



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 09:49 PM 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
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

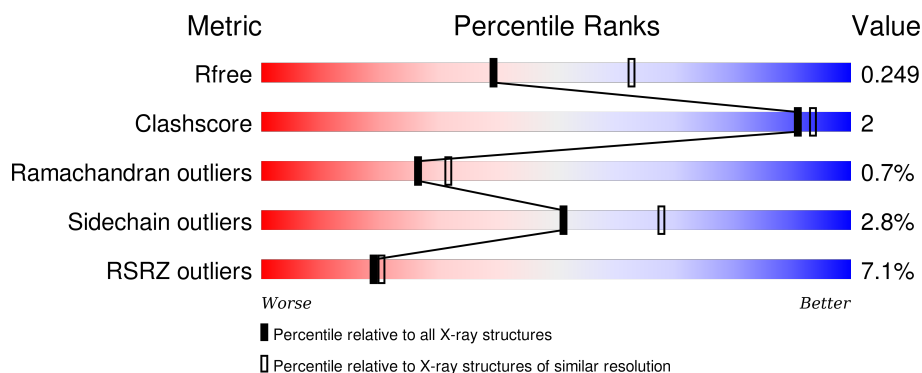
1 Overall quality at a glance ⓘ

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}	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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 ≥ 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 style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 88%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 88% 6% . . </div> </div>
1	B	422	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 1%, green 88%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> % 88% 6% . . </div> </div>
1	C	422	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 86%, yellow 9%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 86% 9% . . </div> </div>
1	D	422	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 87%, yellow 7%, grey 6%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 87% 7% . . </div> </div>
1	E	422	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 87%, yellow 8%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> 87% 8% . . </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	422	<div><div>%</div><div><div></div><div>88%</div><div>6%</div><div></div><div></div></div><div></div></div>
1	G	422	<div><div>3%</div><div><div></div><div>87%</div><div>8%</div><div></div><div></div></div><div></div></div>
1	H	422	<div><div>5%</div><div><div></div><div>89%</div><div>5%</div><div></div><div></div></div><div></div></div>
1	I	422	<div><div>30%</div><div><div></div><div>90%</div><div></div><div></div><div></div></div><div></div></div>
1	J	422	<div><div>27%</div><div><div></div><div>81%</div><div></div><div></div><div></div></div><div></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

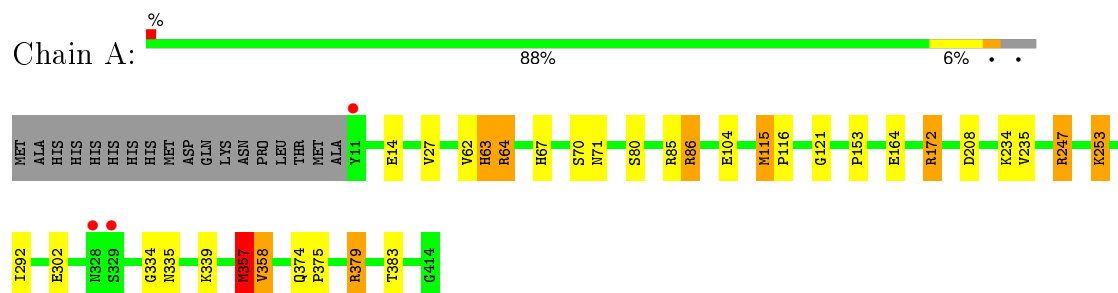
- Molecule 3 is water.

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

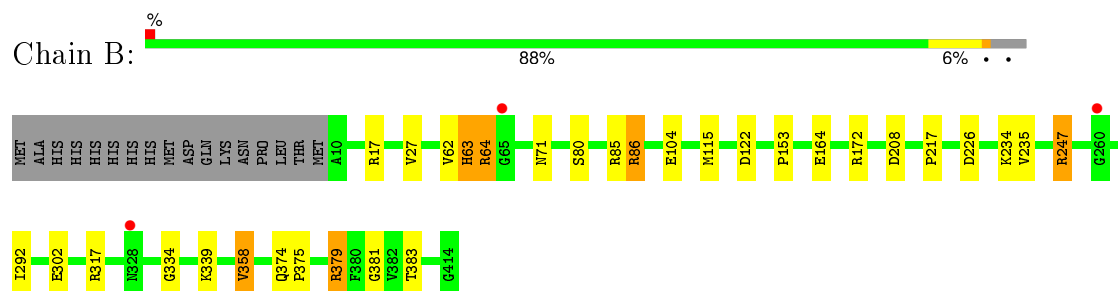
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

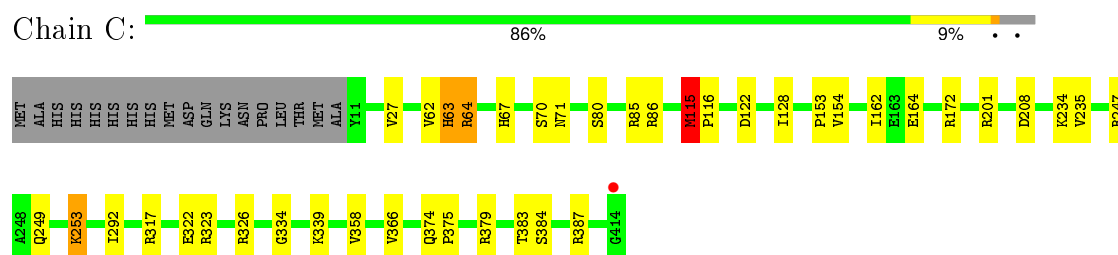
- Molecule 1: Aminotransferase



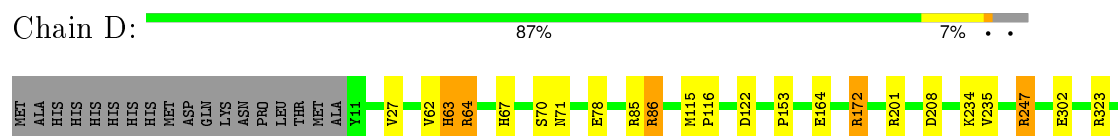
- Molecule 1: Aminotransferase



- Molecule 1: Aminotransferase



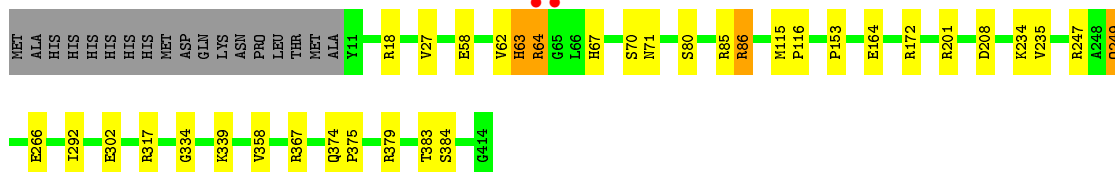
- Molecule 1: Aminotransferase

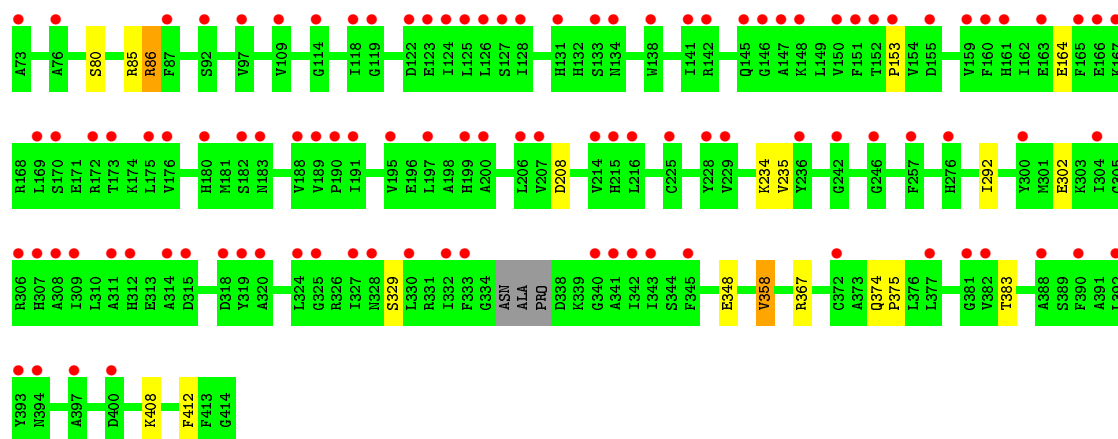




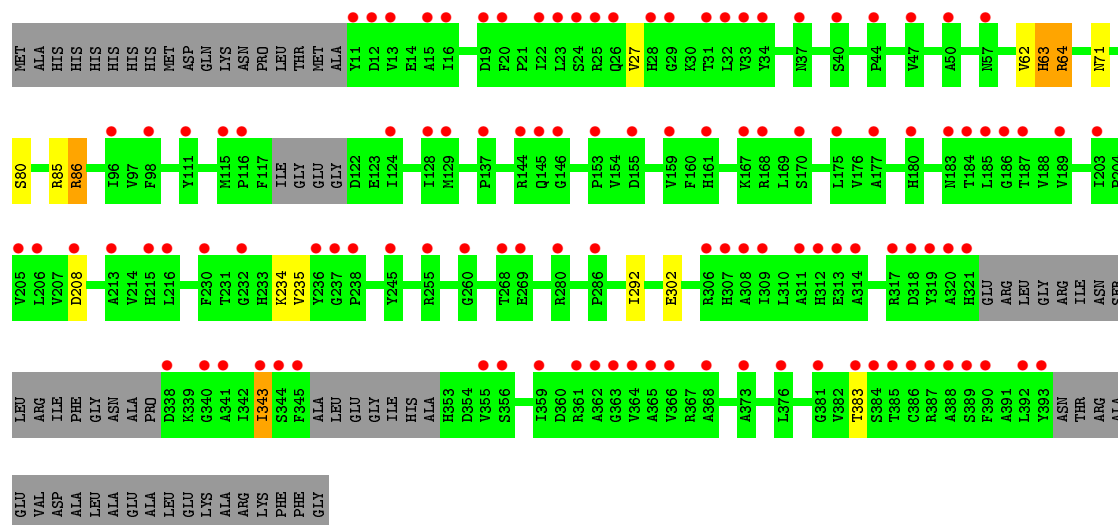
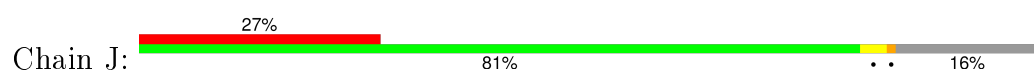
• Molecule 1: Aminotransferase

Chain E: 87% 8% . .





• Molecule 1: Aminotransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	34.6	Xtriage
Anisotropy	1.233	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 178357 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	30371	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	3023	21	0
1	B	3110	0	3014	16	0
1	C	3118	0	3025	16	0
1	D	3131	0	3050	17	0
1	E	3083	0	2952	12	0
1	F	3097	0	2974	15	0
1	G	3041	0	2898	16	0
1	H	3041	0	2919	10	0
1	I	2764	0	2423	9	0
1	J	2508	0	2183	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	28461	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:H:115:MET:HB3	1:H:116:PRO:HD3	1.77	0.67
1:A:115:MET:HB3	1:A:116:PRO:HD3	1.74	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: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:B:62:VAL:O	1:B:64:ARG:N	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:C:62:VAL:O	1:C:64:ARG:N	2.30	0.60
1:A:121:GLY:C	1:A:172:ARG:HH21	2.04	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:H:122:ASP:OD1	1:H:172:ARG:NH1	2.34	0.59
1:F:62:VAL:O	1:F:64:ARG:N	2.32	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:F:334:GLY:O	1:F:339:LYS:NZ	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:GLY:O	1:A: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:B:63:HIS:O	1:B:64:ARG:C	2.48	0.52
1:A:357:MET:HG2	1:F:361:ARG:HG3	1.91	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:C:128:ILE:CG2	1:C:154:VAL:HG22	2.46	0.44
1:A:67:HIS:CE1	1:A:70:SER:HB2	2.53	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:G:63:HIS:O	1:G:64:ARG:C	2.56	0.43
1:A:80:SER:OG	1:A:292:ILE:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:66:LEU:N	1:G:66:LEU:HD12	2.33	0.43
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: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:J:80:SER:OG	1:J:292:ILE:HA	2.19	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: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:I:86:ARG:HD2	1:I:302:GLU:OE2	2.20	0.42
1:E:80:SER:OG	1:E:292:ILE:HA	2.20	0.42
1:J:208:ASP:OD2	1:J:234:LLP:N1	2.52	0.42
1:H:374:GLN:HB2	1:H:375:PRO:HD3	2.01	0.42
1:I:80:SER:OG	1:I:292:ILE:HA	2.20	0.42
1:F:67:HIS:CE1	1:F:70:SER:HB2	2.54	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:374:GLN:HB2	1:G:375:PRO:HD3	2.01	0.42
1:G:80:SER:OG	1:G:292:ILE:HA	2.20	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%)	26	32
1	B	402/422 (95%)	389 (97%)	10 (2%)	3 (1%)	26	32
1	C	401/422 (95%)	388 (97%)	10 (2%)	3 (1%)	26	32
1	D	402/422 (95%)	388 (96%)	11 (3%)	3 (1%)	26	32
1	E	401/422 (95%)	388 (97%)	10 (2%)	3 (1%)	26	32
1	F	402/422 (95%)	389 (97%)	10 (2%)	3 (1%)	26	32
1	G	400/422 (95%)	387 (97%)	10 (2%)	3 (1%)	24	28
1	H	395/422 (94%)	384 (97%)	10 (2%)	1 (0%)	46	57
1	I	391/422 (93%)	380 (97%)	10 (3%)	1 (0%)	46	57
1	J	347/422 (82%)	335 (96%)	9 (3%)	3 (1%)	21	25
All	All	3944/4220 (94%)	3818 (97%)	100 (2%)	26 (1%)	26	32

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%)	43	60
1	B	311/341 (91%)	303 (97%)	8 (3%)	54	70
1	C	313/341 (92%)	303 (97%)	10 (3%)	46	63
1	D	316/341 (93%)	307 (97%)	9 (3%)	51	68
1	E	305/341 (89%)	295 (97%)	10 (3%)	45	61
1	F	308/341 (90%)	299 (97%)	9 (3%)	50	66
1	G	297/341 (87%)	288 (97%)	9 (3%)	48	65
1	H	300/341 (88%)	293 (98%)	7 (2%)	58	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	I	233/341 (68%)	229 (98%)	4 (2%)	68	81
1	J	215/341 (63%)	210 (98%)	5 (2%)	58	74
All	All	2910/3410 (85%)	2828 (97%)	82 (3%)	51	68

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	23,24,25	3.50	4 (17%)	28,32,34	1.14	2 (7%)
1	LLP	B	234	1	23,24,25	2.95	5 (21%)	28,32,34	1.39	6 (21%)
1	LLP	C	234	1	23,24,25	3.15	5 (21%)	28,32,34	1.22	3 (10%)
1	LLP	D	234	1	23,24,25	3.43	5 (21%)	28,32,34	1.34	4 (14%)
1	LLP	E	234	1	23,24,25	2.73	6 (26%)	28,32,34	1.29	4 (14%)
1	LLP	F	234	1	23,24,25	3.03	5 (21%)	28,32,34	1.30	4 (14%)
1	LLP	G	234	1	23,24,25	3.50	5 (21%)	28,32,34	1.25	5 (17%)
1	LLP	H	234	1	23,24,25	3.48	5 (21%)	28,32,34	1.27	6 (21%)
1	LLP	I	234	1	23,24,25	3.38	5 (21%)	28,32,34	1.21	4 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	LLP	J	234	1	23,24,25	3.27	5 (21%)	28,32,34	1.34	4 (14%)

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 (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	234	LLP	CB-CA	-2.27	1.51	1.53
1	E	234	LLP	CB-CA	-2.26	1.51	1.53
1	I	234	LLP	C4-C4'	2.09	1.50	1.46
1	D	234	LLP	C4-C4'	2.10	1.50	1.46
1	C	234	LLP	C4-C4'	2.44	1.50	1.46
1	H	234	LLP	C4-C4'	2.46	1.51	1.46
1	E	234	LLP	C4-C4'	2.73	1.51	1.46
1	G	234	LLP	C4-C4'	2.98	1.51	1.46
1	J	234	LLP	C4-C4'	3.13	1.52	1.46
1	C	234	LLP	C4-C5	3.46	1.46	1.42
1	B	234	LLP	C4-C4'	3.65	1.53	1.46
1	E	234	LLP	C4-C5	3.88	1.47	1.42
1	H	234	LLP	C4-C5	4.27	1.47	1.42
1	F	234	LLP	C4-C5	4.39	1.47	1.42
1	B	234	LLP	C4-C3	4.65	1.46	1.40
1	E	234	LLP	C4-C3	4.79	1.46	1.40
1	I	234	LLP	C4-C5	4.82	1.48	1.42
1	A	234	LLP	C4-C5	4.85	1.48	1.42
1	J	234	LLP	C4-C5	4.87	1.48	1.42
1	G	234	LLP	C4-C5	5.02	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	234	LLP	C4-C3	5.14	1.47	1.40
1	D	234	LLP	C4-C5	5.15	1.48	1.42
1	B	234	LLP	C4-C5	5.20	1.49	1.42
1	B	234	LLP	C4'-NZ	5.20	1.43	1.27
1	J	234	LLP	C4-C3	5.49	1.47	1.40
1	F	234	LLP	C4'-NZ	5.78	1.44	1.27
1	A	234	LLP	C4-C3	5.80	1.48	1.40
1	D	234	LLP	C4'-NZ	5.85	1.45	1.27
1	J	234	LLP	C4'-NZ	5.86	1.45	1.27
1	A	234	LLP	C4'-NZ	5.87	1.45	1.27
1	D	234	LLP	C4-C3	5.94	1.48	1.40
1	I	234	LLP	C4'-NZ	5.98	1.45	1.27
1	H	234	LLP	C4'-NZ	6.04	1.45	1.27
1	E	234	LLP	C4'-NZ	6.04	1.45	1.27
1	C	234	LLP	C4'-NZ	6.07	1.45	1.27
1	G	234	LLP	C4'-NZ	6.11	1.45	1.27
1	I	234	LLP	C4-C3	6.31	1.48	1.40
1	G	234	LLP	C4-C3	6.39	1.48	1.40
1	H	234	LLP	C4-C3	6.52	1.49	1.40
1	F	234	LLP	C4-C3	6.84	1.49	1.40
1	E	234	LLP	C3-C2	8.78	1.46	1.40
1	F	234	LLP	C3-C2	9.67	1.47	1.40
1	B	234	LLP	C3-C2	10.10	1.47	1.40
1	C	234	LLP	C3-C2	11.77	1.48	1.40
1	J	234	LLP	C3-C2	11.81	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 (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	234	LLP	C3-C4-C5	-2.61	116.15	118.11
1	J	234	LLP	C4-C4'-NZ	-2.45	111.41	125.06
1	H	234	LLP	O-C-CA	-2.43	119.17	125.49
1	B	234	LLP	C3-C4-C5	-2.40	116.31	118.11
1	D	234	LLP	C4-C4'-NZ	-2.40	111.72	125.06
1	E	234	LLP	C4-C4'-NZ	-2.39	111.74	125.06
1	B	234	LLP	C4-C4'-NZ	-2.33	112.07	125.06
1	G	234	LLP	C4-C4'-NZ	-2.32	112.13	125.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	234	LLP	O-C-CA	-2.32	119.44	125.49
1	C	234	LLP	C4-C4'-NZ	-2.28	112.38	125.06
1	G	234	LLP	O-C-CA	-2.24	119.66	125.49
1	I	234	LLP	C4-C4'-NZ	-2.22	112.73	125.06
1	I	234	LLP	O-C-CA	-2.21	119.74	125.49
1	F	234	LLP	O-C-CA	-2.19	119.78	125.49
1	F	234	LLP	C4-C4'-NZ	-2.18	112.94	125.06
1	G	234	LLP	C3-C4-C5	-2.17	116.48	118.11
1	H	234	LLP	C4-C4'-NZ	-2.16	113.06	125.06
1	D	234	LLP	C3-C4-C5	-2.15	116.49	118.11
1	A	234	LLP	C4-C4'-NZ	-2.13	113.19	125.06
1	H	234	LLP	C3-C4-C5	-2.11	116.53	118.11
1	B	234	LLP	O-C-CA	-2.08	120.07	125.49
1	E	234	LLP	O3-C3-C2	2.03	121.19	117.66
1	H	234	LLP	C6-N1-C2	2.08	123.53	119.28
1	H	234	LLP	OP2-P-OP1	2.09	117.29	110.58
1	A	234	LLP	OP2-P-OP1	2.14	117.46	110.58
1	F	234	LLP	OP2-P-OP1	2.15	117.49	110.58
1	J	234	LLP	OP2-P-OP1	2.18	117.61	110.58
1	E	234	LLP	OP2-P-OP1	2.19	117.62	110.58
1	I	234	LLP	OP2-P-OP1	2.21	117.68	110.58
1	H	234	LLP	O3-C3-C2	2.22	121.53	117.66
1	G	234	LLP	OP2-P-OP1	2.24	117.78	110.58
1	C	234	LLP	OP2-P-OP1	2.24	117.79	110.58
1	D	234	LLP	OP2-P-OP1	2.29	117.95	110.58
1	B	234	LLP	OP2-P-OP1	2.30	117.98	110.58
1	J	234	LLP	C6-N1-C2	2.30	123.97	119.28
1	I	234	LLP	C6-N1-C2	2.39	124.15	119.28
1	B	234	LLP	C6-N1-C2	2.43	124.24	119.28
1	G	234	LLP	O3-C3-C2	2.43	121.89	117.66
1	D	234	LLP	O3-C3-C2	2.62	122.22	117.66
1	E	234	LLP	C6-N1-C2	2.72	124.83	119.28
1	B	234	LLP	O3-C3-C2	2.73	122.40	117.66
1	F	234	LLP	C6-N1-C2	3.29	125.99	119.28

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
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, 95th 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 ²)	Q<0.9
1	A	403/422 (95%)	-0.01	3 (0%) 89 90	39, 52, 68, 79	0
1	B	404/422 (95%)	0.03	3 (0%) 89 90	39, 50, 65, 80	0
1	C	403/422 (95%)	-0.06	1 (0%) 95 96	43, 54, 65, 71	0
1	D	403/422 (95%)	-0.01	0 100 100	41, 49, 60, 67	0
1	E	403/422 (95%)	-0.05	2 (0%) 91 92	40, 52, 68, 77	0
1	F	403/422 (95%)	0.07	3 (0%) 89 90	41, 55, 72, 82	0
1	G	402/422 (95%)	0.24	13 (3%) 51 54	51, 63, 87, 105	0
1	H	399/422 (94%)	0.34	19 (4%) 34 37	55, 69, 81, 89	0
1	I	397/422 (94%)	1.68	126 (31%) 1 0	66, 89, 125, 143	0
1	J	355/422 (84%)	1.68	113 (31%) 1 0	70, 85, 106, 116	0
All	All	3972/4220 (94%)	0.37	283 (7%) 19 20	39, 58, 98, 143	0

All (283) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	126	LEU	12.0
1	J	203	ILE	7.9
1	I	76	ALA	7.6
1	J	373	ALA	7.4
1	I	304	ILE	7.2
1	J	33	VAL	6.7
1	J	314	ALA	6.7
1	J	320	ALA	6.6
1	I	214	VAL	6.5
1	I	341	ALA	6.5
1	J	187	THR	6.4
1	I	173	THR	6.4
1	J	20	PHE	6.3

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Mol	Chain	Res	Type	RSRZ
1	I	127	SER	6.3
1	I	123	GLU	6.2
1	I	125	LEU	6.1
1	J	186	GLY	6.0
1	I	309	ILE	6.0
1	I	215	HIS	5.9
1	I	191	ILE	5.8
1	I	382	VAL	5.7
1	I	381	GLY	5.7
1	I	393	TYR	5.6
1	I	216	LEU	5.4
1	I	397	ALA	5.4
1	J	364	VAL	5.4
1	I	56	ALA	5.4
1	I	182	SER	5.4
1	I	170	SER	5.3
1	I	118	ILE	5.2
1	I	172	ARG	5.2
1	I	150	VAL	5.2
1	J	189	VAL	5.1
1	J	319	TYR	5.1
1	J	44	PRO	5.1
1	J	216	LEU	5.0
1	J	31	THR	5.0
1	I	161	HIS	5.0
1	J	362	ALA	5.0
1	I	13	VAL	5.0
1	J	359	ILE	4.9
1	J	24	SER	4.8
1	H	13	VAL	4.8
1	I	169	LEU	4.8
1	J	177	ALA	4.8
1	I	146	GLY	4.7
1	J	363	GLY	4.7
1	J	390	PHE	4.6
1	J	387	ARG	4.5
1	J	318	ASP	4.5
1	J	12	ASP	4.4
1	I	200	ALA	4.4
1	J	268	THR	4.3
1	I	343	ILE	4.3
1	I	312	HIS	4.3

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Mol	Chain	Res	Type	RSRZ
1	J	185	LEU	4.2
1	J	183	ASN	4.1
1	I	124	ILE	4.1
1	J	269	GLU	4.1
1	H	15	ALA	4.1
1	J	28	HIS	4.1
1	I	318	ASP	4.1
1	I	176	VAL	4.1
1	J	159	VAL	4.0
1	J	366	VAL	4.0
1	J	40	SER	4.0
1	H	304	ILE	4.0
1	I	390	PHE	4.0
1	J	381	GLY	4.0
1	J	344	SER	4.0
1	J	11	TYR	4.0
1	J	356	SER	4.0
1	I	138	TRP	4.0
1	J	313	GLU	3.9
1	I	69	LEU	3.9
1	I	342	ILE	3.9
1	J	29	GLY	3.9
1	I	324	LEU	3.9
1	I	67	HIS	3.8
1	J	365	ALA	3.8
1	J	385	THR	3.8
1	G	325	GLY	3.8
1	J	26	GLN	3.8
1	H	414	GLY	3.7
1	I	148	LYS	3.7
1	I	145	GLN	3.7
1	I	152	THR	3.7
1	J	50	ALA	3.7
1	J	311	ALA	3.7
1	I	63	HIS	3.6
1	I	114	GLY	3.6
1	J	389	SER	3.6
1	I	319	TYR	3.6
1	I	188	VAL	3.5
1	I	199	HIS	3.5
1	I	52	THR	3.5
1	J	368	ALA	3.5

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Mol	Chain	Res	Type	RSRZ
1	I	327	ILE	3.5
1	J	146	GLY	3.5
1	G	413	PHE	3.5
1	H	305	GLY	3.5
1	J	16	ILE	3.5
1	J	128	ILE	3.5
1	I	159	VAL	3.5
1	I	392	LEU	3.4
1	J	137	PRO	3.4
1	J	392	LEU	3.4
1	I	308	ALA	3.4
1	I	155	ASP	3.3
1	J	355	VAL	3.3
1	J	341	ALA	3.3
1	J	116	PRO	3.3
1	J	340	GLY	3.3
1	I	314	ALA	3.3
1	I	19	ASP	3.3
1	I	388	ALA	3.3
1	J	386	CYS	3.2
1	J	206	LEU	3.2
1	I	147	ALA	3.2
1	I	59	TYR	3.1
1	J	338	ASP	3.1
1	I	311	ALA	3.1
1	I	180	HIS	3.1
1	H	11	TYR	3.1
1	G	349	GLY	3.1
1	I	333	PHE	3.1
1	I	330	LEU	3.1
1	J	343	ILE	3.1
1	I	189	VAL	3.1
1	I	34	TYR	3.0
1	I	372	CYS	3.0
1	I	51	VAL	3.0
1	I	175	LEU	3.0
1	I	166	GLU	3.0
1	J	19	ASP	3.0
1	I	128	ILE	3.0
1	J	124	ILE	3.0
1	A	328	ASN	3.0
1	J	111	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	I	97	VAL	3.0
1	I	345	PHE	3.0
1	I	153	PRO	3.0
1	I	377	LEU	2.9
1	I	15	ALA	2.9
1	J	34	TYR	2.9
1	G	352	ALA	2.9
1	J	345	PHE	2.9
1	B	328	ASN	2.9
1	I	119	GLY	2.9
1	H	23	LEU	2.9
1	H	399	VAL	2.9
1	J	115	MET	2.9
1	J	317	ARG	2.9
1	J	13	VAL	2.8
1	I	73	ALA	2.8
1	C	414	GLY	2.8
1	I	151	PHE	2.8
1	I	165	PHE	2.8
1	I	142	ARG	2.8
1	I	315	ASP	2.8
1	J	155	ASP	2.8
1	I	32	LEU	2.8
1	I	225	CYS	2.8
1	I	21	PRO	2.8
1	G	410	ARG	2.8
1	I	122	ASP	2.8
1	J	307	HIS	2.8
1	I	197	LEU	2.7
1	J	25	ARG	2.7
1	J	37	ASN	2.7
1	J	393	TYR	2.7
1	I	190	PRO	2.7
1	J	384	SER	2.7
1	J	144	ARG	2.7
1	G	411	LYS	2.7
1	G	409	ALA	2.7
1	I	228	TYR	2.7
1	I	300	TYR	2.7
1	H	16	ILE	2.7
1	I	141	ILE	2.7
1	J	180	HIS	2.7

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Mol	Chain	Res	Type	RSRZ
1	I	109	VAL	2.7
1	I	332	ILE	2.6
1	E	65	GLY	2.6
1	J	32	LEU	2.6
1	I	55	TYR	2.6
1	J	184	THR	2.6
1	G	328	ASN	2.6
1	I	43	LYS	2.6
1	H	48	ILE	2.6
1	J	383	THR	2.5
1	I	60	ALA	2.5
1	J	361	ARG	2.5
1	J	309	ILE	2.5
1	I	41	ALA	2.5
1	H	391	ALA	2.5
1	I	242	GLY	2.5
1	I	394	ASN	2.5
1	J	308	ALA	2.5
1	J	153	PRO	2.5
1	J	23	LEU	2.5
1	J	161	HIS	2.5
1	B	65	GLY	2.5
1	G	326	ARG	2.5
1	J	98	PHE	2.5
1	J	215	HIS	2.5
1	I	320	ALA	2.5
1	I	183	ASN	2.4
1	J	15	ALA	2.4
1	G	65	GLY	2.4
1	H	393	TYR	2.4
1	J	321	HIS	2.4
1	I	70	SER	2.4
1	J	96	ILE	2.4
1	I	195	VAL	2.4
1	J	213	ALA	2.4
1	H	57	ASN	2.4
1	I	167	LYS	2.4
1	H	309	ILE	2.4
1	H	308	ALA	2.3
1	I	325	GLY	2.3
1	J	168	ARG	2.3
1	I	306	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	87	PHE	2.3
1	J	280	ARG	2.3
1	I	340	GLY	2.3
1	J	230	PHE	2.3
1	A	11	TYR	2.3
1	J	236	TYR	2.3
1	J	47	VAL	2.3
1	J	238	PRO	2.3
1	J	22	ILE	2.2
1	J	312	HIS	2.2
1	I	236	TYR	2.2
1	J	376	LEU	2.2
1	I	92	SER	2.2
1	I	134	ASN	2.2
1	I	58	GLU	2.2
1	E	64	ARG	2.2
1	I	42	GLN	2.2
1	J	145	GLN	2.2
1	F	243	VAL	2.2
1	I	246	GLY	2.2
1	J	175	LEU	2.2
1	I	133	SER	2.2
1	I	17	ARG	2.2
1	I	276	HIS	2.1
1	I	307	HIS	2.1
1	J	205	VAL	2.1
1	B	260	GLY	2.1
1	F	414	GLY	2.1
1	I	160	PHE	2.1
1	G	28	HIS	2.1
1	J	232	GLY	2.1
1	H	394	ASN	2.1
1	I	131	HIS	2.1
1	A	329	SER	2.1
1	J	129	MET	2.1
1	J	57	ASN	2.1
1	J	237	GLY	2.1
1	J	260	GLY	2.1
1	I	328	ASN	2.1
1	H	316	LEU	2.1
1	I	206	LEU	2.1
1	J	170	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	I	72	ALA	2.1
1	J	388	ALA	2.1
1	G	154	VAL	2.1
1	J	255	ARG	2.1
1	I	257	PHE	2.1
1	H	24	SER	2.1
1	F	328	ASN	2.0
1	H	17	ARG	2.0
1	I	207	VAL	2.0
1	J	245	TYR	2.0
1	I	400	ASP	2.0
1	J	208	ASP	2.0
1	J	167	LYS	2.0
1	I	229	VAL	2.0
1	I	163	GLU	2.0
1	J	306	ARG	2.0
1	J	286	PRO	2.0
1	G	380	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95th 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(Å 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, 95th 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(\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.