WORLDWIDE wwPDB PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 13, 2017 – 06:39 pm GMT

PDB ID	:	1WMG
Title	:	Crystal structure of the UNC5H2 death domain
Authors	:	Handa, N.; Murayama, K.; Shirouzu, M.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2004-07-09
Resolution	:	2.10 Å(reported)

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

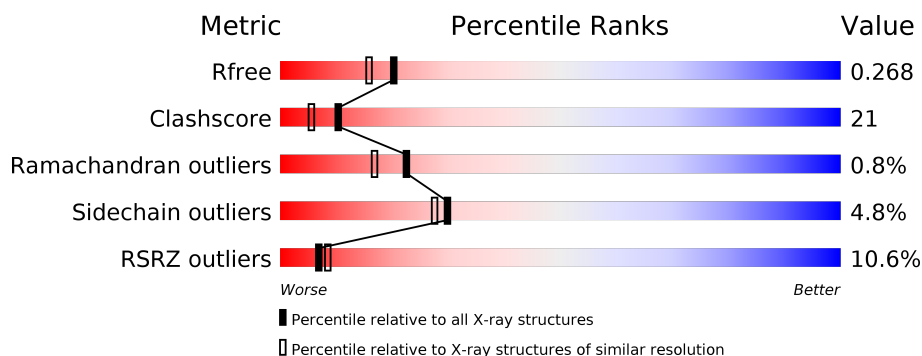|		
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 2.10 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	Percentile Ranks	Value
Rfree		0.268
Clashscore		21
Ramachandran outliers		0.8%
Sidechain outliers		4.8%
RSRZ outliers		10.6%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (2.10-2.10)

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	103	9% / 59% / 27% / • / 13%
1	B	103	3% / 52% / 24% / • / 19%
1	C	103	4% / 63% / 20% / • / 15%
1	D	103	% / 56% / 22% / 5% / 17%
1	E	103	12% / 60% / 22% / • / 15%
1	F	103	23% / 42% / 38% / 5% / 16%

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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	SO3	E	1005	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4298 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 netrin receptor Unc5h2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	90	Total	C	N	O	S	Se	0	0	0
			700	438	120	137	1	4			
1	B	83	Total	C	N	O	S	Se	0	0	0
			647	408	112	122	1	4			
1	C	88	Total	C	N	O	S	Se	0	0	0
			688	432	118	133	1	4			
1	D	86	Total	C	N	O	S	Se	0	0	0
			671	423	115	128	1	4			
1	E	88	Total	C	N	O	S	Se	0	0	0
			688	432	118	133	1	4			
1	F	87	Total	C	N	O	S	Se	0	0	0
			676	423	117	131	1	4			

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	847	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
A	848	SER	-	CLONING ARTIFACT	UNP Q8K1S3
A	849	SER	-	CLONING ARTIFACT	UNP Q8K1S3
A	850	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
A	851	SER	-	CLONING ARTIFACT	UNP Q8K1S3
A	852	SER	-	CLONING ARTIFACT	UNP Q8K1S3
A	853	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
A	889	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
A	930	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
A	935	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
A	939	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
A	944	SER	-	CLONING ARTIFACT	UNP Q8K1S3
A	945	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
A	946	PRO	-	CLONING ARTIFACT	UNP Q8K1S3
A	947	SER	-	CLONING ARTIFACT	UNP Q8K1S3
A	948	SER	-	CLONING ARTIFACT	UNP Q8K1S3
A	949	GLY	-	CLONING ARTIFACT	UNP Q8K1S3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	847	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
B	848	SER	-	CLONING ARTIFACT	UNP Q8K1S3
B	849	SER	-	CLONING ARTIFACT	UNP Q8K1S3
B	850	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
B	851	SER	-	CLONING ARTIFACT	UNP Q8K1S3
B	852	SER	-	CLONING ARTIFACT	UNP Q8K1S3
B	853	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
B	889	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
B	930	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
B	935	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
B	939	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
B	944	SER	-	CLONING ARTIFACT	UNP Q8K1S3
B	945	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
B	946	PRO	-	CLONING ARTIFACT	UNP Q8K1S3
B	947	SER	-	CLONING ARTIFACT	UNP Q8K1S3
B	948	SER	-	CLONING ARTIFACT	UNP Q8K1S3
B	949	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
C	847	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
C	848	SER	-	CLONING ARTIFACT	UNP Q8K1S3
C	849	SER	-	CLONING ARTIFACT	UNP Q8K1S3
C	850	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
C	851	SER	-	CLONING ARTIFACT	UNP Q8K1S3
C	852	SER	-	CLONING ARTIFACT	UNP Q8K1S3
C	853	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
C	889	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
C	930	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
C	935	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
C	939	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
C	944	SER	-	CLONING ARTIFACT	UNP Q8K1S3
C	945	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
C	946	PRO	-	CLONING ARTIFACT	UNP Q8K1S3
C	947	SER	-	CLONING ARTIFACT	UNP Q8K1S3
C	948	SER	-	CLONING ARTIFACT	UNP Q8K1S3
C	949	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
D	847	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
D	848	SER	-	CLONING ARTIFACT	UNP Q8K1S3
D	849	SER	-	CLONING ARTIFACT	UNP Q8K1S3
D	850	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
D	851	SER	-	CLONING ARTIFACT	UNP Q8K1S3
D	852	SER	-	CLONING ARTIFACT	UNP Q8K1S3
D	853	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
D	889	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3

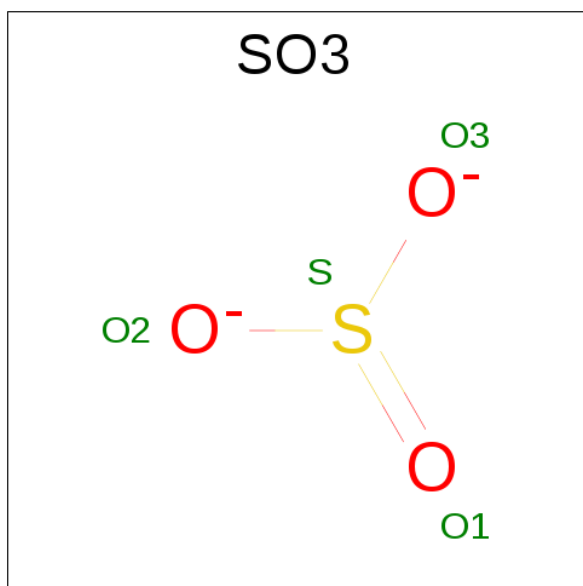*Continued on next page...*

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Chain	Residue	Modelled	Actual	Comment	Reference
D	930	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
D	935	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
D	939	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
D	944	SER	-	CLONING ARTIFACT	UNP Q8K1S3
D	945	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
D	946	PRO	-	CLONING ARTIFACT	UNP Q8K1S3
D	947	SER	-	CLONING ARTIFACT	UNP Q8K1S3
D	948	SER	-	CLONING ARTIFACT	UNP Q8K1S3
D	949	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
E	847	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
E	848	SER	-	CLONING ARTIFACT	UNP Q8K1S3
E	849	SER	-	CLONING ARTIFACT	UNP Q8K1S3
E	850	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
E	851	SER	-	CLONING ARTIFACT	UNP Q8K1S3
E	852	SER	-	CLONING ARTIFACT	UNP Q8K1S3
E	853	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
E	889	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
E	930	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
E	935	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
E	939	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
E	944	SER	-	CLONING ARTIFACT	UNP Q8K1S3
E	945	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
E	946	PRO	-	CLONING ARTIFACT	UNP Q8K1S3
E	947	SER	-	CLONING ARTIFACT	UNP Q8K1S3
E	948	SER	-	CLONING ARTIFACT	UNP Q8K1S3
E	949	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
F	847	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
F	848	SER	-	CLONING ARTIFACT	UNP Q8K1S3
F	849	SER	-	CLONING ARTIFACT	UNP Q8K1S3
F	850	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
F	851	SER	-	CLONING ARTIFACT	UNP Q8K1S3
F	852	SER	-	CLONING ARTIFACT	UNP Q8K1S3
F	853	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
F	889	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
F	930	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
F	935	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
F	939	MSE	MET	MODIFIED RESIDUE	UNP Q8K1S3
F	944	SER	-	CLONING ARTIFACT	UNP Q8K1S3
F	945	GLY	-	CLONING ARTIFACT	UNP Q8K1S3
F	946	PRO	-	CLONING ARTIFACT	UNP Q8K1S3
F	947	SER	-	CLONING ARTIFACT	UNP Q8K1S3
F	948	SER	-	CLONING ARTIFACT	UNP Q8K1S3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	949	GLY	-	CLONING ARTIFACT	UNP Q8K1S3

- Molecule 2 is SULFITE ION (three-letter code: SO3) (formula: O_3S).

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

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
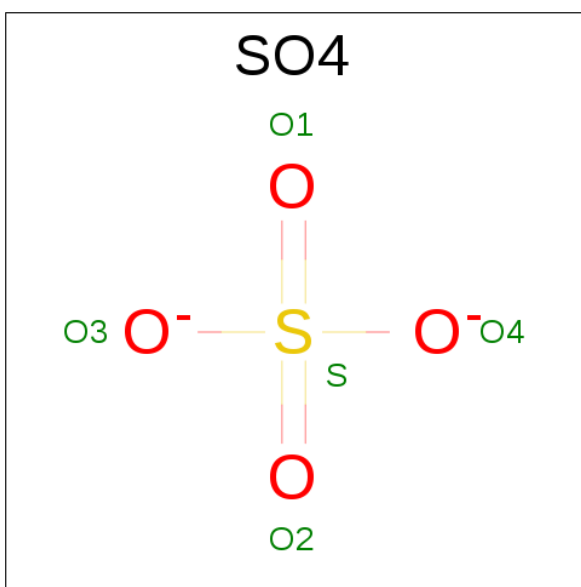
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total 5	O 4	S 1	0	0
3	F	1	Total 5	O 4	S 1	0	0
3	C	1	Total 5	O 4	S 1	0	0

• Molecule 4 is water.

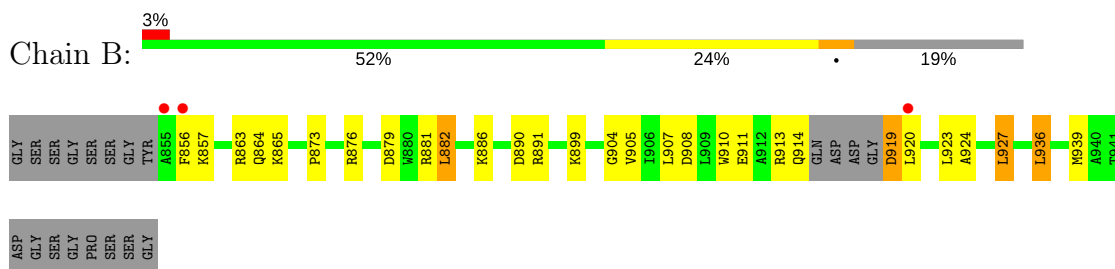| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	43	Total 43	O 43	0	0
4	B	40	Total 40	O 40	0	0
4	C	27	Total 27	O 27	0	0
4	D	41	Total 41	O 41	0	0
4	E	27	Total 27	O 27	0	0
4	F	7	Total 7	O 7	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA 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.
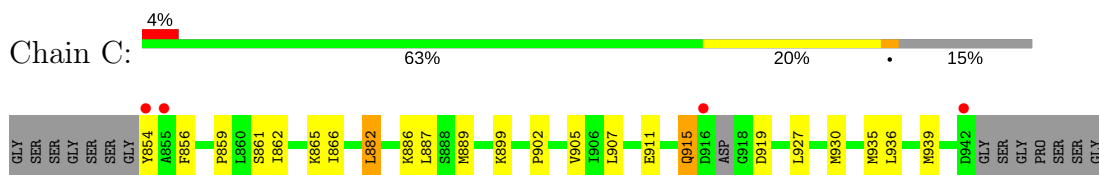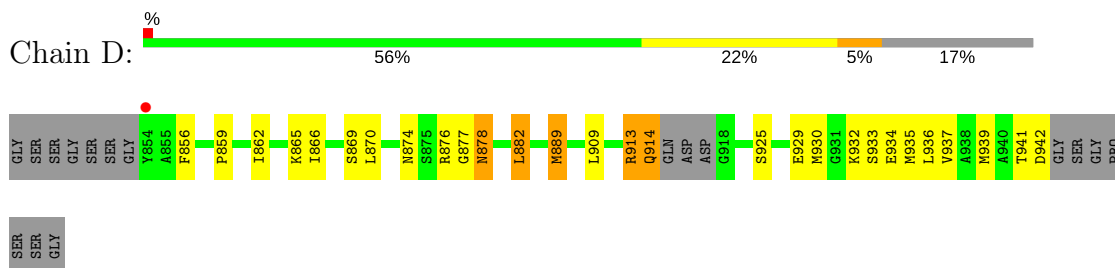
- Molecule 1: netrin receptor Unc5h2

Chain A:

- Molecule 1: netrin receptor Unc5h2

Chain B:

- Molecule 1: netrin receptor Unc5h2

Chain C:

- Molecule 1: netrin receptor Unc5h2

Chain D:

- Molecule 1: netrin receptor Unc5h2

Chain E:

12%

60%

22%

•

15%

GLY SER SER GLY SER SER GLY Y854 A855 F856 P859 L860 S861 I862 R863 Q864 K865 R876 L883 K886 D890 R891 N894 Y895 T898 K899 V905 I906 L907 E911 Q915 D916 D917 G918 D919 A926 L927 E928 E929 M930 S933 E934 M935 L936 V937 T941 ASP

GLY SER GLY PRO SER GLY

• Molecule 1: netrin receptor Unc5h2

Chain F:

23%

42%

38%

5%

16%

GLY SER SER GLY SER SER GLY TYR A855 F856 K857 I858 P859 L860 S861 I862 R863 Q864 K865 S868 D871 A872 S875 R876 G877 W880 R881 L882 Q885 K886 L887 S888 M889 D890 N894 T898 K899 A900 S901 G904 V905 I906 L907 D908 L909 W910 E911 A912 R913 Q914 Q915 D916

D917 G918 D919 L920 A924 L927 M930 S933 E934 M935 L936 V937 A938 M939 A940 T941 ASP GLY SER GLY PRO SER SER GLY

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	124.88Å 47.21Å 121.18Å 90.00° 119.56° 90.00°	Depositor
Resolution (Å)	39.78 – 2.10 39.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	93.8 (39.78-2.10) 97.5 (39.78-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.86 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.269 0.234 , 0.268	Depositor DCC
R_{free} test set	1736 reflections (4.92%)	DCC
Wilson B-factor (Å^2)	28.9	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 64.6	EDS
L-test for twinning[2]	$< |L| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4298	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: SO3, 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	0.40	0/707	0.56	0/947
1	B	0.41	0/652	0.62	0/871
1	C	0.36	0/694	0.63	0/928
1	D	0.42	0/677	0.59	1/905 (0.1%)
1	E	0.34	0/695	0.53	0/931
1	F	0.32	0/682	0.53	0/913
All	All	0.38	0/4107	0.58	1/5495 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	889	MSE	CG-SE-CE	-5.46	86.89	98.90

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	700	0	693	30	0
1	B	647	0	657	31	0
1	C	688	0	685	23	0
1	D	671	0	673	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	688	0	686	30	0
1	F	676	0	677	41	0
2	A	4	0	0	0	0
2	C	8	0	0	0	0
2	D	8	0	0	0	0
2	E	8	0	0	2	0
3	C	5	0	0	0	0
3	E	5	0	0	0	0
3	F	5	0	0	0	0
4	A	43	0	0	2	0
4	B	40	0	0	0	0
4	C	27	0	0	0	0
4	D	41	0	0	0	0
4	E	27	0	0	2	0
4	F	7	0	0	2	0
All	All	4298	0	4071	170	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 21.

The worst 5 of 170 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:E:899:LYS:HG3	1:E:905:VAL:HG21	1.36	1.07
1:F:889:MSE:HE1	1:F:906:ILE:HG23	1.30	1.06
1:B:914:GLN:HE22	1:B:919:ASP:HB3	1.18	1.02
1:F:920:LEU:H	1:F:920:LEU:HD12	1.28	0.97
1:A:899:LYS:HG3	1:A:905:VAL:HG21	1.45	0.96

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	88/103 (85%)	82 (93%)	5 (6%)	1 (1%)	17	11
1	B	79/103 (77%)	75 (95%)	4 (5%)	0	100	100
1	C	84/103 (82%)	80 (95%)	4 (5%)	0	100	100
1	D	82/103 (80%)	81 (99%)	1 (1%)	0	100	100
1	E	86/103 (84%)	80 (93%)	4 (5%)	2 (2%)	7	3
1	F	85/103 (82%)	72 (85%)	12 (14%)	1 (1%)	15	9
All	All	504/618 (82%)	470 (93%)	30 (6%)	4 (1%)	22	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	914	GLN
1	E	918	GLY
1	F	856	PHE
1	E	917	ASP

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	75/79 (95%)	73 (97%)	2 (3%)	50	54
1	B	70/79 (89%)	65 (93%)	5 (7%)	17	13
1	C	74/79 (94%)	72 (97%)	2 (3%)	50	54
1	D	72/79 (91%)	68 (94%)	4 (6%)	25	21
1	E	74/79 (94%)	73 (99%)	1 (1%)	71	78
1	F	73/79 (92%)	66 (90%)	7 (10%)	10	6
All	All	438/474 (92%)	417 (95%)	21 (5%)	30	27

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	878	ASN

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W O R L D W I D E
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PROTEIN DATA BANK

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Mol	Chain	Res	Type
1	D	913	ARG
1	F	890	ASP
1	C	915	GLN
1	F	901	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	874	ASN
1	D	878	ASN
1	F	864	GLN
1	C	915	GLN
1	E	915	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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

10 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
2	SO3	A	1001	-	1,3,3	0.77	0	0,3,3	0.00	-
2	SO3	C	1003	-	1,3,3	0.82	0	0,3,3	0.00	-
2	SO3	C	1004	-	1,3,3	0.83	0	0,3,3	0.00	-
3	SO4	C	2003	-	4,4,4	1.87	1 (25%)	6,6,6	0.85	0
2	SO3	D	1002	-	1,3,3	0.64	0	0,3,3	0.00	-
2	SO3	D	1006	-	1,3,3	0.72	0	0,3,3	0.00	-
2	SO3	E	1005	-	1,3,3	0.80	0	0,3,3	0.00	-
2	SO3	E	1007	-	1,3,3	0.89	0	0,3,3	0.00	-
3	SO4	E	2001	-	4,4,4	1.89	1 (25%)	6,6,6	0.83	0
3	SO4	F	2002	-	4,4,4	1.86	1 (25%)	6,6,6	0.85	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	SO3	A	1001	-	-	0/0/0/0	0/0/0/0
2	SO3	C	1003	-	-	0/0/0/0	0/0/0/0
2	SO3	C	1004	-	-	0/0/0/0	0/0/0/0
3	SO4	C	2003	-	-	0/0/0/0	0/0/0/0
2	SO3	D	1002	-	-	0/0/0/0	0/0/0/0
2	SO3	D	1006	-	-	0/0/0/0	0/0/0/0
2	SO3	E	1005	-	-	0/0/0/0	0/0/0/0
2	SO3	E	1007	-	-	0/0/0/0	0/0/0/0
3	SO4	E	2001	-	-	0/0/0/0	0/0/0/0
3	SO4	F	2002	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2002	SO4	O1-S	3.16	1.62	1.45
3	E	2001	SO4	O1-S	3.20	1.63	1.45
3	C	2003	SO4	O1-S	3.23	1.63	1.45

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 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1005	SO3	2	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	86/103 (83%)	0.67	9 (10%)	7	9	24, 35, 77, 84	0
1	B	79/103 (76%)	0.48	3 (3%)	41	48	21, 32, 58, 71	0
1	C	84/103 (81%)	0.67	4 (4%)	31	37	24, 39, 63, 73	0
1	D	82/103 (79%)	0.28	1 (1%)	79	82	19, 33, 53, 64	0
1	E	84/103 (81%)	0.81	12 (14%)	3	4	27, 47, 68, 76	0
1	F	83/103 (80%)	1.57	24 (28%)	1	1	40, 65, 86, 87	0
All	All	498/618 (80%)	0.75	53 (10%)	7	8	19, 40, 77, 87	0

The worst 5 of 53 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	860	LEU	9.5
1	C	855	ALA	8.0
1	B	855	ALA	7.8
1	F	855	ALA	7.3
1	E	918	GLY	6.9

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 carbohydrates 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. 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, 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	LLDF	B-factors(Å^2)	Q<0.9
2	SO3	A	1001	4/4	0.96	0.13	-0.90	54,55,55,57	0
2	SO3	E	1007	4/4	0.83	0.18	-	88,88,89,89	0
2	SO3	C	1003	4/4	0.89	0.13	-	85,86,86,86	0
2	SO3	E	1005	4/4	0.93	0.14	-	67,67,67,68	0
2	SO3	D	1002	4/4	0.93	0.17	-	81,81,81,82	0
3	SO4	F	2002	5/5	0.93	0.13	-	75,76,77,77	0
2	SO3	C	1004	4/4	0.95	0.14	-	73,73,73,73	0
2	SO3	D	1006	4/4	0.96	0.15	-	69,69,69,70	0
3	SO4	C	2003	5/5	0.97	0.08	-	49,50,52,52	0
3	SO4	E	2001	5/5	0.95	0.12	-	75,75,76,76	0

6.5 Other polymers ⓘ

There are no such residues in this entry.