.45
1:BBB:113:TRP:CG	2:BBB:201:4IR:H9A	2.53	0.44
1:DDD:23:ASN:HB3	1:DDD:164:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CCC:108:GLY:HA2	1:CCC:126:TRP:O	2.18	0.44
1:DDD:48:GLY:O	1:DDD:49:ALA:HB3	2.17	0.44
1:BBB:30:ILE:O	1:BBB:41:GLY:HA3	2.18	0.44
1:BBB:150:GLU:H	1:BBB:150:GLU:CD	2.26	0.43
1:DDD:33:ALA:HB1	1:DDD:94:TYR:CE1	2.53	0.43
1:BBB:150:GLU:CD	1:BBB:150:GLU:N	2.76	0.43
1:AAA:22:TYR:O	1:AAA:164:PHE:HA	2.19	0.43
1:CCC:22:TYR:O	1:CCC:164:PHE:HA	2.18	0.43
1:CCC:115:ASN:HD22	1:CCC:115:ASN:C	2.27	0.43
1:DDD:107[B]:LEU:HD11	1:DDD:109:TRP:HZ3	1.83	0.43
1:CCC:107:LEU:HD12	1:CCC:107:LEU:C	2.44	0.42
1:BBB:44:GLU:HA	1:BBB:86:SER:O	2.19	0.42
1:BBB:21:TRP:HB3	1:BBB:164:PHE:HB3	2.01	0.42
1:AAA:113:TRP:CG	2:AAA:201:4IR:H9A	2.55	0.41
1:AAA:23:ASN:HB3	1:AAA:164:PHE:CD1	2.56	0.41
1:CCC:13:ASP:O	1:CCC:17:ILE:HG13	2.20	0.41
1:AAA:107:LEU:C	1:AAA:107:LEU:CD1	2.93	0.41
1:CCC:21:TRP:HB3	1:CCC:164:PHE:HB3	2.03	0.41
1:BBB:90:LEU:C	1:BBB:90:LEU:HD12	2.46	0.41
1:AAA:107:LEU:HD12	1:AAA:107:LEU:O	2.21	0.40
1:CCC:142:TRP:CZ2	1:CCC:160:GLY:HA3	2.56	0.40
1:DDD:137:ARG:HH11	1:DDD:163:THR:HG21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AAA	118/194 (61%)	114 (97%)	4 (3%)	0	100	100
1	BBB	123/194 (63%)	118 (96%)	5 (4%)	0	100	100
1	CCC	121/194 (62%)	119 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	DDD	120/194 (62%)	118 (98%)	2 (2%)	0	100 100
All	All	482/776 (62%)	469 (97%)	13 (3%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	AAA	88/140 (63%)	87 (99%)	1 (1%)	65 57
1	BBB	91/140 (65%)	91 (100%)	0	100 100
1	CCC	90/140 (64%)	87 (97%)	3 (3%)	33 18
1	DDD	90/140 (64%)	90 (100%)	0	100 100
All	All	359/560 (64%)	355 (99%)	4 (1%)	65 57

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	107	LEU
1	CCC	107	LEU
1	CCC	115	ASN
1	CCC	163[A]	THR

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 oligosaccharides 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	4IR	DDD	201	-	31,48,49	3.20	10 (32%)	47,97,104	3.09	18 (38%)
2	4IR	BBB	201	-	31,48,49	3.17	10 (32%)	47,97,104	3.05	21 (44%)
2	4IR	AAA	201	-	31,48,49	3.12	10 (32%)	47,97,104	2.97	19 (40%)
2	4IR	CCC	201	-	31,48,49	3.08	9 (29%)	47,97,104	2.65	19 (40%)

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	4IR	DDD	201	-	-	4/20/186/204	0/10/9/9
2	4IR	BBB	201	-	-	4/20/186/204	0/10/9/9
2	4IR	AAA	201	-	-	6/20/186/204	0/10/9/9
2	4IR	CCC	201	-	-	4/20/186/204	0/10/9/9

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	CCC	201	4IR	O2-C10	9.42	1.42	1.23
2	BBB	201	4IR	O2-C10	9.19	1.41	1.23
2	DDD	201	4IR	O2-C10	9.17	1.41	1.23
2	AAA	201	4IR	O2-C10	8.78	1.41	1.23
2	DDD	201	4IR	O1-C1	8.10	1.40	1.23
2	AAA	201	4IR	C1-N2	7.80	1.48	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	BBB	201	4IR	C1-N2	7.62	1.47	1.35
2	BBB	201	4IR	O1-C1	7.28	1.38	1.23
2	CCC	201	4IR	O1-C1	7.14	1.38	1.23
2	AAA	201	4IR	O1-C1	7.00	1.38	1.23
2	DDD	201	4IR	C1-N1	6.84	1.46	1.35
2	DDD	201	4IR	C1-N2	6.44	1.46	1.35
2	CCC	201	4IR	C16-S2	-6.31	1.67	1.76
2	AAA	201	4IR	C16-S2	-6.05	1.68	1.76
2	CCC	201	4IR	C1-N1	6.01	1.45	1.35
2	BBB	201	4IR	C16-S2	-5.98	1.68	1.76
2	DDD	201	4IR	C16-S2	-5.68	1.68	1.76
2	CCC	201	4IR	C1-N2	5.40	1.44	1.35
2	AAA	201	4IR	C1-N1	5.37	1.44	1.35
2	BBB	201	4IR	C1-N1	5.02	1.43	1.35
2	BBB	201	4IR	C13-C16	3.00	1.43	1.38
2	BBB	201	4IR	S2-N4	2.64	1.66	1.60
2	AAA	201	4IR	C5-S1	-2.62	1.78	1.82
2	BBB	201	4IR	C13-C12	2.54	1.43	1.38
2	CCC	201	4IR	C13-C16	2.43	1.42	1.38
2	DDD	201	4IR	C5-S1	-2.41	1.78	1.82
2	BBB	201	4IR	C2-N1	2.30	1.49	1.46
2	CCC	201	4IR	O3-S2	2.23	1.46	1.43
2	DDD	201	4IR	C2-N1	2.20	1.49	1.46
2	AAA	201	4IR	C13-C16	2.19	1.42	1.38
2	AAA	201	4IR	C15-C14	2.16	1.42	1.38
2	BBB	201	4IR	O3-S2	2.16	1.45	1.43
2	DDD	201	4IR	C4-N2	2.15	1.49	1.45
2	CCC	201	4IR	C14-C11	2.10	1.42	1.39
2	AAA	201	4IR	O3-S2	2.09	1.45	1.43
2	DDD	201	4IR	C13-C16	2.06	1.42	1.38
2	DDD	201	4IR	C15-C16	2.03	1.42	1.38
2	AAA	201	4IR	C12-C11	2.02	1.42	1.39
2	CCC	201	4IR	C15-C16	2.01	1.42	1.38

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	BBB	201	4IR	O4-S2-O3	-10.06	103.22	119.52
2	DDD	201	4IR	C4-C2-N1	8.09	111.03	102.43
2	DDD	201	4IR	O4-S2-O3	-7.73	107.00	119.52
2	AAA	201	4IR	C4-C2-N1	7.69	110.60	102.43
2	AAA	201	4IR	O4-S2-O3	-7.04	108.11	119.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	DDD	201	4IR	C2-N1-C1	-7.03	103.30	112.46
2	CCC	201	4IR	C11-N3-C10	-6.85	115.52	127.50
2	AAA	201	4IR	C4-N2-C1	-6.74	106.33	112.62
2	AAA	201	4IR	C2-N1-C1	-6.63	103.82	112.46
2	BBB	201	4IR	C11-N3-C10	-6.53	116.06	127.50
2	BBB	201	4IR	C4-C2-N1	6.24	109.06	102.43
2	DDD	201	4IR	C3-C2-N1	-6.05	105.34	113.03
2	AAA	201	4IR	N2-C1-N1	5.47	113.89	108.76
2	DDD	201	4IR	N2-C1-N1	5.45	113.87	108.76
2	CCC	201	4IR	C4-C2-N1	5.24	108.00	102.43
2	DDD	201	4IR	C11-N3-C10	-5.17	118.44	127.50
2	DDD	201	4IR	C4-N2-C1	-5.17	107.80	112.62
2	CCC	201	4IR	O4-S2-O3	-4.95	111.50	119.52
2	BBB	201	4IR	O3-S2-N4	4.88	118.41	109.67
2	AAA	201	4IR	C11-N3-C10	-4.80	119.10	127.50
2	CCC	201	4IR	C2-N1-C1	-4.78	106.23	112.46
2	CCC	201	4IR	C4-N2-C1	-4.78	108.17	112.62
2	BBB	201	4IR	C15-C16-C13	-4.66	113.93	120.44
2	BBB	201	4IR	C9-C10-N3	4.63	122.74	114.59
2	AAA	201	4IR	C9-C10-N3	4.62	122.72	114.59
2	CCC	201	4IR	C3-C2-N1	-4.55	107.25	113.03
2	BBB	201	4IR	C2-N1-C1	-4.55	106.54	112.46
2	BBB	201	4IR	C12-C13-C16	4.39	124.00	119.45
2	AAA	201	4IR	C3-C2-N1	-4.38	107.47	113.03
2	BBB	201	4IR	C13-C16-S2	4.26	124.24	119.76
2	DDD	201	4IR	C9-C10-N3	4.24	122.07	114.59
2	DDD	201	4IR	C15-C16-S2	4.07	124.04	119.76
2	DDD	201	4IR	C15-C16-C13	-4.05	114.79	120.44
2	CCC	201	4IR	C9-C10-N3	3.90	121.46	114.59
2	BBB	201	4IR	C3-C2-N1	-3.82	108.17	113.03
2	CCC	201	4IR	N2-C1-N1	3.81	112.34	108.76
2	CCC	201	4IR	O3-S2-N4	-3.81	102.86	109.67
2	DDD	201	4IR	C12-C13-C16	3.79	123.37	119.45
2	BBB	201	4IR	C14-C15-C16	3.78	123.36	119.45
2	CCC	201	4IR	C12-C13-C16	3.78	123.36	119.45
2	AAA	201	4IR	O1-C1-N1	-3.69	120.64	125.94
2	BBB	201	4IR	O2-C10-N3	-3.68	116.92	123.63
2	AAA	201	4IR	C14-C15-C16	3.57	123.14	119.45
2	AAA	201	4IR	C15-C16-C13	-3.45	115.62	120.44
2	CCC	201	4IR	C15-C16-C13	-3.32	115.82	120.44
2	AAA	201	4IR	C6-C5-S1	-3.23	103.69	112.64
2	AAA	201	4IR	O2-C10-C9	-3.02	116.49	122.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	AAA	201	4IR	C12-C13-C16	3.00	122.55	119.45
2	BBB	201	4IR	O1-C1-N1	-2.95	121.70	125.94
2	DDD	201	4IR	O4-S2-C16	2.95	111.78	108.05
2	CCC	201	4IR	O3-S2-C16	2.93	111.75	108.05
2	BBB	201	4IR	C4-N2-C1	-2.93	109.89	112.62
2	BBB	201	4IR	O3-S2-C16	2.92	111.74	108.05
2	AAA	201	4IR	C13-C16-S2	2.91	122.82	119.76
2	CCC	201	4IR	C5-C4-C2	-2.81	105.68	108.94
2	DDD	201	4IR	C14-C15-C16	2.74	122.28	119.45
2	CCC	201	4IR	C13-C16-S2	2.70	122.60	119.76
2	DDD	201	4IR	C22-C17-C18	2.60	128.79	119.83
2	AAA	201	4IR	C8-C9-C10	-2.53	106.16	113.26
2	AAA	201	4IR	O3-S2-C16	2.48	111.19	108.05
2	BBB	201	4IR	C14-C11-C12	-2.46	115.67	119.03
2	DDD	201	4IR	O2-C10-C9	-2.41	117.62	122.02
2	BBB	201	4IR	C5-C4-N2	2.36	115.24	113.13
2	AAA	201	4IR	O4-S2-C16	2.34	111.00	108.05
2	BBB	201	4IR	C22-C17-C18	2.32	127.81	119.83
2	CCC	201	4IR	O2-C10-C9	-2.31	117.80	122.02
2	BBB	201	4IR	C23-C18-C17	2.28	127.69	119.83
2	BBB	201	4IR	C8-C9-C10	-2.24	106.99	113.26
2	DDD	201	4IR	C7-C6-C5	2.21	118.34	113.86
2	DDD	201	4IR	C5-C4-C2	-2.20	106.38	108.94
2	CCC	201	4IR	C2-C4-N2	2.19	105.02	102.67
2	AAA	201	4IR	C2-C4-N2	2.18	105.02	102.67
2	DDD	201	4IR	O1-C1-N2	-2.17	122.82	125.94
2	CCC	201	4IR	C16-S2-N4	2.17	110.74	107.40
2	CCC	201	4IR	C8-C9-C10	-2.10	107.38	113.26
2	CCC	201	4IR	C3-S1-C5	-2.05	85.67	89.89
2	BBB	201	4IR	N2-C1-N1	2.02	110.66	108.76

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	BBB	201	4IR	S1-C5-C6-C7
2	BBB	201	4IR	C4-C5-C6-C7
2	BBB	201	4IR	C15-C16-S2-O3
2	BBB	201	4IR	C13-C16-S2-O3
2	DDD	201	4IR	C13-C16-S2-O4
2	DDD	201	4IR	C15-C16-S2-O4
2	AAA	201	4IR	C13-C16-S2-O3

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Mol	Chain	Res	Type	Atoms
2	CCC	201	4IR	C15-C16-S2-O3
2	CCC	201	4IR	C13-C16-S2-O3
2	AAA	201	4IR	C15-C16-S2-O3
2	AAA	201	4IR	S1-C5-C6-C7
2	CCC	201	4IR	C27-N4-S2-O4
2	AAA	201	4IR	C13-C16-S2-N4
2	DDD	201	4IR	C15-C16-S2-N4
2	AAA	201	4IR	C15-C16-S2-N4
2	DDD	201	4IR	C13-C16-S2-N4
2	AAA	201	4IR	C12-C11-N3-C10
2	CCC	201	4IR	C13-C16-S2-N4

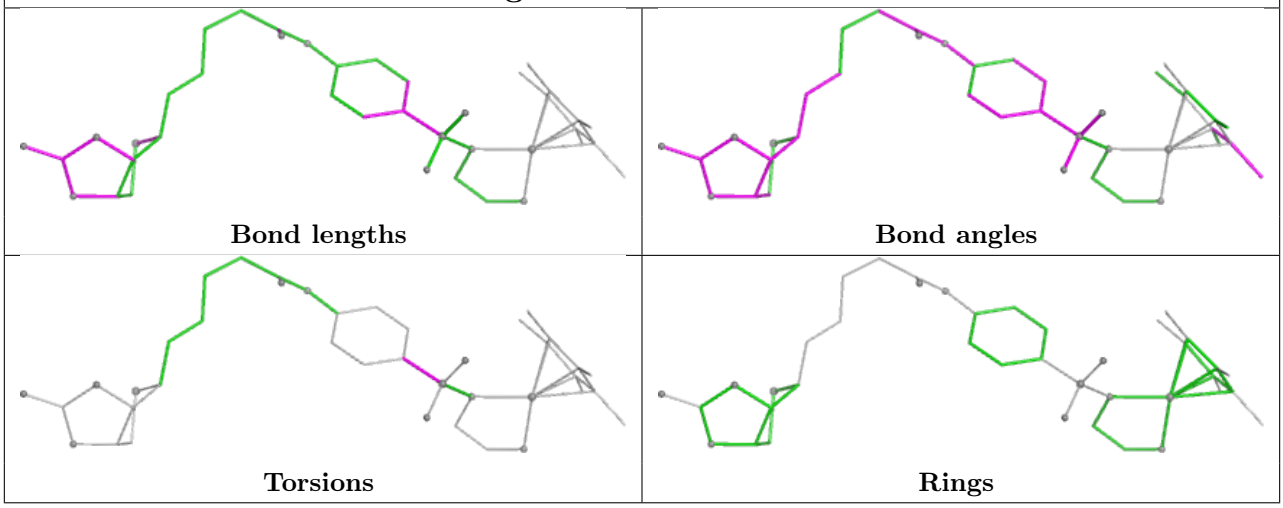
There are no ring outliers.

3 monomers are involved in 6 short contacts:

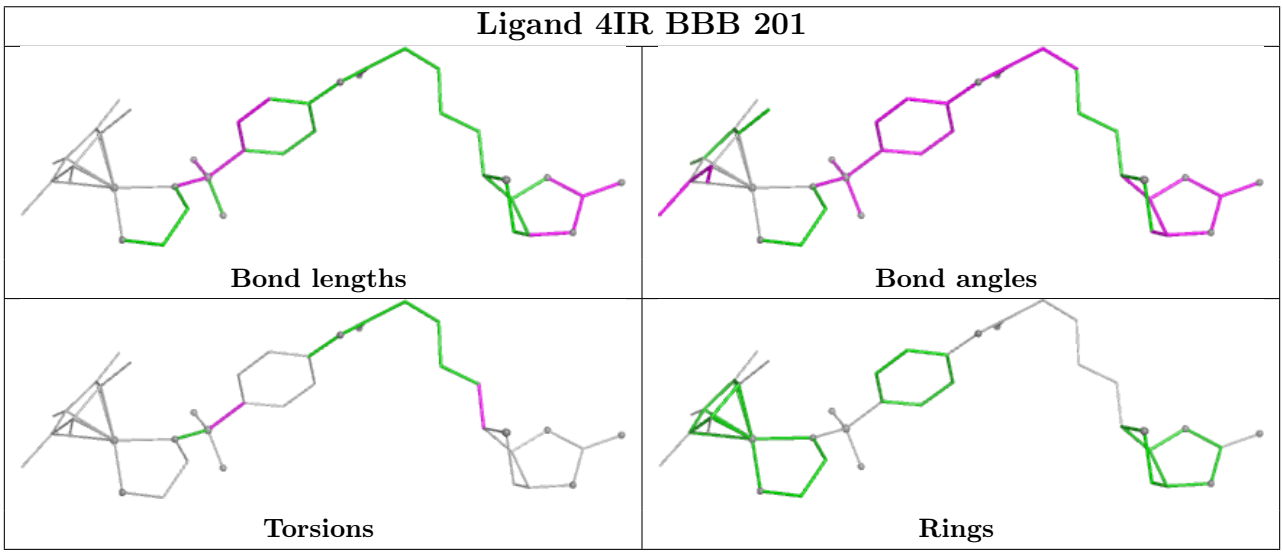
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	201	4IR	3	0
2	AAA	201	4IR	1	0
2	CCC	201	4IR	2	0

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 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.

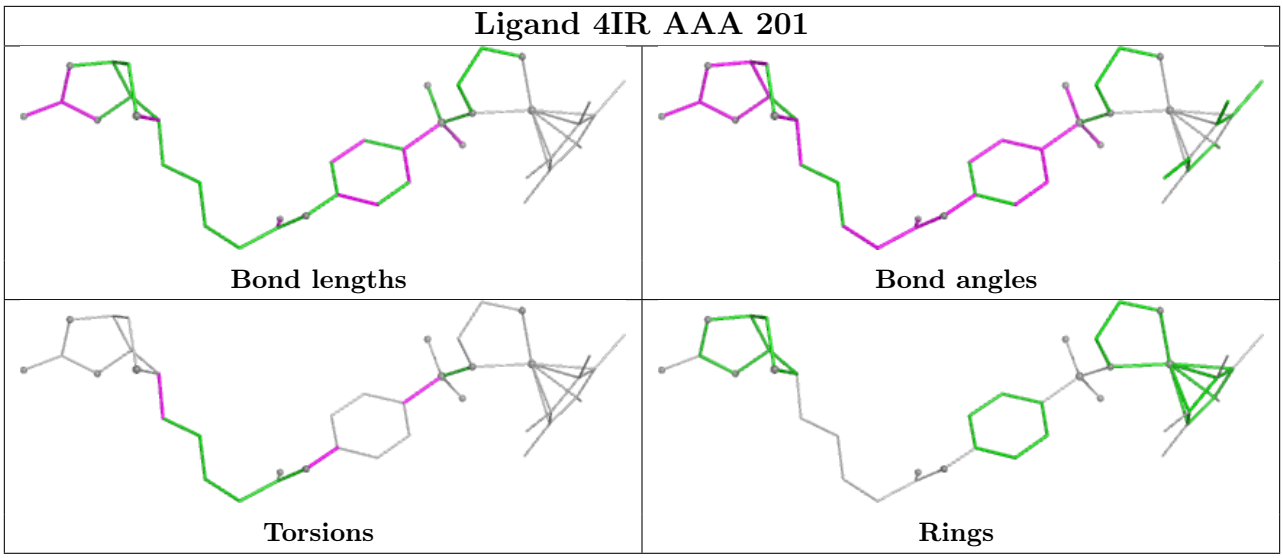
Ligand 4IR DDD 201



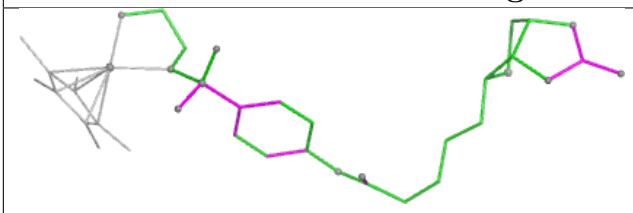
Ligand 4IR BBB 201



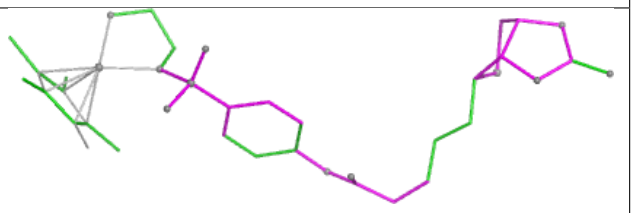
Ligand 4IR AAA 201



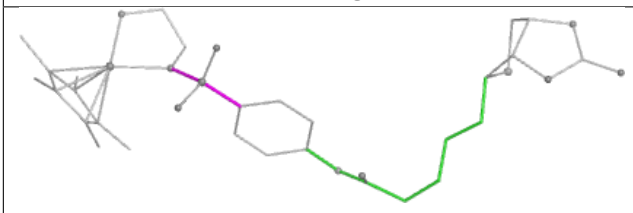
Ligand 4IR CCC 201



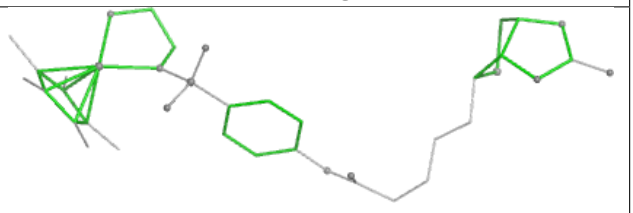
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	122/194 (62%)	0.11	7 (5%)	29	32	14, 22, 46, 56	0
1	BBB	125/194 (64%)	0.16	11 (8%)	15	15	12, 22, 52, 66	2 (1%)
1	CCC	123/194 (63%)	0.17	7 (5%)	29	32	12, 22, 48, 65	2 (1%)
1	DDD	122/194 (62%)	0.19	8 (6%)	24	26	13, 23, 47, 62	2 (1%)
All	All	492/776 (63%)	0.16	33 (6%)	24	26	12, 22, 51, 66	6 (1%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	AAA	49	ALA	5.4
1	DDD	49	ALA	3.9
1	CCC	84	ALA	3.9
1	CCC	13	ASP	3.9
1	BBB	84	ALA	3.6
1	CCC	167	VAL	3.5
1	DDD	167	VAL	3.5
1	CCC	49	ALA	3.5
1	DDD	84	ALA	3.3
1	BBB	167	VAL	3.1
1	DDD	133	GLY	3.0
1	BBB	117	TYR	2.9
1	BBB	51	ALA	2.9
1	CCC	168	LYS	2.9
1	BBB	13	ASP	2.8
1	CCC	50	GLY	2.8
1	AAA	84	ALA	2.7
1	BBB	150	GLU	2.7
1	BBB	85	GLU	2.6
1	DDD	100	THR	2.6
1	AAA	117	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	BBB	100	THR	2.5
1	BBB	49	ALA	2.4
1	BBB	168	LYS	2.4
1	DDD	117	TYR	2.3
1	AAA	13	ASP	2.3
1	AAA	134	ALA	2.2
1	AAA	135	GLU	2.2
1	BBB	134	ALA	2.2
1	AAA	100	THR	2.1
1	DDD	168	LYS	2.1
1	CCC	36	ASP	2.1
1	DDD	36	ASP	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 oligosaccharides in this entry.

6.4 Ligands (i)

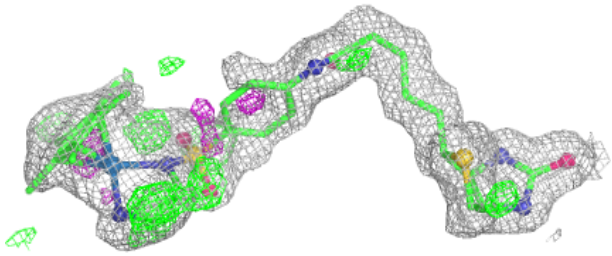
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

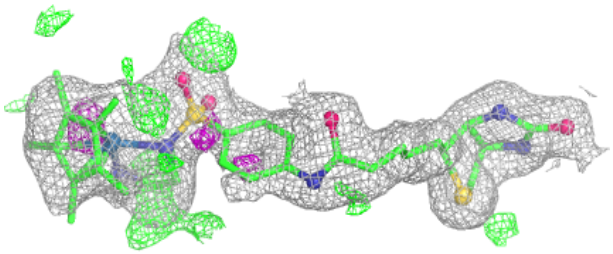
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	4IR	BBB	201	40/41	0.96	0.13	14,38,52,54	1
2	4IR	AAA	201	40/41	0.98	0.10	15,31,43,47	1
2	4IR	CCC	201	40/41	0.98	0.10	14,32,42,43	1
2	4IR	DDD	201	40/41	0.98	0.11	15,30,42,44	1

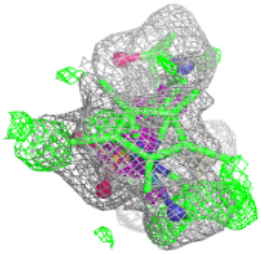
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around 4IR BBB 201:

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

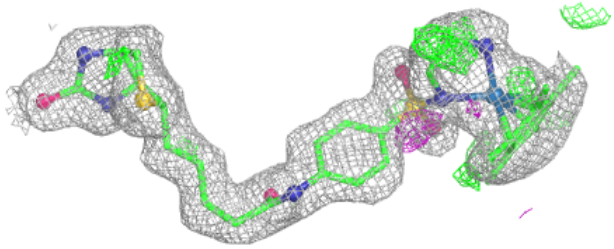


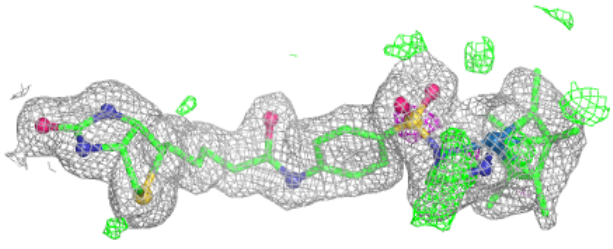


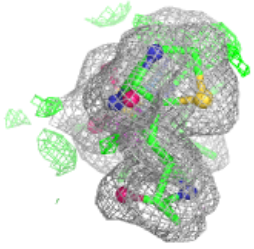


Electron density around 4IR AAA 201:

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

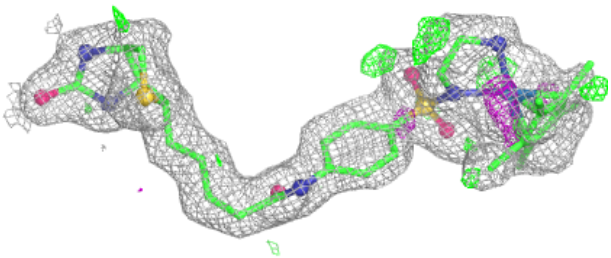


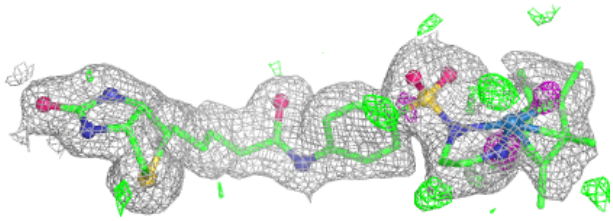


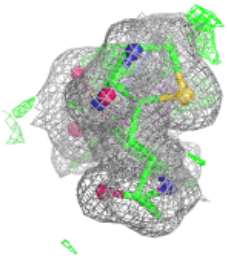


Electron density around 4IR CCC 201:

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

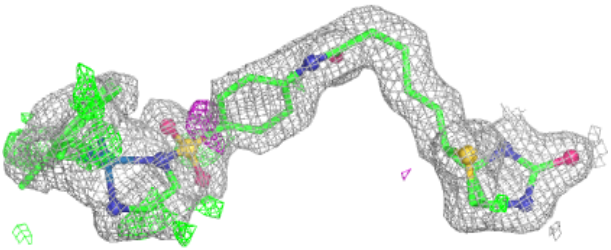


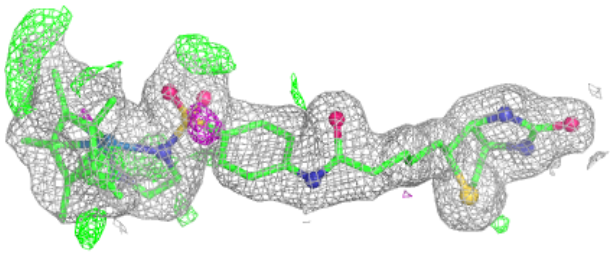


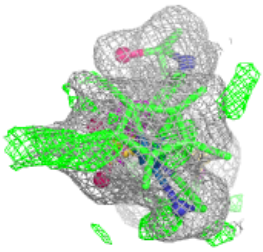


Electron density around 4IR DDD 201:

$2mF_o$-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.