



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2024 – 07:41 PM EDT

PDB ID : 3SZI  
Title : Structure of apo shwanavidin (P21 form)  
Authors : Livnah, O.; Meir, A.  
Deposited on : 2011-07-19  
Resolution : 1.40 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	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
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)	:	2.37.1

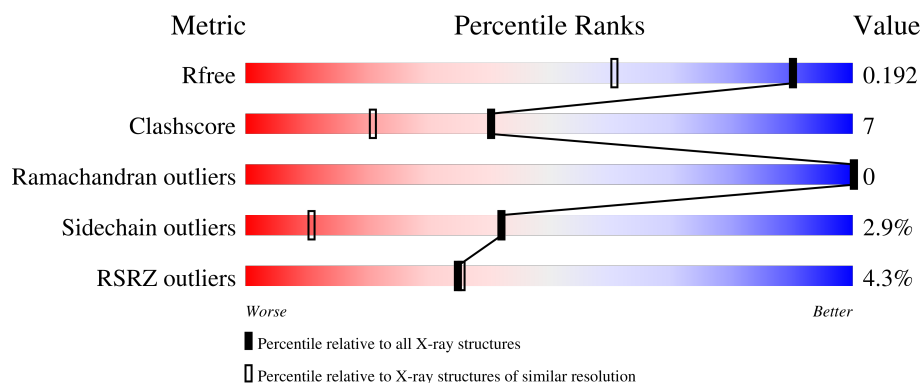
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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	122	<div> <div>5%</div> <div> <div></div> <div>88%</div> <div>7%</div> <div>• •</div> </div> </div>
1	B	122	<div> <div>4%</div> <div> <div></div> <div>79%</div> <div>11%</div> <div>• 7%</div> </div> </div>
1	C	122	<div> <div>2%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• •</div> </div> </div>
1	D	122	<div> <div>3%</div> <div> <div></div> <div>84%</div> <div>11%</div> <div>• •</div> </div> </div>
1	E	122	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	122	<div><div></div><div>8%</div><div>83%</div><div>11%</div><div></div><div></div></div>
1	G	122	<div><div></div><div>2%</div><div>80%</div><div>16%</div><div></div><div></div></div>
1	H	122	<div><div></div><div>4%</div><div>89%</div><div>7%</div><div></div><div></div></div>
1	I	122	<div><div></div><div>4%</div><div>83%</div><div>13%</div><div></div><div></div></div>
1	J	122	<div><div></div><div>3%</div><div>87%</div><div>11%</div><div></div><div></div></div>
1	K	122	<div><div></div><div>3%</div><div>89%</div><div>7%</div><div></div><div></div></div>
1	L	122	<div><div></div><div>4%</div><div>84%</div><div>13%</div><div></div><div></div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12423 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 Avidin/streptavidin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	117	Total	C	N	O	S	4	12	0
			933	590	150	190	3			
1	B	113	Total	C	N	O	S	5	9	0
			896	573	145	175	3			
1	C	117	Total	C	N	O	S	4	7	0
			909	573	148	185	3			
1	D	120	Total	C	N	O	S	5	6	0
			923	583	150	186	4			
1	E	118	Total	C	N	O	S	14	6	0
			914	577	149	185	3			
1	F	117	Total	C	N	O	S	2	7	0
			915	580	148	184	3			
1	G	119	Total	C	N	O	S	4	8	0
			931	592	151	184	4			
1	H	117	Total	C	N	O	S	6	4	0
			902	572	148	179	3			
1	I	117	Total	C	N	O	S	7	11	0
			927	592	148	184	3			
1	K	117	Total	C	N	O	S	13	6	0
			912	579	148	181	4			
1	J	119	Total	C	N	O	S	3	8	0
			927	588	150	185	4			
1	L	120	Total	C	N	O	S	7	8	0
			934	590	151	189	4			

There are 24 discrepancies between the modelled and reference sequences:

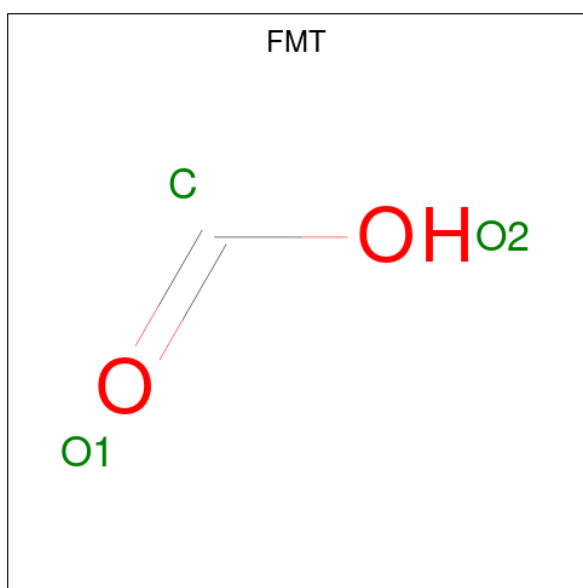
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	EXPRESSION TAG	UNP Q12QS6
A	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
B	1	MET	-	EXPRESSION TAG	UNP Q12QS6
B	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
C	1	MET	-	EXPRESSION TAG	UNP Q12QS6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
D	1	MET	-	EXPRESSION TAG	UNP Q12QS6
D	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
E	1	MET	-	EXPRESSION TAG	UNP Q12QS6
E	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
F	1	MET	-	EXPRESSION TAG	UNP Q12QS6
F	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
G	1	MET	-	EXPRESSION TAG	UNP Q12QS6
G	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
H	1	MET	-	EXPRESSION TAG	UNP Q12QS6
H	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
I	1	MET	-	EXPRESSION TAG	UNP Q12QS6
I	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
K	1	MET	-	EXPRESSION TAG	UNP Q12QS6
K	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
J	1	MET	-	EXPRESSION TAG	UNP Q12QS6
J	2	ALA	-	EXPRESSION TAG	UNP Q12QS6
L	1	MET	-	EXPRESSION TAG	UNP Q12QS6
L	2	ALA	-	EXPRESSION TAG	UNP Q12QS6

- Molecule 2 is FORMIC ACID (three-letter code: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total C O 3 1 2	0	0
2	H	1	Total C O 3 1 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	I	1	Total	C	O	0	0
			3	1	2		
2	K	1	Total	C	O	0	0
			3	1	2		
2	K	1	Total	C	O	0	0
			3	1	2		
2	J	1	Total	C	O	0	0
			3	1	2		

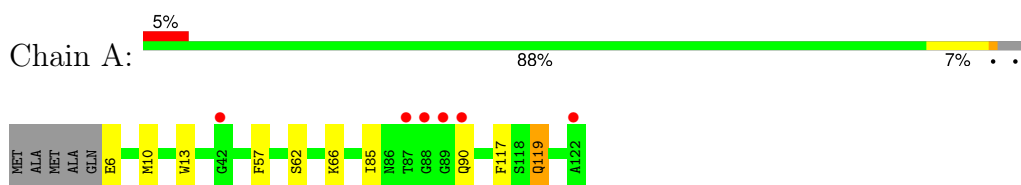
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	121	Total	O	0	0
			121	121		
3	B	122	Total	O	0	0
			122	122		
3	C	126	Total	O	0	0
			126	126		
3	D	111	Total	O	0	0
			111	111		
3	E	117	Total	O	0	0
			117	117		
3	F	91	Total	O	0	0
			91	91		
3	G	129	Total	O	0	0
			129	129		
3	H	92	Total	O	0	0
			92	92		
3	I	108	Total	O	0	0
			108	108		
3	K	121	Total	O	0	0
			121	121		
3	J	127	Total	O	0	0
			127	127		
3	L	117	Total	O	0	0
			117	117		

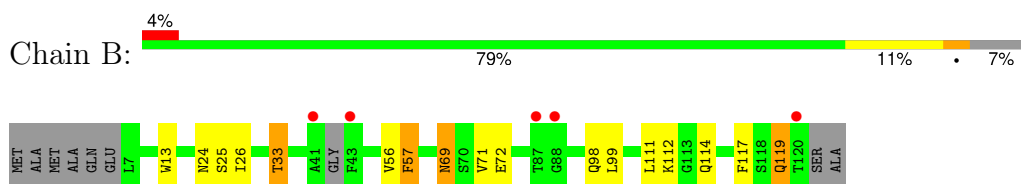
### 3 Residue-property plots [i](#)

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.

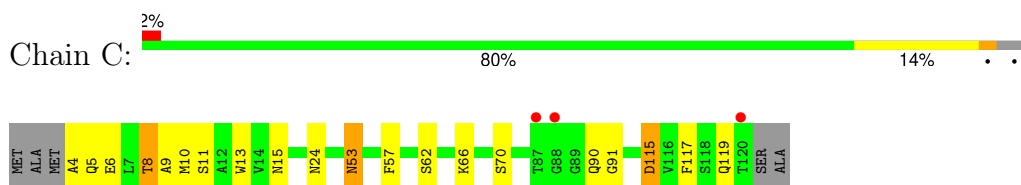
- Molecule 1: Avidin/streptavidin



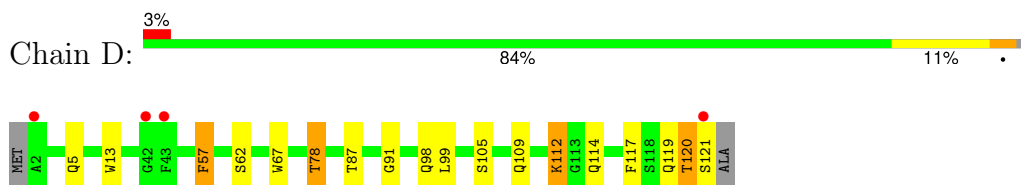
- Molecule 1: Avidin/streptavidin



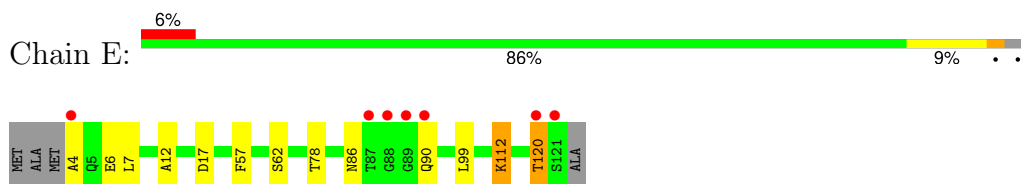
- Molecule 1: Avidin/streptavidin



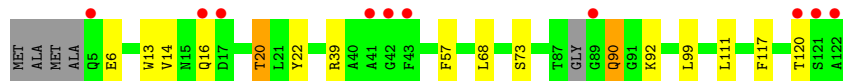
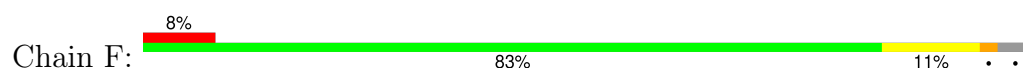
- Molecule 1: Avidin/streptavidin



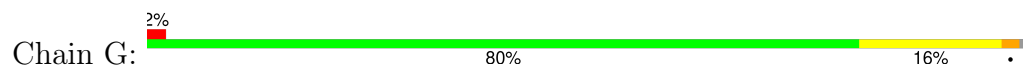
- Molecule 1: Avidin/streptavidin



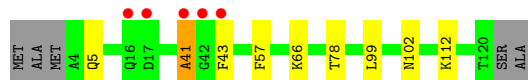
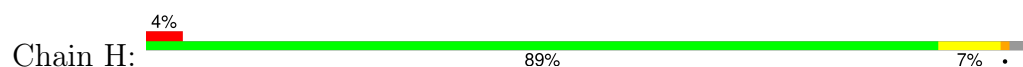
- Molecule 1: Avidin/streptavidin



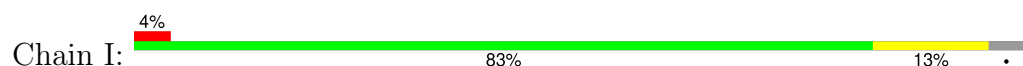
- Molecule 1: Avidin/streptavidin



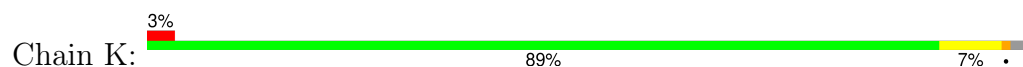
- Molecule 1: Avidin/streptavidin



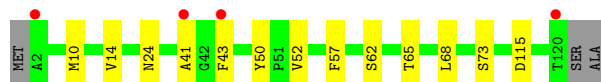
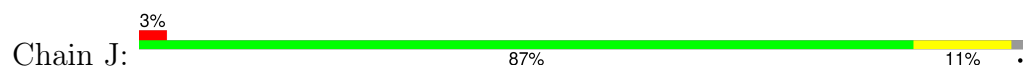
- Molecule 1: Avidin/streptavidin



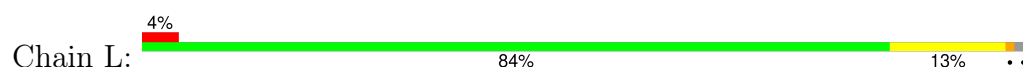
- Molecule 1: Avidin/streptavidin



- Molecule 1: Avidin/streptavidin



- Molecule 1: Avidin/streptavidin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	67.52Å 110.56Å 84.20Å 90.00° 93.93° 90.00°	Depositor
Resolution (Å)	83.92 – 1.40 42.73 – 1.40	Depositor EDS
% Data completeness (in resolution range)	97.3 (83.92-1.40) 97.3 (42.73-1.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.92 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.157 , 0.192 0.157 , 0.192	Depositor DCC
$R_{free}$ test set	11813 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	15.2	Xtriage
Anisotropy	0.231	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 57.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.41 % 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 2.6504e-03. 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: FMT

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	1/993 (0.1%)	0.69	0/1351
1	B	0.59	1/943 (0.1%)	0.72	0/1284
1	C	0.79	1/951 (0.1%)	0.70	0/1296
1	D	0.59	0/962	0.78	3/1311 (0.2%)
1	E	0.74	2/953 (0.2%)	0.89	5/1299 (0.4%)
1	F	0.53	0/953	0.73	2/1298 (0.2%)
1	G	0.57	1/973 (0.1%)	0.68	0/1325
1	H	0.74	1/935 (0.1%)	0.76	2/1275 (0.2%)
1	I	0.54	1/981 (0.1%)	0.74	2/1338 (0.1%)
1	J	0.55	0/972	0.69	0/1325
1	K	1.33	4/950 (0.4%)	0.85	5/1293 (0.4%)
1	L	0.85	2/979 (0.2%)	0.75	2/1332 (0.2%)
All	All	0.74	14/11545 (0.1%)	0.75	21/15727 (0.1%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	6	GLU	CD-OE1	-24.00	0.99	1.25
1	K	6	GLU	CD-OE2	22.80	1.50	1.25
1	L	6	GLU	CG-CD	-18.55	1.24	1.51
1	C	6	GLU	CD-OE2	-17.64	1.06	1.25
1	H	41	ALA	CA-CB	15.66	1.85	1.52
1	K	90	GLN	CD-NE2	-15.59	0.93	1.32
1	A	6	GLU	CD-OE2	-11.35	1.13	1.25
1	E	112	LYS	CD-CE	-11.31	1.23	1.51
1	L	92	LYS	CG-CD	8.86	1.82	1.52
1	E	86	ASN	CG-OD1	-8.83	1.04	1.24
1	K	112	LYS	CD-CE	8.67	1.73	1.51
1	B	114	GLN	CD-NE2	6.17	1.48	1.32
1	G	90	GLN	CB-CG	-5.72	1.37	1.52
1	I	87	THR	CA-CB	-5.50	1.39	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	41	ALA	N-CA-CB	-9.04	97.44	110.10
1	E	6	GLU	CG-CD-OE2	9.02	136.35	118.30
1	E	6	GLU	CG-CD-OE1	-8.96	100.39	118.30
1	K	90	GLN	OE1-CD-NE2	8.71	141.93	121.90
1	I	87	THR	N-CA-CB	8.71	126.84	110.30
1	L	92	LYS	CB-CG-CD	-8.55	89.37	111.60
1	K	90	GLN	CG-CD-NE2	-8.40	96.53	116.70
1	K	6	GLU	CG-CD-OE1	8.21	134.71	118.30
1	K	6	GLU	CG-CD-OE2	-8.17	101.96	118.30
1	E	90	GLN	N-CA-CB	8.04	125.08	110.60
1	E	86	ASN	OD1-CG-ND2	7.93	140.13	121.90
1	H	41	ALA	CB-CA-C	-7.91	98.23	110.10
1	I	87	THR	CA-CB-CG2	6.72	121.81	112.40
1	F	90	GLN	CG-CD-OE1	-6.54	108.53	121.60
1	D	120	THR	CB-CA-C	-6.53	93.98	111.60
1	D	112	LYS	CD-CE-NZ	-6.19	97.46	111.70
1	K	112	LYS	CD-CE-NZ	6.00	125.50	111.70
1	E	86	ASN	CB-CG-ND2	-5.99	102.32	116.70
1	F	90	GLN	OE1-CD-NE2	5.26	134.00	121.90
1	D	87	THR	CA-CB-CG2	5.20	119.68	112.40
1	L	6	GLU	CB-CG-CD	5.15	128.11	114.20

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	933	0	909	7	0
1	B	896	0	883	14	0
1	C	909	0	870	15	0
1	D	923	0	890	19	0
1	E	914	0	876	7	0
1	F	915	0	884	20	0
1	G	931	0	910	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	902	0	868	8	0
1	I	927	0	915	19	0
1	J	927	0	902	11	0
1	K	912	0	883	5	0
1	L	934	0	905	21	0
2	D	3	0	1	0	0
2	H	3	0	1	0	0
2	I	3	0	1	0	0
2	J	3	0	1	0	0
2	K	6	0	2	0	0
3	A	121	0	0	1	0
3	B	122	0	0	1	0
3	C	126	0	0	2	0
3	D	111	0	0	2	0
3	E	117	0	0	3	1
3	F	91	0	0	3	0
3	G	129	0	0	7	1
3	H	92	0	0	1	0
3	I	108	0	0	3	0
3	J	127	0	0	3	0
3	K	121	0	0	1	0
3	L	117	0	0	4	0
All	All	12423	0	10701	155	1

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 7.

All (155) 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:D:78:THR:HG22	1:D:99[B]:LEU:HD23	1.42	1.02
1:G:41:ALA:HA	3:G:308:HOH:O	1.58	1.02
1:D:67:TRP:HE1	1:D:78:THR:HG23	1.21	1.01
1:D:91:GLY:H	1:D:119:GLN:HE21	1.19	0.91
1:D:67:TRP:HE1	1:D:78:THR:CG2	1.90	0.85
1:L:20[A]:THR:HG22	1:L:39:ARG:HH12	1.42	0.84
1:B:13:TRP:CZ3	1:B:119:GLN:HG2	2.14	0.82
1:L:20[A]:THR:HG23	1:L:22:TYR:CE1	2.13	0.82
1:F:20[A]:THR:HG23	1:F:39:ARG:HH12	1.45	0.82
1:D:78:THR:HG21	3:D:325:HOH:O	1.80	0.81
1:F:20[A]:THR:CG2	1:F:39:ARG:HH12	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:20[A]:THR:HG21	1:L:22:TYR:OH	1.81	0.80
1:G:105:SER:H	1:G:109:GLN:HE22	1.28	0.78
1:I:99[A]:LEU:HD23	1:I:111:LEU:HD12	1.65	0.78
1:J:14[A]:VAL:HG13	3:J:348:HOH:O	1.85	0.77
1:I:14[B]:VAL:HG23	1:I:120:THR:HG21	1.68	0.76
1:D:67:TRP:NE1	1:D:78:THR:HG23	2.00	0.74
1:G:105:SER:H	1:G:109:GLN:NE2	1.85	0.74
1:F:14:VAL:CG1	1:F:120:THR:HG21	2.17	0.74
1:E:120:THR:HG23	3:L:275:HOH:O	1.88	0.74
1:C:15:ASN:HB2	1:C:115[B]:ASP:OD2	1.88	0.73
1:D:105:SER:H	1:D:109:GLN:HE22	1.34	0.73
1:I:14[B]:VAL:CG2	1:I:120:THR:HG21	2.18	0.72
1:B:98:GLN:HE21	1:B:112[B]:LYS:HE3	1.55	0.71
1:C:8:THR:HG23	1:C:9:ALA:O	1.91	0.71
1:G:34:GLY:C	1:G:52[A]:VAL:HG12	2.12	0.69
1:D:62[A]:SER:OG	3:D:410:HOH:O	2.09	0.69
1:F:14:VAL:HG11	1:F:120:THR:HG21	1.73	0.69
1:L:20[A]:THR:CG2	1:L:39:ARG:HH12	2.05	0.69
1:A:10:MET:HA	1:C:70[B]:SER:OG	1.93	0.69
1:F:14:VAL:HG12	1:F:120:THR:CG2	2.23	0.69
1:I:14[B]:VAL:HG23	1:I:120:THR:CG2	2.22	0.69
1:L:20[A]:THR:HG21	1:L:22:TYR:CZ	2.28	0.69
1:C:91:GLY:H	1:C:119:GLN:HE21	1.39	0.68
1:G:62[B]:SER:OG	3:G:329:HOH:O	2.11	0.67
1:A:62[A]:SER:OG	3:A:321:HOH:O	2.12	0.67
1:G:14[A]:VAL:HG13	3:G:236:HOH:O	1.94	0.67
1:L:20[A]:THR:HG22	1:L:39:ARG:NH1	2.09	0.66
1:L:20[A]:THR:CG2	1:L:22:TYR:CE1	2.78	0.66
1:C:91:GLY:H	1:C:119:GLN:NE2	1.94	0.66
1:E:62[A]:SER:OG	3:E:317:HOH:O	2.14	0.65
1:J:68:LEU:HD13	1:J:73:SER:HB2	1.78	0.65
1:D:98:GLN:HE21	1:D:112:LYS:HE2	1.60	0.64
1:B:112[B]:LYS:NZ	3:B:221:HOH:O	2.29	0.64
1:D:105:SER:H	1:D:109:GLN:NE2	1.94	0.64
1:F:14:VAL:HG12	1:F:120:THR:HG23	1.78	0.64
1:L:62[B]:SER:OG	3:L:314:HOH:O	2.15	0.62
1:D:91:GLY:H	1:D:119:GLN:NE2	1.93	0.62
1:F:68:LEU:CD1	1:F:73:SER:HB2	2.30	0.62
1:C:5:GLN:H	1:C:119:GLN:NE2	1.96	0.62
1:D:121:SER:HA	1:I:71[A]:VAL:HG23	1.82	0.62
1:I:21[A]:LEU:CD1	1:I:23:ILE:HG13	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:119:GLN:O	1:G:120:THR:HB	2.00	0.61
1:B:69:ASN:C	1:B:69:ASN:HD22	2.05	0.60
1:F:14:VAL:CG1	1:F:120:THR:CG2	2.78	0.59
1:I:21[A]:LEU:HD11	1:I:23:ILE:HG12	1.83	0.59
1:B:99[A]:LEU:HD23	1:B:111:LEU:HD12	1.83	0.59
1:D:5:GLN:H	1:D:119:GLN:HE22	1.49	0.58
1:H:5:GLN:NE2	3:H:377:HOH:O	2.21	0.58
1:E:12:ALA:HB3	1:E:120:THR:HG21	1.85	0.58
1:G:59:THR:H	1:H:102:ASN:ND2	2.00	0.58
1:G:14[B]:VAL:HG23	1:G:120:THR:O	2.03	0.58
1:G:15:ASN:HD22	1:G:16:GLN:N	2.02	0.58
1:F:68:LEU:HD13	1:F:73:SER:HB2	1.86	0.57
1:D:5:GLN:H	1:D:119:GLN:NE2	2.03	0.57
1:G:15:ASN:HD22	1:G:17:ASP:H	1.52	0.57
1:E:4:ALA:N	3:E:247:HOH:O	2.38	0.56
1:L:20[A]:THR:CG2	1:L:22:TYR:CZ	2.88	0.56
1:J:115:ASP:OD1	3:J:317:HOH:O	2.18	0.56
1:I:62[B]:SER:OG	3:I:408:HOH:O	2.17	0.56
1:B:26:ILE:HG21	1:B:56[A]:VAL:HG21	1.88	0.55
1:G:96:LEU:HD13	1:H:112:LYS:HZ1	1.70	0.55
1:I:21[A]:LEU:HD11	1:I:23:ILE:CG1	2.36	0.55
1:C:8:THR:HG22	1:C:11:SER:HB3	1.89	0.55
1:H:41:ALA:O	1:H:43:PHE:CD2	2.59	0.55
1:J:10:MET:HE2	1:J:24:ASN:O	2.07	0.55
1:E:78:THR:OG1	1:E:99[B]:LEU:HD23	2.07	0.54
1:G:114:GLN:HG3	3:G:211:HOH:O	2.07	0.54
1:B:98:GLN:NE2	1:B:112[B]:LYS:HE3	2.22	0.53
1:E:120:THR:HG21	1:L:71:VAL:HG12	1.90	0.53
1:E:17:ASP:O	3:E:313:HOH:O	2.19	0.52
1:I:21[A]:LEU:HD12	1:I:23:ILE:HG13	1.92	0.52
1:C:5:GLN:H	1:C:119:GLN:HE22	1.57	0.51
1:J:10:MET:CE	1:J:24:ASN:O	2.58	0.51
1:F:99[A]:LEU:HD23	1:F:111:LEU:HD12	1.92	0.51
1:K:13:TRP:HB3	1:K:117:PHE:HB3	1.93	0.50
1:G:96:LEU:CD1	1:H:112:LYS:HZ1	2.25	0.50
1:L:10:MET:HE2	1:L:24:ASN:O	2.12	0.50
1:B:25:SER:OG	1:B:33:THR:HB	2.12	0.50
1:K:78:THR:OG1	1:K:99[A]:LEU:HD13	2.11	0.50
1:I:21[A]:LEU:CD1	1:I:23:ILE:CG1	2.90	0.49
1:F:20[A]:THR:CG2	1:F:39:ARG:NH1	2.70	0.49
1:C:62[B]:SER:OG	3:C:325:HOH:O	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:4:ALA:HA	1:C:119:GLN:HE22	1.79	0.48
1:B:69:ASN:ND2	1:B:71:VAL:H	2.11	0.48
1:F:20[B]:THR:HG21	3:F:235:HOH:O	2.14	0.48
1:L:20[A]:THR:HG23	1:L:22:TYR:HE1	1.75	0.47
1:F:20[A]:THR:HG21	3:F:235:HOH:O	2.14	0.47
1:B:13:TRP:HB3	1:B:117:PHE:HB3	1.97	0.47
1:F:16:GLN:HB2	3:F:290:HOH:O	2.14	0.47
1:L:8:THR:CG2	3:L:308:HOH:O	2.63	0.47
1:L:78:THR:OG1	1:L:99[A]:LEU:HD13	2.14	0.47
1:L:92:LYS:HG2	1:L:117:PHE:O	2.14	0.46
1:J:50:TYR:HB3	1:J:65[A]:THR:CG2	2.46	0.46
1:F:92:LYS:HB3	1:F:92:LYS:HE2	1.38	0.46
1:K:3:MET:SD	1:K:3:MET:N	2.88	0.46
1:G:15:ASN:ND2	1:G:17:ASP:H	2.12	0.46
1:G:112[A]:LYS:NZ	3:G:325:HOH:O	2.48	0.46
1:J:68:LEU:CD1	1:J:73:SER:HB2	2.44	0.46
1:B:24[A]:ASN:HB3	1:B:33:THR:HG22	1.98	0.46
1:G:52[A]:VAL:HG23	1:G:64[A]:SER:O	2.16	0.46
1:K:78:THR:OG1	1:K:99[B]:LEU:HD23	2.17	0.45
1:L:13:TRP:HB3	1:L:117:PHE:HB3	1.97	0.45
1:C:24[B]:ASN:ND2	3:C:302:HOH:O	2.49	0.45
1:G:10:MET:HE2	1:G:24:ASN:O	2.17	0.45
1:J:41:ALA:O	1:J:43:PHE:CD1	2.69	0.45
1:J:52:VAL:HG22	1:J:65[A]:THR:OG1	2.16	0.44
1:J:62[B]:SER:OG	3:J:423:HOH:O	2.21	0.44
1:A:13:TRP:CH2	1:A:119[A]:GLN:HG3	2.52	0.44
1:F:20[B]:THR:HG23	1:F:39:ARG:HH12	1.81	0.44
1:K:6:GLU:HG2	3:K:339:HOH:O	2.17	0.44
1:C:53:ASN:C	1:C:53:ASN:HD22	2.20	0.44
1:D:121:SER:CA	1:I:71[A]:VAL:HG23	2.47	0.43
1:A:10:MET:CA	1:C:70[B]:SER:OG	2.65	0.43
1:L:99[A]:LEU:HD23	1:L:111:LEU:HD12	1.99	0.43
1:A:66:LYS:HE3	1:B:57:PHE:CG	2.53	0.43
1:F:13:TRP:HB3	1:F:117:PHE:HB3	2.00	0.43
1:G:10:MET:CE	1:G:24:ASN:O	2.67	0.43
1:I:4:ALA:HB3	1:I:86:ASN:OD1	2.18	0.43
1:L:99[A]:LEU:HB3	1:L:111:LEU:HB2	2.00	0.42
1:L:8:THR:HG23	1:L:9:ALA:O	2.20	0.42
1:B:69:ASN:ND2	1:B:72:GLU:H	2.17	0.42
1:F:20[B]:THR:HG23	1:F:39:ARG:NH1	2.35	0.42
1:G:46:GLN:NE2	3:G:308:HOH:O	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:41:ALA:O	1:J:43:PHE:HD1	2.02	0.42
1:C:66:LYS:HE3	1:D:57:PHE:CG	2.55	0.41
1:D:13:TRP:HB3	1:D:117:PHE:HB3	2.01	0.41
1:F:20[B]:THR:OG1	1:F:22:TYR:CE1	2.65	0.41
1:G:96:LEU:HD13	1:H:112:LYS:NZ	2.35	0.41
1:B:13:TRP:CH2	1:B:119:GLN:HG2	2.55	0.41
1:G:14[A]:VAL:HG11	3:G:291:HOH:O	2.21	0.41
1:G:57:PHE:CG	1:H:66:LYS:HE3	2.55	0.41
1:A:13:TRP:HB3	1:A:117:PHE:HB3	2.03	0.41
1:C:13:TRP:HB3	1:C:117:PHE:HB3	2.03	0.41
1:H:78:THR:OG1	1:H:99[A]:LEU:HD13	2.21	0.41
1:I:114[A]:GLN:HG3	3:I:311:HOH:O	2.20	0.41
1:D:121:SER:O	1:I:71[B]:VAL:HG13	2.21	0.40
1:I:5:GLN:HB3	1:I:119:GLN:HB3	2.03	0.40
1:D:121:SER:C	1:I:71[A]:VAL:HG23	2.42	0.40
1:L:8:THR:HG21	3:L:308:HOH:O	2.22	0.40
1:I:114[A]:GLN:CG	3:I:311:HOH:O	2.70	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:313:HOH:O	3:G:238:HOH:O[1_455]	2.11	0.09

## 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	128/122 (105%)	124 (97%)	4 (3%)	0	100	100
1	B	118/122 (97%)	117 (99%)	1 (1%)	0	100	100
1	C	122/122 (100%)	122 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	124/122 (102%)	123 (99%)	1 (1%)	0	100	100
1	E	122/122 (100%)	121 (99%)	1 (1%)	0	100	100
1	F	120/122 (98%)	118 (98%)	2 (2%)	0	100	100
1	G	125/122 (102%)	125 (100%)	0	0	100	100
1	H	119/122 (98%)	119 (100%)	0	0	100	100
1	I	126/122 (103%)	125 (99%)	1 (1%)	0	100	100
1	J	125/122 (102%)	123 (98%)	2 (2%)	0	100	100
1	K	119/122 (98%)	117 (98%)	2 (2%)	0	100	100
1	L	126/122 (103%)	124 (98%)	2 (2%)	0	100	100
All	All	1474/1464 (101%)	1458 (99%)	16 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	110/100 (110%)	105 (96%)	5 (4%)	27	4
1	B	104/100 (104%)	100 (96%)	4 (4%)	33	6
1	C	104/100 (104%)	97 (93%)	7 (7%)	16	1
1	D	105/100 (105%)	101 (96%)	4 (4%)	33	6
1	E	104/100 (104%)	100 (96%)	4 (4%)	33	6
1	F	105/100 (105%)	100 (95%)	5 (5%)	25	4
1	G	106/100 (106%)	104 (98%)	2 (2%)	57	25
1	H	101/100 (101%)	100 (99%)	1 (1%)	76	53
1	I	108/100 (108%)	106 (98%)	2 (2%)	57	25
1	J	106/100 (106%)	105 (99%)	1 (1%)	78	58
1	K	104/100 (104%)	103 (99%)	1 (1%)	76	53
1	L	107/100 (107%)	106 (99%)	1 (1%)	78	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1264/1200 (105%)	1227 (97%)	37 (3%)	42 11

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	PHE
1	A	85	ILE
1	A	90	GLN
1	A	119[A]	GLN
1	A	119[B]	GLN
1	B	33	THR
1	B	57	PHE
1	B	69	ASN
1	B	119	GLN
1	C	8	THR
1	C	10	MET
1	C	53	ASN
1	C	57	PHE
1	C	90	GLN
1	C	115[A]	ASP
1	C	115[B]	ASP
1	D	57	PHE
1	D	78	THR
1	D	114	GLN
1	D	120	THR
1	E	7	LEU
1	E	57	PHE
1	E	112	LYS
1	E	120	THR
1	F	6	GLU
1	F	20[A]	THR
1	F	20[B]	THR
1	F	57	PHE
1	F	90	GLN
1	G	15	ASN
1	G	57	PHE
1	H	57	PHE
1	I	57	PHE
1	I	85	ILE
1	K	57	PHE
1	J	57	PHE
1	L	57	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	69	ASN
1	B	90	GLN
1	B	98	GLN
1	C	5	GLN
1	C	53	ASN
1	C	119	GLN
1	D	98	GLN
1	D	109	GLN
1	D	119	GLN
1	E	5	GLN
1	E	16	GLN
1	E	98	GLN
1	F	5	GLN
1	G	5	GLN
1	G	15	ASN
1	G	98	GLN
1	G	109	GLN
1	H	46	GLN
1	H	102	ASN
1	K	5	GLN
1	K	90	GLN
1	J	5	GLN
1	J	24	ASN
1	L	5	GLN
1	L	24	ASN

### 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	FMT	D	201	-	2,2,2	0.70	0	1,1,1	0.24	0
2	FMT	H	201	-	2,2,2	0.69	0	1,1,1	0.20	0
2	FMT	J	201	-	2,2,2	0.78	0	1,1,1	0.36	0
2	FMT	I	201	-	2,2,2	0.62	0	1,1,1	0.29	0
2	FMT	K	202	-	2,2,2	0.66	0	1,1,1	0.18	0
2	FMT	K	201	-	2,2,2	0.66	0	1,1,1	0.13	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 ⓘ

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(Å²)	Q<0.9	
1	A	117/122 (95%)	-0.19	6 (5%)	28	27	11, 15, 27, 34	2 (1%)
1	B	113/122 (92%)	-0.31	5 (4%)	34	34	11, 16, 28, 35	4 (3%)
1	C	117/122 (95%)	-0.40	3 (2%)	56	55	10, 14, 22, 32	3 (2%)
1	D	120/122 (98%)	-0.22	4 (3%)	46	46	10, 14, 27, 31	3 (2%)
1	E	118/122 (96%)	-0.31	7 (5%)	22	20	12, 16, 26, 40	5 (4%)
1	F	117/122 (95%)	-0.01	10 (8%)	10	9	12, 19, 32, 36	2 (1%)
1	G	119/122 (97%)	-0.39	3 (2%)	57	57	11, 15, 23, 29	1 (0%)
1	H	117/122 (95%)	-0.12	5 (4%)	35	35	13, 18, 28, 35	3 (2%)
1	I	117/122 (95%)	-0.18	5 (4%)	35	35	11, 16, 28, 35	3 (2%)
1	J	119/122 (97%)	-0.38	4 (3%)	45	44	12, 15, 25, 27	2 (1%)
1	K	117/122 (95%)	-0.27	4 (3%)	45	44	11, 15, 30, 37	5 (4%)
1	L	120/122 (98%)	-0.21	5 (4%)	36	37	10, 14, 27, 33	4 (3%)
All	All	1411/1464 (96%)	-0.25	61 (4%)	35	35	10, 16, 28, 40	37 (2%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	43	PHE	8.9
1	F	42	GLY	7.1
1	H	41	ALA	6.8
1	F	43	PHE	5.9
1	F	121	SER	5.7
1	A	89	GLY	5.3
1	B	88	GLY	5.3
1	G	2	ALA	5.0
1	I	4	ALA	4.9
1	K	3	MET	4.7
1	E	88	GLY	4.6

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Mol	Chain	Res	Type	RSRZ
1	E	87	THR	4.4
1	D	2	ALA	4.4
1	F	41	ALA	4.3
1	J	43	PHE	4.1
1	H	42	GLY	4.0
1	F	89	GLY	3.9
1	I	88	GLY	3.7
1	G	120	THR	3.6
1	D	121	SER	3.6
1	L	88	GLY	3.5
1	L	43	PHE	3.4
1	A	90	GLN	3.4
1	H	16	GLN	3.3
1	D	43	PHE	3.3
1	B	120	THR	3.3
1	E	121	SER	3.2
1	J	41	ALA	3.2
1	H	17	ASP	3.2
1	A	122	ALA	3.2
1	B	43	PHE	3.1
1	I	43	PHE	3.0
1	G	43	PHE	3.0
1	A	87	THR	2.9
1	F	122	ALA	2.9
1	C	120	THR	2.9
1	A	88	GLY	2.8
1	E	90	GLN	2.8
1	E	4	ALA	2.7
1	K	4	ALA	2.7
1	I	86	ASN	2.7
1	J	120	THR	2.6
1	A	42	GLY	2.6
1	J	2	ALA	2.6
1	L	3	MET	2.6
1	E	120	THR	2.6
1	E	89	GLY	2.5
1	L	4	ALA	2.4
1	C	88	GLY	2.4
1	K	120	THR	2.3
1	D	42	GLY	2.3
1	L	122	ALA	2.3
1	B	87	THR	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	5	GLN	2.2
1	B	41	ALA	2.1
1	C	87	THR	2.1
1	F	17	ASP	2.1
1	K	41	ALA	2.1
1	F	16	GLN	2.0
1	F	120	THR	2.0
1	I	87	THR	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( $\text{\AA}^2$ )	Q<0.9
2	FMT	K	202	3/3	0.52	0.12	37,37,38,38	0
2	FMT	K	201	3/3	0.68	0.12	27,27,27,28	0
2	FMT	H	201	3/3	0.70	0.11	41,41,41,42	0
2	FMT	I	201	3/3	0.82	0.10	33,33,33,34	0
2	FMT	D	201	3/3	0.85	0.10	37,37,37,37	0
2	FMT	J	201	3/3	0.90	0.11	30,30,30,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.