



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 02:38 PM EDT

PDB ID : 5Z0Q / pdb_00005z0q
Title : Crystal Structure of OvoB
Authors : Cai, Y.J.; Huang, P.; Wu, L.; Zhou, J.H.; Liu, P.H.
Deposited on : 2017-12-20
Resolution : 2.77 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

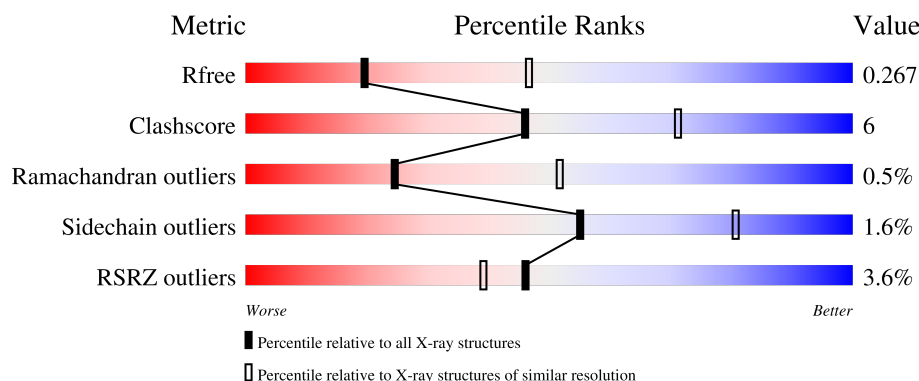
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	389	2% 81% 15% ..
1	B	389	2% 85% 12% ..
1	C	389	2% 85% 12% .
1	D	389	2% 84% 12% ..
1	E	389	2% 82% 15% ..

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Mol	Chain	Length	Quality of chain
1	F	389	3% 80% 17%
1	G	389	3% 78% 18%
1	H	389	7% 77% 18%
1	I	389	3% 83% 13%
1	J	389	4% 80% 16%
1	K	389	4% 82% 14%
1	L	389	7% 76% 20%

2 Entry composition

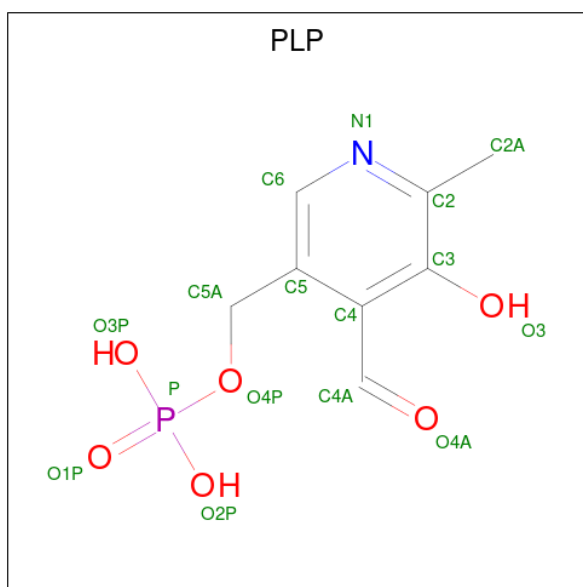
There are 2 unique types of molecules in this entry. The entry contains 36073 atoms, of which 0 are hydrogens and 0 are deuteriums.

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, class I and II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	379	Total	C	N	O	S	0	0	0
			3006	1907	544	542	13			
1	A	376	Total	C	N	O	S	0	0	0
			2984	1893	541	537	13			
1	B	379	Total	C	N	O	S	0	0	0
			3006	1907	544	542	13			
1	D	378	Total	C	N	O	S	0	0	0
			2995	1898	543	541	13			
1	E	378	Total	C	N	O	S	0	0	0
			2995	1898	543	541	13			
1	F	379	Total	C	N	O	S	0	0	0
			3006	1907	544	542	13			
1	G	379	Total	C	N	O	S	0	0	0
			3006	1907	544	542	13			
1	H	378	Total	C	N	O	S	0	0	0
			2999	1903	543	539	14			
1	I	375	Total	C	N	O	S	0	0	0
			2973	1884	540	536	13			
1	J	375	Total	C	N	O	S	0	0	0
			2973	1884	540	536	13			
1	K	376	Total	C	N	O	S	0	0	0
			2984	1893	541	537	13			
1	L	374	Total	C	N	O	S	0	0	0
			2966	1880	539	534	13			

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: C₈H₁₀NO₆P).

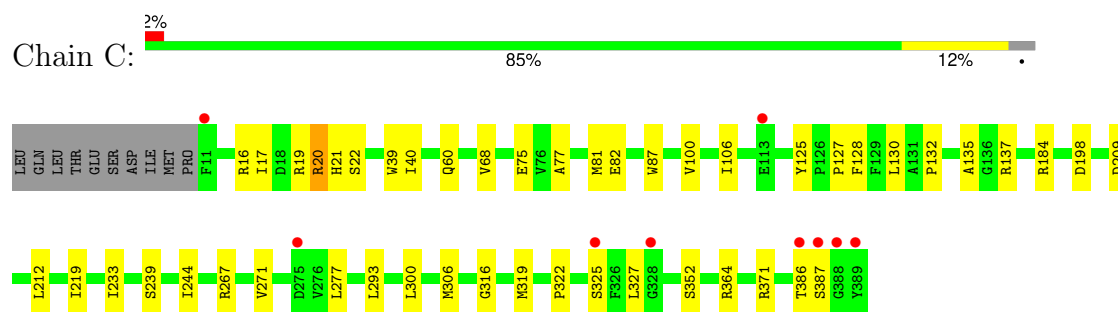


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	E	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	F	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	G	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	H	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	I	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	J	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	K	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	L	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

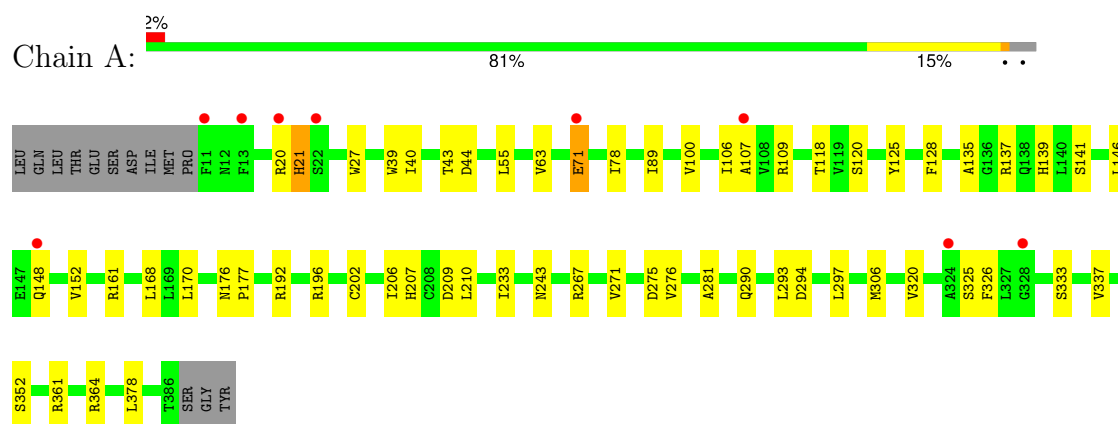
3 Residue-property plots [i](#)

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.

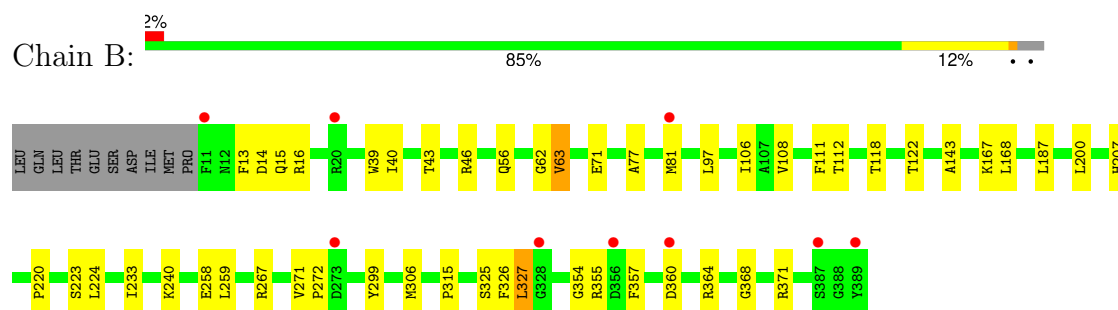
- Molecule 1: Aminotransferase, class I and II



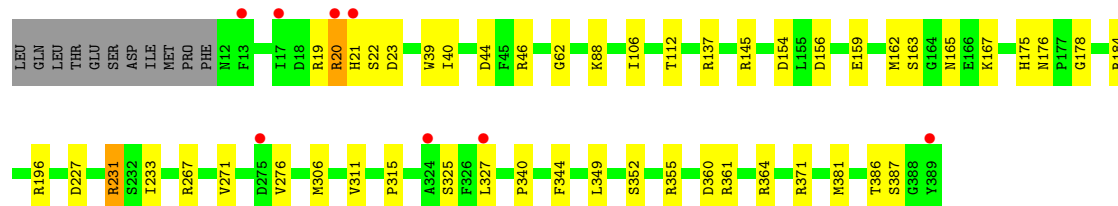
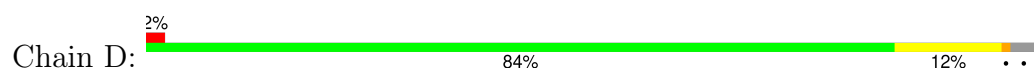
- Molecule 1: Aminotransferase, class I and II



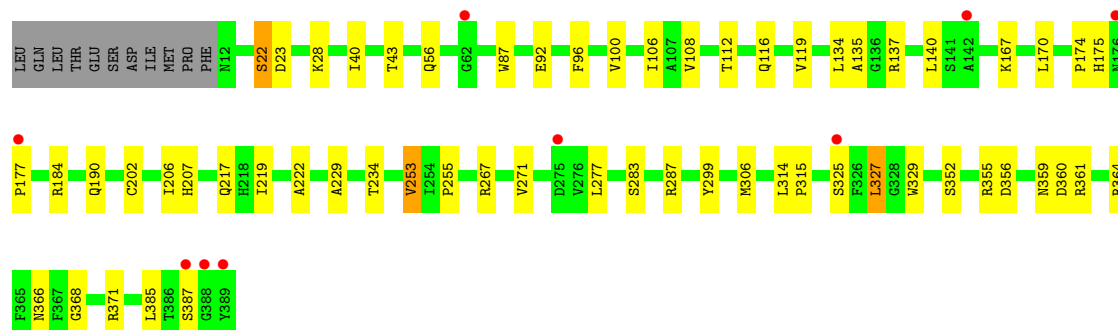
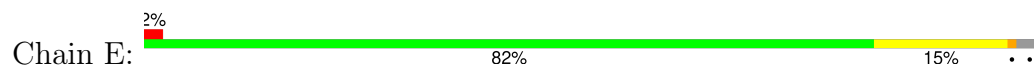
- Molecule 1: Aminotransferase, class I and II



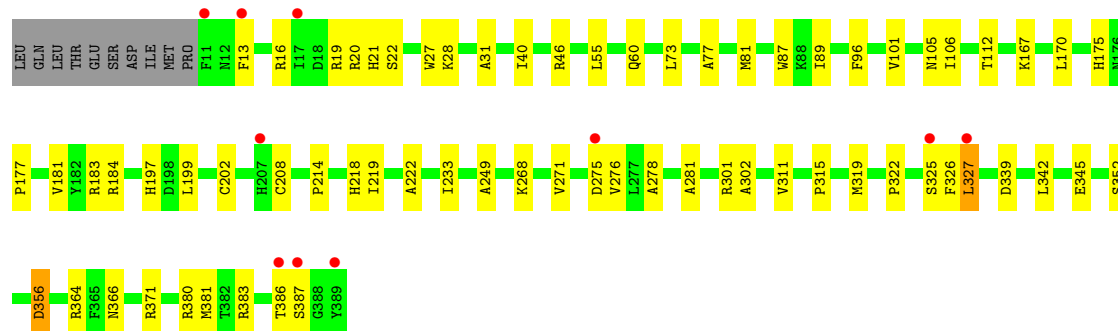
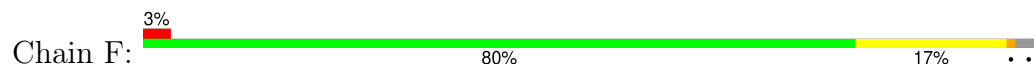
- Molecule 1: Aminotransferase, class I and II



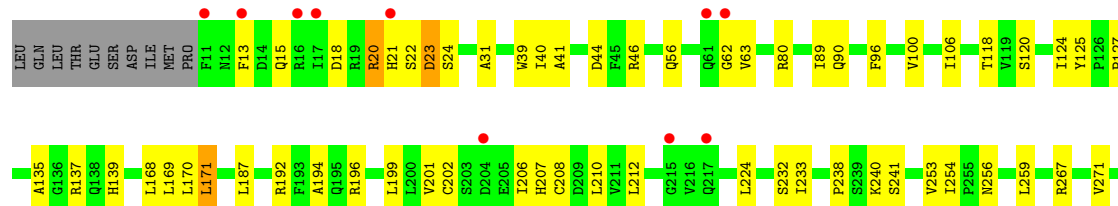
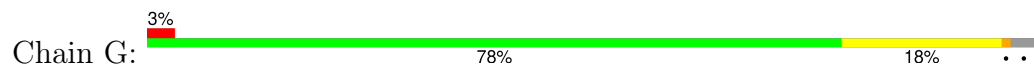
- Molecule 1: Aminotransferase, class I and II



- Molecule 1: Aminotransferase, class I and II

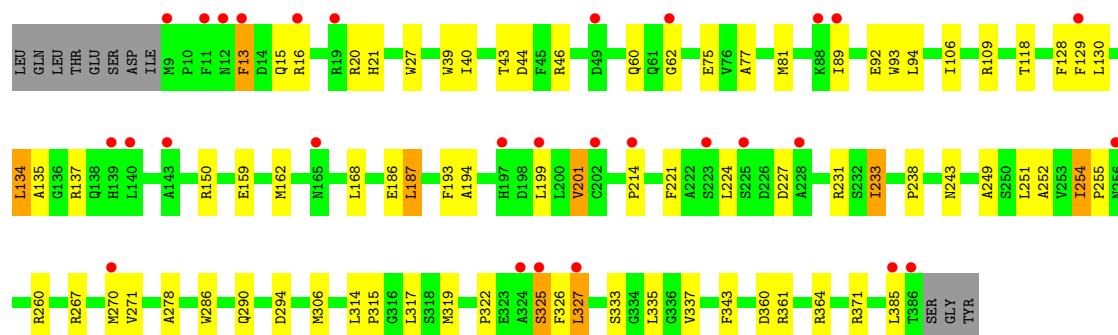
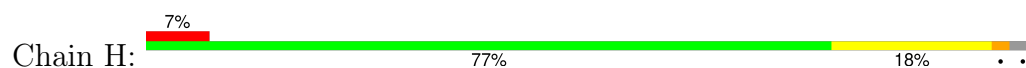


- Molecule 1: Aminotransferase, class I and II

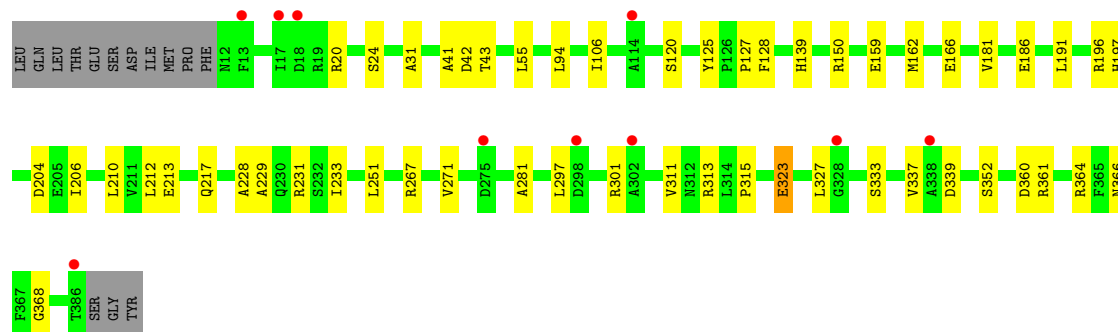
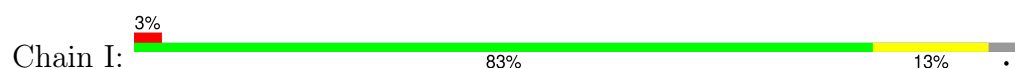




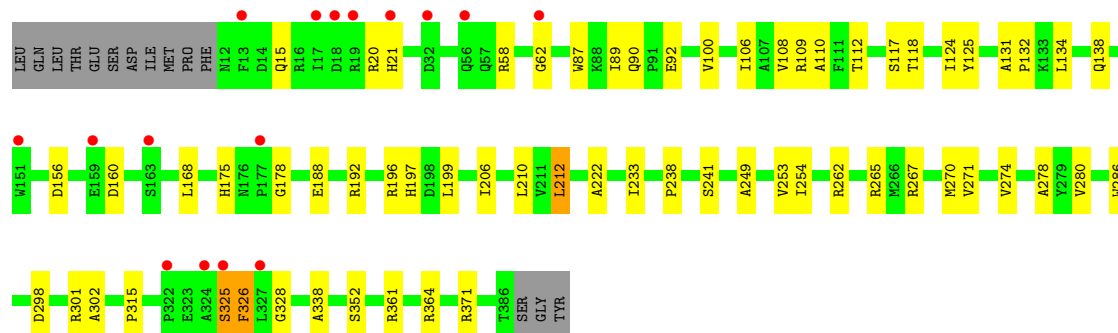
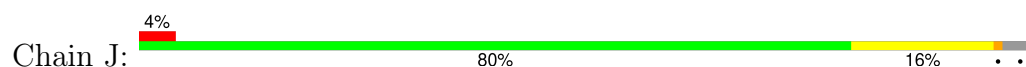
- Molecule 1: Aminotransferase, class I and II



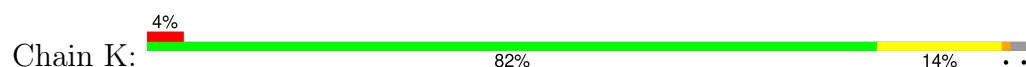
- Molecule 1: Aminotransferase, class I and II

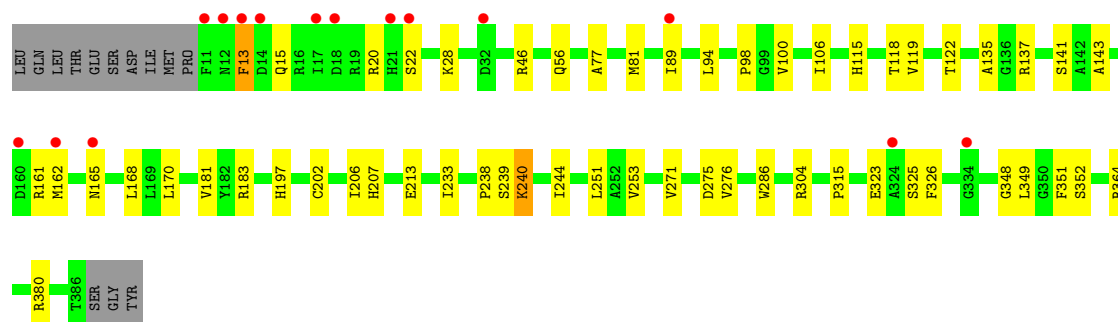


- Molecule 1: Aminotransferase, class I and II

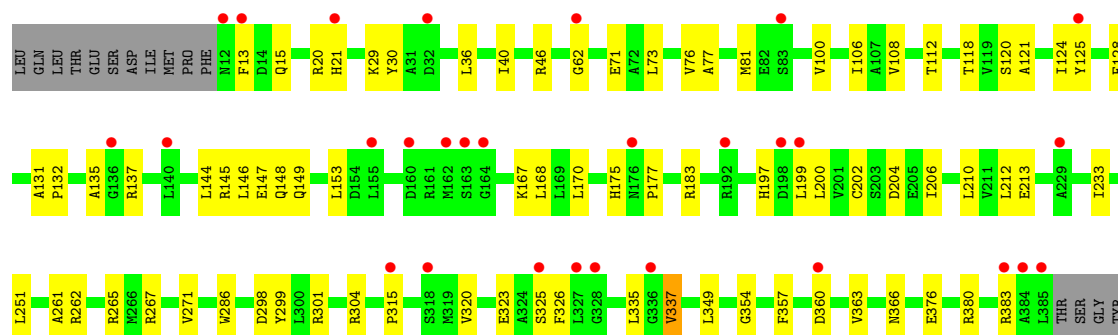
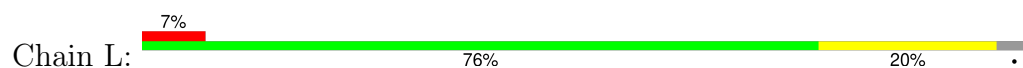


- Molecule 1: Aminotransferase, class I and II





• Molecule 1: Aminotransferase, class I and II



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	58.12Å 133.59Å 165.70Å 89.39° 84.58° 86.56°	Depositor
Resolution (Å)	42.97 – 2.77 42.97 – 2.77	Depositor EDS
% Data completeness (in resolution range)	90.1 (42.97-2.77) 92.3 (42.97-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.73Å)	Xtriage
Refinement program	PHENIX (1.12_2829)	Depositor
R, R_{free}	0.210 , 0.267 0.211 , 0.267	Depositor DCC
R_{free} test set	5835 reflections (4.44%)	wwPDB-VP
Wilson B-factor (Å ²)	44.4	Xtriage
Anisotropy	0.132	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 33.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	36073	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.11% 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: PLP

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	0.11	0/3056	0.31	0/4144
1	B	0.11	0/3079	0.30	0/4175
1	C	0.11	0/3079	0.32	0/4175
1	D	0.10	0/3067	0.31	0/4159
1	E	0.10	0/3067	0.30	0/4159
1	F	0.10	0/3079	0.32	0/4175
1	G	0.11	0/3079	0.33	0/4175
1	H	0.11	0/3072	0.34	0/4166
1	I	0.10	0/3044	0.30	0/4128
1	J	0.10	0/3044	0.34	0/4128
1	K	0.10	0/3056	0.30	0/4144
1	L	0.11	0/3037	0.34	0/4118
All	All	0.11	0/36759	0.32	0/49846

There are no bond length outliers.

There are no bond angle outliers.

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	2984	0	2941	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3006	0	2958	29	0
1	C	3006	0	2958	26	0
1	D	2995	0	2949	27	0
1	E	2995	0	2949	35	0
1	F	3006	0	2958	42	0
1	G	3006	0	2957	42	0
1	H	2999	0	2957	50	0
1	I	2973	0	2932	34	0
1	J	2973	0	2932	34	0
1	K	2984	0	2941	29	0
1	L	2966	0	2926	50	0
2	A	15	0	7	0	0
2	B	15	0	7	0	0
2	C	15	0	7	1	0
2	D	15	0	7	1	0
2	E	15	0	7	0	0
2	F	15	0	7	0	0
2	G	15	0	7	0	0
2	H	15	0	7	0	0
2	I	15	0	7	0	0
2	J	15	0	7	0	0
2	K	15	0	7	0	0
2	L	15	0	7	1	0
All	All	36073	0	35442	415	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 6.

All (415) 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:G:267:ARG:HG3	1:G:271:VAL:HB	1.67	0.77
1:A:78:ILE:HD13	1:A:89:ILE:HG13	1.68	0.76
1:D:46:ARG:HG3	1:G:62:GLY:HA3	1.69	0.74
1:D:227:ASP:OD1	1:D:231:ARG:NH1	2.23	0.71
1:F:214:PRO:HB3	1:I:301:ARG:HH22	1.56	0.70
1:L:145:ARG:NH2	1:L:147:GLU:OE2	2.24	0.70
1:C:106:ILE:HD11	1:C:271:VAL:HG21	1.73	0.69
1:B:327:LEU:HD13	1:B:364:ARG:HD2	1.74	0.69
1:H:62:GLY:HA3	1:L:46:ARG:HG3	1.73	0.69
1:I:212:LEU:O	1:I:301:ARG:NH2	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:ARG:HB3	1:F:219:ILE:HD13	1.76	0.68
1:K:106:ILE:HD11	1:K:271:VAL:HG21	1.75	0.68
1:G:106:ILE:HD11	1:G:271:VAL:HG21	1.76	0.67
1:E:22:SER:OG	1:E:23:ASP:N	2.25	0.67
1:H:233:ILE:HD13	1:H:254:ILE:HG12	1.78	0.65
1:H:118:THR:HG22	1:H:168:LEU:HB3	1.78	0.65
1:H:46:ARG:HG3	1:L:62:GLY:HA3	1.79	0.64
1:J:106:ILE:HD11	1:J:271:VAL:HG21	1.79	0.64
1:F:106:ILE:HG12	1:J:270:MET:HE3	1.79	0.64
1:H:187:LEU:HB3	1:H:224:LEU:HD11	1.79	0.64
1:B:97:LEU:HD23	1:B:267:ARG:HE	1.63	0.63
1:L:118:THR:HG22	1:L:168:LEU:HB3	1.80	0.63
1:F:301:ARG:HH12	1:I:301:ARG:NH1	1.95	0.63
1:I:333:SER:HB3	1:I:361:ARG:HH11	1.63	0.63
1:H:233:ILE:HD11	1:H:252:ALA:HB1	1.81	0.63
1:A:118:THR:HG22	1:A:168:LEU:HB3	1.81	0.63
1:G:327:LEU:HD13	1:G:364:ARG:HD2	1.80	0.63
1:J:20:ARG:HA	1:J:21:HIS:C	2.23	0.63
1:H:135:ALA:O	1:H:137:ARG:NH1	2.31	0.63
1:J:118:THR:HG22	1:J:168:LEU:HB3	1.81	0.62
1:G:40:ILE:O	1:G:366:ASN:ND2	2.31	0.62
1:I:106:ILE:HD11	1:I:271:VAL:HG21	1.80	0.62
1:F:106:ILE:HD11	1:F:271:VAL:HG21	1.82	0.62
1:B:106:ILE:HD11	1:B:271:VAL:HG21	1.82	0.61
1:D:175:HIS:HD2	1:D:178:GLY:H	1.49	0.61
1:A:120:SER:HB3	1:A:139:HIS:CE1	2.36	0.61
1:E:267:ARG:HG3	1:E:271:VAL:HB	1.81	0.61
1:H:267:ARG:HG2	1:H:271:VAL:HB	1.83	0.61
1:J:267:ARG:HG2	1:J:271:VAL:HB	1.83	0.61
1:J:298:ASP:OD1	1:J:301:ARG:NH2	2.33	0.60
1:L:106:ILE:HD11	1:L:271:VAL:HG21	1.83	0.60
1:A:107:ALA:O	1:A:109:ARG:N	2.32	0.60
1:F:181:VAL:O	1:F:183:ARG:NH1	2.34	0.60
1:C:352:SER:HB2	1:C:364:ARG:HB3	1.82	0.60
1:H:92:GLU:O	1:H:260:ARG:NH1	2.35	0.60
1:J:156:ASP:OD1	1:J:196:ARG:NH2	2.33	0.60
1:D:20:ARG:HH12	1:D:44:ASP:HA	1.67	0.60
1:B:16:ARG:HH11	1:B:46:ARG:HB3	1.66	0.60
1:E:40:ILE:O	1:E:366:ASN:ND2	2.35	0.60
1:H:270:MET:HE3	1:L:106:ILE:HG12	1.84	0.60
1:K:22:SER:O	1:K:28:LYS:NZ	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:267:ARG:HG2	1:C:271:VAL:HB	1.85	0.59
1:J:90:GLN:NE2	1:J:92:GLU:OE2	2.33	0.59
1:J:117:SER:HB3	1:J:138:GLN:HB2	1.84	0.59
1:E:234:THR:HB	1:E:253:VAL:HG22	1.85	0.59
1:F:112:THR:HG22	1:F:167:LYS:HB3	1.84	0.59
1:F:311:VAL:HG22	1:F:381:MET:HE1	1.86	0.58
1:H:337:VAL:O	1:H:361:ARG:NH2	2.35	0.58
1:G:96:PHE:O	1:G:267:ARG:NH2	2.36	0.58
1:G:100:VAL:HG21	1:G:206:ILE:HG21	1.85	0.58
1:H:106:ILE:HD11	1:H:271:VAL:HG21	1.85	0.58
1:A:337:VAL:O	1:A:361:ARG:NH1	2.37	0.57
1:K:181:VAL:O	1:K:183:ARG:NH1	2.37	0.57
1:H:254:ILE:HB	1:H:260:ARG:HB2	1.84	0.57
1:K:213:GLU:HG2	1:K:304:ARG:HH12	1.68	0.57
1:D:352:SER:HB2	1:D:364:ARG:HB3	1.87	0.57
1:J:175:HIS:HD2	1:J:178:GLY:H	1.53	0.57
1:J:233:ILE:HG13	1:J:254:ILE:HG12	1.86	0.56
1:C:209:ASP:HB3	1:C:293:LEU:HD21	1.87	0.56
1:A:63:VAL:HG11	1:I:20:ARG:HH21	1.69	0.56
1:D:159:GLU:HA	1:D:162:MET:HG3	1.87	0.56
1:F:20:ARG:HA	1:F:21:HIS:C	2.30	0.56
1:C:19:ARG:HG3	1:C:21:HIS:HB2	1.86	0.56
1:L:212:LEU:HD11	1:L:325:SER:HB3	1.87	0.56
1:I:267:ARG:HG2	1:I:271:VAL:HB	1.88	0.56
1:C:135:ALA:O	1:C:137:ARG:NH1	2.39	0.55
1:D:267:ARG:HG2	1:D:271:VAL:HB	1.87	0.55
1:G:20:ARG:HA	1:G:21:HIS:C	2.32	0.55
1:G:170:LEU:HD23	1:G:202:CYS:HB3	1.88	0.55
1:A:141:SER:O	1:A:161:ARG:NH2	2.35	0.55
1:I:20:ARG:NH1	1:I:24:SER:OG	2.40	0.55
1:G:120:SER:HB3	1:G:139:HIS:CE1	2.42	0.55
1:L:125:TYR:HB3	1:L:128:PHE:HD1	1.71	0.55
1:B:43:THR:HG22	1:B:368:GLY:HA3	1.88	0.55
1:D:112:THR:HG22	1:D:167:LYS:HB3	1.88	0.55
1:F:40:ILE:O	1:F:366:ASN:ND2	2.40	0.54
1:H:306:MET:HE1	1:H:371:ARG:HH21	1.72	0.54
1:D:106:ILE:HD11	1:D:271:VAL:HG21	1.89	0.54
1:E:299:TYR:OH	1:E:371:ARG:N	2.35	0.54
1:H:20:ARG:HA	1:H:21:HIS:C	2.33	0.54
1:L:135:ALA:O	1:L:137:ARG:NH2	2.42	0.53
1:L:100:VAL:HG21	1:L:206:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:125:TYR:HB3	1:L:128:PHE:CD1	2.44	0.53
1:E:355:ARG:HB2	1:E:360:ASP:HB3	1.90	0.53
1:G:233:ILE:HG23	1:G:254:ILE:HG12	1.91	0.53
1:J:58:ARG:HG2	1:J:280:VAL:HG21	1.90	0.53
1:L:267:ARG:HG2	1:L:271:VAL:HB	1.90	0.53
1:A:125:TYR:HB3	1:A:128:PHE:HD2	1.73	0.53
1:J:338:ALA:O	1:J:361:ARG:NH2	2.41	0.53
1:K:141:SER:O	1:K:161:ARG:NH2	2.38	0.53
1:L:120:SER:HB3	1:L:170:LEU:HB2	1.91	0.53
1:C:306:MET:HE1	1:C:371:ARG:HD3	1.91	0.52
1:B:14:ASP:HA	1:B:16:ARG:NH2	2.24	0.52
1:C:184:ARG:HH11	1:C:219:ILE:HD13	1.73	0.52
1:A:43:THR:O	1:A:243:ASN:ND2	2.41	0.52
1:A:146:LEU:HD11	1:A:320:VAL:HG11	1.91	0.52
1:E:283:SER:OG	1:E:287:ARG:NH1	2.42	0.52
1:G:311:VAL:HG22	1:G:381:MET:HE1	1.92	0.52
1:A:192:ARG:O	1:A:196:ARG:HG2	2.10	0.52
1:J:160:ASP:OD1	1:J:160:ASP:N	2.41	0.52
1:H:249:ALA:HB2	1:H:278:ALA:HB1	1.91	0.52
1:C:100:VAL:HB	2:C:401:PLP:H6	1.90	0.52
1:E:108:VAL:O	1:E:112:THR:OG1	2.27	0.52
1:D:311:VAL:HG22	1:D:381:MET:HE1	1.92	0.52
1:G:135:ALA:O	1:G:137:ARG:NH1	2.43	0.52
1:K:207:HIS:CE1	1:K:240:LYS:HD3	2.46	0.51
1:E:306:MET:HE1	1:E:371:ARG:HD3	1.91	0.51
1:A:135:ALA:O	1:A:137:ARG:NH1	2.43	0.51
1:H:319:MET:HE2	1:H:322:PRO:HD3	1.92	0.51
1:K:94:LEU:HD22	1:K:251:LEU:HD12	1.93	0.51
1:E:100:VAL:HG21	1:E:206:ILE:HD12	1.93	0.51
1:F:73:LEU:HD22	1:F:96:PHE:HE1	1.75	0.51
1:I:120:SER:HB3	1:I:139:HIS:CE1	2.45	0.51
1:A:63:VAL:HG11	1:I:20:ARG:NH2	2.26	0.51
1:E:170:LEU:HD23	1:E:202:CYS:HB3	1.93	0.51
1:A:55:LEU:HD21	1:A:281:ALA:HB2	1.91	0.51
1:A:20:ARG:NH1	1:A:44:ASP:OD1	2.43	0.51
1:H:333:SER:HB3	1:H:361:ARG:HB3	1.93	0.51
1:I:210:LEU:HA	1:I:297:LEU:HD21	1.93	0.51
1:F:352:SER:HB2	1:F:364:ARG:HB3	1.93	0.51
1:H:290:GLN:NE2	1:H:294:ASP:OD1	2.41	0.51
1:K:118:THR:HG22	1:K:168:LEU:HB3	1.92	0.51
1:A:106:ILE:HD11	1:A:271:VAL:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:100:VAL:HG21	1:J:206:ILE:HD12	1.92	0.50
1:L:167:LYS:HE3	1:L:200:LEU:HD13	1.93	0.50
1:G:23:ASP:OD1	1:G:23:ASP:N	2.42	0.50
1:L:204:ASP:OD2	2:L:401:PLP:N1	2.45	0.50
1:C:68:VAL:HG11	1:E:28:LYS:HD3	1.92	0.50
1:D:20:ARG:HA	1:D:21:HIS:C	2.37	0.50
1:E:106:ILE:HD11	1:E:271:VAL:HG21	1.94	0.50
1:E:174:PRO:HD2	1:E:207:HIS:HB2	1.94	0.50
1:L:108:VAL:O	1:L:112:THR:OG1	2.30	0.50
1:D:112:THR:O	1:D:137:ARG:NH1	2.45	0.50
1:C:125:TYR:HB3	1:C:128:PHE:CD1	2.47	0.50
1:K:115:HIS:O	1:K:165:ASN:ND2	2.27	0.50
1:C:16:ARG:HE	1:C:17:ILE:H	1.59	0.49
1:A:125:TYR:HB3	1:A:128:PHE:CD2	2.47	0.49
1:H:150:ARG:NH2	1:H:186:GLU:OE2	2.45	0.49
1:I:43:THR:HG22	1:I:368:GLY:HA3	1.93	0.49
1:F:327:LEU:HD13	1:F:364:ARG:HD2	1.94	0.49
1:C:20:ARG:HA	1:C:21:HIS:C	2.38	0.49
1:G:118:THR:HG22	1:G:168:LEU:HB3	1.94	0.49
1:H:13:PHE:CE1	1:H:15:GLN:HB2	2.47	0.49
1:F:249:ALA:HB2	1:F:278:ALA:HB1	1.94	0.49
1:H:128:PHE:C	1:H:130:LEU:H	2.21	0.49
1:I:159:GLU:OE1	1:I:197:HIS:NE2	2.43	0.49
1:K:100:VAL:HG21	1:K:206:ILE:HG21	1.95	0.49
1:I:150:ARG:NH2	1:I:186:GLU:OE2	2.46	0.49
1:J:302:ALA:HB3	1:J:371:ARG:HH12	1.78	0.48
1:G:194:ALA:HA	1:G:199:LEU:HD12	1.95	0.48
1:I:42:ASP:H	1:I:366:ASN:HD21	1.59	0.48
1:H:238:PRO:HB3	1:H:286:TRP:NE1	2.29	0.48
1:E:175:HIS:CD2	1:E:177:PRO:HD2	2.49	0.48
1:G:256:ASN:HD22	1:G:259:LEU:HG	1.79	0.48
1:H:159:GLU:HG2	1:H:193:PHE:HE1	1.79	0.48
1:L:40:ILE:O	1:L:366:ASN:ND2	2.47	0.48
1:I:204:ASP:OD1	1:I:206:ILE:HG12	2.14	0.48
1:L:131:ALA:HB3	1:L:132:PRO:HD3	1.96	0.48
1:A:267:ARG:HG3	1:A:271:VAL:HB	1.96	0.48
1:C:239:SER:HA	1:C:244:ILE:HG13	1.96	0.48
1:D:176:ASN:ND2	2:D:401:PLP:O3	2.47	0.48
1:G:192:ARG:HB3	1:G:196:ARG:NH1	2.29	0.48
1:B:108:VAL:O	1:B:112:THR:OG1	2.31	0.47
1:C:60:GLN:OE1	1:E:56:GLN:NE2	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:41:ALA:HB1	1:G:240:LYS:HE3	1.96	0.47
1:A:20:ARG:HD3	1:A:27:TRP:CD1	2.50	0.47
1:F:301:ARG:HH12	1:I:301:ARG:CZ	2.26	0.47
1:H:89:ILE:HG21	1:H:94:LEU:HD21	1.96	0.47
1:E:96:PHE:O	1:E:267:ARG:NH2	2.47	0.47
1:F:77:ALA:O	1:F:81:MET:HG2	2.14	0.47
1:H:77:ALA:O	1:H:81:MET:HG2	2.13	0.47
1:J:89:ILE:HD12	1:J:253:VAL:HG11	1.96	0.47
1:J:262:ARG:HG3	1:J:265:ARG:HH21	1.77	0.47
1:B:354:GLY:HA2	1:B:357:PHE:HD2	1.80	0.47
1:I:94:LEU:HD22	1:I:251:LEU:HD13	1.97	0.47
1:I:311:VAL:C	1:I:313:ARG:H	2.21	0.47
1:B:77:ALA:O	1:B:81:MET:HG2	2.15	0.47
1:G:39:TRP:CG	1:G:40:ILE:H	2.33	0.47
1:H:227:ASP:O	1:H:231:ARG:HG2	2.14	0.47
1:L:175:HIS:ND1	1:L:177:PRO:O	2.44	0.47
1:A:206:ILE:HG23	1:A:207:HIS:CD2	2.49	0.47
1:L:170:LEU:HD23	1:L:202:CYS:HB3	1.96	0.47
1:E:119:VAL:HG22	1:E:140:LEU:HB3	1.96	0.47
1:E:327:LEU:HD22	1:E:364:ARG:NE	2.30	0.46
1:H:92:GLU:HB3	1:H:260:ARG:HH12	1.78	0.46
1:F:87:TRP:CE2	1:F:89:ILE:HD11	2.50	0.46
1:F:175:HIS:ND1	1:F:177:PRO:O	2.42	0.46
1:I:360:ASP:OD1	1:I:360:ASP:N	2.48	0.46
1:L:298:ASP:OD1	1:L:301:ARG:NH1	2.48	0.46
1:J:210:LEU:HD21	1:J:241:SER:HA	1.97	0.46
1:D:19:ARG:NH2	1:D:20:ARG:H	2.12	0.46
1:E:184:ARG:HG3	1:E:219:ILE:HD13	1.97	0.46
1:F:275:ASP:OD1	1:F:276:VAL:N	2.48	0.46
1:L:197:HIS:HB2	1:L:199:LEU:HG	1.98	0.46
1:I:181:VAL:HG23	1:I:323:GLU:HB2	1.97	0.46
1:L:128:PHE:CD2	1:L:170:LEU:HB3	2.50	0.46
1:K:162:MET:HE2	1:K:197:HIS:ND1	2.30	0.46
1:L:354:GLY:HA2	1:L:357:PHE:HD2	1.80	0.46
1:C:386:THR:HG23	1:C:387:SER:HB3	1.98	0.46
1:B:220:PRO:O	1:B:223:SER:OG	2.32	0.46
1:G:306:MET:HE1	1:G:371:ARG:HD3	1.98	0.46
1:L:183:ARG:NH2	1:L:323:GLU:OE2	2.49	0.46
1:L:213:GLU:OE2	1:L:304:ARG:NH1	2.46	0.46
1:B:14:ASP:HA	1:B:16:ARG:HH22	1.81	0.45
1:F:22:SER:O	1:F:28:LYS:NZ	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:183:ARG:NH2	1:K:323:GLU:OE2	2.49	0.45
1:J:197:HIS:HB2	1:J:199:LEU:HG	1.97	0.45
1:K:13:PHE:CE1	1:K:15:GLN:HB3	2.51	0.45
1:A:128:PHE:CD1	1:A:170:LEU:HB3	2.52	0.45
1:A:170:LEU:HD23	1:A:202:CYS:HB3	1.99	0.45
1:L:146:LEU:HD11	1:L:320:VAL:HG11	1.98	0.45
1:A:148:GLN:HE22	1:A:152:VAL:HG11	1.81	0.45
1:D:306:MET:HE1	1:D:371:ARG:HD3	1.99	0.45
1:G:210:LEU:HD21	1:G:241:SER:HA	1.98	0.45
1:H:20:ARG:HH11	1:H:27:TRP:CD1	2.34	0.45
1:J:249:ALA:HB2	1:J:278:ALA:HB1	1.98	0.45
1:D:20:ARG:HB3	1:D:22:SER:OG	2.16	0.45
1:D:344:PHE:HB3	1:D:349:LEU:HB2	1.98	0.45
1:H:306:MET:HE3	1:H:306:MET:HB2	1.84	0.45
1:F:386:THR:HA	1:F:387:SER:HA	1.59	0.45
1:G:106:ILE:HD13	1:G:267:ARG:HB2	1.99	0.45
1:H:109:ARG:HH22	1:H:134:LEU:HD22	1.82	0.45
1:B:325:SER:OG	1:B:326:PHE:N	2.49	0.45
1:H:43:THR:O	1:H:243:ASN:ND2	2.49	0.45
1:H:327:LEU:HD22	1:H:364:ARG:NE	2.31	0.45
1:L:29:LYS:HE3	1:L:30:TYR:CZ	2.52	0.45
1:C:20:ARG:HB3	1:C:22:SER:OG	2.16	0.45
1:A:210:LEU:HA	1:A:297:LEU:HD21	1.98	0.45
1:B:62:GLY:HA3	1:K:46:ARG:HD2	1.98	0.45
1:F:301:ARG:HH22	1:I:301:ARG:CZ	2.30	0.45
1:L:15:GLN:HG2	1:L:299:TYR:CE1	2.52	0.45
1:D:145:ARG:NH2	1:D:154:ASP:OD2	2.49	0.45
1:A:325:SER:OG	1:A:326:PHE:N	2.49	0.45
1:L:360:ASP:OD1	1:L:360:ASP:N	2.49	0.45
1:F:302:ALA:HB3	1:F:371:ARG:HH21	1.81	0.44
1:L:335:LEU:HB3	1:L:337:VAL:HG23	1.98	0.44
1:C:212:LEU:HD11	1:C:325:SER:OG	2.17	0.44
1:B:63:VAL:HG21	1:K:20:ARG:HD3	1.99	0.44
1:D:163:SER:OG	1:D:165:ASN:OD1	2.35	0.44
1:L:121:ALA:HB2	1:L:153:LEU:HD22	1.98	0.44
1:D:386:THR:HA	1:D:387:SER:HA	1.58	0.44
1:F:20:ARG:HD3	1:F:27:TRP:CD1	2.52	0.44
1:F:268:LYS:HD2	1:J:134:LEU:HD11	1.98	0.44
1:J:352:SER:HB2	1:J:364:ARG:HB3	1.99	0.44
1:L:262:ARG:NH2	1:L:265:ARG:HD2	2.32	0.44
1:A:352:SER:HB2	1:A:364:ARG:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:13:PHE:HE1	1:H:15:GLN:HB2	1.80	0.44
1:B:13:PHE:CE1	1:B:15:GLN:HB2	2.52	0.44
1:D:39:TRP:CG	1:D:40:ILE:H	2.36	0.44
1:G:89:ILE:HD12	1:G:253:VAL:HG11	1.98	0.44
1:H:20:ARG:NH1	1:H:44:ASP:OD1	2.50	0.44
1:J:131:ALA:HB3	1:J:132:PRO:HD3	1.99	0.44
1:L:124:ILE:HG12	1:L:125:TYR:H	1.83	0.44
1:B:56:GLN:OE1	1:K:56:GLN:HG2	2.17	0.44
1:E:177:PRO:O	1:E:329:TRP:HB2	2.18	0.44
1:E:352:SER:HB2	1:E:364:ARG:HB3	2.00	0.44
1:G:201:VAL:O	1:G:233:ILE:HD12	2.17	0.44
1:H:94:LEU:HD22	1:H:251:LEU:HD21	1.99	0.44
1:I:337:VAL:HG12	1:I:339:ASP:H	1.82	0.44
1:D:340:PRO:HD3	1:D:361:ARG:NH2	2.33	0.44
1:F:319:MET:HE2	1:F:322:PRO:HD3	1.99	0.44
1:H:194:ALA:O	1:H:231:ARG:NH2	2.51	0.44
1:K:122:THR:HG23	1:K:143:ALA:HA	1.98	0.44
1:F:13:PHE:CE2	1:F:16:ARG:HG2	2.53	0.44
1:G:13:PHE:CZ	1:G:15:GLN:HB2	2.53	0.44
1:G:325:SER:HA	1:G:326:PHE:HA	1.83	0.44
1:H:270:MET:HE2	1:H:270:MET:HB3	1.89	0.44
1:I:55:LEU:HD21	1:I:281:ALA:HB2	2.00	0.44
1:J:238:PRO:HB3	1:J:286:TRP:NE1	2.32	0.44
1:L:325:SER:HA	1:L:326:PHE:HA	1.82	0.44
1:B:39:TRP:CG	1:B:40:ILE:H	2.35	0.44
1:K:239:SER:HA	1:K:244:ILE:HG13	2.00	0.44
1:C:132:PRO:HB3	1:C:137:ARG:HB2	2.00	0.43
1:A:100:VAL:HG21	1:A:206:ILE:HD12	2.00	0.43
1:A:106:ILE:HD13	1:A:267:ARG:HB2	1.99	0.43
1:G:20:ARG:HB3	1:G:22:SER:OG	2.17	0.43
1:K:89:ILE:HD12	1:K:253:VAL:HG11	2.00	0.43
1:C:300:LEU:HD13	1:C:325:SER:HB3	2.00	0.43
1:H:201:VAL:HG21	1:H:221:PHE:HE2	1.83	0.43
1:I:159:GLU:OE2	1:I:196:ARG:NH1	2.52	0.43
1:J:108:VAL:O	1:J:112:THR:OG1	2.24	0.43
1:J:188:GLU:O	1:J:192:ARG:HG3	2.18	0.43
1:I:333:SER:HB3	1:I:361:ARG:HD2	2.00	0.43
1:K:170:LEU:HD23	1:K:202:CYS:HB3	2.01	0.43
1:L:13:PHE:CE1	1:L:15:GLN:HB2	2.53	0.43
1:A:20:ARG:HA	1:A:21:HIS:C	2.43	0.43
1:A:128:PHE:HD1	1:A:170:LEU:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:ASN:HA	1:A:177:PRO:HA	1.87	0.43
1:G:201:VAL:O	1:G:232:SER:HA	2.19	0.43
1:L:73:LEU:HA	1:L:76:VAL:HG12	2.01	0.43
1:D:62:GLY:HA3	1:G:46:ARG:HG3	2.00	0.43
1:E:92:GLU:CD	1:E:92:GLU:H	2.27	0.43
1:K:325:SER:OG	1:K:326:PHE:N	2.48	0.43
1:G:207:HIS:CE1	1:G:240:LYS:HE2	2.53	0.43
1:G:20:ARG:HH21	1:G:44:ASP:HA	1.83	0.43
1:K:348:GLY:O	1:K:380:ARG:NH1	2.49	0.43
1:L:128:PHE:HD2	1:L:170:LEU:HB3	1.83	0.43
1:C:277:LEU:HD13	1:E:277:LEU:HD13	2.00	0.43
1:A:39:TRP:CG	1:A:40:ILE:H	2.37	0.43
1:A:71:GLU:CD	1:A:71:GLU:H	2.27	0.43
1:B:112:THR:HG22	1:B:167:LYS:HB3	2.00	0.43
1:B:272:PRO:HG3	1:K:98:PRO:HG2	2.01	0.43
1:E:359:ASN:OD1	1:E:361:ARG:HD3	2.18	0.43
1:F:28:LYS:HA	1:F:31:ALA:HB2	2.01	0.43
1:G:124:ILE:HG12	1:G:125:TYR:H	1.83	0.43
1:I:229:ALA:C	1:I:231:ARG:H	2.27	0.43
1:L:349:LEU:HD21	1:L:380:ARG:HB2	2.01	0.43
1:D:88:LYS:H	1:D:88:LYS:HD2	1.84	0.42
1:I:352:SER:HB2	1:I:364:ARG:HB3	2.00	0.42
1:B:299:TYR:OH	1:B:371:ARG:N	2.39	0.42
1:E:43:THR:HG22	1:E:368:GLY:HA3	2.00	0.42
1:F:101:VAL:O	1:F:105:ASN:ND2	2.47	0.42
1:I:191:LEU:HD11	1:I:228:ALA:HB2	2.01	0.42
1:L:144:LEU:HD11	1:L:175:HIS:CE1	2.54	0.42
1:B:122:THR:HG23	1:B:143:ALA:HA	2.01	0.42
1:A:306:MET:HE3	1:A:378:LEU:HD12	2.02	0.42
1:B:111:PHE:HB3	1:B:200:LEU:HD12	2.00	0.42
1:B:118:THR:HG22	1:B:168:LEU:HB3	2.01	0.42
1:D:184:ARG:NH2	1:E:217:GLN:OE1	2.46	0.42
1:E:87:TRP:CZ2	1:E:222:ALA:HB3	2.54	0.42
1:E:385:LEU:C	1:E:387:SER:HA	2.45	0.42
1:G:238:PRO:HB3	1:G:286:TRP:NE1	2.34	0.42
1:H:60:GLN:O	1:L:46:ARG:NH1	2.45	0.42
1:H:314:LEU:HD22	1:H:385:LEU:HD12	2.01	0.42
1:H:337:VAL:HG11	1:H:343:PHE:HB2	2.00	0.42
1:K:275:ASP:OD1	1:K:276:VAL:N	2.53	0.42
1:L:20:ARG:HA	1:L:21:HIS:C	2.44	0.42
1:H:93:TRP:CD1	1:H:255:PRO:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:258:GLU:O	1:B:259:LEU:HB2	2.20	0.42
1:G:212:LEU:HD12	1:G:304:ARG:HD3	2.01	0.42
1:K:238:PRO:HB3	1:K:286:TRP:NE1	2.35	0.42
1:C:127:PRO:HA	1:C:130:LEU:HB2	2.00	0.42
1:A:333:SER:HB3	1:A:361:ARG:HB3	2.02	0.42
1:J:124:ILE:HG13	1:J:125:TYR:N	2.35	0.42
1:D:156:ASP:OD1	1:D:196:ARG:NH2	2.53	0.42
1:F:339:ASP:HB3	1:F:342:LEU:HB3	2.02	0.42
1:B:39:TRP:CG	1:B:40:ILE:N	2.87	0.42
1:K:135:ALA:O	1:K:137:ARG:NH1	2.52	0.42
1:E:116:GLN:NE2	1:E:167:LYS:HD2	2.35	0.42
1:G:80:ARG:NH2	1:G:290:GLN:OE1	2.43	0.42
1:H:16:ARG:NH2	1:H:46:ARG:HD2	2.35	0.42
1:H:194:ALA:HA	1:H:199:LEU:HD12	2.02	0.42
1:H:201:VAL:HG21	1:H:221:PHE:CE2	2.55	0.42
1:L:251:LEU:HD21	1:L:286:TRP:HZ3	1.85	0.42
1:A:361:ARG:HA	1:A:361:ARG:HD3	1.78	0.41
1:B:187:LEU:HB3	1:B:224:LEU:HD11	2.02	0.41
1:L:210:LEU:HB3	1:L:325:SER:OG	2.20	0.41
1:E:135:ALA:O	1:E:137:ARG:NH1	2.53	0.41
1:F:325:SER:HA	1:F:326:PHE:HA	1.85	0.41
1:A:209:ASP:HB3	1:A:293:LEU:HD21	2.01	0.41
1:A:290:GLN:NE2	1:A:294:ASP:OD1	2.53	0.41
1:B:355:ARG:HG2	1:B:360:ASP:HA	2.02	0.41
1:F:46:ARG:HG3	1:J:62:GLY:HA3	2.02	0.41
1:F:87:TRP:CZ2	1:F:222:ALA:HB3	2.54	0.41
1:L:13:PHE:C	1:L:15:GLN:H	2.29	0.41
1:C:82:GLU:HA	1:C:87:TRP:H	1.86	0.41
1:D:355:ARG:HB2	1:D:360:ASP:HB3	2.01	0.41
1:K:352:SER:HB2	1:K:364:ARG:HB3	2.03	0.41
1:L:148:GLN:O	1:L:149:GLN:HG2	2.20	0.41
1:A:275:ASP:OD1	1:A:276:VAL:N	2.53	0.41
1:E:314:LEU:HD13	1:E:385:LEU:HD12	2.02	0.41
1:F:197:HIS:HB2	1:F:199:LEU:HG	2.03	0.41
1:F:208:CYS:HB2	1:F:218:HIS:CG	2.56	0.41
1:I:213:GLU:HG3	1:I:323:GLU:HB3	2.02	0.41
1:J:212:LEU:O	1:J:301:ARG:NH1	2.54	0.41
1:A:120:SER:HB2	1:A:170:LEU:HB2	2.03	0.41
1:H:360:ASP:OD1	1:H:360:ASP:N	2.53	0.41
1:L:77:ALA:O	1:L:81:MET:HG2	2.21	0.41
1:C:77:ALA:O	1:C:81:MET:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:207:HIS:CE1	1:B:240:LYS:HD3	2.56	0.41
1:F:356:ASP:N	1:F:356:ASP:OD1	2.54	0.41
1:H:39:TRP:CG	1:H:40:ILE:H	2.38	0.41
1:I:125:TYR:CD2	1:I:127:PRO:HD2	2.55	0.41
1:J:325:SER:CB	1:J:326:PHE:HA	2.50	0.41
1:L:36:LEU:HD11	1:L:376:GLU:OE1	2.21	0.41
1:E:190:GLN:H	1:E:190:GLN:HG2	1.70	0.41
1:G:20:ARG:HD2	1:G:24:SER:HB2	2.01	0.41
1:J:87:TRP:CZ2	1:J:222:ALA:HB3	2.55	0.41
1:C:39:TRP:CG	1:C:40:ILE:H	2.38	0.41
1:C:319:MET:HE2	1:C:322:PRO:HD3	2.01	0.41
1:E:229:ALA:HB1	1:E:255:PRO:HG2	2.03	0.41
1:F:19:ARG:HG3	1:F:21:HIS:HB3	2.03	0.41
1:F:342:LEU:HA	1:F:345:GLU:HG2	2.03	0.41
1:G:39:TRP:CG	1:G:40:ILE:N	2.89	0.41
1:G:125:TYR:CD2	1:G:127:PRO:HD2	2.55	0.41
1:G:275:ASP:OD1	1:G:276:VAL:N	2.54	0.41
1:H:317:LEU:HD21	1:H:335:LEU:HD11	2.03	0.41
1:J:270:MET:HE2	1:J:270:MET:HB3	1.98	0.41
1:K:77:ALA:O	1:K:81:MET:HG2	2.21	0.41
1:L:15:GLN:HG2	1:L:299:TYR:HE1	1.86	0.41
1:L:261:ALA:O	1:L:265:ARG:HG3	2.20	0.41
1:E:356:ASP:OD1	1:E:356:ASP:N	2.54	0.41
1:F:170:LEU:HD23	1:F:202:CYS:HB3	2.02	0.41
1:G:169:LEU:HG	1:G:171:LEU:HD13	2.02	0.41
1:H:325:SER:HA	1:H:326:PHE:HA	1.81	0.41
1:I:162:MET:HE2	1:I:166:GLU:HG2	2.02	0.41
1:F:184:ARG:NH2	1:I:217:GLN:OE1	2.54	0.40
1:G:187:LEU:HB3	1:G:224:LEU:HD11	2.02	0.40
1:I:125:TYR:HB3	1:I:128:PHE:CD1	2.57	0.40
1:K:349:LEU:HB3	1:K:351:PHE:CZ	2.56	0.40
1:A:39:TRP:CG	1:A:40:ILE:N	2.89	0.40
1:F:380:ARG:HG2	1:F:383:ARG:HH12	1.86	0.40
1:B:306:MET:HE1	1:B:371:ARG:HD2	2.03	0.40
1:F:55:LEU:HD21	1:F:281:ALA:HB2	2.04	0.40
1:J:110:ALA:O	1:J:262:ARG:HD2	2.21	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	374/389 (96%)	352 (94%)	22 (6%)	0	100	100
1	B	377/389 (97%)	358 (95%)	18 (5%)	1 (0%)	36	63
1	C	377/389 (97%)	360 (96%)	16 (4%)	1 (0%)	36	63
1	D	376/389 (97%)	359 (96%)	15 (4%)	2 (0%)	24	52
1	E	376/389 (97%)	358 (95%)	17 (4%)	1 (0%)	36	63
1	F	377/389 (97%)	360 (96%)	16 (4%)	1 (0%)	36	63
1	G	377/389 (97%)	347 (92%)	26 (7%)	4 (1%)	11	32
1	H	376/389 (97%)	347 (92%)	25 (7%)	4 (1%)	11	32
1	I	373/389 (96%)	345 (92%)	25 (7%)	3 (1%)	16	40
1	J	373/389 (96%)	350 (94%)	21 (6%)	2 (0%)	24	52
1	K	374/389 (96%)	352 (94%)	20 (5%)	2 (0%)	24	52
1	L	372/389 (96%)	344 (92%)	27 (7%)	1 (0%)	36	63
All	All	4502/4668 (96%)	4232 (94%)	248 (6%)	22 (0%)	24	52

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	63	VAL
1	H	129	PHE
1	H	214	PRO
1	I	41	ALA
1	I	315	PRO
1	J	315	PRO
1	K	315	PRO
1	L	315	PRO
1	B	315	PRO
1	D	325	SER
1	E	315	PRO
1	G	31	ALA

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Mol	Chain	Res	Type
1	G	315	PRO
1	H	13	PHE
1	I	31	ALA
1	C	316	GLY
1	G	18	ASP
1	K	13	PHE
1	D	315	PRO
1	H	315	PRO
1	F	315	PRO
1	J	328	GLY

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	313/325 (96%)	310 (99%)	3 (1%)	68	86
1	B	315/325 (97%)	311 (99%)	4 (1%)	61	83
1	C	315/325 (97%)	310 (98%)	5 (2%)	55	81
1	D	314/325 (97%)	308 (98%)	6 (2%)	50	78
1	E	314/325 (97%)	309 (98%)	5 (2%)	55	81
1	F	315/325 (97%)	311 (99%)	4 (1%)	61	83
1	G	315/325 (97%)	307 (98%)	8 (2%)	42	73
1	H	315/325 (97%)	306 (97%)	9 (3%)	37	70
1	I	312/325 (96%)	309 (99%)	3 (1%)	68	86
1	J	312/325 (96%)	306 (98%)	6 (2%)	50	78
1	K	313/325 (96%)	310 (99%)	3 (1%)	68	86
1	L	311/325 (96%)	306 (98%)	5 (2%)	55	81
All	All	3764/3900 (96%)	3703 (98%)	61 (2%)	55	81

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	ARG
1	C	75	GLU
1	C	198	ASP
1	C	233	ILE
1	C	327	LEU
1	A	21	HIS
1	A	71	GLU
1	A	233	ILE
1	B	63	VAL
1	B	71	GLU
1	B	233	ILE
1	B	327	LEU
1	D	20	ARG
1	D	23	ASP
1	D	231	ARG
1	D	233	ILE
1	D	276	VAL
1	D	327	LEU
1	E	22	SER
1	E	134	LEU
1	E	253	VAL
1	E	325	SER
1	E	327	LEU
1	F	60	GLN
1	F	233	ILE
1	F	327	LEU
1	F	356	ASP
1	G	20	ARG
1	G	23	ASP
1	G	56	GLN
1	G	90	GLN
1	G	171	LEU
1	G	208	CYS
1	G	325	SER
1	G	327	LEU
1	H	75	GLU
1	H	134	LEU
1	H	162	MET
1	H	187	LEU
1	H	201	VAL
1	H	233	ILE
1	H	254	ILE
1	H	325	SER

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Mol	Chain	Res	Type
1	H	327	LEU
1	I	233	ILE
1	I	323	GLU
1	I	327	LEU
1	J	15	GLN
1	J	109	ARG
1	J	212	LEU
1	J	274	VAL
1	J	325	SER
1	J	326	PHE
1	K	119	VAL
1	K	233	ILE
1	K	240	LYS
1	L	71	GLU
1	L	233	ILE
1	L	337	VAL
1	L	363	VAL
1	L	383	ARG

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

Mol	Chain	Res	Type
1	C	372	GLN
1	A	12	ASN
1	A	61	GLN
1	A	176	ASN
1	B	217	GLN
1	D	176	ASN
1	D	190	GLN
1	D	218	HIS
1	D	296	GLN
1	E	12	ASN
1	E	176	ASN
1	E	230	GLN
1	F	90	GLN
1	G	379	GLN
1	H	56	GLN
1	H	243	ASN
1	H	264	ASN
1	I	312	ASN
1	J	60	GLN
1	J	312	ASN

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Mol	Chain	Res	Type
1	J	372	GLN
1	K	60	GLN
1	K	61	GLN
1	K	312	ASN
1	K	379	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	PLP	J	401	1	15,15,16	1.10	2 (13%)	21,22,23	1.07	2 (9%)
2	PLP	E	401	1	15,15,16	1.10	2 (13%)	21,22,23	1.10	2 (9%)
2	PLP	A	401	1	15,15,16	1.17	2 (13%)	21,22,23	1.25	2 (9%)
2	PLP	I	401	1	15,15,16	1.09	1 (6%)	21,22,23	1.06	2 (9%)
2	PLP	L	401	1	15,15,16	1.08	2 (13%)	21,22,23	1.07	2 (9%)
2	PLP	C	401	1	15,15,16	1.10	2 (13%)	21,22,23	1.10	2 (9%)
2	PLP	F	401	1	15,15,16	1.08	2 (13%)	21,22,23	1.15	2 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PLP	B	401	1	15,15,16	1.12	2 (13%)	21,22,23	1.11	2 (9%)
2	PLP	D	401	1	15,15,16	1.13	2 (13%)	21,22,23	1.22	2 (9%)
2	PLP	G	401	1	15,15,16	1.12	2 (13%)	21,22,23	1.17	2 (9%)
2	PLP	H	401	1	15,15,16	1.11	2 (13%)	21,22,23	1.11	2 (9%)
2	PLP	K	401	1	15,15,16	1.07	2 (13%)	21,22,23	1.26	3 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	J	401	1	-	2/6/6/8	0/1/1/1
2	PLP	E	401	1	-	0/6/6/8	0/1/1/1
2	PLP	A	401	1	-	1/6/6/8	0/1/1/1
2	PLP	I	401	1	-	2/6/6/8	0/1/1/1
2	PLP	L	401	1	-	0/6/6/8	0/1/1/1
2	PLP	C	401	1	-	0/6/6/8	0/1/1/1
2	PLP	F	401	1	-	1/6/6/8	0/1/1/1
2	PLP	B	401	1	-	0/6/6/8	0/1/1/1
2	PLP	D	401	1	-	3/6/6/8	0/1/1/1
2	PLP	G	401	1	-	1/6/6/8	0/1/1/1
2	PLP	H	401	1	-	1/6/6/8	0/1/1/1
2	PLP	K	401	1	-	1/6/6/8	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C2-N1	3.01	1.39	1.33
2	G	401	PLP	C2-N1	2.73	1.38	1.33
2	D	401	PLP	C2-N1	2.69	1.38	1.33
2	E	401	PLP	C2-N1	2.66	1.38	1.33
2	H	401	PLP	C2-N1	2.66	1.38	1.33
2	B	401	PLP	C2-N1	2.65	1.38	1.33
2	C	401	PLP	C2-N1	2.64	1.38	1.33
2	F	401	PLP	C2-N1	2.64	1.38	1.33
2	I	401	PLP	C2-N1	2.63	1.38	1.33
2	J	401	PLP	C2-N1	2.63	1.38	1.33
2	K	401	PLP	C2-N1	2.59	1.38	1.33
2	L	401	PLP	C2-N1	2.57	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	PLP	C6-N1	2.21	1.38	1.34
2	B	401	PLP	C6-N1	2.09	1.38	1.34
2	H	401	PLP	C6-N1	2.09	1.38	1.34
2	D	401	PLP	C6-N1	2.07	1.38	1.34
2	K	401	PLP	C6-N1	2.07	1.38	1.34
2	G	401	PLP	C6-N1	2.06	1.38	1.34
2	J	401	PLP	C6-N1	2.04	1.38	1.34
2	L	401	PLP	C6-N1	2.04	1.38	1.34
2	E	401	PLP	C6-N1	2.02	1.38	1.34
2	F	401	PLP	C6-N1	2.00	1.38	1.34
2	C	401	PLP	C6-N1	2.00	1.38	1.34

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	PLP	C6-C5-C4	3.08	120.62	118.10
2	A	401	PLP	C5-C6-N1	-2.83	119.22	123.83
2	K	401	PLP	C6-C5-C4	2.77	120.36	118.10
2	F	401	PLP	C6-C5-C4	2.66	120.28	118.10
2	F	401	PLP	C5-C6-N1	-2.46	119.83	123.83
2	G	401	PLP	C5-C6-N1	-2.45	119.85	123.83
2	K	401	PLP	C5-C6-N1	-2.40	119.92	123.83
2	B	401	PLP	C5-C6-N1	-2.40	119.92	123.83
2	D	401	PLP	C5-C6-N1	-2.40	119.93	123.83
2	G	401	PLP	C6-C5-C4	2.39	120.06	118.10
2	J	401	PLP	C5-C6-N1	-2.37	119.98	123.83
2	I	401	PLP	C5-C6-N1	-2.36	119.99	123.83
2	K	401	PLP	C4A-C4-C5	-2.33	118.53	120.94
2	C	401	PLP	C5-C6-N1	-2.31	120.07	123.83
2	L	401	PLP	C5-C6-N1	-2.31	120.08	123.83
2	H	401	PLP	C5-C6-N1	-2.30	120.09	123.83
2	E	401	PLP	C5-C6-N1	-2.29	120.10	123.83
2	D	401	PLP	C6-C5-C4	2.28	119.96	118.10
2	I	401	PLP	C6-C5-C4	2.28	119.96	118.10
2	L	401	PLP	C6-C5-C4	2.26	119.95	118.10
2	H	401	PLP	C6-C5-C4	2.22	119.91	118.10
2	C	401	PLP	C6-C5-C4	2.21	119.91	118.10
2	B	401	PLP	C6-C5-C4	2.21	119.91	118.10
2	J	401	PLP	C6-C5-C4	2.15	119.86	118.10
2	E	401	PLP	C6-C5-C4	2.14	119.85	118.10

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	PLP	C5A-O4P-P-O1P
2	D	401	PLP	C5A-O4P-P-O2P
2	G	401	PLP	C5A-O4P-P-O2P
2	I	401	PLP	C5A-O4P-P-O2P
2	J	401	PLP	C5A-O4P-P-O1P
2	D	401	PLP	C5A-O4P-P-O3P
2	I	401	PLP	C5A-O4P-P-O3P
2	J	401	PLP	C5A-O4P-P-O2P
2	A	401	PLP	C5A-O4P-P-O1P
2	F	401	PLP	C5A-O4P-P-O2P
2	H	401	PLP	C5A-O4P-P-O2P
2	K	401	PLP	C5A-O4P-P-O3P

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	L	401	PLP	1	0
2	C	401	PLP	1	0
2	D	401	PLP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	376/389 (96%)	0.16	9 (2%) 59 52	21, 33, 51, 63	0
1	B	379/389 (97%)	0.25	9 (2%) 59 52	22, 34, 56, 71	0
1	C	379/389 (97%)	0.14	9 (2%) 59 52	21, 31, 48, 78	0
1	D	378/389 (97%)	0.21	8 (2%) 63 56	22, 34, 52, 87	0
1	E	378/389 (97%)	0.23	9 (2%) 59 52	22, 34, 53, 75	0
1	F	379/389 (97%)	0.38	10 (2%) 57 49	26, 41, 58, 82	0
1	G	379/389 (97%)	0.39	12 (3%) 50 43	22, 39, 59, 72	0
1	H	378/389 (97%)	0.76	29 (7%) 19 15	32, 50, 68, 87	0
1	I	375/389 (96%)	0.37	10 (2%) 56 48	24, 42, 61, 74	0
1	J	375/389 (96%)	0.61	16 (4%) 40 33	29, 49, 68, 89	0
1	K	376/389 (96%)	0.29	15 (3%) 42 36	25, 38, 59, 84	0
1	L	374/389 (96%)	0.78	29 (7%) 19 15	28, 51, 73, 89	0
All	All	4526/4668 (96%)	0.38	165 (3%) 46 39	21, 40, 63, 89	0

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	325	SER	7.9
1	H	11	PHE	6.5
1	E	389	TYR	6.0
1	F	325	SER	5.9
1	L	164	GLY	5.7
1	C	389	TYR	5.6
1	H	89	ILE	5.4
1	A	324	ALA	5.2
1	L	325	SER	4.6
1	G	17	ILE	4.5
1	C	387	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	E	176	ASN	4.4
1	H	325	SER	4.2
1	J	325	SER	4.2
1	D	17	ILE	4.2
1	K	11	PHE	4.0
1	L	163	SER	3.9
1	D	324	ALA	3.9
1	C	325	SER	3.6
1	E	325	SER	3.6
1	L	328	GLY	3.6
1	L	384	ALA	3.5
1	L	385	LEU	3.4
1	E	177	PRO	3.4
1	K	13	PHE	3.4
1	J	327	LEU	3.3
1	J	17	ILE	3.2
1	L	155	LEU	3.2
1	K	160	ASP	3.2
1	K	21	HIS	3.2
1	B	387	SER	3.2
1	I	17	ILE	3.2
1	K	17	ILE	3.1
1	K	22	SER	3.1
1	H	256	ASN	3.1
1	J	18	ASP	3.1
1	D	20	ARG	3.1
1	F	207	HIS	3.0
1	J	21	HIS	3.0
1	D	389	TYR	3.0
1	A	148	GLN	3.0
1	F	389	TYR	3.0
1	H	16	ARG	3.0
1	D	13	PHE	3.0
1	B	20	ARG	2.9
1	K	165	ASN	2.9
1	L	21	HIS	2.9
1	E	388	GLY	2.9
1	G	11	PHE	2.9
1	I	13	PHE	2.9
1	K	89	ILE	2.8
1	G	215	GLY	2.8
1	K	32	ASP	2.8

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Mol	Chain	Res	Type	RSRZ
1	L	327	LEU	2.8
1	A	22	SER	2.8
1	H	62	GLY	2.8
1	L	162	MET	2.8
1	G	62	GLY	2.7
1	F	275	ASP	2.7
1	B	389	TYR	2.7
1	E	62	GLY	2.7
1	K	324	ALA	2.7
1	F	327	LEU	2.7
1	B	11	PHE	2.7
1	H	140	LEU	2.6
1	J	159	GLU	2.6
1	L	136	GLY	2.6
1	H	165	ASN	2.6
1	F	13	PHE	2.6
1	J	19	ARG	2.6
1	C	328	GLY	2.5
1	H	13	PHE	2.5
1	B	356	ASP	2.5
1	H	49	ASP	2.5
1	K	18	ASP	2.5
1	H	88	LYS	2.5
1	G	21	HIS	2.5
1	H	223	SER	2.5
1	G	16	ARG	2.5
1	I	18	ASP	2.5
1	I	298	ASP	2.5
1	I	328	GLY	2.5
1	H	228	ALA	2.5
1	J	163	SER	2.5
1	C	388	GLY	2.5
1	C	11	PHE	2.5
1	L	13	PHE	2.5
1	E	275	ASP	2.4
1	H	129	PHE	2.4
1	H	386	THR	2.4
1	F	387	SER	2.4
1	L	318	SER	2.4
1	C	275	ASP	2.4
1	A	328	GLY	2.4
1	E	142	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	11	PHE	2.4
1	L	192	ARG	2.4
1	J	324	ALA	2.4
1	H	327	LEU	2.3
1	F	386	THR	2.3
1	J	322	PRO	2.3
1	L	315	PRO	2.3
1	A	20	ARG	2.3
1	L	229	ALA	2.3
1	F	17	ILE	2.3
1	H	19	ARG	2.3
1	L	383	ARG	2.3
1	D	327	LEU	2.3
1	C	113	GLU	2.3
1	I	275	ASP	2.3
1	L	62	GLY	2.3
1	D	275	ASP	2.3
1	H	9	MET	2.2
1	H	214	PRO	2.2
1	H	199	LEU	2.2
1	H	385	LEU	2.2
1	A	107	ALA	2.2
1	J	151	TRP	2.2
1	J	13	PHE	2.2
1	I	338	ALA	2.2
1	L	125	TYR	2.2
1	K	334	GLY	2.2
1	L	160	ASP	2.2
1	H	12	ASN	2.2
1	J	56	GLN	2.2
1	B	273	ASP	2.2
1	J	32	ASP	2.2
1	H	197	HIS	2.2
1	C	386	THR	2.1
1	G	61	GLN	2.1
1	H	270	MET	2.1
1	D	21	HIS	2.1
1	E	387	SER	2.1
1	H	202	CYS	2.1
1	K	12	ASN	2.1
1	L	32	ASP	2.1
1	L	198	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	L	360	ASP	2.1
1	G	318	SER	2.1
1	H	225	SER	2.1
1	H	324	ALA	2.1
1	I	302	ALA	2.1
1	A	71	GLU	2.1
1	G	217	GLN	2.1
1	K	162	MET	2.1
1	L	140	LEU	2.1
1	A	13	PHE	2.1
1	B	360	ASP	2.1
1	G	204	ASP	2.1
1	K	14	ASP	2.1
1	I	114	ALA	2.1
1	L	83	SER	2.1
1	I	386	THR	2.1
1	L	199	LEU	2.1
1	L	12	ASN	2.1
1	A	11	PHE	2.1
1	B	81	MET	2.0
1	J	177	PRO	2.0
1	J	62	GLY	2.0
1	G	13	PHE	2.0
1	H	143	ALA	2.0
1	H	139	HIS	2.0
1	B	328	GLY	2.0
1	L	176	ASN	2.0
1	L	336	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
2	PLP	H	401	15/16	0.83	0.13	46,55,63,70	0
2	PLP	I	401	15/16	0.85	0.12	35,48,62,74	0
2	PLP	G	401	15/16	0.86	0.14	42,47,55,60	0
2	PLP	K	401	15/16	0.86	0.12	40,47,55,56	0
2	PLP	L	401	15/16	0.86	0.11	42,50,57,68	0
2	PLP	E	401	15/16	0.89	0.10	35,41,50,65	0
2	PLP	F	401	15/16	0.91	0.09	42,49,56,59	0
2	PLP	J	401	15/16	0.91	0.10	43,53,59,61	0
2	PLP	D	401	15/16	0.91	0.10	34,41,50,50	0
2	PLP	B	401	15/16	0.91	0.10	30,43,48,55	0
2	PLP	C	401	15/16	0.92	0.10	34,41,46,47	0
2	PLP	A	401	15/16	0.92	0.09	32,41,49,50	0

6.5 Other polymers [i](#)

There are no such residues in this entry.