



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 13, 2024 – 10:31 AM EST

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 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 ⓘ 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	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

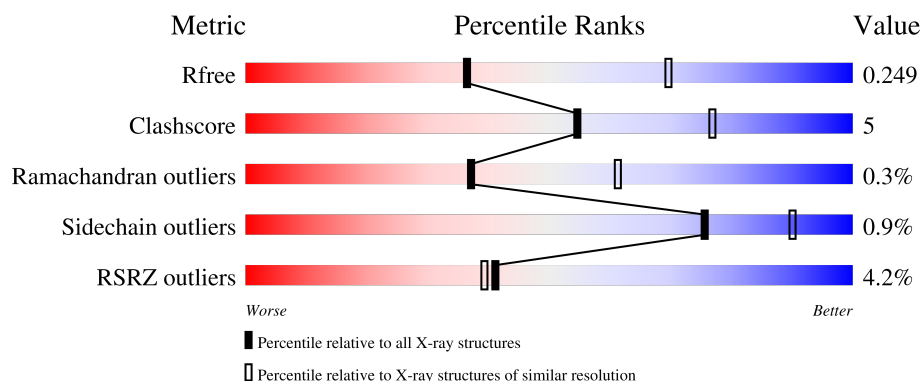
1 Overall quality at a glance

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}	164625	3333 (2.70-2.70)
Clashscore	180529	3684 (2.70-2.70)
Ramachandran outliers	177936	3633 (2.70-2.70)
Sidechain outliers	177891	3633 (2.70-2.70)
RSRZ outliers	164620	3333 (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 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 $\leq 5\%$. 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	 3% 78% 15% 6%
1	D	325	 % 87% 9% •
1	E	325	 6% 82% 13% • 5%

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Mol	Chain	Length	Quality of chain
2	F	43	<div><div><div></div><div></div><div></div></div><div>5%28%70%</div></div>
2	G	43	<div><div><div></div><div></div><div></div></div><div>9%33%65%</div></div>
2	H	43	<div><div><div></div><div></div><div></div></div><div>5%40%60%</div></div>
2	I	43	<div><div><div></div><div></div><div></div></div><div>7%33%65%</div></div>
2	J	43	<div><div><div></div><div></div><div></div></div><div>5%28%70%</div></div>

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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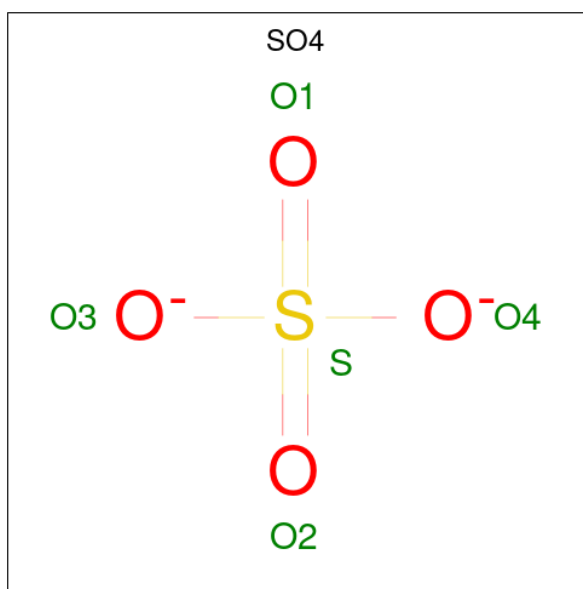
Chain	Residue	Modelled	Actual	Comment	Reference
H	365	SER	-	expression tag	UNP Q86UE4
H	366	THR	-	expression tag	UNP Q86UE4
H	367	GLY	-	expression tag	UNP Q86UE4
H	368	ASN	-	expression tag	UNP Q86UE4
H	369	ALA	-	expression tag	UNP Q86UE4
H	370	SER	-	expression tag	UNP Q86UE4
H	371	ASP	-	expression tag	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: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

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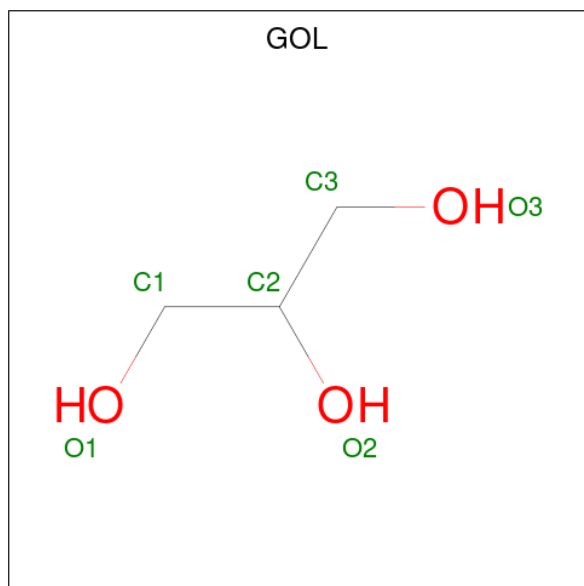
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

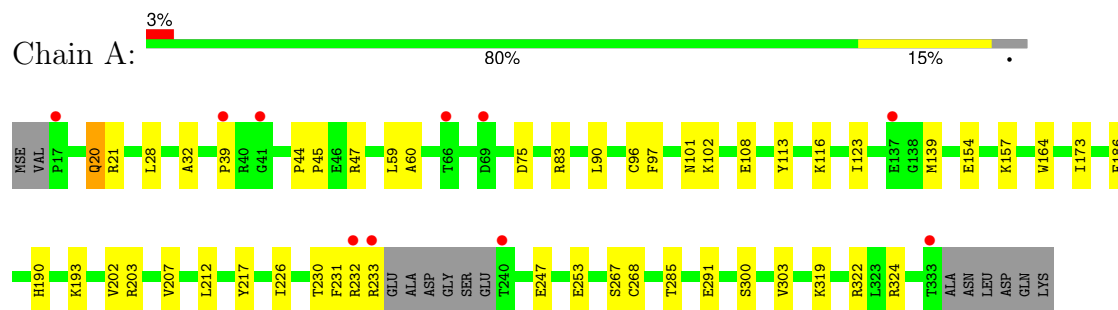
- Molecule 6 is water.

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

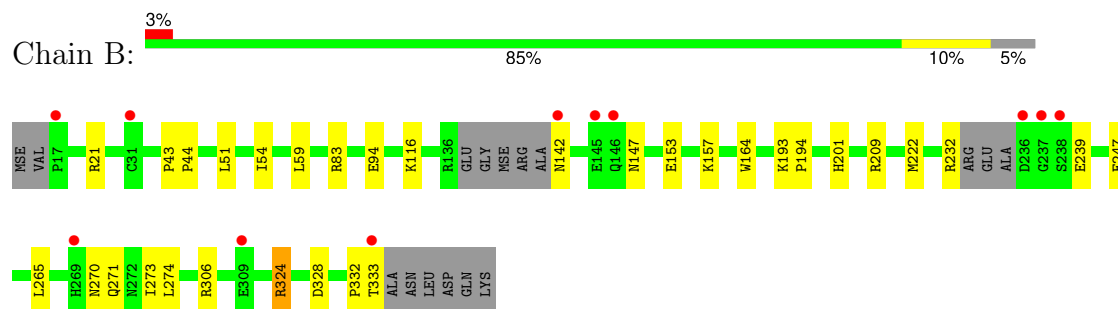
3 Residue-property plots

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.

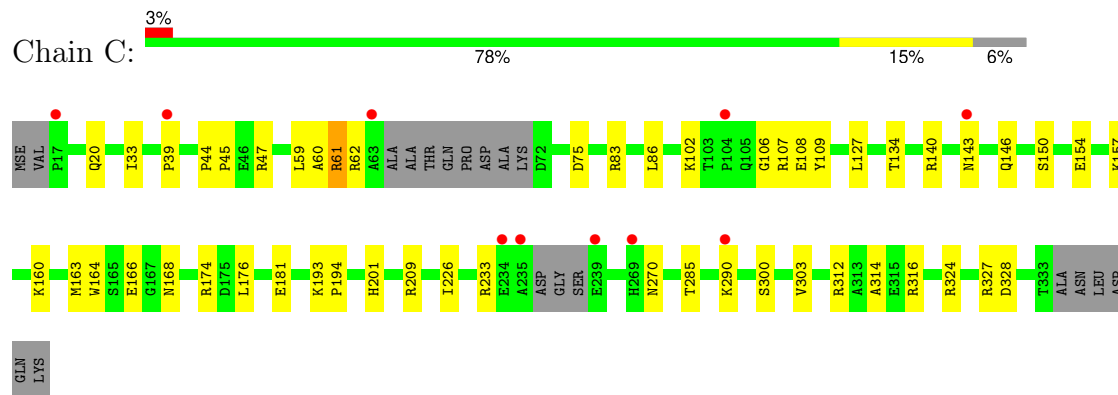
- Molecule 1: Staphylococcal nuclease domain-containing protein 1



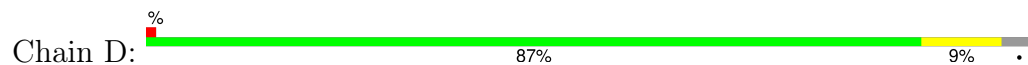
- Molecule 1: Staphylococcal nuclease domain-containing protein 1



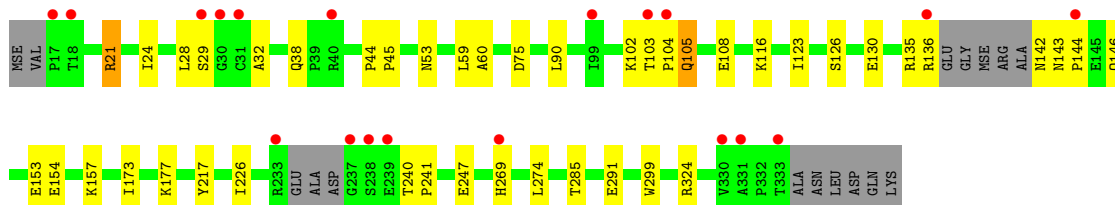
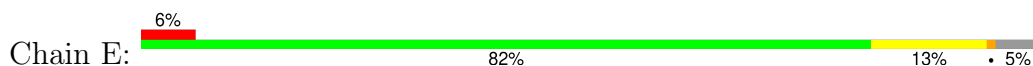
- Molecule 1: Staphylococcal nuclease domain-containing protein 1



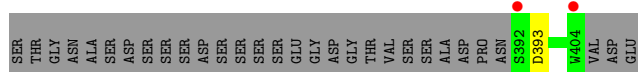
- Molecule 1: Staphylococcal nuclease domain-containing protein 1



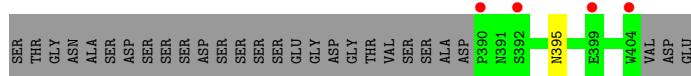
- Molecule 1: Staphylococcal nuclease domain-containing protein 1



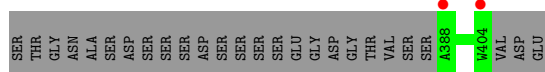
- Molecule 2: Protein LYRIC



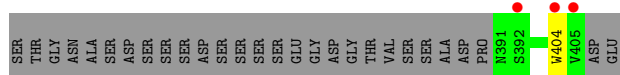
- Molecule 2: Protein LYRIC



- Molecule 2: Protein LYRIC



- Molecule 2: Protein LYRIC



- Molecule 2: Protein LYRIC



SER	THR	GLY	ASN	ALA	SER	ASP	SER	SER	SER	SER	SER	SER	SER	SER	GLU	GLY	ASP	GLY	THR	VAL	SER	SER	ALA	ASP	PRO	ASN	S392	+	W404	VAL	ASP	GLU
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4 Data and refinement statistics

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) 92.7 (45.07-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1690)	Depositor
R, R_{free}	0.190 , 0.248 0.195 , 0.249	Depositor DCC
R_{free} test set	2000 reflections (3.38%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.720	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 46.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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 3.30% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, GOL, CS

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 [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	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.

The worst 5 of 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

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%)	37	61
1	B	304/325 (94%)	296 (97%)	6 (2%)	2 (1%)	19	42
1	C	301/325 (93%)	290 (96%)	10 (3%)	1 (0%)	37	61
1	D	308/325 (95%)	301 (98%)	6 (2%)	1 (0%)	37	61
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%)	37	61

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 ⓘ

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%)	79	91
1	B	260/266 (98%)	259 (100%)	1 (0%)	89	96
1	C	257/266 (97%)	252 (98%)	5 (2%)	52	79
1	D	260/266 (98%)	260 (100%)	0	100	100
1	E	255/266 (96%)	252 (99%)	3 (1%)	67	86
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%)	6	16
All	All	1351/1505 (90%)	1339 (99%)	12 (1%)	75	90

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	270	ASN
1	E	21	ARG
2	J	404	TRP
1	E	105	GLN
1	C	61	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

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

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 oligosaccharides 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	$\# Z > 2$
5	GOL	D	403	-	5,5,5	0.37	0	5,5,5	0.38	0
3	SO4	A	401	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	E	401	-	4,4,4	0.23	0	6,6,6	0.07	0
5	GOL	E	403	-	5,5,5	0.37	0	5,5,5	0.30	0
5	GOL	B	404	-	5,5,5	0.36	0	5,5,5	0.27	0
3	SO4	B	401	-	4,4,4	0.24	0	6,6,6	0.06	0
3	SO4	D	401	-	4,4,4	0.24	0	6,6,6	0.07	0
3	SO4	C	401	-	4,4,4	0.24	0	6,6,6	0.07	0
5	GOL	B	403	-	5,5,5	0.37	0	5,5,5	0.31	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
5	GOL	D	403	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	E	403	-	-	2/4/4/4	-
5	GOL	B	404	-	-	4/4/4/4	-
5	GOL	B	403	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 8 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	403	GOL	O1-C1-C2-C3
5	B	404	GOL	O1-C1-C2-C3
5	B	404	GOL	C1-C2-C3-O3
5	B	404	GOL	O2-C2-C3-O3
5	E	403	GOL	C1-C2-C3-O3

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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, 95th 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%)	0.07	10 (3%) 49 47	18, 50, 95, 127	1 (0%)
1	B	305/325 (93%)	-0.12	11 (3%) 46 45	14, 42, 88, 122	1 (0%)
1	C	301/325 (92%)	0.08	10 (3%) 49 47	16, 47, 90, 126	1 (0%)
1	D	306/325 (94%)	0.01	4 (1%) 74 74	17, 48, 91, 115	1 (0%)
1	E	305/325 (93%)	0.18	19 (6%) 28 26	31, 50, 101, 153	0
2	F	13/43 (30%)	0.57	2 (15%) 6 6	49, 64, 95, 117	0
2	G	15/43 (34%)	1.10	4 (26%) 2 2	40, 57, 108, 124	0
2	H	17/43 (39%)	0.82	2 (11%) 10 10	36, 63, 105, 106	0
2	I	15/43 (34%)	1.14	3 (20%) 3 4	44, 61, 114, 124	0
2	J	13/43 (30%)	0.53	2 (15%) 6 6	46, 57, 86, 104	0
All	All	1596/1840 (86%)	0.08	67 (4%) 41 39	14, 48, 97, 153	4 (0%)

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	404	TRP	5.0
2	I	404	TRP	5.0
1	B	17	PRO	4.3
1	B	31	CYS	4.3
1	E	17	PRO	3.8

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th 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
4	CS	A	402	1/1	0.54	0.23	194,194,194,194	0
4	CS	B	402	1/1	0.65	0.20	208,208,208,208	0
3	SO4	E	401	5/5	0.66	0.29	132,135,139,139	0
5	GOL	E	403	6/6	0.66	0.24	74,79,89,92	0
3	SO4	A	401	5/5	0.68	0.14	146,148,151,152	0
5	GOL	B	403	6/6	0.69	0.21	69,93,94,95	0
5	GOL	D	403	6/6	0.71	0.21	73,85,90,93	0
4	CS	C	402	1/1	0.73	0.15	202,202,202,202	0
5	GOL	B	404	6/6	0.74	0.23	58,81,90,90	0
4	CS	E	402	1/1	0.75	0.17	202,202,202,202	0
4	CS	D	402	1/1	0.83	0.16	173,173,173,173	0
3	SO4	B	401	5/5	0.84	0.24	121,131,133,136	0
3	SO4	C	401	5/5	0.84	0.22	101,101,104,106	0
3	SO4	D	401	5/5	0.91	0.15	106,107,111,112	0

6.5 Other polymers [i](#)

There are no such residues in this entry.