



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:55 PM UTC

PDB ID : 4W91 / pdb_00004w91
Title : Crystal structure of a cysteine desulfurase SufS from *Brucella suis* bound to PLP
Authors : 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:

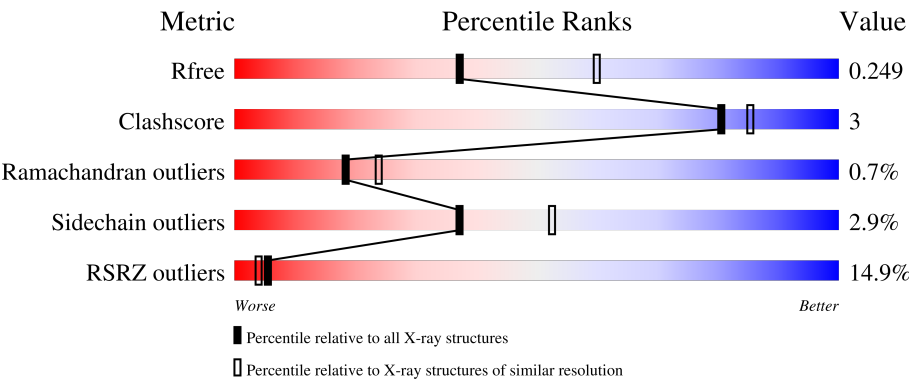
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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}	180053	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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 $\leq 5\%$. 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	2% 87% 6% . . .
1	B	422	2% 88% 6% . . .
1	C	422	2% 86% 7% . . .
1	D	422	% 86% 8% . . .
1	E	422	2% 88% 6% . . .

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Mol	Chain	Length	Quality of chain
1	F	422	2% 87% 7%
1	G	422	5% 86% 7% 5%
1	H	422	4% 88% 6% 5%
1	I	422	62% 90% 6%
1	J	422	59% 81% 16%

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 (CCD ID: 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 1	Cl 1	0	0
2	I	1	Total 1	Cl 1	0	0

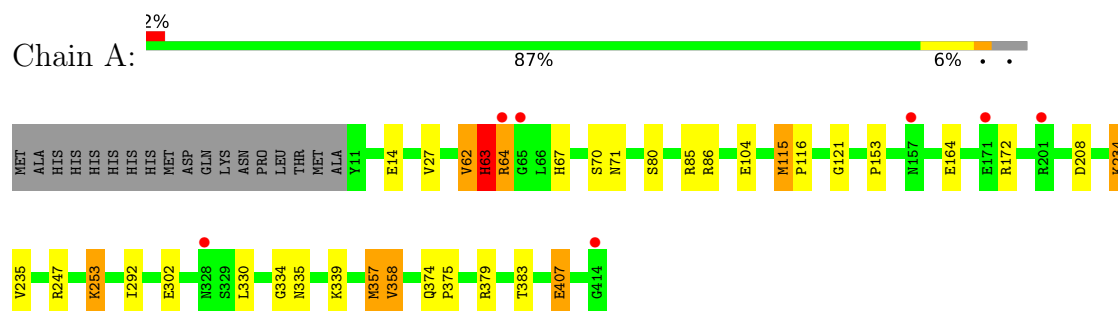
- Molecule 3 is water.

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

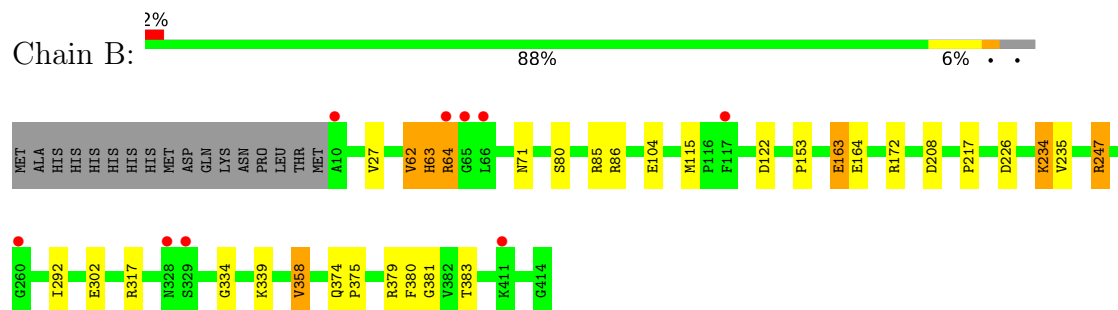
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, 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.

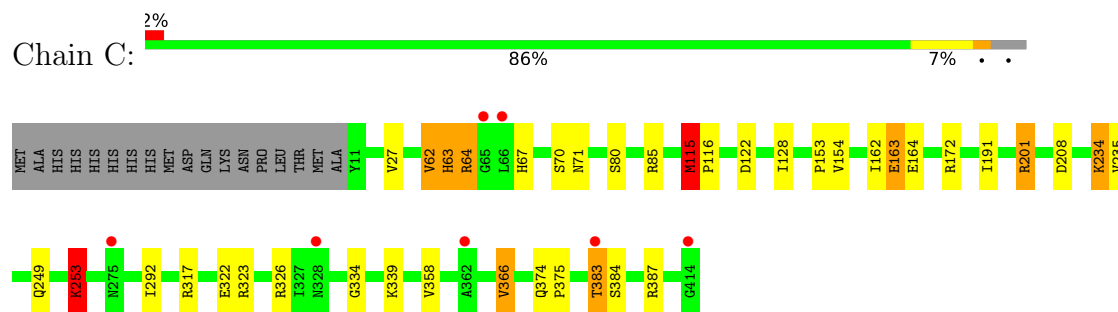
• Molecule 1: Aminotransferase



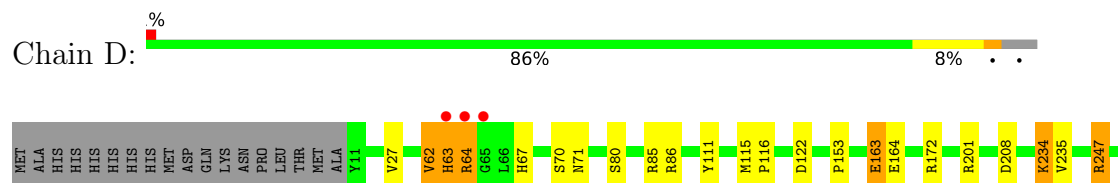
• Molecule 1: Aminotransferase



• Molecule 1: Aminotransferase

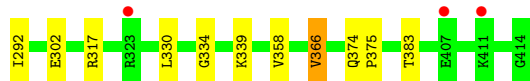
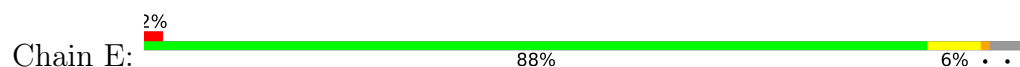


• Molecule 1: Aminotransferase

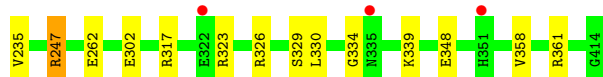
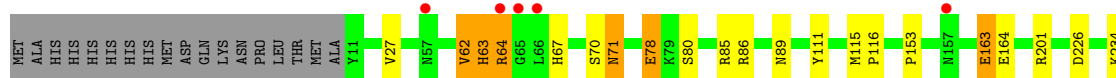
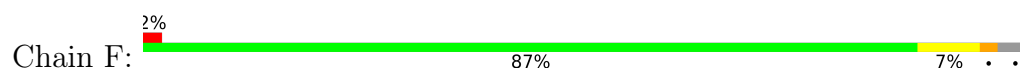




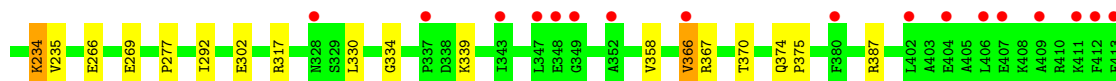
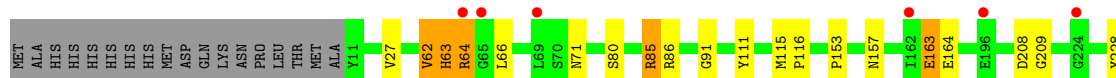
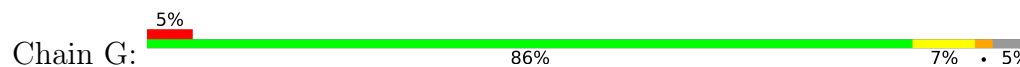
• Molecule 1: Aminotransferase



• Molecule 1: Aminotransferase

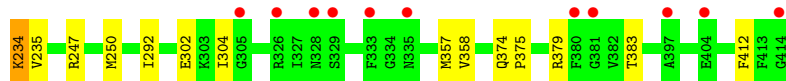
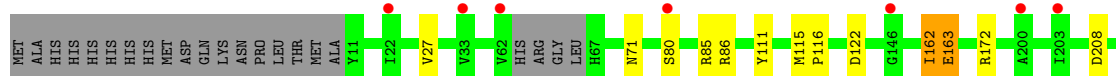
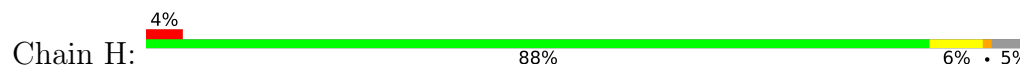


• Molecule 1: Aminotransferase

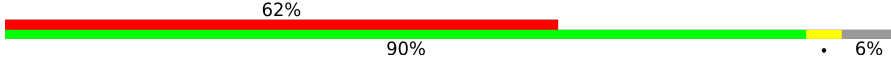


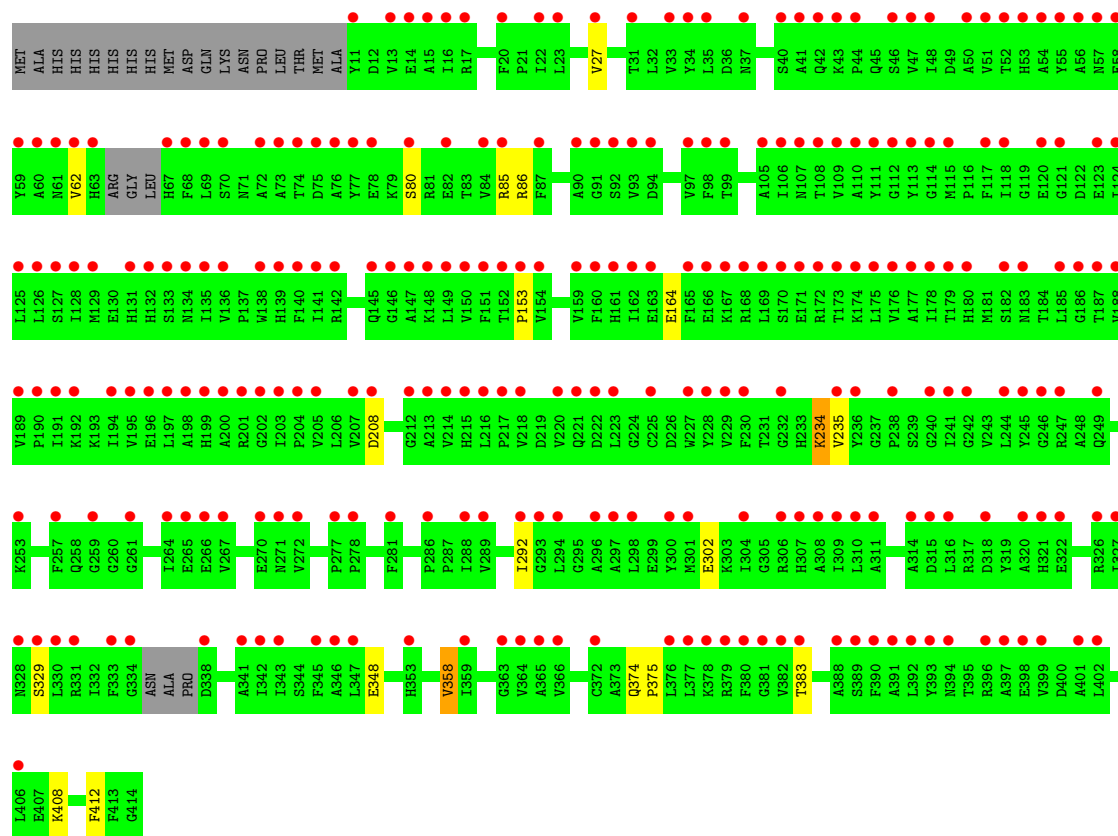
GLY

• Molecule 1: Aminotransferase



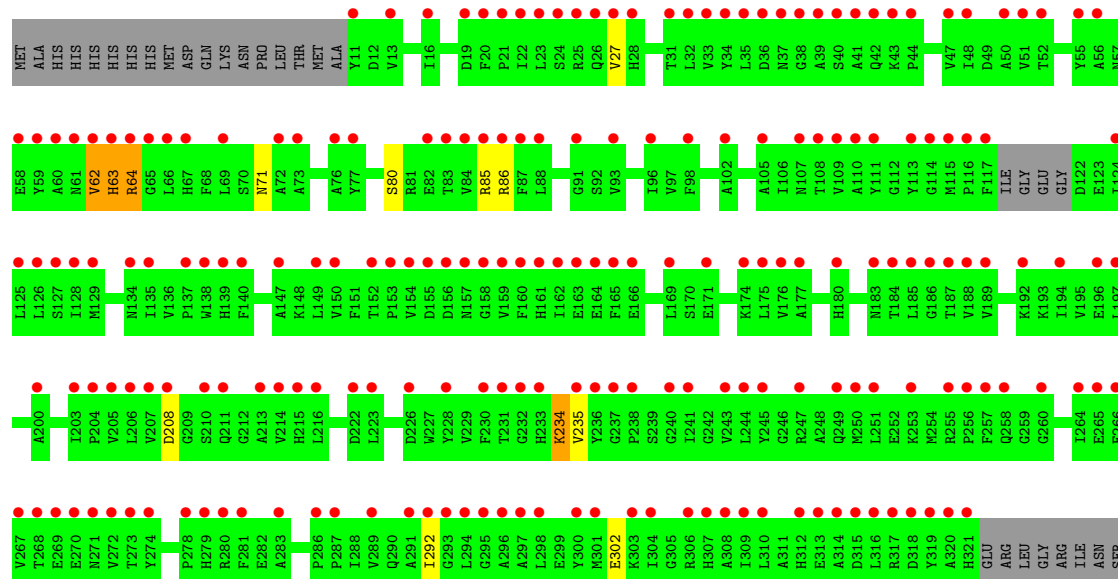
• Molecule 1: Aminotransferase

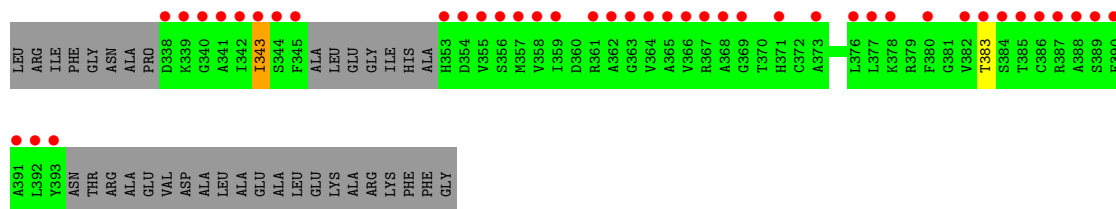
Chain I: 



• Molecule 1: Aminotransferase

Chain J: 





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 50.00 – 2.45	Depositor EDS
% Data completeness (in resolution range)	96.5 (50.00-2.45) 96.4 (50.00-2.45)	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 (4.84%)	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)	0.33 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 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	0.77	1/3168 (0.0%)	0.88	2/4301 (0.0%)
1	B	0.78	0/3155	0.86	1/4284 (0.0%)
1	C	0.81	1/3163 (0.0%)	0.90	8/4293 (0.2%)
1	D	0.82	2/3179 (0.1%)	0.89	2/4312 (0.0%)
1	E	0.79	0/3128	0.90	3/4254 (0.1%)
1	F	0.78	1/3146 (0.0%)	0.88	2/4277 (0.0%)
1	G	0.71	1/3084 (0.0%)	0.88	3/4201 (0.1%)
1	H	0.71	0/3084	0.89	4/4194 (0.1%)
1	I	0.69	0/2794	0.88	1/3822 (0.0%)
1	J	0.68	0/2538	0.89	2/3472 (0.1%)
All	All	0.76	6/30439 (0.0%)	0.88	28/41410 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	277	PRO	C-O	-7.31	1.18	1.25
1	A	63	HIS	N-CA	6.19	1.54	1.46
1	C	383	THR	C-O	5.18	1.30	1.24
1	G	277	PRO	C-O	-5.15	1.20	1.25
1	D	80	SER	N-CA	5.13	1.52	1.46
1	F	80	SER	CA-CB	5.05	1.61	1.53

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	343	ILE	CB-CA-C	10.78	123.56	110.73
1	G	366	VAL	N-CA-CB	-8.19	103.27	112.45
1	H	162	ILE	N-CA-CB	7.94	121.34	110.54
1	I	62	VAL	N-CA-C	7.29	119.14	112.43
1	G	62	VAL	N-CA-C	7.05	118.87	112.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	62	VAL	N-CA-C	6.99	118.86	112.43
1	D	62	VAL	N-CA-C	6.89	118.71	112.17
1	B	62	VAL	N-CA-C	6.65	118.55	112.43
1	E	62	VAL	N-CA-C	6.58	118.86	111.88
1	A	62	VAL	N-CA-C	6.48	118.32	112.17
1	C	201	ARG	NE-CZ-NH2	6.45	125.00	119.20
1	C	366	VAL	N-CA-CB	-6.26	103.75	112.52
1	J	62	VAL	N-CA-C	6.07	118.32	111.88
1	E	366	VAL	N-CA-CB	-5.97	104.16	112.52
1	H	162	ILE	CB-CA-C	-5.88	104.20	112.14
1	A	407	GLU	CB-CG-CD	5.86	122.56	112.60
1	C	191	ILE	N-CA-C	5.84	116.62	110.72
1	H	304	ILE	CG1-CB-CG2	5.73	127.90	110.70
1	E	247	ARG	CG-CD-NE	5.70	124.54	112.00
1	C	384	SER	CA-CB-OG	-5.68	99.73	111.10
1	D	247	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	C	62	VAL	N-CA-C	5.46	117.67	111.88
1	G	367	ARG	CD-NE-CZ	-5.43	116.79	124.40
1	F	71	ASN	N-CA-C	5.42	116.87	111.07
1	C	253	LYS	CB-CG-CD	5.41	123.75	111.30
1	C	201	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	C	115	MET	CG-SD-CE	5.12	112.16	100.90
1	H	250	MET	CG-SD-CE	5.07	112.05	100.90

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	22	0
1	B	3110	0	3012	20	0
1	C	3118	0	3023	18	0
1	D	3131	0	3048	21	0
1	E	3083	0	2950	15	0
1	F	3097	0	2972	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	G	3041	0	2896	20	0
1	H	3041	0	2917	13	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	149	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 3.

All (149) 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:A:121:GLY:C	1:A:172:ARG:HH21	2.04	0.65
1:B:379:ARG:O	1:D:381:GLY:HA2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:357:MET:HE2	1:F:361:ARG:HG2	1.85	0.57
1:B:63:HIS:O	1:B:64:ARG:C	2.48	0.57
1:F:226:ASP:HA	1:F:247:ARG:HD3	1.87	0.56
1:F:163:GLU:H	1:F:163:GLU:CD	2.14	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:D:111:TYR:HA	1:D:115:MET:HE2	1.90	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:63:HIS:O	1:E:64:ARG:C	2.52	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
1:F:334:GLY:O	1:F:339:LYS:NZ	2.41	0.53
1:J:63:HIS:O	1:J:64:ARG:C	2.51	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:HIS:O	1:A:64:ARG:C	2.52	0.51
1:E:334:GLY:O	1:E:339:LYS:NZ	2.41	0.51
1:G:334:GLY:O	1:G:339:LYS:NZ	2.42	0.51
1:E:111:TYR:HA	1:E:115:MET:HE2	1.93	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:H:111:TYR:HA	1:H:115:MET:HE2	1.94	0.50
1:D:63:HIS:O	1:D:64:ARG:C	2.53	0.50
1:F:111:TYR:HA	1:F:115:MET:HE2	1.92	0.50
1:F:63:HIS:O	1:F:64:ARG:C	2.54	0.49
1:G:111:TYR:HA	1:G:115:MET:HE2	1.92	0.49
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:C:63:HIS:O	1:C:64:ARG:C	2.55	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:G:63:HIS:O	1:G:64:ARG:C	2.56	0.47
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:G:208:ASP:OD2	1:G:234:LLP:N1	2.47	0.46
1:E:249:GLN:CD	1:E:249:GLN:H	2.24	0.46
1:D:86:ARG:HD2	1:D:302:GLU:OE2	2.15	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:D:357:MET:C	1:D:357:MET:SD	2.99	0.45
1:G:269:GLU:CD	1:H:379:ARG:HH11	2.25	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:H:163:GLU:H	1:H:163:GLU:CD	2.26	0.44
1:C:374:GLN:HB2	1:C:375:PRO:HD3	2.00	0.44
1:E:330:LEU:C	1:E:330:LEU:HD23	2.42	0.44
1:E:374:GLN:HB2	1:E:375:PRO:HD3	2.00	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:B:62:VAL:C	1:B:64:ARG:N	2.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:PHE:C	1:D:381:GLY:HA3	2.43	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:G:66:LEU:HD12	1:G:66:LEU:N	2.33	0.43
1:H:357:MET:C	1:H:357:MET:SD	3.01	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:D:163:GLU:H	1:D:163:GLU:CD	2.26	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:G:62:VAL:C	1:G:64:ARG:N	2.77	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:B:163:GLU:H	1:B:163:GLU:CD	2.27	0.42
1:C:62:VAL:C	1:C:64:ARG:N	2.78	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:D:62:VAL:C	1:D:64:ARG:N	2.77	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:C:163:GLU:H	1:C:163:GLU:CD	2.27	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:F:62:VAL:C	1:F:64:ARG:N	2.79	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:E:62:VAL:C	1:E:64:ARG:N	2.79	0.41
1:A:374:GLN:HB2	1:A:375:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:ARG:C	1:B:379:ARG:HD3	2.45	0.41
1:F:330:LEU:HD23	1:F:330:LEU:C	2.46	0.41
1:G:330:LEU:C	1:G:330:LEU:HD23	2.46	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:G:163:GLU:H	1:G:163:GLU:CD	2.29	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:A:330:LEU:C	1:A:330:LEU:HD23	2.46	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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	18	24
1	B	402/422 (95%)	389 (97%)	10 (2%)	3 (1%)	18	24
1	C	401/422 (95%)	388 (97%)	10 (2%)	3 (1%)	18	24
1	D	402/422 (95%)	388 (96%)	11 (3%)	3 (1%)	18	24
1	E	401/422 (95%)	388 (97%)	10 (2%)	3 (1%)	18	24
1	F	402/422 (95%)	389 (97%)	10 (2%)	3 (1%)	18	24
1	G	400/422 (95%)	387 (97%)	10 (2%)	3 (1%)	16	20
1	H	395/422 (94%)	384 (97%)	10 (2%)	1 (0%)	36	45
1	I	391/422 (93%)	380 (97%)	10 (3%)	1 (0%)	36	45
1	J	347/422 (82%)	335 (96%)	9 (3%)	3 (1%)	14	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	3944/4220 (94%)	3818 (97%)	100 (2%)	26 (1%)	18 24

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
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%)	300 (96%)	12 (4%)	29	43
1	B	311/341 (91%)	303 (97%)	8 (3%)	40	55
1	C	313/341 (92%)	302 (96%)	11 (4%)	32	46
1	D	316/341 (93%)	305 (96%)	11 (4%)	32	46
1	E	305/341 (89%)	296 (97%)	9 (3%)	36	51
1	F	308/341 (90%)	298 (97%)	10 (3%)	34	49
1	G	297/341 (87%)	289 (97%)	8 (3%)	39	54
1	H	300/341 (88%)	293 (98%)	7 (2%)	44	59
1	I	233/341 (68%)	229 (98%)	4 (2%)	53	67
1	J	215/341 (63%)	210 (98%)	5 (2%)	44	59
All	All	2910/3410 (85%)	2825 (97%)	85 (3%)	37	52

All (85) 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	A	407	GLU
1	B	27	VAL
1	B	71	ASN
1	B	85	ARG
1	B	115	MET
1	B	163	GLU
1	B	247	ARG
1	B	358	VAL
1	B	383	THR
1	C	27	VAL
1	C	71	ASN
1	C	85	ARG
1	C	115	MET

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Mol	Chain	Res	Type
1	C	162	ILE
1	C	163	GLU
1	C	201	ARG
1	C	253	LYS
1	C	323	ARG
1	C	358	VAL
1	C	383	THR
1	D	27	VAL
1	D	71	ASN
1	D	85	ARG
1	D	163	GLU
1	D	201[A]	ARG
1	D	201[B]	ARG
1	D	247	ARG
1	D	323	ARG
1	D	329	SER
1	D	358	VAL
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	366	VAL
1	E	383	THR
1	F	27	VAL
1	F	71	ASN
1	F	78	GLU
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	358	VAL
1	G	27	VAL
1	G	71	ASN
1	G	85	ARG
1	G	157	ASN
1	G	163	GLU

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Mol	Chain	Res	Type
1	G	266	GLU
1	G	358	VAL
1	G	370	THR
1	H	27	VAL
1	H	71	ASN
1	H	85	ARG
1	H	162	ILE
1	H	163	GLU
1	H	358	VAL
1	H	383	THR
1	I	27	VAL
1	I	85	ARG
1	I	358	VAL
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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	211	GLN
1	A	221	GLN
1	A	353	HIS
1	B	89	ASN
1	B	145	GLN
1	C	45	GLN
1	C	89	ASN
1	C	211	GLN
1	D	45	GLN
1	D	89	ASN
1	D	221	GLN
1	D	328	ASN
1	E	45	GLN
1	E	221	GLN
1	F	45	GLN
1	F	221	GLN
1	H	67	HIS
1	H	89	ASN
1	H	211	GLN

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Mol	Chain	Res	Type
1	H	221	GLN
1	H	353	HIS
1	I	89	ASN
1	I	221	GLN
1	J	221	GLN
1	J	371	HIS

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	I	234	1	23,24,25	2.55	4 (17%)	25,32,34	1.41	3 (12%)
1	LLP	H	234	1	23,24,25	2.58	5 (21%)	25,32,34	1.44	4 (16%)
1	LLP	C	234	1	23,24,25	2.33	5 (21%)	25,32,34	1.32	3 (12%)
1	LLP	J	234	1	23,24,25	2.47	5 (21%)	25,32,34	1.52	5 (20%)
1	LLP	A	234	1	23,24,25	2.62	4 (17%)	25,32,34	1.40	2 (8%)
1	LLP	E	234	1	23,24,25	2.11	5 (21%)	25,32,34	1.49	3 (12%)
1	LLP	G	234	1	23,24,25	2.65	5 (21%)	25,32,34	1.40	4 (16%)
1	LLP	F	234	1	23,24,25	2.33	5 (21%)	25,32,34	1.46	4 (16%)
1	LLP	B	234	1	23,24,25	2.28	5 (21%)	25,32,34	1.63	5 (20%)
1	LLP	D	234	1	23,24,25	2.59	4 (17%)	25,32,34	1.62	5 (20%)

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	I	234	1	-	2/16/17/19	0/1/1/1
1	LLP	H	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	J	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	G	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	B	234	1	-	2/16/17/19	0/1/1/1
1	LLP	D	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	8.59	1.49	1.41
1	H	234	LLP	C3-C2	8.36	1.49	1.41
1	D	234	LLP	C3-C2	8.21	1.49	1.41
1	G	234	LLP	C3-C2	8.20	1.49	1.41
1	I	234	LLP	C3-C2	7.90	1.49	1.41
1	J	234	LLP	C3-C2	7.68	1.48	1.41
1	C	234	LLP	C3-C2	7.65	1.48	1.41
1	B	234	LLP	C3-C2	6.54	1.47	1.41
1	F	234	LLP	C3-C2	6.25	1.47	1.41
1	E	234	LLP	C3-C2	5.66	1.46	1.41
1	G	234	LLP	C4'-NZ	5.55	1.45	1.27
1	C	234	LLP	C4'-NZ	5.52	1.45	1.27
1	E	234	LLP	C4'-NZ	5.49	1.45	1.27
1	H	234	LLP	C4'-NZ	5.49	1.45	1.27
1	I	234	LLP	C4'-NZ	5.43	1.45	1.27
1	A	234	LLP	C4'-NZ	5.34	1.45	1.27
1	J	234	LLP	C4'-NZ	5.33	1.45	1.27
1	D	234	LLP	C4'-NZ	5.32	1.45	1.27
1	F	234	LLP	C4'-NZ	5.26	1.44	1.27
1	B	234	LLP	C4-C5	5.06	1.49	1.42
1	F	234	LLP	C4-C3	5.01	1.49	1.41
1	D	234	LLP	C4-C5	5.00	1.48	1.42
1	G	234	LLP	C4-C5	4.88	1.48	1.42
1	H	234	LLP	C4-C3	4.77	1.49	1.41
1	B	234	LLP	C4'-NZ	4.75	1.43	1.27
1	J	234	LLP	C4-C5	4.73	1.48	1.42
1	A	234	LLP	C4-C5	4.71	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	234	LLP	C4-C5	4.69	1.48	1.42
1	G	234	LLP	C4-C3	4.67	1.48	1.41
1	I	234	LLP	C4-C3	4.61	1.48	1.41
1	D	234	LLP	C4-C3	4.32	1.48	1.41
1	F	234	LLP	C4-C5	4.26	1.47	1.42
1	A	234	LLP	C4-C3	4.22	1.48	1.41
1	H	234	LLP	C4-C5	4.14	1.47	1.42
1	J	234	LLP	C4-C3	3.98	1.47	1.41
1	E	234	LLP	C4-C5	3.76	1.47	1.42
1	C	234	LLP	C4-C3	3.71	1.47	1.41
1	E	234	LLP	C4-C3	3.44	1.46	1.41
1	C	234	LLP	C4-C5	3.36	1.46	1.42
1	B	234	LLP	C4-C3	3.34	1.46	1.41
1	B	234	LLP	C4-C4'	3.01	1.53	1.46
1	J	234	LLP	C4-C4'	2.59	1.52	1.46
1	G	234	LLP	C4-C4'	2.46	1.51	1.46
1	E	234	LLP	C4-C4'	2.26	1.51	1.46
1	F	234	LLP	C6-C5	2.13	1.41	1.37
1	H	234	LLP	C4-C4'	2.04	1.51	1.46
1	C	234	LLP	C4-C4'	2.02	1.50	1.46

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	234	LLP	C4-C3-C2	-4.98	117.34	120.14
1	B	234	LLP	C4-C3-C2	-4.44	117.64	120.14
1	A	234	LLP	C4-C3-C2	-4.36	117.69	120.14
1	G	234	LLP	C4-C3-C2	-3.85	117.97	120.14
1	F	234	LLP	C6-N1-C2	3.75	125.99	119.20
1	H	234	LLP	C4-C3-C2	-3.74	118.04	120.14
1	E	234	LLP	C4-C3-C2	-3.73	118.04	120.14
1	I	234	LLP	C4-C3-C2	-3.70	118.06	120.14
1	J	234	LLP	C4-C3-C2	-3.57	118.13	120.14
1	C	234	LLP	C4-C3-C2	-3.16	118.37	120.14
1	E	234	LLP	C6-N1-C2	3.11	124.83	119.20
1	F	234	LLP	C4-C3-C2	-2.79	118.57	120.14
1	B	234	LLP	C6-N1-C2	2.78	124.24	119.20
1	J	234	LLP	C4-C4'-NZ	-2.74	111.41	124.04
1	I	234	LLP	C6-N1-C2	2.73	124.15	119.20
1	D	234	LLP	C4-C4'-NZ	-2.67	111.72	124.04
1	E	234	LLP	C4-C4'-NZ	-2.67	111.74	124.04
1	J	234	LLP	C3-C4-C5	-2.65	116.15	118.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	234	LLP	C6-N1-C2	2.63	123.97	119.20
1	B	234	LLP	C4-C4'-NZ	-2.59	112.07	124.04
1	G	234	LLP	C4-C4'-NZ	-2.58	112.13	124.04
1	C	234	LLP	C4-C4'-NZ	-2.53	112.38	124.04
1	B	234	LLP	C3-C4-C5	-2.45	116.31	118.28
1	I	234	LLP	C4-C4'-NZ	-2.45	112.73	124.04
1	F	234	LLP	C4-C4'-NZ	-2.41	112.94	124.04
1	H	234	LLP	C6-N1-C2	2.39	123.53	119.20
1	H	234	LLP	C4-C4'-NZ	-2.38	113.06	124.04
1	A	234	LLP	C4-C4'-NZ	-2.35	113.19	124.04
1	B	234	LLP	O3-C3-C2	2.33	122.40	117.58
1	D	234	LLP	O3-C3-C2	2.24	122.22	117.58
1	G	234	LLP	C3-C4-C5	-2.23	116.48	118.28
1	D	234	LLP	C3-C4-C5	-2.22	116.49	118.28
1	F	234	LLP	C3-C2-N1	-2.19	118.19	120.96
1	H	234	LLP	C3-C4-C5	-2.18	116.53	118.28
1	D	234	LLP	C6-N1-C2	2.09	122.98	119.20
1	G	234	LLP	O3-C3-C2	2.08	121.89	117.58
1	C	234	LLP	C6-N1-C2	2.03	122.88	119.20
1	J	234	LLP	OP2-P-OP4	-2.02	101.40	106.67

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
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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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 ⓘ

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%)	0.35	7 (1%) 69 71	30, 52, 68, 79	2 (0%)
1	B	404/422 (95%)	0.36	9 (2%) 62 64	39, 50, 65, 80	0
1	C	403/422 (95%)	0.22	7 (1%) 69 71	43, 54, 65, 71	0
1	D	403/422 (95%)	0.23	5 (1%) 76 78	35, 49, 60, 67	1 (0%)
1	E	403/422 (95%)	0.31	7 (1%) 69 71	40, 52, 68, 77	0
1	F	403/422 (95%)	0.41	8 (1%) 65 66	38, 55, 72, 82	1 (0%)
1	G	402/422 (95%)	0.78	23 (5%) 29 26	51, 63, 87, 105	0
1	H	399/422 (94%)	0.80	18 (4%) 38 37	55, 69, 81, 89	0
1	I	397/422 (94%)	2.50	260 (65%) 0 0	66, 89, 125, 143	0
1	J	355/422 (84%)	2.63	248 (69%) 0 0	70, 85, 106, 116	0
All	All	3972/4220 (94%)	0.84	592 (14%) 5 4	30, 58, 98, 143	4 (0%)

All (592) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	126	LEU	9.6
1	I	152	THR	6.6
1	I	338	ASP	6.0
1	I	76	ALA	5.9
1	I	125	LEU	5.8
1	I	341	ALA	5.7
1	J	364	VAL	5.5
1	J	354	ASP	5.5
1	J	365	ALA	5.3
1	G	65	GLY	5.3
1	I	191	ILE	5.3
1	J	345	PHE	5.2
1	E	65	GLY	5.2

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Mol	Chain	Res	Type	RSRZ
1	J	44	PRO	5.2
1	I	150	VAL	5.1
1	I	124	ILE	5.1
1	J	203	ILE	5.1
1	J	128	ILE	5.0
1	J	373	ALA	5.0
1	I	214	VAL	4.9
1	I	315	ASP	4.9
1	I	171	GLU	4.9
1	J	387	ARG	4.9
1	I	41	ALA	4.8
1	I	203	ILE	4.8
1	I	73	ALA	4.8
1	I	127	SER	4.8
1	J	359	ILE	4.8
1	I	11	TYR	4.8
1	I	55	TYR	4.8
1	J	271	ASN	4.8
1	J	392	LEU	4.7
1	I	97	VAL	4.7
1	J	158	GLY	4.7
1	J	353	HIS	4.7
1	I	289	VAL	4.7
1	J	187	THR	4.6
1	J	33	VAL	4.6
1	I	58	GLU	4.6
1	I	63	HIS	4.6
1	J	319	TYR	4.6
1	I	194	ILE	4.6
1	J	342	ILE	4.6
1	J	343	ILE	4.6
1	J	216	LEU	4.5
1	J	357	MET	4.5
1	J	361	ARG	4.5
1	J	117	PHE	4.5
1	I	228	TYR	4.5
1	I	51	VAL	4.5
1	I	57	ASN	4.5
1	J	40	SER	4.5
1	J	341	ALA	4.5
1	I	190	PRO	4.4
1	J	50	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	J	268	THR	4.4
1	J	177	ALA	4.4
1	J	389	SER	4.4
1	J	156	ASP	4.3
1	I	223	LEU	4.3
1	I	309	ILE	4.3
1	J	48	ILE	4.2
1	I	189	VAL	4.2
1	J	291	ALA	4.2
1	I	333	PHE	4.2
1	I	160	PHE	4.2
1	J	362	ALA	4.2
1	J	344	SER	4.1
1	J	304	ILE	4.1
1	J	355	VAL	4.1
1	I	180	HIS	4.1
1	J	73	ALA	4.1
1	J	58	GLU	4.1
1	J	393	TYR	4.1
1	J	175	LEU	4.1
1	I	168	ARG	4.1
1	J	186	GLY	4.0
1	F	351[A]	HIS	4.0
1	J	20	PHE	4.0
1	J	137	PRO	4.0
1	J	269	GLU	4.0
1	I	141	ILE	4.0
1	I	310	LEU	4.0
1	J	185	LEU	4.0
1	J	206	LEU	4.0
1	J	176	VAL	4.0
1	I	249	GLN	4.0
1	I	123	GLU	3.9
1	J	385	THR	3.9
1	I	117	PHE	3.9
1	I	200	ALA	3.9
1	J	318	ASP	3.9
1	I	215	HIS	3.9
1	J	174	LYS	3.9
1	I	334	GLY	3.9
1	I	48	ILE	3.9
1	I	153	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	I	393	TYR	3.9
1	J	34	TYR	3.9
1	A	65	GLY	3.9
1	I	149	LEU	3.9
1	J	388	ALA	3.8
1	I	118	ILE	3.8
1	J	238	PRO	3.8
1	J	236	TYR	3.8
1	J	356	SER	3.8
1	J	52	THR	3.8
1	I	383	THR	3.8
1	I	172	ARG	3.8
1	I	87	PHE	3.8
1	I	59	TYR	3.8
1	J	382	VAL	3.7
1	I	376	LEU	3.7
1	J	183	ASN	3.7
1	J	213	ALA	3.7
1	C	383	THR	3.7
1	I	397	ALA	3.7
1	I	78	GLU	3.7
1	I	270	GLU	3.7
1	J	125	LEU	3.7
1	I	113	TYR	3.7
1	I	129	MET	3.7
1	I	364	VAL	3.7
1	J	31	THR	3.7
1	J	296	ALA	3.7
1	J	88	LEU	3.7
1	I	47	VAL	3.6
1	J	366	VAL	3.6
1	J	127	SER	3.6
1	J	368	ALA	3.6
1	I	390	PHE	3.6
1	J	23	LEU	3.6
1	I	16	ILE	3.6
1	I	372	CYS	3.6
1	J	47	VAL	3.6
1	J	376	LEU	3.6
1	I	22	ILE	3.6
1	I	292	ILE	3.6
1	J	222	ASP	3.6

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Mol	Chain	Res	Type	RSRZ
1	I	242	GLY	3.6
1	I	68	PHE	3.6
1	J	278	PRO	3.6
1	I	151	PHE	3.6
1	J	230	PHE	3.6
1	J	315	ASP	3.6
1	J	207	VAL	3.5
1	J	300	TYR	3.5
1	A	64	ARG	3.5
1	I	50	ALA	3.5
1	I	162	ILE	3.5
1	J	98	PHE	3.5
1	I	77	TYR	3.5
1	I	177	ALA	3.5
1	I	227	TRP	3.5
1	I	281	PHE	3.5
1	J	306	ARG	3.5
1	I	236	TYR	3.5
1	F	65	GLY	3.5
1	G	224	GLY	3.5
1	J	37	ASN	3.5
1	J	164	GLU	3.5
1	I	173	THR	3.5
1	J	66	LEU	3.5
1	J	153	PRO	3.5
1	J	240	GLY	3.5
1	J	257	PHE	3.5
1	I	67	HIS	3.5
1	I	176	VAL	3.4
1	J	138	TRP	3.4
1	J	214	VAL	3.4
1	E	64	ARG	3.4
1	J	21	PRO	3.4
1	I	90	ALA	3.4
1	J	309	ILE	3.4
1	I	175	LEU	3.4
1	G	328	ASN	3.3
1	J	32	LEU	3.3
1	J	298	LEU	3.3
1	I	93	VAL	3.3
1	C	65	GLY	3.3
1	J	16	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	124	ILE	3.3
1	J	314	ALA	3.3
1	J	223	LEU	3.3
1	I	201	ARG	3.3
1	I	229	VAL	3.3
1	J	159	VAL	3.3
1	J	307	HIS	3.3
1	I	128	ILE	3.3
1	I	70	SER	3.3
1	J	245	TYR	3.3
1	I	216	LEU	3.3
1	J	51	VAL	3.3
1	G	349	GLY	3.3
1	J	363	GLY	3.3
1	I	147	ALA	3.3
1	J	208	ASP	3.2
1	I	142	ARG	3.2
1	I	307	HIS	3.2
1	I	159	VAL	3.2
1	J	115	MET	3.2
1	J	289	VAL	3.2
1	J	292	ILE	3.2
1	J	390	PHE	3.2
1	I	204	PRO	3.2
1	J	169	LEU	3.2
1	I	138	TRP	3.2
1	I	165	PHE	3.2
1	C	66	LEU	3.2
1	I	23	LEU	3.2
1	I	183	ASN	3.2
1	D	65	GLY	3.2
1	I	33	VAL	3.2
1	B	10	ALA	3.2
1	I	169	LEU	3.2
1	I	197	LEU	3.2
1	J	166	GLU	3.2
1	B	65	GLY	3.2
1	I	235	VAL	3.2
1	I	72	ALA	3.1
1	I	92	SER	3.1
1	I	182	SER	3.1
1	J	160	PHE	3.1

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Mol	Chain	Res	Type	RSRZ
1	I	267	VAL	3.1
1	I	382	VAL	3.1
1	J	11	TYR	3.1
1	J	188	VAL	3.1
1	J	249	GLN	3.1
1	I	80	SER	3.1
1	I	133	SER	3.1
1	I	178	ILE	3.1
1	I	60	ALA	3.1
1	J	39	ALA	3.1
1	J	43	LYS	3.1
1	I	186	GLY	3.1
1	J	274	TYR	3.1
1	H	328	ASN	3.1
1	I	328	ASN	3.1
1	I	247	ARG	3.1
1	I	346	ALA	3.0
1	I	53	HIS	3.0
1	J	215	HIS	3.0
1	J	312	HIS	3.0
1	I	44	PRO	3.0
1	I	347	LEU	3.0
1	J	294	LEU	3.0
1	J	377	LEU	3.0
1	B	260	GLY	3.0
1	I	293	GLY	3.0
1	I	288	ILE	3.0
1	I	163	GLU	3.0
1	J	266	GLU	3.0
1	I	225	CYS	3.0
1	J	281	PHE	3.0
1	I	62	VAL	3.0
1	I	56	ALA	3.0
1	I	196	GLU	3.0
1	I	257	PHE	3.0
1	J	243	VAL	3.0
1	I	213	ALA	3.0
1	J	25	ARG	3.0
1	I	329	SER	3.0
1	I	217	PRO	2.9
1	E	66	LEU	2.9
1	J	113	TYR	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	316	LEU	2.9
1	J	339	LYS	2.9
1	I	380	PHE	2.9
1	I	40	SER	2.9
1	I	136	VAL	2.9
1	I	195	VAL	2.9
1	J	76	ALA	2.9
1	I	167	LYS	2.9
1	B	66	LEU	2.9
1	I	318	ASP	2.9
1	I	389	SER	2.9
1	J	134	ASN	2.9
1	J	320	ALA	2.9
1	I	316	LEU	2.9
1	I	245	TYR	2.9
1	I	98	PHE	2.9
1	J	162	ILE	2.9
1	E	411	LYS	2.9
1	J	35	LEU	2.9
1	H	380	PHE	2.9
1	I	140	PHE	2.9
1	I	345	PHE	2.9
1	J	369	GLY	2.9
1	I	134	ASN	2.8
1	J	109	VAL	2.8
1	I	198	ALA	2.8
1	I	377	LEU	2.8
1	J	42	GLN	2.8
1	I	322	GLU	2.8
1	D	64	ARG	2.8
1	I	399	VAL	2.8
1	J	108	THR	2.8
1	J	184	THR	2.8
1	J	386	CYS	2.8
1	I	222	ASP	2.8
1	J	196	GLU	2.8
1	I	238	PRO	2.8
1	J	205	VAL	2.8
1	I	311	ALA	2.8
1	I	392	LEU	2.8
1	J	149	LEU	2.8
1	J	129	MET	2.8

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Mol	Chain	Res	Type	RSRZ
1	J	255	ARG	2.8
1	J	378	LYS	2.8
1	I	220	VAL	2.8
1	J	150	VAL	2.8
1	G	352	ALA	2.8
1	I	391	ALA	2.8
1	I	378	LYS	2.8
1	I	304	ILE	2.7
1	I	327	ILE	2.7
1	J	194	ILE	2.7
1	J	241	ILE	2.7
1	I	46	SER	2.7
1	I	170	SER	2.7
1	J	384	SER	2.7
1	J	84	VAL	2.7
1	I	166	GLU	2.7
1	I	94	ASP	2.7
1	J	232	GLY	2.7
1	J	380	PHE	2.7
1	I	111	TYR	2.7
1	J	24	SER	2.7
1	C	362	ALA	2.7
1	I	110	ALA	2.7
1	J	60	ALA	2.7
1	I	306	ARG	2.7
1	J	270	GLU	2.7
1	H	203	ILE	2.7
1	J	204	PRO	2.7
1	I	366	VAL	2.7
1	J	192	LYS	2.7
1	J	272	VAL	2.7
1	J	180	HIS	2.7
1	C	414	GLY	2.7
1	I	202	GLY	2.7
1	I	230	PHE	2.7
1	J	27	VAL	2.7
1	J	64	ARG	2.7
1	J	72	ALA	2.7
1	G	347	LEU	2.6
1	I	188	VAL	2.6
1	J	69	LEU	2.6
1	H	404	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	I	187	THR	2.6
1	I	314	ALA	2.6
1	J	59	TYR	2.6
1	J	19	ASP	2.6
1	J	226	ASP	2.6
1	J	87	PHE	2.6
1	J	96	ILE	2.6
1	J	86	ARG	2.6
1	I	244	LEU	2.6
1	I	271	ASN	2.6
1	E	265	GLU	2.6
1	I	266	GLU	2.6
1	J	152	THR	2.6
1	J	200	ALA	2.6
1	J	273	THR	2.6
1	I	114	GLY	2.6
1	J	287	PRO	2.6
1	F	66	LEU	2.6
1	I	69	LEU	2.6
1	H	62	VAL	2.6
1	J	62	VAL	2.6
1	J	210	SER	2.6
1	I	108	THR	2.6
1	I	308	ALA	2.6
1	J	111	TYR	2.6
1	E	323	ARG	2.6
1	I	379	ARG	2.6
1	J	338	ASP	2.6
1	I	342	ILE	2.6
1	A	171	GLU	2.6
1	I	330	LEU	2.6
1	I	205	VAL	2.6
1	J	161	HIS	2.6
1	J	317	ARG	2.5
1	H	305	GLY	2.5
1	I	145	GLN	2.5
1	I	394	ASN	2.5
1	J	157	ASN	2.5
1	J	371	HIS	2.5
1	J	85	ARG	2.5
1	I	240	GLY	2.5
1	I	246	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	J	286	PRO	2.5
1	J	295	GLY	2.5
1	I	20	PHE	2.5
1	I	13	VAL	2.5
1	I	27	VAL	2.5
1	I	107	ASN	2.5
1	I	109	VAL	2.5
1	I	253	LYS	2.5
1	J	358	VAL	2.5
1	I	297	ALA	2.5
1	I	212	GLY	2.5
1	I	75	ASP	2.5
1	J	163	GLU	2.5
1	H	333	PHE	2.5
1	I	294	LEU	2.5
1	I	272	VAL	2.5
1	J	235	VAL	2.5
1	J	321	HIS	2.5
1	A	201[A]	ARG	2.5
1	J	247	ARG	2.5
1	I	52	THR	2.5
1	J	55	TYR	2.5
1	I	106	ILE	2.5
1	I	406	LEU	2.5
1	B	117	PHE	2.5
1	A	157	ASN	2.5
1	J	56	ALA	2.5
1	G	411	LYS	2.4
1	I	34	TYR	2.4
1	I	320	ALA	2.4
1	I	192	LYS	2.4
1	I	381	GLY	2.4
1	J	260	GLY	2.4
1	J	310	LEU	2.4
1	J	233	HIS	2.4
1	G	412	PHE	2.4
1	J	301	MET	2.4
1	J	110	ALA	2.4
1	J	256	PRO	2.4
1	J	303	LYS	2.4
1	J	313	GLU	2.4
1	I	221	GLN	2.4

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Mol	Chain	Res	Type	RSRZ
1	J	367	ARG	2.4
1	J	61	ASN	2.4
1	I	15	ALA	2.4
1	I	105	ALA	2.4
1	F	322	GLU	2.4
1	I	120	GLU	2.4
1	I	259	GLY	2.4
1	J	22	ILE	2.4
1	I	154	VAL	2.4
1	J	154	VAL	2.4
1	J	107	ASN	2.4
1	H	326	ARG	2.3
1	I	326	ARG	2.3
1	I	131	HIS	2.3
1	I	353	HIS	2.3
1	J	28	HIS	2.3
1	F	157	ASN	2.3
1	I	14	GLU	2.3
1	J	147	ALA	2.3
1	F	64	ARG	2.3
1	J	293	GLY	2.3
1	G	406	LEU	2.3
1	I	135	ILE	2.3
1	I	241	ILE	2.3
1	J	197	LEU	2.3
1	I	115	MET	2.3
1	I	301	MET	2.3
1	G	413	PHE	2.3
1	I	82	GLU	2.3
1	J	82	GLU	2.3
1	C	275	ASN	2.3
1	J	391	ALA	2.3
1	B	64	ARG	2.3
1	J	280	ARG	2.3
1	J	91	GLY	2.3
1	J	63	HIS	2.3
1	I	185	LEU	2.3
1	I	148	LYS	2.3
1	I	300	TYR	2.3
1	J	93	VAL	2.3
1	J	228	TYR	2.3
1	J	267	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	H	381	GLY	2.3
1	I	232	GLY	2.3
1	J	211	GLN	2.3
1	H	80	SER	2.3
1	G	69	LEU	2.3
1	I	359	ILE	2.3
1	J	244	LEU	2.3
1	I	174	LYS	2.3
1	H	33	VAL	2.3
1	I	207	VAL	2.3
1	J	189	VAL	2.3
1	H	335	ASN	2.2
1	I	85	ARG	2.3
1	J	308	ALA	2.2
1	J	258	GLN	2.2
1	J	340	GLY	2.2
1	I	264	ILE	2.2
1	I	208	ASP	2.2
1	J	265	GLU	2.2
1	G	366	VAL	2.2
1	I	331	ARG	2.2
1	J	41	ALA	2.2
1	J	105	ALA	2.2
1	I	74	THR	2.2
1	J	237	GLY	2.2
1	I	402	LEU	2.2
1	J	135	ILE	2.2
1	J	264	ILE	2.2
1	I	277	PRO	2.2
1	I	37	ASN	2.2
1	I	54	ALA	2.2
1	J	253	LYS	2.2
1	I	112	GLY	2.2
1	I	121	GLY	2.2
1	I	146	GLY	2.2
1	J	38	GLY	2.2
1	I	17	ARG	2.2
1	I	278	PRO	2.2
1	I	218	VAL	2.2
1	B	328	ASN	2.2
1	C	328	ASN	2.2
1	H	200	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	61	ASN	2.2
1	I	99	THR	2.2
1	A	414	GLY	2.2
1	H	414	GLY	2.2
1	G	337	PRO	2.2
1	J	140	PHE	2.2
1	J	165	PHE	2.2
1	I	199	HIS	2.1
1	I	91	GLY	2.1
1	I	179	THR	2.1
1	J	83	THR	2.1
1	J	231	THR	2.1
1	G	343	ILE	2.1
1	G	404	GLU	2.1
1	I	265	GLU	2.1
1	J	36	ASP	2.1
1	J	155	ASP	2.1
1	I	286	PRO	2.1
1	A	328	ASN	2.1
1	I	298	LEU	2.1
1	J	383	THR	2.1
1	G	64	ARG	2.1
1	J	77	TYR	2.1
1	H	329	SER	2.1
1	J	139	HIS	2.1
1	J	250	MET	2.1
1	J	13	VAL	2.1
1	J	26	GLN	2.1
1	H	397	ALA	2.1
1	I	401	ALA	2.1
1	J	297	ALA	2.1
1	D	414	GLY	2.1
1	I	261	GLY	2.1
1	I	363	GLY	2.1
1	H	22	ILE	2.1
1	I	42	GLN	2.1
1	I	84	VAL	2.1
1	I	365	ALA	2.1
1	I	388	ALA	2.1
1	J	283	ALA	2.1
1	F	335	ASN	2.1
1	I	35	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	114	GLY	2.1
1	G	348	GLU	2.1
1	G	162	ILE	2.1
1	B	411	LYS	2.1
1	B	329	SER	2.1
1	J	116	PRO	2.1
1	J	279	HIS	2.1
1	G	409	ALA	2.0
1	J	102	ALA	2.0
1	J	251	LEU	2.0
1	H	146	GLY	2.0
1	J	171	GLU	2.0
1	D	383	THR	2.0
1	I	31	THR	2.0
1	I	43	LYS	2.0
1	I	343	ILE	2.0
1	G	380	PHE	2.0
1	I	396	ARG	2.0
1	E	407	GLU	2.0
1	G	196	GLU	2.0
1	G	402	LEU	2.0
1	I	296	ALA	2.0
1	G	407	GLU	2.0
1	I	398	GLU	2.0
1	J	126	LEU	2.0
1	F	57	ASN	2.0
1	J	65	GLY	2.0
1	D	63	HIS	2.0
1	I	132	HIS	2.0
1	I	139	HIS	2.0
1	I	161	HIS	2.0
1	I	321	HIS	2.0
1	J	67	HIS	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. 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	B-factors($\text{\AA}^2$)	Q<0.9
1	LLP	I	234	24/25	0.87	0.17	72,75,80,82	0
1	LLP	J	234	24/25	0.89	0.17	75,77,79,80	0
1	LLP	G	234	24/25	0.96	0.09	54,57,59,59	0
1	LLP	H	234	24/25	0.96	0.09	54,56,59,61	0
1	LLP	E	234	24/25	0.97	0.08	41,42,44,45	0
1	LLP	A	234	24/25	0.97	0.08	40,43,44,45	0
1	LLP	B	234	24/25	0.97	0.07	38,40,41,41	0
1	LLP	C	234	24/25	0.97	0.09	44,46,47,47	0
1	LLP	D	234	24/25	0.97	0.07	41,41,42,43	0
1	LLP	F	234	24/25	0.98	0.07	42,44,46,47	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	CL	C	501	1/1	0.78	0.21	86,86,86,86	0
2	CL	H	501	1/1	0.82	0.23	71,71,71,71	0
2	CL	E	501	1/1	0.87	0.20	72,72,72,72	0
2	CL	I	501	1/1	0.87	0.21	79,79,79,79	0
2	CL	D	501	1/1	0.88	0.14	52,52,52,52	0
2	CL	B	501	1/1	0.88	0.21	69,69,69,69	0
2	CL	A	501	1/1	0.90	0.22	69,69,69,69	0

6.5 Other polymers [i](#)

There are no such residues in this entry.