



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:43 PM UTC

PDB ID : 1FUN / pdb\_00001fun  
Title : SUPEROXIDE DISMUTASE MUTANT WITH LYS 136 REPLACED BY GLU, CYS 6 REPLACED BY ALA AND CYS 111 REPLACED BY SER (K136E, C6A, C111S)  
Authors : Lo, T.P.; Tainer, J.A.; Getzoff, E.D.  
Deposited on : 1998-07-23  
Resolution : 2.85 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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

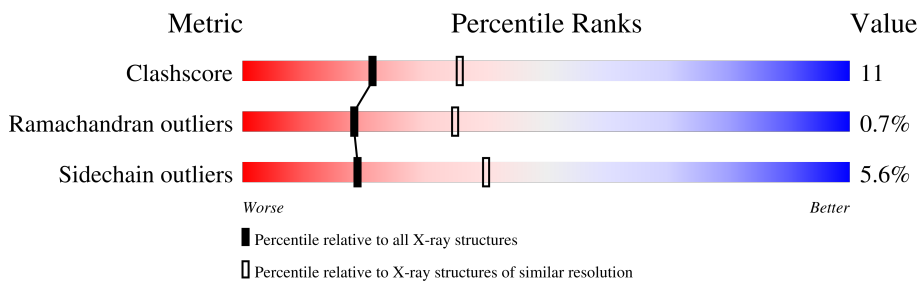
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)



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  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

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	

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Mol	Chain	Length	Quality of chain
1	I	153	 76% 21% .
1	J	153	 61% 37% .

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11354 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
			Total	C	N	O	S			
1	A	153	1109	678	202	227	2	0	0	0
1	F	153	1109	678	202	227	2	0	0	0
1	B	153	1109	678	202	227	2	0	0	0
1	G	153	1109	678	202	227	2	0	0	0
1	C	153	1109	678	202	227	2	0	0	0
1	H	153	1109	678	202	227	2	0	0	0
1	D	153	1109	678	202	227	2	0	0	0
1	I	153	1109	678	202	227	2	0	0	0
1	E	153	1109	678	202	227	2	0	0	0
1	J	153	1109	678	202	227	2	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	ALA	CYS	engineered mutation	UNP P00441
A	111	SER	CYS	engineered mutation	UNP P00441
A	136	GLU	LYS	engineered mutation	UNP P00441
F	6	ALA	CYS	engineered mutation	UNP P00441
F	111	SER	CYS	engineered mutation	UNP P00441
F	136	GLU	LYS	engineered mutation	UNP P00441
B	6	ALA	CYS	engineered mutation	UNP P00441
B	111	SER	CYS	engineered mutation	UNP P00441
B	136	GLU	LYS	engineered mutation	UNP P00441

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Chain	Residue	Modelled	Actual	Comment	Reference
G	6	ALA	CYS	engineered mutation	UNP P00441
G	111	SER	CYS	engineered mutation	UNP P00441
G	136	GLU	LYS	engineered mutation	UNP P00441
C	6	ALA	CYS	engineered mutation	UNP P00441
C	111	SER	CYS	engineered mutation	UNP P00441
C	136	GLU	LYS	engineered mutation	UNP P00441
H	6	ALA	CYS	engineered mutation	UNP P00441
H	111	SER	CYS	engineered mutation	UNP P00441
H	136	GLU	LYS	engineered mutation	UNP P00441
D	6	ALA	CYS	engineered mutation	UNP P00441
D	111	SER	CYS	engineered mutation	UNP P00441
D	136	GLU	LYS	engineered mutation	UNP P00441
I	6	ALA	CYS	engineered mutation	UNP P00441
I	111	SER	CYS	engineered mutation	UNP P00441
I	136	GLU	LYS	engineered mutation	UNP P00441
E	6	ALA	CYS	engineered mutation	UNP P00441
E	111	SER	CYS	engineered mutation	UNP P00441
E	136	GLU	LYS	engineered mutation	UNP P00441
J	6	ALA	CYS	engineered mutation	UNP P00441
J	111	SER	CYS	engineered mutation	UNP P00441
J	136	GLU	LYS	engineered mutation	UNP P00441

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

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

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



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

- Molecule 5 is water.

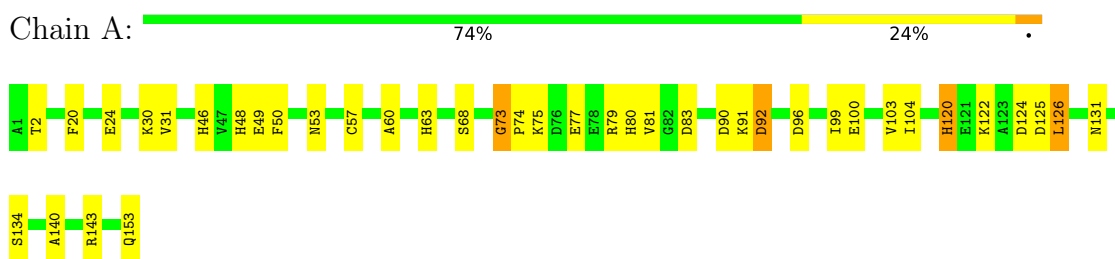
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	17	Total	O	0	0
			17	17		
5	F	37	Total	O	0	0
			37	37		
5	B	32	Total	O	0	0
			32	32		
5	G	33	Total	O	0	0
			33	33		
5	C	21	Total	O	0	0
			21	21		
5	H	43	Total	O	0	0
			43	43		
5	D	8	Total	O	0	0
			8	8		
5	I	25	Total	O	0	0
			25	25		
5	E	8	Total	O	0	0
			8	8		
5	J	15	Total	O	0	0
			15	15		

### 3 Residue-property plots [i](#)

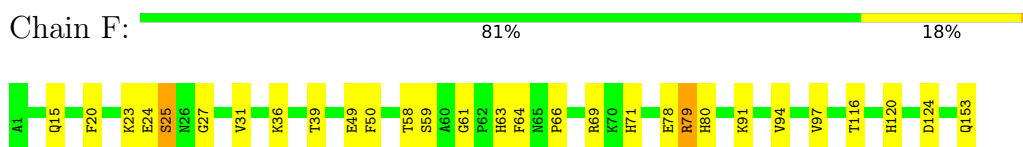
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

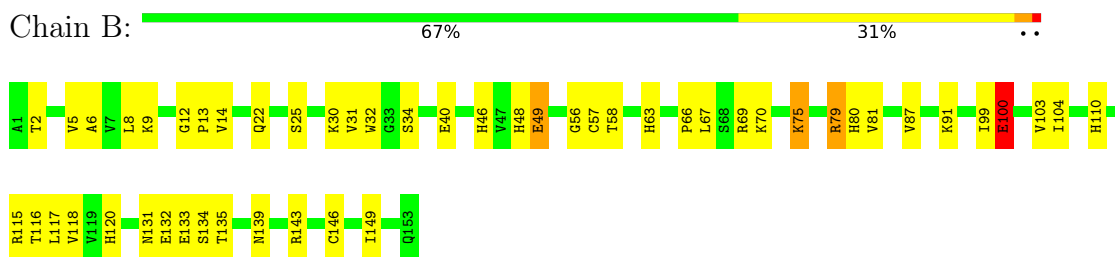
- Molecule 1: SUPEROXIDE DISMUTASE



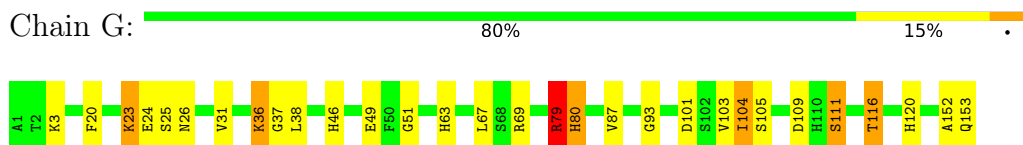
- Molecule 1: SUPEROXIDE DISMUTASE



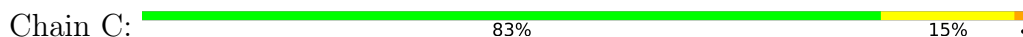
- Molecule 1: SUPEROXIDE DISMUTASE



- Molecule 1: SUPEROXIDE DISMUTASE



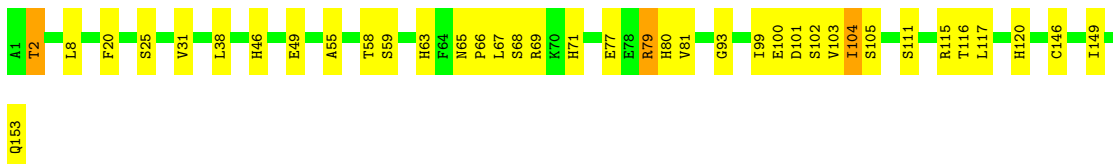
- Molecule 1: SUPEROXIDE DISMUTASE





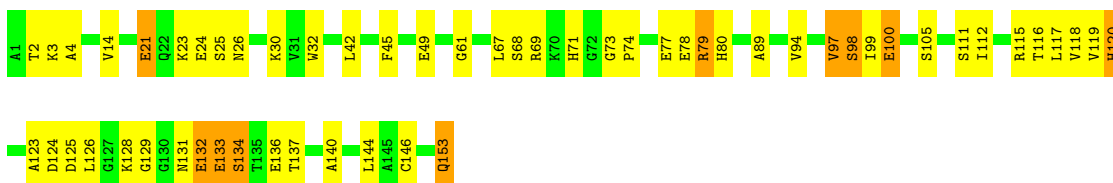
- Molecule 1: SUPEROXIDE DISMUTASE

Chain H: 75% 23%



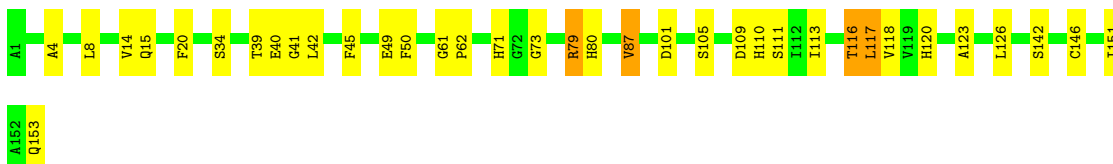
- Molecule 1: SUPEROXIDE DISMUTASE

Chain D: 63% 30% 7%



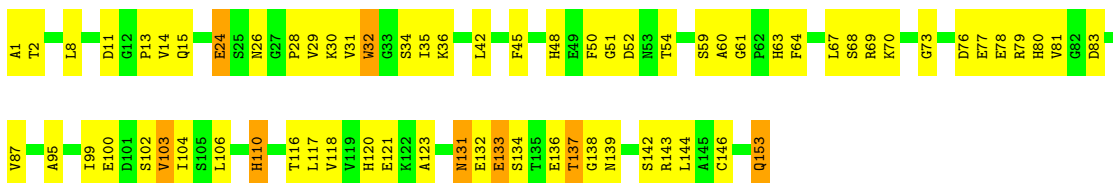
- Molecule 1: SUPEROXIDE DISMUTASE

Chain I: 76% 21%



- Molecule 1: SUPEROXIDE DISMUTASE

Chain E: 55% 40% 5%



- Molecule 1: SUPEROXIDE DISMUTASE

Chain J: 61% 37%





## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	205.20Å 167.00Å 145.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.85	Depositor
% Data completeness (in resolution range)	100.0 (8.00-2.85)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.189 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	11354	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

## 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, CU, 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	0.66	0/1127	1.12	7/1520 (0.5%)
1	B	0.74	0/1127	1.14	10/1520 (0.7%)
1	C	0.73	0/1127	1.10	3/1520 (0.2%)
1	D	0.65	0/1127	1.10	8/1520 (0.5%)
1	E	0.64	0/1127	1.10	9/1520 (0.6%)
1	F	0.79	0/1127	1.13	8/1520 (0.5%)
1	G	0.81	1/1127 (0.1%)	1.15	7/1520 (0.5%)
1	H	0.78	0/1127	1.16	6/1520 (0.4%)
1	I	0.69	0/1127	1.12	10/1520 (0.7%)
1	J	0.62	0/1127	1.17	7/1520 (0.5%)
All	All	0.71	1/11270 (0.0%)	1.13	75/15200 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	103	VAL	CA-CB	-5.31	1.47	1.54

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	49	GLU	N-CA-C	12.51	124.65	111.14
1	J	49	GLU	N-CA-C	12.27	124.19	111.07
1	H	49	GLU	N-CA-C	10.35	122.56	111.28
1	F	49	GLU	N-CA-C	9.53	121.36	110.97
1	E	103	VAL	N-CA-C	-9.08	104.00	111.81
1	I	49	GLU	N-CA-C	8.82	120.51	111.07
1	D	49	GLU	N-CA-C	8.73	120.72	111.03
1	B	49	GLU	N-CA-C	8.49	120.16	111.07
1	E	77	GLU	N-CA-C	-8.32	102.72	113.12
1	C	85	GLY	N-CA-C	8.26	121.26	111.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	77	GLU	N-CA-C	-7.72	102.81	111.07
1	A	49	GLU	N-CA-C	7.15	119.74	111.02
1	I	142	SER	N-CA-C	6.70	119.18	110.53
1	A	77	GLU	N-CA-C	-6.69	102.61	111.24
1	H	120	HIS	N-CA-C	6.66	120.25	110.59
1	H	2	THR	N-CA-C	-6.65	105.69	113.88
1	A	2	THR	N-CA-C	-6.42	105.99	113.88
1	D	120	HIS	N-CA-C	6.41	118.80	110.53
1	A	92	ASP	N-CA-C	-6.38	105.63	113.41
1	G	116	THR	N-CA-C	6.38	118.91	108.52
1	J	25	SER	N-CA-C	-6.31	104.40	111.28
1	B	100	GLU	N-CA-C	-6.26	97.61	108.69
1	I	41	GLY	N-CA-C	6.20	119.28	111.85
1	F	120	HIS	N-CA-C	6.16	119.97	110.42
1	F	116	THR	N-CA-C	6.09	118.66	108.73
1	I	117	LEU	N-CA-C	-6.03	99.87	109.76
1	C	77	GLU	N-CA-C	-6.02	106.48	113.88
1	H	77	GLU	N-CA-C	-5.91	104.92	111.36
1	G	120	HIS	N-CA-C	5.86	119.14	110.46
1	D	2	THR	N-CA-C	-5.86	106.16	113.55
1	G	104	ILE	CB-CA-C	-5.76	105.26	111.59
1	F	61	GLY	CA-C-N	5.73	127.00	119.84
1	F	61	GLY	C-N-CA	5.73	127.00	119.84
1	F	97	VAL	N-CA-C	5.72	116.97	109.58
1	D	61	GLY	CA-C-N	5.71	126.98	119.84
1	D	61	GLY	C-N-CA	5.71	126.98	119.84
1	J	120	HIS	N-CA-C	5.70	118.89	110.46
1	B	13	PRO	N-CA-C	5.68	121.01	113.57
1	E	120	HIS	N-CA-C	5.67	119.20	110.42
1	A	120	HIS	N-CA-C	5.59	118.74	110.46
1	G	80	HIS	N-CA-C	-5.59	103.15	110.53
1	B	32	TRP	N-CA-C	5.58	118.28	108.75
1	I	14	VAL	N-CA-C	5.57	116.78	109.21
1	A	50	PHE	N-CA-C	5.53	119.11	110.32
1	B	110	HIS	N-CA-C	-5.45	104.19	111.87
1	B	120	HIS	N-CA-C	5.45	118.80	110.36
1	D	97	VAL	N-CA-C	5.43	116.13	108.36
1	B	12	GLY	CA-C-N	5.43	124.94	119.19
1	B	12	GLY	C-N-CA	5.43	124.94	119.19
1	D	4	ALA	N-CA-C	-5.42	101.06	109.24
1	F	124	ASP	N-CA-C	-5.40	100.50	109.46
1	J	104	ILE	N-CA-C	-5.34	102.70	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	14	VAL	N-CA-C	5.33	115.87	108.84
1	E	32	TRP	N-CA-C	5.32	117.07	109.14
1	I	120	HIS	N-CA-C	5.31	118.29	110.59
1	H	104	ILE	CB-CA-C	-5.31	105.75	111.59
1	G	79	ARG	CG-CD-NE	5.29	123.65	112.00
1	B	117	LEU	N-CA-C	-5.25	101.14	109.96
1	I	87	VAL	N-CA-C	-5.24	100.93	108.48
1	G	87	VAL	N-CA-C	-5.24	101.53	108.96
1	J	124	ASP	N-CA-C	-5.19	102.17	109.96
1	E	2	THR	N-CA-C	-5.19	105.80	111.82
1	F	23	LYS	N-CA-C	5.17	117.66	111.71
1	D	124	ASP	N-CA-C	-5.14	102.25	109.96
1	I	61	GLY	CA-C-N	5.13	126.47	120.98
1	I	61	GLY	C-N-CA	5.13	126.47	120.98
1	H	117	LEU	N-CA-C	-5.11	100.97	109.46
1	G	49	GLU	N-CA-C	5.09	121.65	110.80
1	E	24	GLU	N-CA-C	-5.09	101.45	109.50
1	E	87	VAL	N-CA-C	-5.08	100.58	108.81
1	J	106	LEU	N-CA-C	-5.06	106.70	112.92
1	I	116	THR	N-CA-C	5.05	117.47	109.24
1	E	61	GLY	CA-C-N	5.03	125.50	120.52
1	E	61	GLY	C-N-CA	5.03	125.50	120.52
1	A	73	GLY	N-CA-C	-5.02	105.92	112.10

There are no chirality outliers.

There are no planarity outliers.

## 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	1109	0	1070	21	0
1	B	1109	0	1070	29	0
1	C	1109	0	1070	13	0
1	D	1109	0	1070	38	0
1	E	1109	0	1070	45	0
1	F	1109	0	1070	15	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	1109	0	1070	15	0
1	H	1109	0	1070	18	0
1	I	1109	0	1070	20	0
1	J	1109	0	1070	33	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
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
5	A	17	0	0	0	0
5	B	32	0	0	0	0
5	C	21	0	0	0	0
5	D	8	0	0	0	0
5	E	8	0	0	1	0
5	F	37	0	0	1	0
5	G	33	0	0	0	0
5	H	43	0	0	0	0
5	I	25	0	0	0	0
5	J	15	0	0	0	0
All	All	11354	0	10700	238	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 11.

All (238) 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:E:70:LYS:HE2	1:E:78:GLU:HG2	1.52	0.91
1:E:81:VAL:HG13	1:E:103:VAL:HG12	1.51	0.90
1:D:69:ARG:HB3	1:D:78:GLU:HG3	1.57	0.85
1:C:8:LEU:O	1:C:9:LYS:HD2	1.80	0.82
1:E:131:ASN:O	1:E:134:SER:HB3	1.84	0.78
1:G:79:ARG:HG3	1:G:79:ARG:HH11	1.52	0.75
1:D:136:GLU:HG3	1:D:137:THR:HG23	1.70	0.74
1:B:75:LYS:HB2	1:I:153:GLN:NE2	2.04	0.73
1:F:91:LYS:H	1:F:91:LYS:HD2	1.53	0.72
1:A:131:ASN:HB3	1:A:134:SER:HB2	1.71	0.72
1:D:79:ARG:HG3	1:D:79:ARG:HH11	1.53	0.71
1:D:74:PRO:HA	1:D:79:ARG:HE	1.58	0.67
1:D:126:LEU:O	1:D:128:LYS:HD3	1.94	0.67
1:I:73:GLY:HA2	1:I:126:LEU:HD22	1.77	0.67
1:C:2:THR:HB	1:C:22:GLN:O	1.96	0.65
1:D:153:GLN:HG2	1:I:50:PHE:CZ	2.31	0.65
1:A:120:HIS:HB3	1:A:140:ALA:O	1.95	0.65
1:D:71:HIS:HB2	1:D:80:HIS:CE1	2.33	0.64
1:E:70:LYS:HG2	1:E:78:GLU:HG3	1.78	0.63
1:J:87:VAL:HG11	1:J:97:VAL:HG22	1.80	0.63
1:B:118:VAL:HG11	1:B:143:ARG:HG2	1.81	0.62
1:B:70:LYS:HD2	1:B:135:THR:HB	1.80	0.62
1:D:73:GLY:HA2	1:D:126:LEU:HD22	1.81	0.62
1:J:14:VAL:HA	1:J:36:LYS:O	1.99	0.62
1:B:99:ILE:HG22	1:B:100:GLU:N	2.14	0.61
1:A:153:GLN:HB2	1:F:50:PHE:CZ	2.35	0.61
1:C:7:VAL:HG12	1:C:9:LYS:HD3	1.80	0.61
1:J:3:LYS:HG3	1:J:4:ALA:H	1.65	0.61
1:D:131:ASN:OD1	1:D:134:SER:HB2	2.01	0.60
1:D:30:LYS:HG2	1:D:100:GLU:HG3	1.84	0.60
1:E:13:PRO:O	1:E:15:GLN:HG2	2.01	0.60
1:E:35:ILE:HD11	1:E:45:PHE:HE1	1.66	0.60
1:D:79:ARG:HG3	1:D:79:ARG:NH1	2.15	0.60
1:J:24:GLU:HB2	1:J:27:GLY:HA3	1.82	0.60
1:B:31:VAL:HB	1:B:99:ILE:HB	1.84	0.59
1:F:71:HIS:HB2	1:F:80:HIS:CE1	2.37	0.59
1:J:115:ARG:O	1:J:148:VAL:HA	2.03	0.59
1:B:118:VAL:HG22	1:B:146:CYS:HB3	1.84	0.59
1:J:79:ARG:NH2	1:J:103:VAL:HB	2.18	0.59
1:I:71:HIS:HB2	1:I:80:HIS:CE1	2.38	0.58
1:E:70:LYS:HG2	1:E:78:GLU:CG	2.32	0.58
1:E:70:LYS:CE	1:E:78:GLU:HG2	2.29	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:THR:HG23	5:F:280:HOH:O	2.03	0.58
1:E:70:LYS:HE2	1:E:78:GLU:CG	2.29	0.58
1:J:92:ASP:O	1:J:94:VAL:HG23	2.03	0.57
1:E:52:ASP:O	1:E:59:SER:HB2	2.03	0.57
1:A:131:ASN:O	1:A:134:SER:HB3	2.05	0.57
1:A:73:GLY:HA2	1:A:126:LEU:HD22	1.87	0.57
1:J:74:PRO:HG2	1:J:75:LYS:HD2	1.88	0.56
1:H:116:THR:CG2	1:H:146:CYS:HB2	2.36	0.56
1:E:8:LEU:HD21	1:E:117:LEU:HD23	1.86	0.56
1:D:89:ALA:HA	1:D:94:VAL:O	2.06	0.55
1:A:57:CYS:O	1:A:143:ARG:NH1	2.38	0.55
1:A:99:ILE:HG22	1:A:100:GLU:N	2.19	0.55
1:F:63:HIS:HE1	1:F:71:HIS:CE1	2.23	0.55
1:C:49:GLU:O	1:C:115:ARG:HD3	2.07	0.54
1:E:134:SER:HA	1:E:139:ASN:OD1	2.07	0.54
1:I:45:PHE:HB2	1:I:87:VAL:HG13	1.90	0.54
1:B:2:THR:HG23	1:B:22:GLN:O	2.07	0.54
1:A:81:VAL:HG13	1:A:103:VAL:HG12	1.88	0.54
1:I:109:ASP:OD2	1:I:110:HIS:HD2	1.91	0.54
1:J:3:LYS:HG3	1:J:4:ALA:N	2.23	0.54
1:J:13:PRO:O	1:J:15:GLN:HG2	2.08	0.54
1:D:3:LYS:HG2	1:D:21:GLU:HG3	1.90	0.53
1:H:115:ARG:O	1:H:149:ILE:HG13	2.09	0.53
1:J:1:ALA:N	1:J:106:LEU:O	2.40	0.53
1:F:79:ARG:HD3	1:F:80:HIS:O	2.09	0.53
1:D:112:ILE:HA	1:D:115:ARG:HD2	1.91	0.53
1:J:116:THR:CG2	1:J:146:CYS:HB2	2.39	0.53
1:I:8:LEU:O	1:I:15:GLN:HA	2.09	0.53
1:J:31:VAL:HB	1:J:99:ILE:HB	1.91	0.52
1:D:69:ARG:HE	1:D:78:GLU:CD	2.17	0.52
1:D:136:GLU:HG3	1:D:137:THR:N	2.24	0.52
1:G:36:LYS:HG2	1:G:37:GLY:N	2.23	0.52
1:D:120:HIS:HB3	1:D:140:ALA:O	2.10	0.52
1:E:63:HIS:CE1	1:E:137:THR:HA	2.44	0.52
1:H:65:ASN:ND2	1:H:68:SER:HA	2.25	0.52
1:E:64:PHE:HZ	1:E:110:HIS:HA	1.75	0.52
1:D:136:GLU:HG3	1:D:137:THR:H	1.75	0.52
1:E:48:HIS:NE2	1:E:63:HIS:HD2	2.08	0.52
1:H:20:PHE:CD1	1:H:31:VAL:HG22	2.45	0.51
1:B:75:LYS:NZ	1:I:153:GLN:H	2.08	0.51
1:J:24:GLU:HB2	1:J:27:GLY:CA	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:PRO:HG2	1:A:75:LYS:HG2	1.91	0.51
1:G:38:LEU:O	1:G:93:GLY:HA2	2.09	0.51
1:E:42:LEU:HB2	1:E:123:ALA:HB2	1.93	0.51
1:E:79:ARG:HH21	1:E:83:ASP:H	1.57	0.51
1:E:134:SER:O	1:E:138:GLY:HA2	2.11	0.51
1:I:45:PHE:CZ	1:I:117:LEU:HD21	2.45	0.50
1:E:14:VAL:HG21	1:E:144:LEU:HB3	1.92	0.50
1:B:48:HIS:CE1	1:B:63:HIS:HD2	2.29	0.50
1:G:20:PHE:CD1	1:G:31:VAL:HG22	2.46	0.50
1:J:8:LEU:HA	1:J:146:CYS:O	2.11	0.50
1:B:8:LEU:O	1:B:9:LYS:HG3	2.11	0.50
1:D:116:THR:CG2	1:D:146:CYS:HB2	2.42	0.50
1:I:116:THR:CG2	1:I:146:CYS:HB2	2.41	0.50
1:J:60:ALA:HB3	1:J:143:ARG:HH11	1.76	0.50
1:A:60:ALA:HB3	1:A:143:ARG:NH1	2.27	0.50
1:D:79:ARG:HH11	1:D:79:ARG:CG	2.24	0.50
1:B:99:ILE:CG2	1:B:100:GLU:N	2.74	0.50
1:B:67:LEU:O	1:B:69:ARG:HG2	2.12	0.49
1:B:75:LYS:HZ3	1:I:153:GLN:H	1.58	0.49
1:B:49:GLU:O	1:B:115:ARG:HG2	2.11	0.49
1:E:153:GLN:HB2	1:J:50:PHE:CE1	2.47	0.49
1:A:153:GLN:HB2	1:F:50:PHE:CE1	2.47	0.49
1:J:87:VAL:CG1	1:J:97:VAL:HG22	2.41	0.49
1:F:20:PHE:CD2	1:F:31:VAL:HG22	2.48	0.49
1:E:30:LYS:HG2	1:E:32:TRP:CE3	2.48	0.49
1:A:31:VAL:HB	1:A:99:ILE:HB	1.94	0.49
1:G:46:HIS:ND1	1:G:63:HIS:CE1	2.80	0.49
1:I:4:ALA:HB3	1:I:20:PHE:HB2	1.95	0.48
1:E:28:PRO:HB3	1:E:102:SER:OG	2.13	0.48
1:H:66:PRO:HD2	1:H:81:VAL:HG23	1.94	0.48
1:H:79:ARG:HH22	1:H:101:ASP:CG	2.21	0.48
1:F:24:GLU:O	1:F:27:GLY:N	2.41	0.48
1:E:83:ASP:HB3	5:E:209:HOH:O	2.12	0.48
1:J:112:ILE:HD12	1:J:149:ILE:HD13	1.96	0.48
1:F:91:LYS:H	1:F:91:LYS:CD	2.22	0.48
1:G:105:SER:O	1:G:111:SER:HA	2.14	0.48
1:E:31:VAL:HB	1:E:99:ILE:HB	1.95	0.48
1:E:117:LEU:O	1:E:146:CYS:HA	2.14	0.48
1:J:60:ALA:HB3	1:J:143:ARG:NH1	2.29	0.48
1:B:48:HIS:CE1	1:B:63:HIS:CD2	3.03	0.47
1:E:121:GLU:HB2	1:E:142:SER:OG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:39:THR:O	1:J:89:ALA:HB3	2.14	0.47
1:A:124:ASP:C	1:A:126:LEU:H	2.22	0.47
1:E:24:GLU:HB2	1:E:26:ASN:OD1	2.14	0.47
1:B:46:HIS:ND1	1:B:63:HIS:NE2	2.62	0.47
1:G:79:ARG:HG3	1:G:80:HIS:O	2.14	0.47
1:E:99:ILE:HG22	1:E:100:GLU:N	2.28	0.47
1:H:79:ARG:HD3	1:H:80:HIS:O	2.14	0.47
1:F:36:LYS:HD2	1:F:94:VAL:HG22	1.97	0.47
1:H:46:HIS:ND1	1:H:63:HIS:NE2	2.63	0.47
1:B:79:ARG:HD3	1:B:80:HIS:O	2.14	0.47
1:D:42:LEU:HB2	1:D:123:ALA:HB2	1.97	0.47
1:E:29:VAL:HG21	1:E:104:ILE:HG13	1.97	0.47
1:E:133:GLU:HA	1:E:136:GLU:HB2	1.96	0.47
1:E:51:GLY:HA2	1:E:116:THR:OG1	2.15	0.47
1:J:4:ALA:HB3	1:J:20:PHE:HB2	1.98	0.47
1:H:81:VAL:HG13	1:H:103:VAL:HG12	1.97	0.46
1:E:67:LEU:HB2	1:E:69:ARG:HG2	1.96	0.46
1:A:20:PHE:HA	1:A:30:LYS:O	2.14	0.46
1:C:50:PHE:CZ	1:H:153:GLN:HB2	2.51	0.46
1:D:98:SER:O	1:D:99:ILE:HG13	2.16	0.46
1:D:45:PHE:CZ	1:D:117:LEU:HD21	2.50	0.46
1:G:67:LEU:HB2	1:G:69:ARG:HG2	1.98	0.46
1:E:80:HIS:HB2	1:E:83:ASP:CG	2.40	0.46
1:E:116:THR:HG22	1:E:146:CYS:HB2	1.98	0.46
1:J:22:GLN:HB2	1:J:29:VAL:HG13	1.97	0.46
1:C:23:LYS:HE2	1:C:28:PRO:HD2	1.98	0.46
1:B:133:GLU:HA	1:B:133:GLU:OE1	2.16	0.46
1:H:116:THR:HG23	1:H:146:CYS:HB2	1.98	0.46
1:D:125:ASP:CG	1:D:129:GLY:HA3	2.40	0.46
1:B:115:ARG:O	1:B:149:ILE:HG13	2.16	0.46
1:B:133:GLU:HB3	1:B:139:ASN:ND2	2.30	0.46
1:E:1:ALA:N	1:E:106:LEU:O	2.49	0.46
1:F:79:ARG:CD	1:F:80:HIS:O	2.64	0.46
1:H:38:LEU:O	1:H:93:GLY:HA2	2.15	0.46
1:I:105:SER:O	1:I:111:SER:HA	2.16	0.45
1:E:35:ILE:HD11	1:E:45:PHE:CE1	2.50	0.45
1:D:32:TRP:HA	1:D:97:VAL:O	2.17	0.45
1:J:46:HIS:HB3	1:J:82:GLY:O	2.15	0.45
1:G:101:ASP:OD2	1:G:104:ILE:HG12	2.16	0.45
1:J:10:GLY:C	1:J:12:GLY:H	2.24	0.45
1:C:79:ARG:HD3	1:C:80:HIS:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:24:GLU:C	1:D:26:ASN:H	2.25	0.45
1:D:69:ARG:HB3	1:D:78:GLU:CG	2.39	0.45
1:D:80:HIS:HE1	1:D:136:GLU:O	1.98	0.45
1:D:105:SER:O	1:D:111:SER:HA	2.17	0.45
1:J:105:SER:O	1:J:111:SER:HA	2.17	0.45
1:B:70:LYS:HD3	1:B:70:LYS:HA	1.84	0.45
1:C:23:LYS:HZ2	1:C:23:LYS:N	2.14	0.45
1:C:46:HIS:ND1	1:C:63:HIS:CE1	2.84	0.45
1:A:131:ASN:HB3	1:A:134:SER:CB	2.45	0.45
1:B:81:VAL:HG13	1:B:103:VAL:HG12	1.99	0.45
1:I:118:VAL:HG22	1:I:146:CYS:HB3	1.99	0.45
1:E:54:THR:HG22	1:J:17:ILE:HD13	1.99	0.44
1:E:118:VAL:HG11	1:E:143:ARG:HG2	1.98	0.44
1:F:69:ARG:HD2	1:F:78:GLU:OE1	2.16	0.44
1:G:23:LYS:H	1:G:23:LYS:HD3	1.83	0.44
1:J:47:VAL:HG11	1:J:112:ILE:HG22	1.99	0.44
1:I:116:THR:HG22	1:I:118:VAL:HG23	2.00	0.44
1:A:48:HIS:CE1	1:A:63:HIS:HD2	2.36	0.44
1:G:23:LYS:H	1:G:23:LYS:CD	2.30	0.44
1:B:81:VAL:HG12	1:B:104:ILE:HG22	1.99	0.44
1:B:56:GLY:O	1:B:58:THR:N	2.50	0.43
1:D:119:VAL:O	1:D:119:VAL:HG13	2.18	0.43
1:C:42:LEU:HB2	1:C:123:ALA:HB2	2.01	0.43
1:D:73:GLY:CA	1:D:126:LEU:HD22	2.47	0.43
1:E:110:HIS:CD2	1:E:110:HIS:N	2.87	0.43
1:A:122:LYS:HB2	1:A:140:ALA:C	2.43	0.43
1:D:132:GLU:O	1:D:133:GLU:C	2.61	0.43
1:B:116:THR:HG22	1:B:118:VAL:HG23	2.00	0.43
1:G:46:HIS:ND1	1:G:63:HIS:NE2	2.66	0.43
1:I:79:ARG:HH22	1:I:101:ASP:CG	2.26	0.43
1:D:125:ASP:OD2	1:D:129:GLY:HA3	2.19	0.43
1:A:90:ASP:OD1	1:A:92:ASP:HB2	2.18	0.43
1:C:5:VAL:HG22	1:C:6:ALA:N	2.32	0.42
1:H:8:LEU:HD23	1:H:146:CYS:C	2.44	0.42
1:D:14:VAL:HG21	1:D:144:LEU:HB3	2.01	0.42
1:D:24:GLU:O	1:D:26:ASN:N	2.52	0.42
1:I:113:ILE:HD12	1:I:151:ILE:HG12	2.01	0.42
1:D:118:VAL:HG22	1:D:146:CYS:HB3	2.02	0.42
1:B:116:THR:CG2	1:B:146:CYS:HB2	2.49	0.42
1:E:50:PHE:O	1:E:60:ALA:HA	2.19	0.42
1:J:8:LEU:HD21	1:J:117:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:55:ALA:O	1:H:58:THR:HB	2.19	0.42
1:B:131:ASN:O	1:B:134:SER:HB3	2.20	0.42
1:J:118:VAL:HG11	1:J:143:ARG:HG2	2.01	0.42
1:G:3:LYS:HB3	1:G:3:LYS:HE2	1.83	0.42
1:E:116:THR:CG2	1:E:146:CYS:HB2	2.49	0.42
1:J:45:PHE:O	1:J:84:LEU:HB2	2.20	0.42
1:E:73:GLY:O	1:E:76:ASP:HB2	2.19	0.41
1:G:51:GLY:HA2	1:G:116:THR:OG1	2.21	0.41
1:C:46:HIS:CE1	1:C:63:HIS:CE1	3.08	0.41
1:D:128:LYS:HE2	1:D:128:LYS:HB2	1.85	0.41
1:I:45:PHE:HZ	1:I:117:LEU:HD21	1.85	0.41
1:C:20:PHE:CD2	1:C:31:VAL:HG22	2.55	0.41
1:D:67:LEU:O	1:D:69:ARG:N	2.53	0.41
1:A:80:HIS:HB2	1:A:83:ASP:CG	2.45	0.41
1:F:64:PHE:CE1	1:F:66:PRO:HD3	2.55	0.41
1:E:34:SER:HA	1:E:95:ALA:O	2.20	0.41
1:J:3:LYS:CG	1:J:4:ALA:N	2.83	0.41
1:B:5:VAL:HG22	1:B:6:ALA:N	2.36	0.41
1:A:99:ILE:CG2	1:A:100:GLU:N	2.84	0.41
1:I:39:THR:O	1:I:40:GLU:C	2.64	0.41
1:E:36:LYS:HE3	1:E:36:LYS:HB2	1.68	0.41
1:B:66:PRO:HD2	1:B:81:VAL:HG23	2.03	0.41
1:H:71:HIS:HB2	1:H:80:HIS:CE1	2.56	0.41
1:I:42:LEU:HB2	1:I:123:ALA:HB2	2.03	0.41
1:H:99:ILE:HG22	1:H:100:GLU:N	2.35	0.40
1:A:125:ASP:O	1:A:126:LEU:C	2.64	0.40
1:H:105:SER:O	1:H:111:SER:HA	2.21	0.40
1:G:3:LYS:HB3	1:G:152:ALA:HB3	2.04	0.40
1:H:104:ILE:O	1:H:104:ILE:HG13	2.20	0.40
1:E:64:PHE:CZ	1:E:110:HIS:HA	2.56	0.40
1:J:71:HIS:HB2	1:J:80:HIS:CE1	2.57	0.40
1:F:24:GLU:O	1:F:25:SER:C	2.64	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries

of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	151/153 (99%)	141 (93%)	9 (6%)	1 (1%)	18	35
1	B	151/153 (99%)	136 (90%)	13 (9%)	2 (1%)	9	21
1	C	151/153 (99%)	143 (95%)	8 (5%)	0	100	100
1	D	151/153 (99%)	136 (90%)	12 (8%)	3 (2%)	6	13
1	E	151/153 (99%)	141 (93%)	10 (7%)	0	100	100
1	F	151/153 (99%)	143 (95%)	7 (5%)	1 (1%)	18	35
1	G	151/153 (99%)	140 (93%)	8 (5%)	3 (2%)	6	13
1	H	151/153 (99%)	146 (97%)	5 (3%)	0	100	100
1	I	151/153 (99%)	144 (95%)	7 (5%)	0	100	100
1	J	151/153 (99%)	135 (89%)	15 (10%)	1 (1%)	18	35
All	All	1510/1530 (99%)	1405 (93%)	94 (6%)	11 (1%)	18	35

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	126	LEU
1	G	25	SER
1	D	25	SER
1	D	68	SER
1	F	25	SER
1	B	57	CYS
1	B	40	GLU
1	G	26	ASN
1	G	109	ASP
1	D	77	GLU
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%)	109 (93%)	8 (7%)	14	30
1	B	117/117 (100%)	108 (92%)	9 (8%)	12	25
1	C	117/117 (100%)	111 (95%)	6 (5%)	21	43
1	D	117/117 (100%)	108 (92%)	9 (8%)	12	25
1	E	117/117 (100%)	109 (93%)	8 (7%)	14	30
1	F	117/117 (100%)	112 (96%)	5 (4%)	26	50
1	G	117/117 (100%)	111 (95%)	6 (5%)	21	43
1	H	117/117 (100%)	110 (94%)	7 (6%)	17	36
1	I	117/117 (100%)	114 (97%)	3 (3%)	40	65
1	J	117/117 (100%)	113 (97%)	4 (3%)	32	58
All	All	1170/1170 (100%)	1105 (94%)	65 (6%)	19	40

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	GLU
1	A	46	HIS
1	A	53	ASN
1	A	68	SER
1	A	79	ARG
1	A	91	LYS
1	A	96	ASP
1	A	104	ILE
1	F	15	GLN
1	F	58	THR
1	F	59	SER
1	F	79	ARG
1	F	153	GLN
1	B	25	SER
1	B	30	LYS
1	B	34	SER
1	B	75	LYS
1	B	79	ARG
1	B	87	VAL
1	B	91	LYS
1	B	100	GLU
1	B	132	GLU
1	G	23	LYS
1	G	24	GLU

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	36	LYS
1	G	79	ARG
1	G	111	SER
1	G	153	GLN
1	C	3	LYS
1	C	23	LYS
1	C	59	SER
1	C	79	ARG
1	C	107	SER
1	C	132	GLU
1	H	2	THR
1	H	25	SER
1	H	59	SER
1	H	67	LEU
1	H	69	ARG
1	H	79	ARG
1	H	102	SER
1	D	21	GLU
1	D	23	LYS
1	D	79	ARG
1	D	98	SER
1	D	100	GLU
1	D	132	GLU
1	D	133	GLU
1	D	134	SER
1	D	153	GLN
1	I	34	SER
1	I	62	PRO
1	I	79	ARG
1	E	11	ASP
1	E	68	SER
1	E	110	HIS
1	E	131	ASN
1	E	132	GLU
1	E	133	GLU
1	E	137	THR
1	E	153	GLN
1	J	26	ASN
1	J	46	HIS
1	J	67	LEU
1	J	142	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	F	53	ASN
1	B	15	GLN
1	B	53	ASN
1	B	139	ASN
1	G	53	ASN
1	C	15	GLN
1	C	19	ASN
1	C	53	ASN
1	D	19	ASN
1	D	65	ASN
1	D	153	GLN
1	I	53	ASN
1	I	110	HIS
1	I	153	GLN
1	E	53	ASN
1	E	63	HIS
1	E	110	HIS
1	J	53	ASN
1	J	110	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 oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 20 are monoatomic - leaving 1 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	200	-	4,4,4	0.18	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.