Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2026 – 07:27 am BST

PDB ID	:	1OA0 / pdb_00001oa0
Title	:	REDUCED HYBRID CLUSTER PROTEIN FROM DESULFOVIBRIO DESULFURICANS X-RAY STRUCTURE AT 1.25A RESOLUTION
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Deposited on	:	2002-12-23
Resolution	:	1.25 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 (i) 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 (i)) were used in the production of this report:

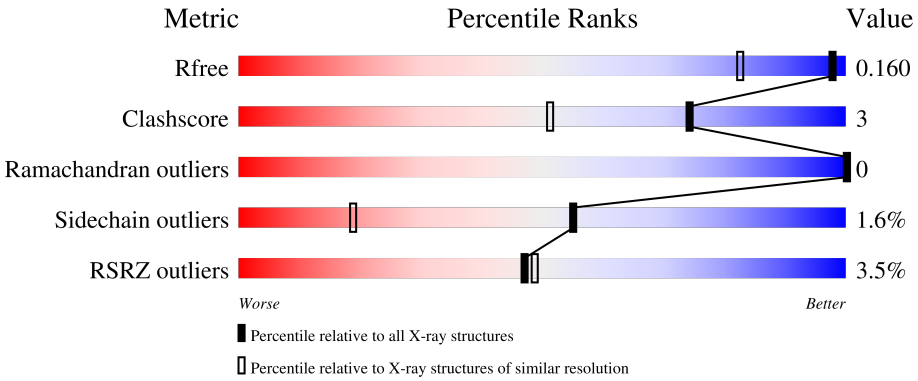
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.25 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	1693 (1.28-1.24)
Clashscore	190562	1730 (1.28-1.24)
Ramachandran outliers	187476	1695 (1.28-1.24)
Sidechain outliers	187428	1694 (1.28-1.24)
RSRZ outliers	180081	1693 (1.28-1.24)

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 <=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	544	3% 93% 6% ·
1	B	544	4% 94% 5% ·

2 Entry composition

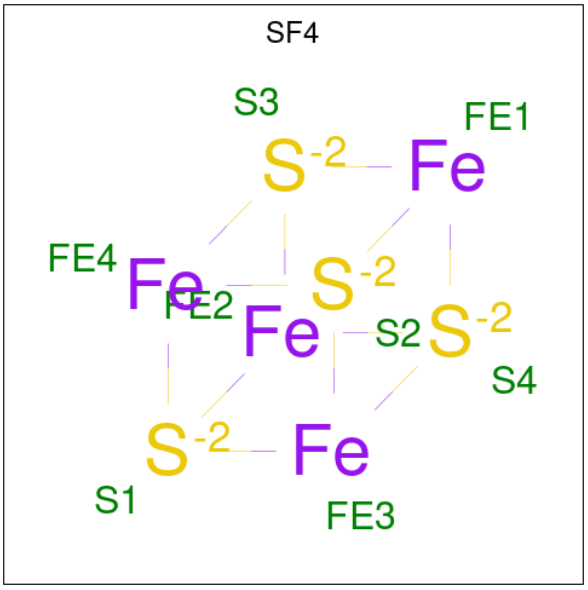
There are 5 unique types of molecules in this entry. The entry contains 10655 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PRISMANE PROTEIN.

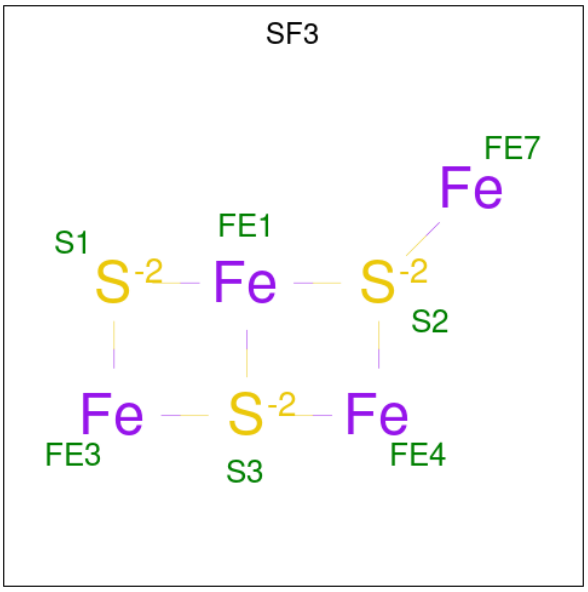
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	544	Total	C	N	O	S	0	18	1
			4171	2656	702	790	23			
1	B	544	Total	C	N	O	S	0	22	1
			4178	2660	702	792	24			

- Molecule 2 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



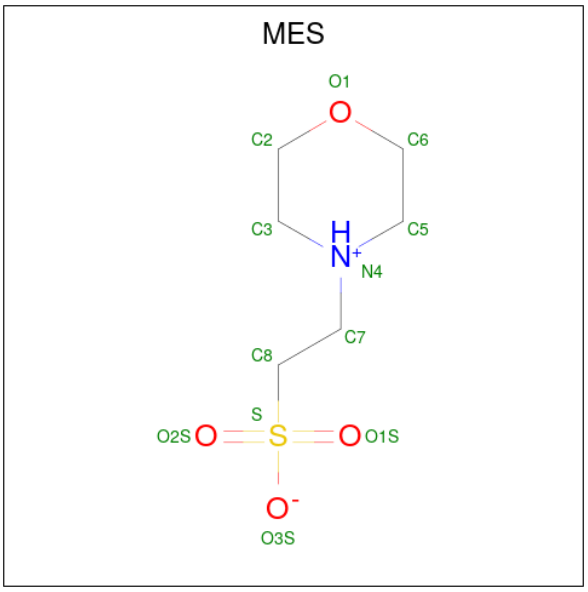
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	Fe	S	0	0
			8	4	4		
2	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 3 is FE4-S3 CLUSTER (CCD ID: SF3) (formula: Fe_4S_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Fe S 7 4 3	0	0
3	B	1	Total Fe S 7 4 3	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O S 12 6 1 4 1	0	0

- Molecule 5 is water.

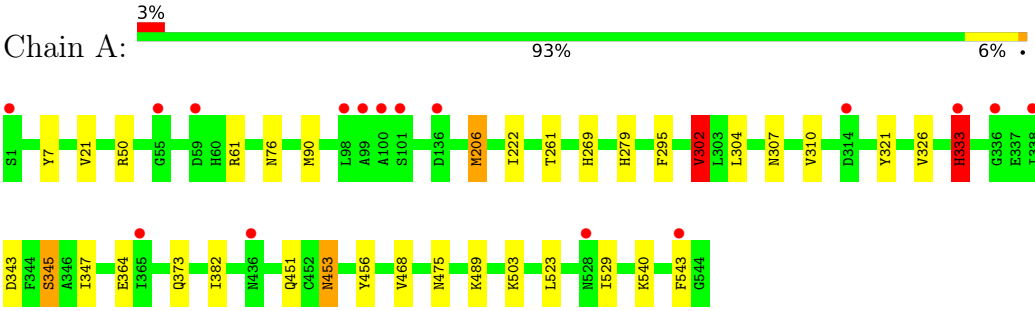
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1178	Total O 1178 1178	0	0
5	B	1086	Total O 1086 1086	0	0

3 Residue-property plots (i)

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.

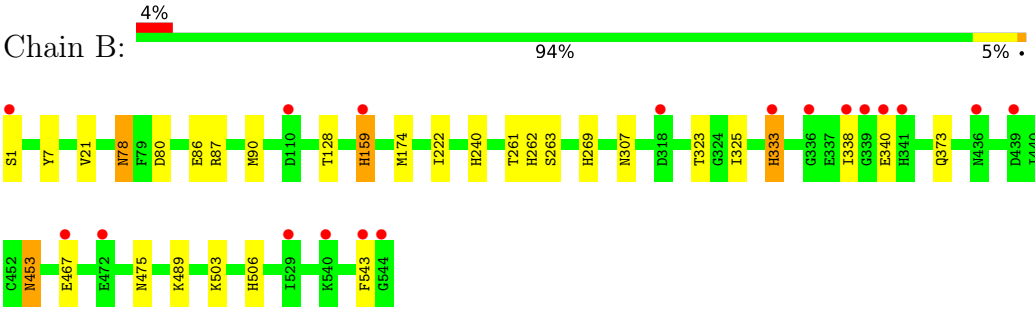
• Molecule 1: PRISMANE PROTEIN

Chain A:



• Molecule 1: PRISMANE PROTEIN

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	57.75Å 61.99Å 72.80Å 82.72° 73.74° 87.44°	Depositor
Resolution (Å)	29.49 – 1.25 29.49 – 1.25	Depositor EDS
% Data completeness (in resolution range)	92.7 (29.49-1.25) 92.7 (29.49-1.25)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.66 (at 1.25Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.133 , 0.150 0.144 , 0.160	Depositor DCC
R_{free} test set	6123 reflections (2.48%)	wwPDB-VP
Wilson B-factor (Å^2)	6.9	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 43.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	10655	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MES, SF3, SF4

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	0.87	13/4345 (0.3%)	0.77	3/5890 (0.1%)
1	B	0.79	7/4388 (0.2%)	0.79	5/5942 (0.1%)
All	All	0.83	20/8733 (0.2%)	0.78	8/11832 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	333	HIS	CE1-NE2	25.77	1.58	1.32
1	A	333	HIS	CE1-NE2	22.12	1.54	1.32
1	A	333	HIS	CG-ND1	18.78	1.58	1.38
1	B	333	HIS	CG-CD2	17.52	1.55	1.35
1	A	341	HIS	CE1-NE2	15.35	1.47	1.32
1	B	333	HIS	CG-ND1	13.44	1.53	1.38
1	A	333	HIS	CD2-NE2	13.21	1.52	1.37
1	B	333	HIS	CD2-NE2	10.82	1.49	1.37
1	A	279	HIS	ND1-CE1	10.23	1.42	1.32
1	A	333	HIS	CB-CG	9.30	1.63	1.50
1	A	341	HIS	CG-ND1	8.67	1.47	1.38
1	A	341	HIS	CG-CD2	8.43	1.45	1.35
1	A	302[A]	VAL	CA-CB	7.74	1.64	1.54
1	A	302[B]	VAL	CA-CB	7.74	1.64	1.54
1	A	302[C]	VAL	CA-CB	7.74	1.64	1.54
1	B	543	PHE	C-N	-6.89	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	PHE	C-N	-6.87	1.23	1.33
1	B	159	HIS	CE1-NE2	6.61	1.39	1.32
1	B	506	HIS	CE1-NE2	6.53	1.39	1.32
1	A	206	MET	SD-CE	-5.28	1.66	1.79

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	333	HIS	CG-CD2-NE2	-13.70	93.50	107.20
1	B	333	HIS	CE1-NE2-CD2	9.76	118.76	109.00
1	A	333	HIS	ND1-CE1-NE2	-7.70	100.70	108.40
1	B	333	HIS	ND1-CE1-NE2	-6.91	101.49	108.40
1	B	333	HIS	ND1-CG-CD2	6.75	112.85	106.10
1	B	333	HIS	CB-CG-CD2	-5.88	123.55	131.20
1	A	333	HIS	CA-CB-CG	5.72	119.52	113.80
1	A	76	ASN	N-CA-C	5.34	119.08	112.24

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	364[A]	GLU	Mainchain
1	A	364[B]	GLU	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4171	0	4201	24	0
1	B	4178	0	4206	25	0
2	A	8	0	0	0	0
2	B	8	0	0	0	0
3	A	7	0	0	0	0
3	B	7	0	0	0	0
4	A	12	0	13	3	0
5	A	1178	0	0	9	1
5	B	1086	0	0	3	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	10655	0	8420	52	1

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 3.

All (52) 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)
4:A:602:MES:H22	5:A:3177:HOH:O	1.70	0.92
1:A:326:VAL:O	1:A:333:HIS:CE1	2.30	0.85
1:A:475:ASN:HD21	1:A:503:LYS:H	1.31	0.77
1:A:333:HIS:ND1	5:A:2880:HOH:O	2.23	0.71
4:A:602:MES:C2	5:A:3177:HOH:O	2.34	0.68
1:B:338[A]:ILE:HD11	1:B:340[A]:GLU:HG2	1.77	0.67
1:B:475:ASN:HD21	1:B:503:LYS:H	1.41	0.66
1:B:1:SER:N	5:B:2004:HOH:O	2.29	0.65
1:A:310[C]:VAL:HG22	5:A:2285:HOH:O	1.97	0.63
1:A:382:ILE:HD13	1:A:468:VAL:HG11	1.80	0.62
1:B:338[A]:ILE:CD1	1:B:340[A]:GLU:HG2	2.31	0.60
4:A:602:MES:H51	5:A:2954:HOH:O	2.02	0.59
1:A:307:ASN:HD21	1:A:489:LYS:NZ	2.01	0.59
1:B:307:ASN:HD21	1:B:489:LYS:NZ	2.02	0.58
1:A:540:LYS:NZ	5:A:3168:HOH:O	2.34	0.57
1:A:451:GLN:HE21	1:A:453:ASN:HD21	1.52	0.57
1:B:78:ASN:HD22	1:B:80:ASP:H	1.50	0.57
1:B:451:GLN:HE21	1:B:453:ASN:HD21	1.53	0.56
1:A:475:ASN:ND2	1:A:503:LYS:H	2.01	0.55
1:B:78:ASN:ND2	1:B:80:ASP:H	2.04	0.55
1:B:222:ILE:H	1:B:373:GLN:HE21	1.56	0.54
1:B:475:ASN:ND2	1:B:503:LYS:H	2.07	0.52
1:A:50:ARG:HG2	5:A:2201:HOH:O	2.08	0.51
1:A:222:ILE:H	1:A:373:GLN:HE21	1.59	0.51
1:B:323:THR:HA	1:B:333:HIS:CE1	2.46	0.51
1:A:523:LEU:HB3	1:A:529:ILE:HD12	1.93	0.50
1:B:78:ASN:HD21	1:B:80:ASP:HB3	1.78	0.48
1:B:261:THR:OG1	1:B:269:HIS:HE1	1.97	0.48
1:B:159:HIS:HE1	1:B:240:HIS:HB2	1.78	0.48
1:B:338[B]:ILE:CD1	1:B:340[B]:GLU:HG2	2.43	0.48
1:B:307:ASN:HD21	1:B:489:LYS:HZ1	1.63	0.47
1:A:333:HIS:CE1	5:A:2880:HOH:O	2.67	0.46
1:A:302[A]:VAL:CG2	1:A:304:LEU:CD2	2.94	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:ASP:OD1	1:A:345[A]:SER:HB3	2.16	0.46
1:A:302[A]:VAL:HG23	1:A:304:LEU:CD2	2.46	0.45
1:A:321:TYR:CD2	1:A:347[B]:ILE:HG12	2.52	0.44
1:B:159:HIS:CE1	1:B:240:HIS:HB2	2.52	0.44
1:A:261:THR:OG1	1:A:269:HIS:HE1	2.01	0.44
1:A:302[B]:VAL:HG12	1:A:304:LEU:CD2	2.47	0.44
1:B:87:ARG:HA	1:B:90[A]:MET:HE3	1.99	0.43
1:A:206:MET:HB3	1:A:456:TYR:HB2	2.00	0.43
1:B:86:GLU:HG3	1:B:90[A]:MET:HE2	2.00	0.43
1:B:451:GLN:NE2	1:B:453:ASN:HD21	2.16	0.43
1:A:342:LYS:HE3	5:A:2894:HOH:O	2.18	0.43
1:B:338[B]:ILE:HD11	1:B:340[B]:GLU:CG	2.49	0.43
1:A:295:PHE:CE2	1:A:302[C]:VAL:HG11	2.55	0.42
1:B:262:HIS:CE1	1:B:263:SER:HB2	2.54	0.42
1:B:128:THR:HG23	5:B:2423:HOH:O	2.20	0.42
1:A:451:GLN:NE2	1:A:453:ASN:HD21	2.16	0.41
1:B:333:HIS:HD2	5:B:2399:HOH:O	2.04	0.41
1:B:325:ILE:HD12	1:B:325:ILE:C	2.46	0.41
1:A:343:ASP:OD1	1:A:345[B]:SER:OG	2.31	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:2851:HOH:O	5:B:2004:HOH:O[1_454]	2.15	0.05

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	563/544 (104%)	551 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	567/544 (104%)	554 (98%)	13 (2%)	0	100 100
All	All	1130/1088 (104%)	1105 (98%)	25 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	450/433 (104%)	435 (97%)	15 (3%)	33 4
1	B	457/433 (106%)	448 (98%)	9 (2%)	48 12
All	All	907/866 (105%)	883 (97%)	24 (3%)	55 7

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	TYR
1	A	21[A]	VAL
1	A	21[B]	VAL
1	A	21[C]	VAL
1	A	61[A]	ARG
1	A	61[B]	ARG
1	A	90[A]	MET
1	A	90[B]	MET
1	A	302[A]	VAL
1	A	302[B]	VAL
1	A	302[C]	VAL
1	A	333	HIS
1	A	345[A]	SER
1	A	345[B]	SER
1	A	453	ASN
1	B	7	TYR
1	B	21[A]	VAL
1	B	21[B]	VAL

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Mol	Chain	Res	Type
1	B	21[C]	VAL
1	B	78	ASN
1	B	174[A]	MET
1	B	174[B]	MET
1	B	453	ASN
1	B	467	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	34	GLN
1	A	219	HIS
1	A	269	HIS
1	A	283	ASN
1	A	286	ASN
1	A	307	ASN
1	A	333	HIS
1	A	373	GLN
1	A	451	GLN
1	A	475	ASN
1	A	518	ASN
1	B	78	ASN
1	B	159	HIS
1	B	269	HIS
1	B	283	ASN
1	B	307	ASN
1	B	333	HIS
1	B	373	GLN
1	B	451	GLN
1	B	475	ASN

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)

5 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	$\#\|Z\| > 2$
4	MES	A	602	-	12,12,12	1.76	1 (8%)	14,16,16	0.71	0
3	SF3	B	1545	1	0,8,8	-	-	-		
2	SF4	B	1544	1	0,12,12	-	-	-		
2	SF4	A	600	1	0,12,12	-	-	-		
3	SF3	A	601	1	0,8,8	-	-	-		

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
4	MES	A	602	-	-	0/6/14/14	0/1/1/1
3	SF3	B	1545	1	-	-	0/2/2/2
2	SF4	B	1544	1	-	-	0/6/5/5
2	SF4	A	600	1	-	-	0/6/5/5
3	SF3	A	601	1	-	-	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	602	MES	O3S-S	-4.82	1.30	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 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	602	MES	3	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	544/544 (100%)	0.00	18 (3%)	49	51	3, 7, 14, 20	18 (3%)
1	B	544/544 (100%)	0.09	20 (3%)	45	47	3, 8, 15, 21	22 (4%)
All	All	1088/1088 (100%)	0.05	38 (3%)	47	49	3, 7, 14, 21	40 (3%)

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	338[A]	ILE	6.7
1	A	333	HIS	6.3
1	B	336	GLY	4.6
1	A	1	SER	4.5
1	A	100	ALA	4.5
1	B	333	HIS	3.9
1	B	544	GLY	3.9
1	B	543	PHE	3.8
1	B	340[A]	GLU	3.7
1	A	341	HIS	3.5
1	B	339	GLY	3.3
1	A	336	GLY	3.3
1	A	436	ASN	3.3
1	B	472	GLU	3.0
1	A	136	ASP	2.9
1	A	528[A]	ASN	2.9
1	A	338	ILE	2.9
1	B	441	GLY	2.8
1	B	442	GLY	2.8
1	A	543	PHE	2.8
1	A	101	SER	2.7
1	B	341	HIS	2.6
1	A	55	GLY	2.6
1	B	439	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	365	ILE	2.6
1	A	99	ALA	2.5
1	B	159	HIS	2.5
1	A	314	ASP	2.5
1	B	318	ASP	2.4
1	B	540	LYS	2.3
1	A	98	LEU	2.2
1	B	436	ASN	2.2
1	B	467	GLU	2.2
1	A	59	ASP	2.1
1	B	1	SER	2.1
1	B	110	ASP	2.1
1	B	529	ILE	2.1
1	A	339	GLY	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 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(Å^2)	Q<0.9
4	MES	A	602	12/12	0.82	0.17	20,20,20,20	0
2	SF4	B	1544	8/8	1.00	0.01	3,3,3,3	0
3	SF3	A	601	7/7	1.00	0.01	3,4,5,7	0
3	SF3	B	1545	7/7	1.00	0.01	4,4,5,7	0
2	SF4	A	600	8/8	1.00	0.01	3,4,4,4	0

6.5 Other polymers (i)

There are no such residues in this entry.