Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 07:43 am BST

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)

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

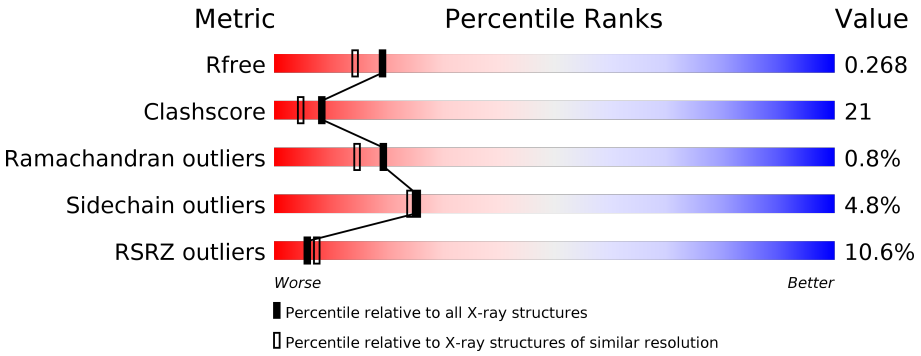
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	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%

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

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

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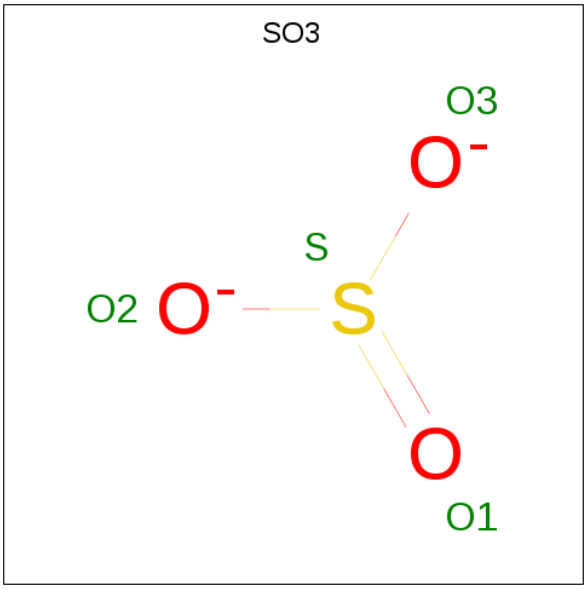
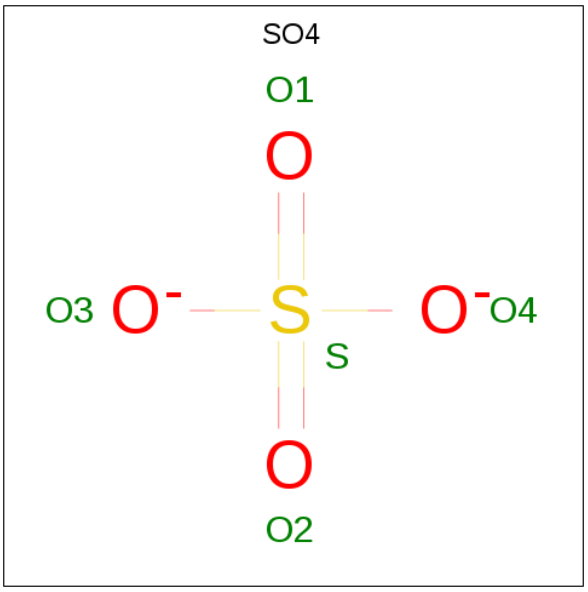
Chain	Residue	Modelled	Actual	Comment	Reference
F	949	GLY	-	CLONING ARTIFACT	UNP Q8K1S3

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



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

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



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

- Molecule 4 is water.

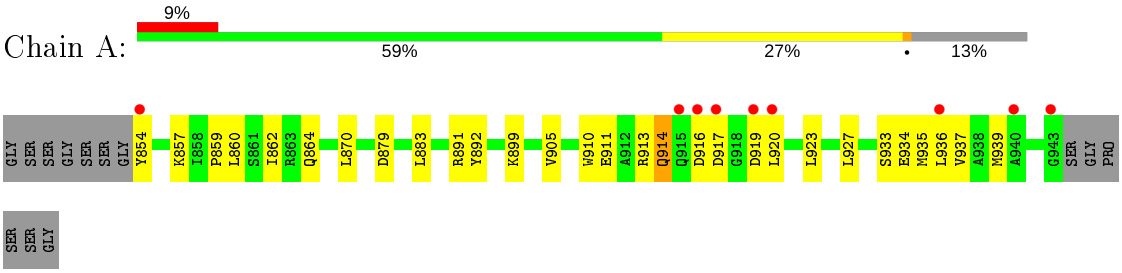
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	43	Total O 43 43	0	0
4	B	40	Total O 40 40	0	0
4	C	27	Total O 27 27	0	0
4	D	41	Total O 41 41	0	0
4	E	27	Total O 27 27	0	0
4	F	7	Total O 7 7	0	0

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 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.

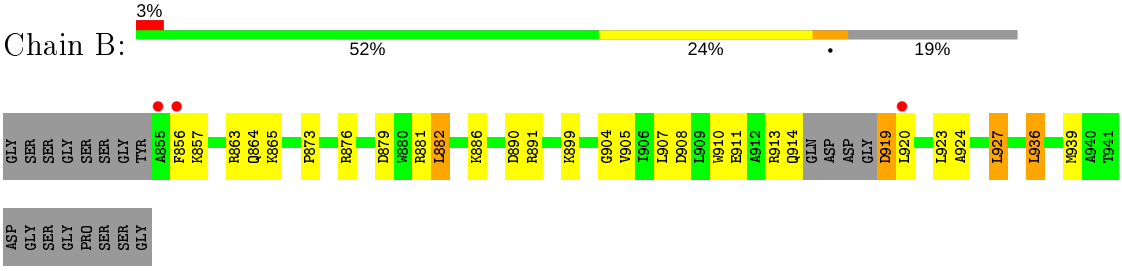
- Molecule 1: netrin receptor Unc5h2

Chain A:



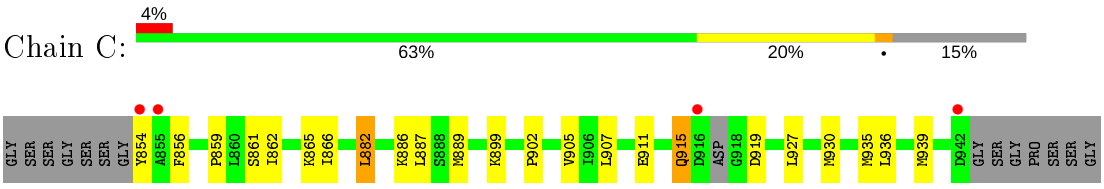
- Molecule 1: netrin receptor Unc5h2

Chain B:



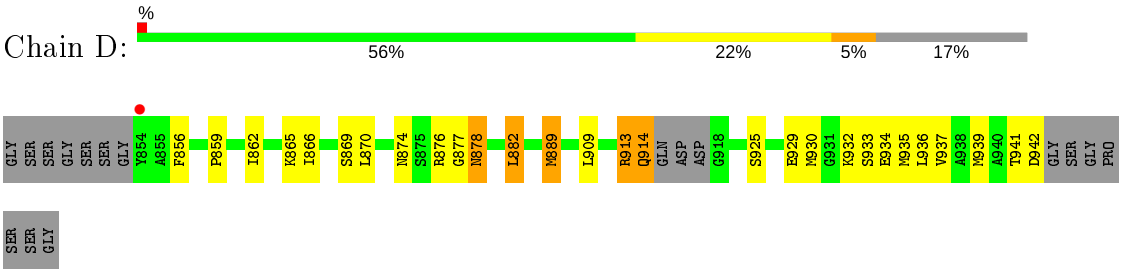
- Molecule 1: netrin receptor Unc5h2

Chain C:



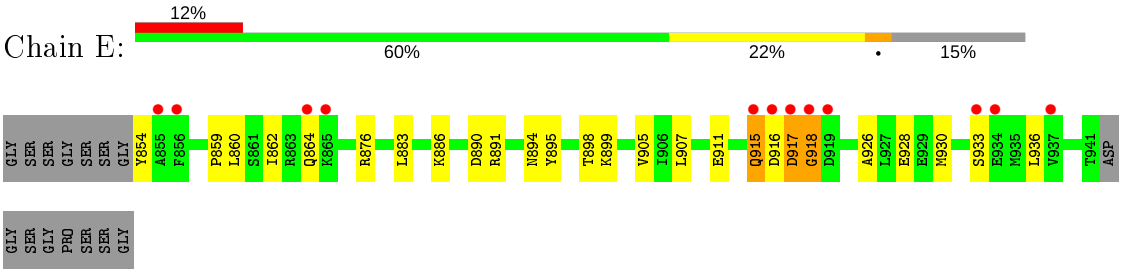
- Molecule 1: netrin receptor Unc5h2

Chain D:



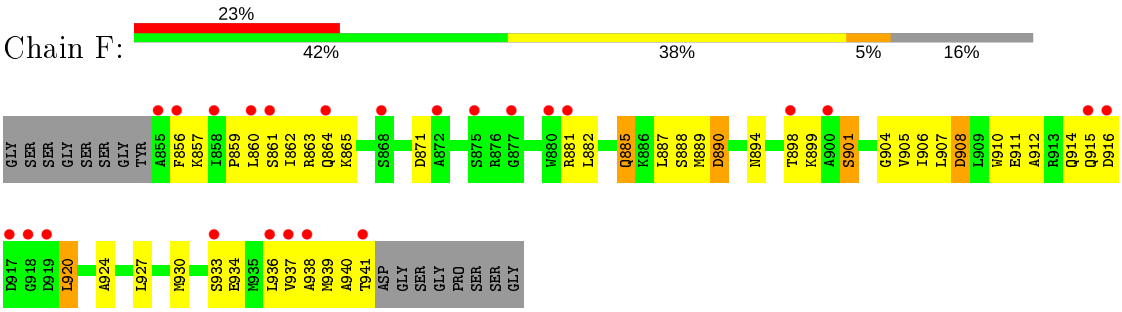
- Molecule 1: netrin receptor Unc5h2

Chain E:



• Molecule 1: netrin receptor Unc5h2

Chain F:



4 Data and refinement statistics (i)

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	3403 reflections (4.97%)	wwPDB-VP
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.*

[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(^{o})	Ideal(^{o})
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.

All (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
1:A:859:PRO:HG2	1:A:862:ILE:HD12	1.50	0.93
1:B:927:LEU:HD23	1:B:939:MSE:HE1	1.52	0.91
1:F:860:LEU:H	1:F:860:LEU:HD22	1.37	0.89
1:B:914:GLN:NE2	1:B:919:ASP:HB3	1.89	0.87
1:B:910:TRP:HZ2	1:B:920:LEU:HA	1.43	0.82
1:F:936:LEU:HA	1:F:939:MSE:HE3	1.64	0.78
1:A:935:MSE:HE2	1:A:935:MSE:HA	1.65	0.78
1:E:926:ALA:C	1:E:930:MSE:HE3	2.04	0.77
1:D:874:ASN:HD21	1:D:876:ARG:HB2	1.52	0.75
1:E:915:GLN:HA	1:E:915:GLN:HE21	1.51	0.74
1:C:915:GLN:HE21	1:C:915:GLN:HA	1.52	0.74
1:C:859:PRO:HG2	1:C:862:ILE:HD12	1.70	0.74
1:C:866:ILE:HG12	1:C:935:MSE:HE2	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:899:LYS:HG3	1:C:905:VAL:HG21	1.69	0.74
1:D:859:PRO:HG2	1:D:862:ILE:HD12	1.69	0.73
1:B:910:TRP:CZ2	1:B:920:LEU:HA	2.21	0.73
1:F:871:ASP:OD1	1:F:901:SER:HB2	1.87	0.73
1:E:926:ALA:O	1:E:930:MSE:HE3	1.88	0.72
1:A:913:ARG:HB3	1:B:891:ARG:NH2	2.04	0.71
1:C:936:LEU:HA	1:C:939:MSE:HE3	1.72	0.71
1:A:910:TRP:HZ2	1:A:920:LEU:HA	1.57	0.69
1:E:883:LEU:HD12	1:E:930:MSE:HE1	1.73	0.69
1:C:882:LEU:HB3	1:C:930:MSE:HE3	1.75	0.68
1:E:864:GLN:HG3	4:E:71:HOH:O	1.94	0.68
1:F:907:LEU:O	1:F:911:GLU:HG3	1.95	0.67
1:E:886:LYS:HD2	1:E:930:MSE:HE2	1.77	0.66
1:F:882:LEU:HB3	1:F:930:MSE:HE3	1.79	0.65
1:E:883:LEU:CD1	1:E:930:MSE:HE1	2.28	0.64
1:E:891:ARG:HG2	2:E:1005:SO3:O2	1.98	0.63
1:D:934:GLU:H	1:D:934:GLU:CD	2.02	0.63
1:A:913:ARG:HB3	1:B:891:ARG:HH22	1.63	0.63
1:E:876:ARG:NH2	4:E:30:HOH:O	2.32	0.62
1:D:935:MSE:O	1:D:939:MSE:HG3	1.99	0.62
1:F:898:THR:HG22	1:F:898:THR:O	1.99	0.62
1:F:920:LEU:H	1:F:920:LEU:CD1	2.06	0.62
1:F:899:LYS:HD2	1:F:905:VAL:HG11	1.81	0.62
1:B:899:LYS:HG3	1:B:905:VAL:HG21	1.82	0.61
1:A:913:ARG:HD2	1:B:891:ARG:CZ	2.30	0.61
1:B:882:LEU:HD22	1:B:886:LYS:HE2	1.82	0.61
1:B:914:GLN:HE22	1:B:919:ASP:CB	2.03	0.60
1:A:854:TYR:HD2	1:A:857:LYS:HE2	1.66	0.60
1:F:881:ARG:HD2	4:F:134:HOH:O	2.02	0.60
1:F:885:GLN:HE21	1:F:885:GLN:HA	1.66	0.59
1:C:887:LEU:CB	1:C:889:MSE:HE3	2.33	0.59
1:B:923:LEU:O	1:B:927:LEU:HD22	2.03	0.58
1:B:863:ARG:NH2	1:B:908:ASP:OD1	2.36	0.58
1:F:933:SER:O	1:F:937:VAL:HG13	2.04	0.58
1:A:935:MSE:CE	1:A:935:MSE:HA	2.33	0.58
1:D:889:MSE:HE1	1:D:909:LEU:CB	2.34	0.58
1:A:891:ARG:HG2	1:B:913:ARG:HG3	1.86	0.58
1:F:860:LEU:H	1:F:860:LEU:CD2	2.15	0.57
1:B:873:PRO:O	1:B:876:ARG:HG3	2.05	0.56
1:B:936:LEU:HD12	1:C:936:LEU:HB3	1.88	0.56
1:D:925:SER:O	1:D:929:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:939:MSE:O	1:F:940:ALA:HA	2.06	0.56
1:D:889:MSE:HE1	1:D:909:LEU:HB2	1.88	0.56
1:A:913:ARG:HD2	1:B:891:ARG:NH2	2.21	0.56
1:F:861:SER:O	1:F:865:LYS:HG3	2.06	0.55
1:A:920:LEU:HD23	1:A:920:LEU:O	2.06	0.55
1:C:899:LYS:O	1:C:902:PRO:HD3	2.08	0.54
1:F:862:ILE:HD12	1:F:939:MSE:HA	1.88	0.54
1:C:854:TYR:C	1:C:856:PHE:N	2.61	0.54
1:A:870:LEU:O	1:A:879:ASP:HB2	2.08	0.53
1:B:891:ARG:HH21	1:B:891:ARG:HG2	1.73	0.53
1:D:874:ASN:ND2	1:D:878:ASN:H	2.06	0.53
1:D:889:MSE:SE	1:D:913:ARG:NH2	2.91	0.53
1:A:933:SER:O	1:A:936:LEU:HG	2.08	0.53
1:D:941:THR:O	1:D:942:ASP:HB2	2.09	0.53
1:A:854:TYR:CD2	1:A:857:LYS:HE2	2.44	0.52
1:A:911:GLU:O	1:A:914:GLN:HB2	2.08	0.52
1:A:934:GLU:HG2	4:A:88:HOH:O	2.08	0.52
1:C:887:LEU:HB2	1:C:889:MSE:HE3	1.91	0.52
1:D:932:LYS:HB3	1:D:935:MSE:HE3	1.91	0.51
1:D:932:LYS:O	1:D:936:LEU:HG	2.11	0.51
1:E:864:GLN:NE2	1:E:864:GLN:HA	2.25	0.51
1:A:936:LEU:HD13	1:F:936:LEU:HD13	1.92	0.51
1:E:933:SER:HA	1:E:936:LEU:HD12	1.93	0.51
1:F:904:GLY:O	1:F:908:ASP:OD1	2.28	0.51
1:D:874:ASN:HD22	1:D:877:GLY:N	2.09	0.51
1:F:859:PRO:HG2	1:F:862:ILE:CG1	2.41	0.51
1:C:919:ASP:N	1:C:919:ASP:OD2	2.44	0.50
1:A:936:LEU:HA	1:A:939:MSE:HE3	1.93	0.50
1:F:865:LYS:HD3	1:F:938:ALA:HB1	1.92	0.50
1:A:933:SER:HA	1:A:936:LEU:HG	1.93	0.49
1:F:885:GLN:HE21	1:F:885:GLN:CA	2.23	0.49
1:F:937:VAL:HG23	1:F:938:ALA:N	2.27	0.49
1:C:854:TYR:C	1:C:856:PHE:H	2.15	0.49
1:A:859:PRO:CG	1:A:862:ILE:HD12	2.33	0.49
1:E:864:GLN:HE21	1:E:864:GLN:HA	1.78	0.48
1:E:915:GLN:HA	1:E:915:GLN:NE2	2.25	0.48
1:D:856:PHE:CD2	1:D:914:GLN:HB3	2.49	0.48
1:C:887:LEU:HB3	1:C:889:MSE:HE3	1.95	0.48
1:C:861:SER:O	1:C:865:LYS:HG3	2.13	0.48
1:D:882:LEU:HD13	1:D:930:MSE:HG2	1.94	0.48
1:E:895:TYR:O	1:E:898:THR:HB	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:924:ALA:HA	1:F:927:LEU:HD12	1.96	0.47
1:D:874:ASN:HD22	1:D:877:GLY:H	1.61	0.47
1:E:926:ALA:HB1	1:E:930:MSE:CE	2.44	0.47
1:D:874:ASN:ND2	1:D:876:ARG:HB2	2.26	0.47
1:A:936:LEU:HD12	1:A:937:VAL:N	2.30	0.47
1:F:863:ARG:NH2	4:F:129:HOH:O	2.47	0.47
1:B:879:ASP:OD1	1:B:881:ARG:NH1	2.49	0.46
1:E:860:LEU:O	1:E:860:LEU:HD23	2.15	0.46
1:D:862:ILE:O	1:D:866:ILE:HG13	2.15	0.46
1:E:917:ASP:O	1:E:918:GLY:C	2.54	0.46
1:F:910:TRP:HH2	1:F:920:LEU:HA	1.80	0.46
1:E:854:TYR:CE1	1:F:894:ASN:HB3	2.51	0.46
1:B:863:ARG:NH2	1:B:904:GLY:O	2.49	0.46
1:C:899:LYS:HB3	1:C:899:LYS:NZ	2.30	0.46
1:C:927:LEU:HD12	1:C:939:MSE:CE	2.46	0.46
1:C:882:LEU:O	1:C:886:LYS:HG2	2.16	0.45
1:A:892:TYR:CE1	1:B:913:ARG:HD3	2.51	0.45
1:E:859:PRO:CG	1:E:862:ILE:HD12	2.47	0.45
1:F:889:MSE:HB2	1:F:889:MSE:HE3	1.82	0.45
1:A:919:ASP:HB3	4:A:107:HOH:O	2.17	0.45
1:C:936:LEU:HD23	1:C:939:MSE:HE3	1.99	0.44
1:D:870:LEU:HD21	1:D:932:LYS:HE3	2.00	0.44
1:B:927:LEU:CD2	1:B:939:MSE:HE1	2.35	0.44
1:E:859:PRO:HG2	1:E:862:ILE:HD12	1.99	0.44
1:E:907:LEU:O	1:E:911:GLU:HG3	2.17	0.44
1:F:915:GLN:HG3	1:F:916:ASP:OD2	2.18	0.44
1:A:870:LEU:HD12	1:A:883:LEU:HD22	2.00	0.44
1:D:889:MSE:HE3	1:D:889:MSE:HB3	1.86	0.44
1:B:907:LEU:O	1:B:911:GLU:HG3	2.17	0.44
1:D:865:LYS:HD3	1:D:939:MSE:HG2	2.00	0.44
1:F:916:ASP:N	1:F:916:ASP:OD2	2.50	0.44
1:B:856:PHE:CG	1:B:857:LYS:N	2.86	0.44
1:E:933:SER:O	1:E:936:LEU:HB2	2.18	0.44
1:F:888:SER:HA	1:F:890:ASP:OD1	2.18	0.43
1:B:936:LEU:HA	1:B:939:MSE:HE3	2.00	0.43
1:D:869:SER:HB3	1:D:935:MSE:HE2	1.99	0.43
1:C:859:PRO:CG	1:C:862:ILE:HD12	2.45	0.43
1:F:889:MSE:HE1	1:F:906:ILE:CG2	2.22	0.43
1:E:899:LYS:CG	1:E:905:VAL:HG21	2.27	0.43
1:F:927:LEU:CD1	1:F:939:MSE:HE1	2.48	0.43
1:E:915:GLN:HE21	1:E:915:GLN:CA	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:916:ASP:C	1:E:918:GLY:H	2.22	0.43
1:E:928:GLU:HB2	1:E:936:LEU:HD11	2.00	0.43
1:D:859:PRO:CG	1:D:862:ILE:HD12	2.45	0.42
1:F:862:ILE:CD1	1:F:939:MSE:HA	2.48	0.42
1:A:892:TYR:HE1	1:B:913:ARG:HD3	1.83	0.42
1:F:860:LEU:O	1:F:864:GLN:HG3	2.19	0.42
1:D:889:MSE:SE	1:D:913:ARG:HH21	2.53	0.42
1:A:923:LEU:O	1:A:927:LEU:HD22	2.20	0.42
1:D:869:SER:CB	1:D:935:MSE:HE2	2.49	0.42
1:F:865:LYS:CD	1:F:938:ALA:HB1	2.50	0.42
1:A:916:ASP:O	1:A:917:ASP:C	2.58	0.42
1:F:859:PRO:HG2	1:F:862:ILE:HG13	2.01	0.42
1:B:891:ARG:CG	1:B:891:ARG:HH21	2.33	0.42
1:E:864:GLN:CA	1:E:864:GLN:HE21	2.30	0.42
1:A:920:LEU:HD13	1:F:941:THR:CG2	2.50	0.42
1:D:941:THR:O	1:D:942:ASP:CB	2.68	0.42
1:F:934:GLU:O	1:F:937:VAL:HG22	2.20	0.42
1:B:857:LYS:HB3	1:B:857:LYS:HE2	1.91	0.41
1:B:924:ALA:O	1:B:936:LEU:HD21	2.20	0.41
1:B:882:LEU:CD2	1:B:886:LYS:HE2	2.49	0.41
1:C:907:LEU:O	1:C:911:GLU:HG3	2.19	0.41
1:C:915:GLN:HA	1:C:915:GLN:NE2	2.28	0.41
1:B:864:GLN:OE1	1:B:865:LYS:HD2	2.21	0.41
1:C:927:LEU:HD12	1:C:939:MSE:HE1	2.03	0.41
1:D:933:SER:O	1:D:937:VAL:HG23	2.21	0.41
1:E:890:ASP:HB3	2:E:1005:SO3:O3	2.20	0.41
1:F:910:TRP:O	1:F:914:GLN:HG2	2.21	0.41
1:D:878:ASN:HA	1:D:878:ASN:HD22	1.65	0.40
1:E:894:ASN:HB2	1:F:912:ALA:HB1	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	88/103 (85%)	82 (93%)	5 (6%)	1 (1%)	14 9
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%)	6 2
1	F	85/103 (82%)	72 (85%)	12 (14%)	1 (1%)	13 8
All	All	504/618 (82%)	470 (93%)	30 (6%)	4 (1%)	19 15

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 (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	75/79 (95%)	73 (97%)	2 (3%)	44 48
1	B	70/79 (89%)	65 (93%)	5 (7%)	14 11
1	C	74/79 (94%)	72 (97%)	2 (3%)	44 48
1	D	72/79 (91%)	68 (94%)	4 (6%)	21 18
1	E	74/79 (94%)	73 (99%)	1 (1%)	67 73
1	F	73/79 (92%)	66 (90%)	7 (10%)	8 5
All	All	438/474 (92%)	417 (95%)	21 (5%)	25 24

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	860	LEU

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Mol	Chain	Res	Type
1	A	864	GLN
1	B	882	LEU
1	B	890	ASP
1	B	919	ASP
1	B	927	LEU
1	B	936	LEU
1	C	882	LEU
1	C	915	GLN
1	D	878	ASN
1	D	882	LEU
1	D	913	ARG
1	D	914	GLN
1	E	915	GLN
1	F	857	LYS
1	F	885	GLN
1	F	887	LEU
1	F	890	ASP
1	F	901	SER
1	F	908	ASP
1	F	920	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	864	GLN
1	A	878	ASN
1	A	894	ASN
1	B	885	GLN
1	B	914	GLN
1	C	915	GLN
1	D	874	ASN
1	D	878	ASN
1	D	914	GLN
1	E	864	GLN
1	E	894	ASN
1	E	915	GLN
1	F	864	GLN
1	F	885	GLN
1	F	894	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

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	$\#\|Z\| > 2$
3	SO4	F	2002	-	4,4,4	1.88	2 (50%)	6,6,6	0.88	0
2	SO3	E	1007	-	1,3,3	0.92	0	0,3,3	0.00	-
2	SO3	C	1003	-	1,3,3	0.84	0	0,3,3	0.00	-
2	SO3	E	1005	-	1,3,3	0.82	0	0,3,3	0.00	-
2	SO3	D	1002	-	1,3,3	0.65	0	0,3,3	0.00	-
2	SO3	A	1001	-	1,3,3	0.78	0	0,3,3	0.00	-
2	SO3	C	1004	-	1,3,3	0.85	0	0,3,3	0.00	-
2	SO3	D	1006	-	1,3,3	0.73	0	0,3,3	0.00	-
3	SO4	C	2003	-	4,4,4	1.88	2 (50%)	6,6,6	0.88	0
3	SO4	E	2001	-	4,4,4	1.90	2 (50%)	6,6,6	0.86	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2003	SO4	O1-S	3.17	1.63	1.46
3	E	2001	SO4	O1-S	3.13	1.63	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	2002	SO4	O1-S	3.10	1.62	1.46
3	E	2001	SO4	O3-S	-2.12	1.30	1.47
3	F	2002	SO4	O3-S	-2.07	1.30	1.47
3	C	2003	SO4	O3-S	-2.01	1.31	1.47

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 (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	86/103 (83%)	0.67	9 (10%) 6 8	24, 35, 77, 84	0
1	B	79/103 (76%)	0.48	3 (3%) 40 46	21, 32, 58, 71	0
1	C	84/103 (81%)	0.67	4 (4%) 30 36	24, 39, 63, 73	0
1	D	82/103 (79%)	0.29	1 (1%) 79 82	19, 33, 53, 64	0
1	E	84/103 (81%)	0.82	12 (14%) 2 3	27, 47, 68, 76	0
1	F	83/103 (80%)	1.57	24 (28%) 0 0	40, 65, 86, 87	0
All	All	498/618 (80%)	0.75	53 (10%) 6 7	19, 40, 77, 87	0

All (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	7.7
1	F	855	ALA	7.3
1	E	918	GLY	6.9
1	A	916	ASP	6.4
1	B	856	PHE	6.0
1	E	855	ALA	5.7
1	A	917	ASP	5.7
1	B	920	LEU	5.5
1	C	854	TYR	5.2
1	F	856	PHE	4.7
1	F	877	GLY	4.7
1	E	917	ASP	4.6
1	C	942	ASP	4.4
1	A	854	TYR	4.3
1	D	854	TYR	4.3
1	E	933	SER	4.2
1	A	919	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	F	916	ASP	4.0
1	E	937	VAL	4.0
1	F	938	ALA	4.0
1	A	915	GLN	3.9
1	E	934	GLU	3.8
1	C	916	ASP	3.8
1	E	856	PHE	3.3
1	F	868	SER	3.2
1	E	919	ASP	3.2
1	F	875	SER	3.2
1	F	872	ALA	3.1
1	F	936	LEU	3.1
1	E	915	GLN	3.1
1	F	917	ASP	3.1
1	A	943	GLY	2.9
1	F	864	GLN	2.9
1	F	915	GLN	2.9
1	A	936	LEU	2.9
1	F	918	GLY	2.9
1	F	898	THR	2.8
1	F	937	VAL	2.7
1	E	916	ASP	2.7
1	F	858	ILE	2.7
1	F	933	SER	2.6
1	A	940	ALA	2.5
1	F	880	TRP	2.5
1	A	920	LEU	2.4
1	F	919	ASP	2.4
1	E	865	LYS	2.3
1	E	864	GLN	2.2
1	F	900	ALA	2.2
1	F	861	SER	2.2
1	F	941	THR	2.2
1	F	881	ARG	2.1

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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
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
3	SO4	F	2002	5/5	0.93	0.13	75,76,77,77	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
2	SO3	C	1004	4/4	0.95	0.14	73,73,73,73	0
3	SO4	E	2001	5/5	0.95	0.12	75,75,76,76	0
2	SO3	D	1006	4/4	0.96	0.15	69,69,69,70	0
2	SO3	A	1001	4/4	0.96	0.13	54,55,55,57	0
3	SO4	C	2003	5/5	0.97	0.08	49,50,52,52	0

6.5 Other polymers (i)

There are no such residues in this entry.