



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:15 PM GMT

PDB ID : 1UXL  
Title : I113T MUTANT OF HUMAN SOD1  
Authors : Hough, M.A.; Grossmann, J.G.; Antonyuk, S.V.; Strange, R.W.; Doucette, P.A.; Rodriguez, J.A.; Whitson, L.J.; Hart, P.J.; Hayward, L.J.; Valentine, J.S.; Hasnain, S.S.  
Deposited on : 2004-02-25  
Resolution : 1.60 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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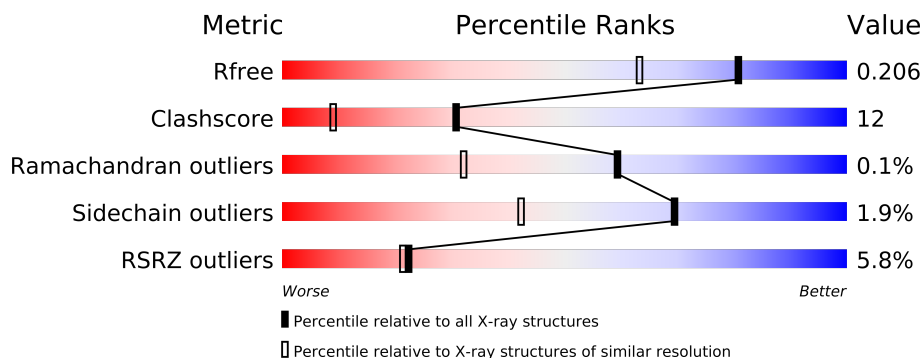
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 1.60 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))
$R_{free}$	66092	1872 (1.60-1.60)
Clashscore	79885	2199 (1.60-1.60)
Ramachandran outliers	78287	2126 (1.60-1.60)
Sidechain outliers	78261	2125 (1.60-1.60)
RSRZ outliers	66119	1872 (1.60-1.60)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	153	
1	B	153	
1	C	153	
1	D	153	
1	E	153	
1	F	153	
1	G	153	
1	H	153	
1	I	153	
1	J	153	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	CU	G	154	-	X
4	SO4	B	156	-	X
4	SO4	C	157	-	X
4	SO4	D	156	-	X
4	SO4	E	156	-	X
4	SO4	F	156	-	X
4	SO4	H	156	-	X
4	SO4	I	156	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 13831 atoms, of which 0 are hydrogen and 0 are deuterium.

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
1	A	153	Total	C	N	O	S	22	10	0
			1158	706	210	237	5			
1	B	153	Total	C	N	O	S	7	5	0
			1141	694	210	232	5			
1	C	153	Total	C	N	O	S	13	2	0
			1113	679	203	226	5			
1	D	153	Total	C	N	O	S	23	8	0
			1134	691	205	234	4			
1	E	153	Total	C	N	O	S	22	0	0
			1109	677	203	225	4			
1	F	153	Total	C	N	O	S	3	6	0
			1129	688	206	231	4			
1	G	153	Total	C	N	O	S	12	2	0
			1115	682	203	226	4			
1	H	153	Total	C	N	O	S	13	12	0
			1162	705	210	243	4			
1	I	153	Total	C	N	O	S	17	5	0
			1146	701	209	231	5			
1	J	153	Total	C	N	O	S	25	3	0
			1116	682	203	227	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	THR	ILE	ENGINEERED MUTATION	UNP P00441
B	113	THR	ILE	ENGINEERED MUTATION	UNP P00441
C	113	THR	ILE	ENGINEERED MUTATION	UNP P00441
D	113	THR	ILE	ENGINEERED MUTATION	UNP P00441
E	113	THR	ILE	ENGINEERED MUTATION	UNP P00441
F	113	THR	ILE	ENGINEERED MUTATION	UNP P00441
G	113	THR	ILE	ENGINEERED MUTATION	UNP P00441
H	113	THR	ILE	ENGINEERED MUTATION	UNP P00441
I	113	THR	ILE	ENGINEERED MUTATION	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
J	113	THR	ILE	ENGINEERED MUTATION	UNP P00441

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

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

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

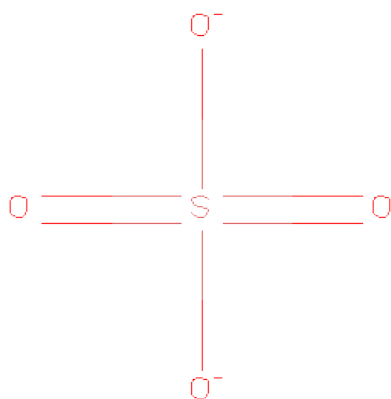
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Zn 1 1	0	0
3	J	1	Total Zn 1 1	0	0
3	D	1	Total Zn 1 1	0	0
3	E	1	Total Zn 1 1	0	0
3	H	1	Total Zn 1 1	0	0
3	B	1	Total Zn 1 1	0	0
3	I	1	Total Zn 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		
4	D	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	F	1	Total	O	S	0	0
			5	4	1		
4	H	1	Total	O	S	0	0
			5	4	1		
4	I	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is water.

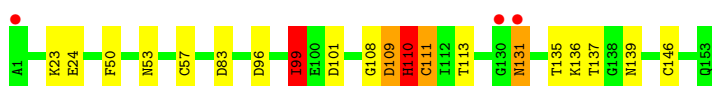
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	248	Total 248	O 248	0	0
5	B	197	Total 197	O 197	0	0
5	C	263	Total 263	O 263	0	0
5	D	178	Total 178	O 178	0	0
5	E	179	Total 179	O 179	0	0
5	F	304	Total 304	O 304	0	0
5	G	270	Total 270	O 270	0	0
5	H	316	Total 316	O 316	0	0
5	I	246	Total 246	O 246	0	0
5	J	246	Total 246	O 246	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: SUPEROXIDE DISMUTASE [CU-ZN]

Chain A: 



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain B: 



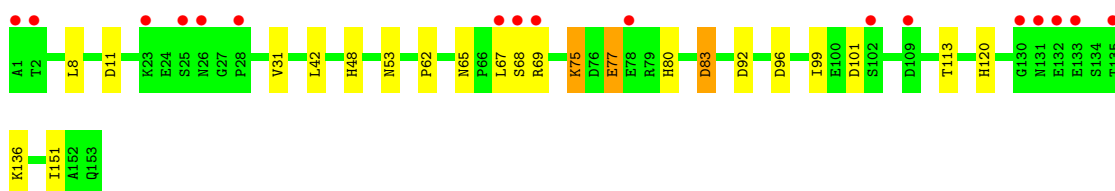
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain C: 



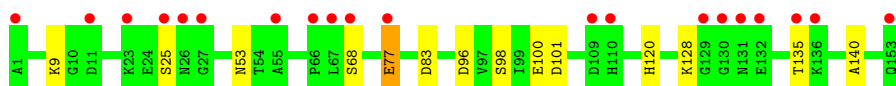
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain D: 



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain E: 



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain F: 





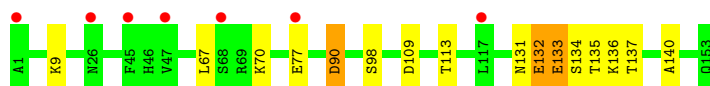
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain G:



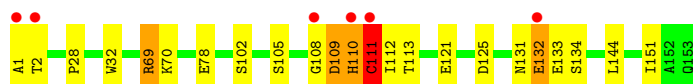
- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain H:



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain I:



- Molecule 1: SUPEROXIDE DISMUTASE [CU-ZN]

Chain J:



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	166.04Å 203.55Å 144.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.60 23.99 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.6 (20.00-1.60) 99.6 (23.99-1.60)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.45 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.170 , 0.196 0.182 , 0.206	Depositor DCC
$R_{free}$ test set	15965 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	18.7	Xtriage
Anisotropy	0.204	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 59.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 316398 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13831	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.64	2/1200 (0.2%)	1.29	14/1619 (0.9%)
1	B	0.86	1/1162 (0.1%)	0.98	10/1563 (0.6%)
1	C	0.58	1/1140 (0.1%)	0.90	4/1537 (0.3%)
1	D	0.47	0/1188	0.90	7/1602 (0.4%)
1	E	0.46	1/1127 (0.1%)	0.79	3/1519 (0.2%)
1	F	0.56	0/1173	0.86	1/1581 (0.1%)
1	G	0.61	1/1142 (0.1%)	0.83	1/1540 (0.1%)
1	H	1.10	2/1221 (0.2%)	1.02	3/1647 (0.2%)
1	I	0.77	3/1175 (0.3%)	1.09	9/1586 (0.6%)
1	J	0.56	1/1148 (0.1%)	0.88	4/1548 (0.3%)
All	All	0.69	12/11676 (0.1%)	0.97	56/15742 (0.4%)

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	3
1	I	0	1
All	All	0	4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	133[A]	GLU	C-N	23.15	1.87	1.34
1	H	133[B]	GLU	C-N	23.15	1.87	1.34
1	B	107	SER	C-N	22.68	1.73	1.33
1	I	111[A]	CYS	C-N	13.17	1.64	1.34
1	I	111[B]	CYS	C-N	13.17	1.64	1.34
1	G	70	LYS	CD-CE	9.74	1.75	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	24	GLU	CG-CD	9.67	1.66	1.51
1	A	99[A]	ILE	C-N	7.37	1.50	1.34
1	A	99[B]	ILE	C-N	7.37	1.50	1.34
1	E	77	GLU	CB-CG	6.31	1.64	1.52
1	C	77	GLU	CG-CD	-5.65	1.43	1.51
1	I	70	LYS	CD-CE	5.10	1.64	1.51

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	110[A]	HIS	O-C-N	-17.30	95.02	122.70
1	A	110[B]	HIS	O-C-N	-17.30	95.02	122.70
1	I	111[A]	CYS	O-C-N	-16.54	96.23	122.70
1	I	111[B]	CYS	O-C-N	-16.54	96.23	122.70
1	H	133[A]	GLU	O-C-N	-13.81	100.60	122.70
1	H	133[B]	GLU	O-C-N	-13.81	100.60	122.70
1	A	110[A]	HIS	C-N-CA	12.65	153.32	121.70
1	A	110[B]	HIS	C-N-CA	12.65	153.32	121.70
1	A	110[A]	HIS	CA-C-N	11.04	141.49	117.20
1	A	110[B]	HIS	CA-C-N	11.04	141.49	117.20
1	B	107	SER	C-N-CA	-9.91	101.48	122.30
1	D	83	ASP	CB-CG-OD1	8.61	126.05	118.30
1	I	111[A]	CYS	CA-C-N	8.54	135.99	117.20
1	I	111[B]	CYS	CA-C-N	8.54	135.99	117.20
1	H	90	ASP	CB-CG-OD2	8.21	125.69	118.30
1	B	111[A]	CYS	N-CA-CB	-7.86	96.45	110.60
1	B	111[B]	CYS	N-CA-CB	-7.86	96.45	110.60
1	A	99[A]	ILE	CA-C-N	-7.69	100.28	117.20
1	A	99[B]	ILE	CA-C-N	-7.69	100.28	117.20
1	B	132	GLU	N-CA-CB	-6.96	98.07	110.60
1	A	99[A]	ILE	O-C-N	6.80	133.58	122.70
1	A	99[B]	ILE	O-C-N	6.80	133.58	122.70
1	B	83	ASP	CB-CG-OD2	6.26	123.93	118.30
1	A	101[A]	ASP	CB-CG-OD2	5.94	123.65	118.30
1	A	101[B]	ASP	CB-CG-OD2	5.94	123.65	118.30
1	C	83	ASP	CB-CG-OD2	5.80	123.52	118.30
1	D	77	GLU	CA-C-O	5.78	132.24	120.10
1	C	109	ASP	CB-CG-OD2	5.75	123.48	118.30
1	B	79	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	D	101	ASP	CB-CG-OD2	5.63	123.36	118.30
1	A	96	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	96	ASP	CB-CG-OD2	5.58	123.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	101	ASP	CB-CG-OD2	5.56	123.30	118.30
1	D	77	GLU	CA-C-N	-5.52	105.06	117.20
1	G	70	LYS	CG-CD-CE	-5.48	95.46	111.90
1	J	96	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	11	ASP	CB-CG-OD2	5.38	123.14	118.30
1	J	92	ASP	CB-CG-OD2	5.37	123.13	118.30
1	C	92	ASP	CB-CG-OD2	5.37	123.13	118.30
1	E	96	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	101	ASP	CB-CG-OD2	5.33	123.10	118.30
1	I	125	ASP	CB-CG-OD1	5.26	123.03	118.30
1	E	83	ASP	CB-CG-OD2	5.25	123.03	118.30
1	D	92	ASP	CB-CG-OD2	5.24	123.02	118.30
1	I	111[A]	CYS	N-CA-CB	-5.24	101.17	110.60
1	I	111[B]	CYS	N-CA-CB	-5.24	101.17	110.60
1	A	83	ASP	CB-CG-OD2	5.24	123.01	118.30
1	B	92	ASP	CB-CG-OD2	5.23	123.01	118.30
1	I	109[A]	ASP	CB-CG-OD2	5.22	123.00	118.30
1	I	109[B]	ASP	CB-CG-OD2	5.22	123.00	118.30
1	B	11	ASP	CB-CG-OD2	5.15	122.94	118.30
1	F	115	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	C	96	ASP	CB-CG-OD2	5.08	122.87	118.30
1	J	109	ASP	CB-CG-OD2	5.05	122.85	118.30
1	B	125	ASP	CB-CG-OD2	5.05	122.84	118.30
1	J	24	GLU	CB-CG-CD	-5.03	100.62	114.20

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109[A]	ASP	Sidechain
1	A	110[A]	HIS	Mainchain
1	A	99[A]	ILE	Mainchain
1	I	111[A]	CYS	Mainchain

## 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1158	0	1118	26	0
1	B	1141	0	1093	33	0
1	C	1113	0	1077	30	0
1	D	1134	0	1093	24	0
1	E	1109	0	1073	9	0
1	F	1129	0	1092	22	0
1	G	1115	0	1083	16	0
1	H	1162	0	1107	25	0
1	I	1146	0	1099	52	1
1	J	1116	0	1084	12	0
2	A	2	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
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	5	0	0	1	0
4	B	5	0	0	1	0
4	C	5	0	0	2	0
4	D	5	0	0	7	0
4	E	5	0	0	1	0
4	F	5	0	0	2	0
4	H	5	0	0	1	0
4	I	5	0	0	0	0
5	A	248	0	0	21	1
5	B	197	0	0	17	0
5	C	263	0	0	22	2
5	D	178	0	0	15	2
5	E	179	0	0	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	304	0	0	20	0
5	G	270	0	0	16	1
5	H	316	0	0	16	0
5	I	246	0	0	30	0
5	J	246	0	0	10	2
All	All	13831	0	10919	254	5

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 12.

All (254) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:107:SER:C	1:B:108[A]:GLY:N	1.73	1.39
1:H:133[A]:GLU:C	1:H:134:SER:N	1.87	1.28
4:F:156:SO4:O4	5:F:2301:HOH:O	1.52	1.25
4:C:157:SO4:O2	5:C:2263:HOH:O	1.55	1.24
1:A:53:ASN:ND2	5:A:2119:HOH:O	1.68	1.24
4:F:156:SO4:O2	5:F:2302:HOH:O	1.55	1.21
1:I:111[B]:CYS:HA	1:I:112:ILE:N	1.54	1.20
1:I:102:SER:HB3	5:I:2182:HOH:O	1.46	1.15
1:B:23:LYS:HE3	5:B:2042:HOH:O	1.44	1.14
1:F:1:ALA:HB1	5:F:2005:HOH:O	1.45	1.14
1:E:53:ASN:HB3	5:E:2078:HOH:O	1.49	1.12
1:B:30:LYS:HB2	5:B:2015:HOH:O	1.51	1.10
1:B:110[B]:HIS:O	5:B:2157:HOH:O	1.68	1.10
1:I:1:ALA:HB2	5:I:2004:HOH:O	1.52	1.09
1:B:111[A]:CYS:C	1:B:112:ILE:N	2.07	1.08
1:F:24:GLU:HG2	5:F:2071:HOH:O	1.54	1.07
1:C:109:ASP:HA	5:C:2203:HOH:O	1.54	1.06
4:H:156:SO4:O3	5:H:2313:HOH:O	1.72	1.06
1:I:111[B]:CYS:CA	1:I:112:ILE:N	2.10	1.05
1:D:62:PRO:HG2	5:D:2086:HOH:O	1.54	1.03
1:I:131:ASN:ND2	1:I:134:SER:H	1.55	1.03
1:B:107:SER:C	1:B:108[B]:GLY:N	2.13	1.02
1:H:133[B]:GLU:HG2	5:H:2288:HOH:O	1.59	1.01
1:A:136:LYS:HB3	5:A:2223:HOH:O	1.61	1.01
1:F:113[B]:THR:HG21	5:F:2236:HOH:O	1.59	0.99
1:C:113[B]:THR:HG21	5:C:2201:HOH:O	1.62	0.99
1:A:113[B]:THR:HG21	5:A:2187:HOH:O	1.63	0.98
1:B:3:LYS:HE2	5:B:2034:HOH:O	1.62	0.98
1:I:109[B]:ASP:O	1:I:111[B]:CYS:N	1.98	0.97
1:H:132[A]:GLU:O	1:H:135[A]:THR:OG1	1.83	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:111[B]:CYS:SG	1:A:113[B]:THR:HG23	2.06	0.95
1:A:135:THR:HG22	5:A:2141:HOH:O	1.66	0.94
1:I:131:ASN:HD21	1:I:134:SER:N	1.67	0.92
1:A:110[B]:HIS:HB3	5:A:2198:HOH:O	1.67	0.92
1:A:53:ASN:HB3	5:A:2117:HOH:O	1.67	0.92
1:I:131:ASN:HD21	1:I:134:SER:H	1.14	0.90
4:D:156:SO4:O3	5:D:2178:HOH:O	1.90	0.89
1:H:113[B]:THR:HG21	5:H:2237:HOH:O	1.73	0.89
1:F:32:TRP:CD1	5:F:2092:HOH:O	2.25	0.88
1:D:53[B]:ASN:OD1	5:D:2071:HOH:O	1.91	0.87
4:D:156:SO4:O4	5:D:2176:HOH:O	1.93	0.86
1:I:32[A]:TRP:CH2	5:I:2047:HOH:O	2.31	0.83
1:D:69:ARG:HG2	5:D:2089:HOH:O	1.78	0.82
1:I:108:GLY:O	1:I:111[A]:CYS:HB3	1.80	0.82
1:J:90:ASP:HB3	5:J:2160:HOH:O	1.78	0.82
1:D:53[A]:ASN:OD1	5:D:2074:HOH:O	1.96	0.82
1:B:131[B]:ASN:OD1	5:B:2173:HOH:O	1.97	0.81
1:B:78:GLU:HA	5:B:2110:HOH:O	1.81	0.81
1:I:111[B]:CYS:C	1:I:112:ILE:N	2.30	0.81
1:B:107:SER:C	1:B:108[A]:GLY:CA	2.50	0.80
1:I:2:THR:HG22	5:I:2006:HOH:O	1.80	0.80
1:I:1:ALA:CB	5:I:2004:HOH:O	2.17	0.79
1:I:132:GLU:HG3	5:I:2224:HOH:O	1.82	0.79
1:A:24:GLU:HB3	5:A:2052:HOH:O	1.82	0.79
1:A:137:THR:HG23	5:A:2223:HOH:O	1.83	0.79
1:J:9:LYS:HD2	5:J:2014:HOH:O	1.83	0.78
1:E:100:GLU:HG2	5:E:2132:HOH:O	1.82	0.78
1:H:77:GLU:HG3	5:H:2189:HOH:O	1.83	0.78
1:D:77:GLU:HA	5:D:2105:HOH:O	1.85	0.78
1:C:132:GLU:CD	1:C:132:GLU:H	1.89	0.76
1:J:100:GLU:OE2	5:J:2170:HOH:O	2.03	0.76
1:G:135:THR:HB	5:G:2068:HOH:O	1.85	0.76
1:I:1:ALA:HA	5:I:2002:HOH:O	1.86	0.76
1:I:32[A]:TRP:HH2	5:I:2047:HOH:O	1.64	0.75
1:F:26:ASN:HB2	5:F:2076:HOH:O	1.84	0.75
1:I:109[A]:ASP:HB2	5:I:2191:HOH:O	1.86	0.75
4:B:156:SO4:O4	5:B:2197:HOH:O	2.03	0.75
1:I:131:ASN:ND2	1:I:134:SER:N	2.29	0.74
1:D:69:ARG:HD3	5:D:2100:HOH:O	1.85	0.74
1:I:69:ARG:NH1	1:I:78:GLU:OE1	2.20	0.74
1:A:109[B]:ASP:N	5:A:2195:HOH:O	2.21	0.73
1:I:109[B]:ASP:C	1:I:111[B]:CYS:H	1.89	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:132[A]:GLU:OE1	1:H:132[A]:GLU:N	2.22	0.72
1:G:135:THR:CB	5:G:2068:HOH:O	2.36	0.72
1:A:131:ASN:HD21	1:A:139:ASN:HD21	1.35	0.72
1:B:128:LYS:HE2	5:B:2170:HOH:O	1.89	0.72
1:G:77:GLU:CG	5:G:2152:HOH:O	2.37	0.72
1:C:132:GLU:HG3	5:C:2236:HOH:O	1.89	0.71
1:I:131:ASN:HD22	1:I:133:GLU:N	1.88	0.70
1:I:2:THR:HG21	5:I:2020:HOH:O	1.89	0.70
1:A:99[A]:ILE:HD13	5:A:2155:HOH:O	1.90	0.70
1:D:65:ASN:OD1	5:D:2087:HOH:O	2.10	0.70
1:G:53:ASN:ND2	5:G:2127:HOH:O	2.25	0.69
1:D:48:HIS:CE1	4:D:156:SO4:O1	2.46	0.69
1:C:111[A]:CYS:SG	5:C:2210:HOH:O	2.49	0.69
1:I:1:ALA:C	5:I:2006:HOH:O	2.31	0.68
1:C:69:ARG:NH1	5:C:2150:HOH:O	2.26	0.68
1:I:113[A]:THR:HG21	5:I:2189:HOH:O	1.92	0.68
1:I:132:GLU:CG	5:I:2224:HOH:O	2.39	0.68
1:I:2:THR:CG2	5:I:2006:HOH:O	2.37	0.68
1:B:79:ARG:HD3	1:B:80:HIS:O	1.93	0.68
1:C:39:THR:O	1:C:43:HIS:HE1	1.77	0.68
1:J:30:LYS:HG2	5:J:2170:HOH:O	1.93	0.67
1:D:53[A]:ASN:ND2	5:D:2072:HOH:O	2.03	0.67
1:C:111[A]:CYS:HB3	5:C:2210:HOH:O	1.95	0.67
1:I:105:SER:O	1:I:111[B]:CYS:HB2	1.94	0.66
1:D:48:HIS:NE2	4:D:156:SO4:O1	2.29	0.65
1:G:121:GLU:HG3	5:G:2256:HOH:O	1.97	0.65
1:I:132:GLU:CD	1:I:133:GLU:H	2.00	0.65
1:A:110[B]:HIS:N	5:A:2195:HOH:O	2.22	0.65
1:D:113[B]:THR:HG21	1:D:151:ILE:HG13	1.80	0.64
1:G:113[B]:THR:HG21	5:G:2217:HOH:O	1.98	0.64
1:B:30:LYS:CE	5:B:2054:HOH:O	2.46	0.64
1:F:70:LYS:HE2	5:F:2183:HOH:O	1.97	0.64
1:F:70:LYS:CE	5:F:2183:HOH:O	2.47	0.63
1:F:27:GLY:HA2	5:F:2078:HOH:O	1.98	0.63
1:B:57:CYS:HG	1:B:146:CYS:CB	2.12	0.63
1:G:121:GLU:CG	5:G:2256:HOH:O	2.46	0.63
1:H:109[B]:ASP:OD2	5:H:2245:HOH:O	2.14	0.62
1:B:79:ARG:CD	1:B:80:HIS:O	2.48	0.61
1:G:121:GLU:CD	5:G:2256:HOH:O	2.38	0.61
1:C:23:LYS:HG3	5:C:2068:HOH:O	2.00	0.61
1:C:136:LYS:HD3	5:C:2239:HOH:O	2.01	0.61
1:I:109[A]:ASP:N	5:I:2192:HOH:O	2.34	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:75:LYS:HD3	5:I:2125:HOH:O	2.01	0.60
1:A:109[B]:ASP:CG	5:A:2193:HOH:O	2.40	0.59
1:C:136:LYS:CD	5:C:2239:HOH:O	2.49	0.59
1:F:25:SER:HB2	5:F:2082:HOH:O	2.02	0.59
1:I:102:SER:CB	5:I:2182:HOH:O	2.23	0.59
1:B:30:LYS:HE2	5:B:2054:HOH:O	2.03	0.58
1:I:1:ALA:N	5:I:2001:HOH:O	2.32	0.57
1:G:135:THR:CG2	5:G:2068:HOH:O	2.53	0.57
1:A:108[B]:GLY:C	5:A:2195:HOH:O	2.41	0.57
1:B:32:TRP:NE1	5:B:2055:HOH:O	2.33	0.57
1:E:98:SER:OG	1:F:21:GLU:OE1	2.17	0.56
1:I:131:ASN:HD22	1:I:133:GLU:H	1.53	0.56
1:C:109:ASP:OD1	1:C:109:ASP:O	2.22	0.56
1:G:135:THR:HG22	5:G:2068:HOH:O	2.05	0.56
1:H:132[A]:GLU:OE2	5:H:2281:HOH:O	2.17	0.56
1:B:32:TRP:CZ2	5:B:2055:HOH:O	2.58	0.56
1:I:132:GLU:CB	5:I:2224:HOH:O	2.54	0.56
1:H:133[A]:GLU:HG3	1:H:133[A]:GLU:O	2.06	0.56
1:C:128:LYS:NZ	5:C:2230:HOH:O	2.25	0.56
1:G:70:LYS:CD	5:G:2156:HOH:O	2.54	0.55
1:B:108[A]:GLY:O	1:B:111[A]:CYS:HB3	2.05	0.55
1:B:107:SER:CA	1:B:108[A]:GLY:N	2.67	0.55
1:H:137:THR:HB	5:H:2291:HOH:O	2.05	0.55
1:I:109[B]:ASP:C	1:I:111[B]:CYS:N	2.51	0.55
1:I:109[A]:ASP:HA	5:I:2192:HOH:O	2.06	0.55
1:I:132:GLU:CD	5:I:2225:HOH:O	2.44	0.55
1:B:75:LYS:CD	5:I:2125:HOH:O	2.53	0.55
1:I:69:ARG:CG	1:I:69:ARG:HH11	2.20	0.55
1:H:132[A]:GLU:CB	5:H:2284:HOH:O	2.53	0.54
1:I:2:THR:N	5:I:2006:HOH:O	2.40	0.54
1:I:69:ARG:NH1	1:I:69:ARG:HG2	2.23	0.54
1:I:113[B]:THR:HG21	1:I:151:ILE:HG13	1.88	0.54
1:A:136:LYS:CB	5:A:2223:HOH:O	2.37	0.54
1:D:113[A]:THR:HG21	5:D:2137:HOH:O	2.07	0.54
1:E:9:LYS:CE	5:E:2019:HOH:O	2.54	0.53
1:G:77:GLU:HG3	5:G:2152:HOH:O	2.03	0.53
1:D:67:LEU:HA	5:D:2090:HOH:O	2.06	0.53
1:A:109[B]:ASP:HB2	5:A:2196:HOH:O	2.09	0.53
1:I:109[A]:ASP:CB	5:I:2191:HOH:O	2.51	0.53
1:C:132:GLU:CD	1:C:132:GLU:N	2.58	0.53
1:J:110:HIS:ND1	5:J:2187:HOH:O	2.34	0.52
1:G:27:GLY:HA2	5:G:2062:HOH:O	2.08	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:30:LYS:HG3	5:F:2088:HOH:O	2.09	0.52
1:C:132:GLU:CG	5:C:2236:HOH:O	2.52	0.51
1:D:80:HIS:HB2	1:D:83:ASP:CG	2.30	0.51
1:E:9:LYS:HE2	5:E:2019:HOH:O	2.10	0.51
1:I:109[A]:ASP:CA	5:I:2192:HOH:O	2.59	0.51
1:I:111[B]:CYS:CB	1:I:112:ILE:N	2.63	0.51
1:G:77:GLU:HG2	5:G:2152:HOH:O	2.06	0.50
1:A:99[B]:ILE:HD11	5:A:2155:HOH:O	0.61	0.50
1:B:32:TRP:CE2	5:B:2055:HOH:O	2.64	0.50
1:H:132[A]:GLU:CD	1:H:132[A]:GLU:N	2.65	0.50
1:J:30:LYS:CG	5:J:2170:HOH:O	2.54	0.50
1:A:110[B]:HIS:HE1	5:A:2197:HOH:O	1.95	0.50
1:J:30:LYS:CE	5:J:2170:HOH:O	2.60	0.50
1:C:108:GLY:O	1:C:111[B]:CYS:HB3	2.12	0.49
1:C:69:ARG:HD3	5:C:2149:HOH:O	2.10	0.49
1:C:43:HIS:HD2	1:C:120:HIS:O	1.96	0.49
1:F:32:TRP:NE1	5:F:2092:HOH:O	2.39	0.49
1:B:108[A]:GLY:O	1:B:111[A]:CYS:CB	2.61	0.49
1:F:26:ASN:HA	5:F:2083:HOH:O	2.11	0.49
1:D:80:HIS:HE1	1:D:136:LYS:O	1.96	0.49
1:A:99[B]:ILE:CD1	5:A:2155:HOH:O	0.81	0.49
1:D:75:LYS:HE2	5:D:2097:HOH:O	2.13	0.49
1:H:133[A]:GLU:C	1:H:136:LYS:H	2.16	0.48
1:A:57:CYS:CB	1:A:146:CYS:HG	2.21	0.48
1:C:69:ARG:HD3	5:C:2166:HOH:O	2.13	0.48
1:I:121:GLU:HA	1:I:144:LEU:HD11	1.95	0.48
1:B:30:LYS:NZ	5:B:2054:HOH:O	2.47	0.48
5:G:2181:HOH:O	1:H:131[B]:ASN:HB3	2.14	0.47
1:H:77:GLU:CG	5:H:2189:HOH:O	2.50	0.47
1:E:140:ALA:HB3	5:E:2158:HOH:O	2.15	0.47
1:B:23:LYS:HE2	5:B:2035:HOH:O	2.14	0.47
1:J:30:LYS:NZ	5:J:2170:HOH:O	2.43	0.47
1:F:25:SER:CA	5:F:2082:HOH:O	2.62	0.47
1:C:1:ALA:HB2	1:C:23:LYS:HD3	1.97	0.47
4:A:156:SO4:O4	5:A:2248:HOH:O	2.16	0.47
1:H:133[A]:GLU:CD	5:H:2288:HOH:O	2.52	0.46
1:C:120:HIS:HE1	4:C:157:SO4:O3	1.98	0.46
1:H:132[A]:GLU:HB2	5:H:2284:HOH:O	2.15	0.46
1:H:70:LYS:HB3	1:H:135[B]:THR:HG22	1.98	0.46
1:I:131:ASN:ND2	1:I:133:GLU:N	2.61	0.46
1:C:136:LYS:NZ	5:C:2239:HOH:O	2.46	0.46
1:F:32:TRP:HD1	5:F:2092:HOH:O	1.77	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:2:THR:HG21	5:C:2039:HOH:O	2.16	0.45
1:B:30:LYS:HG2	1:B:32:TRP:CE3	2.51	0.45
1:C:132:GLU:CD	5:C:2236:HOH:O	2.54	0.45
1:B:80:HIS:HE1	1:B:136:LYS:O	1.99	0.45
1:F:111:CYS:SG	1:F:113[B]:THR:HG23	2.56	0.45
1:D:77:GLU:CA	5:D:2105:HOH:O	2.36	0.45
1:F:25:SER:HA	5:F:2082:HOH:O	2.17	0.44
1:I:132:GLU:CD	1:I:133:GLU:N	2.68	0.44
1:F:132:GLU:HG3	1:H:98:SER:CB	2.47	0.44
1:B:105:SER:O	1:B:111[B]:CYS:HA	2.17	0.44
1:C:109:ASP:OD1	1:C:109:ASP:C	2.55	0.44
1:C:23:LYS:HD2	5:C:2058:HOH:O	2.17	0.44
1:H:133[A]:GLU:C	1:H:134:SER:CA	2.80	0.43
1:B:79:ARG:NH2	1:B:101:ASP:OD1	2.41	0.43
1:D:48:HIS:HE1	4:D:156:SO4:S	2.40	0.43
1:A:110[B]:HIS:CB	5:A:2198:HOH:O	2.38	0.43
1:D:120:HIS:NE2	4:D:156:SO4:O1	2.51	0.43
1:J:1:ALA:N	5:J:2001:HOH:O	2.45	0.43
1:I:28:PRO:HB3	5:I:2182:HOH:O	2.16	0.43
1:F:26:ASN:N	5:F:2082:HOH:O	2.35	0.43
1:H:133[B]:GLU:CG	5:H:2288:HOH:O	2.37	0.43
1:B:128:LYS:NZ	5:B:2108:HOH:O	2.51	0.43
1:J:122:LYS:NZ	5:J:2197:HOH:O	2.42	0.43
1:D:69:ARG:N	5:D:2089:HOH:O	2.51	0.42
1:D:67:LEU:O	1:D:68:SER:HB2	2.18	0.42
1:H:67:LEU:HD21	5:H:2251:HOH:O	2.19	0.42
1:C:131:ASN:ND2	5:C:2234:HOH:O	2.51	0.42
1:C:69:ARG:NE	5:C:2149:HOH:O	2.50	0.42
1:I:105:SER:OG	5:I:2188:HOH:O	2.22	0.42
1:D:48:HIS:CE1	4:D:156:SO4:S	3.13	0.42
1:E:68:SER:HA	5:E:2092:HOH:O	2.20	0.42
1:B:3:LYS:NZ	5:B:2004:HOH:O	2.52	0.41
1:H:9:LYS:HG2	5:H:2015:HOH:O	2.20	0.41
1:B:107:SER:N	1:B:111[B]:CYS:HB2	2.35	0.41
1:C:23:LYS:CG	5:C:2068:HOH:O	2.61	0.41
1:H:9:LYS:HD3	5:H:2014:HOH:O	2.20	0.41
1:C:2:THR:HG23	5:C:2052:HOH:O	2.20	0.41
1:A:109[B]:ASP:HB2	5:A:2193:HOH:O	2.21	0.41
1:I:2:THR:CG2	5:I:2054:HOH:O	2.68	0.41
1:D:31:VAL:HB	1:D:99:ILE:HB	2.01	0.41
1:H:140:ALA:HB3	5:H:2291:HOH:O	2.20	0.41
1:F:26:ASN:ND2	5:F:2080:HOH:O	2.51	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:I:132:GLU:HB3	5:I:2224:HOH:O	2.17	0.41
1:G:77:GLU:HG3	5:G:2065:HOH:O	2.20	0.41
1:I:110[B]:HIS:N	5:I:2190:HOH:O	2.54	0.41
1:E:68:SER:CA	5:E:2092:HOH:O	2.69	0.40
1:G:122:LYS:HE3	1:G:139:ASN:O	2.20	0.40
1:A:50:PHE:CE1	1:F:153:GLN:HB3	2.57	0.40
1:E:120:HIS:HE1	4:E:156:SO4:O2	2.04	0.40
1:F:132:GLU:HG2	5:F:2275:HOH:O	2.22	0.40

All (5) 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	Distance(Å)	Clash(Å)
5:G:2100:HOH:O	5:G:2100:HOH:O[3_755]	0.36	1.84
1:I:110[B]:HIS:CB	5:D:2090:HOH:O[3_755]	2.03	0.17
5:C:2229:HOH:O	5:J:2141:HOH:O[5_545]	2.15	0.05
5:A:2075:HOH:O	5:D:2152:HOH:O[5_445]	2.18	0.02
5:C:2231:HOH:O	5:J:2215:HOH:O[5_545]	2.19	0.01

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	161/153 (105%)	159 (99%)	2 (1%)	0	100	100
1	B	156/153 (102%)	156 (100%)	0	0	100	100
1	C	153/153 (100%)	153 (100%)	0	0	100	100
1	D	159/153 (104%)	156 (98%)	3 (2%)	0	100	100
1	E	151/153 (99%)	150 (99%)	1 (1%)	0	100	100
1	F	157/153 (103%)	156 (99%)	1 (1%)	0	100	100
1	G	153/153 (100%)	151 (99%)	2 (1%)	0	100	100
1	H	163/153 (106%)	163 (100%)	0	0	100	100
1	I	156/153 (102%)	154 (99%)	0	2 (1%)	18	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	154/153 (101%)	154 (100%)	0	0	100	100
All	All	1563/1530 (102%)	1552 (99%)	9 (1%)	2 (0%)	59	32

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	110[A]	HIS
1	I	110[B]	HIS

### 5.3.2 Protein sidechains ⓘ

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	127/118 (108%)	123 (97%)	4 (3%)	52	21
1	B	122/118 (103%)	117 (96%)	5 (4%)	41	13
1	C	120/118 (102%)	118 (98%)	2 (2%)	73	47
1	D	126/118 (107%)	124 (98%)	2 (2%)	75	50
1	E	118/118 (100%)	114 (97%)	4 (3%)	49	19
1	F	124/118 (105%)	123 (99%)	1 (1%)	89	78
1	G	120/118 (102%)	120 (100%)	0	100	100
1	H	130/118 (110%)	127 (98%)	3 (2%)	63	32
1	I	123/118 (104%)	119 (97%)	4 (3%)	50	20
1	J	121/118 (102%)	119 (98%)	2 (2%)	73	47
All	All	1231/1180 (104%)	1204 (98%)	27 (2%)	69	34

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LYS
1	A	111[A]	CYS
1	A	111[B]	CYS
1	A	131	ASN
1	B	75	LYS

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Mol	Chain	Res	Type
1	B	79	ARG
1	B	91	LYS
1	B	111[A]	CYS
1	B	111[B]	CYS
1	C	2	THR
1	C	132	GLU
1	D	42	LEU
1	D	75	LYS
1	E	25	SER
1	E	77	GLU
1	E	128	LYS
1	E	135	THR
1	F	26	ASN
1	H	90	ASP
1	H	132[A]	GLU
1	H	132[B]	GLU
1	I	69	ARG
1	I	111[A]	CYS
1	I	111[B]	CYS
1	I	132	GLU
1	J	24	GLU
1	J	29	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	131	ASN
1	B	139	ASN
1	C	43	HIS
1	E	53	ASN
1	F	110	HIS
1	F	153	GLN
1	I	131	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

Of 29 ligands modelled in this entry, 21 are monoatomic - leaving 8 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	A	156	-	4,4,4	0.43	0	6,6,6	0.47	0
4	SO4	B	156	2	4,4,4	0.43	0	6,6,6	0.33	0
4	SO4	C	157	-	4,4,4	0.71	0	6,6,6	0.19	0
4	SO4	D	156	2	4,4,4	0.45	0	6,6,6	0.47	0
4	SO4	E	156	-	4,4,4	0.28	0	6,6,6	0.50	0
4	SO4	F	156	-	4,4,4	1.08	1 (25%)	6,6,6	0.28	0
4	SO4	H	156	-	4,4,4	1.21	1 (25%)	6,6,6	0.37	0
4	SO4	I	156	-	4,4,4	0.29	0	6,6,6	0.26	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
4	SO4	A	156	-	-	0/0/0/0	0/0/0/0
4	SO4	B	156	2	-	0/0/0/0	0/0/0/0
4	SO4	C	157	-	-	0/0/0/0	0/0/0/0
4	SO4	D	156	2	-	0/0/0/0	0/0/0/0
4	SO4	E	156	-	-	0/0/0/0	0/0/0/0
4	SO4	F	156	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SO4	H	156	-	-	0/0/0/0	0/0/0/0
4	SO4	I	156	-	-	0/0/0/0	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	156	SO4	O1-S	-2.24	1.39	1.47
4	F	156	SO4	O1-S	-2.15	1.40	1.47

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	153/153 (100%)	0.05	3 (1%) 62 62	10, 14, 22, 30	9 (5%)
1	B	153/153 (100%)	0.85	20 (13%) 4 3	13, 19, 30, 37	4 (2%)
1	C	153/153 (100%)	-0.02	1 (0%) 84 87	9, 13, 20, 26	7 (4%)
1	D	153/153 (100%)	0.87	17 (11%) 6 5	13, 19, 31, 36	7 (4%)
1	E	153/153 (100%)	0.56	20 (13%) 4 3	11, 19, 29, 34	6 (3%)
1	F	153/153 (100%)	0.10	5 (3%) 44 42	9, 12, 21, 28	4 (2%)
1	G	153/153 (100%)	0.11	6 (3%) 37 36	7, 13, 22, 26	7 (4%)
1	H	153/153 (100%)	0.09	7 (4%) 31 30	8, 12, 21, 25	6 (3%)
1	I	153/153 (100%)	0.02	6 (3%) 37 36	9, 15, 26, 30	9 (5%)
1	J	153/153 (100%)	0.17	4 (2%) 53 52	9, 16, 24, 29	12 (7%)
All	All	1530/1530 (100%)	0.28	89 (5%) 22 21	7, 15, 26, 37	71 (4%)

All (89) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	1	ALA	6.6
1	I	1	ALA	5.6
1	E	1	ALA	5.1
1	J	25	SER	5.1
1	B	129	GLY	4.9
1	D	26	ASN	4.9
1	D	132[A]	GLU	4.8
1	E	130	GLY	4.8
1	J	1	ALA	4.6
1	B	1	ALA	4.6
1	E	132	GLU	4.5
1	F	26	ASN	4.4
1	E	26	ASN	4.3

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Mol	Chain	Res	Type	RSRZ
1	D	109	ASP	4.1
1	B	135	THR	4.1
1	D	67	LEU	4.1
1	E	109	ASP	3.9
1	D	28	PRO	3.9
1	B	131[A]	ASN	3.8
1	E	11	ASP	3.8
1	D	68	SER	3.7
1	D	131[A]	ASN	3.6
1	A	130	GLY	3.6
1	G	26	ASN	3.6
1	E	25	SER	3.5
1	B	130	GLY	3.4
1	B	77	GLU	3.4
1	E	55	ALA	3.3
1	E	67	LEU	3.3
1	E	23	LYS	3.3
1	D	78	GLU	3.3
1	D	23	LYS	3.3
1	D	102	SER	3.2
1	B	70	LYS	3.2
1	A	131	ASN	3.2
1	H	1	ALA	3.1
1	A	1	ALA	3.1
1	D	130	GLY	3.1
1	B	91	LYS	3.1
1	E	27	GLY	3.1
1	G	1	ALA	3.1
1	F	1	ALA	3.1
1	D	25	SER	3.0
1	I	111[A]	CYS	3.0
1	D	135	THR	2.9
1	G	45	PHE	2.9
1	B	69	ARG	2.9
1	D	69	ARG	2.9
1	B	109[A]	ASP	2.9
1	J	92	ASP	2.9
1	H	26[A]	ASN	2.8
1	E	135	THR	2.8
1	J	91	LYS	2.8
1	E	68	SER	2.8
1	F	45	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	68	SER	2.7
1	E	131	ASN	2.7
1	E	77	GLU	2.7
1	E	110	HIS	2.7
1	B	128	LYS	2.7
1	E	129	GLY	2.7
1	E	66	PRO	2.6
1	F	117	LEU	2.6
1	B	67	LEU	2.5
1	D	133[A]	GLU	2.5
1	B	92	ASP	2.5
1	F	84	LEU	2.4
1	C	109	ASP	2.4
1	D	2	THR	2.3
1	I	2	THR	2.3
1	I	108	GLY	2.3
1	H	117	LEU	2.3
1	B	127	GLY	2.3
1	G	25	SER	2.3
1	I	110[A]	HIS	2.2
1	B	111[A]	CYS	2.2
1	B	117	LEU	2.2
1	E	153	GLN	2.2
1	G	117	LEU	2.2
1	B	133	GLU	2.2
1	H	77	GLU	2.1
1	H	68	SER	2.1
1	E	136	LYS	2.1
1	I	132	GLU	2.1
1	G	84	LEU	2.1
1	H	45	PHE	2.1
1	H	47	VAL	2.1
1	B	134	SER	2.1
1	B	132	GLU	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 carbohydrates in this entry.

## 6.4 Ligands ⓘ

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<sup>th</sup> 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	D	156	5/5	0.23	6.23	15,26,30,31	5
4	SO4	I	156	5/5	0.24	5.56	38,41,43,44	0
4	SO4	E	156	5/5	0.21	5.48	32,33,34,34	5
4	SO4	H	156	5/5	0.28	4.75	15,21,25,26	5
4	SO4	C	157	5/5	0.19	4.28	24,27,30,31	5
2	CU	G	154	1/1	0.23	3.99	14,14,14,14	1
4	SO4	F	156	5/5	0.18	2.87	14,19,21,22	5
4	SO4	B	156	5/5	0.24	2.78	26,26,28,28	5
2	CU	D	154	1/1	0.12	1.23	21,21,21,21	0
3	ZN	G	155	1/1	0.09	-0.23	12,12,12,12	0
4	SO4	A	156	5/5	0.08	-0.31	21,23,29,30	5
3	ZN	H	155	1/1	0.08	-0.43	12,12,12,12	0
3	ZN	F	155	1/1	0.08	-0.80	12,12,12,12	0
3	ZN	E	155	1/1	0.09	-0.80	17,17,17,17	0
2	CU	E	154	1/1	0.08	-0.82	30,30,30,30	0
3	ZN	C	155	1/1	0.06	-1.02	12,12,12,12	0
2	CU	B	154	1/1	0.08	-1.19	24,24,24,24	0
3	ZN	J	155	1/1	0.03	-1.36	13,13,13,13	0
3	ZN	D	155	1/1	0.09	-1.64	21,21,21,21	0
3	ZN	B	155	1/1	0.09	-1.92	18,18,18,18	0
2	CU	F	154	1/1	0.09	-2.06	23,23,23,23	0
3	ZN	A	155	1/1	0.05	-2.06	14,14,14,14	0
2	CU	I	154	1/1	0.03	-2.08	24,24,24,24	0
2	CU	C	154	1/1	0.06	-2.14	25,25,25,25	0
2	CU	J	154	1/1	0.02	-2.15	22,22,22,22	0
2	CU	A	154[B]	1/1	0.05	-2.19	11,11,11,11	1
2	CU	H	154	1/1	0.06	-2.55	22,22,22,22	0
2	CU	A	154[A]	1/1	0.05	-2.80	17,17,17,17	1
3	ZN	I	155	1/1	0.02	-2.90	13,13,13,13	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.