



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 06:05 am GMT

PDB ID : 4W91  
Title : Crystal structure of a cysteine desulfurase SufS from *Brucella suis* bound to PLP  
Authors : Seattle Structural Genomics Center for Infectious Disease  
Deposited on : 2014-08-26  
Resolution : 2.45 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

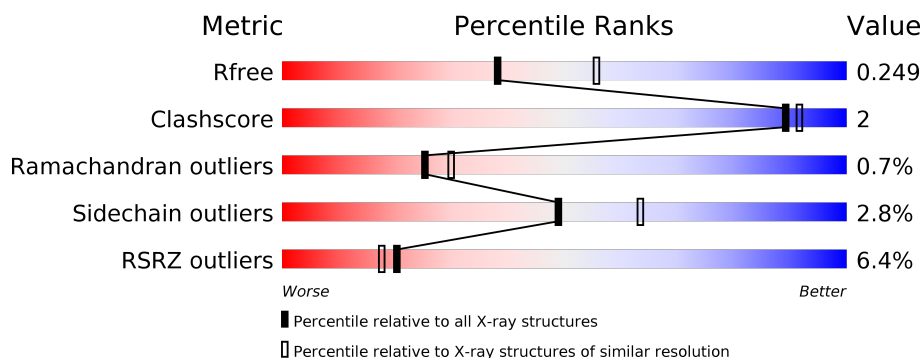
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	100719	1119 (2.48-2.44)
Clashscore	112137	1193 (2.48-2.44)
Ramachandran outliers	110173	1185 (2.48-2.44)
Sidechain outliers	110143	1185 (2.48-2.44)
RSRZ outliers	101464	1126 (2.48-2.44)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	422	<div> <div></div> <div>88% 6% . .</div> </div>
1	B	422	<div> <div></div> <div>88% 6% . .</div> </div>
1	C	422	<div> <div></div> <div>86% 9% . .</div> </div>
1	D	422	<div> <div></div> <div>87% 7% . .</div> </div>
1	E	422	<div> <div></div> <div>87% 8% . .</div> </div>
1	F	422	<div> <div></div> <div>88% 6% . .</div> </div>

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Mol	Chain	Length	Quality of chain
1	G	422	<div><div></div><div>3%</div><div>87%</div><div>8%</div><div>• 5%</div></div>
1	H	422	<div><div></div><div>4%</div><div>89%</div><div>5%</div><div>5%</div></div>
1	I	422	<div><div></div><div>28%</div><div>90%</div><div>• 6%</div></div>
1	J	422	<div><div></div><div>24%</div><div>81%</div><div>• • 16%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 30371 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 Aminotransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	404	Total	C	N	O	P	S	0	2	0
			3117	1974	558	573	1	11			
1	B	405	Total	C	N	O	P	S	0	0	0
			3110	1970	555	574	1	10			
1	C	404	Total	C	N	O	P	S	0	0	0
			3118	1973	558	576	1	10			
1	D	404	Total	C	N	O	P	S	0	1	0
			3131	1982	560	577	1	11			
1	E	404	Total	C	N	O	P	S	0	0	0
			3083	1952	548	572	1	10			
1	F	404	Total	C	N	O	P	S	0	1	0
			3097	1961	552	573	1	10			
1	G	403	Total	C	N	O	P	S	0	0	0
			3041	1931	536	563	1	10			
1	H	400	Total	C	N	O	P	S	0	0	0
			3041	1927	542	560	1	11			
1	I	398	Total	C	N	O	P	S	0	0	0
			2764	1728	501	525	1	9			
1	J	356	Total	C	N	O	P	S	0	0	0
			2508	1575	449	474	1	9			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP D0BBJ1
A	-6	ALA	-	expression tag	UNP D0BBJ1
A	-5	HIS	-	expression tag	UNP D0BBJ1
A	-4	HIS	-	expression tag	UNP D0BBJ1
A	-3	HIS	-	expression tag	UNP D0BBJ1
A	-2	HIS	-	expression tag	UNP D0BBJ1
A	-1	HIS	-	expression tag	UNP D0BBJ1
A	0	HIS	-	expression tag	UNP D0BBJ1
B	-7	MET	-	initiating methionine	UNP D0BBJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-6	ALA	-	expression tag	UNP D0BBJ1
B	-5	HIS	-	expression tag	UNP D0BBJ1
B	-4	HIS	-	expression tag	UNP D0BBJ1
B	-3	HIS	-	expression tag	UNP D0BBJ1
B	-2	HIS	-	expression tag	UNP D0BBJ1
B	-1	HIS	-	expression tag	UNP D0BBJ1
B	0	HIS	-	expression tag	UNP D0BBJ1
C	-7	MET	-	initiating methionine	UNP D0BBJ1
C	-6	ALA	-	expression tag	UNP D0BBJ1
C	-5	HIS	-	expression tag	UNP D0BBJ1
C	-4	HIS	-	expression tag	UNP D0BBJ1
C	-3	HIS	-	expression tag	UNP D0BBJ1
C	-2	HIS	-	expression tag	UNP D0BBJ1
C	-1	HIS	-	expression tag	UNP D0BBJ1
C	0	HIS	-	expression tag	UNP D0BBJ1
D	-7	MET	-	initiating methionine	UNP D0BBJ1
D	-6	ALA	-	expression tag	UNP D0BBJ1
D	-5	HIS	-	expression tag	UNP D0BBJ1
D	-4	HIS	-	expression tag	UNP D0BBJ1
D	-3	HIS	-	expression tag	UNP D0BBJ1
D	-2	HIS	-	expression tag	UNP D0BBJ1
D	-1	HIS	-	expression tag	UNP D0BBJ1
D	0	HIS	-	expression tag	UNP D0BBJ1
E	-7	MET	-	initiating methionine	UNP D0BBJ1
E	-6	ALA	-	expression tag	UNP D0BBJ1
E	-5	HIS	-	expression tag	UNP D0BBJ1
E	-4	HIS	-	expression tag	UNP D0BBJ1
E	-3	HIS	-	expression tag	UNP D0BBJ1
E	-2	HIS	-	expression tag	UNP D0BBJ1
E	-1	HIS	-	expression tag	UNP D0BBJ1
E	0	HIS	-	expression tag	UNP D0BBJ1
F	-7	MET	-	initiating methionine	UNP D0BBJ1
F	-6	ALA	-	expression tag	UNP D0BBJ1
F	-5	HIS	-	expression tag	UNP D0BBJ1
F	-4	HIS	-	expression tag	UNP D0BBJ1
F	-3	HIS	-	expression tag	UNP D0BBJ1
F	-2	HIS	-	expression tag	UNP D0BBJ1
F	-1	HIS	-	expression tag	UNP D0BBJ1
F	0	HIS	-	expression tag	UNP D0BBJ1
G	-7	MET	-	initiating methionine	UNP D0BBJ1
G	-6	ALA	-	expression tag	UNP D0BBJ1
G	-5	HIS	-	expression tag	UNP D0BBJ1

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-4	HIS	-	expression tag	UNP D0BBJ1
G	-3	HIS	-	expression tag	UNP D0BBJ1
G	-2	HIS	-	expression tag	UNP D0BBJ1
G	-1	HIS	-	expression tag	UNP D0BBJ1
G	0	HIS	-	expression tag	UNP D0BBJ1
H	-7	MET	-	initiating methionine	UNP D0BBJ1
H	-6	ALA	-	expression tag	UNP D0BBJ1
H	-5	HIS	-	expression tag	UNP D0BBJ1
H	-4	HIS	-	expression tag	UNP D0BBJ1
H	-3	HIS	-	expression tag	UNP D0BBJ1
H	-2	HIS	-	expression tag	UNP D0BBJ1
H	-1	HIS	-	expression tag	UNP D0BBJ1
H	0	HIS	-	expression tag	UNP D0BBJ1
I	-7	MET	-	initiating methionine	UNP D0BBJ1
I	-6	ALA	-	expression tag	UNP D0BBJ1
I	-5	HIS	-	expression tag	UNP D0BBJ1
I	-4	HIS	-	expression tag	UNP D0BBJ1
I	-3	HIS	-	expression tag	UNP D0BBJ1
I	-2	HIS	-	expression tag	UNP D0BBJ1
I	-1	HIS	-	expression tag	UNP D0BBJ1
I	0	HIS	-	expression tag	UNP D0BBJ1
J	-7	MET	-	initiating methionine	UNP D0BBJ1
J	-6	ALA	-	expression tag	UNP D0BBJ1
J	-5	HIS	-	expression tag	UNP D0BBJ1
J	-4	HIS	-	expression tag	UNP D0BBJ1
J	-3	HIS	-	expression tag	UNP D0BBJ1
J	-2	HIS	-	expression tag	UNP D0BBJ1
J	-1	HIS	-	expression tag	UNP D0BBJ1
J	0	HIS	-	expression tag	UNP D0BBJ1

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0
2	H	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	I	1	Total Cl 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	1	Total 1	Cl 1	0	0
2	A	1	Total 1	Cl 1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	46	Total 46	O 46	0	0
3	B	52	Total 52	O 52	0	0
3	C	38	Total 38	O 38	0	0
3	D	54	Total 54	O 54	0	0
3	E	41	Total 41	O 41	0	0
3	F	49	Total 49	O 49	0	0
3	G	41	Total 41	O 41	0	0
3	H	28	Total 28	O 28	0	0
3	I	2	Total 2	O 2	0	0
3	J	3	Total 3	O 3	0	0



- Molecule 1: Aminotransferase

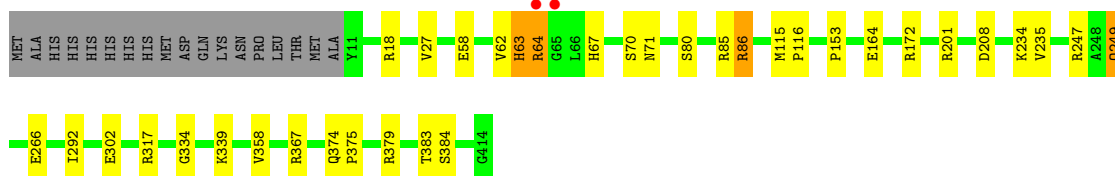






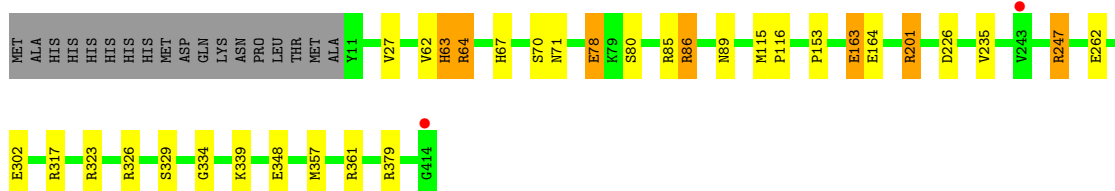
• Molecule 1: Aminotransferase

Chain E: 87% 8%



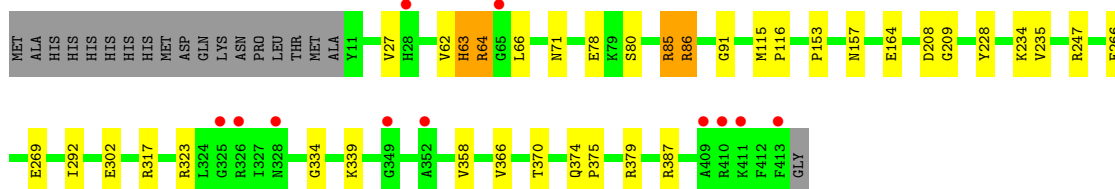
• Molecule 1: Aminotransferase

Chain F: 88% 6%



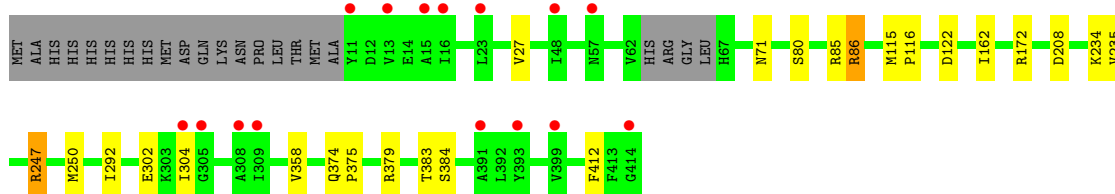
• Molecule 1: Aminotransferase

Chain G: 3% 87% 8% 5%



• Molecule 1: Aminotransferase

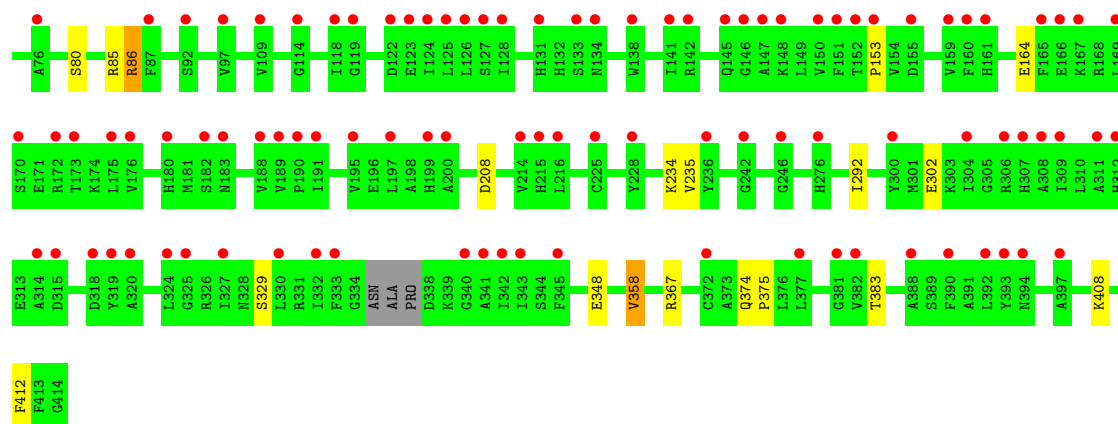
Chain H: 4% 89% 5% 5%



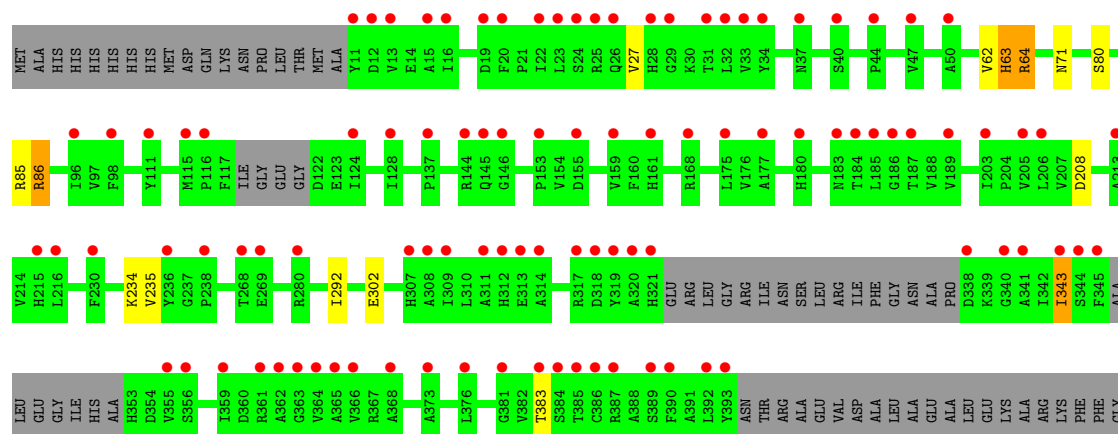
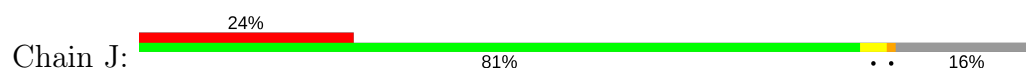
• Molecule 1: Aminotransferase

Chain I: 28% 90% 6%





● Molecule 1: Aminotransferase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.85Å 121.91Å 133.72Å 111.49° 106.53° 89.81°	Depositor
Resolution (Å)	50.00 – 2.45 48.39 – 2.45	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.45) 84.4 (48.39-2.45)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, $R_{free}$	0.237 , 0.252 0.231 , 0.249	Depositor DCC
$R_{free}$ test set	8955 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	34.6	Xtriage
Anisotropy	1.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.1	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	0.93	EDS
Total number of atoms	30371	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: LLP, CL

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	0.57	0/3168	0.77	7/4301 (0.2%)
1	B	0.58	0/3155	0.70	3/4284 (0.1%)
1	C	0.60	2/3163 (0.1%)	0.75	7/4293 (0.2%)
1	D	0.62	1/3179 (0.0%)	0.73	4/4312 (0.1%)
1	E	0.59	0/3128	0.76	11/4254 (0.3%)
1	F	0.58	1/3146 (0.0%)	0.71	3/4277 (0.1%)
1	G	0.52	1/3084 (0.0%)	0.70	3/4201 (0.1%)
1	H	0.52	0/3084	0.73	5/4194 (0.1%)
1	I	0.48	0/2794	0.66	2/3822 (0.1%)
1	J	0.47	0/2538	0.64	3/3472 (0.1%)
All	All	0.56	5/30439 (0.0%)	0.72	48/41410 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	78	GLU	CD-OE2	5.69	1.31	1.25
1	G	78	GLU	CD-OE2	5.55	1.31	1.25
1	F	80	SER	CA-CB	5.49	1.61	1.52
1	C	384	SER	CA-CB	-5.25	1.45	1.52
1	C	384	SER	CB-OG	-5.04	1.35	1.42

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	ARG	NE-CZ-NH1	10.86	125.73	120.30
1	C	201	ARG	NE-CZ-NH2	9.40	125.00	120.30
1	A	379	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	D	247	ARG	NE-CZ-NH1	-8.82	115.89	120.30
1	A	247	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	247	ARG	NE-CZ-NH1	8.52	124.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	247	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	C	201	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	E	18	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	F	78	GLU	OE1-CD-OE2	-7.83	113.91	123.30
1	H	247	ARG	NE-CZ-NH2	-7.51	116.54	120.30
1	H	304	ILE	CG1-CB-CG2	7.50	127.90	111.40
1	C	115	MET	CG-SD-CE	7.47	112.16	100.20
1	H	250	MET	CG-SD-CE	7.40	112.05	100.20
1	E	247	ARG	NE-CZ-NH1	-7.03	116.78	120.30
1	C	247	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	B	86	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	E	172	ARG	NE-CZ-NH2	-6.65	116.98	120.30
1	E	172	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	D	86	ARG	NE-CZ-NH2	-6.35	117.12	120.30
1	J	86	ARG	NE-CZ-NH2	-6.35	117.13	120.30
1	A	357	MET	CG-SD-CE	6.25	110.20	100.20
1	H	247	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	E	247	ARG	CG-CD-NE	6.07	124.54	111.80
1	J	343	ILE	CB-CA-C	5.98	123.56	111.60
1	C	86	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	F	86	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	E	367	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	G	247	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	J	86	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	86	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	E	86	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	E	247	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	B	86	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	I	367	ARG	NE-CZ-NH1	5.37	122.99	120.30
1	G	247	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	E	18	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	D	172	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	E	58	GLU	CB-CA-C	5.28	120.95	110.40
1	I	86	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	17	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	F	201	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	H	86	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	A	172	ARG	CG-CD-NE	-5.10	101.09	111.80
1	D	247	ARG	NE-CZ-NH2	5.09	122.84	120.30
1	E	172	ARG	CD-NE-CZ	5.08	130.71	123.60
1	C	86	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	G	86	ARG	NE-CZ-NH2	-5.04	117.78	120.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3117	0	3021	21	0
1	B	3110	0	3012	16	0
1	C	3118	0	3023	16	0
1	D	3131	0	3048	17	0
1	E	3083	0	2950	12	0
1	F	3097	0	2972	15	0
1	G	3041	0	2896	16	0
1	H	3041	0	2917	10	0
1	I	2764	0	2421	9	0
1	J	2508	0	2181	5	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	H	1	0	0	0	0
2	I	1	0	0	0	0
3	A	46	0	0	1	0
3	B	52	0	0	1	0
3	C	38	0	0	0	0
3	D	54	0	0	0	0
3	E	41	0	0	0	0
3	F	49	0	0	0	0
3	G	41	0	0	1	0
3	H	28	0	0	2	0
3	I	2	0	0	0	0
3	J	3	0	0	0	0
All	All	30371	0	28441	126	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 2.

All (126) 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:F:78:GLU:HA	1:F:78:GLU:OE1	1.67	0.94
1:H:247:ARG:HD3	3:H:621:HOH:O	1.81	0.79
1:C:115:MET:HB3	1:C:116:PRO:HD3	1.75	0.69
1:D:115:MET:HB3	1:D:116:PRO:HD3	1.76	0.68
1:A:115:MET:HB3	1:A:116:PRO:HD3	1.74	0.67
1:H:115:MET:HB3	1:H:116:PRO:HD3	1.77	0.67
1:F:115:MET:HB3	1:F:116:PRO:HD3	1.76	0.66
1:E:115:MET:HB3	1:E:116:PRO:HD3	1.77	0.66
1:C:249:GLN:O	1:C:253:LYS:HG2	1.97	0.65
1:G:115:MET:HB3	1:G:116:PRO:HD3	1.76	0.65
1:B:379:ARG:O	1:D:381:GLY:HA2	1.96	0.64
1:F:323:ARG:HA	1:F:326:ARG:HD2	1.81	0.63
1:B:62:VAL:O	1:B:64:ARG:N	2.32	0.63
1:D:62:VAL:O	1:D:64:ARG:N	2.32	0.63
1:D:414:GLY:O	1:I:408:LYS:NZ	2.32	0.63
1:E:62:VAL:O	1:E:64:ARG:N	2.33	0.62
1:A:62:VAL:O	1:A:64:ARG:N	2.33	0.61
1:H:247:ARG:CD	3:H:621:HOH:O	2.45	0.61
1:D:412:PHE:CZ	1:I:358:VAL:HG13	2.36	0.60
1:C:122:ASP:OD1	1:C:172:ARG:NH1	2.33	0.60
1:A:121:GLY:C	1:A:172:ARG:HH21	2.04	0.60
1:C:62:VAL:O	1:C:64:ARG:N	2.30	0.60
1:G:62:VAL:O	1:G:64:ARG:N	2.32	0.59
1:B:122:ASP:OD1	1:B:172:ARG:NH1	2.35	0.59
1:J:62:VAL:O	1:J:64:ARG:N	2.35	0.59
1:F:62:VAL:O	1:F:64:ARG:N	2.32	0.59
1:H:122:ASP:OD1	1:H:172:ARG:NH1	2.34	0.59
1:B:381:GLY:HA2	1:D:379:ARG:O	2.04	0.58
1:F:226:ASP:HA	1:F:247:ARG:HD3	1.87	0.56
1:I:153:PRO:HG2	1:I:164:GLU:HG2	1.89	0.55
1:G:366:VAL:HG22	1:G:387:ARG:O	2.07	0.55
1:D:358:VAL:HG13	1:I:412:PHE:CZ	2.41	0.55
1:B:153:PRO:HG2	1:B:164:GLU:HG2	1.89	0.55
1:C:366:VAL:HG22	1:C:387:ARG:O	2.08	0.54
1:F:153:PRO:HG2	1:F:164:GLU:HG2	1.89	0.54
1:E:153:PRO:HG2	1:E:164:GLU:HG2	1.89	0.54
1:G:153:PRO:HG2	1:G:164:GLU:HG2	1.90	0.53
1:A:357:MET:HG3	1:A:358:VAL:N	2.23	0.53
1:E:334:GLY:O	1:E:339:LYS:NZ	2.41	0.53
1:A:153:PRO:HG2	1:A:164:GLU:HG2	1.90	0.53
1:A:334:GLY:O	1:A:339:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:334:GLY:O	1:F:339:LYS:NZ	2.41	0.53
1:B:334:GLY:O	1:B:339:LYS:NZ	2.41	0.52
1:I:329:SER:OG	1:I:348:GLU:CB	2.57	0.52
1:A:357:MET:HG2	1:F:361:ARG:HG3	1.91	0.52
1:B:63:HIS:O	1:B:64:ARG:C	2.48	0.52
1:D:153:PRO:HG2	1:D:164:GLU:HG2	1.92	0.52
1:A:335:ASN:HB2	3:A:632:HOH:O	2.08	0.52
1:A:86:ARG:HG3	1:G:91:GLY:O	2.10	0.51
1:G:334:GLY:O	1:G:339:LYS:NZ	2.42	0.51
1:F:163:GLU:H	1:F:163:GLU:CD	2.14	0.51
1:B:358:VAL:HG13	1:H:412:PHE:CZ	2.46	0.51
1:C:153:PRO:HG2	1:C:164:GLU:HG2	1.93	0.50
1:A:208:ASP:OD2	1:A:234:LLP:N1	2.45	0.50
1:C:334:GLY:O	1:C:339:LYS:NZ	2.42	0.50
1:D:122:ASP:OD1	1:D:172:ARG:NH2	2.39	0.49
1:D:208:ASP:OD2	1:D:234:LLP:N1	2.46	0.49
1:E:63:HIS:O	1:E:64:ARG:C	2.52	0.49
1:F:329:SER:OG	1:F:348:GLU:CB	2.60	0.48
1:D:339:LYS:NZ	1:D:342:ILE:O	2.46	0.48
1:J:63:HIS:O	1:J:64:ARG:C	2.51	0.48
1:C:322:GLU:OE2	1:C:326:ARG:NH1	2.46	0.47
1:C:208:ASP:OD2	1:C:234:LLP:N1	2.47	0.47
1:A:63:HIS:O	1:A:64:ARG:C	2.52	0.46
1:G:208:ASP:OD2	1:G:234:LLP:N1	2.47	0.46
1:D:86:ARG:HD2	1:D:302:GLU:OE2	2.15	0.46
1:D:63:HIS:O	1:D:64:ARG:C	2.53	0.46
1:F:86:ARG:HD2	1:F:302:GLU:OE2	2.16	0.45
1:H:208:ASP:OD2	1:H:234:LLP:N1	2.49	0.45
1:F:63:HIS:O	1:F:64:ARG:C	2.54	0.45
1:A:67:HIS:CE1	1:A:70:SER:HB2	2.53	0.44
1:C:128:ILE:CG2	1:C:154:VAL:HG22	2.46	0.44
1:B:208:ASP:OD2	1:B:234:LLP:N1	2.50	0.44
1:C:374:GLN:HB2	1:C:375:PRO:HD3	2.00	0.44
1:E:374:GLN:HB2	1:E:375:PRO:HD3	2.00	0.44
1:C:63:HIS:O	1:C:64:ARG:C	2.55	0.44
1:B:217:PRO:HD2	3:B:641:HOH:O	2.18	0.44
1:A:86:ARG:HD2	1:A:302:GLU:OE2	2.17	0.44
1:I:208:ASP:OD2	1:I:234:LLP:N1	2.51	0.44
1:G:86:ARG:HD2	1:G:302:GLU:OE2	2.18	0.44
1:A:80:SER:OG	1:A:292:ILE:HA	2.18	0.43
1:G:63:HIS:O	1:G:64:ARG:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:SER:OG	1:C:292:ILE:HA	2.19	0.43
1:E:208:ASP:OD2	1:E:234:LLP:N1	2.52	0.43
1:G:66:LEU:N	1:G:66:LEU:HD12	2.33	0.43
1:D:339:LYS:HD3	1:D:340:GLY:O	2.18	0.43
1:A:121:GLY:CA	1:A:172:ARG:HH21	2.32	0.43
1:G:317:ARG:HD2	1:G:339:LYS:HG2	2.01	0.43
1:A:121:GLY:HA3	1:A:172:ARG:HH21	1.83	0.43
1:A:104:GLU:OE2	1:B:104:GLU:OE2	2.37	0.43
1:B:374:GLN:HB2	1:B:375:PRO:HD3	2.00	0.43
1:J:80:SER:OG	1:J:292:ILE:HA	2.19	0.43
1:B:80:SER:OG	1:B:292:ILE:HA	2.19	0.42
1:C:317:ARG:HD2	1:C:339:LYS:HG2	2.01	0.42
1:G:85:ARG:NH2	3:G:510:HOH:O	2.51	0.42
1:C:67:HIS:CE1	1:C:70:SER:HB2	2.55	0.42
1:E:80:SER:OG	1:E:292:ILE:HA	2.20	0.42
1:H:374:GLN:HB2	1:H:375:PRO:HD3	2.01	0.42
1:I:86:ARG:HD2	1:I:302:GLU:OE2	2.20	0.42
1:J:208:ASP:OD2	1:J:234:LLP:N1	2.52	0.42
1:F:67:HIS:CE1	1:F:70:SER:HB2	2.54	0.42
1:I:80:SER:OG	1:I:292:ILE:HA	2.20	0.42
1:E:86:ARG:HD2	1:E:302:GLU:OE2	2.19	0.42
1:C:253:LYS:HG2	1:C:253:LYS:H	1.64	0.42
1:D:374:GLN:HB2	1:D:375:PRO:HD3	2.01	0.42
1:G:80:SER:OG	1:G:292:ILE:HA	2.20	0.42
1:G:374:GLN:HB2	1:G:375:PRO:HD3	2.01	0.42
1:B:86:ARG:HD2	1:B:302:GLU:OE2	2.20	0.41
1:D:67:HIS:CE1	1:D:70:SER:HB2	2.55	0.41
1:E:249:GLN:H	1:E:249:GLN:CD	2.24	0.41
1:A:115:MET:HB3	1:A:116:PRO:CD	2.47	0.41
1:F:317:ARG:HD2	1:F:339:LYS:HG2	2.02	0.41
1:B:317:ARG:HD2	1:B:339:LYS:HG2	2.01	0.41
1:A:374:GLN:HB2	1:A:375:PRO:HD3	2.03	0.41
1:H:86:ARG:HD2	1:H:302:GLU:OE2	2.20	0.41
1:I:374:GLN:HB2	1:I:375:PRO:HD3	2.03	0.41
1:E:317:ARG:HD2	1:E:339:LYS:HG2	2.01	0.41
1:E:67:HIS:CE1	1:E:70:SER:HB2	2.56	0.41
1:D:357:MET:SD	1:D:357:MET:C	2.99	0.41
1:G:209:GLY:HA3	1:G:228:TYR:CZ	2.56	0.40
1:H:80:SER:OG	1:H:292:ILE:HA	2.20	0.40
1:B:226:ASP:HA	1:B:247:ARG:HG3	2.02	0.40
1:J:86:ARG:HD2	1:J:302:GLU:OE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:MET:HE1	1:F:357:MET:O	2.21	0.40
1:G:269:GLU:CD	1:H:379:ARG:HH11	2.25	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	403/422 (96%)	390 (97%)	10 (2%)	3 (1%)	25	30
1	B	402/422 (95%)	389 (97%)	10 (2%)	3 (1%)	25	30
1	C	401/422 (95%)	388 (97%)	10 (2%)	3 (1%)	25	30
1	D	402/422 (95%)	388 (96%)	11 (3%)	3 (1%)	25	30
1	E	401/422 (95%)	388 (97%)	10 (2%)	3 (1%)	25	30
1	F	402/422 (95%)	389 (97%)	10 (2%)	3 (1%)	25	30
1	G	400/422 (95%)	387 (97%)	10 (2%)	3 (1%)	22	26
1	H	395/422 (94%)	384 (97%)	10 (2%)	1 (0%)	44	55
1	I	391/422 (93%)	380 (97%)	10 (3%)	1 (0%)	44	55
1	J	347/422 (82%)	335 (96%)	9 (3%)	3 (1%)	20	23
All	All	3944/4220 (94%)	3818 (97%)	100 (2%)	26 (1%)	25	30

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	B	64	ARG
1	C	64	ARG
1	D	64	ARG
1	E	64	ARG

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Mol	Chain	Res	Type
1	F	64	ARG
1	G	64	ARG
1	J	64	ARG
1	E	63	HIS
1	J	63	HIS
1	B	63	HIS
1	C	63	HIS
1	D	63	HIS
1	F	63	HIS
1	G	63	HIS
1	A	63	HIS
1	C	235	VAL
1	B	235	VAL
1	D	235	VAL
1	F	235	VAL
1	G	235	VAL
1	H	235	VAL
1	I	235	VAL
1	J	235	VAL
1	A	235	VAL
1	E	235	VAL

### 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	312/341 (92%)	301 (96%)	11 (4%)	41	56
1	B	311/341 (91%)	303 (97%)	8 (3%)	51	66
1	C	313/341 (92%)	303 (97%)	10 (3%)	44	58
1	D	316/341 (93%)	307 (97%)	9 (3%)	49	63
1	E	305/341 (89%)	295 (97%)	10 (3%)	43	57
1	F	308/341 (90%)	299 (97%)	9 (3%)	48	61
1	G	297/341 (87%)	288 (97%)	9 (3%)	46	60
1	H	300/341 (88%)	293 (98%)	7 (2%)	56	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	233/341 (68%)	229 (98%)	4 (2%)	66	78
1	J	215/341 (63%)	210 (98%)	5 (2%)	56	70
All	All	2910/3410 (85%)	2828 (97%)	82 (3%)	49	63

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	GLU
1	A	27	VAL
1	A	71	ASN
1	A	85	ARG
1	A	115	MET
1	A	247	ARG
1	A	253	LYS
1	A	357	MET
1	A	358	VAL
1	A	379	ARG
1	A	383	THR
1	B	27	VAL
1	B	71	ASN
1	B	85	ARG
1	B	115	MET
1	B	247	ARG
1	B	358	VAL
1	B	379	ARG
1	B	383	THR
1	C	27	VAL
1	C	71	ASN
1	C	85	ARG
1	C	115	MET
1	C	162	ILE
1	C	253	LYS
1	C	323	ARG
1	C	358	VAL
1	C	379	ARG
1	C	383	THR
1	D	27	VAL
1	D	71	ASN
1	D	85	ARG
1	D	201[A]	ARG
1	D	201[B]	ARG

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Mol	Chain	Res	Type
1	D	247	ARG
1	D	323	ARG
1	D	379	ARG
1	D	383	THR
1	E	27	VAL
1	E	71	ASN
1	E	85	ARG
1	E	201	ARG
1	E	249	GLN
1	E	266	GLU
1	E	358	VAL
1	E	379	ARG
1	E	383	THR
1	E	384	SER
1	F	27	VAL
1	F	71	ASN
1	F	85	ARG
1	F	89	ASN
1	F	163	GLU
1	F	201	ARG
1	F	247	ARG
1	F	262	GLU
1	F	379	ARG
1	G	27	VAL
1	G	71	ASN
1	G	85	ARG
1	G	157	ASN
1	G	266	GLU
1	G	323	ARG
1	G	358	VAL
1	G	370	THR
1	G	379	ARG
1	H	27	VAL
1	H	71	ASN
1	H	85	ARG
1	H	162	ILE
1	H	358	VAL
1	H	383	THR
1	H	384	SER
1	I	27	VAL
1	I	85	ARG
1	I	358	VAL

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Mol	Chain	Res	Type
1	I	383	THR
1	J	27	VAL
1	J	71	ASN
1	J	85	ARG
1	J	343	ILE
1	J	383	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	335	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

10 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	LLP	A	234	1	24,24,25	3.37	4 (16%)	28,32,34	1.31	2 (7%)
1	LLP	B	234	1	24,24,25	2.90	6 (25%)	28,32,34	1.54	5 (17%)
1	LLP	C	234	1	24,24,25	3.03	5 (20%)	28,32,34	1.28	3 (10%)
1	LLP	D	234	1	24,24,25	3.29	5 (20%)	28,32,34	1.51	4 (14%)
1	LLP	E	234	1	24,24,25	2.64	6 (25%)	28,32,34	1.40	3 (10%)
1	LLP	F	234	1	24,24,25	2.85	5 (20%)	28,32,34	1.38	3 (10%)
1	LLP	G	234	1	24,24,25	3.36	5 (20%)	28,32,34	1.36	3 (10%)
1	LLP	H	234	1	24,24,25	3.32	5 (20%)	28,32,34	1.38	5 (17%)
1	LLP	I	234	1	24,24,25	3.24	5 (20%)	28,32,34	1.33	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	LLP	J	234	1	24,24,25	3.15	5 (20%)	28,32,34	1.43	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	A	234	1	-	0/15/17/19	0/1/1/1
1	LLP	B	234	1	-	0/15/17/19	0/1/1/1
1	LLP	C	234	1	-	0/15/17/19	0/1/1/1
1	LLP	D	234	1	-	0/15/17/19	0/1/1/1
1	LLP	E	234	1	-	0/15/17/19	0/1/1/1
1	LLP	F	234	1	-	0/15/17/19	0/1/1/1
1	LLP	G	234	1	-	0/15/17/19	0/1/1/1
1	LLP	H	234	1	-	0/15/17/19	0/1/1/1
1	LLP	I	234	1	-	0/15/17/19	0/1/1/1
1	LLP	J	234	1	-	0/15/17/19	0/1/1/1

All (51) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	234	LLP	C6-C5	2.02	1.41	1.37
1	I	234	LLP	C4-C4'	2.10	1.50	1.46
1	D	234	LLP	C4-C4'	2.11	1.50	1.46
1	E	234	LLP	CA-C	2.11	1.53	1.50
1	C	234	LLP	C4-C4'	2.43	1.50	1.46
1	H	234	LLP	C4-C4'	2.45	1.51	1.46
1	E	234	LLP	C4-C4'	2.71	1.51	1.46
1	B	234	LLP	CA-C	2.74	1.53	1.50
1	G	234	LLP	C4-C4'	2.95	1.51	1.46
1	J	234	LLP	C4-C4'	3.09	1.52	1.46
1	B	234	LLP	C4-C3	3.54	1.46	1.40
1	B	234	LLP	C4-C4'	3.59	1.53	1.46
1	C	234	LLP	C4-C5	3.62	1.46	1.42
1	E	234	LLP	C4-C3	3.64	1.46	1.40
1	C	234	LLP	C4-C3	3.91	1.47	1.40
1	E	234	LLP	C4-C5	4.06	1.47	1.42
1	J	234	LLP	C4-C3	4.18	1.47	1.40
1	A	234	LLP	C4-C3	4.43	1.48	1.40
1	H	234	LLP	C4-C5	4.47	1.47	1.42
1	D	234	LLP	C4-C3	4.53	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	234	LLP	C4-C5	4.60	1.47	1.42
1	I	234	LLP	C4-C3	4.82	1.48	1.40
1	G	234	LLP	C4-C3	4.88	1.48	1.40
1	H	234	LLP	C4-C3	4.98	1.49	1.40
1	I	234	LLP	C4-C5	5.06	1.48	1.42
1	A	234	LLP	C4-C5	5.08	1.48	1.42
1	J	234	LLP	C4-C5	5.11	1.48	1.42
1	F	234	LLP	C4-C3	5.23	1.49	1.40
1	G	234	LLP	C4-C5	5.27	1.48	1.42
1	D	234	LLP	C4-C5	5.40	1.48	1.42
1	B	234	LLP	C4'-NZ	5.41	1.43	1.27
1	B	234	LLP	C4-C5	5.46	1.49	1.42
1	F	234	LLP	C4'-NZ	6.01	1.44	1.27
1	D	234	LLP	C4'-NZ	6.08	1.45	1.27
1	J	234	LLP	C4'-NZ	6.10	1.45	1.27
1	A	234	LLP	C4'-NZ	6.10	1.45	1.27
1	I	234	LLP	C4'-NZ	6.21	1.45	1.27
1	H	234	LLP	C4'-NZ	6.28	1.45	1.27
1	E	234	LLP	C4'-NZ	6.28	1.45	1.27
1	C	234	LLP	C4'-NZ	6.31	1.45	1.27
1	G	234	LLP	C4'-NZ	6.35	1.45	1.27
1	E	234	LLP	C3-C2	8.79	1.46	1.40
1	F	234	LLP	C3-C2	9.68	1.47	1.40
1	B	234	LLP	C3-C2	10.11	1.47	1.40
1	C	234	LLP	C3-C2	11.77	1.48	1.40
1	J	234	LLP	C3-C2	11.82	1.48	1.40
1	I	234	LLP	C3-C2	12.14	1.49	1.40
1	G	234	LLP	C3-C2	12.59	1.49	1.40
1	D	234	LLP	C3-C2	12.61	1.49	1.40
1	H	234	LLP	C3-C2	12.83	1.49	1.40
1	A	234	LLP	C3-C2	13.17	1.49	1.40

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	234	LLP	C4-C3-C2	-4.57	117.34	120.15
1	B	234	LLP	C4-C3-C2	-4.08	117.64	120.15
1	A	234	LLP	C4-C3-C2	-4.01	117.69	120.15
1	G	234	LLP	C4-C3-C2	-3.55	117.97	120.15
1	H	234	LLP	C4-C3-C2	-3.44	118.04	120.15
1	E	234	LLP	C4-C3-C2	-3.44	118.04	120.15
1	I	234	LLP	C4-C3-C2	-3.41	118.06	120.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	234	LLP	C4-C3-C2	-3.29	118.13	120.15
1	C	234	LLP	C4-C3-C2	-2.91	118.37	120.15
1	J	234	LLP	C3-C4-C5	-2.75	116.15	118.24
1	J	234	LLP	C4-C4'-NZ	-2.73	111.41	124.66
1	D	234	LLP	C4-C4'-NZ	-2.66	111.72	124.66
1	E	234	LLP	C4-C4'-NZ	-2.66	111.74	124.66
1	B	234	LLP	C4-C4'-NZ	-2.59	112.07	124.66
1	G	234	LLP	C4-C4'-NZ	-2.58	112.13	124.66
1	F	234	LLP	C4-C3-C2	-2.58	118.57	120.15
1	B	234	LLP	C3-C4-C5	-2.54	116.31	118.24
1	C	234	LLP	C4-C4'-NZ	-2.53	112.38	124.66
1	I	234	LLP	C4-C4'-NZ	-2.46	112.73	124.66
1	F	234	LLP	C4-C4'-NZ	-2.41	112.94	124.66
1	H	234	LLP	C4-C4'-NZ	-2.39	113.06	124.66
1	A	234	LLP	C4-C4'-NZ	-2.36	113.19	124.66
1	G	234	LLP	C3-C4-C5	-2.31	116.48	118.24
1	D	234	LLP	C3-C4-C5	-2.30	116.49	118.24
1	H	234	LLP	C3-C4-C5	-2.25	116.53	118.24
1	H	234	LLP	O-C-CA	-2.12	119.17	125.02
1	C	234	LLP	O-C-CA	-2.02	119.44	125.02
1	J	234	LLP	OP2-P-OP4	-2.01	101.40	106.73
1	D	234	LLP	O3-C3-C2	2.12	122.22	117.78
1	B	234	LLP	O3-C3-C2	2.21	122.40	117.78
1	H	234	LLP	C6-N1-C2	2.22	123.53	119.26
1	J	234	LLP	C6-N1-C2	2.45	123.97	119.26
1	I	234	LLP	C6-N1-C2	2.54	124.15	119.26
1	B	234	LLP	C6-N1-C2	2.59	124.24	119.26
1	E	234	LLP	C6-N1-C2	2.89	124.83	119.26
1	F	234	LLP	C6-N1-C2	3.50	125.99	119.26

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	234	LLP	1	0
1	B	234	LLP	1	0
1	C	234	LLP	1	0
1	D	234	LLP	1	0
1	E	234	LLP	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	G	234	LLP	1	0
1	H	234	LLP	1	0
1	I	234	LLP	1	0
1	J	234	LLP	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 7 are monoatomic - leaving 0 for Mogul analysis.

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(Å <sup>2</sup> )	Q<0.9
1	A	403/422 (95%)	-0.06	3 (0%) 87 89	39, 52, 68, 79	0
1	B	404/422 (95%)	-0.03	3 (0%) 87 89	39, 50, 65, 80	0
1	C	403/422 (95%)	-0.11	1 (0%) 94 95	43, 54, 65, 71	0
1	D	403/422 (95%)	-0.07	0 100 100	41, 49, 60, 67	0
1	E	403/422 (95%)	-0.10	2 (0%) 90 92	40, 52, 68, 77	0
1	F	403/422 (95%)	0.01	2 (0%) 90 92	41, 55, 72, 82	0
1	G	402/422 (95%)	0.18	11 (2%) 55 50	51, 63, 87, 105	0
1	H	399/422 (94%)	0.27	15 (3%) 41 38	55, 69, 81, 89	0
1	I	397/422 (94%)	1.57	118 (29%) 1 0	66, 89, 125, 143	0
1	J	355/422 (84%)	1.57	100 (28%) 1 0	70, 85, 106, 116	0
All	All	3972/4220 (94%)	0.31	255 (6%) 20 17	39, 58, 98, 143	0

All (255) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	126	LEU	11.6
1	J	203	ILE	7.6
1	I	76	ALA	7.2
1	J	373	ALA	7.1
1	I	304	ILE	7.0
1	J	33	VAL	6.4
1	J	314	ALA	6.4
1	J	320	ALA	6.3
1	I	214	VAL	6.2
1	I	341	ALA	6.2
1	J	187	THR	6.2
1	I	173	THR	6.1
1	J	20	PHE	6.1

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Mol	Chain	Res	Type	RSRZ
1	I	127	SER	6.0
1	I	123	GLU	6.0
1	I	125	LEU	5.9
1	I	309	ILE	5.8
1	J	186	GLY	5.7
1	I	215	HIS	5.7
1	I	191	ILE	5.6
1	I	382	VAL	5.5
1	I	381	GLY	5.4
1	I	393	TYR	5.4
1	I	216	LEU	5.2
1	I	182	SER	5.2
1	I	170	SER	5.2
1	I	397	ALA	5.2
1	J	364	VAL	5.1
1	I	56	ALA	5.1
1	I	118	ILE	5.0
1	I	172	ARG	5.0
1	I	150	VAL	4.9
1	J	319	TYR	4.9
1	J	189	VAL	4.9
1	J	216	LEU	4.8
1	I	161	HIS	4.8
1	J	31	THR	4.8
1	J	44	PRO	4.8
1	J	362	ALA	4.8
1	I	13	VAL	4.7
1	J	359	ILE	4.7
1	J	24	SER	4.6
1	I	169	LEU	4.6
1	H	13	VAL	4.6
1	J	177	ALA	4.5
1	I	146	GLY	4.5
1	J	390	PHE	4.4
1	J	363	GLY	4.4
1	J	387	ARG	4.3
1	J	318	ASP	4.3
1	J	12	ASP	4.2
1	I	200	ALA	4.2
1	J	268	THR	4.1
1	I	312	HIS	4.1
1	I	343	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	J	185	LEU	4.0
1	J	183	ASN	4.0
1	J	269	GLU	3.9
1	I	124	ILE	3.9
1	J	28	HIS	3.9
1	J	40	SER	3.9
1	I	390	PHE	3.9
1	H	15	ALA	3.9
1	I	318	ASP	3.9
1	I	176	VAL	3.9
1	H	304	ILE	3.8
1	J	344	SER	3.8
1	J	159	VAL	3.8
1	J	366	VAL	3.8
1	J	11	TYR	3.8
1	I	138	TRP	3.8
1	J	356	SER	3.8
1	J	381	GLY	3.8
1	J	313	GLU	3.8
1	I	69	LEU	3.8
1	I	342	ILE	3.7
1	I	67	HIS	3.7
1	I	324	LEU	3.7
1	J	29	GLY	3.7
1	J	365	ALA	3.6
1	J	385	THR	3.6
1	J	26	GLN	3.6
1	G	325	GLY	3.6
1	I	148	LYS	3.6
1	I	145	GLN	3.5
1	H	414	GLY	3.5
1	I	152	THR	3.5
1	I	63	HIS	3.5
1	J	50	ALA	3.5
1	J	311	ALA	3.5
1	J	389	SER	3.4
1	I	114	GLY	3.4
1	I	319	TYR	3.4
1	I	199	HIS	3.4
1	G	413	PHE	3.4
1	I	327	ILE	3.4
1	I	188	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	I	52	THR	3.3
1	J	368	ALA	3.3
1	J	146	GLY	3.3
1	J	16	ILE	3.3
1	J	128	ILE	3.3
1	H	305	GLY	3.3
1	I	159	VAL	3.3
1	I	392	LEU	3.3
1	J	392	LEU	3.3
1	J	137	PRO	3.2
1	I	308	ALA	3.2
1	J	355	VAL	3.2
1	I	155	ASP	3.2
1	J	341	ALA	3.1
1	J	116	PRO	3.1
1	I	314	ALA	3.1
1	J	340	GLY	3.1
1	I	19	ASP	3.1
1	I	388	ALA	3.1
1	J	206	LEU	3.0
1	I	59	TYR	3.0
1	J	386	CYS	3.0
1	I	180	HIS	3.0
1	I	147	ALA	3.0
1	H	11	TYR	3.0
1	I	333	PHE	3.0
1	J	338	ASP	3.0
1	I	311	ALA	3.0
1	I	330	LEU	2.9
1	J	343	ILE	2.9
1	G	349	GLY	2.9
1	I	34	TYR	2.9
1	I	189	VAL	2.9
1	I	166	GLU	2.9
1	I	175	LEU	2.9
1	J	111	TYR	2.9
1	I	51	VAL	2.9
1	I	372	CYS	2.9
1	A	328	ASN	2.9
1	I	128	ILE	2.9
1	J	124	ILE	2.9
1	J	19	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	I	345	PHE	2.8
1	I	97	VAL	2.8
1	J	34	TYR	2.8
1	I	377	LEU	2.8
1	J	345	PHE	2.8
1	I	15	ALA	2.8
1	B	328	ASN	2.8
1	I	153	PRO	2.8
1	G	352	ALA	2.8
1	H	23	LEU	2.7
1	J	317	ARG	2.7
1	I	119	GLY	2.7
1	H	399	VAL	2.7
1	I	151	PHE	2.7
1	I	165	PHE	2.7
1	J	115	MET	2.7
1	J	13	VAL	2.7
1	I	73	ALA	2.7
1	I	142	ARG	2.7
1	C	414	GLY	2.7
1	I	32	LEU	2.6
1	G	410	ARG	2.6
1	I	315	ASP	2.6
1	J	155	ASP	2.6
1	J	307	HIS	2.6
1	I	225	CYS	2.6
1	J	25	ARG	2.6
1	J	393	TYR	2.6
1	J	37	ASN	2.6
1	I	122	ASP	2.6
1	I	197	LEU	2.6
1	I	21	PRO	2.6
1	J	384	SER	2.6
1	G	411	LYS	2.6
1	J	144	ARG	2.6
1	I	228	TYR	2.6
1	I	300	TYR	2.6
1	J	180	HIS	2.6
1	I	190	PRO	2.5
1	H	16	ILE	2.5
1	I	141	ILE	2.5
1	G	409	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	I	332	ILE	2.5
1	I	55	TYR	2.5
1	I	109	VAL	2.5
1	J	32	LEU	2.5
1	E	65	GLY	2.5
1	I	43	LYS	2.5
1	J	184	THR	2.5
1	G	328	ASN	2.5
1	J	361	ARG	2.4
1	H	48	ILE	2.4
1	J	383	THR	2.4
1	I	60	ALA	2.4
1	I	394	ASN	2.4
1	J	161	HIS	2.4
1	J	309	ILE	2.4
1	J	98	PHE	2.4
1	G	326	ARG	2.4
1	I	41	ALA	2.4
1	J	23	LEU	2.4
1	J	215	HIS	2.3
1	H	391	ALA	2.3
1	J	308	ALA	2.3
1	I	242	GLY	2.3
1	J	153	PRO	2.3
1	B	65	GLY	2.3
1	I	183	ASN	2.3
1	H	393	TYR	2.3
1	I	320	ALA	2.3
1	J	321	HIS	2.3
1	I	70	SER	2.3
1	J	15	ALA	2.3
1	G	65	GLY	2.3
1	J	96	ILE	2.3
1	H	57	ASN	2.3
1	I	167	LYS	2.3
1	I	195	VAL	2.2
1	J	213	ALA	2.2
1	H	309	ILE	2.2
1	J	168	ARG	2.2
1	I	306	ARG	2.2
1	H	308	ALA	2.2
1	I	87	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	325	GLY	2.2
1	J	230	PHE	2.2
1	J	280	ARG	2.2
1	A	11	TYR	2.1
1	J	236	TYR	2.1
1	J	312	HIS	2.1
1	I	236	TYR	2.1
1	J	22	ILE	2.1
1	J	376	LEU	2.1
1	I	340	GLY	2.1
1	J	47	VAL	2.1
1	J	145	GLN	2.1
1	J	238	PRO	2.1
1	E	64	ARG	2.1
1	I	58	GLU	2.1
1	I	92	SER	2.1
1	I	134	ASN	2.1
1	I	42	GLN	2.1
1	J	175	LEU	2.1
1	F	243	VAL	2.1
1	I	133	SER	2.1
1	I	246	GLY	2.1
1	I	17	ARG	2.1
1	I	276	HIS	2.0
1	I	307	HIS	2.0
1	I	160	PHE	2.0
1	G	28	HIS	2.0
1	F	414	GLY	2.0
1	I	131	HIS	2.0
1	A	329	SER	2.0
1	J	205	VAL	2.0
1	B	260	GLY	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	LLP	H	234	24/25	0.96	0.16	-	54,56,59,61	0
1	LLP	I	234	24/25	0.89	0.22	-	72,75,80,82	0
1	LLP	F	234	24/25	0.98	0.17	-	42,44,46,47	0
1	LLP	J	234	24/25	0.90	0.22	-	75,77,79,80	0
1	LLP	C	234	24/25	0.97	0.15	-	44,46,47,47	0
1	LLP	A	234	24/25	0.97	0.14	-	40,43,44,45	0
1	LLP	G	234	24/25	0.97	0.15	-	54,57,59,59	0
1	LLP	D	234	24/25	0.97	0.17	-	41,41,42,43	0
1	LLP	E	234	24/25	0.98	0.15	-	41,42,44,45	0
1	LLP	B	234	24/25	0.98	0.16	-	38,40,41,41	0

### 6.3 Carbohydrates [i](#)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CL	I	501	1/1	0.84	0.17	-	79,79,79,79	0
2	CL	C	501	1/1	0.85	0.14	-	86,86,86,86	0
2	CL	B	501	1/1	0.81	0.22	-	69,69,69,69	0
2	CL	E	501	1/1	0.82	0.20	-	72,72,72,72	0
2	CL	D	501	1/1	0.87	0.17	-	52,52,52,52	0
2	CL	H	501	1/1	0.70	0.15	-	71,71,71,71	0
2	CL	A	501	1/1	0.85	0.18	-	69,69,69,69	0

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

There are no such residues in this entry.