



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 25, 2020 – 04:43 PM BST

PDB ID : 4B3E
Title : Structure of copper-zinc superoxide dismutase complexed with bicarbonate.
Authors : Strange, R.W.; Hough, M.A.; Antonyuk, S.V.; Hasnain, S.S.
Deposited on : 2012-07-23
Resolution : 2.15 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 : 2.13
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) : 2.13

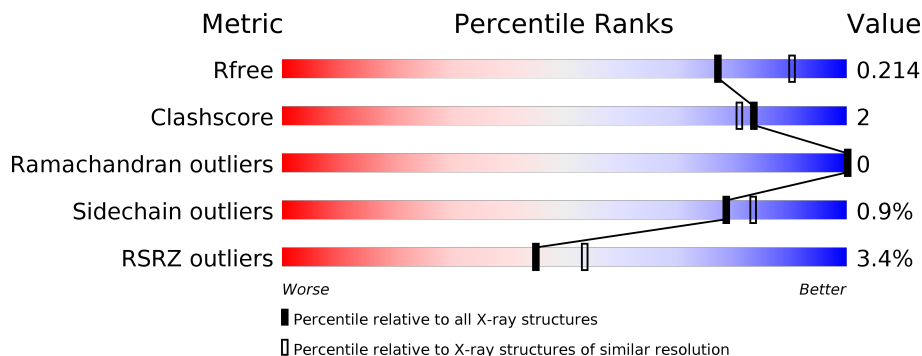
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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.



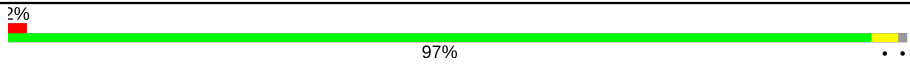
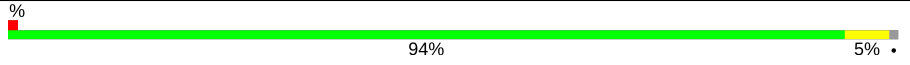
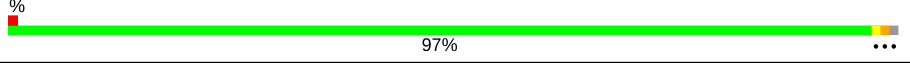
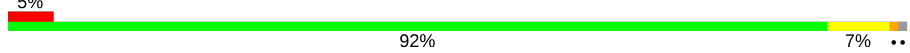
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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 $\leq 5\%$. 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	154	<div style="display: flex; align-items: center;"> <div style="width: 3%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 92%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">3% 95% 5% .</p>
1	B	154	<div style="display: flex; align-items: center;"> <div style="width: 5%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 87%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 7%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">5% 92% 7% ..</p>
1	C	154	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 94%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">94% 5% .</p>
1	D	154	<div style="display: flex; align-items: center;"> <div style="width: 6%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 91%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 3%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">6% 97% ..</p>
1	E	154	<div style="display: flex; align-items: center;"> <div style="width: 9%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 89%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 2%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">9% 98% ..</p>
1	F	154	<div style="display: flex; align-items: center;"> <div style="width: 0%; height: 10px; background-color: red; margin-right: 5px;"></div> <div style="width: 94%; height: 10px; background-color: green; margin-right: 5px;"></div> <div style="width: 5%; height: 10px; background-color: yellow; margin-right: 5px;"></div> <div style="width: 1%; height: 10px; background-color: grey;"></div> </div> <p style="text-align: center;">% 94% 5% .</p>

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Mol	Chain	Length	Quality of chain
1	G	154	 2% 97% ..
1	H	154	 % 94% 5% .
1	I	154	 % 97% ...
1	J	154	 5% 92% 7% ..

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12812 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 [CU-ZN].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	153	1115	682	204	225	4	0	1	0
1	B	153	1110	679	203	224	4	0	0	0
1	C	153	1126	691	203	228	4	0	3	0
1	D	153	1116	683	203	226	4	0	1	0
1	E	153	1110	679	203	224	4	0	0	0
1	F	153	1118	686	203	225	4	0	2	0
1	G	153	1110	679	203	224	4	0	0	0
1	H	153	1113	681	203	225	4	1	1	0
1	I	153	1110	679	203	224	4	0	0	0
1	J	153	1110	679	203	224	4	1	0	0

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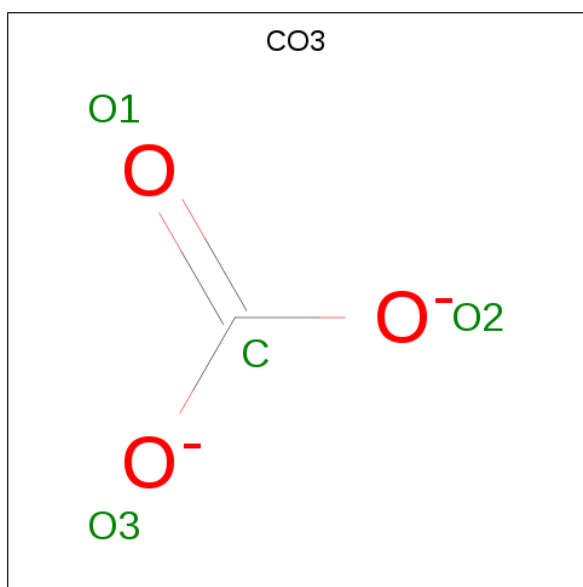
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	H	1	Total Cu 1 1	0	0
2	B	1	Total Cu 1 1	0	0
2	I	1	Total Cu 1 1	0	0
2	C	1	Total Cu 1 1	0	0
2	A	1	Total Cu 1 1	0	0
2	F	1	Total Cu 1 1	0	0

- 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 CARBONATE ION (three-letter code: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 1 3	0	0
4	B	1	Total C O 4 1 3	0	0
4	C	1	Total C O 4 1 3	0	0
4	D	1	Total C O 4 1 3	0	0
4	E	1	Total C O 4 1 3	0	0
4	F	1	Total C O 4 1 3	0	0
4	G	1	Total C O 4 1 3	0	0
4	H	1	Total C O 4 1 3	0	0
4	I	1	Total C O 4 1 3	0	0
4	J	1	Total C O 4 1 3	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	166	Total	O	0	0
			166	166		
6	B	126	Total	O	0	0
			126	126		
6	C	199	Total	O	0	0
			199	199		
6	D	120	Total	O	0	0
			120	120		
6	E	111	Total	O	0	0
			111	111		
6	F	238	Total	O	0	0
			238	238		
6	G	187	Total	O	0	0
			187	187		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	152	Total 153	O 153	0	1
6	I	167	Total 168	O 168	0	1
6	J	121	Total 121	O 121	0	0

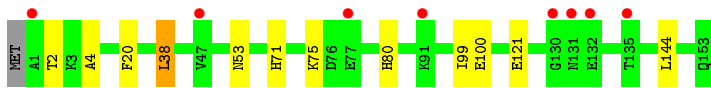
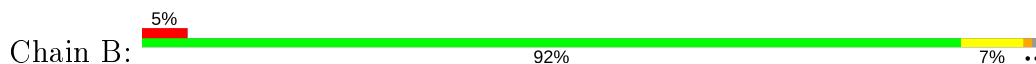
3 Residue-property plots [i](#)

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: SUPEROXIDE DISMUTASE [CU-ZN]



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



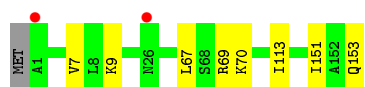
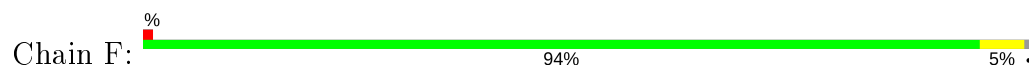
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



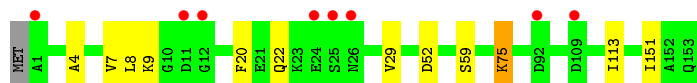
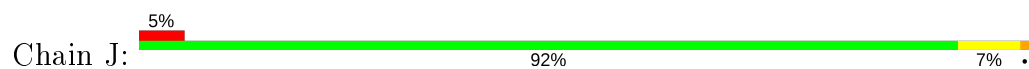
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	165.99Å 203.11Å 144.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.15 19.98 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.4 (20.00-2.15) 94.6 (19.98-2.15)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.06 (at 2.15Å)	Xtrriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.175 , 0.215 0.176 , 0.214	Depositor DCC
R_{free} test set	6298 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	25.2	Xtrriage
Anisotropy	0.075	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.42 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12812	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, CU, CO3

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	0.62	0/1136	0.69	0/1531
1	B	0.57	0/1128	0.67	1/1520 (0.1%)
1	C	0.62	0/1153	0.70	0/1554
1	D	0.54	0/1137	0.63	0/1532
1	E	0.55	0/1128	0.64	0/1520
1	F	0.64	0/1142	0.69	0/1539
1	G	0.67	0/1128	0.71	0/1520
1	H	0.68	1/1134 (0.1%)	0.85	1/1528 (0.1%)
1	I	0.61	0/1128	0.67	0/1520
1	J	1.05	1/1128 (0.1%)	0.78	1/1520 (0.1%)
All	All	0.67	2/11342 (0.0%)	0.71	3/15284 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	75	LYS	CE-NZ	-29.56	0.75	1.49
1	H	70	LYS	CE-NZ	6.34	1.64	1.49

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	70	LYS	CD-CE-NZ	17.77	152.56	111.70
1	J	75	LYS	CD-CE-NZ	17.28	151.44	111.70
1	B	38	LEU	CA-CB-CG	5.01	126.82	115.30

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	1115	0	1083	10	0
1	B	1110	0	1077	6	0
1	C	1126	0	1098	6	0
1	D	1116	0	1083	0	0
1	E	1110	0	1077	0	0
1	F	1118	0	1093	17	0
1	G	1110	0	1077	1	1
1	H	1113	0	1082	7	0
1	I	1110	0	1077	2	0
1	J	1110	0	1077	8	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	1	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
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	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	4	0	0	0	0
4	E	4	0	0	0	0
4	F	4	0	0	0	0
4	G	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	H	4	0	0	0	0
4	I	4	0	0	0	0
4	J	4	0	0	0	0
5	F	10	0	0	0	0
5	G	5	0	0	0	0
5	J	10	0	0	1	1
6	A	166	0	0	1	0
6	B	126	0	0	2	1
6	C	199	0	0	3	1
6	D	120	0	0	0	0
6	E	111	0	0	2	0
6	F	238	0	0	6	0
6	G	187	0	0	1	1
6	H	153	0	0	7	0
6	I	168	0	0	2	0
6	J	121	0	0	2	0
All	All	12812	0	10824	52	3

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 (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)
1:H:1:ALA:HB1	6:H:2004:HOH:O	1.30	1.31
1:F:113:ILE:HD13	1:F:151[B]:ILE:HG22	1.36	1.03
6:I:2154:HOH:O	5:J:1155:SO4:O4	1.75	1.03
6:E:2050:HOH:O	1:J:7:VAL:HG23	1.71	0.90
2:H:154:CU:CU	6:H:2065:HOH:O	1.31	0.81
1:I:132:GLU:O	1:I:135:THR:HG22	1.86	0.75
1:A:115:ARG:HG2	1:F:151[B]:ILE:HD11	1.70	0.74
1:H:1:ALA:HB3	6:H:2005:HOH:O	1.87	0.73
6:E:2075:HOH:O	1:F:153:GLN:OE1	2.08	0.72
1:B:75:LYS:NZ	6:B:2078:HOH:O	2.23	0.71
1:J:75:LYS:HE2	6:J:2069:HOH:O	1.90	0.70
1:H:122:LYS:NZ	6:H:2132:HOH:O	2.25	0.69
1:C:1:ALA:HB2	1:C:23:LYS:HD3	1.78	0.64
1:B:53:ASN:HB2	6:B:2057:HOH:O	1.97	0.64
1:C:1:ALA:HB2	1:C:23:LYS:CD	2.29	0.62
1:J:52:ASP:O	1:J:59:SER:HB2	1.98	0.62
1:G:70:LYS:NZ	6:G:2111:HOH:O	2.33	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:70:LYS:HD2	6:F:2134:HOH:O	2.03	0.58
1:A:115:ARG:NH1	1:F:151[B]:ILE:HD11	2.19	0.58
1:C:2:THR:HG21	6:C:2040:HOH:O	2.05	0.57
1:C:131:ASN:ND2	6:C:2178:HOH:O	2.22	0.54
1:B:121:GLU:HA	1:B:144:LEU:HD11	1.89	0.54
1:A:135:THR:HG22	6:A:2152:HOH:O	2.08	0.54
1:C:77[A]:GLU:HG3	6:C:2122:HOH:O	2.09	0.52
1:A:115:ARG:CZ	1:F:151[B]:ILE:HD11	2.38	0.52
1:H:132:GLU:HG2	1:H:136:LYS:HE3	1.92	0.51
1:H:63:HIS:NE2	6:H:2065:HOH:O	2.12	0.50
1:F:113:ILE:HD13	1:F:151[B]:ILE:CG2	2.25	0.50
1:H:69:ARG:NH1	6:H:2095:HOH:O	2.46	0.49
1:F:69:ARG:HD2	6:F:2131:HOH:O	2.15	0.47
1:H:46:HIS:ND1	6:H:2065:HOH:O	2.35	0.47
1:B:4:ALA:HB3	1:B:20:PHE:HB2	1.98	0.46
1:C:113[B]:ILE:HG21	1:C:151:ILE:HG13	1.98	0.46
1:F:7:VAL:HG23	6:F:2013:HOH:O	2.17	0.45
1:J:75:LYS:HE3	6:J:2070:HOH:O	2.17	0.44
1:A:2:THR:HG23	1:A:106:LEU:HD12	1.99	0.44
1:J:4:ALA:HB3	1:J:20:PHE:HB2	1.98	0.44
1:I:63:HIS:NE2	6:I:2068:HOH:O	2.12	0.44
1:B:71:HIS:HB2	1:B:80:HIS:CE1	2.53	0.44
1:F:69:ARG:CZ	6:F:2131:HOH:O	2.66	0.43
1:J:113:ILE:HD13	1:J:151:ILE:HG12	2.00	0.43
1:J:22:GLN:HB2	1:J:29:VAL:HG22	2.00	0.43
1:A:50:PHE:CE1	1:F:153:GLN:HB3	2.54	0.42
1:J:7:VAL:HG11	1:J:9:LYS:HE3	2.01	0.41
1:A:115:ARG:CG	1:F:151[B]:ILE:HD11	2.46	0.41
1:A:115:ARG:NH1	1:F:151[B]:ILE:CD1	2.82	0.41
1:F:9:LYS:NZ	6:F:2016:HOH:O	2.39	0.41
1:A:115:ARG:CZ	1:F:151[B]:ILE:CD1	2.99	0.41
1:F:113:ILE:HD13	1:F:151[A]:ILE:HG12	2.03	0.40
1:F:67:LEU:HD21	6:F:2184:HOH:O	2.21	0.40
1:A:31:VAL:HB	1:A:99:ILE:HB	2.04	0.40
1:B:99:ILE:HG22	1:B:100:GLU:N	2.36	0.40

All (3) 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)
6:B:2023:HOH:O	6:G:2006:HOH:O[4_566]	1.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:1154:SO4:O2	6:C:2128:HOH:O[5_455]	1.90	0.30
1:G:26:ASN:ND2	1:G:67:LEU:CD2[3_755]	2.18	0.02

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%)	152 (100%)	0	0	100	100
1	B	151/154 (98%)	147 (97%)	4 (3%)	0	100	100
1	C	154/154 (100%)	153 (99%)	1 (1%)	0	100	100
1	D	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
1	E	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
1	F	153/154 (99%)	151 (99%)	2 (1%)	0	100	100
1	G	151/154 (98%)	148 (98%)	3 (2%)	0	100	100
1	H	152/154 (99%)	149 (98%)	3 (2%)	0	100	100
1	I	151/154 (98%)	151 (100%)	0	0	100	100
1	J	151/154 (98%)	149 (99%)	2 (1%)	0	100	100
All	All	1518/1540 (99%)	1497 (99%)	21 (1%)	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	119/119 (100%)	119 (100%)	0	100	100
1	B	118/119 (99%)	116 (98%)	2 (2%)	60	65
1	C	121/119 (102%)	120 (99%)	1 (1%)	81	86
1	D	119/119 (100%)	116 (98%)	3 (2%)	47	49
1	E	118/119 (99%)	116 (98%)	2 (2%)	60	65
1	F	120/119 (101%)	120 (100%)	0	100	100
1	G	118/119 (99%)	117 (99%)	1 (1%)	81	86
1	H	119/119 (100%)	119 (100%)	0	100	100
1	I	118/119 (99%)	117 (99%)	1 (1%)	81	86
1	J	118/119 (99%)	117 (99%)	1 (1%)	81	86
All	All	1188/1190 (100%)	1177 (99%)	11 (1%)	78	83

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2	THR
1	B	38	LEU
1	C	59	SER
1	D	42	LEU
1	D	98	SER
1	D	107	SER
1	E	23	LYS
1	E	59	SER
1	G	2	THR
1	I	135	THR
1	J	8	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 35 ligands modelled in this entry, 20 are monoatomic - leaving 15 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
5	SO4	F	1155	-	4,4,4	0.39	0	6,6,6	0.28	0
5	SO4	F	1154	-	4,4,4	0.47	0	6,6,6	0.75	0
5	SO4	G	1154	-	4,4,4	0.42	0	6,6,6	0.35	0
4	CO3	H	156	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	I	156	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	D	156	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	G	156	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	J	156	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	E	156	-	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	J	1155	-	4,4,4	0.33	0	6,6,6	0.16	0
4	CO3	C	156	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	F	156	-	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	A	156	2	0,3,3	0.00	-	0,3,3	0.00	-
4	CO3	B	156	2	0,3,3	0.00	-	0,3,3	0.00	-
5	SO4	J	1154	-	4,4,4	0.38	0	6,6,6	0.26	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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	J	1155	SO4	1	0
5	J	1154	SO4	0	1

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	153/154 (99%)	-0.17	5 (3%) 46 55	14, 22, 41, 55	4 (2%)
1	B	153/154 (99%)	0.18	8 (5%) 27 35	19, 35, 61, 82	3 (1%)
1	C	153/154 (99%)	-0.33	0 100 100	13, 20, 31, 42	2 (1%)
1	D	153/154 (99%)	0.19	10 (6%) 18 25	20, 33, 67, 82	2 (1%)
1	E	153/154 (99%)	0.28	14 (9%) 9 13	22, 34, 60, 82	2 (1%)
1	F	153/154 (99%)	-0.34	2 (1%) 77 82	12, 17, 27, 39	3 (1%)
1	G	153/154 (99%)	-0.30	3 (1%) 65 72	13, 18, 31, 48	2 (1%)
1	H	153/154 (99%)	-0.32	1 (0%) 87 91	12, 17, 32, 47	3 (1%)
1	I	153/154 (99%)	-0.28	1 (0%) 87 91	15, 22, 39, 51	5 (3%)
1	J	153/154 (99%)	-0.06	8 (5%) 27 35	18, 28, 43, 59	7 (4%)
All	All	1530/1540 (99%)	-0.11	52 (3%) 45 53	12, 24, 49, 82	33 (2%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1	ALA	5.9
1	B	131	ASN	5.5
1	A	131	ASN	4.5
1	J	26	ASN	4.3
1	E	132	GLU	4.3
1	B	132	GLU	4.3
1	D	131	ASN	4.3
1	E	25	SER	4.1
1	D	130	GLY	4.0
1	A	1	ALA	3.9
1	E	77	GLU	3.9
1	G	26	ASN	3.9
1	E	11	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	J	1	ALA	3.8
1	F	26	ASN	3.7
1	A	130	GLY	3.7
1	D	1	ALA	3.5
1	E	109	ASP	3.5
1	D	25	SER	3.5
1	J	109	ASP	3.3
1	B	135	THR	3.3
1	D	135	THR	3.3
1	E	133	GLU	3.3
1	G	1	ALA	3.2
1	H	26	ASN	3.2
1	E	26	ASN	3.1
1	D	132	GLU	3.1
1	B	91	LYS	3.1
1	E	130	GLY	3.0
1	E	131	ASN	3.0
1	B	47	VAL	3.0
1	J	25	SER	2.6
1	D	26	ASN	2.6
1	E	23	LYS	2.6
1	E	27	GLY	2.5
1	B	77	GLU	2.5
1	D	109	ASP	2.4
1	G	25	SER	2.3
1	J	24	GLU	2.3
1	A	129	GLY	2.3
1	D	23	LYS	2.2
1	B	130	GLY	2.2
1	I	117	LEU	2.2
1	J	11	ASP	2.2
1	A	132	GLU	2.2
1	J	12	GLY	2.1
1	J	92	ASP	2.1
1	E	1	ALA	2.1
1	F	1	ALA	2.1
1	E	107	SER	2.0
1	D	133	GLU	2.0
1	E	108	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 monosaccharides 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(\AA^2)	Q<0.9
4	CO3	D	156	4/4	0.79	0.31	34,36,36,38	4
5	SO4	J	1154	5/5	0.82	0.20	39,40,45,45	5
4	CO3	I	156	4/4	0.83	0.21	52,57,59,59	0
5	SO4	J	1155	5/5	0.84	0.34	60,61,64,64	5
4	CO3	H	156	4/4	0.85	0.18	42,43,44,47	0
4	CO3	C	156	4/4	0.86	0.15	50,53,53,55	0
4	CO3	J	156	4/4	0.89	0.20	52,55,56,58	0
5	SO4	F	1154	5/5	0.90	0.16	47,56,58,61	0
4	CO3	F	156	4/4	0.91	0.14	43,43,44,46	0
5	SO4	G	1154	5/5	0.93	0.22	34,36,41,42	5
5	SO4	F	1155	5/5	0.95	0.11	68,68,76,78	0
4	CO3	A	156	4/4	0.95	0.11	30,33,34,36	0
4	CO3	E	156	4/4	0.95	0.12	39,40,40,40	4
4	CO3	G	156	4/4	0.96	0.34	25,26,27,27	4
4	CO3	B	156	4/4	0.96	0.14	33,34,34,36	4
2	CU	E	154	1/1	0.97	0.09	35,35,35,35	1
2	CU	D	154	1/1	0.98	0.12	25,25,25,25	1
2	CU	B	154	1/1	0.98	0.10	32,32,32,32	1
2	CU	G	154	1/1	0.98	0.09	19,19,19,19	1
2	CU	C	154	1/1	0.99	0.06	29,29,29,29	0
3	ZN	B	155	1/1	0.99	0.08	30,30,30,30	1
3	ZN	D	155	1/1	0.99	0.03	40,40,40,40	0
2	CU	F	154	1/1	0.99	0.10	27,27,27,27	0
2	CU	A	154	1/1	0.99	0.05	30,30,30,30	0
2	CU	J	154	1/1	0.99	0.05	33,33,33,33	0
3	ZN	H	155	1/1	1.00	0.07	14,14,14,14	0
3	ZN	I	155	1/1	1.00	0.05	19,19,19,19	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	F	155	1/1	1.00	0.05	13,13,13,13	0
3	ZN	A	155	1/1	1.00	0.06	22,22,22,22	0
3	ZN	J	155	1/1	1.00	0.04	20,20,20,20	0
2	CU	H	154	1/1	1.00	0.01	28,28,28,28	0
2	CU	I	154	1/1	1.00	0.03	28,28,28,28	0
3	ZN	C	155	1/1	1.00	0.06	17,17,17,17	0
3	ZN	E	155	1/1	1.00	0.04	35,35,35,35	0
3	ZN	G	155	1/1	1.00	0.06	13,13,13,13	0

6.5 Other polymers [i](#)

There are no such residues in this entry.