Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:01 PM GMT

PDB ID	:	4QMG
Title	:	The Structure of MTDH-SND1 Complex Reveals Novel Cancer-Promoting Interactions
Authors	:	Guo, F.; Stanevich, V.; Wan, L.; Satyshur, K.; Kang, Y.; Xing, Y.
Deposited on	:	2014-06-16
Resolution	:	2.70 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
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:

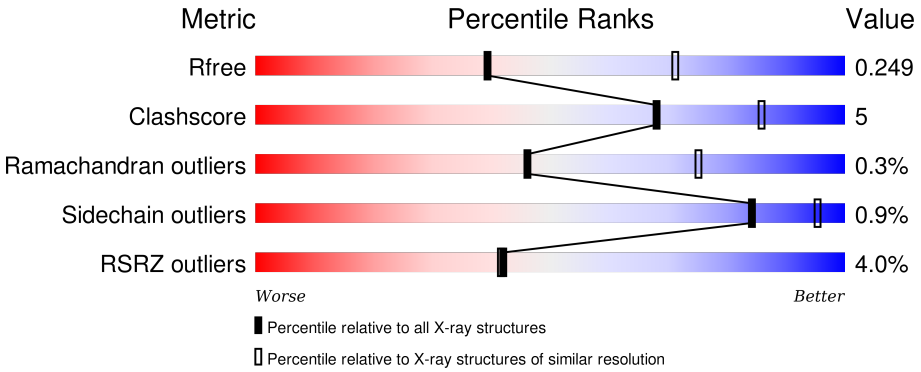
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	325	3% 80% 15% •
1	B	325	3% 85% 10% 5%
1	C	325	2% 78% 15% 6%
1	D	325	4% 87% 9% •
1	E	325	4% 82% 13% • 5%

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Mol	Chain	Length	Quality of chain
2	F	43	2% 28% 70%
2	G	43	2% 33% 65%
2	H	43	12% 40% 60%
2	I	43	9% 33% 65%
2	J	43	2% 28% 70%

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	A	401	-	-	-	X
3	SO4	B	401	-	-	-	X
3	SO4	D	401	-	-	-	X
3	SO4	E	401	-	-	-	X
5	GOL	B	404	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 13224 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 Staphylococcal nuclease domain-containing protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	311	Total	C	N	O	S	Se	0	1	0
			2478	1552	466	449	6	5			
1	B	309	Total	C	N	O	S	Se	0	1	0
			2454	1538	458	448	6	4			
1	C	306	Total	C	N	O	S	Se	0	1	0
			2438	1528	459	440	6	5			
1	D	311	Total	C	N	O	S	Se	0	1	0
			2468	1547	460	450	6	5			
1	E	309	Total	C	N	O	S	Se	0	0	0
			2429	1525	452	442	6	4			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	15	MSE	-	EXPRESSION TAG	UNP Q7KZF4
B	15	MSE	-	EXPRESSION TAG	UNP Q7KZF4
C	15	MSE	-	EXPRESSION TAG	UNP Q7KZF4
D	15	MSE	-	EXPRESSION TAG	UNP Q7KZF4
E	15	MSE	-	EXPRESSION TAG	UNP Q7KZF4

- Molecule 2 is a protein called Protein LYRIC.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	F	13	Total	C	N	O	0	0	0
			111	71	18	22			
2	G	15	Total	C	N	O	0	0	0
			126	80	21	25			
2	H	17	Total	C	N	O	0	0	0
			139	87	23	29			
2	I	15	Total	C	N	O	0	0	0
			126	80	21	25			
2	J	13	Total	C	N	O	0	0	0
			111	71	18	22			

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	365	SER	-	EXPRESSION TAG	UNP Q86UE4
F	366	THR	-	EXPRESSION TAG	UNP Q86UE4
F	367	GLY	-	EXPRESSION TAG	UNP Q86UE4
F	368	ASN	-	EXPRESSION TAG	UNP Q86UE4
F	369	ALA	-	EXPRESSION TAG	UNP Q86UE4
F	370	SER	-	EXPRESSION TAG	UNP Q86UE4
F	371	ASP	-	EXPRESSION TAG	UNP Q86UE4
F	372	SER	-	EXPRESSION TAG	UNP Q86UE4
F	373	SER	-	EXPRESSION TAG	UNP Q86UE4
F	374	SER	-	EXPRESSION TAG	UNP Q86UE4
F	375	ASP	-	EXPRESSION TAG	UNP Q86UE4
F	376	SER	-	EXPRESSION TAG	UNP Q86UE4
F	377	SER	-	EXPRESSION TAG	UNP Q86UE4
F	378	SER	-	EXPRESSION TAG	UNP Q86UE4
F	379	SER	-	EXPRESSION TAG	UNP Q86UE4
F	380	GLU	-	EXPRESSION TAG	UNP Q86UE4
F	381	GLY	-	EXPRESSION TAG	UNP Q86UE4
F	382	ASP	-	EXPRESSION TAG	UNP Q86UE4
F	383	GLY	-	EXPRESSION TAG	UNP Q86UE4
F	384	THR	-	EXPRESSION TAG	UNP Q86UE4
F	385	VAL	-	EXPRESSION TAG	UNP Q86UE4
G	365	SER	-	EXPRESSION TAG	UNP Q86UE4
G	366	THR	-	EXPRESSION TAG	UNP Q86UE4
G	367	GLY	-	EXPRESSION TAG	UNP Q86UE4
G	368	ASN	-	EXPRESSION TAG	UNP Q86UE4
G	369	ALA	-	EXPRESSION TAG	UNP Q86UE4
G	370	SER	-	EXPRESSION TAG	UNP Q86UE4
G	371	ASP	-	EXPRESSION TAG	UNP Q86UE4
G	372	SER	-	EXPRESSION TAG	UNP Q86UE4
G	373	SER	-	EXPRESSION TAG	UNP Q86UE4
G	374	SER	-	EXPRESSION TAG	UNP Q86UE4
G	375	ASP	-	EXPRESSION TAG	UNP Q86UE4
G	376	SER	-	EXPRESSION TAG	UNP Q86UE4
G	377	SER	-	EXPRESSION TAG	UNP Q86UE4
G	378	SER	-	EXPRESSION TAG	UNP Q86UE4
G	379	SER	-	EXPRESSION TAG	UNP Q86UE4
G	380	GLU	-	EXPRESSION TAG	UNP Q86UE4
G	381	GLY	-	EXPRESSION TAG	UNP Q86UE4
G	382	ASP	-	EXPRESSION TAG	UNP Q86UE4
G	383	GLY	-	EXPRESSION TAG	UNP Q86UE4
G	384	THR	-	EXPRESSION TAG	UNP Q86UE4
G	385	VAL	-	EXPRESSION TAG	UNP Q86UE4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	365	SER	-	EXPRESSION TAG	UNP Q86UE4
H	366	THR	-	EXPRESSION TAG	UNP Q86UE4
H	367	GLY	-	EXPRESSION TAG	UNP Q86UE4
H	368	ASN	-	EXPRESSION TAG	UNP Q86UE4
H	369	ALA	-	EXPRESSION TAG	UNP Q86UE4
H	370	SER	-	EXPRESSION TAG	UNP Q86UE4
H	371	ASP	-	EXPRESSION TAG	UNP Q86UE4
H	372	SER	-	EXPRESSION TAG	UNP Q86UE4
H	373	SER	-	EXPRESSION TAG	UNP Q86UE4
H	374	SER	-	EXPRESSION TAG	UNP Q86UE4
H	375	ASP	-	EXPRESSION TAG	UNP Q86UE4
H	376	SER	-	EXPRESSION TAG	UNP Q86UE4
H	377	SER	-	EXPRESSION TAG	UNP Q86UE4
H	378	SER	-	EXPRESSION TAG	UNP Q86UE4
H	379	SER	-	EXPRESSION TAG	UNP Q86UE4
H	380	GLU	-	EXPRESSION TAG	UNP Q86UE4
H	381	GLY	-	EXPRESSION TAG	UNP Q86UE4
H	382	ASP	-	EXPRESSION TAG	UNP Q86UE4
H	383	GLY	-	EXPRESSION TAG	UNP Q86UE4
H	384	THR	-	EXPRESSION TAG	UNP Q86UE4
H	385	VAL	-	EXPRESSION TAG	UNP Q86UE4
I	365	SER	-	EXPRESSION TAG	UNP Q86UE4
I	366	THR	-	EXPRESSION TAG	UNP Q86UE4
I	367	GLY	-	EXPRESSION TAG	UNP Q86UE4
I	368	ASN	-	EXPRESSION TAG	UNP Q86UE4
I	369	ALA	-	EXPRESSION TAG	UNP Q86UE4
I	370	SER	-	EXPRESSION TAG	UNP Q86UE4
I	371	ASP	-	EXPRESSION TAG	UNP Q86UE4
I	372	SER	-	EXPRESSION TAG	UNP Q86UE4
I	373	SER	-	EXPRESSION TAG	UNP Q86UE4
I	374	SER	-	EXPRESSION TAG	UNP Q86UE4
I	375	ASP	-	EXPRESSION TAG	UNP Q86UE4
I	376	SER	-	EXPRESSION TAG	UNP Q86UE4
I	377	SER	-	EXPRESSION TAG	UNP Q86UE4
I	378	SER	-	EXPRESSION TAG	UNP Q86UE4
I	379	SER	-	EXPRESSION TAG	UNP Q86UE4
I	380	GLU	-	EXPRESSION TAG	UNP Q86UE4
I	381	GLY	-	EXPRESSION TAG	UNP Q86UE4
I	382	ASP	-	EXPRESSION TAG	UNP Q86UE4
I	383	GLY	-	EXPRESSION TAG	UNP Q86UE4
I	384	THR	-	EXPRESSION TAG	UNP Q86UE4
I	385	VAL	-	EXPRESSION TAG	UNP Q86UE4

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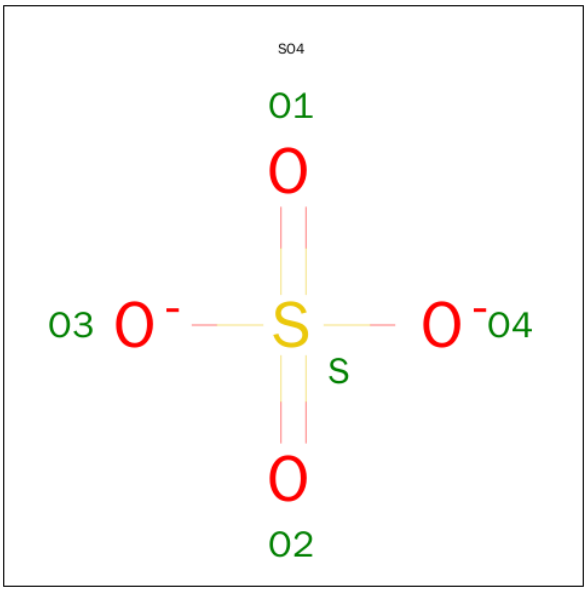
Chain	Residue	Modelled	Actual	Comment	Reference
J	365	SER	-	EXPRESSION TAG	UNP Q86UE4
J	366	THR	-	EXPRESSION TAG	UNP Q86UE4
J	367	GLY	-	EXPRESSION TAG	UNP Q86UE4
J	368	ASN	-	EXPRESSION TAG	UNP Q86UE4
J	369	ALA	-	EXPRESSION TAG	UNP Q86UE4
J	370	SER	-	EXPRESSION TAG	UNP Q86UE4
J	371	ASP	-	EXPRESSION TAG	UNP Q86UE4
J	372	SER	-	EXPRESSION TAG	UNP Q86UE4
J	373	SER	-	EXPRESSION TAG	UNP Q86UE4
J	374	SER	-	EXPRESSION TAG	UNP Q86UE4
J	375	ASP	-	EXPRESSION TAG	UNP Q86UE4
J	376	SER	-	EXPRESSION TAG	UNP Q86UE4
J	377	SER	-	EXPRESSION TAG	UNP Q86UE4
J	378	SER	-	EXPRESSION TAG	UNP Q86UE4
J	379	SER	-	EXPRESSION TAG	UNP Q86UE4
J	380	GLU	-	EXPRESSION TAG	UNP Q86UE4
J	381	GLY	-	EXPRESSION TAG	UNP Q86UE4
J	382	ASP	-	EXPRESSION TAG	UNP Q86UE4
J	383	GLY	-	EXPRESSION TAG	UNP Q86UE4
J	384	THR	-	EXPRESSION TAG	UNP Q86UE4
J	385	VAL	-	EXPRESSION TAG	UNP Q86UE4

- 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

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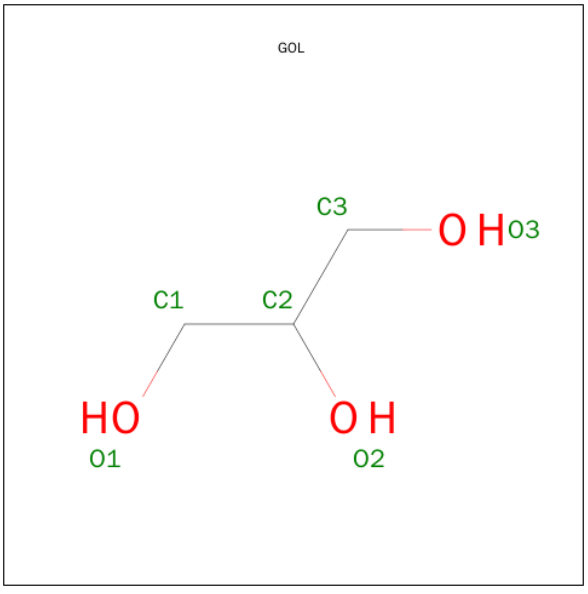
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	C	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	E	1	Total O S 5 4 1	0	0

- Molecule 4 is CESIUM ION (three-letter code: CS) (formula: Cs).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cs 1 1	0	0
4	A	1	Total Cs 1 1	0	0
4	D	1	Total Cs 1 1	0	0
4	C	1	Total Cs 1 1	0	0
4	E	1	Total Cs 1 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	E	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

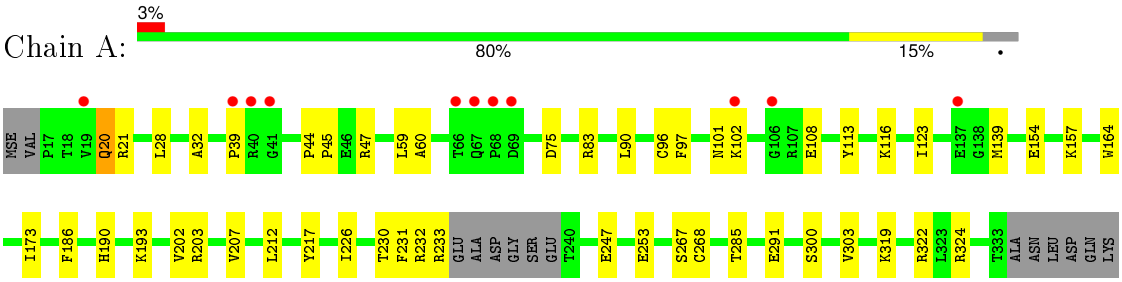
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	48	Total O 48 48	0	0
6	F	3	Total O 3 3	0	0
6	B	73	Total O 73 73	0	0
6	C	53	Total O 53 53	0	0
6	H	7	Total O 7 7	0	0
6	D	51	Total O 51 51	0	0
6	I	4	Total O 4 4	0	0
6	E	45	Total O 45 45	0	0
6	J	6	Total O 6 6	0	0

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.

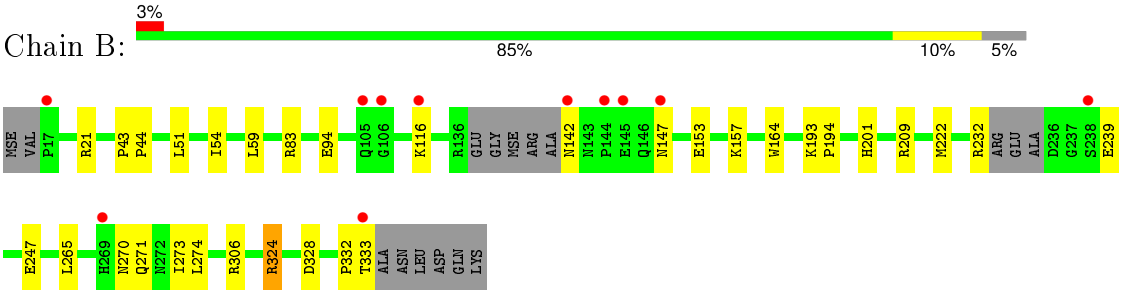
- Molecule 1: Staphylococcal nuclease domain-containing protein 1

Chain A:



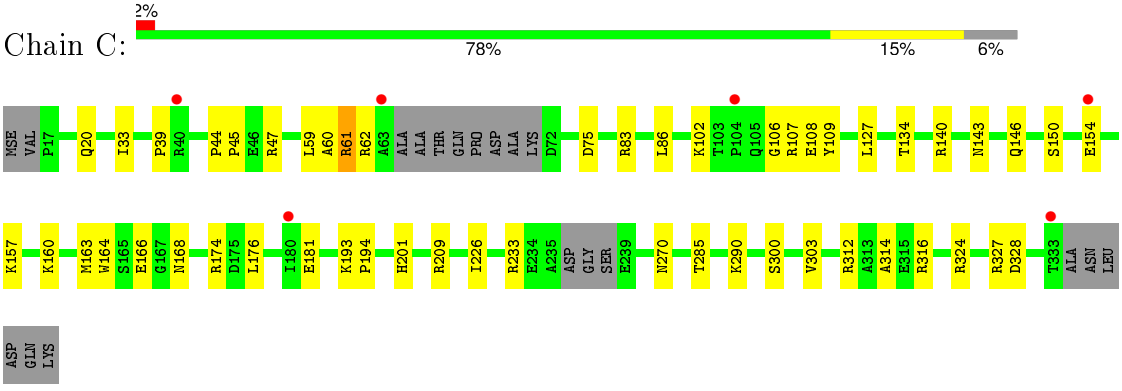
- Molecule 1: Staphylococcal nuclease domain-containing protein 1

Chain B:



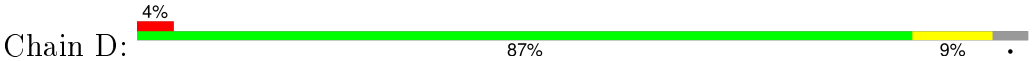
- Molecule 1: Staphylococcal nuclease domain-containing protein 1

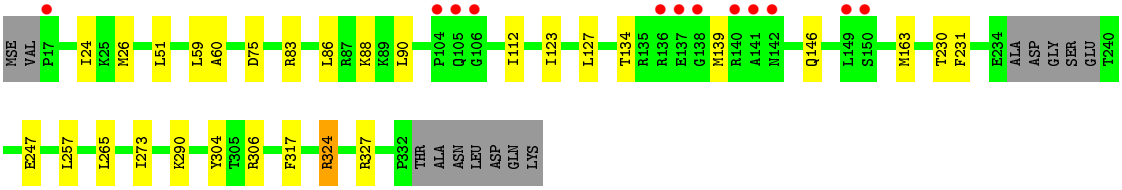
Chain C:



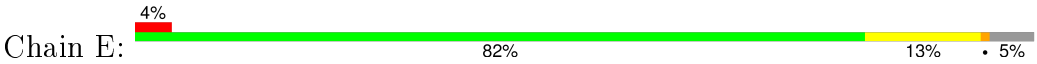
- Molecule 1: Staphylococcal nuclease domain-containing protein 1

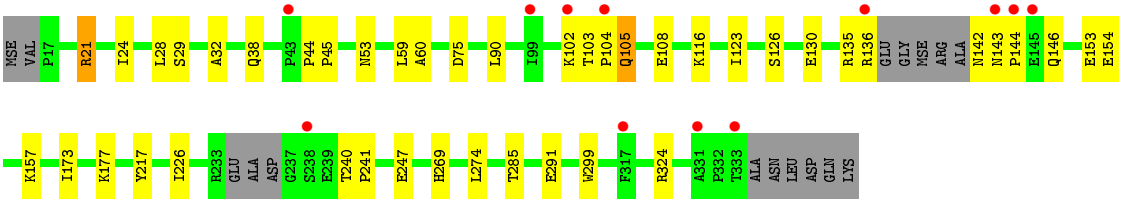
Chain D:



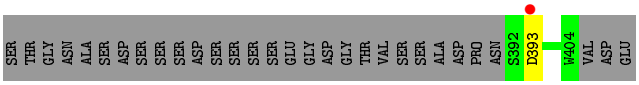


• Molecule 1: Staphylococcal nuclease domain-containing protein 1

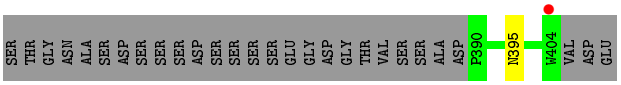




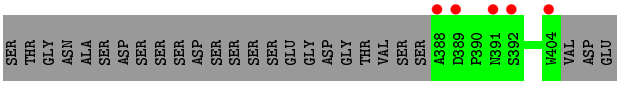
• Molecule 2: Protein LYRIC



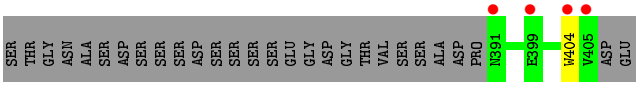
• Molecule 2: Protein LYRIC



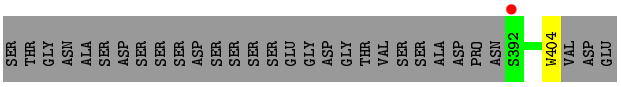
• Molecule 2: Protein LYRIC



• Molecule 2: Protein LYRIC



• Molecule 2: Protein LYRIC


SER
THR
GLY
ASN
ALA
SER
ASP
SER
SER
SER
ASP
SER
SER
SER
SER
GLU
GLY
ASP
GLY
THR
VAL
SER
SER
ALA
ASP
PRO
ASN
S392
W4O4
VAL
ASP
GLU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.83Å 65.72Å 135.84Å 90.00° 96.31° 90.00°	Depositor
Resolution (Å)	45.07 – 2.70 45.07 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.07-2.70) 92.8 (45.07-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$< I/\sigma(I) >$ [1]	2.59 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.190 , 0.248 0.193 , 0.249	Depositor DCC
R_{free} test set	3876 reflections (3.39%)	DCC
Wilson B-factor (Å^2)	42.8	Xtriage
Anisotropy	0.692	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	1 of 58969 reflections (0.002%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	13224	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.31% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CS, GOL, 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	0.24	0/2523	0.43	0/3399
1	B	0.22	0/2499	0.43	0/3369
1	C	0.21	0/2481	0.41	0/3340
1	D	0.21	0/2513	0.40	0/3387
1	E	0.21	0/2473	0.41	0/3336
2	F	0.19	0/117	0.33	0/162
2	G	0.21	0/133	0.35	0/184
2	H	0.19	0/146	0.33	0/203
2	I	0.19	0/132	0.45	0/183
2	J	0.18	0/117	0.34	0/162
All	All	0.22	0/13134	0.41	0/17725

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2478	0	2496	29	0
1	B	2454	0	2462	19	0
1	C	2438	0	2450	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2468	0	2473	18	0
1	E	2429	0	2434	26	0
2	F	111	0	82	1	0
2	G	126	0	96	1	0
2	H	139	0	104	0	0
2	I	126	0	97	2	0
2	J	111	0	82	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
3	D	5	0	0	0	0
3	E	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
5	B	12	0	16	0	0
5	D	6	0	8	0	0
5	E	6	0	8	0	0
6	A	48	0	0	0	0
6	B	73	0	0	0	0
6	C	53	0	0	0	0
6	D	51	0	0	0	0
6	E	45	0	0	0	0
6	F	3	0	0	0	0
6	H	7	0	0	0	0
6	I	4	0	0	0	0
6	J	6	0	0	0	0
All	All	13224	0	12808	122	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 5.

All (122) 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:88:LYS:HG3	2:I:404:TRP:HE1	1.40	0.86
1:E:21:ARG:NH1	1:E:116:LYS:O	2.10	0.84
1:D:26:MSE:HE2	1:D:257:LEU:HD21	1.68	0.76
1:B:59:LEU:HD11	1:B:83:ARG:HG3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:53:ASN:HA	1:E:136:ARG:HE	1.58	0.69
1:A:59:LEU:HD11	1:A:83:ARG:HG3	1.76	0.68
1:A:47:ARG:NH1	1:A:108:GLU:OE2	2.27	0.67
1:A:21:ARG:NH2	1:A:116:LYS:O	2.28	0.67
1:B:270:ASN:CG	1:B:271:GLN:H	1.96	0.66
1:A:319:LYS:O	1:A:322:ARG:NH1	2.28	0.66
1:C:60:ALA:N	1:C:75:ASP:OD1	2.29	0.65
1:E:105:GLN:H	1:E:105:GLN:CD	2.00	0.64
1:A:203:ARG:HB2	1:A:207:VAL:HG13	1.81	0.62
1:C:61:ARG:HD3	1:C:62:ARG:N	2.14	0.62
1:C:61:ARG:HD3	1:C:62:ARG:H	1.65	0.61
1:C:102:LYS:HD3	1:C:108:GLU:HG2	1.83	0.60
1:D:90:LEU:HD21	1:D:123:ILE:HD11	1.83	0.59
1:A:60:ALA:N	1:A:75:ASP:OD1	2.35	0.58
1:A:193:LYS:NZ	1:B:328:ASP:OD2	2.38	0.57
1:B:232:ARG:O	1:B:239:GLU:N	2.38	0.57
1:A:324:ARG:HH11	2:F:393:ASP:HA	1.68	0.57
1:D:230:THR:OG1	1:D:231:PHE:N	2.38	0.56
1:B:324:ARG:NH1	2:G:395:ASN:HD21	2.03	0.56
1:D:88:LYS:HG3	2:I:404:TRP:NE1	2.17	0.56
1:B:142:ASN:HA	1:B:147:ASN:HD21	1.71	0.55
1:B:153:GLU:HG2	1:B:157:LYS:HE3	1.88	0.55
1:C:150:SER:O	1:C:154:GLU:HG3	2.06	0.55
1:A:20:GLN:HG3	1:A:97:PHE:CE2	2.43	0.54
1:E:24:ILE:HG13	1:E:90:LEU:HB3	1.90	0.54
1:C:75:ASP:OD2	1:C:174:ARG:NH1	2.38	0.53
1:C:174:ARG:NH2	3:C:401:SO4:O4	2.41	0.53
1:D:59:LEU:HD11	1:D:83:ARG:HG3	1.91	0.53
1:C:290:LYS:HE2	1:C:314:ALA:HA	1.91	0.53
1:B:51:LEU:HD23	1:B:54:ILE:HD11	1.91	0.52
1:E:103:THR:HB	1:E:104:PRO:HD2	1.92	0.52
1:C:134:THR:HG23	1:C:163:MSE:SE	2.59	0.52
1:D:247:GLU:N	1:D:247:GLU:OE1	2.42	0.52
1:E:28:LEU:HB2	1:E:32:ALA:HB3	1.92	0.52
1:A:101:ASN:OD1	1:A:102:LYS:N	2.43	0.51
1:D:60:ALA:N	1:D:75:ASP:OD1	2.42	0.50
1:E:135:ARG:NE	1:E:153:GLU:OE1	2.44	0.50
1:C:59:LEU:HD11	1:C:83:ARG:HG3	1.92	0.50
1:D:139:MSE:HE3	1:D:146:GLN:HB3	1.94	0.49
1:C:20:GLN:HE22	1:C:47:ARG:NH1	2.11	0.49
1:E:102:LYS:HG3	1:E:108:GLU:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:ARG:C	1:A:233:ARG:HD3	2.34	0.48
1:E:53:ASN:HA	1:E:136:ARG:NE	2.27	0.48
1:D:324:ARG:O	1:D:327:ARG:HG2	2.13	0.48
1:C:47:ARG:NH2	1:C:108:GLU:OE1	2.46	0.48
1:E:142:ASN:HB3	1:E:146:GLN:HB3	1.96	0.48
1:A:139:MSE:HE3	1:E:38:GLN:HG3	1.95	0.48
1:C:143:ASN:HB2	1:C:146:GLN:H	1.78	0.47
1:A:28:LEU:HB2	1:A:32:ALA:HB3	1.96	0.47
1:C:107:ARG:NH1	1:C:109:TYR:OH	2.48	0.47
1:C:201[B]:HIS:HB3	1:C:209:ARG:HB2	1.95	0.47
1:D:24:ILE:HG13	1:D:90:LEU:HB3	1.96	0.47
1:D:265:LEU:HD22	1:D:273:ILE:HG21	1.96	0.47
1:D:86:LEU:HD11	1:D:127:LEU:HD11	1.95	0.47
1:D:290:LYS:HG3	1:D:317:PHE:CD1	2.51	0.46
1:A:75:ASP:HB2	1:A:173:ILE:HG23	1.98	0.46
1:A:291:GLU:O	1:A:324:ARG:HD3	2.16	0.46
1:A:230:THR:OG1	1:A:231:PHE:N	2.49	0.46
1:A:247:GLU:N	1:A:247:GLU:OE1	2.48	0.46
1:A:157:LYS:HD3	1:A:164:TRP:CE3	2.51	0.45
1:D:134:THR:HG23	1:D:163:MSE:SE	2.65	0.45
1:E:154:GLU:HA	1:E:157:LYS:HG3	1.98	0.45
1:C:86:LEU:HD11	1:C:127:LEU:HD11	1.97	0.45
1:B:270:ASN:CG	1:B:271:GLN:N	2.66	0.45
1:B:247:GLU:N	1:B:247:GLU:OE1	2.47	0.45
1:C:300:SER:O	1:C:303:VAL:HG22	2.17	0.45
1:C:20:GLN:HE22	1:C:47:ARG:HH12	1.65	0.45
1:D:304:TYR:CZ	1:D:306:ARG:HB2	2.52	0.45
1:B:222:MSE:HG3	1:B:274:LEU:HD23	1.99	0.44
1:E:60:ALA:N	1:E:75:ASP:OD1	2.45	0.44
1:A:96:CYS:SG	1:A:113:TYR:HB2	2.57	0.44
1:E:177:LYS:HD2	1:E:217:TYR:CE1	2.53	0.44
1:B:21:ARG:HD3	1:B:116:LYS:HG3	2.00	0.44
1:E:226:ILE:HD13	1:E:285:THR:HG23	2.00	0.44
1:C:176:LEU:HD23	1:C:176:LEU:HA	1.87	0.44
1:E:90:LEU:HD21	1:E:123:ILE:HD11	2.01	0.43
1:A:226:ILE:HD13	1:A:285:THR:HG23	2.01	0.43
1:E:291:GLU:O	1:E:324:ARG:HD3	2.18	0.43
1:C:157:LYS:HE2	1:C:157:LYS:HB3	1.89	0.43
1:B:157:LYS:HE2	1:B:164:TRP:CH2	2.53	0.43
1:E:75:ASP:HB2	1:E:173:ILE:HG23	2.00	0.43
1:A:300:SER:O	1:A:303:VAL:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:201[A]:HIS:HB2	1:C:209:ARG:HB2	2.00	0.43
1:B:43:PRO:HA	1:B:44:PRO:HD3	1.86	0.43
1:A:212:LEU:HB2	1:A:217:TYR:HB2	2.00	0.43
1:A:44:PRO:HA	1:A:45:PRO:HD3	1.85	0.42
1:E:103:THR:HB	1:E:105:GLN:HE22	1.85	0.42
1:C:327:ARG:HG3	1:C:328:ASP:N	2.34	0.42
1:C:102:LYS:HE3	1:C:106:GLY:HA2	2.01	0.42
1:B:21:ARG:NE	1:B:94:GLU:OE2	2.47	0.42
1:C:157:LYS:HG2	1:C:164:TRP:CD2	2.55	0.42
1:C:160:LYS:HE2	1:C:166:GLU:HG2	2.02	0.42
1:B:201[B]:HIS:HB3	1:B:209:ARG:HB2	2.01	0.42
1:D:123:ILE:HA	1:D:123:ILE:HD13	1.86	0.42
1:A:154:GLU:OE2	1:A:157:LYS:NZ	2.42	0.41
1:B:265:LEU:HD22	1:B:273:ILE:HG21	2.02	0.41
1:A:90:LEU:HD21	1:A:123:ILE:HD11	2.00	0.41
1:E:274:LEU:HD21	1:E:299:TRP:CH2	2.56	0.41
1:A:202:VAL:HB	1:A:253:GLU:HG3	2.01	0.41
1:E:247:GLU:N	1:E:247:GLU:OE1	2.51	0.41
1:C:168:ASN:N	1:C:168:ASN:OD1	2.52	0.41
1:C:312:ARG:O	1:C:316:ARG:HG3	2.20	0.41
1:C:226:ILE:HD13	1:C:285:THR:HG23	2.03	0.41
1:C:44:PRO:HA	1:C:45:PRO:HD3	1.87	0.41
1:E:240:THR:HA	1:E:241:PRO:HD3	1.93	0.41
1:A:157:LYS:HG2	1:A:164:TRP:CD2	2.56	0.41
1:B:193:LYS:HA	1:B:194:PRO:HD3	1.94	0.41
1:D:51:LEU:HD21	1:D:112:ILE:HD12	2.01	0.41
1:A:267:SER:OG	1:A:268:CYS:N	2.52	0.41
1:A:186:PHE:O	1:A:190:HIS:ND1	2.50	0.40
1:C:33:ILE:HD11	1:C:86:LEU:HD13	2.03	0.40
1:C:39:PRO:HB3	1:C:44:PRO:HD3	2.01	0.40
1:E:44:PRO:HA	1:E:45:PRO:HD3	1.91	0.40
1:E:143:ASN:HB2	1:E:144:PRO:HD2	2.02	0.40
1:B:306:ARG:HA	1:B:306:ARG:HD3	1.88	0.40
1:C:193:LYS:HA	1:C:194:PRO:HD3	1.93	0.40
1:E:126:SER:O	1:E:130:GLU:HG2	2.21	0.40
1:E:29:SER:HB2	1:E:59:LEU:HB2	2.03	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	A	308/325 (95%)	295 (96%)	12 (4%)	1 (0%)	46	75
1	B	304/325 (94%)	296 (97%)	6 (2%)	2 (1%)	26	55
1	C	301/325 (93%)	290 (96%)	10 (3%)	1 (0%)	46	75
1	D	308/325 (95%)	301 (98%)	6 (2%)	1 (0%)	46	75
1	E	303/325 (93%)	290 (96%)	13 (4%)	0	100	100
2	F	11/43 (26%)	10 (91%)	1 (9%)	0	100	100
2	G	13/43 (30%)	12 (92%)	1 (8%)	0	100	100
2	H	15/43 (35%)	14 (93%)	1 (7%)	0	100	100
2	I	13/43 (30%)	13 (100%)	0	0	100	100
2	J	11/43 (26%)	10 (91%)	1 (9%)	0	100	100
All	All	1587/1840 (86%)	1531 (96%)	51 (3%)	5 (0%)	46	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	324	ARG
1	C	324	ARG
1	B	324	ARG
1	B	332	PRO
1	A	39	PRO

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	262/266 (98%)	260 (99%)	2 (1%)	86 96
1	B	260/266 (98%)	259 (100%)	1 (0%)	93 98
1	C	257/266 (97%)	252 (98%)	5 (2%)	65 88
1	D	260/266 (98%)	260 (100%)	0	100 100
1	E	255/266 (96%)	252 (99%)	3 (1%)	78 93
2	F	10/35 (29%)	10 (100%)	0	100 100
2	G	12/35 (34%)	12 (100%)	0	100 100
2	H	13/35 (37%)	13 (100%)	0	100 100
2	I	12/35 (34%)	12 (100%)	0	100 100
2	J	10/35 (29%)	9 (90%)	1 (10%)	9 22
All	All	1351/1505 (90%)	1339 (99%)	12 (1%)	84 95

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	232	ARG
1	B	333	THR
1	C	61	ARG
1	C	140	ARG
1	C	181	GLU
1	C	233	ARG
1	C	270	ASN
1	E	21	ARG
1	E	105	GLN
1	E	269	HIS
2	J	404	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	B	147	ASN
2	G	395	ASN
1	C	20	GLN
1	D	38	GLN
1	E	270	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 5 are monoatomic - leaving 9 for Mogul analysis.

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	401	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	B	401	-	4,4,4	0.23	0	6,6,6	0.07	0
5	GOL	B	403	-	5,5,5	0.34	0	5,5,5	0.23	0
5	GOL	B	404	-	5,5,5	0.32	0	5,5,5	0.24	0
3	SO4	C	401	-	4,4,4	0.22	0	6,6,6	0.08	0
3	SO4	D	401	-	4,4,4	0.23	0	6,6,6	0.08	0
5	GOL	D	403	-	5,5,5	0.35	0	5,5,5	0.29	0
3	SO4	E	401	-	4,4,4	0.23	0	6,6,6	0.07	0
5	GOL	E	403	-	5,5,5	0.34	0	5,5,5	0.25	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	SO4	A	401	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	B	401	-	-	0/0/0/0	0/0/0/0
5	GOL	B	403	-	-	0/4/4/4	0/0/0/0
5	GOL	B	404	-	-	0/4/4/4	0/0/0/0
3	SO4	C	401	-	-	0/0/0/0	0/0/0/0
3	SO4	D	401	-	-	0/0/0/0	0/0/0/0
5	GOL	D	403	-	-	0/4/4/4	0/0/0/0
3	SO4	E	401	-	-	0/0/0/0	0/0/0/0
5	GOL	E	403	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	401	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	306/325 (94%)	0.16	11 (3%)	46	46	32, 50, 95, 127	0
1	B	305/325 (93%)	0.10	11 (3%)	46	46	25, 42, 88, 122	0
1	C	301/325 (92%)	0.08	6 (1%)	68	69	26, 47, 90, 126	0
1	D	306/325 (94%)	0.15	12 (3%)	43	43	30, 48, 91, 115	0
1	E	305/325 (93%)	0.23	12 (3%)	43	43	31, 50, 101, 153	0
2	F	13/43 (30%)	0.36	1 (7%)	16	14	49, 64, 95, 117	0
2	G	15/43 (34%)	0.53	1 (6%)	21	19	40, 57, 108, 125	0
2	H	17/43 (39%)	1.03	5 (29%)	1	0	36, 63, 105, 106	0
2	I	15/43 (34%)	0.82	4 (26%)	1	1	44, 61, 114, 124	0
2	J	13/43 (30%)	0.43	1 (7%)	16	14	46, 57, 86, 104	0
All	All	1596/1840 (86%)	0.17	64 (4%)	42	41	25, 48, 97, 153	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	142	ASN	4.5
1	E	99	ILE	4.4
1	E	144	PRO	4.3
1	A	66	THR	4.2
1	D	106	GLY	4.1
1	E	102	LYS	4.0
2	H	388	ALA	3.8
2	G	404	TRP	3.6
1	C	104	PRO	3.5
1	B	17	PRO	3.4
1	E	333	THR	3.4
1	A	69	ASP	3.3
2	I	404	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	63	ALA	3.2
1	A	68	PRO	3.2
1	A	106	GLY	3.1
1	A	67	GLN	3.1
1	E	143	ASN	3.1
2	H	391	ASN	3.0
1	E	43	PRO	3.0
2	H	389	ASP	2.9
1	A	39	PRO	2.9
1	B	333	THR	2.8
1	D	104	PRO	2.8
1	D	136	ARG	2.8
1	A	41	GLY	2.8
2	J	392	SER	2.8
1	C	40	ARG	2.8
1	C	180	ILE	2.7
1	D	141	ALA	2.7
1	E	331	ALA	2.7
1	B	144	PRO	2.7
1	A	40	ARG	2.6
1	E	145	GLU	2.6
1	D	137	GLU	2.6
1	A	137	GLU	2.5
1	C	154	GLU	2.5
1	D	140	ARG	2.4
1	D	149	LEU	2.4
1	B	269	HIS	2.4
1	D	138	GLY	2.4
2	H	404	TRP	2.3
1	E	238	SER	2.3
1	D	142	ASN	2.3
1	A	102	LYS	2.3
1	E	136	ARG	2.3
1	E	317	PHE	2.2
1	D	105	GLN	2.2
2	I	405	VAL	2.2
2	I	399	GLU	2.2
2	H	392	SER	2.2
2	I	391	ASN	2.2
1	A	19	VAL	2.1
1	D	150	SER	2.1
1	E	104	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	147	ASN	2.1
1	B	116	LYS	2.1
1	C	333	THR	2.1
1	B	106	GLY	2.1
1	B	145	GLU	2.1
1	D	17	PRO	2.1
1	B	105	GLN	2.0
1	B	238	SER	2.0
2	F	393	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 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	A	401	5/5	0.69	0.52	7.82	146,148,151,152	0
3	SO4	D	401	5/5	0.94	0.36	7.41	106,107,111,112	0
3	SO4	E	401	5/5	0.77	0.34	6.16	132,135,139,139	0
3	SO4	B	401	5/5	0.81	0.32	4.01	121,131,133,136	0
5	GOL	B	404	6/6	0.81	0.31	3.68	58,81,90,90	0
3	SO4	C	401	5/5	0.91	0.19	1.36	101,101,104,106	0
5	GOL	B	403	6/6	0.81	0.30	-	69,93,94,95	0
4	CS	B	402	1/1	0.49	0.12	-	208,208,208,208	0
4	CS	C	402	1/1	0.66	0.08	-	202,202,202,202	0
5	GOL	E	403	6/6	0.72	0.30	-	74,79,89,92	0
4	CS	E	402	1/1	0.75	0.07	-	202,202,202,202	0
4	CS	A	402	1/1	0.70	0.23	-	194,194,194,194	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	CS	D	402	1/1	0.75	0.09	-	173,173,173,173	0
5	GOL	D	403	6/6	0.78	0.25	-	73,85,90,93	0

6.5 Other polymers (i)

There are no such residues in this entry.