wwPDB X-ray Structure Validation Summary Report (i)

Nov 15, 2022 – 03:20 pm GMT

PDB ID	:	6YYO
Title	:	Structure of Cathepsin S in complex with Compound 1
Authors	:	Wagener, M.; Schade, M.; Merla, B.; Hars, U.; Kueckelhaus, S.Q.
Deposited on	:	2020-05-05
Resolution	:	1.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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:

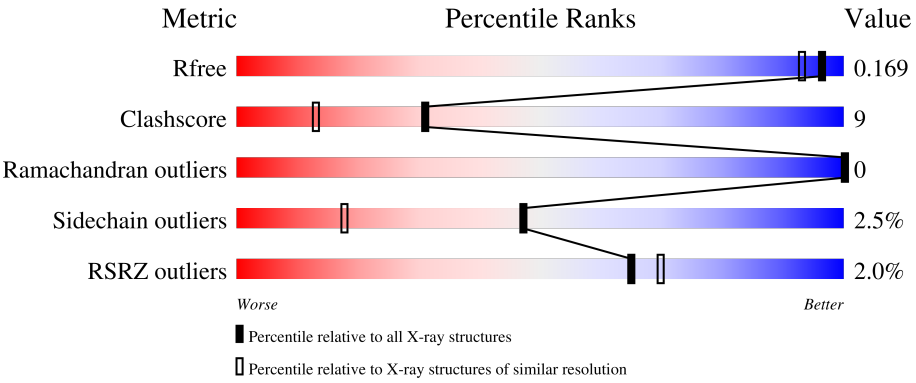
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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	225	3% 85% 12%
1	BBB	225	% 89% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	BBB	303	-	-	X	-
3	EDO	BBB	316	-	-	X	-
3	EDO	BBB	322	-	-	X	-
6	FLC	BBB	302	-	X	X	-

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 4477 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.

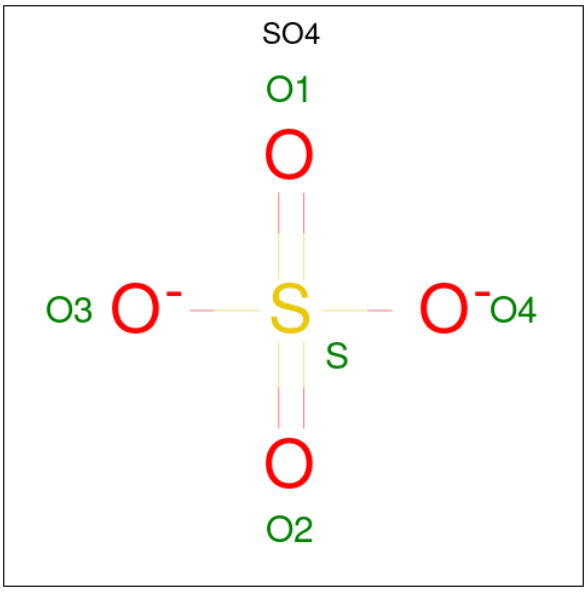
- Molecule 1 is a protein called Cathepsin S.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	AAA	220	Total	C	N	O	S	0	12	0
			1786	1132	304	338	12			
1	BBB	220	Total	C	N	O	S	0	14	0
			1799	1143	308	336	12			

There are 12 discrepancies between the modelled and reference sequences:

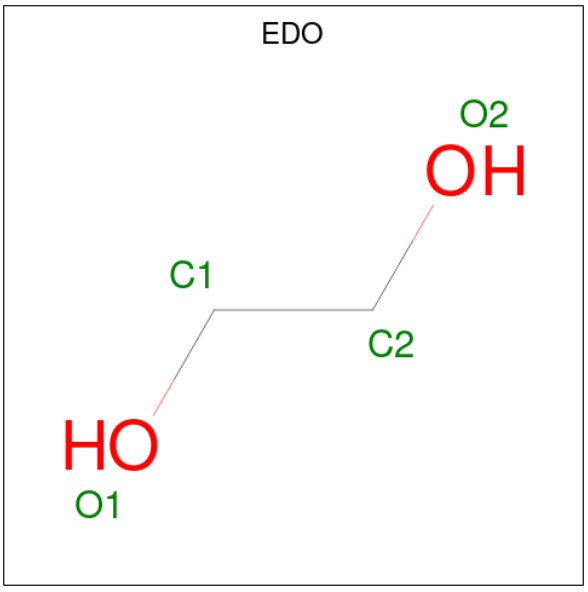
Chain	Residue	Modelled	Actual	Comment	Reference
AAA	218	HIS	-	expression tag	UNP P25774
AAA	219	HIS	-	expression tag	UNP P25774
AAA	220	HIS	-	expression tag	UNP P25774
AAA	221	HIS	-	expression tag	UNP P25774
AAA	222	HIS	-	expression tag	UNP P25774
AAA	223	HIS	-	expression tag	UNP P25774
BBB	218	HIS	-	expression tag	UNP P25774
BBB	219	HIS	-	expression tag	UNP P25774
BBB	220	HIS	-	expression tag	UNP P25774
BBB	221	HIS	-	expression tag	UNP P25774
BBB	222	HIS	-	expression tag	UNP P25774
BBB	223	HIS	-	expression tag	UNP P25774

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	AAA	1	Total O S 5 4 1	0	0
2	BBB	1	Total O S 5 4 1	0	0
2	BBB	1	Total O S 5 4 1	0	0
2	BBB	1	Total O S 5 4 1	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	AAA	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0

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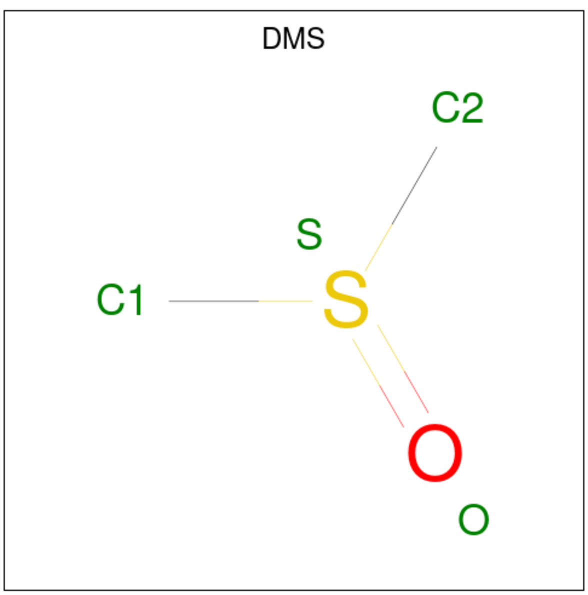
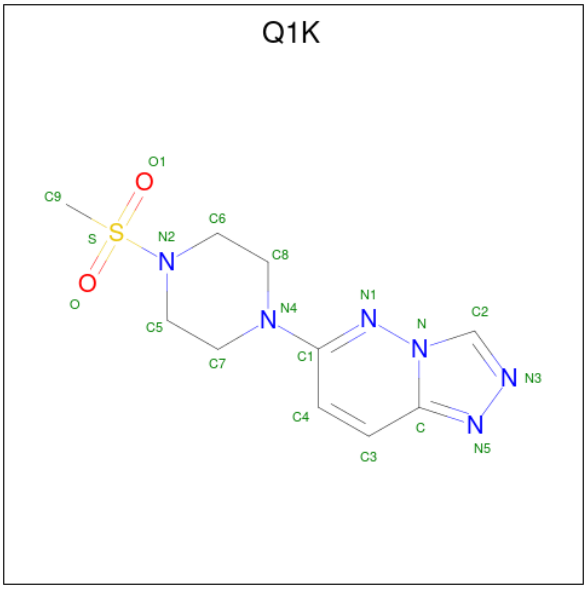
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0
3	BBB	1	Total C O 4 2 2	0	0

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



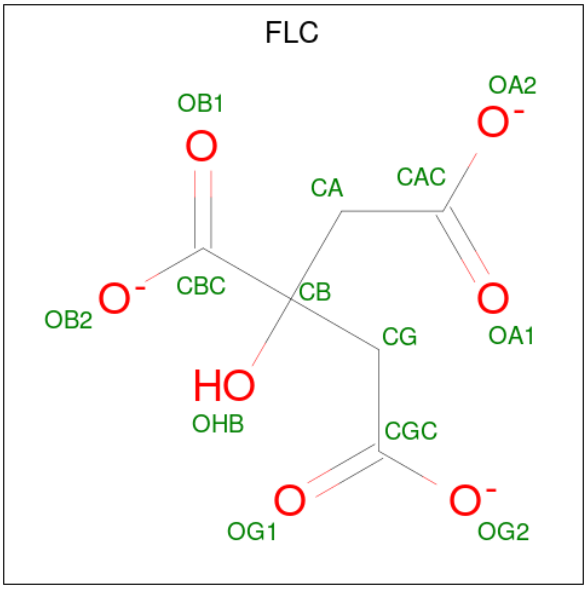
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	AAA	1	Total C O S 4 2 1 1	0	0

- Molecule 5 is 6-(4-methylsulfonylpiperazin-1-yl)-[1,2,4]triazolo[4,3-b]pyridazine (three-letter code: Q1K) (formula: $C_{10}H_{14}N_6O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	AAA	1	Total	C	N	O	S	0	0
			19	10	6	2	1		
5	BBB	1	Total	C	N	O	S	0	0
			19	10	6	2	1		

- Molecule 6 is CITRATE ANION (three-letter code: FLC) (formula: $C_6H_5O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	BBB	1	Total C O 13 6 7	0	0

- Molecule 7 is water.

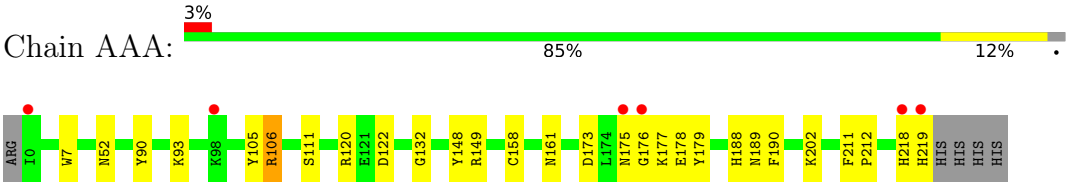
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	AAA	346	Total O 347 347	0	1
7	BBB	342	Total O 342 342	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

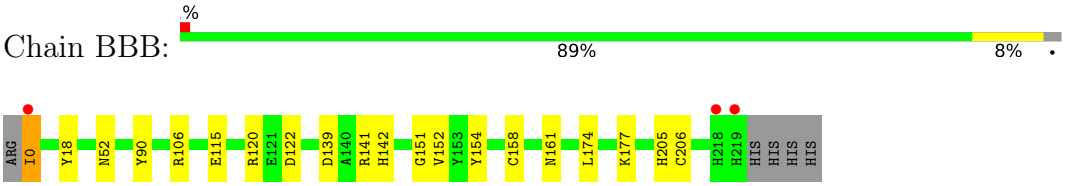
• Molecule 1: Cathepsin S

Chain AAA:



• Molecule 1: Cathepsin S

Chain BBB:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	85.46Å 85.46Å 150.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.30 – 1.50 28.28 – 1.50	Depositor EDS
% Data completeness (in resolution range)	97.3 (28.30-1.50) 97.4 (28.28-1.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.137 , 0.169 0.138 , 0.169	Depositor DCC
R_{free} test set	4406 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	15.6	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	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	0.97	EDS
Total number of atoms	4477	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.77% 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: EDO, Q1K, DMS, FLC, SO4

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	0.82	0/1861	0.94	4/2515 (0.2%)
1	BBB	0.81	2/1884 (0.1%)	0.96	2/2544 (0.1%)
All	All	0.81	2/3745 (0.1%)	0.95	6/5059 (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	AAA	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	BBB	115[A]	GLU	CD-OE2	-5.02	1.20	1.25
1	BBB	115[B]	GLU	CD-OE2	-5.02	1.20	1.25

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	BBB	106	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	BBB	106	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	AAA	105	TYR	CB-CG-CD1	5.53	124.32	121.00
1	AAA	106[A]	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	AAA	106[B]	ARG	NE-CZ-NH1	5.15	122.88	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	AAA	190	PHE	Mainchain

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	1786	0	1726	29	0
1	BBB	1799	0	1756	20	0
2	AAA	5	0	0	1	0
2	BBB	15	0	0	3	0
3	AAA	56	0	83	6	2
3	BBB	72	0	106	20	0
4	AAA	4	0	6	0	0
5	AAA	19	0	0	0	0
5	BBB	19	0	0	0	0
6	BBB	13	0	5	4	0
7	AAA	347	0	0	13	2
7	BBB	342	0	0	21	2
All	All	4477	0	3682	68	5

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.

The worst 5 of 68 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:AAA:173[B]:ASP:OD1	1:AAA:176[B]:GLY:N	1.68	1.26
1:AAA:120[A]:ARG:NH1	7:AAA:606:HOH:O	1.72	1.22
1:AAA:189:ASN:ND2	7:AAA:607:HOH:O	1.73	1.21
1:AAA:173[B]:ASP:OD1	1:AAA:176[B]:GLY:CA	1.95	1.15
2:BBB:303:SO4:O1	7:BBB:404:HOH:O	1.64	1.14

All (5) 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)
7:AAA:848:HOH:O	7:AAA:848:HOH:O[5_555]	1.43	0.77
3:AAA:302:EDO:O2	3:AAA:302:EDO:O2[5_555]	1.56	0.64
7:AAA:710:HOH:O	7:BBB:422:HOH:O[8_655]	1.71	0.49
3:AAA:302:EDO:O1	3:AAA:302:EDO:O1[5_555]	1.94	0.26
7:BBB:510:HOH:O	7:BBB:510:HOH:O[6_565]	2.07	0.13

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	230/225 (102%)	226 (98%)	4 (2%)	0	100	100
1	BBB	232/225 (103%)	228 (98%)	4 (2%)	0	100	100
All	All	462/450 (103%)	454 (98%)	8 (2%)	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	192/186 (103%)	187 (97%)	5 (3%)	46	16
1	BBB	195/186 (105%)	191 (98%)	4 (2%)	53	23
All	All	387/372 (104%)	378 (98%)	9 (2%)	47	20

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	BBB	90	TYR
1	BBB	158	CYS
1	AAA	158	CYS
1	AAA	177	LYS
1	BBB	0	ILE

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)

40 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	$\#\|Z\| > 2$
3	EDO	BBB	305	-	3,3,3	0.74	0	2,2,2	0.68	0
2	SO4	BBB	303	-	4,4,4	0.54	0	6,6,6	0.37	0
3	EDO	BBB	319	-	3,3,3	0.33	0	2,2,2	0.35	0
3	EDO	AAA	309	-	3,3,3	0.76	0	2,2,2	0.19	0
3	EDO	AAA	302	-	3,3,3	0.12	0	2,2,2	0.28	0
2	SO4	BBB	304	-	4,4,4	0.34	0	6,6,6	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	Q1K	AAA	317	-	17,21,21	2.76	6 (35%)	21,31,31	2.33	10 (47%)
3	EDO	BBB	306	-	3,3,3	0.11	0	2,2,2	0.60	0
3	EDO	BBB	317	-	3,3,3	0.38	0	2,2,2	0.64	0
3	EDO	AAA	308	-	3,3,3	0.57	0	2,2,2	0.77	0
3	EDO	AAA	313	-	3,3,3	0.66	0	2,2,2	0.38	0
3	EDO	AAA	304	-	3,3,3	0.16	0	2,2,2	0.18	0
3	EDO	AAA	307	-	3,3,3	0.52	0	2,2,2	0.51	0
3	EDO	BBB	320	-	3,3,3	0.56	0	2,2,2	0.52	0
3	EDO	BBB	321	-	3,3,3	0.07	0	2,2,2	0.12	0
3	EDO	AAA	305	-	3,3,3	0.32	0	2,2,2	0.32	0
3	EDO	AAA	316	-	3,3,3	0.27	0	2,2,2	0.42	0
3	EDO	BBB	315	-	3,3,3	0.11	0	2,2,2	0.36	0
3	EDO	AAA	314	-	3,3,3	0.35	0	2,2,2	0.11	0
3	EDO	BBB	307	-	3,3,3	0.47	0	2,2,2	0.17	0
3	EDO	AAA	310	-	3,3,3	0.37	0	2,2,2	0.55	0
6	FLC	BBB	302	-	12,12,12	1.46	3 (25%)	17,17,17	3.24	6 (35%)
4	DMS	AAA	306	-	3,3,3	0.32	0	3,3,3	0.34	0
3	EDO	BBB	312	-	3,3,3	0.36	0	2,2,2	0.48	0
2	SO4	AAA	301	-	4,4,4	0.26	0	6,6,6	0.30	0
3	EDO	BBB	309	-	3,3,3	0.40	0	2,2,2	0.29	0
2	SO4	BBB	301	-	4,4,4	2.03	2 (50%)	6,6,6	1.17	1 (16%)
3	EDO	BBB	314	-	3,3,3	0.39	0	2,2,2	0.33	0
3	EDO	AAA	311	-	3,3,3	0.34	0	2,2,2	0.60	0
3	EDO	BBB	318	-	3,3,3	0.69	0	2,2,2	0.99	0
3	EDO	AAA	303	-	3,3,3	0.21	0	2,2,2	0.04	0
3	EDO	BBB	311	-	3,3,3	0.11	0	2,2,2	0.53	0
3	EDO	AAA	315	-	3,3,3	0.25	0	2,2,2	0.48	0
3	EDO	BBB	316	-	3,3,3	0.89	0	2,2,2	0.58	0
5	Q1K	BBB	323	-	17,21,21	2.11	6 (35%)	21,31,31	3.48	11 (52%)
3	EDO	BBB	308	-	3,3,3	0.07	0	2,2,2	0.31	0
3	EDO	BBB	313	-	3,3,3	0.85	0	2,2,2	0.91	0
3	EDO	BBB	322	-	3,3,3	0.20	0	2,2,2	0.18	0
3	EDO	BBB	310	-	3,3,3	0.19	0	2,2,2	0.28	0
3	EDO	AAA	312	-	3,3,3	0.28	0	2,2,2	0.26	0

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
3	EDO	BBB	305	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	EDO	BBB	319	-	-	0/1/1/1	-
3	EDO	AAA	309	-	-	1/1/1/1	-
3	EDO	AAA	302	-	-	0/1/1/1	-
5	Q1K	AAA	317	-	-	0/10/20/20	0/3/3/3
3	EDO	BBB	306	-	-	0/1/1/1	-
3	EDO	BBB	317	-	-	0/1/1/1	-
3	EDO	AAA	308	-	-	1/1/1/1	-
3	EDO	AAA	313	-	-	0/1/1/1	-
3	EDO	AAA	304	-	-	1/1/1/1	-
3	EDO	AAA	307	-	-	0/1/1/1	-
3	EDO	BBB	320	-	-	1/1/1/1	-
3	EDO	BBB	321	-	-	0/1/1/1	-
3	EDO	AAA	305	-	-	1/1/1/1	-
3	EDO	AAA	316	-	-	1/1/1/1	-
3	EDO	BBB	315	-	-	1/1/1/1	-
3	EDO	AAA	314	-	-	1/1/1/1	-
3	EDO	BBB	307	-	-	0/1/1/1	-
3	EDO	AAA	310	-	-	0/1/1/1	-
6	FLC	BBB	302	-	-	9/16/16/16	-
3	EDO	BBB	312	-	-	1/1/1/1	-
3	EDO	BBB	309	-	-	0/1/1/1	-
3	EDO	BBB	314	-	-	0/1/1/1	-
3	EDO	AAA	311	-	-	0/1/1/1	-
3	EDO	BBB	318	-	-	0/1/1/1	-
3	EDO	AAA	303	-	-	0/1/1/1	-
3	EDO	BBB	311	-	-	0/1/1/1	-
3	EDO	AAA	315	-	-	1/1/1/1	-
3	EDO	BBB	316	-	-	1/1/1/1	-
5	Q1K	BBB	323	-	-	0/10/20/20	0/3/3/3
3	EDO	BBB	308	-	-	1/1/1/1	-
3	EDO	BBB	313	-	-	0/1/1/1	-
3	EDO	BBB	322	-	-	0/1/1/1	-
3	EDO	BBB	310	-	-	1/1/1/1	-
3	EDO	AAA	312	-	-	1/1/1/1	-

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	AAA	317	Q1K	C1-N1	6.91	1.42	1.32
5	AAA	317	Q1K	N3-N5	-5.89	1.26	1.37
5	BBB	323	Q1K	C1-N1	4.76	1.39	1.32
5	AAA	317	Q1K	C6-N2	3.27	1.51	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	BBB	323	Q1K	S-N2	-3.23	1.59	1.63

The worst 5 of 28 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	BBB	323	Q1K	O1-S-N2	-8.71	99.73	107.03
6	BBB	302	FLC	OB1-CBC-CB	-7.96	110.98	122.25
5	BBB	323	Q1K	C4-C3-C	-6.86	111.45	119.76
6	BBB	302	FLC	OB2-CBC-CB	6.51	124.36	113.05
6	BBB	302	FLC	CA-CB-CBC	5.18	121.24	110.11

There are no chirality outliers.

5 of 24 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	BBB	302	FLC	CG-CB-CBC-OB2
6	BBB	302	FLC	OHB-CB-CBC-OB1
6	BBB	302	FLC	OHB-CB-CBC-OB2
6	BBB	302	FLC	CBC-CB-CG-CGC
6	BBB	302	FLC	CG-CB-CBC-OB1

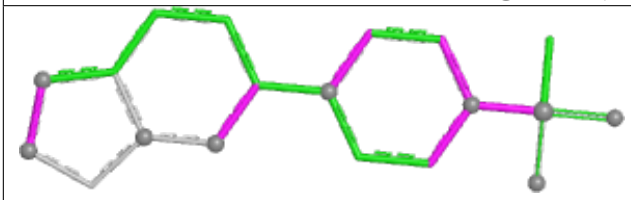
There are no ring outliers.

15 monomers are involved in 35 short contacts:

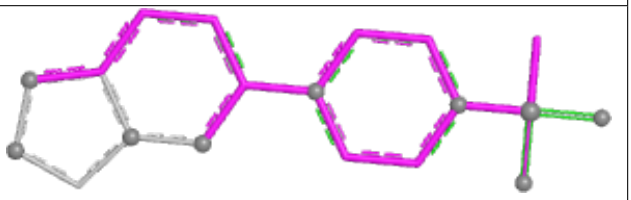
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	BBB	303	SO4	2	0
3	AAA	302	EDO	1	2
3	BBB	317	EDO	1	0
3	AAA	308	EDO	2	0
3	AAA	304	EDO	1	0
3	BBB	320	EDO	3	0
3	BBB	315	EDO	3	0
6	BBB	302	FLC	4	0
2	AAA	301	SO4	1	0
2	BBB	301	SO4	1	0
3	AAA	311	EDO	1	0
3	BBB	318	EDO	1	0
3	AAA	315	EDO	1	0
3	BBB	316	EDO	5	0
3	BBB	322	EDO	7	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.

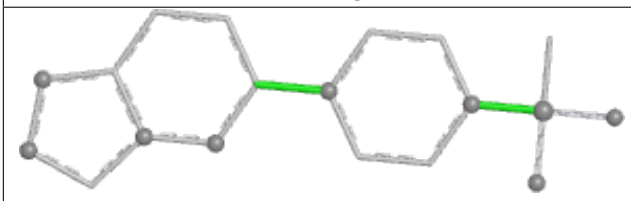
Ligand Q1K AAA 317



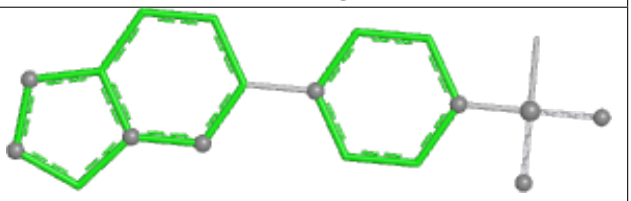
Bond lengths



Bond angles

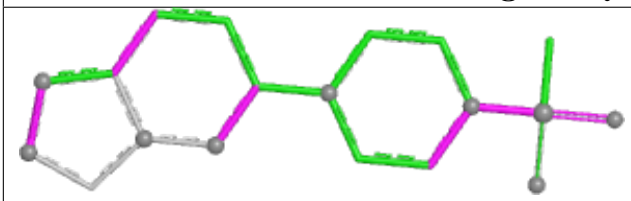


Torsions

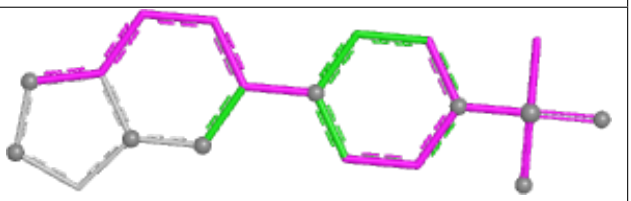


Rings

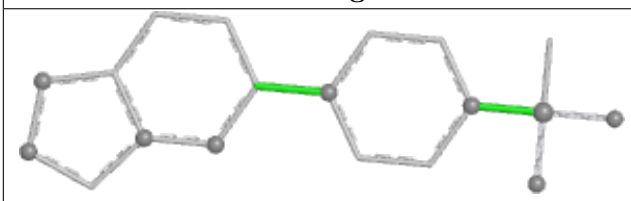
Ligand Q1K BBB 323



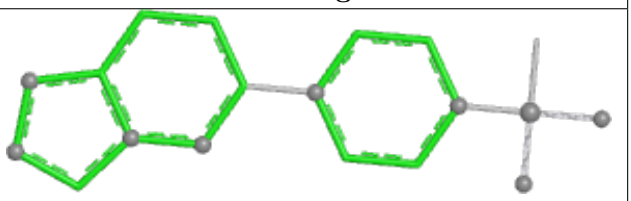
Bond lengths



Bond angles



Torsions



Rings

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	220/225 (97%)	-0.31	6 (2%)	54	59	11, 16, 28, 69	0
1	BBB	220/225 (97%)	-0.31	3 (1%)	75	79	11, 16, 25, 50	0
All	All	440/450 (97%)	-0.31	9 (2%)	65	70	11, 16, 26, 69	0

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	BBB	0	ILE	8.1
1	AAA	219	HIS	7.8
1	AAA	0	ILE	7.0
1	BBB	219	HIS	5.2
1	AAA	218	HIS	3.4

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

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

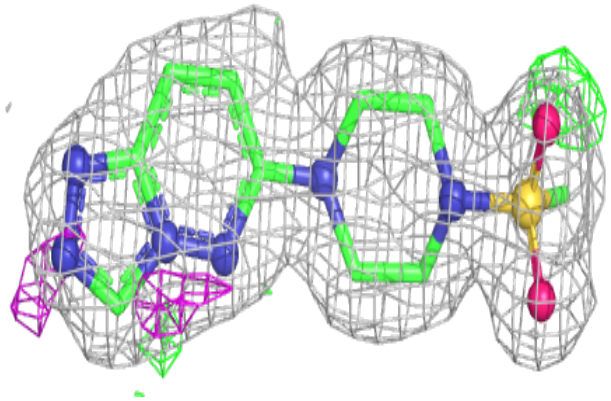
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	EDO	AAA	316	4/4	0.57	0.21	55,56,57,58	0
3	EDO	AAA	313	4/4	0.73	0.25	41,46,48,53	0
3	EDO	AAA	314	4/4	0.76	0.14	51,52,53,54	0
3	EDO	AAA	305	4/4	0.76	0.15	49,50,50,52	0
3	EDO	BBB	316	4/4	0.78	0.15	34,36,37,37	0
6	FLC	BBB	302	13/13	0.81	0.16	29,30,32,33	13
3	EDO	BBB	321	4/4	0.84	0.15	54,56,58,60	0
3	EDO	BBB	313	4/4	0.86	0.15	29,35,36,37	0
3	EDO	AAA	311	4/4	0.86	0.14	28,31,33,35	0
3	EDO	AAA	308	4/4	0.86	0.19	25,31,33,42	0
3	EDO	BBB	312	4/4	0.86	0.18	38,39,39,40	0
3	EDO	BBB	305	4/4	0.87	0.11	30,38,42,44	0
3	EDO	BBB	319	4/4	0.87	0.22	31,36,39,42	0
3	EDO	BBB	310	4/4	0.88	0.23	50,51,52,53	0
3	EDO	BBB	311	4/4	0.88	0.09	41,42,44,44	0
2	SO4	BBB	303	5/5	0.88	0.20	31,34,35,35	5
2	SO4	AAA	301	5/5	0.88	0.17	26,27,30,32	5
3	EDO	BBB	307	4/4	0.89	0.10	35,36,38,38	0
3	EDO	AAA	315	4/4	0.89	0.12	27,29,30,34	0
3	EDO	BBB	318	4/4	0.89	0.15	30,35,36,39	0
3	EDO	BBB	309	4/4	0.90	0.16	29,35,37,41	0
3	EDO	AAA	310	4/4	0.90	0.15	26,30,33,34	0
3	EDO	AAA	304	4/4	0.91	0.12	38,43,45,51	0
3	EDO	BBB	320	4/4	0.91	0.19	32,32,38,42	0
3	EDO	BBB	317	4/4	0.91	0.11	27,35,39,44	0
3	EDO	BBB	322	4/4	0.91	0.23	35,35,36,41	0
3	EDO	AAA	302	4/4	0.91	0.18	47,56,58,61	0
3	EDO	BBB	308	4/4	0.92	0.15	38,38,40,40	4
3	EDO	AAA	312	4/4	0.93	0.12	33,41,41,47	0
3	EDO	AAA	307	4/4	0.94	0.07	30,30,31,35	0
2	SO4	BBB	304	5/5	0.94	0.25	78,81,84,85	0
3	EDO	AAA	309	4/4	0.94	0.10	30,35,36,36	0
3	EDO	BBB	314	4/4	0.94	0.11	30,34,35,35	0
4	DMS	AAA	306	4/4	0.95	0.21	42,48,51,52	0
3	EDO	BBB	315	4/4	0.95	0.10	27,36,37,42	0
3	EDO	AAA	303	4/4	0.96	0.09	22,26,29,33	0
3	EDO	BBB	306	4/4	0.96	0.18	21,29,31,39	0
5	Q1K	AAA	317	19/19	0.97	0.07	19,22,33,38	0
5	Q1K	BBB	323	19/19	0.97	0.07	18,22,31,31	0
2	SO4	BBB	301	5/5	0.97	0.11	44,45,46,50	5

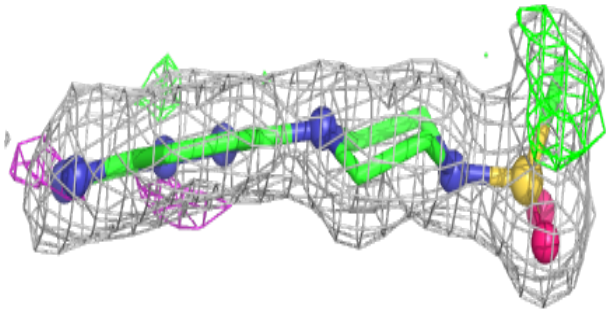
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

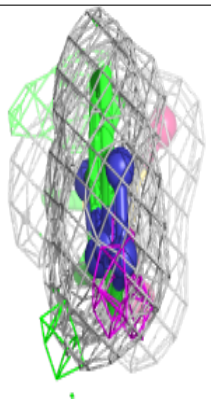
orientation to approximate a three-dimensional view.

Electron density around Q1K AAA 317:

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

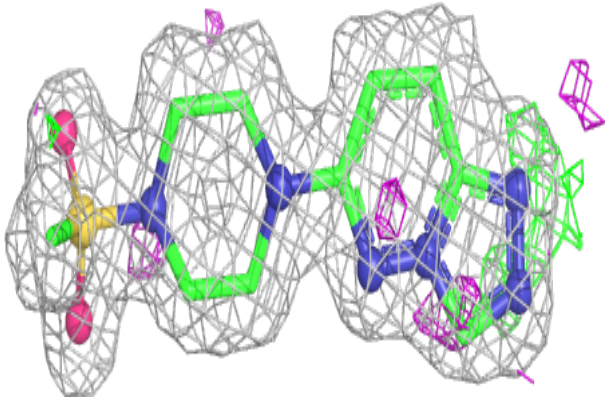


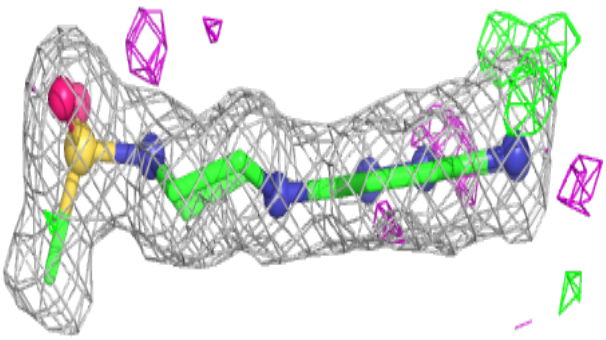


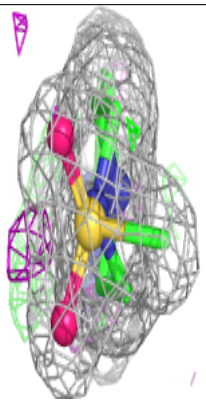


Electron density around Q1K BBB 323:

$2mF_o$-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.