



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 08:39 PM UTC

PDB ID : 1WMG / pdb_00001wmg
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 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:

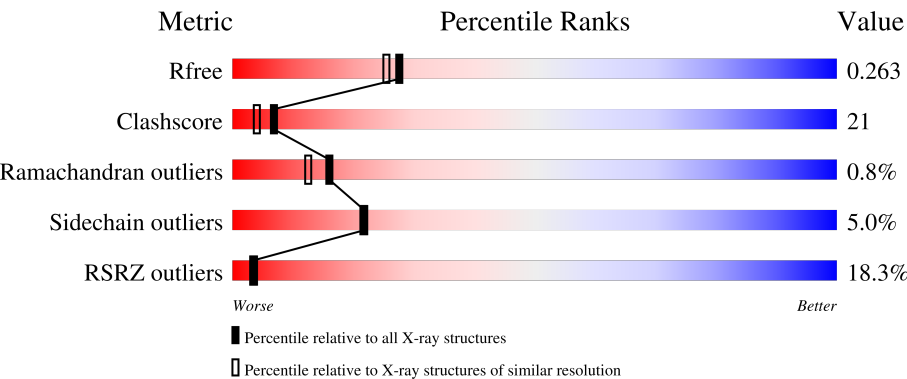
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 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	103	13% 59% 27% • 13%
1	B	103	6% 50% 24% 6% 19%
1	C	103	10% 59% 23% •• 15%
1	D	103	3% 55% 21% 7% 17%
1	E	103	21% 58% 25% • 15%

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Mol	Chain	Length	Quality of chain
1	F	103	

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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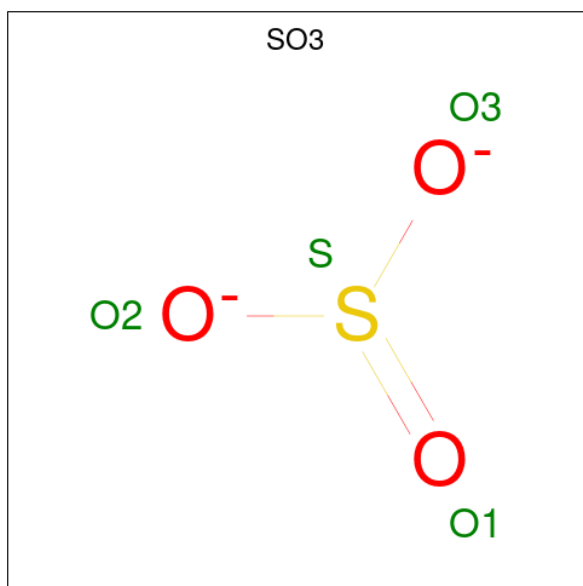
Chain	Residue	Modelled	Actual	Comment	Reference
D	930	MSE	MET	modified residue	UNP Q8K1S3
D	935	MSE	MET	modified residue	UNP Q8K1S3
D	939	MSE	MET	modified residue	UNP Q8K1S3
D	944	SER	-	cloning artifact	UNP Q8K1S3
D	945	GLY	-	cloning artifact	UNP Q8K1S3
D	946	PRO	-	cloning artifact	UNP Q8K1S3
D	947	SER	-	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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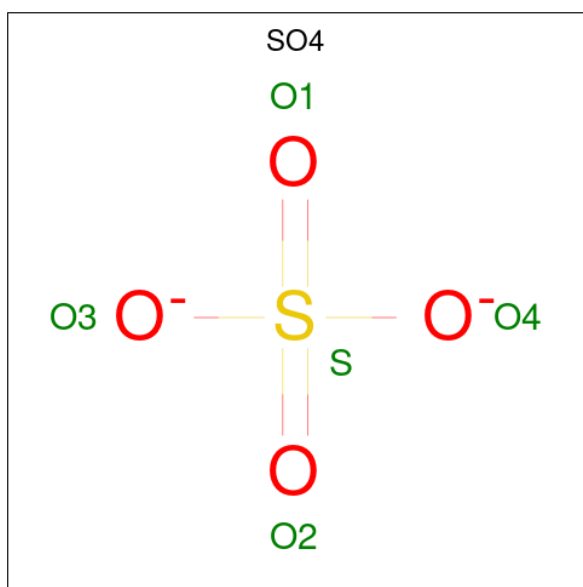
Chain	Residue	Modelled	Actual	Comment	Reference
F	949	GLY	-	cloning artifact	UNP Q8K1S3

- Molecule 2 is SULFITE ION (CCD ID: SO3) (formula: O₃S).



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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

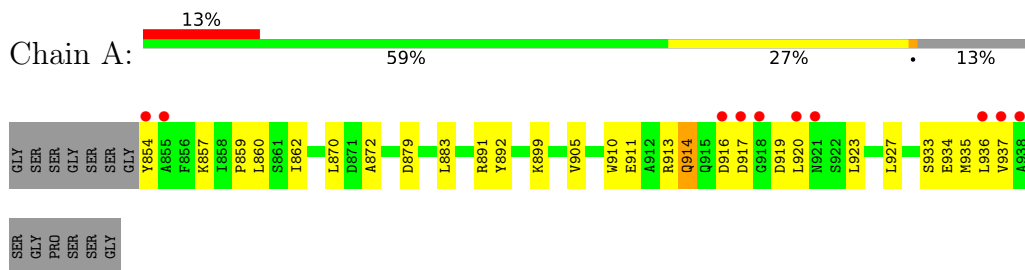
- Molecule 4 is water.

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

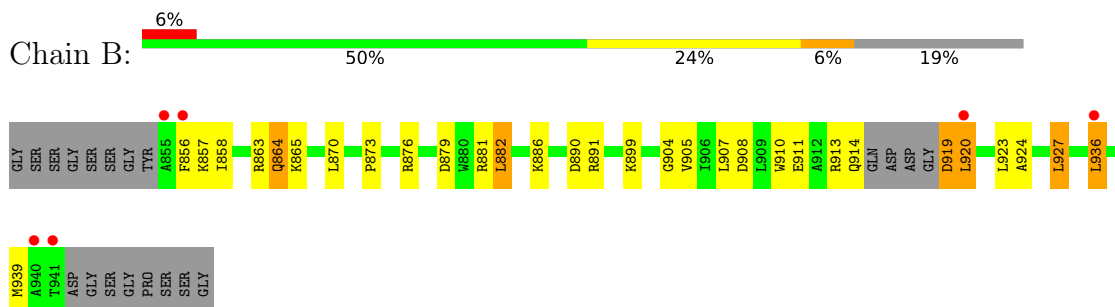
3 Residue-property plots

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.

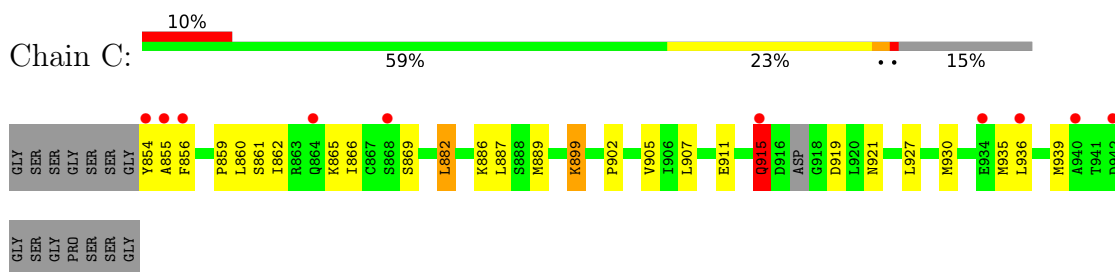
- Molecule 1: netrin receptor Unc5h2



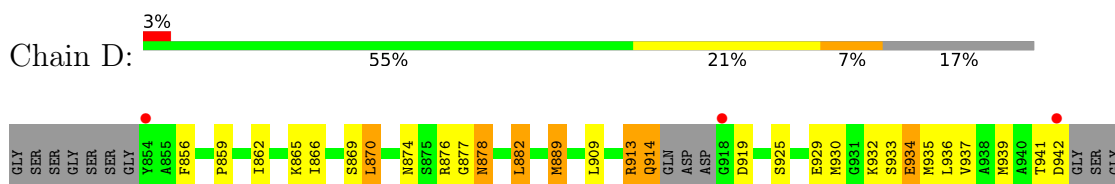
- Molecule 1: netrin receptor Unc5h2



- Molecule 1: netrin receptor Unc5h2

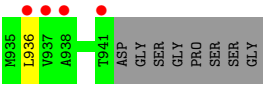
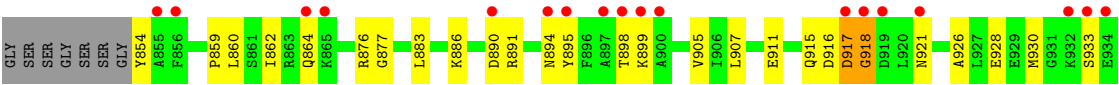


- Molecule 1: netrin receptor Unc5h2

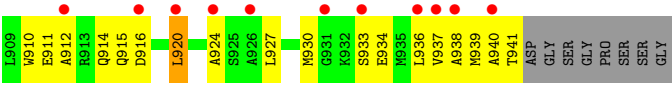
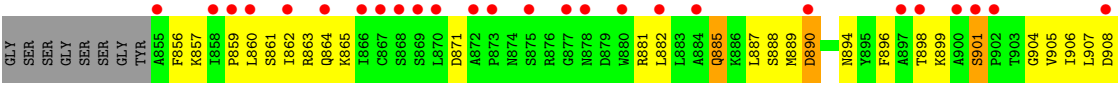


PRO
SER
SER
GLY

● Molecule 1: netrin receptor Unc5h2



● Molecule 1: netrin receptor Unc5h2



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) 95.3 (39.78-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.86 (at 2.10Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.269 0.223 , 0.263	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)	0.39 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.009 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, SO3

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	0.49	0/707	0.89	1/947 (0.1%)
1	B	0.54	0/652	0.97	3/871 (0.3%)
1	C	0.44	0/694	0.98	4/928 (0.4%)
1	D	0.52	0/677	0.93	3/905 (0.3%)
1	E	0.42	0/695	0.84	2/931 (0.2%)
1	F	0.37	0/682	0.88	0/913
All	All	0.47	0/4107	0.92	13/5495 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	915	GLN	N-CA-C	-6.13	100.86	109.69
1	C	921	ASN	N-CA-C	6.04	118.35	111.11
1	B	870	LEU	N-CA-C	5.88	119.71	112.54
1	C	855	ALA	N-CA-C	-5.79	105.92	112.87
1	A	872	ALA	N-CA-C	5.71	117.69	109.48
1	E	921	ASN	N-CA-C	5.58	117.83	111.02
1	B	920	LEU	N-CA-C	-5.56	106.33	113.01
1	D	919	ASP	N-CA-C	5.53	117.41	108.34
1	D	889	MSE	CG-SE-CE	-5.47	86.89	98.92
1	E	877	GLY	N-CA-C	-5.41	107.52	115.30
1	D	870	LEU	N-CA-C	5.28	119.72	113.28
1	B	858	ILE	CB-CA-C	-5.02	106.27	110.94
1	C	869	SER	N-CA-C	5.00	116.55	111.14

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	32	0
1	C	688	0	685	23	0
1	D	671	0	673	28	0
1	E	688	0	686	32	0
1	F	676	0	677	42	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	174	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 (174) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:926:ALA:C	1:E:930:MSE:HE3	2.04	0.82
1:F:936:LEU:HA	1:F:939:MSE:HE3	1.64	0.78
1:A:935:MSE:HA	1:A:935:MSE:HE2	1.65	0.78
1:D:874:ASN:HD21	1:D:876:ARG:HB2	1.52	0.75
1:E:915:GLN:HE21	1:E:915:GLN:HA	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
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:D:934:GLU:H	1:D:934:GLU:CD	2.02	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: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:O	1:F:898:THR:HG22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HA	1:A:935:MSE:CE	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
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:O	1:A:920:LEU:HD23	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:A:870:LEU:O	1:A:879:ASP:HB2	2.08	0.53
1:B:891:ARG:HG2	1:B:891:ARG:HH21	1.73	0.53
1:C:854:TYR:C	1:C:856:PHE:H	2.15	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:C:854:TYR:C	1:C:856:PHE:N	2.61	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:917:ASP:O	1:E:918:GLY:C	2.54	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:D:941:THR:O	1:D:942:ASP:HB2	2.09	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:859:PRO:CG	1:A:862:ILE:HD12	2.33	0.49
1:E:864:GLN:HA	1:E:864:GLN:HE21	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
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:E:916:ASP:C	1:E:918:GLY:H	2.22	0.47
1:A:936:LEU:HD12	1:A:937:VAL:N	2.30	0.47
1:C:919:ASP:OD2	1:C:919:ASP:N	2.44	0.47
1:A:916:ASP:O	1:A:917:ASP:C	2.58	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:HD23	1:E:860:LEU:O	2.15	0.46
1:D:862:ILE:O	1:D:866:ILE:HG13	2.15	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:B:914:GLN:CD	1:B:919:ASP:HB3	2.41	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:HE3	1:F:889:MSE:HB2	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:HB3	1:D:889:MSE:HE3	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:916:ASP:OD2	1:F:916:ASP:N	2.50	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:E:860:LEU:HD23	1:E:860:LEU:C	2.45	0.42
1:F:865:LYS:CD	1:F:938:ALA:HB1	2.50	0.42
1:F:859:PRO:HG2	1:F:862:ILE:HG13	2.01	0.42
1:A:920:LEU:HD13	1:F:941:THR:CG2	2.50	0.42
1:B:891:ARG:HH21	1:B:891:ARG:CG	2.33	0.42
1:E:864:GLN:HE21	1:E:864:GLN:CA	2.30	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:E:916:ASP:C	1:E:918:GLY:N	2.78	0.41
1:F:896:PHE:C	1:F:898:THR:H	2.29	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:878:ASN:HD22	1:D:878:ASN:HA	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%)	11	8
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%)	5	2
1	F	85/103 (82%)	72 (85%)	12 (14%)	1 (1%)	10	7
All	All	504/618 (82%)	470 (93%)	30 (6%)	4 (1%)	16	12

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%)	74 (99%)	1 (1%)	61	69
1	B	70/79 (89%)	64 (91%)	6 (9%)	10	7
1	C	74/79 (94%)	70 (95%)	4 (5%)	20	18
1	D	72/79 (91%)	67 (93%)	5 (7%)	14	12
1	E	74/79 (94%)	74 (100%)	0	100	100
1	F	73/79 (92%)	67 (92%)	6 (8%)	10	8
All	All	438/474 (92%)	416 (95%)	22 (5%)	22	22

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	860	LEU
1	B	864	GLN
1	B	882	LEU
1	B	890	ASP
1	B	919	ASP
1	B	927	LEU
1	B	936	LEU
1	C	860	LEU
1	C	882	LEU
1	C	899	LYS
1	C	915	GLN
1	D	878	ASN
1	D	882	LEU
1	D	913	ARG
1	D	914	GLN
1	D	934	GLU
1	F	857	LYS
1	F	885	GLN
1	F	887	LEU
1	F	890	ASP
1	F	901	SER
1	F	920	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	E	1007	-	1,3,3	0.91	0	0,3,3	-	-
3	SO4	E	2001	-	4,4,4	1.88	2 (50%)	6,6,6	0.79	0
2	SO3	D	1006	-	1,3,3	0.73	0	0,3,3	-	-
2	SO3	C	1004	-	1,3,3	0.84	0	0,3,3	-	-
2	SO3	D	1002	-	1,3,3	0.65	0	0,3,3	-	-
2	SO3	E	1005	-	1,3,3	0.81	0	0,3,3	-	-
3	SO4	F	2002	-	4,4,4	1.85	2 (50%)	6,6,6	0.81	0
2	SO3	A	1001	-	1,3,3	0.78	0	0,3,3	-	-
3	SO4	C	2003	-	4,4,4	1.86	2 (50%)	6,6,6	0.82	0
2	SO3	C	1003	-	1,3,3	0.83	0	0,3,3	-	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2003	SO4	O1-S	3.09	1.63	1.44
3	E	2001	SO4	O1-S	3.06	1.63	1.44
3	F	2002	SO4	O1-S	3.02	1.62	1.44
3	E	2001	SO4	O3-S	-2.15	1.30	1.48
3	F	2002	SO4	O3-S	-2.10	1.30	1.48
3	C	2003	SO4	O3-S	-2.04	1.31	1.48

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, 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%)	0.82	13 (15%) 5 5	24, 35, 77, 84	0
1	B	79/103 (76%)	0.49	6 (7%) 20 21	21, 32, 58, 71	0
1	C	84/103 (81%)	0.86	10 (11%) 9 9	24, 39, 63, 73	0
1	D	82/103 (79%)	0.44	3 (3%) 45 47	19, 33, 53, 64	0
1	E	84/103 (81%)	1.30	22 (26%) 1 1	27, 47, 68, 76	0
1	F	83/103 (80%)	2.03	37 (44%) 0 1	40, 65, 86, 87	0
All	All	498/618 (80%)	0.99	91 (18%) 3 3	19, 40, 77, 87	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	918	GLY	5.5
1	F	936	LEU	5.2
1	F	860	LEU	4.8
1	B	856	PHE	4.7
1	E	934	GLU	4.5
1	F	868	SER	4.4
1	A	938	ALA	4.4
1	A	940	ALA	4.3
1	B	920	LEU	4.2
1	F	870	LEU	4.1
1	C	855	ALA	4.0
1	B	855	ALA	4.0
1	E	855	ALA	3.9
1	E	900	ALA	3.9
1	F	858	ILE	3.8
1	F	877	GLY	3.8
1	A	917	ASP	3.7
1	F	900	ALA	3.7
1	F	933	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	942	ASP	3.5
1	A	943	GLY	3.5
1	F	901	SER	3.4
1	B	940	ALA	3.4
1	F	880	TRP	3.4
1	C	854	TYR	3.4
1	E	941	THR	3.4
1	F	862	ILE	3.3
1	F	869	SER	3.2
1	E	938	ALA	3.2
1	D	942	ASP	3.2
1	A	941	THR	3.2
1	A	937	VAL	3.2
1	F	872	ALA	3.2
1	A	936	LEU	3.2
1	F	898	THR	3.1
1	F	897	ALA	3.1
1	A	920	LEU	3.1
1	E	933	SER	3.1
1	B	941	THR	3.0
1	F	859	PRO	3.0
1	D	854	TYR	3.0
1	E	937	VAL	2.9
1	F	902	PRO	2.9
1	F	938	ALA	2.8
1	F	866	ILE	2.8
1	C	936	LEU	2.8
1	F	916	ASP	2.7
1	F	855	ALA	2.7
1	F	920	LEU	2.7
1	C	934	GLU	2.7
1	E	865	LYS	2.7
1	A	854	TYR	2.6
1	C	915	GLN	2.6
1	C	940	ALA	2.6
1	D	918	GLY	2.5
1	C	856	PHE	2.5
1	F	937	VAL	2.5
1	E	936	LEU	2.5
1	E	856	PHE	2.5
1	F	940	ALA	2.5
1	E	864	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	898	THR	2.4
1	F	926	ALA	2.4
1	F	878	ASN	2.4
1	A	855	ALA	2.4
1	F	912	ALA	2.4
1	E	917	ASP	2.4
1	E	890	ASP	2.3
1	F	864	GLN	2.3
1	E	897	ALA	2.3
1	A	916	ASP	2.3
1	A	918	GLY	2.3
1	F	873	PRO	2.2
1	E	899	LYS	2.2
1	E	895	TYR	2.2
1	E	919	ASP	2.2
1	F	931	GLY	2.2
1	C	868	SER	2.2
1	F	882	LEU	2.1
1	B	936	LEU	2.1
1	E	932	LYS	2.1
1	E	894	ASN	2.1
1	C	864	GLN	2.1
1	F	875	SER	2.1
1	F	867	CYS	2.1
1	A	921	ASN	2.0
1	F	908	ASP	2.0
1	F	884	ALA	2.0
1	F	924	ALA	2.0
1	E	921	ASN	2.0
1	F	890	ASP	2.0

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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	SO3	E	1007	4/4	0.69	0.12	88,88,89,89	0
2	SO3	C	1003	4/4	0.76	0.13	85,86,86,86	0
2	SO3	C	1004	4/4	0.82	0.14	73,73,73,73	0
2	SO3	E	1005	4/4	0.85	0.17	67,67,67,68	0
2	SO3	D	1002	4/4	0.85	0.13	81,81,81,82	0
3	SO4	F	2002	5/5	0.88	0.09	75,76,77,77	0
3	SO4	E	2001	5/5	0.91	0.10	75,75,76,76	0
2	SO3	A	1001	4/4	0.94	0.12	54,55,55,57	0
2	SO3	D	1006	4/4	0.94	0.09	69,69,69,70	0
3	SO4	C	2003	5/5	0.96	0.08	49,50,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.