



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 10, 2024 – 09:25 PM EST

PDB ID : 2P32  
Title : Crystal structure of the C-terminal 10 kDa subdomain from *C. elegans* Hsp70  
Authors : Worrall, L.J.; Walkinshaw, M.D.  
Deposited on : 2007-03-08  
Resolution : 3.20 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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
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) : 2.36

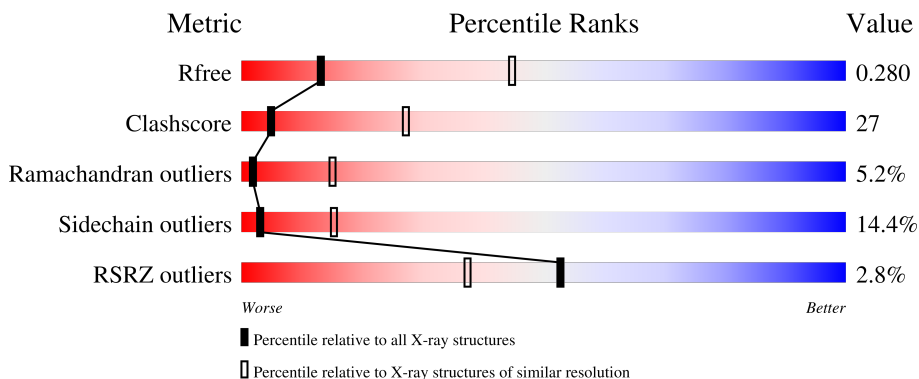
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.20 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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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  $\leq 5\%$ . 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	120	
1	B	120	
1	C	120	
1	D	120	
1	E	120	

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Mol	Chain	Length	Quality of chain
1	F	120	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	A	1	-	-	-	X
2	SO4	B	6	-	-	-	X
2	SO4	C	2	-	-	-	X
2	SO4	D	4	-	-	-	X
2	SO4	E	3	-	-	-	X
2	SO4	F	5	-	-	-	X

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4002 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 Heat shock 70 kDa protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	82	662	415	109	136	2	0	0	0
1	B	82	662	415	109	136	2	0	0	0
1	C	82	662	415	109	136	2	0	0	0
1	D	82	662	415	109	136	2	0	0	0
1	E	82	662	415	109	136	2	0	0	0
1	F	82	662	415	109	136	2	0	0	0

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	521	MET	-	cloning artifact	UNP P09446
A	522	GLY	-	cloning artifact	UNP P09446
A	523	SER	-	cloning artifact	UNP P09446
A	524	SER	-	cloning artifact	UNP P09446
A	525	HIS	-	expression tag	UNP P09446
A	526	HIS	-	expression tag	UNP P09446
A	527	HIS	-	expression tag	UNP P09446
A	528	HIS	-	expression tag	UNP P09446
A	529	HIS	-	expression tag	UNP P09446
A	530	HIS	-	expression tag	UNP P09446
A	531	SER	-	cloning artifact	UNP P09446
A	532	SER	-	cloning artifact	UNP P09446
A	533	GLY	-	cloning artifact	UNP P09446
A	534	LEU	-	cloning artifact	UNP P09446
A	535	VAL	-	cloning artifact	UNP P09446
A	536	PRO	-	cloning artifact	UNP P09446
A	537	ARG	-	cloning artifact	UNP P09446

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Chain	Residue	Modelled	Actual	Comment	Reference
A	538	GLY	-	cloning artifact	UNP P09446
A	539	SER	-	cloning artifact	UNP P09446
A	540	HIS	-	cloning artifact	UNP P09446
A	541	MET	-	cloning artifact	UNP P09446
B	521	MET	-	cloning artifact	UNP P09446
B	522	GLY	-	cloning artifact	UNP P09446
B	523	SER	-	cloning artifact	UNP P09446
B	524	SER	-	cloning artifact	UNP P09446
B	525	HIS	-	expression tag	UNP P09446
B	526	HIS	-	expression tag	UNP P09446
B	527	HIS	-	expression tag	UNP P09446
B	528	HIS	-	expression tag	UNP P09446
B	529	HIS	-	expression tag	UNP P09446
B	530	HIS	-	expression tag	UNP P09446
B	531	SER	-	cloning artifact	UNP P09446
B	532	SER	-	cloning artifact	UNP P09446
B	533	GLY	-	cloning artifact	UNP P09446
B	534	LEU	-	cloning artifact	UNP P09446
B	535	VAL	-	cloning artifact	UNP P09446
B	536	PRO	-	cloning artifact	UNP P09446
B	537	ARG	-	cloning artifact	UNP P09446
B	538	GLY	-	cloning artifact	UNP P09446
B	539	SER	-	cloning artifact	UNP P09446
B	540	HIS	-	cloning artifact	UNP P09446
B	541	MET	-	cloning artifact	UNP P09446
C	521	MET	-	cloning artifact	UNP P09446
C	522	GLY	-	cloning artifact	UNP P09446
C	523	SER	-	cloning artifact	UNP P09446
C	524	SER	-	cloning artifact	UNP P09446
C	525	HIS	-	expression tag	UNP P09446
C	526	HIS	-	expression tag	UNP P09446
C	527	HIS	-	expression tag	UNP P09446
C	528	HIS	-	expression tag	UNP P09446
C	529	HIS	-	expression tag	UNP P09446
C	530	HIS	-	expression tag	UNP P09446
C	531	SER	-	cloning artifact	UNP P09446
C	532	SER	-	cloning artifact	UNP P09446
C	533	GLY	-	cloning artifact	UNP P09446
C	534	LEU	-	cloning artifact	UNP P09446
C	535	VAL	-	cloning artifact	UNP P09446
C	536	PRO	-	cloning artifact	UNP P09446
C	537	ARG	-	cloning artifact	UNP P09446

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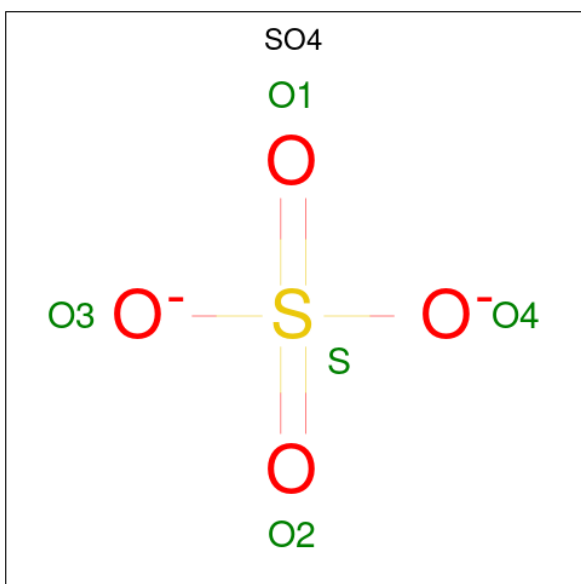
Chain	Residue	Modelled	Actual	Comment	Reference
C	538	GLY	-	cloning artifact	UNP P09446
C	539	SER	-	cloning artifact	UNP P09446
C	540	HIS	-	cloning artifact	UNP P09446
C	541	MET	-	cloning artifact	UNP P09446
D	521	MET	-	cloning artifact	UNP P09446
D	522	GLY	-	cloning artifact	UNP P09446
D	523	SER	-	cloning artifact	UNP P09446
D	524	SER	-	cloning artifact	UNP P09446
D	525	HIS	-	expression tag	UNP P09446
D	526	HIS	-	expression tag	UNP P09446
D	527	HIS	-	expression tag	UNP P09446
D	528	HIS	-	expression tag	UNP P09446
D	529	HIS	-	expression tag	UNP P09446
D	530	HIS	-	expression tag	UNP P09446
D	531	SER	-	cloning artifact	UNP P09446
D	532	SER	-	cloning artifact	UNP P09446
D	533	GLY	-	cloning artifact	UNP P09446
D	534	LEU	-	cloning artifact	UNP P09446
D	535	VAL	-	cloning artifact	UNP P09446
D	536	PRO	-	cloning artifact	UNP P09446
D	537	ARG	-	cloning artifact	UNP P09446
D	538	GLY	-	cloning artifact	UNP P09446
D	539	SER	-	cloning artifact	UNP P09446
D	540	HIS	-	cloning artifact	UNP P09446
D	541	MET	-	cloning artifact	UNP P09446
E	521	MET	-	cloning artifact	UNP P09446
E	522	GLY	-	cloning artifact	UNP P09446
E	523	SER	-	cloning artifact	UNP P09446
E	524	SER	-	cloning artifact	UNP P09446
E	525	HIS	-	expression tag	UNP P09446
E	526	HIS	-	expression tag	UNP P09446
E	527	HIS	-	expression tag	UNP P09446
E	528	HIS	-	expression tag	UNP P09446
E	529	HIS	-	expression tag	UNP P09446
E	530	HIS	-	expression tag	UNP P09446
E	531	SER	-	cloning artifact	UNP P09446
E	532	SER	-	cloning artifact	UNP P09446
E	533	GLY	-	cloning artifact	UNP P09446
E	534	LEU	-	cloning artifact	UNP P09446
E	535	VAL	-	cloning artifact	UNP P09446
E	536	PRO	-	cloning artifact	UNP P09446
E	537	ARG	-	cloning artifact	UNP P09446

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Chain	Residue	Modelled	Actual	Comment	Reference
E	538	GLY	-	cloning artifact	UNP P09446
E	539	SER	-	cloning artifact	UNP P09446
E	540	HIS	-	cloning artifact	UNP P09446
E	541	MET	-	cloning artifact	UNP P09446
F	521	MET	-	cloning artifact	UNP P09446
F	522	GLY	-	cloning artifact	UNP P09446
F	523	SER	-	cloning artifact	UNP P09446
F	524	SER	-	cloning artifact	UNP P09446
F	525	HIS	-	expression tag	UNP P09446
F	526	HIS	-	expression tag	UNP P09446
F	527	HIS	-	expression tag	UNP P09446
F	528	HIS	-	expression tag	UNP P09446
F	529	HIS	-	expression tag	UNP P09446
F	530	HIS	-	expression tag	UNP P09446
F	531	SER	-	cloning artifact	UNP P09446
F	532	SER	-	cloning artifact	UNP P09446
F	533	GLY	-	cloning artifact	UNP P09446
F	534	LEU	-	cloning artifact	UNP P09446
F	535	VAL	-	cloning artifact	UNP P09446
F	536	PRO	-	cloning artifact	UNP P09446
F	537	ARG	-	cloning artifact	UNP P09446
F	538	GLY	-	cloning artifact	UNP P09446
F	539	SER	-	cloning artifact	UNP P09446
F	540	HIS	-	cloning artifact	UNP P09446
F	541	MET	-	cloning artifact	UNP P09446

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



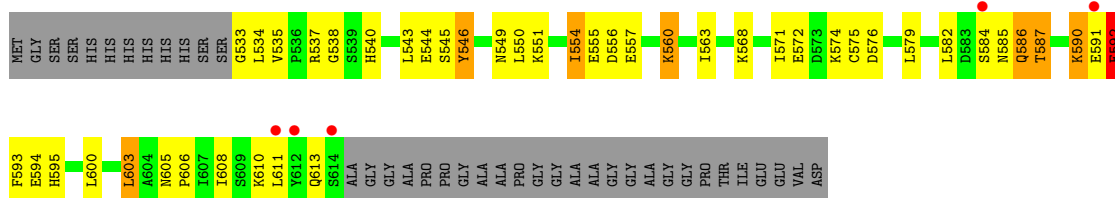
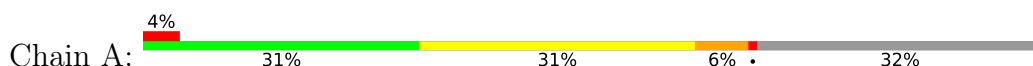
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		
2	D	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	F	1	Total	O	S	0	0
			5	4	1		



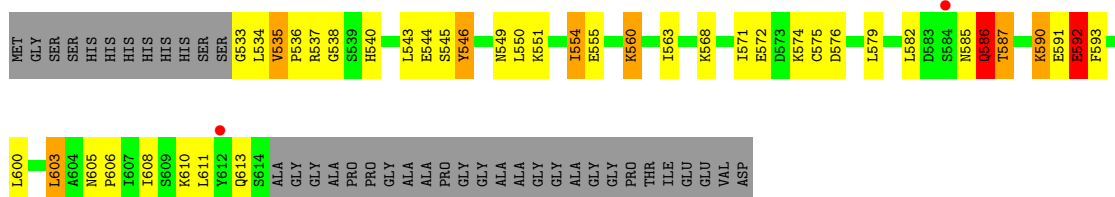
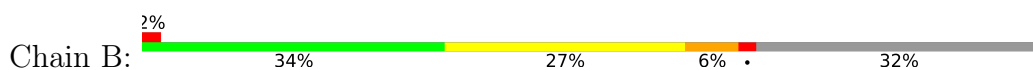
### 3 Residue-property plots [i](#)

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.

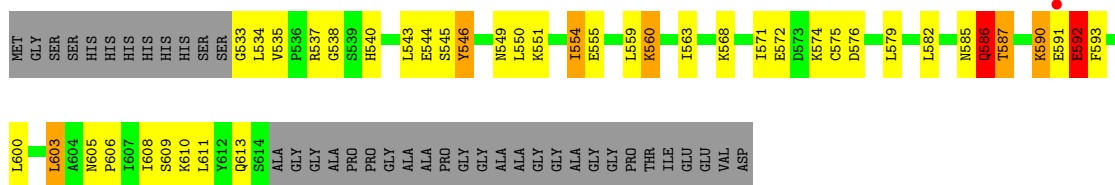
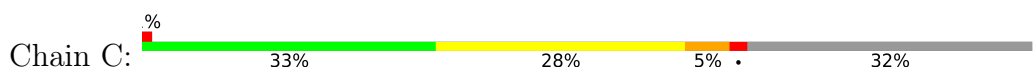
- Molecule 1: Heat shock 70 kDa protein A



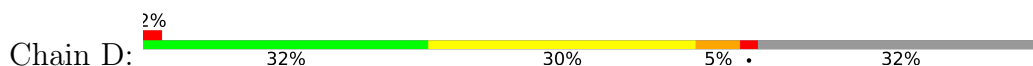
- Molecule 1: Heat shock 70 kDa protein A

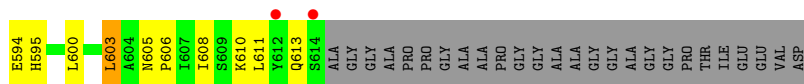


- Molecule 1: Heat shock 70 kDa protein A

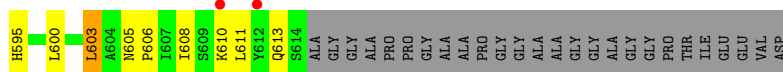


- Molecule 1: Heat shock 70 kDa protein A

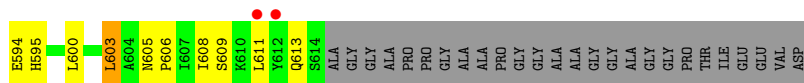
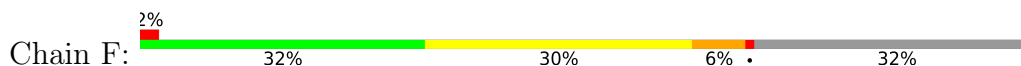




• Molecule 1: Heat shock 70 kDa protein A



• Molecule 1: Heat shock 70 kDa protein A



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.93Å 138.93Å 100.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.00 – 3.20 35.99 – 3.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (36.00-3.20) 96.7 (35.99-3.20)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.89 (at 3.18Å)	Xtrriage
Refinement program	REFMAC refmac_5.2.0019	Depositor
R, $R_{free}$	0.268 , 0.282 0.270 , 0.280	Depositor DCC
$R_{free}$ test set	820 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	86.3	Xtrriage
Anisotropy	0.239	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 126.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	4002	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	104.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.59 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1203e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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

<sup>2</sup>Theoretical 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: 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	0.85	0/672	0.84	0/900
1	B	0.83	0/672	0.83	0/900
1	C	0.89	0/672	0.84	0/900
1	D	0.88	0/672	0.85	0/900
1	E	0.86	0/672	0.91	1/900 (0.1%)
1	F	0.82	0/672	0.84	0/900
All	All	0.86	0/4032	0.85	1/5400 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	535	VAL	CG1-CB-CG2	9.93	126.79	110.90

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	662	0	649	37	0
1	B	662	0	649	40	0
1	C	662	0	649	41	0
1	D	662	0	649	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	662	0	649	38	0
1	F	662	0	649	39	0
2	A	5	0	0	0	0
2	B	5	0	0	1	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
2	E	5	0	0	0	0
2	F	5	0	0	0	0
All	All	4002	0	3894	217	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 27.

All (217) 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:C:585:ASN:O	1:C:587:THR:N	1.95	1.00
1:B:590:LYS:O	1:B:592:GLU:N	1.96	0.97
1:A:590:LYS:O	1:A:592:GLU:N	1.98	0.96
1:C:590:LYS:O	1:C:592:GLU:N	1.98	0.96
1:D:590:LYS:O	1:D:592:GLU:N	1.98	0.96
1:E:590:LYS:O	1:E:592:GLU:N	1.97	0.95
1:F:585:ASN:O	1:F:587:THR:N	2.00	0.95
1:F:590:LYS:O	1:F:592:GLU:N	1.99	0.93
1:D:585:ASN:O	1:D:587:THR:N	2.00	0.93
1:B:585:ASN:O	1:B:587:THR:N	2.02	0.92
1:A:585:ASN:O	1:A:587:THR:N	2.04	0.90
1:E:585:ASN:O	1:E:587:THR:N	2.05	0.89
1:C:537:ARG:NH1	1:D:579:LEU:HD22	2.06	0.70
1:B:579:LEU:HD22	1:E:537:ARG:NH1	2.07	0.70
1:E:608:ILE:HD12	1:E:608:ILE:C	2.12	0.69
1:A:579:LEU:HD22	1:F:537:ARG:NH1	2.08	0.68
1:A:534:LEU:HD22	1:A:587:THR:HG22	1.75	0.68
1:F:608:ILE:C	1:F:608:ILE:HD12	2.17	0.66
1:B:537:ARG:NH1	1:E:579:LEU:HD22	2.11	0.65
1:D:608:ILE:HD12	1:D:608:ILE:C	2.17	0.65
1:C:534:LEU:HD22	1:C:587:THR:HG22	1.80	0.63
1:D:534:LEU:HD22	1:D:587:THR:HG22	1.79	0.63
1:E:534:LEU:HD22	1:E:587:THR:HG22	1.80	0.63
1:B:534:LEU:HD22	1:B:587:THR:HG22	1.80	0.62
1:A:537:ARG:NH1	1:F:579:LEU:HD22	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:608:ILE:HD12	1:B:608:ILE:C	2.19	0.62
1:A:579:LEU:HD22	1:F:537:ARG:HH11	1.64	0.61
1:B:579:LEU:HD22	1:E:537:ARG:HH11	1.64	0.61
1:F:534:LEU:HD22	1:F:587:THR:HG22	1.81	0.61
1:D:574:LYS:HG3	1:D:603:LEU:HD12	1.83	0.61
1:F:574:LYS:HG3	1:F:603:LEU:HD12	1.82	0.60
1:A:574:LYS:HG3	1:A:603:LEU:HD12	1.83	0.60
1:A:608:ILE:C	1:A:608:ILE:HD12	2.21	0.60
1:E:537:ARG:O	1:E:538:GLY:C	2.40	0.60
1:B:574:LYS:HG3	1:B:603:LEU:HD12	1.83	0.60
1:E:575:CYS:O	1:E:579:LEU:HD12	2.02	0.59
1:E:574:LYS:HG3	1:E:603:LEU:HD12	1.85	0.59
1:C:537:ARG:HH11	1:D:579:LEU:HD22	1.67	0.58
1:B:537:ARG:O	1:B:538:GLY:C	2.40	0.58
1:C:608:ILE:C	1:C:608:ILE:HD12	2.23	0.58
1:A:571:ILE:HG22	1:A:572:GLU:N	2.18	0.58
1:B:540:HIS:HE1	1:B:582:LEU:O	1.86	0.58
1:B:575:CYS:O	1:B:579:LEU:HD12	2.04	0.58
1:C:611:LEU:O	1:C:613:GLN:N	2.34	0.57
1:D:610:LYS:O	1:D:613:GLN:NE2	2.34	0.57
1:D:537:ARG:O	1:D:538:GLY:C	2.43	0.57
1:A:575:CYS:O	1:A:579:LEU:HD12	2.04	0.56
1:F:537:ARG:O	1:F:538:GLY:C	2.43	0.56
1:B:590:LYS:O	1:B:593:PHE:N	2.39	0.56
1:C:579:LEU:HD22	1:D:537:ARG:NH1	2.20	0.56
1:E:551:LYS:HE3	1:E:576:ASP:OD1	2.04	0.56
1:A:600:LEU:C	1:A:600:LEU:HD23	2.26	0.56
1:B:537:ARG:HH11	1:E:579:LEU:HD22	1.70	0.56
1:C:574:LYS:HG3	1:C:603:LEU:HD12	1.88	0.56
1:A:537:ARG:HH11	1:F:579:LEU:HD22	1.70	0.55
1:C:551:LYS:HE3	1:C:576:ASP:OD1	2.06	0.55
1:F:600:LEU:C	1:F:600:LEU:HD23	2.27	0.55
1:E:600:LEU:C	1:E:600:LEU:HD23	2.27	0.55
1:A:537:ARG:O	1:A:538:GLY:C	2.45	0.55
1:E:540:HIS:HE1	1:E:582:LEU:O	1.90	0.54
1:D:590:LYS:O	1:D:593:PHE:N	2.41	0.54
1:D:600:LEU:HD23	1:D:600:LEU:C	2.27	0.54
1:D:534:LEU:CD2	1:D:587:THR:HG22	2.38	0.54
1:E:590:LYS:O	1:E:593:PHE:N	2.42	0.53
1:D:575:CYS:O	1:D:579:LEU:HD12	2.08	0.53
1:C:537:ARG:O	1:C:538:GLY:C	2.46	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:LEU:CD2	1:A:587:THR:HG22	2.39	0.53
1:D:554:ILE:HG23	1:D:568:LYS:HG3	1.91	0.52
1:F:575:CYS:O	1:F:579:LEU:HD12	2.08	0.52
1:D:571:ILE:HG22	1:D:572:GLU:N	2.23	0.52
1:C:540:HIS:HE1	1:C:582:LEU:O	1.91	0.52
1:E:554:ILE:HG23	1:E:568:LYS:HG3	1.91	0.52
1:D:611:LEU:O	1:D:613:GLN:N	2.39	0.52
1:A:554:ILE:HG23	1:A:568:LYS:HG3	1.92	0.52
1:B:534:LEU:CD2	1:B:587:THR:HG22	2.40	0.52
1:B:551:LYS:HE3	1:B:576:ASP:OD1	2.10	0.52
1:C:550:LEU:HD11	1:C:600:LEU:HD21	1.92	0.52
1:E:611:LEU:O	1:E:613:GLN:N	2.37	0.52
1:F:554:ILE:HG23	1:F:568:LYS:HG3	1.92	0.51
1:D:551:LYS:HE3	1:D:576:ASP:OD1	2.10	0.51
1:A:551:LYS:HE3	1:A:576:ASP:OD1	2.10	0.51
1:B:543:LEU:O	1:B:544:GLU:C	2.49	0.51
1:F:590:LYS:O	1:F:593:PHE:N	2.44	0.51
1:C:600:LEU:C	1:C:600:LEU:HD23	2.32	0.50
1:C:554:ILE:HG23	1:C:568:LYS:HG3	1.94	0.50
1:A:546:TYR:CE1	1:A:550:LEU:HD11	2.47	0.50
1:A:590:LYS:O	1:A:593:PHE:N	2.44	0.50
1:D:546:TYR:CE1	1:D:550:LEU:HD11	2.47	0.50
1:F:550:LEU:HD11	1:F:600:LEU:HD21	1.93	0.50
1:C:575:CYS:O	1:C:579:LEU:HD12	2.12	0.49
1:D:584:SER:HB2	1:E:586:GLN:OE1	2.12	0.49
1:F:550:LEU:CD1	1:F:600:LEU:HD21	2.42	0.49
1:A:545:SER:O	1:A:549:ASN:ND2	2.43	0.49
1:C:550:LEU:CD1	1:C:600:LEU:HD21	2.42	0.49
1:C:590:LYS:HA	1:C:593:PHE:HB3	1.95	0.49
1:F:551:LYS:HE3	1:F:576:ASP:OD1	2.12	0.49
1:C:590:LYS:O	1:C:593:PHE:N	2.46	0.49
1:F:611:LEU:O	1:F:613:GLN:N	2.37	0.49
1:D:590:LYS:C	1:D:592:GLU:N	2.66	0.48
1:B:554:ILE:HG23	1:B:568:LYS:HG3	1.94	0.48
1:A:540:HIS:HE1	1:A:582:LEU:O	1.97	0.48
1:A:610:LYS:O	1:A:613:GLN:NE2	2.36	0.48
1:F:540:HIS:HE1	1:F:582:LEU:O	1.95	0.48
1:A:549:ASN:O	1:A:550:LEU:C	2.52	0.48
1:B:590:LYS:HA	1:B:593:PHE:HB3	1.96	0.48
1:C:534:LEU:CD2	1:C:587:THR:HG22	2.41	0.48
1:C:579:LEU:HD22	1:D:537:ARG:HH11	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:546:TYR:CE1	1:C:550:LEU:HD11	2.48	0.48
1:F:546:TYR:CE1	1:F:550:LEU:HD11	2.48	0.48
1:B:571:ILE:HG22	1:B:572:GLU:N	2.28	0.48
1:E:610:LYS:O	1:E:613:GLN:NE2	2.36	0.48
1:F:534:LEU:CD2	1:F:587:THR:HG22	2.44	0.48
1:E:550:LEU:HD11	1:E:600:LEU:HD21	1.96	0.47
1:B:550:LEU:HD11	1:B:600:LEU:HD21	1.96	0.47
1:B:600:LEU:HD23	1:B:600:LEU:C	2.35	0.47
1:C:549:ASN:O	1:C:550:LEU:C	2.52	0.47
1:C:571:ILE:HG22	1:C:572:GLU:N	2.29	0.47
1:B:545:SER:O	1:B:549:ASN:ND2	2.47	0.47
1:C:545:SER:O	1:C:549:ASN:ND2	2.46	0.47
1:D:543:LEU:O	1:D:544:GLU:C	2.53	0.47
1:B:610:LYS:O	1:B:613:GLN:NE2	2.38	0.47
1:D:549:ASN:O	1:D:550:LEU:C	2.53	0.47
1:D:590:LYS:HA	1:D:593:PHE:HB3	1.96	0.47
1:E:590:LYS:HA	1:E:593:PHE:HB3	1.96	0.47
1:C:590:LYS:C	1:C:592:GLU:N	2.65	0.47
1:A:534:LEU:HD23	1:A:587:THR:O	2.16	0.46
1:D:540:HIS:HE1	1:D:582:LEU:O	1.97	0.46
1:F:590:LYS:C	1:F:592:GLU:N	2.68	0.46
1:E:534:LEU:CD2	1:E:587:THR:HG22	2.46	0.46
1:E:543:LEU:O	1:E:544:GLU:C	2.54	0.46
1:A:590:LYS:HA	1:A:593:PHE:HB3	1.97	0.46
1:F:543:LEU:O	1:F:544:GLU:C	2.54	0.46
1:E:571:ILE:HG22	1:E:572:GLU:N	2.31	0.46
1:E:611:LEU:C	1:E:613:GLN:H	2.18	0.46
1:A:543:LEU:O	1:A:544:GLU:C	2.54	0.46
1:B:535:VAL:HG13	1:B:536:PRO:O	2.16	0.46
1:E:534:LEU:HD23	1:E:587:THR:O	2.16	0.46
1:C:543:LEU:O	1:C:544:GLU:C	2.54	0.45
1:C:554:ILE:CG1	1:C:571:ILE:HG21	2.46	0.45
1:F:590:LYS:HA	1:F:593:PHE:HB3	1.97	0.45
1:B:540:HIS:CE1	1:B:586:GLN:HA	2.52	0.45
1:A:605:ASN:N	1:A:606:PRO:HD2	2.32	0.45
1:D:559:LEU:HD13	1:D:611:LEU:HD21	1.98	0.45
1:A:537:ARG:O	1:A:540:HIS:N	2.49	0.45
1:B:611:LEU:O	1:B:613:GLN:N	2.46	0.45
1:B:540:HIS:CE1	1:B:582:LEU:O	2.68	0.45
1:C:605:ASN:N	1:C:606:PRO:HD2	2.32	0.45
1:D:594:GLU:O	1:D:595:HIS:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:545:SER:O	1:F:549:ASN:ND2	2.48	0.45
1:B:605:ASN:N	1:B:606:PRO:HD2	2.32	0.44
1:F:554:ILE:CG1	1:F:571:ILE:HG21	2.47	0.44
1:F:559:LEU:HD13	1:F:611:LEU:HD21	1.98	0.44
1:C:559:LEU:HD13	1:C:611:LEU:HD21	1.99	0.44
1:F:605:ASN:N	1:F:606:PRO:HD2	2.33	0.44
1:B:585:ASN:C	1:B:587:THR:H	2.18	0.44
1:D:605:ASN:N	1:D:606:PRO:HD2	2.32	0.44
1:E:533:GLY:HA2	1:E:534:LEU:CB	2.48	0.44
1:F:608:ILE:HD12	1:F:609:SER:N	2.32	0.44
1:D:545:SER:O	1:D:549:ASN:ND2	2.48	0.44
1:F:549:ASN:O	1:F:550:LEU:C	2.55	0.44
1:C:540:HIS:CE1	1:C:582:LEU:O	2.71	0.44
1:F:608:ILE:C	1:F:608:ILE:CD1	2.87	0.43
1:D:533:GLY:HA2	1:D:534:LEU:CB	2.49	0.43
1:D:550:LEU:HD11	1:D:600:LEU:HD21	2.01	0.43
1:C:533:GLY:HA2	1:C:534:LEU:CB	2.48	0.43
1:F:594:GLU:O	1:F:595:HIS:C	2.55	0.43
1:B:537:ARG:NH1	2:B:6:SO4:O4	2.51	0.43
1:F:537:ARG:O	1:F:540:HIS:N	2.52	0.43
1:D:585:ASN:O	1:D:586:GLN:C	2.56	0.43
1:C:610:LYS:O	1:C:613:GLN:NE2	2.41	0.43
1:F:571:ILE:HG22	1:F:572:GLU:N	2.34	0.43
1:E:537:ARG:O	1:E:540:HIS:N	2.51	0.43
1:F:554:ILE:HG13	1:F:571:ILE:HG21	2.00	0.43
1:C:554:ILE:HG13	1:C:571:ILE:HG21	1.99	0.42
1:E:540:HIS:CE1	1:E:586:GLN:HA	2.54	0.42
1:C:611:LEU:C	1:C:613:GLN:H	2.20	0.42
1:C:533:GLY:CA	1:C:534:LEU:HB2	2.50	0.42
1:E:549:ASN:O	1:E:550:LEU:C	2.58	0.42
1:A:584:SER:HB2	1:B:586:GLN:OE1	2.19	0.42
1:B:550:LEU:CD1	1:B:600:LEU:HD21	2.49	0.42
1:E:605:ASN:N	1:E:606:PRO:HD2	2.34	0.42
1:F:611:LEU:C	1:F:613:GLN:H	2.20	0.42
1:D:554:ILE:CG1	1:D:571:ILE:HG21	2.50	0.42
1:E:575:CYS:C	1:E:579:LEU:HD12	2.40	0.42
1:F:533:GLY:HA2	1:F:534:LEU:CB	2.49	0.42
1:F:585:ASN:C	1:F:587:THR:H	2.17	0.42
1:A:550:LEU:HD11	1:A:600:LEU:HD21	2.02	0.42
1:C:540:HIS:CE1	1:C:586:GLN:HA	2.55	0.42
1:E:593:PHE:CD2	1:E:593:PHE:C	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:GLY:HA2	1:A:534:LEU:CB	2.49	0.42
1:A:556:ASP:O	1:A:557:GLU:C	2.58	0.42
1:E:533:GLY:CA	1:E:534:LEU:HB2	2.50	0.42
1:A:594:GLU:O	1:A:595:HIS:C	2.58	0.42
1:B:554:ILE:CG1	1:B:571:ILE:HG21	2.50	0.41
1:E:550:LEU:CD1	1:E:600:LEU:HD21	2.50	0.41
1:F:533:GLY:CA	1:F:534:LEU:HB2	2.50	0.41
1:E:594:GLU:O	1:E:595:HIS:C	2.59	0.41
1:B:549:ASN:O	1:B:550:LEU:C	2.56	0.41
1:B:554:ILE:HG13	1:B:571:ILE:HG21	2.03	0.41
1:C:543:LEU:HB3	1:C:582:LEU:HD11	2.02	0.41
1:D:593:PHE:CD2	1:D:593:PHE:C	2.93	0.41
1:A:611:LEU:C	1:A:613:GLN:H	2.24	0.41
1:B:533:GLY:HA2	1:B:534:LEU:CB	2.51	0.41
1:B:546:TYR:CE1	1:B:550:LEU:HD11	2.56	0.41
1:C:603:LEU:HD23	1:C:603:LEU:HA	1.93	0.41
1:A:533:GLY:CA	1:A:534:LEU:HB2	2.52	0.40
1:A:543:LEU:HD12	1:A:543:LEU:HA	1.90	0.40
1:A:575:CYS:C	1:A:579:LEU:HD12	2.41	0.40
1:A:585:ASN:C	1:A:587:THR:H	2.21	0.40
1:B:590:LYS:C	1:B:592:GLU:N	2.67	0.40
1:B:533:GLY:CA	1:B:534:LEU:HB2	2.51	0.40
1:D:533:GLY:CA	1:D:534:LEU:HB2	2.51	0.40
1:B:608:ILE:C	1:B:608:ILE:CD1	2.89	0.40
1:C:537:ARG:O	1:C:540:HIS:N	2.54	0.40
1:E:546:TYR:O	1:E:547:ALA:C	2.59	0.40
1:C:608:ILE:HD12	1:C:609:SER:N	2.37	0.40
1:E:537:ARG:HH11	1:E:537:ARG:HD2	1.79	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	80/120 (67%)	59 (74%)	17 (21%)	4 (5%)	2	16
1	B	80/120 (67%)	58 (72%)	18 (22%)	4 (5%)	2	16
1	C	80/120 (67%)	58 (72%)	18 (22%)	4 (5%)	2	16
1	D	80/120 (67%)	57 (71%)	19 (24%)	4 (5%)	2	16
1	E	80/120 (67%)	59 (74%)	17 (21%)	4 (5%)	2	16
1	F	80/120 (67%)	58 (72%)	17 (21%)	5 (6%)	1	10
All	All	480/720 (67%)	349 (73%)	106 (22%)	25 (5%)	2	15

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	560	LYS
1	A	586	GLN
1	A	591	GLU
1	A	592	GLU
1	B	560	LYS
1	B	586	GLN
1	B	591	GLU
1	B	592	GLU
1	C	560	LYS
1	C	586	GLN
1	C	591	GLU
1	C	592	GLU
1	D	560	LYS
1	D	586	GLN
1	D	591	GLU
1	D	592	GLU
1	E	560	LYS
1	E	586	GLN
1	E	591	GLU
1	E	592	GLU
1	F	560	LYS
1	F	586	GLN
1	F	591	GLU
1	F	592	GLU
1	F	589	GLU

### 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	74/96 (77%)	63 (85%)	11 (15%)	3	14
1	B	74/96 (77%)	63 (85%)	11 (15%)	3	14
1	C	74/96 (77%)	63 (85%)	11 (15%)	3	14
1	D	74/96 (77%)	63 (85%)	11 (15%)	3	14
1	E	74/96 (77%)	65 (88%)	9 (12%)	5	22
1	F	74/96 (77%)	63 (85%)	11 (15%)	3	14
All	All	444/576 (77%)	380 (86%)	64 (14%)	3	15

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	535	VAL
1	A	546	TYR
1	A	554	ILE
1	A	555	GLU
1	A	560	LYS
1	A	563	ILE
1	A	586	GLN
1	A	587	THR
1	A	590	LYS
1	A	592	GLU
1	A	603	LEU
1	B	535	VAL
1	B	546	TYR
1	B	554	ILE
1	B	555	GLU
1	B	560	LYS
1	B	563	ILE
1	B	586	GLN
1	B	587	THR
1	B	590	LYS
1	B	592	GLU
1	B	603	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	535	VAL
1	C	546	TYR
1	C	554	ILE
1	C	555	GLU
1	C	560	LYS
1	C	563	ILE
1	C	586	GLN
1	C	587	THR
1	C	590	LYS
1	C	592	GLU
1	C	603	LEU
1	D	535	VAL
1	D	546	TYR
1	D	554	ILE
1	D	555	GLU
1	D	560	LYS
1	D	563	ILE
1	D	586	GLN
1	D	587	THR
1	D	590	LYS
1	D	592	GLU
1	D	603	LEU
1	E	554	ILE
1	E	555	GLU
1	E	560	LYS
1	E	563	ILE
1	E	586	GLN
1	E	587	THR
1	E	590	LYS
1	E	592	GLU
1	E	603	LEU
1	F	535	VAL
1	F	546	TYR
1	F	554	ILE
1	F	555	GLU
1	F	560	LYS
1	F	563	ILE
1	F	586	GLN
1	F	587	THR
1	F	590	LYS
1	F	592	GLU
1	F	603	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	540	HIS
1	A	586	GLN
1	A	596	GLN
1	B	540	HIS
1	B	586	GLN
1	B	596	GLN
1	C	540	HIS
1	C	586	GLN
1	C	596	GLN
1	C	605	ASN
1	D	540	HIS
1	D	586	GLN
1	D	596	GLN
1	E	540	HIS
1	E	596	GLN
1	F	540	HIS
1	F	586	GLN
1	F	596	GLN

### 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](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	SO4	F	5	-	4,4,4	1.69	1 (25%)	6,6,6	0.63	0
2	SO4	A	1	-	4,4,4	0.21	0	6,6,6	0.36	0
2	SO4	D	4	-	4,4,4	0.23	0	6,6,6	0.38	0
2	SO4	B	6	-	4,4,4	0.18	0	6,6,6	0.31	0
2	SO4	E	3	-	4,4,4	0.22	0	6,6,6	0.54	0
2	SO4	C	2	-	4,4,4	0.74	0	6,6,6	0.56	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	5	SO4	O1-S	2.40	1.59	1.46

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	6	SO4	1	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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	82/120 (68%)	0.43	5 (6%) 21 12	92, 103, 108, 110	0
1	B	82/120 (68%)	0.28	2 (2%) 59 44	92, 103, 108, 110	0
1	C	82/120 (68%)	0.21	1 (1%) 79 67	92, 103, 108, 110	0
1	D	82/120 (68%)	0.23	2 (2%) 59 44	92, 103, 108, 110	0
1	E	82/120 (68%)	0.28	2 (2%) 59 44	92, 103, 108, 110	0
1	F	82/120 (68%)	0.23	2 (2%) 59 44	92, 103, 108, 110	0
All	All	492/720 (68%)	0.28	14 (2%) 53 37	92, 103, 108, 110	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	614	SER	4.3
1	A	612	TYR	4.3
1	A	614	SER	3.8
1	F	611	LEU	3.2
1	E	610	LYS	3.1
1	A	584	SER	2.7
1	B	612	TYR	2.6
1	D	612	TYR	2.5
1	B	584	SER	2.5
1	A	611	LEU	2.4
1	C	591	GLU	2.4
1	F	612	TYR	2.3
1	A	591	GLU	2.2
1	E	612	TYR	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, 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SO4	D	4	5/5	0.15	0.75	154,155,155,156	0
2	SO4	C	2	5/5	0.21	0.79	157,159,159,159	0
2	SO4	A	1	5/5	0.33	0.71	160,161,162,162	0
2	SO4	B	6	5/5	0.42	0.75	173,173,173,173	0
2	SO4	F	5	5/5	0.46	0.60	153,155,155,155	0
2	SO4	E	3	5/5	0.76	0.42	155,155,156,157	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.