Full wwPDB X-ray Structure Validation Report (i)

Dec 28, 2016 – 11:00 AM JST

PDB ID	:	5WRW
Title	:	Structure of human apo-SRP72
Deposited on	:	2016-12-04
Resolution	:	2.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report.

This report is produced by the wwPDB biocuration pipeline after annotation of the structure.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

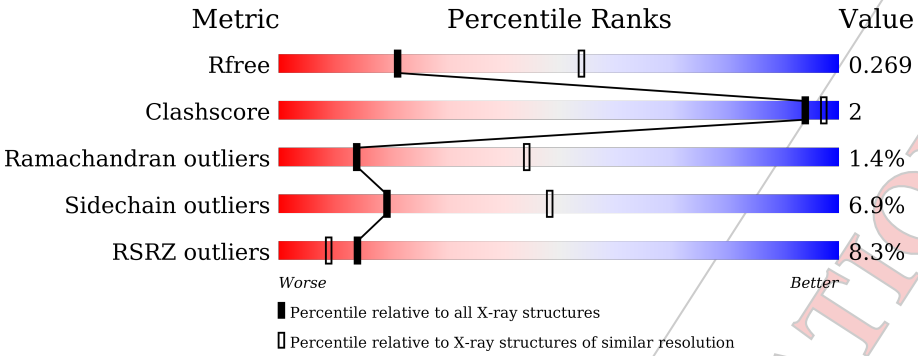
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 2.90 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	163	4% 69% 10% • 20%
1	B	163	4% 70% 7% • 20%
1	C	163	5% 71% 9% • 20%
1	D	163	10% 75% • •• 20%
1	E	163	12% 71% 9% • 20%
1	F	163	6% 75% • •• 20%

2 Entry composition

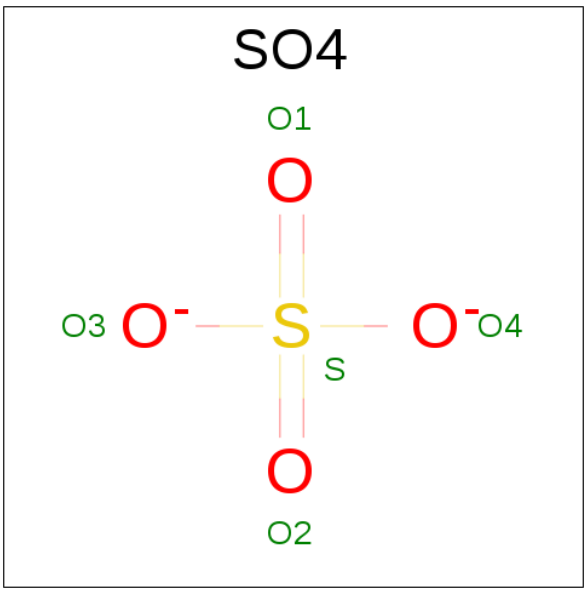
There are 3 unique types of molecules in this entry. The entry contains 6248 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Signal recognition particle subunit SRP72.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	0	0
			1027	645	184	194	4			
1	B	130	Total	C	N	O	S	0	0	0
			1036	651	185	196	4			
1	C	130	Total	C	N	O	S	0	0	0
			1022	642	183	193	4			
1	D	130	Total	C	N	O	S	0	0	0
			998	628	175	191	4			
1	E	130	Total	C	N	O	S	0	0	0
			1028	647	181	196	4			
1	F	130	Total	C	N	O	S	0	1	0
			1038	653	182	199	4			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 3 is water.

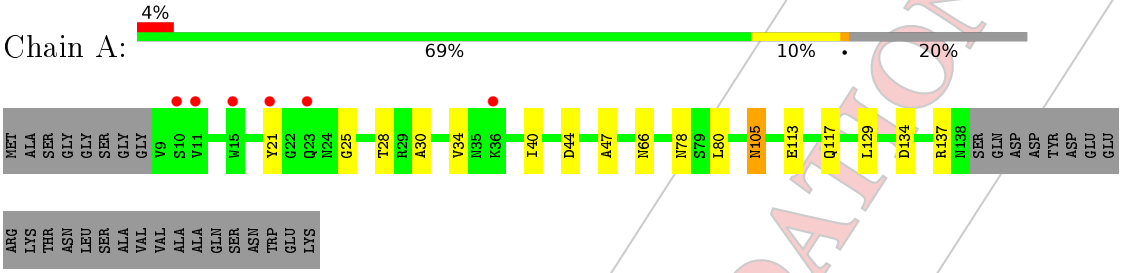
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	26	Total O 26 26	0	0
3	B	16	Total O 16 16	0	0
3	C	24	Total O 24 24	0	0
3	D	4	Total O 4 4	0	0
3	E	6	Total O 6 6	0	0
3	F	13	Total O 13 13	0	0

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 errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

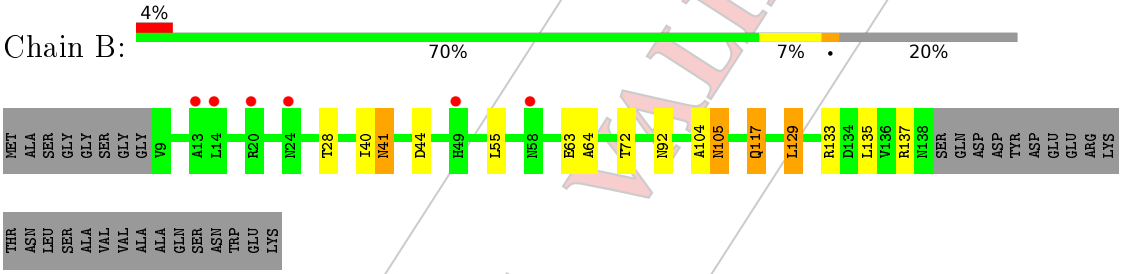
- Molecule 1: Signal recognition particle subunit SRP72

Chain A:



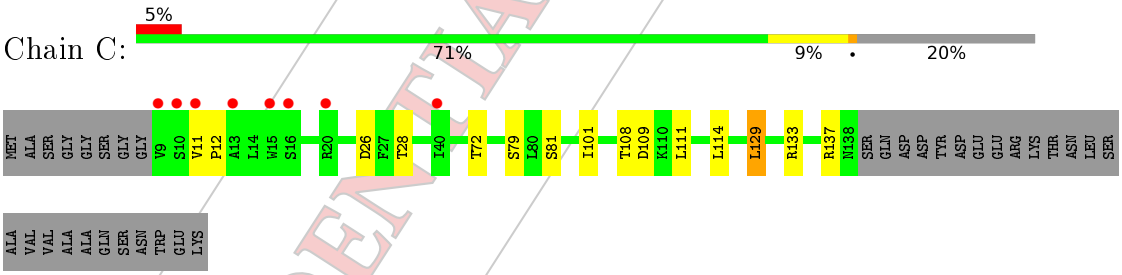
- Molecule 1: Signal recognition particle subunit SRP72

Chain B:



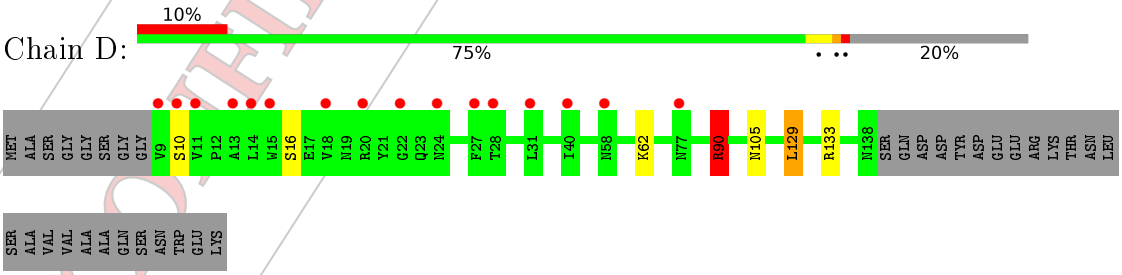
- Molecule 1: Signal recognition particle subunit SRP72

Chain C:



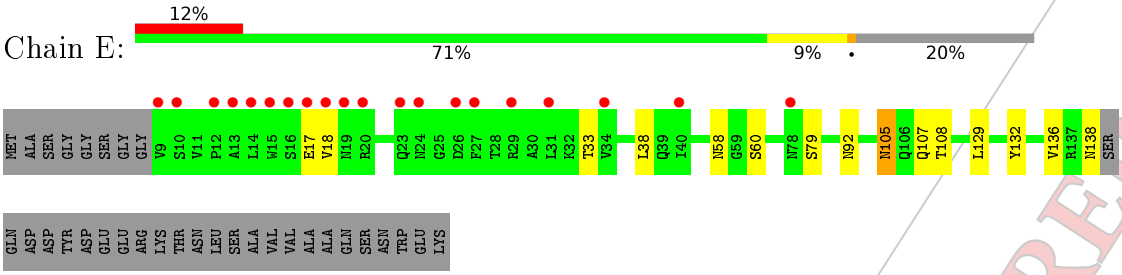
- Molecule 1: Signal recognition particle subunit SRP72

Chain D:



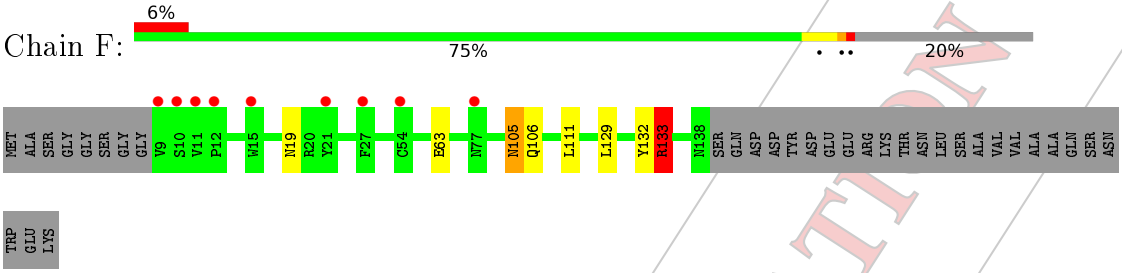
- Molecule 1: Signal recognition particle subunit SRP72

Chain E:



- Molecule 1: Signal recognition particle subunit SRP72

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	83.44Å 123.72Å 150.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.81 – 2.90 49.69 – 2.90	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.81-2.90) 94.9 (49.69-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.61	Depositor
$< I/\sigma(I) >$ [1]	3.56 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.231 , 0.269 0.232 , 0.269	Depositor DCC
R_{free} test set	1683 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	48.6	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 60.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6248	wwPDB-VP
Average B, all atoms (Å^2)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.14% 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: 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	0.56	0/1041	0.71	0/1410
1	B	0.50	0/1050	0.70	0/1422
1	C	0.52	0/1036	0.67	1/1403 (0.1%)
1	D	0.51	0/1011	0.74	3/1373 (0.2%)
1	E	0.52	0/1042	0.69	0/1413
1	F	0.54	0/1055	0.74	3/1430 (0.2%)
All	All	0.53	0/6235	0.71	7/8451 (0.1%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	90	ARG	NE-CZ-NH1	8.42	124.51	120.30
1	F	133	ARG	NE-CZ-NH1	8.09	124.34	120.30
1	D	90	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	F	133	ARG	CG-CD-NE	5.99	124.37	111.80
1	F	133	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	111	LEU	CA-CB-CG	5.50	127.94	115.30
1	D	90	ARG	CG-CD-NE	5.24	122.80	111.80

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	1027	0	1004	5	0
1	B	1036	0	1018	7	0
1	C	1022	0	993	4	0
1	D	998	0	957	3	0
1	E	1028	0	1009	4	0
1	F	1038	0	1021	3	0
2	C	5	0	0	0	0
2	F	5	0	0	0	0
3	A	26	0	0	0	0
3	B	16	0	0	1	0
3	C	24	0	0	0	0
3	D	4	0	0	0	0
3	E	6	0	0	0	0
3	F	13	0	0	0	0
All	All	6248	0	6002	22	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 2.

All (22) 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:A:21:TYR:HB2	1:A:30:ALA:HB2	1.86	0.58
1:F:133:ARG:HG3	1:F:133:ARG:HH11	1.72	0.54
1:A:30:ALA:O	1:A:34:VAL:HG23	2.10	0.52
1:D:90:ARG:HH11	1:D:90:ARG:HG2	1.74	0.51
1:B:55:LEU:HD13	1:B:63:GLU:HG3	1.94	0.49
1:A:117:GLN:HE22	1:B:133:ARG:HH22	1.60	0.48
1:C:11:VAL:HB	1:C:12:PRO:HD3	1.96	0.48
1:D:129:LEU:HD22	1:D:133:ARG:HD2	1.97	0.47
1:B:129:LEU:HD22	1:B:133:ARG:HD2	1.97	0.46
1:A:44:ASP:HB3	1:A:47:ALA:HB3	1.99	0.45
1:E:132:TYR:CZ	1:F:133:ARG:HD2	2.52	0.44
1:A:117:GLN:HE21	1:B:137:ARG:NH1	2.14	0.44
1:B:55:LEU:CB	1:B:64:ALA:HB2	2.48	0.43
1:C:101:ILE:HD11	1:C:114:LEU:HD23	2.01	0.43
1:C:108:THR:OG1	1:C:109:ASP:N	2.52	0.42
1:D:90:ARG:HH11	1:D:90:ARG:CG	2.31	0.42
1:B:117:GLN:HG3	3:B:213:HOH:O	2.19	0.41
1:C:129:LEU:HD22	1:C:133:ARG:HD3	2.02	0.41
1:E:132:TYR:O	1:E:136:VAL:HG12	2.21	0.40
1:E:136:VAL:HG11	1:F:132:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ASN:HB2	1:B:44:ASP:HB2	2.03	0.40
1:E:18:VAL:HB	1:E:33:THR:HG21	2.04	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	128/163 (78%)	117 (91%)	8 (6%)	3 (2%)	8 30
1	B	128/163 (78%)	117 (91%)	8 (6%)	3 (2%)	8 30
1	C	128/163 (78%)	114 (89%)	12 (9%)	2 (2%)	12 40
1	D	128/163 (78%)	120 (94%)	8 (6%)	0	100 100
1	E	128/163 (78%)	118 (92%)	8 (6%)	2 (2%)	12 40
1	F	129/163 (79%)	122 (95%)	6 (5%)	1 (1%)	24 60
All	All	769/978 (79%)	708 (92%)	50 (6%)	11 (1%)	14 44

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	79	SER
1	B	40	ILE
1	B	105	ASN
1	B	104	ALA
1	C	26	ASP
1	C	79	SER
1	F	105	ASN
1	E	105	ASN
1	A	105	ASN
1	A	25	GLY
1	A	40	ILE

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	108/142 (76%)	99 (92%)	9 (8%)	14	38
1	B	110/142 (78%)	102 (93%)	8 (7%)	17	45
1	C	106/142 (75%)	101 (95%)	5 (5%)	32	68
1	D	103/142 (72%)	97 (94%)	6 (6%)	25	58
1	E	110/142 (78%)	100 (91%)	10 (9%)	12	34
1	F	112/142 (79%)	105 (94%)	7 (6%)	22	54
All	All	649/852 (76%)	604 (93%)	45 (7%)	19	48

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28	THR
1	A	66	ASN
1	A	78	ASN
1	A	80	LEU
1	A	105	ASN
1	A	113	GLU
1	A	129	LEU
1	A	134	ASP
1	A	137	ARG
1	B	28	THR
1	B	41	ASN
1	B	72	THR
1	B	92	ASN
1	B	105	ASN
1	B	117	GLN
1	B	129	LEU
1	B	135	LEU
1	C	28	THR
1	C	72	THR
1	C	81	SER
1	C	129	LEU
1	C	137	ARG

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Mol	Chain	Res	Type
1	D	10	SER
1	D	16	SER
1	D	62	LYS
1	D	90	ARG
1	D	105	ASN
1	D	129	LEU
1	E	17	GLU
1	E	38	LEU
1	E	58	ASN
1	E	60	SER
1	E	92	ASN
1	E	105	ASN
1	E	107	GLN
1	E	108	THR
1	E	129	LEU
1	E	138	ASN
1	F	19	ASN
1	F	63	GLU
1	F	105	ASN
1	F	106	GLN
1	F	111	LEU
1	F	129	LEU
1	F	133	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	GLN
1	A	78	ASN
1	A	117	GLN
1	B	78	ASN
1	C	117	GLN
1	D	19	ASN
1	D	39	GLN
1	D	105	ASN
1	D	117	GLN
1	E	39	GLN
1	F	19	ASN
1	F	106	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

2 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	SO4	C	201	-	4,4,4	0.29	0	6,6,6	0.21	0
2	SO4	F	201	-	4,4,4	0.49	0	6,6,6	0.38	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	SO4	C	201	-	-	0/0/0/0	0/0/0/0
2	SO4	F	201	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	130/163 (79%)	0.53	6 (4%) 36 30	21, 59, 103, 109	0
1	B	130/163 (79%)	0.56	6 (4%) 36 30	25, 65, 102, 113	0
1	C	130/163 (79%)	0.46	8 (6%) 24 17	21, 60, 103, 110	0
1	D	130/163 (79%)	0.73	16 (12%) 5 3	24, 69, 115, 121	0
1	E	130/163 (79%)	0.71	20 (15%) 3 1	19, 65, 117, 135	0
1	F	130/163 (79%)	0.44	9 (6%) 20 14	18, 53, 97, 124	0
All	All	780/978 (79%)	0.57	65 (8%) 14 9	18, 62, 108, 135	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	15	TRP	5.0
1	D	9	VAL	5.0
1	D	27	PHE	4.5
1	E	15	TRP	4.4
1	D	13	ALA	4.3
1	E	9	VAL	4.3
1	D	15	TRP	3.9
1	B	14	LEU	3.9
1	D	10	SER	3.7
1	D	14	LEU	3.6
1	E	20	ARG	3.5
1	E	10	SER	3.5
1	C	10	SER	3.4
1	A	11	VAL	3.3
1	D	11	VAL	3.3
1	F	15	TRP	3.3
1	E	12	PRO	3.2
1	F	21	TYR	3.1
1	D	28	THR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	10	SER	3.0
1	D	22	GLY	3.0
1	E	34	VAL	3.0
1	D	24	ASN	3.0
1	E	23	GLN	2.9
1	B	20	ARG	2.9
1	D	18	VAL	2.9
1	E	24	ASN	2.9
1	E	13	ALA	2.9
1	C	40	ILE	2.8
1	D	31	LEU	2.7
1	F	11	VAL	2.7
1	E	17	GLU	2.6
1	A	36	LYS	2.6
1	B	13	ALA	2.6
1	F	27	PHE	2.6
1	B	58	ASN	2.5
1	A	23	GLN	2.5
1	E	27	PHE	2.5
1	E	16	SER	2.4
1	D	58	ASN	2.4
1	F	10	SER	2.4
1	E	29	ARG	2.4
1	E	18	VAL	2.4
1	B	24	ASN	2.3
1	C	16	SER	2.3
1	E	26	ASP	2.3
1	E	31	LEU	2.3
1	E	19	ASN	2.3
1	E	78	ASN	2.2
1	E	40	ILE	2.2
1	F	77	ASN	2.2
1	F	12	PRO	2.2
1	C	15	TRP	2.2
1	C	13	ALA	2.2
1	C	11	VAL	2.2
1	D	40	ILE	2.1
1	B	49	HIS	2.1
1	E	14	LEU	2.1
1	C	20	ARG	2.1
1	C	9	VAL	2.1
1	A	21	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	77	ASN	2.1
1	F	9	VAL	2.1
1	D	20	ARG	2.0
1	F	54	CYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	SO4	C	201	5/5	0.92	0.23	0.94	54,55,58,64	5
2	SO4	F	201	5/5	0.97	0.18	-1.50	51,55,59,60	5

6.5 Other polymers (i)

There are no such residues in this entry.