wwPDB X-ray Structure Validation Summary Report (i)

Dec 15, 2016 – 08:04 PM EST

PDB ID	:	3H6S
Title	:	Structure of clitocypin - cathepsin V complex
Authors	:	Renko, M.; Sabotic, J.; Brzin, J.; Turk, D.
Deposited on	:	2009-04-23
Resolution	:	2.22 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

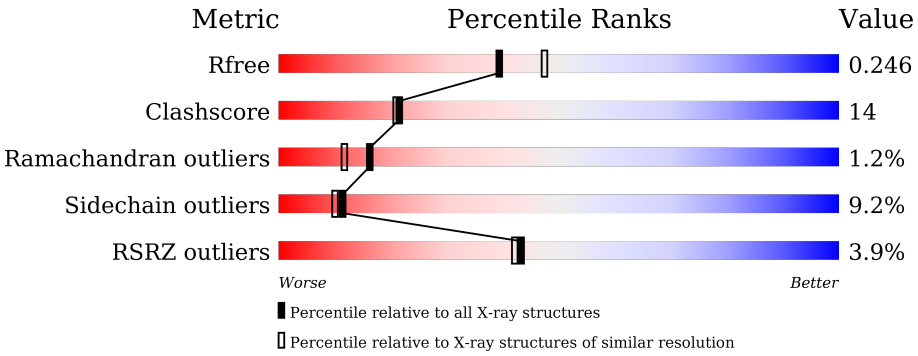
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.22 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}	91344	4405 (2.24-2.20)
Clashscore	102246	5146 (2.24-2.20)
Ramachandran outliers	100387	5065 (2.24-2.20)
Sidechain outliers	100360	5066 (2.24-2.20)
RSRZ outliers	91569	4414 (2.24-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	221	2% 75% 21% •
1	B	221	3% 74% 21% 5%
1	C	221	79% 19% •
1	D	221	6% 74% 23% •
2	E	152	4% 73% 19% 6% •
2	F	152	3% 66% 25% 9% •

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Mol	Chain	Length	Quality of chain
2	G	152	3% 59% 29% 9%
2	H	152	9% 61% 28% 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
3	SO4	F	153	-	X	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12387 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 L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	220	Total	C	N	O	S	7	0	0
			1683	1061	288	324	10			
1	B	220	Total	C	N	O	S	17	0	0
			1683	1061	288	324	10			
1	C	220	Total	C	N	O	S	8	0	0
			1683	1061	288	324	10			
1	D	220	Total	C	N	O	S	11	0	0
			1683	1061	288	324	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	108	GLN	ASN	ENGINEERED	UNP O60911
A	179	ASP	ASN	ENGINEERED	UNP O60911
B	108	GLN	ASN	ENGINEERED	UNP O60911
B	179	ASP	ASN	ENGINEERED	UNP O60911
C	108	GLN	ASN	ENGINEERED	UNP O60911
C	179	ASP	ASN	ENGINEERED	UNP O60911
D	108	GLN	ASN	ENGINEERED	UNP O60911
D	179	ASP	ASN	ENGINEERED	UNP O60911

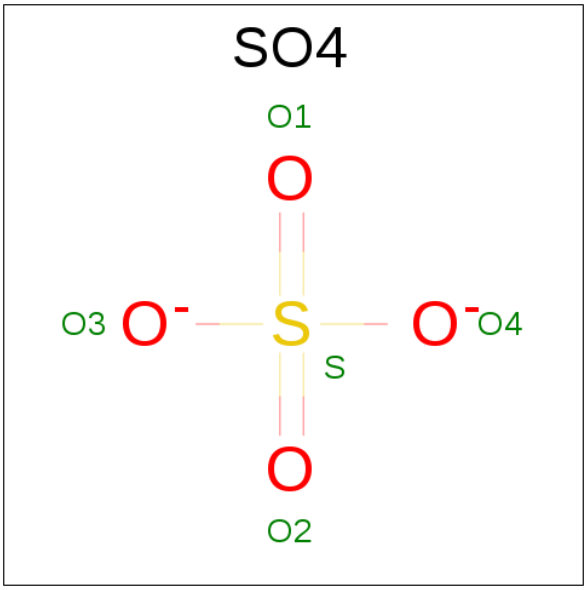
- Molecule 2 is a protein called Clitocypin analog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	152	Total	C	N	O	S	47	0	0
			1192	752	204	233	3			
2	F	152	Total	C	N	O	S	38	0	0
			1192	752	204	233	3			
2	G	152	Total	C	N	O	S	64	0	0
			1192	752	204	233	3			
2	H	152	Total	C	N	O	S	51	0	0
			1192	752	204	233	3			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	82	SME	LEU	ENGINEERED	UNP Q3Y9I6
E	89	SME	ILE	ENGINEERED	UNP Q3Y9I6
F	82	SME	LEU	ENGINEERED	UNP Q3Y9I6
F	89	SME	ILE	ENGINEERED	UNP Q3Y9I6
G	82	SME	LEU	ENGINEERED	UNP Q3Y9I6
G	89	SME	ILE	ENGINEERED	UNP Q3Y9I6
H	82	SME	LEU	ENGINEERED	UNP Q3Y9I6
H	89	SME	ILE	ENGINEERED	UNP Q3Y9I6

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

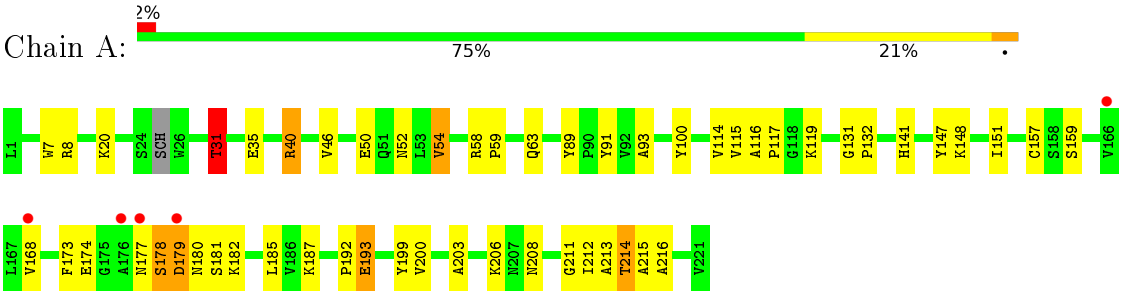
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	169	Total O 169 169	0	0
4	B	124	Total O 124 124	0	0
4	C	174	Total O 174 174	0	0
4	D	97	Total O 97 97	0	0
4	E	85	Total O 85 85	0	0
4	F	81	Total O 81 81	0	0
4	G	64	Total O 64 64	0	0
4	H	63	Total O 63 63	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

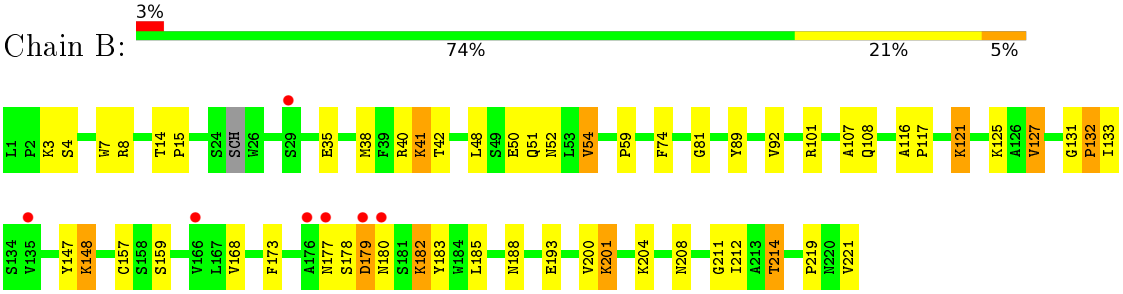
- Molecule 1: Cathepsin L2

Chain A:



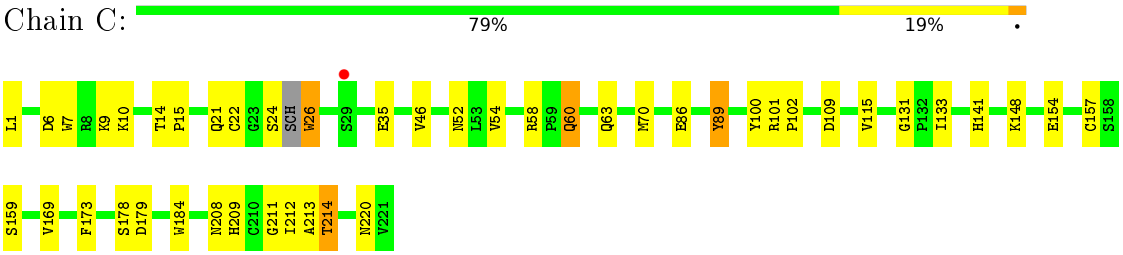
- Molecule 1: Cathepsin L2

Chain B:



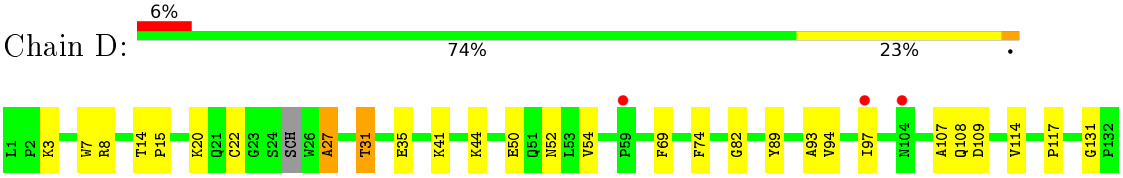
- Molecule 1: Cathepsin L2

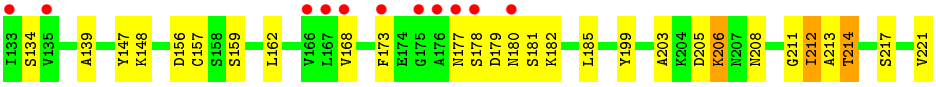
Chain C:



- Molecule 1: Cathepsin L2

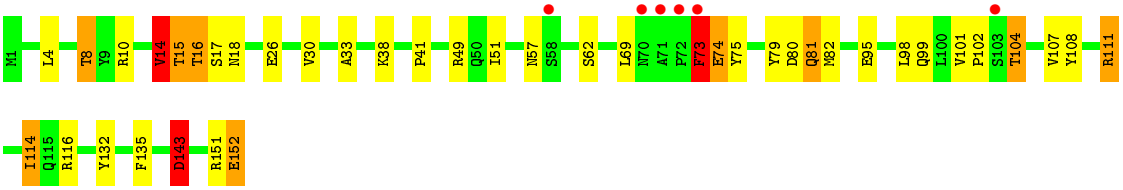
Chain D:





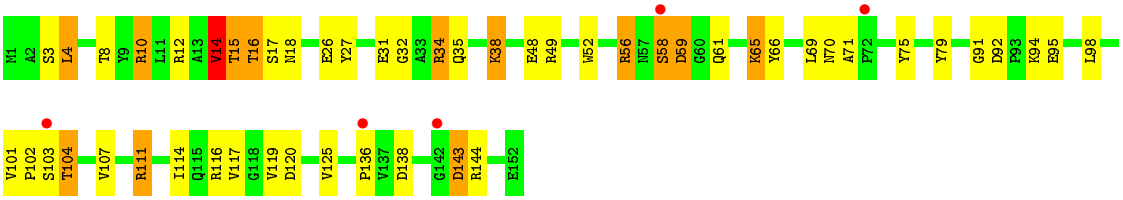
• Molecule 2: Clitocypin analog

Chain E:



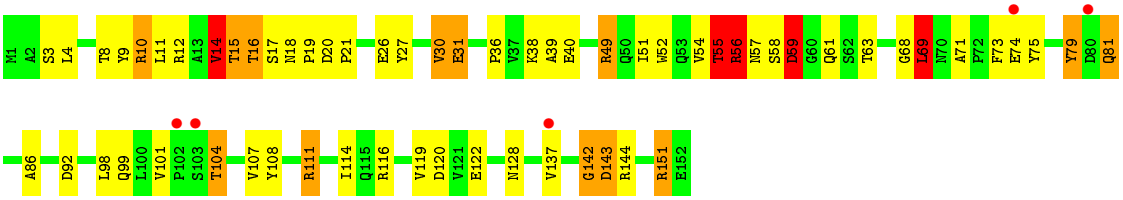
• Molecule 2: Clitocypin analog

Chain F:



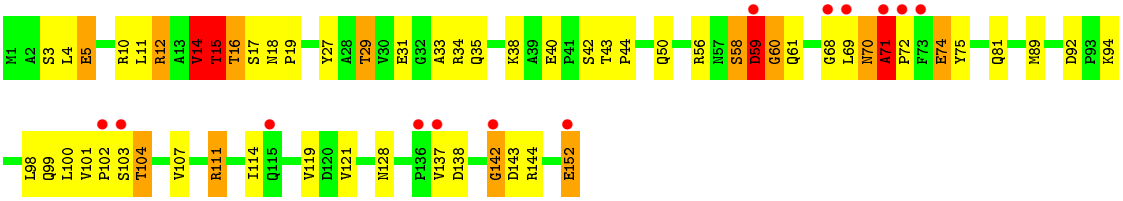
• Molecule 2: Clitocypin analog

Chain G:



• Molecule 2: Clitocypin analog

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	97.18Å 177.76Å 96.18Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.22 27.49 – 2.23	Depositor EDS
% Data completeness (in resolution range)	98.8 (50.00-2.22) 99.2 (27.49-2.23)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.83 (at 2.22Å)	Xtriage
Refinement program	REFMAC5, MAIN	Depositor
R, R_{free}	0.182 , 0.239 0.189 , 0.246	Depositor DCC
R_{free} test set	4098 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	29.5	Xtriage
Anisotropy	0.326	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 51.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.014 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12387	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.26% 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: SME, 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	A	1.26	7/1724 (0.4%)	1.04	3/2328 (0.1%)
1	B	1.15	1/1724 (0.1%)	1.00	3/2328 (0.1%)
1	C	1.31	10/1724 (0.6%)	1.00	0/2328
1	D	1.17	6/1724 (0.3%)	1.02	4/2328 (0.2%)
2	E	1.29	4/1205 (0.3%)	1.24	4/1639 (0.2%)
2	F	1.17	2/1205 (0.2%)	1.26	7/1639 (0.4%)
2	G	1.17	4/1205 (0.3%)	1.30	17/1639 (1.0%)
2	H	1.16	3/1205 (0.2%)	1.25	5/1639 (0.3%)
All	All	1.21	37/11716 (0.3%)	1.12	43/15868 (0.3%)

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	C	0	1
2	G	0	3
All	All	0	4

The worst 5 of 37 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	168	VAL	CB-CG2	8.53	1.70	1.52
1	D	139	ALA	CA-CB	6.96	1.67	1.52
2	E	26	GLU	CG-CD	-6.90	1.41	1.51
1	A	193	GLU	CB-CG	6.74	1.65	1.52
1	C	213	ALA	CA-CB	6.56	1.66	1.52

The worst 5 of 43 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	59	ASP	N-CA-C	-12.84	76.33	111.00
2	G	49	ARG	NE-CZ-NH2	8.77	124.68	120.30
2	F	49	ARG	NE-CZ-NH1	-8.21	116.19	120.30
2	E	14	VAL	CG1-CB-CG2	8.16	123.95	110.90
2	F	49	ARG	NE-CZ-NH2	7.78	124.19	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	89	TYR	Sidechain
2	G	142	GLY	Mainchain
2	G	79	TYR	Sidechain
2	G	86	ALA	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	A	1683	0	1612	36	1
1	B	1683	0	1612	40	1
1	C	1683	0	1612	25	0
1	D	1683	0	1612	33	1
2	E	1192	0	1140	40	2
2	F	1192	0	1140	48	0
2	G	1192	0	1139	55	1
2	H	1192	0	1139	47	2
3	A	5	0	0	0	0
3	B	10	0	0	2	0
3	C	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	1	0
4	A	169	0	0	5	0
4	B	124	0	0	4	0
4	C	174	0	0	4	2
4	D	97	0	0	1	0
4	E	85	0	0	4	0
4	F	81	0	0	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	64	0	0	5	0
4	H	63	0	0	3	0
All	All	12387	0	11006	311	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 14.

The worst 5 of 311 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:ASN:HD21	1:D:214:THR:HG22	0.97	1.14
1:A:177:ASN:HB3	1:A:180:ASN:HB2	1.31	1.09
1:B:177:ASN:HB3	1:B:180:ASN:HB2	1.34	1.07
2:G:16:THR:HG22	2:G:143:ASP:HA	1.43	1.00
1:D:208:ASN:ND2	1:D:214:THR:HG22	1.77	0.98

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)
2:E:116:ARG:NH2	4:C:288:HOH:O[1_455]	1.18	1.02
1:B:108:GLN:OE1	1:D:108:GLN:NE2[2_655]	1.85	0.35
1:A:117:PRO:CG	2:H:114:ILE:CD1[4_455]	2.02	0.18
2:E:116:ARG:CZ	4:C:288:HOH:O[1_455]	2.11	0.09
2:G:69:LEU:CD1	2:H:68:GLY:CA[4_455]	2.14	0.06

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	216/221 (98%)	209 (97%)	7 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	216/221 (98%)	206 (95%)	10 (5%)	0	100 100
1	C	216/221 (98%)	211 (98%)	5 (2%)	0	100 100
1	D	216/221 (98%)	206 (95%)	10 (5%)	0	100 100
2	E	148/152 (97%)	133 (90%)	11 (7%)	4 (3%)	6 3
2	F	148/152 (97%)	139 (94%)	7 (5%)	2 (1%)	14 10
2	G	148/152 (97%)	127 (86%)	16 (11%)	5 (3%)	5 2
2	H	148/152 (97%)	127 (86%)	14 (10%)	7 (5%)	3 1
All	All	1456/1492 (98%)	1358 (93%)	80 (6%)	18 (1%)	16 12

5 of 18 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	69	LEU
2	F	59	ASP
2	G	69	LEU
2	H	5	GLU
2	H	59	ASP

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	178/178 (100%)	168 (94%)	10 (6%)	26 29
1	B	178/178 (100%)	161 (90%)	17 (10%)	10 9
1	C	178/178 (100%)	169 (95%)	9 (5%)	29 33
1	D	178/178 (100%)	166 (93%)	12 (7%)	20 21
2	E	125/125 (100%)	111 (89%)	14 (11%)	7 6
2	F	125/125 (100%)	109 (87%)	16 (13%)	5 4
2	G	125/125 (100%)	109 (87%)	16 (13%)	5 4
2	H	125/125 (100%)	108 (86%)	17 (14%)	5 3
All	All	1212/1212 (100%)	1101 (91%)	111 (9%)	11 10

5 of 111 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	15	THR
2	F	4	LEU
2	H	35	GLN
2	E	16	THR
2	E	98	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 24 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	141	HIS
2	E	18	ASN
2	H	128	ASN
1	C	207	ASN
1	D	180	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

8 non-standard protein/DNA/RNA residues 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	SME	E	82	2	5,7,9	2.45	2 (40%)	4,7,11	2.14	1 (25%)
2	SME	E	89	2	5,7,9	1.92	2 (40%)	4,7,11	1.40	1 (25%)
2	SME	F	82	2	5,7,9	1.82	1 (20%)	4,7,11	1.15	0
2	SME	F	89	2	5,7,9	1.80	2 (40%)	4,7,11	1.73	1 (25%)
2	SME	G	82	2	5,7,9	1.87	2 (40%)	4,7,11	1.21	1 (25%)
2	SME	G	89	2	5,7,9	1.92	2 (40%)	4,7,11	1.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	SME	H	82	2	5,7,9	2.05	2 (40%)	4,7,11	1.68	2 (50%)
2	SME	H	89	2	5,7,9	2.06	2 (40%)	4,7,11	0.92	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
2	SME	E	82	2	-	0/4/6/9	0/0/0/0
2	SME	E	89	2	-	0/4/6/9	0/0/0/0
2	SME	F	82	2	-	0/4/6/9	0/0/0/0
2	SME	F	89	2	-	0/4/6/9	0/0/0/0
2	SME	G	82	2	-	0/4/6/9	0/0/0/0
2	SME	G	89	2	-	0/4/6/9	0/0/0/0
2	SME	H	82	2	-	0/4/6/9	0/0/0/0
2	SME	H	89	2	-	0/4/6/9	0/0/0/0

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	82	SME	CB-CA	-4.40	1.47	1.53
2	F	89	SME	CE-S	2.03	1.90	1.78
2	G	82	SME	CE-S	2.23	1.92	1.78
2	H	82	SME	CE-S	2.65	1.94	1.78
2	G	89	SME	CE-S	2.66	1.94	1.78

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	82	SME	CB-CG-S	-3.62	97.21	113.07
2	E	89	SME	O-C-CA	-2.78	118.26	125.72
2	F	89	SME	O-C-CA	-2.76	118.31	125.72
2	H	82	SME	CB-CA-N	-2.44	103.68	110.54
2	H	82	SME	O-C-CA	-2.13	120.00	125.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	82	SME	2	0
2	H	89	SME	1	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 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	SO4	A	222	-	4,4,4	1.57	1 (25%)	6,6,6	0.57	0
3	SO4	B	222	-	4,4,4	2.19	1 (25%)	6,6,6	0.48	0
3	SO4	B	223	-	4,4,4	1.19	0	6,6,6	0.32	0
3	SO4	C	222	-	4,4,4	1.32	0	6,6,6	0.82	0
3	SO4	D	222	-	4,4,4	1.34	1 (25%)	6,6,6	0.74	0
3	SO4	F	153	-	4,4,4	4.85	3 (75%)	6,6,6	2.72	5 (83%)

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	SO4	A	222	-	-	0/0/0/0	0/0/0/0
3	SO4	B	222	-	-	0/0/0/0	0/0/0/0
3	SO4	B	223	-	-	0/0/0/0	0/0/0/0
3	SO4	C	222	-	-	0/0/0/0	0/0/0/0
3	SO4	D	222	-	-	0/0/0/0	0/0/0/0
3	SO4	F	153	-	-	0/0/0/0	0/0/0/0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	222	SO4	O1-S	2.05	1.54	1.47
3	D	222	SO4	O1-S	2.45	1.55	1.47
3	F	153	SO4	O2-S	3.22	1.58	1.47
3	B	222	SO4	O2-S	3.95	1.61	1.47
3	F	153	SO4	O1-S	5.38	1.66	1.47

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	153	SO4	O2-S-O1	-3.88	96.63	109.59
3	F	153	SO4	O4-S-O1	-2.90	84.99	110.02
3	F	153	SO4	O3-S-O1	-2.19	91.09	110.02
3	F	153	SO4	O4-S-O2	2.57	132.17	110.02
3	F	153	SO4	O4-S-O3	3.06	121.44	109.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	222	SO4	1	0
3	B	223	SO4	1	0
3	F	153	SO4	1	0

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	A	220/221 (99%)	-0.33	5 (2%)	64	63	15, 25, 40, 80	3 (1%)
1	B	220/221 (99%)	-0.13	7 (3%)	51	50	16, 30, 49, 81	8 (3%)
1	C	220/221 (99%)	-0.34	1 (0%)	91	91	15, 24, 38, 53	2 (0%)
1	D	220/221 (99%)	0.01	14 (6%)	23	22	18, 32, 56, 91	4 (1%)
2	E	143/152 (94%)	0.01	6 (4%)	40	39	15, 27, 57, 81	1 (0%)
2	F	144/152 (94%)	-0.24	5 (3%)	48	46	14, 27, 54, 66	1 (0%)
2	G	140/152 (92%)	-0.03	5 (3%)	46	45	19, 32, 60, 67	0
2	H	143/152 (94%)	0.18	13 (9%)	11	11	19, 35, 62, 77	2 (1%)
All	All	1450/1492 (97%)	-0.13	56 (3%)	43	42	14, 28, 55, 91	21 (1%)

The worst 5 of 56 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	72	PRO	6.2
1	A	176	ALA	5.3
2	G	80	ASP	5.3
1	B	176	ALA	4.9
2	H	71	ALA	4.4

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	SME	F	89	8/10	0.86	0.21	-	23,30,36,44	0
2	SME	F	82	8/10	0.74	0.24	-	26,30,34,41	0
2	SME	G	82	8/10	0.67	0.27	-	40,46,51,57	0
2	SME	H	82	8/10	0.79	0.26	-	31,37,38,45	0
2	SME	E	82	8/10	0.77	0.25	-	29,36,41,49	0
2	SME	E	89	8/10	0.84	0.22	-	23,26,39,41	0
2	SME	G	89	8/10	0.87	0.20	-	22,30,34,42	0
2	SME	H	89	8/10	0.87	0.20	-	30,37,46,50	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
3	SO4	F	153	5/5	0.94	0.17	2.17	56,57,61,65	0
3	SO4	A	222	5/5	0.98	0.19	1.54	44,46,51,51	0
3	SO4	C	222	5/5	0.99	0.12	0.72	40,41,46,47	0
3	SO4	B	223	5/5	0.97	0.14	0.55	43,43,48,53	0
3	SO4	D	222	5/5	0.99	0.12	-0.20	39,42,47,49	0
3	SO4	B	222	5/5	0.97	0.10	-0.59	63,64,68,69	0

6.5 Other polymers (i)

There are no such residues in this entry.