Full wwPDB X-ray Structure Validation Report ⓘ

Dec 17, 2023 – 01:07 PM EST

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; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
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
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.

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

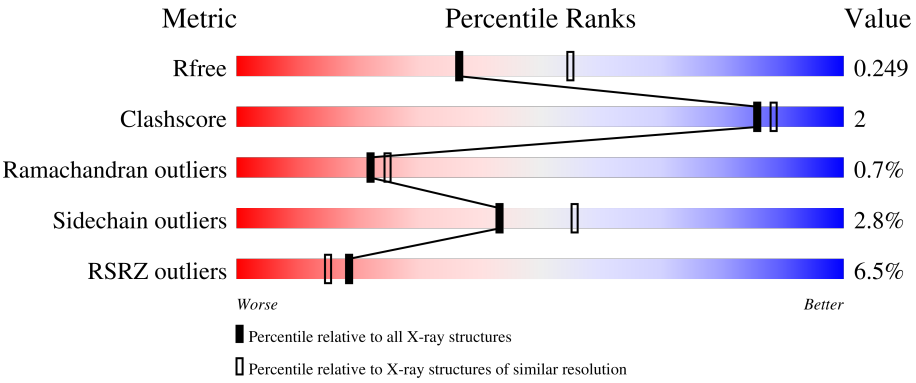
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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}	130704	1544 (2.48-2.44)
Clashscore	141614	1613 (2.48-2.44)
Ramachandran outliers	138981	1598 (2.48-2.44)
Sidechain outliers	138945	1598 (2.48-2.44)
RSRZ outliers	127900	1523 (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 of the lower bar indicate the fraction of residues that contain outliers for >=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 <=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	88% 5%
1	B	422	88% 6%
1	C	422	86% 9%
1	D	422	87% 7%
1	E	422	87% 7%

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Mol	Chain	Length	Quality of chain
1	F	422	88% 6%
1	G	422	3% 87% 8% 5%
1	H	422	4% 89% 5% 5%
1	I	422	28% 90% 6%
1	J	422	24% 81% 16%

2 Entry composition (i)

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	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0
2	C	1	Total Cl 1 1	0	0
2	D	1	Total Cl 1 1	0	0
2	E	1	Total Cl 1 1	0	0

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

- Molecule 3 is water.

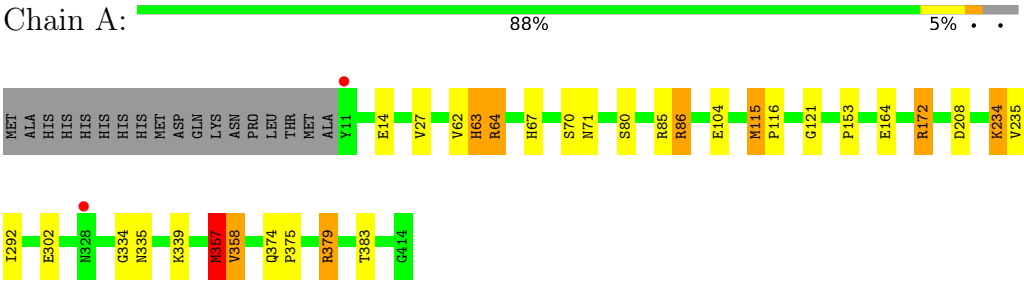
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	46	Total O 46 46	0	0
3	B	52	Total O 52 52	0	0
3	C	38	Total O 38 38	0	0
3	D	54	Total O 54 54	0	0
3	E	41	Total O 41 41	0	0
3	F	49	Total O 49 49	0	0
3	G	41	Total O 41 41	0	0
3	H	28	Total O 28 28	0	0
3	I	2	Total O 2 2	0	0
3	J	3	Total O 3 3	0	0

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.

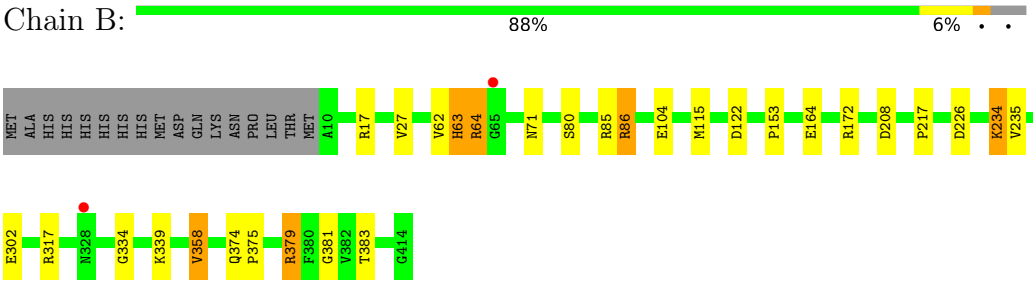
• Molecule 1: Aminotransferase

Chain A:



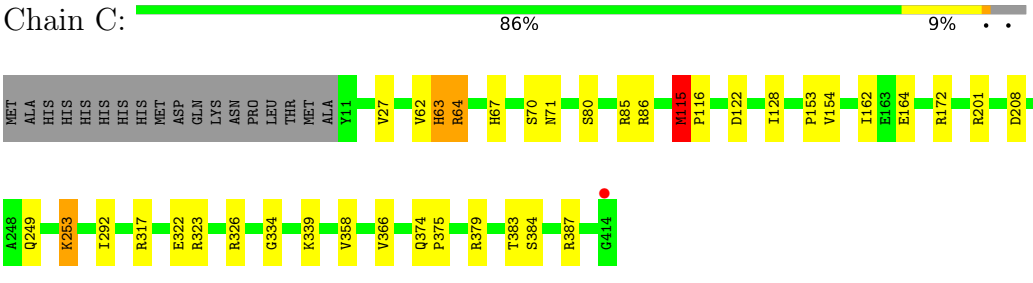
• Molecule 1: Aminotransferase

Chain B:



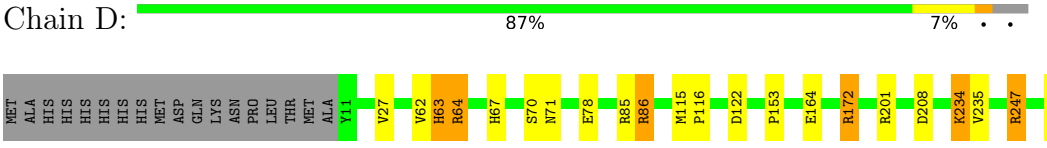
• Molecule 1: Aminotransferase

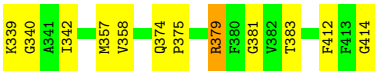
Chain C:



• Molecule 1: Aminotransferase

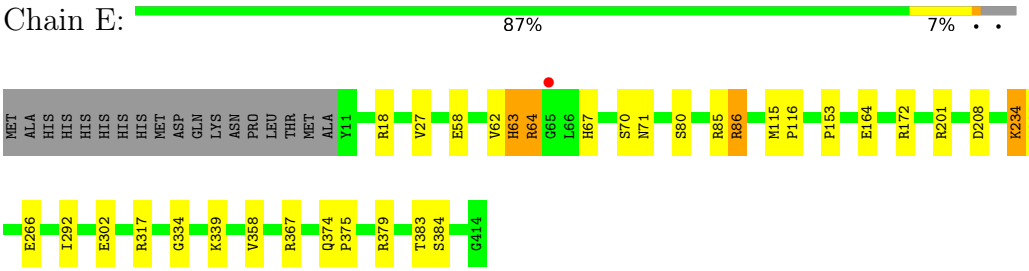
Chain D:





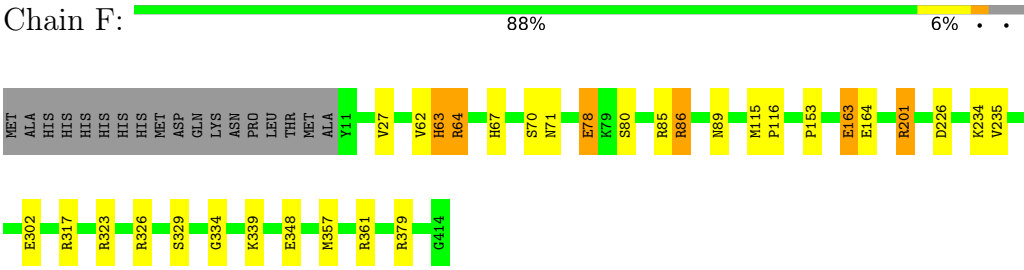
• Molecule 1: Aminotransferase

Chain E:



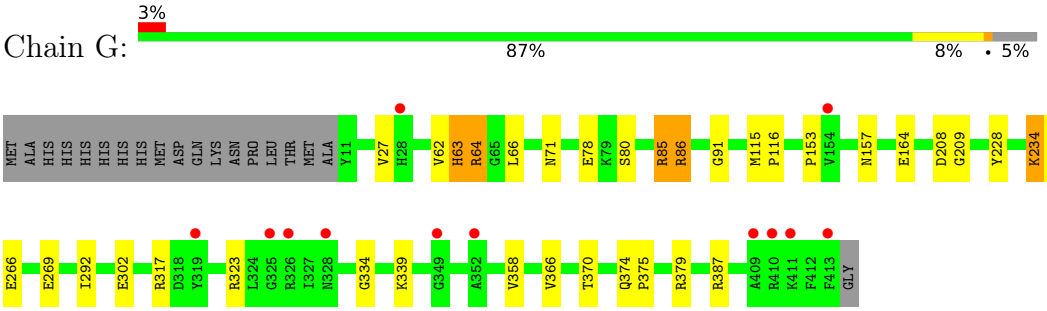
• Molecule 1: Aminotransferase

Chain F:



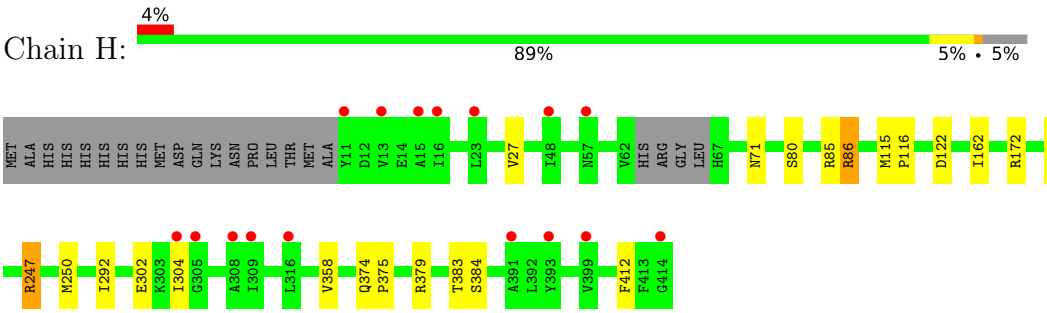
• Molecule 1: Aminotransferase

Chain G:



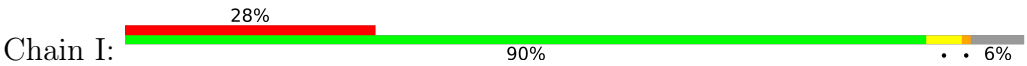
• Molecule 1: Aminotransferase

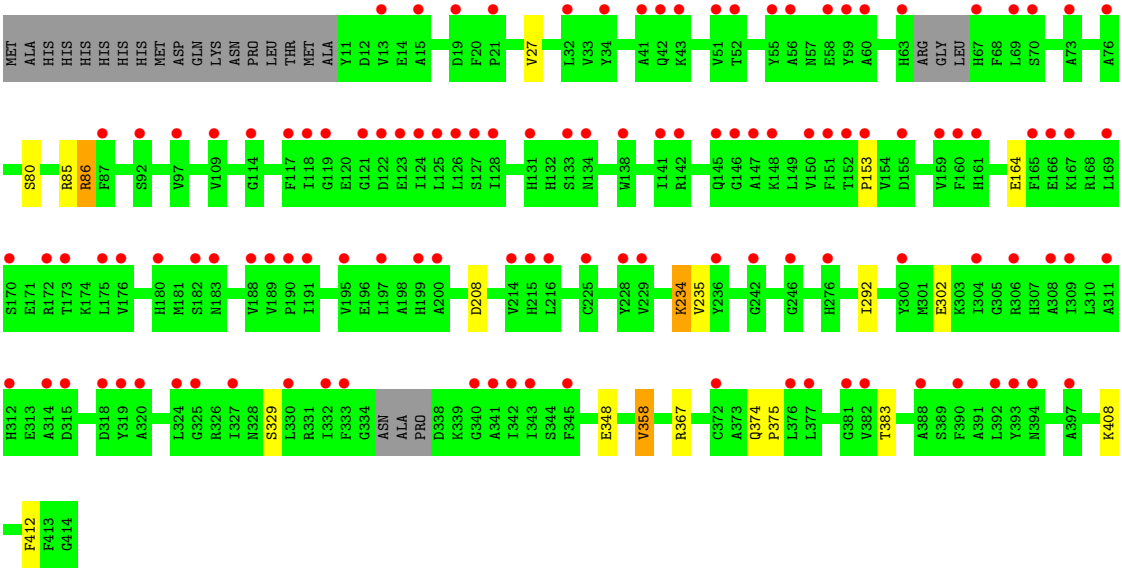
Chain H:



• Molecule 1: Aminotransferase

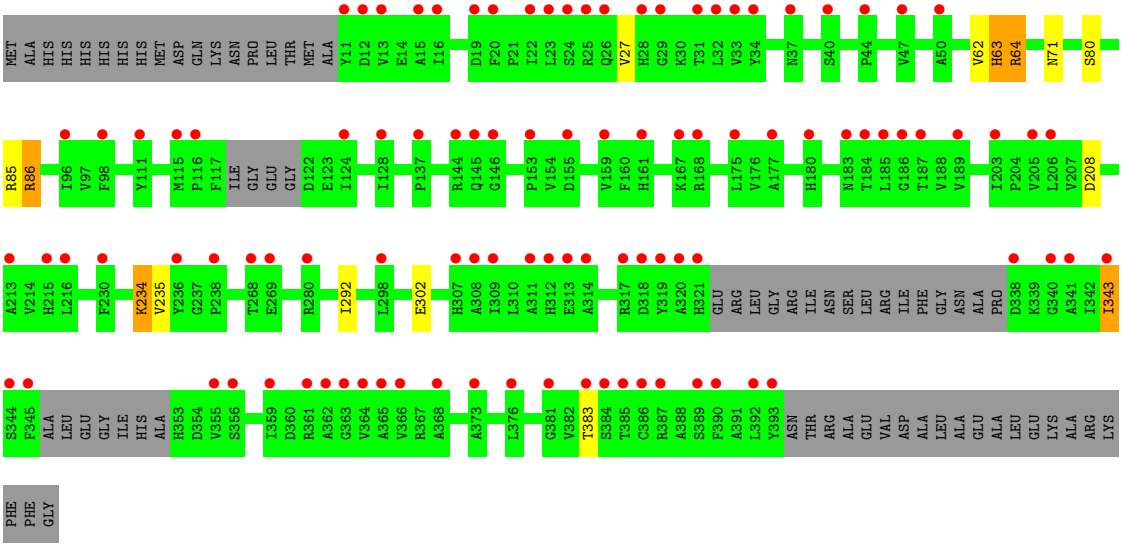
Chain I:





• Molecule 1: Aminotransferase

Chain J:



4 Data and refinement statistics (i)

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) 96.5 (48.39-2.45)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.02%)	wwPDB-VP
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 , 39.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, LLP

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(^{o})	Ideal(^{o})
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(^{o})	Ideal(^{o})
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 (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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:OE1	1:F:78:GLU:HA	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:HD12	1:G:66:LEU:N	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:CD	1:E:249:GLN:H	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:C	1:D:357:MET:SD	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%)	22	25
1	B	402/422 (95%)	389 (97%)	10 (2%)	3 (1%)	22	25
1	C	401/422 (95%)	388 (97%)	10 (2%)	3 (1%)	22	25
1	D	402/422 (95%)	388 (96%)	11 (3%)	3 (1%)	22	25
1	E	401/422 (95%)	388 (97%)	10 (2%)	3 (1%)	22	25
1	F	402/422 (95%)	389 (97%)	10 (2%)	3 (1%)	22	25
1	G	400/422 (95%)	387 (97%)	10 (2%)	3 (1%)	19	22
1	H	395/422 (94%)	384 (97%)	10 (2%)	1 (0%)	41	49
1	I	391/422 (93%)	380 (97%)	10 (3%)	1 (0%)	41	49
1	J	347/422 (82%)	335 (96%)	9 (3%)	3 (1%)	17	19
All	All	3944/4220 (94%)	3818 (97%)	100 (2%)	26 (1%)	22	25

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	312/341 (92%)	301 (96%)	11 (4%)	36	47
1	B	311/341 (91%)	303 (97%)	8 (3%)	46	58
1	C	313/341 (92%)	303 (97%)	10 (3%)	39	50
1	D	316/341 (93%)	307 (97%)	9 (3%)	43	56
1	E	305/341 (89%)	295 (97%)	10 (3%)	38	49
1	F	308/341 (90%)	299 (97%)	9 (3%)	42	53
1	G	297/341 (87%)	288 (97%)	9 (3%)	41	52
1	H	300/341 (88%)	293 (98%)	7 (2%)	50	63

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	I	233/341 (68%)	229 (98%)	4 (2%)	60 73
1	J	215/341 (63%)	210 (98%)	5 (2%)	50 63
All	All	2910/3410 (85%)	2828 (97%)	82 (3%)	43 56

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

Sometimes 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	H	234	1	23,24,25	2.73	5 (21%)	25,32,34	1.41	4 (16%)
1	LLP	F	234	1	23,24,25	2.46	5 (21%)	25,32,34	1.43	3 (12%)
1	LLP	J	234	1	23,24,25	2.61	5 (21%)	25,32,34	1.49	5 (20%)
1	LLP	I	234	1	23,24,25	2.69	4 (17%)	25,32,34	1.37	3 (12%)
1	LLP	B	234	1	23,24,25	2.42	5 (21%)	25,32,34	1.59	5 (20%)
1	LLP	D	234	1	23,24,25	2.73	4 (17%)	25,32,34	1.58	5 (20%)
1	LLP	A	234	1	23,24,25	2.75	4 (17%)	25,32,34	1.36	2 (8%)
1	LLP	E	234	1	23,24,25	2.22	5 (21%)	25,32,34	1.45	3 (12%)
1	LLP	C	234	1	23,24,25	2.44	5 (21%)	25,32,34	1.30	3 (12%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	LLP	G	234	1	23,24,25	2.80	5 (21%)	25,32,34	1.37	4 (16%)

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	H	234	1	-	2/16/17/19	0/1/1/1
1	LLP	F	234	1	-	2/16/17/19	0/1/1/1
1	LLP	J	234	1	-	2/16/17/19	0/1/1/1
1	LLP	I	234	1	-	2/16/17/19	0/1/1/1
1	LLP	B	234	1	-	2/16/17/19	0/1/1/1
1	LLP	D	234	1	-	2/16/17/19	0/1/1/1
1	LLP	A	234	1	-	2/16/17/19	0/1/1/1
1	LLP	E	234	1	-	2/16/17/19	0/1/1/1
1	LLP	C	234	1	-	2/16/17/19	0/1/1/1
1	LLP	G	234	1	-	2/16/17/19	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	234	LLP	C3-C2	8.98	1.49	1.40
1	H	234	LLP	C3-C2	8.74	1.49	1.40
1	D	234	LLP	C3-C2	8.59	1.49	1.40
1	G	234	LLP	C3-C2	8.57	1.49	1.40
1	I	234	LLP	C3-C2	8.26	1.49	1.40
1	J	234	LLP	C3-C2	8.04	1.48	1.40
1	C	234	LLP	C3-C2	8.01	1.48	1.40
1	B	234	LLP	C3-C2	6.85	1.47	1.40
1	F	234	LLP	C3-C2	6.55	1.47	1.40
1	E	234	LLP	C3-C2	5.94	1.46	1.40
1	F	234	LLP	C4-C3	5.68	1.49	1.40
1	B	234	LLP	C4-C5	5.59	1.49	1.42
1	D	234	LLP	C4-C5	5.53	1.48	1.42
1	G	234	LLP	C4'-NZ	5.50	1.45	1.27
1	C	234	LLP	C4'-NZ	5.47	1.45	1.27
1	E	234	LLP	C4'-NZ	5.45	1.45	1.27
1	H	234	LLP	C4'-NZ	5.45	1.45	1.27
1	H	234	LLP	C4-C3	5.42	1.49	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	234	LLP	C4-C5	5.40	1.48	1.42
1	I	234	LLP	C4'-NZ	5.39	1.45	1.27
1	G	234	LLP	C4-C3	5.31	1.48	1.40
1	A	234	LLP	C4'-NZ	5.29	1.45	1.27
1	J	234	LLP	C4'-NZ	5.29	1.45	1.27
1	D	234	LLP	C4'-NZ	5.28	1.45	1.27
1	I	234	LLP	C4-C3	5.24	1.48	1.40
1	J	234	LLP	C4-C5	5.23	1.48	1.42
1	F	234	LLP	C4'-NZ	5.22	1.44	1.27
1	A	234	LLP	C4-C5	5.20	1.48	1.42
1	I	234	LLP	C4-C5	5.18	1.48	1.42
1	D	234	LLP	C4-C3	4.93	1.48	1.40
1	A	234	LLP	C4-C3	4.81	1.48	1.40
1	F	234	LLP	C4-C5	4.71	1.47	1.42
1	B	234	LLP	C4'-NZ	4.71	1.43	1.27
1	H	234	LLP	C4-C5	4.58	1.47	1.42
1	J	234	LLP	C4-C3	4.55	1.47	1.40
1	C	234	LLP	C4-C3	4.26	1.47	1.40
1	E	234	LLP	C4-C5	4.16	1.47	1.42
1	E	234	LLP	C4-C3	3.96	1.46	1.40
1	B	234	LLP	C4-C3	3.85	1.46	1.40
1	C	234	LLP	C4-C5	3.71	1.46	1.42
1	B	234	LLP	C4-C4'	3.37	1.53	1.46
1	J	234	LLP	C4-C4'	2.90	1.52	1.46
1	G	234	LLP	C4-C4'	2.76	1.51	1.46
1	E	234	LLP	C4-C4'	2.52	1.51	1.46
1	H	234	LLP	C4-C4'	2.28	1.51	1.46
1	C	234	LLP	C4-C4'	2.26	1.50	1.46
1	F	234	LLP	C6-C5	2.02	1.41	1.37

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	234	LLP	C4-C3-C2	-4.60	117.34	120.19
1	B	234	LLP	C4-C3-C2	-4.11	117.64	120.19
1	A	234	LLP	C4-C3-C2	-4.03	117.69	120.19
1	F	234	LLP	C6-N1-C2	3.69	125.99	119.17
1	G	234	LLP	C4-C3-C2	-3.58	117.97	120.19
1	H	234	LLP	C4-C3-C2	-3.47	118.04	120.19
1	E	234	LLP	C4-C3-C2	-3.47	118.04	120.19
1	I	234	LLP	C4-C3-C2	-3.44	118.06	120.19
1	J	234	LLP	C4-C3-C2	-3.32	118.13	120.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	234	LLP	C6-N1-C2	3.06	124.83	119.17
1	C	234	LLP	C4-C3-C2	-2.94	118.37	120.19
1	J	234	LLP	C4-C4'-NZ	-2.81	111.41	124.31
1	J	234	LLP	C3-C4-C5	-2.75	116.15	118.26
1	D	234	LLP	C4-C4'-NZ	-2.74	111.72	124.31
1	B	234	LLP	C6-N1-C2	2.74	124.24	119.17
1	E	234	LLP	C4-C4'-NZ	-2.74	111.74	124.31
1	I	234	LLP	C6-N1-C2	2.69	124.15	119.17
1	B	234	LLP	C4-C4'-NZ	-2.67	112.07	124.31
1	G	234	LLP	C4-C4'-NZ	-2.65	112.13	124.31
1	F	234	LLP	C4-C3-C2	-2.61	118.57	120.19
1	C	234	LLP	C4-C4'-NZ	-2.60	112.38	124.31
1	J	234	LLP	C6-N1-C2	2.59	123.97	119.17
1	B	234	LLP	C3-C4-C5	-2.54	116.31	118.26
1	I	234	LLP	C4-C4'-NZ	-2.52	112.73	124.31
1	F	234	LLP	C4-C4'-NZ	-2.48	112.94	124.31
1	H	234	LLP	C4-C4'-NZ	-2.45	113.06	124.31
1	A	234	LLP	C4-C4'-NZ	-2.42	113.19	124.31
1	H	234	LLP	C6-N1-C2	2.35	123.53	119.17
1	G	234	LLP	C3-C4-C5	-2.32	116.48	118.26
1	D	234	LLP	C3-C4-C5	-2.30	116.49	118.26
1	H	234	LLP	C3-C4-C5	-2.26	116.53	118.26
1	B	234	LLP	O3-C3-C2	2.25	122.40	117.49
1	D	234	LLP	O3-C3-C2	2.17	122.22	117.49
1	D	234	LLP	C6-N1-C2	2.06	122.98	119.17
1	G	234	LLP	O3-C3-C2	2.02	121.89	117.49
1	C	234	LLP	C6-N1-C2	2.01	122.88	119.17
1	J	234	LLP	OP2-P-OP4	-2.01	101.40	106.73

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	234	LLP	C4-C4'-NZ-CE
1	B	234	LLP	C4-C4'-NZ-CE
1	C	234	LLP	C4-C4'-NZ-CE
1	D	234	LLP	C4-C4'-NZ-CE
1	E	234	LLP	C4-C4'-NZ-CE
1	F	234	LLP	C4-C4'-NZ-CE
1	G	234	LLP	C4-C4'-NZ-CE
1	H	234	LLP	C4-C4'-NZ-CE
1	I	234	LLP	C4-C4'-NZ-CE

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Mol	Chain	Res	Type	Atoms
1	J	234	LLP	C4-C4'-NZ-CE
1	B	234	LLP	C3-C4-C4'-NZ
1	E	234	LLP	C3-C4-C4'-NZ
1	C	234	LLP	C3-C4-C4'-NZ
1	J	234	LLP	C3-C4-C4'-NZ
1	A	234	LLP	C3-C4-C4'-NZ
1	D	234	LLP	C3-C4-C4'-NZ
1	G	234	LLP	C3-C4-C4'-NZ
1	H	234	LLP	C3-C4-C4'-NZ
1	I	234	LLP	C3-C4-C4'-NZ
1	F	234	LLP	C3-C4-C4'-NZ

There are no ring outliers.

9 monomers are involved in 9 short contacts:

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

5.5 Carbohydrates (i)

There are no monosaccharides 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} 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%)	-0.04	2 (0%) 91 92	39, 52, 68, 79	0
1	B	404/422 (95%)	0.00	2 (0%) 91 92	39, 50, 65, 80	0
1	C	403/422 (95%)	-0.08	1 (0%) 95 95	43, 54, 65, 71	0
1	D	403/422 (95%)	-0.03	0 100 100	41, 49, 60, 67	0
1	E	403/422 (95%)	-0.09	1 (0%) 95 95	40, 52, 68, 77	0
1	F	403/422 (95%)	0.04	1 (0%) 95 95	41, 55, 72, 82	0
1	G	402/422 (95%)	0.21	12 (2%) 50 46	51, 63, 87, 105	0
1	H	399/422 (94%)	0.29	16 (4%) 38 35	55, 69, 81, 89	0
1	I	397/422 (94%)	1.59	120 (30%) 0 0	66, 89, 125, 143	0
1	J	355/422 (84%)	1.62	102 (28%) 0 0	70, 85, 106, 116	0
All	All	3972/4220 (94%)	0.33	257 (6%) 18 15	39, 58, 98, 143	0

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	126	LEU	11.3
1	J	203	ILE	7.5
1	I	304	ILE	7.0
1	J	373	ALA	6.9
1	J	33	VAL	6.9
1	I	76	ALA	6.7
1	J	320	ALA	6.6
1	J	187	THR	6.5
1	J	314	ALA	6.4
1	I	123	GLU	6.3
1	I	173	THR	6.2
1	I	125	LEU	6.2
1	I	127	SER	6.2

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Mol	Chain	Res	Type	RSRZ
1	I	214	VAL	6.1
1	J	186	GLY	6.1
1	J	20	PHE	6.0
1	I	309	ILE	5.7
1	I	215	HIS	5.6
1	I	341	ALA	5.5
1	I	381	GLY	5.5
1	I	170	SER	5.4
1	I	393	TYR	5.3
1	I	216	LEU	5.3
1	I	382	VAL	5.2
1	J	364	VAL	5.2
1	I	191	ILE	5.2
1	I	56	ALA	5.1
1	J	319	TYR	5.1
1	I	150	VAL	5.0
1	I	13	VAL	5.0
1	I	397	ALA	5.0
1	I	182	SER	5.0
1	I	172	ARG	4.9
1	I	161	HIS	4.9
1	J	31	THR	4.9
1	J	189	VAL	4.9
1	I	118	ILE	4.9
1	I	169	LEU	4.8
1	J	44	PRO	4.8
1	J	359	ILE	4.8
1	H	13	VAL	4.7
1	J	24	SER	4.7
1	J	177	ALA	4.7
1	J	362	ALA	4.7
1	J	216	LEU	4.7
1	I	343	ILE	4.5
1	J	363	GLY	4.4
1	J	12	ASP	4.4
1	J	268	THR	4.4
1	J	381	GLY	4.4
1	J	387	ARG	4.4
1	I	146	GLY	4.3
1	J	318	ASP	4.3
1	I	312	HIS	4.2
1	I	124	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	J	28	HIS	4.1
1	I	200	ALA	4.1
1	J	390	PHE	4.1
1	J	183	ASN	4.1
1	J	185	LEU	4.0
1	J	269	GLU	4.0
1	J	366	VAL	3.9
1	J	11	TYR	3.9
1	J	356	SER	3.9
1	I	69	LEU	3.9
1	I	324	LEU	3.9
1	I	176	VAL	3.9
1	I	63	HIS	3.9
1	I	318	ASP	3.9
1	I	145	GLN	3.9
1	H	414	GLY	3.8
1	I	342	ILE	3.8
1	J	344	SER	3.8
1	H	15	ALA	3.8
1	I	138	TRP	3.8
1	J	146	GLY	3.7
1	I	148	LYS	3.7
1	J	29	GLY	3.7
1	J	26	GLN	3.7
1	G	325	GLY	3.7
1	J	385	THR	3.7
1	J	128	ILE	3.6
1	I	67	HIS	3.6
1	J	159	VAL	3.6
1	J	313	GLU	3.6
1	J	40	SER	3.6
1	I	199	HIS	3.6
1	J	311	ALA	3.6
1	I	390	PHE	3.5
1	J	50	ALA	3.5
1	J	365	ALA	3.5
1	I	152	THR	3.5
1	I	327	ILE	3.4
1	J	16	ILE	3.4
1	J	343	ILE	3.4
1	J	355	VAL	3.4
1	J	392	LEU	3.4

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Mol	Chain	Res	Type	RSRZ
1	J	389	SER	3.4
1	H	304	ILE	3.4
1	I	51	VAL	3.4
1	I	114	GLY	3.3
1	G	413	PHE	3.3
1	I	188	VAL	3.3
1	I	388	ALA	3.3
1	I	159	VAL	3.3
1	J	116	PRO	3.3
1	I	155	ASP	3.3
1	J	341	ALA	3.2
1	J	368	ALA	3.2
1	I	147	ALA	3.2
1	I	308	ALA	3.2
1	J	340	GLY	3.2
1	I	319	TYR	3.2
1	I	333	PHE	3.1
1	I	59	TYR	3.1
1	I	180	HIS	3.1
1	J	386	CYS	3.1
1	I	19	ASP	3.1
1	G	352	ALA	3.1
1	H	305	GLY	3.1
1	J	338	ASP	3.1
1	I	330	LEU	3.1
1	I	52	THR	3.1
1	J	137	PRO	3.0
1	G	349	GLY	3.0
1	I	175	LEU	3.0
1	I	392	LEU	3.0
1	H	11	TYR	3.0
1	I	314	ALA	3.0
1	J	13	VAL	3.0
1	J	34	TYR	3.0
1	I	142	ARG	3.0
1	I	97	VAL	2.9
1	J	345	PHE	2.9
1	J	184	THR	2.9
1	I	128	ILE	2.9
1	J	111	TYR	2.9
1	I	151	PHE	2.9
1	J	124	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	206	LEU	2.9
1	I	109	VAL	2.9
1	A	328	ASN	2.9
1	I	166	GLU	2.8
1	I	345	PHE	2.8
1	J	19	ASP	2.8
1	I	119	GLY	2.8
1	J	37	ASN	2.8
1	J	307	HIS	2.8
1	I	377	LEU	2.8
1	J	317	ARG	2.8
1	I	189	VAL	2.7
1	B	328	ASN	2.7
1	I	122	ASP	2.7
1	I	34	TYR	2.7
1	J	25	ARG	2.7
1	J	383	THR	2.7
1	J	155	ASP	2.7
1	I	372	CYS	2.7
1	J	215	HIS	2.7
1	J	115	MET	2.7
1	I	153	PRO	2.7
1	J	32	LEU	2.7
1	I	73	ALA	2.6
1	I	311	ALA	2.6
1	G	411	LYS	2.6
1	H	23	LEU	2.6
1	H	399	VAL	2.6
1	G	409	ALA	2.6
1	I	332	ILE	2.6
1	J	384	SER	2.6
1	I	315	ASP	2.6
1	I	55	TYR	2.6
1	J	180	HIS	2.6
1	I	190	PRO	2.6
1	J	393	TYR	2.6
1	G	410	ARG	2.6
1	I	141	ILE	2.6
1	J	144	ARG	2.6
1	I	15	ALA	2.6
1	I	197	LEU	2.6
1	J	23	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	21	PRO	2.5
1	H	16	ILE	2.5
1	I	165	PHE	2.5
1	C	414	GLY	2.5
1	G	328	ASN	2.5
1	J	361	ARG	2.5
1	I	225	CYS	2.5
1	J	161	HIS	2.5
1	J	15	ALA	2.5
1	J	168	ARG	2.5
1	J	376	LEU	2.5
1	J	153	PRO	2.5
1	G	326	ARG	2.4
1	J	308	ALA	2.4
1	I	246	GLY	2.4
1	H	57	ASN	2.4
1	I	32	LEU	2.4
1	J	309	ILE	2.4
1	I	87	PHE	2.4
1	J	47	VAL	2.4
1	I	228	TYR	2.4
1	I	134	ASN	2.4
1	I	183	ASN	2.4
1	H	393	TYR	2.4
1	H	391	ALA	2.4
1	I	60	ALA	2.4
1	J	238	PRO	2.3
1	I	41	ALA	2.3
1	I	320	ALA	2.3
1	I	43	LYS	2.3
1	H	308	ALA	2.3
1	E	65	GLY	2.3
1	J	312	HIS	2.3
1	I	42	GLN	2.3
1	I	195	VAL	2.3
1	J	96	ILE	2.3
1	I	300	TYR	2.3
1	J	280	ARG	2.2
1	I	131	HIS	2.2
1	J	321	HIS	2.2
1	I	236	TYR	2.2
1	I	242	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	H	48	ILE	2.2
1	I	167	LYS	2.2
1	I	394	ASN	2.2
1	J	145	GLN	2.2
1	A	11	TYR	2.2
1	I	92	SER	2.2
1	J	213	ALA	2.2
1	H	309	ILE	2.2
1	I	58	GLU	2.2
1	J	236	TYR	2.2
1	G	28	HIS	2.1
1	I	70	SER	2.1
1	F	243	VAL	2.1
1	I	229	VAL	2.1
1	I	340	GLY	2.1
1	J	298	LEU	2.1
1	I	121	GLY	2.1
1	I	306	ARG	2.1
1	J	230	PHE	2.1
1	I	325	GLY	2.1
1	J	167	LYS	2.1
1	J	98	PHE	2.1
1	B	65	GLY	2.1
1	G	319	TYR	2.0
1	I	117	PHE	2.0
1	J	175	LEU	2.0
1	G	154	VAL	2.0
1	J	205	VAL	2.0
1	I	133	SER	2.0
1	H	316	LEU	2.0
1	J	22	ILE	2.0
1	I	160	PHE	2.0
1	I	276	HIS	2.0
1	I	376	LEU	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. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
1	LLP	I	234	24/25	0.89	0.22	72,75,80,82	0
1	LLP	J	234	24/25	0.90	0.23	75,77,79,80	0
1	LLP	H	234	24/25	0.96	0.16	54,56,59,61	0
1	LLP	G	234	24/25	0.97	0.15	54,57,59,59	0
1	LLP	A	234	24/25	0.97	0.14	40,43,44,45	0
1	LLP	B	234	24/25	0.97	0.17	38,40,41,41	0
1	LLP	C	234	24/25	0.97	0.15	44,46,47,47	0
1	LLP	E	234	24/25	0.98	0.16	41,42,44,45	0
1	LLP	F	234	24/25	0.98	0.17	42,44,46,47	0
1	LLP	D	234	24/25	0.98	0.17	41,41,42,43	0

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^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CL	H	501	1/1	0.67	0.16	71,71,71,71	0
2	CL	E	501	1/1	0.79	0.18	72,72,72,72	0
2	CL	C	501	1/1	0.80	0.13	86,86,86,86	0
2	CL	B	501	1/1	0.81	0.21	69,69,69,69	0
2	CL	I	501	1/1	0.82	0.18	79,79,79,79	0
2	CL	D	501	1/1	0.84	0.18	52,52,52,52	0
2	CL	A	501	1/1	0.85	0.19	69,69,69,69	0

6.5 Other polymers (i)

There are no such residues in this entry.