wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 01:18 pm BST

PDB ID	:	1SOS
Title	:	ATOMIC STRUCTURES OF WILD-TYPE AND THERMOSTABLE MUTANT RECOMBINANT HUMAN CU, ZN SUPEROXIDE DISMUTASE
Authors	:	Parge, H.E.; Hallewell, R.A.; Tainer, J.A.
Deposited on	:	1992-02-11
Resolution	:	2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 following versions of software and data (see references (i)) were used in the production of this report:

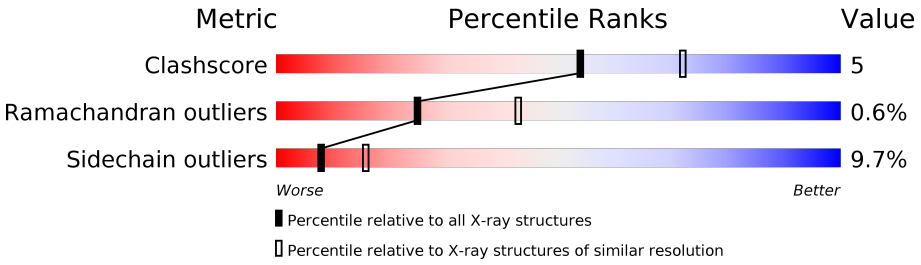
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	154	81% 16%
1	B	154	79% 18%
1	C	154	84% 15%
1	D	154	79% 21%
1	E	154	67% 29%
1	F	154	79% 19%
1	G	154	78% 19%
1	H	154	75% 21%

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Mol	Chain	Length	Quality of chain
1	I	154	
1	J	154	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11649 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 SUPEROXIDE DISMUTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	F	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	B	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	G	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	C	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	H	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	D	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	I	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	E	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			
1	J	154	Total	C	N	O	S	0	0	0
			1112	681	203	226	2			

- Molecule 2 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	G	1	Total	Cu	0	0
			1	1		
2	J	1	Total	Cu	0	0
			1	1		
2	D	1	Total	Cu	0	0
			1	1		
2	E	1	Total	Cu	0	0
			1	1		

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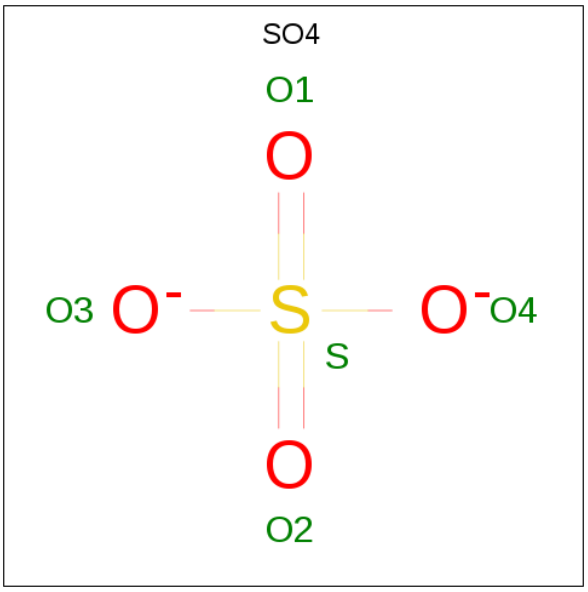
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	A	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	I	1	Total Zn 1 1	0	0
3	C	1	Total Zn 1 1	0	0
3	A	1	Total Zn 1 1	0	0
3	F	1	Total Zn 1 1	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	56	Total O 56 56	0	0
5	F	52	Total O 52 52	0	0
5	B	54	Total O 54 54	0	0
5	G	63	Total O 63 63	0	0
5	C	43	Total O 43 43	0	0
5	H	63	Total O 63 63	0	0
5	D	43	Total O 43 43	0	0
5	I	46	Total O 46 46	0	0
5	E	39	Total O 39 39	0	0
5	J	40	Total O 40 40	0	0

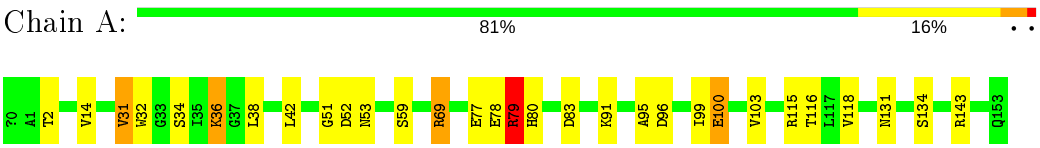
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

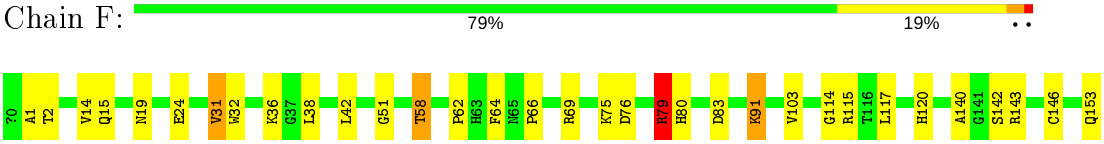
- Molecule 1: SUPEROXIDE DISMUTASE

Chain A:



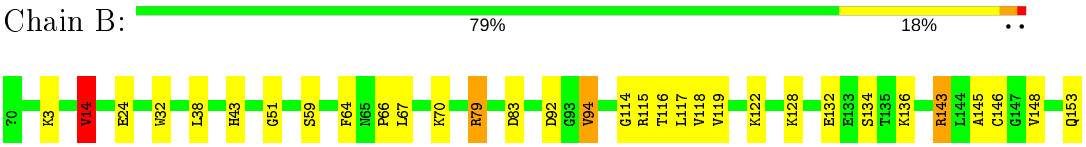
- Molecule 1: SUPEROXIDE DISMUTASE

Chain F:



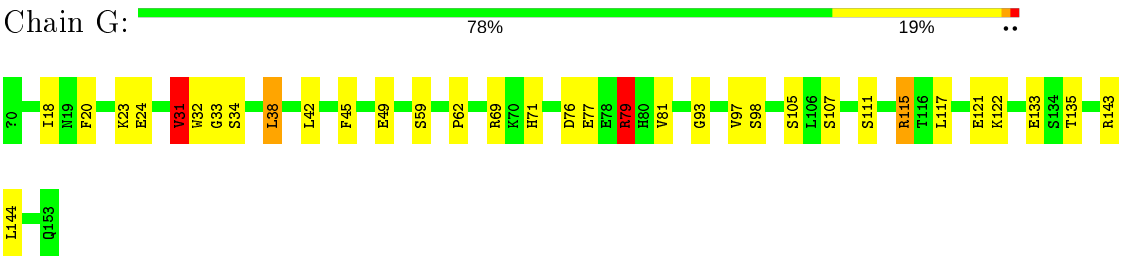
- Molecule 1: SUPEROXIDE DISMUTASE

Chain B:



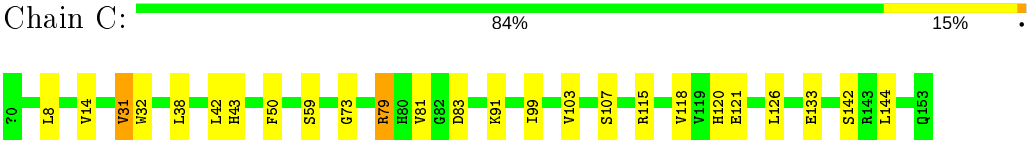
- Molecule 1: SUPEROXIDE DISMUTASE

Chain G:



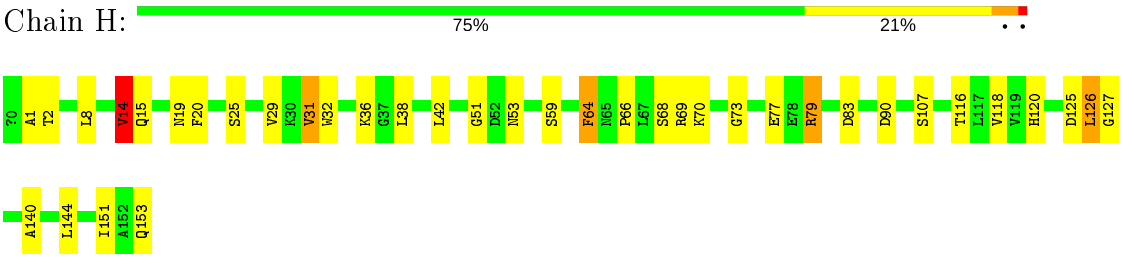
- Molecule 1: SUPEROXIDE DISMUTASE

Chain C:



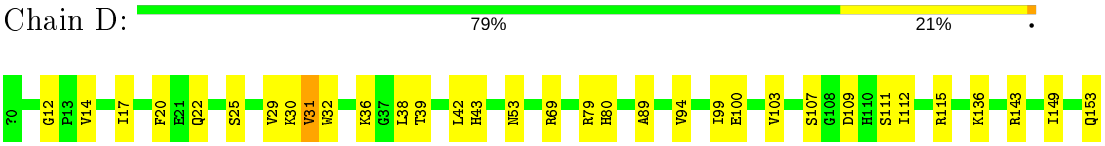
• Molecule 1: SUPEROXIDE DISMUTASE

Chain H:



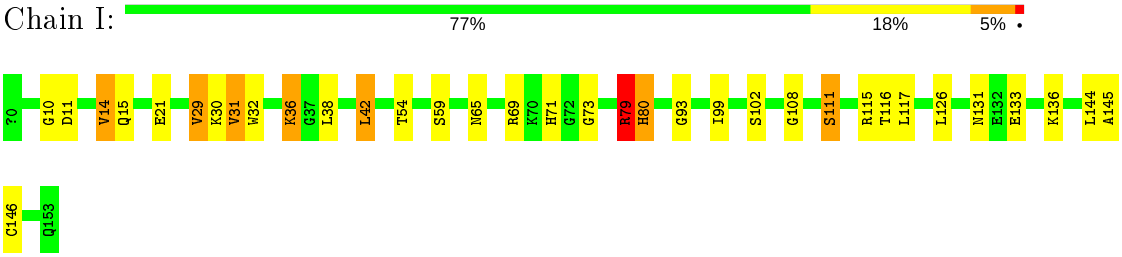
• Molecule 1: SUPEROXIDE DISMUTASE

Chain D:



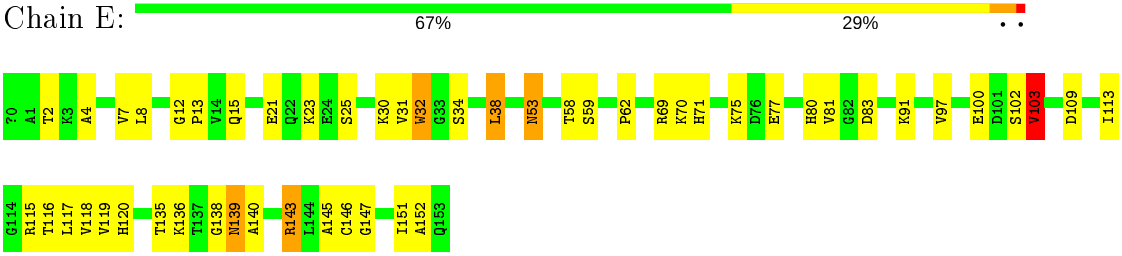
• Molecule 1: SUPEROXIDE DISMUTASE

Chain I:



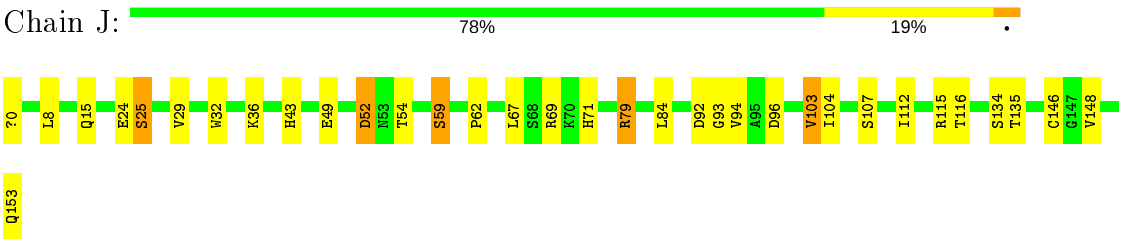
• Molecule 1: SUPEROXIDE DISMUTASE

Chain E:



• Molecule 1: SUPEROXIDE DISMUTASE

Chain J:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	205.20Å 167.00Å 145.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	11649	wwPDB-VP
Average B, all atoms (Å^2)	12.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CU, ACE, 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	0.95	0/1128	1.56	13/1521 (0.9%)
1	B	0.96	0/1128	1.62	13/1521 (0.9%)
1	C	0.97	0/1128	1.60	9/1521 (0.6%)
1	D	0.91	0/1128	1.59	8/1521 (0.5%)
1	E	0.88	0/1128	1.62	16/1521 (1.1%)
1	F	1.02	0/1128	1.60	10/1521 (0.7%)
1	G	0.99	1/1128 (0.1%)	1.62	13/1521 (0.9%)
1	H	1.00	0/1128	1.58	13/1521 (0.9%)
1	I	0.97	0/1128	1.63	14/1521 (0.9%)
1	J	0.92	1/1128 (0.1%)	1.60	8/1521 (0.5%)
All	All	0.96	2/11280 (0.0%)	1.60	117/15210 (0.8%)

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	D	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	31	VAL	CA-CB	5.56	1.66	1.54
1	J	134	SER	CA-CB	-5.14	1.45	1.52

The worst 5 of 117 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	79	ARG	NE-CZ-NH1	14.77	127.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	79	ARG	NE-CZ-NH1	14.72	127.66	120.30
1	H	79	ARG	NE-CZ-NH1	13.18	126.89	120.30
1	D	69	ARG	NE-CZ-NH1	12.39	126.49	120.30
1	D	69	ARG	NE-CZ-NH2	-12.24	114.18	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	12	GLY	Peptide

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	1112	0	1077	9	0
1	B	1112	0	1077	11	0
1	C	1112	0	1077	9	0
1	D	1112	0	1077	10	0
1	E	1112	0	1077	18	0
1	F	1112	0	1077	9	0
1	G	1112	0	1077	11	0
1	H	1112	0	1077	15	0
1	I	1112	0	1077	16	0
1	J	1112	0	1077	11	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	J	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
3	I	1	0	0	0	0
3	J	1	0	0	0	0
4	F	5	0	0	0	0
4	I	5	0	0	0	0
5	A	56	0	0	0	0
5	B	54	0	0	1	0
5	C	43	0	0	1	0
5	D	43	0	0	1	0
5	E	39	0	0	0	0
5	F	52	0	0	1	0
5	G	63	0	0	0	0
5	H	63	0	0	1	0
5	I	46	0	0	1	0
5	J	40	0	0	1	0
All	All	11649	0	10770	116	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 5.

The worst 5 of 116 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:B:119:VAL:HG12	1:B:145:ALA:HB3	1.71	0.72
1:J:0:ACE:H1	1:J:107:SER:HA	1.70	0.72
1:E:70:LYS:HD2	1:E:135:THR:HB	1.72	0.71
1:I:14:VAL:HG22	1:I:145:ALA:HB2	1.73	0.70
1:I:31:VAL:HG13	1:I:99:ILE:HB	1.74	0.69

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	152/154 (99%)	146 (96%)	6 (4%)	0	100 100
1	B	152/154 (99%)	140 (92%)	12 (8%)	0	100 100
1	C	152/154 (99%)	146 (96%)	6 (4%)	0	100 100
1	D	152/154 (99%)	141 (93%)	10 (7%)	1 (1%)	22 39
1	E	152/154 (99%)	139 (91%)	11 (7%)	2 (1%)	12 21
1	F	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22 39
1	G	152/154 (99%)	146 (96%)	6 (4%)	0	100 100
1	H	152/154 (99%)	145 (95%)	6 (4%)	1 (1%)	22 39
1	I	152/154 (99%)	144 (95%)	8 (5%)	0	100 100
1	J	152/154 (99%)	138 (91%)	10 (7%)	4 (3%)	5 8
All	All	1520/1540 (99%)	1430 (94%)	81 (5%)	9 (1%)	25 43

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	126	LEU
1	D	25	SER
1	J	24	GLU
1	J	25	SER
1	J	93	GLY

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	117/117 (100%)	106 (91%)	11 (9%)	8 17
1	B	117/117 (100%)	109 (93%)	8 (7%)	16 30
1	C	117/117 (100%)	108 (92%)	9 (8%)	13 25
1	D	117/117 (100%)	107 (92%)	10 (8%)	10 21
1	E	117/117 (100%)	102 (87%)	15 (13%)	4 8
1	F	117/117 (100%)	103 (88%)	14 (12%)	5 9
1	G	117/117 (100%)	106 (91%)	11 (9%)	8 17
1	H	117/117 (100%)	103 (88%)	14 (12%)	5 9
1	I	117/117 (100%)	105 (90%)	12 (10%)	7 14
1	J	117/117 (100%)	107 (92%)	10 (8%)	10 21
All	All	1170/1170 (100%)	1056 (90%)	114 (10%)	8 16

5 of 114 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	133	GLU
1	H	70	LYS
1	J	29	VAL
1	H	14	VAL
1	H	38	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
1	H	53	ASN
1	I	139	ASN
1	I	110	HIS
1	C	15	GLN
1	D	43	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 22 ligands modelled in this entry, 20 are monoatomic - leaving 2 for Mogul analysis.

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	SO4	F	356	-	4,4,4	0.39	0	6,6,6	0.24	0
4	SO4	I	357	-	4,4,4	0.43	0	6,6,6	0.20	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

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.