



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:25 AM UTC

PDB ID : 1X2H / pdb_00001x2h
Title : Crystal Structure of Lipate-Protein Ligase A from Escherichia coli complexed with lipoic acid
Authors : Fujiwara, K.; Toma, S.; Okamura-Ikeda, K.; Motokawa, Y.; Nakagawa, A.; Taniguchi, H.
Deposited on : 2005-04-23
Resolution : 2.91 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

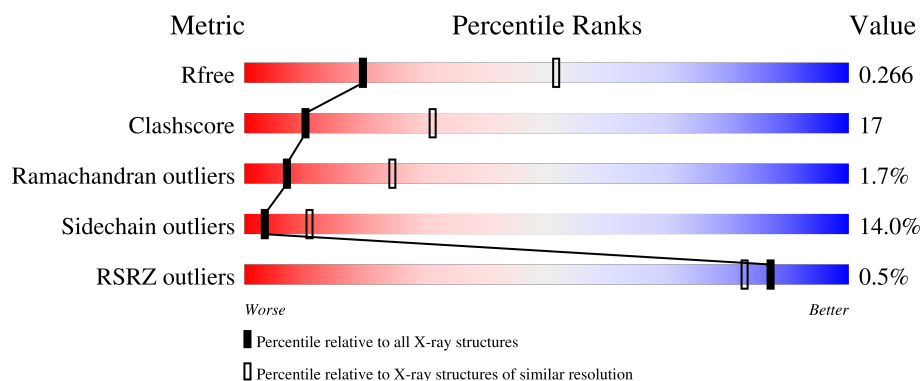
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.91 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	2995 (2.94-2.90)
Clashscore	190562	3213 (2.94-2.90)
Ramachandran outliers	187476	3128 (2.94-2.90)
Sidechain outliers	187428	3130 (2.94-2.90)
RSRZ outliers	180081	2995 (2.94-2.90)

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	337	% 57% 31% 9% ..
1	B	337	64% 28% 6% .
1	C	337	% 56% 36% 9%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7937 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.

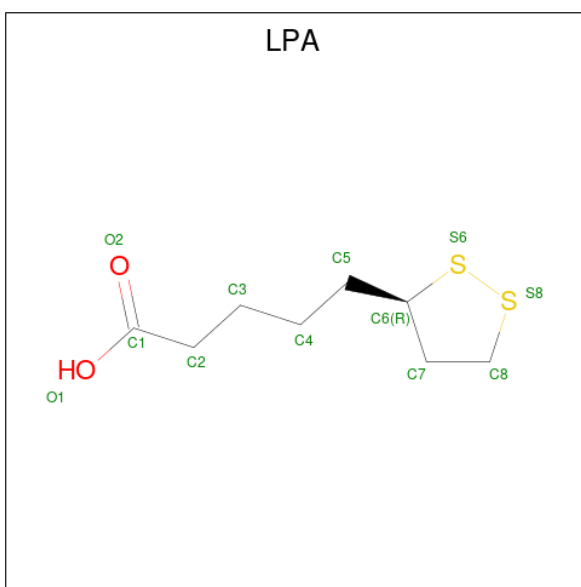
- Molecule 1 is a protein called Lipoate-protein ligase A.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	330	Total	C	N	O	S	Se	0	0	0
			2614	1644	466	493	6	5			
1	B	330	Total	C	N	O	S	Se	0	0	0
			2614	1644	466	493	6	5			
1	C	337	Total	C	N	O	S	Se	0	0	0
			2663	1673	476	503	6	5			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MSE	MET	modified residue	UNP P32099
A	60	MSE	MET	modified residue	UNP P32099
A	89	MSE	MET	modified residue	UNP P32099
A	306	MSE	MET	modified residue	UNP P32099
A	332	MSE	MET	modified residue	UNP P32099
B	27	MSE	MET	modified residue	UNP P32099
B	60	MSE	MET	modified residue	UNP P32099
B	89	MSE	MET	modified residue	UNP P32099
B	306	MSE	MET	modified residue	UNP P32099
B	332	MSE	MET	modified residue	UNP P32099
C	27	MSE	MET	modified residue	UNP P32099
C	60	MSE	MET	modified residue	UNP P32099
C	89	MSE	MET	modified residue	UNP P32099
C	306	MSE	MET	modified residue	UNP P32099
C	332	MSE	MET	modified residue	UNP P32099

- Molecule 2 is LIPOIC ACID (CCD ID: LPA) (formula: C₈H₁₄O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	S	0	0
			12	8	2	2		
2	B	1	Total	C	O	S	0	0
			12	8	2	2		

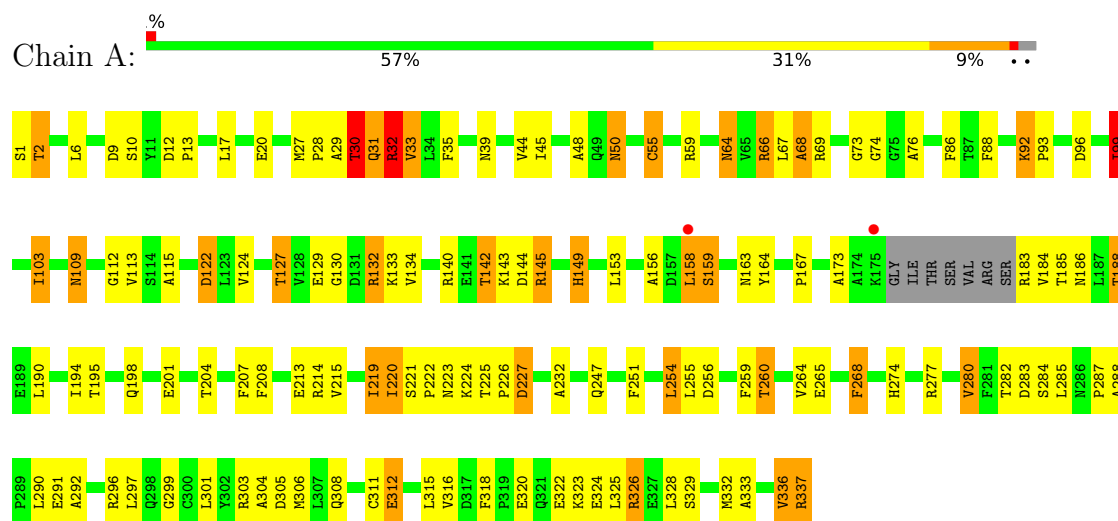
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	11	Total	O	0	0
			11	11		
3	B	8	Total	O	0	0
			8	8		
3	C	3	Total	O	0	0
			3	3		

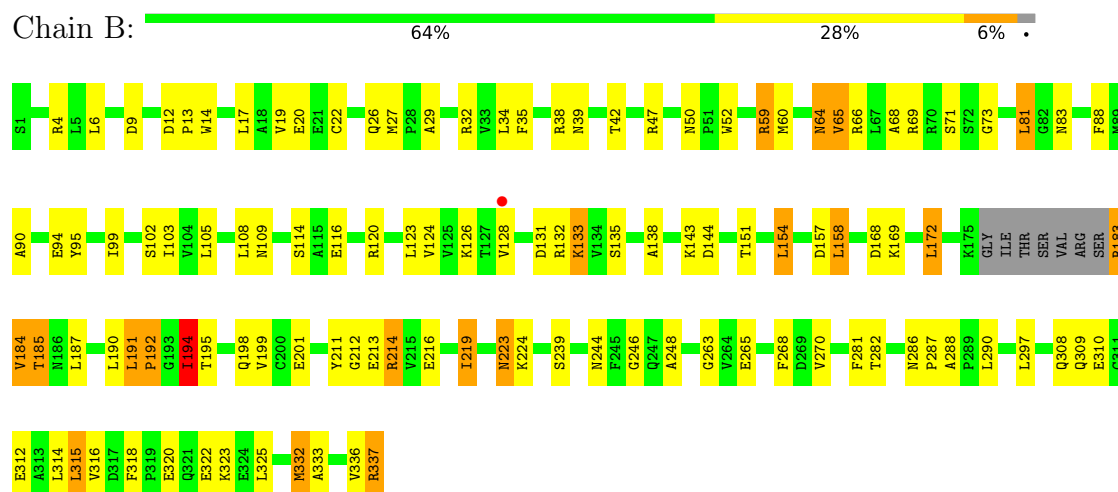
3 Residue-property plots

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: Lipoate-protein ligase A

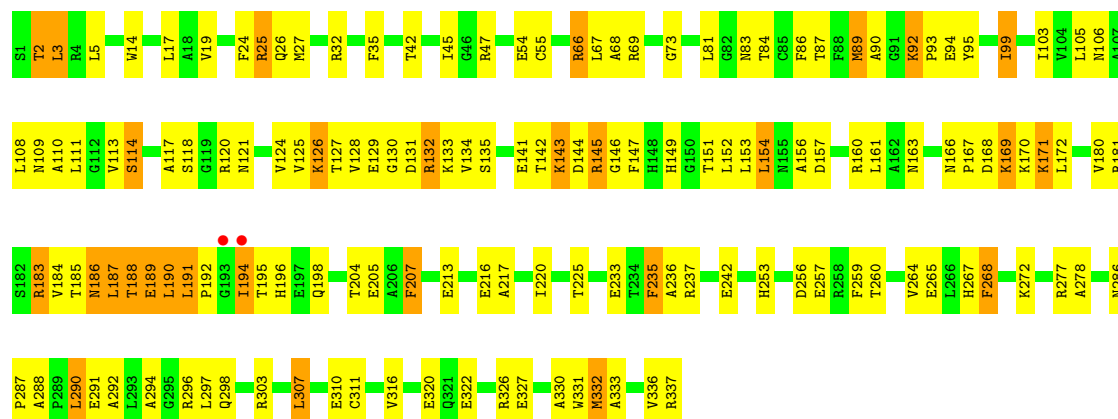


• Molecule 1: Lipoate-protein ligase A



• Molecule 1: Lipoate-protein ligase A





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	83.20Å 111.60Å 289.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	66.67 – 2.91 66.67 – 2.91	Depositor EDS
% Data completeness (in resolution range)	97.1 (66.67-2.91) 97.1 (66.67-2.91)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.97 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.186 , 0.271 0.184 , 0.266	Depositor DCC
R_{free} test set	1572 reflections (5.23%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7937	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: LPA

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	1.22	5/2665 (0.2%)	1.29	24/3601 (0.7%)
1	B	1.14	3/2665 (0.1%)	1.29	18/3601 (0.5%)
1	C	1.11	6/2715 (0.2%)	1.24	15/3670 (0.4%)
All	All	1.16	14/8045 (0.2%)	1.27	57/10872 (0.5%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	MSE	SE-CE	6.75	2.15	1.95
1	C	89	MSE	SE-CE	-6.70	1.75	1.95
1	C	2	THR	CA-CB	6.30	1.64	1.53
1	C	332	MSE	SE-CE	6.16	2.13	1.95
1	A	48	ALA	CA-CB	-5.85	1.45	1.53
1	C	27	MSE	SE-CE	5.78	2.12	1.95
1	B	270	VAL	CA-CB	-5.66	1.47	1.54
1	B	65	VAL	CA-CB	5.56	1.60	1.54
1	A	76	ALA	N-CA	5.38	1.52	1.45
1	A	149	HIS	CA-C	-5.22	1.46	1.52
1	C	19	VAL	CA-CB	-5.19	1.48	1.54
1	A	109	ASN	N-CA	-5.12	1.40	1.46
1	A	68	ALA	CA-CB	-5.10	1.45	1.53
1	C	235	PHE	CA-C	5.01	1.59	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	171	LYS	N-CA-C	-7.24	99.57	110.28
1	B	318	PHE	CA-C-N	-7.07	111.21	119.05
1	B	318	PHE	C-N-CA	-7.07	111.21	119.05
1	A	30	THR	N-CA-C	-6.95	104.61	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	312	GLU	N-CA-C	6.52	120.49	112.54
1	C	55	CYS	N-CA-C	6.47	120.59	110.17
1	C	207	PHE	N-CA-C	-6.46	104.17	111.14
1	B	27	MSE	CA-C-N	-6.44	113.03	119.99
1	B	27	MSE	C-N-CA	-6.44	113.03	119.99
1	A	145	ARG	N-CA-C	6.37	118.75	109.07
1	A	227	ASP	CB-CA-C	6.33	121.90	112.03
1	B	239	SER	CA-C-N	-6.31	113.25	122.65
1	B	239	SER	C-N-CA	-6.31	113.25	122.65
1	A	99	ILE	N-CA-C	6.26	116.37	110.30
1	C	188	THR	N-CA-C	-6.17	105.51	113.16
1	C	156	ALA	N-CA-C	6.15	118.78	108.02
1	C	225	THR	CA-C-N	6.08	126.11	119.90
1	C	225	THR	C-N-CA	6.08	126.11	119.90
1	B	286	ASN	CA-C-N	6.00	127.11	120.45
1	B	286	ASN	C-N-CA	6.00	127.11	120.45
1	A	55	CYS	N-CA-C	5.88	119.30	109.95
1	B	288	ALA	CA-C-N	-5.85	113.59	119.56
1	B	288	ALA	C-N-CA	-5.85	113.59	119.56
1	B	157	ASP	CA-C-N	5.84	128.69	120.28
1	B	157	ASP	C-N-CA	5.84	128.69	120.28
1	A	159	SER	N-CA-C	5.81	119.89	112.34
1	A	221	SER	N-CA-C	-5.77	102.94	108.07
1	A	268	PHE	N-CA-C	5.75	116.88	108.14
1	A	305	ASP	N-CA-C	5.72	117.97	111.11
1	C	145	ARG	N-CA-C	5.67	117.81	109.24
1	A	32	ARG	CA-C-N	-5.54	115.88	123.14
1	A	32	ARG	C-N-CA	-5.54	115.88	123.14
1	B	42	THR	CA-C-N	-5.45	116.04	123.12
1	B	42	THR	C-N-CA	-5.45	116.04	123.12
1	B	268	PHE	N-CA-C	5.41	117.06	108.79
1	A	76	ALA	N-CA-C	5.39	118.89	110.32
1	A	112	GLY	CA-C-N	-5.39	116.51	123.19
1	A	112	GLY	C-N-CA	-5.39	116.51	123.19
1	B	194	ILE	N-CA-C	5.35	120.46	109.34
1	B	248	ALA	CA-C-N	5.33	126.16	119.98
1	B	248	ALA	C-N-CA	5.33	126.16	119.98
1	A	50	ASN	CA-C-N	5.30	124.91	119.56
1	A	50	ASN	C-N-CA	5.30	124.91	119.56
1	C	268	PHE	N-CA-C	5.28	116.56	108.42
1	A	33	VAL	CA-C-N	-5.19	115.83	123.00
1	A	33	VAL	C-N-CA	-5.19	115.83	123.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	106	ASN	N-CA-C	5.12	117.26	111.11
1	A	232	ALA	N-CA-C	-5.11	105.62	111.14
1	A	115	ALA	N-CA-C	-5.10	101.36	108.96
1	C	310	GLU	N-CA-C	-5.09	105.92	111.82
1	C	288	ALA	CA-C-N	-5.08	113.81	119.19
1	C	288	ALA	C-N-CA	-5.08	113.81	119.19
1	C	27	MSE	CA-C-N	-5.03	114.80	120.14
1	C	27	MSE	C-N-CA	-5.03	114.80	120.14
1	A	299	GLY	N-CA-C	-5.03	108.67	115.21
1	A	219	ILE	N-CA-CB	5.02	117.38	111.66
1	A	325	LEU	N-CA-C	5.00	117.11	111.11

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	2614	0	2551	101	0
1	B	2614	0	2551	77	0
1	C	2663	0	2605	104	0
2	A	12	0	13	0	0
2	B	12	0	13	1	0
3	A	11	0	0	2	0
3	B	8	0	0	2	0
3	C	3	0	0	1	0
All	All	7937	0	7733	270	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 17.

All (270) 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:B:332:MSE:SE	1:B:332:MSE:CE	2.15	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:LEU:HD12	1:B:158:LEU:H	1.17	1.04
1:A:282:THR:HG21	1:A:290:LEU:HD12	1.39	1.03
1:C:286:ASN:HB3	3:C:338:HOH:O	1.59	0.99
1:C:89:MSE:HE3	1:C:145:ARG:HB2	1.40	0.99
1:B:83:ASN:HD22	1:B:151:THR:HG21	1.30	0.94
1:A:142:THR:HG23	1:A:143:LYS:H	1.35	0.91
1:A:127:THR:HG22	1:A:129:GLU:H	1.35	0.89
1:A:92:LYS:HB2	1:A:92:LYS:NZ	1.87	0.88
1:A:142:THR:CG2	1:A:143:LYS:N	2.36	0.88
1:C:2:THR:HG22	1:C:213:GLU:OE1	1.76	0.86
1:A:66:ARG:HH21	1:B:64:ASN:HD22	1.23	0.86
1:B:158:LEU:H	1:B:158:LEU:CD1	1.87	0.85
1:B:69:ARG:H	1:B:244:ASN:HD22	1.20	0.84
1:A:142:THR:HG23	1:A:143:LYS:N	1.95	0.82
1:B:337:ARG:HG3	1:B:337:ARG:HH11	1.43	0.81
1:B:183:ARG:HB3	1:B:183:ARG:HH11	1.43	0.80
1:A:132:ARG:HH11	1:A:132:ARG:HB3	1.45	0.79
1:B:158:LEU:HD12	1:B:158:LEU:N	1.97	0.79
1:C:89:MSE:CE	1:C:145:ARG:HB2	2.13	0.78
1:B:183:ARG:HB3	1:B:183:ARG:NH1	1.98	0.78
1:A:2:THR:OG1	1:A:32:ARG:NH1	2.19	0.76
1:B:59:ARG:HH11	1:B:59:ARG:HG2	1.52	0.75
1:B:69:ARG:H	1:B:244:ASN:ND2	1.85	0.74
1:C:127:THR:H	1:C:130:GLY:HA2	1.54	0.71
1:A:127:THR:CG2	1:A:129:GLU:H	2.03	0.71
1:A:158:LEU:HD12	1:A:159:SER:H	1.56	0.71
1:A:66:ARG:NH2	1:B:64:ASN:HD22	1.88	0.70
1:B:154:LEU:HD11	1:B:199:VAL:HG21	1.73	0.69
1:C:142:THR:HG22	1:C:143:LYS:N	2.07	0.69
1:C:303:ARG:O	1:C:307:LEU:HD12	1.92	0.69
1:C:26:GLN:HA	1:C:26:GLN:OE1	1.92	0.69
1:A:127:THR:HG22	1:A:129:GLU:N	2.07	0.69
1:B:123:LEU:HB2	1:B:135:SER:HB3	1.74	0.69
1:B:59:ARG:HH11	1:B:59:ARG:CG	2.05	0.69
1:B:126:LYS:HD3	1:B:131:ASP:OD1	1.92	0.68
1:B:183:ARG:NH1	3:B:346:HOH:O	2.25	0.68
1:C:89:MSE:HE3	1:C:145:ARG:CB	2.20	0.68
1:A:92:LYS:HB2	1:A:92:LYS:HZ2	1.58	0.67
1:B:83:ASN:HB3	1:B:151:THR:CG2	2.25	0.66
1:A:2:THR:HG1	1:A:32:ARG:HH11	1.43	0.66
1:A:132:ARG:HB3	1:A:132:ARG:NH1	2.10	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:VAL:HG12	1:C:336:VAL:O	1.95	0.66
1:A:254:LEU:HD12	1:A:255:LEU:N	2.11	0.66
1:B:191:LEU:O	1:B:192:PRO:C	2.39	0.65
1:C:120:ARG:HB3	1:C:120:ARG:NH1	2.11	0.65
1:A:127:THR:HB	1:A:130:GLY:O	1.97	0.64
1:C:90:ALA:HB3	1:C:95:TYR:HB2	1.78	0.64
1:C:142:THR:HG22	1:C:144:ASP:H	1.61	0.64
1:A:20:GLU:OE2	1:A:149:HIS:ND1	2.31	0.64
1:C:109:ASN:HA	1:C:113:VAL:O	1.98	0.63
1:B:183:ARG:HB3	3:B:346:HOH:O	1.98	0.63
1:C:133:LYS:HD3	1:C:183:ARG:HH21	1.64	0.62
1:B:213:GLU:HG2	1:B:214:ARG:N	2.14	0.62
1:A:204:THR:O	1:A:207:PHE:HB3	2.01	0.61
1:B:47:ARG:HD3	1:B:71:SER:O	2.01	0.61
1:C:89:MSE:HE2	1:C:90:ALA:C	2.24	0.61
1:A:27:MSE:SE	1:A:33:VAL:HG21	2.51	0.61
1:C:2:THR:CG2	1:C:213:GLU:OE1	2.49	0.60
1:C:169:LYS:H	1:C:169:LYS:HD3	1.66	0.60
1:B:312:GLU:O	1:B:315:LEU:HB2	2.00	0.60
1:B:32:ARG:NH2	1:B:94:GLU:OE2	2.24	0.60
1:A:73:GLY:HA3	1:A:287:PRO:HD3	1.83	0.60
1:B:337:ARG:HG3	1:B:337:ARG:NH1	2.17	0.60
1:A:282:THR:CG2	1:A:290:LEU:HD12	2.25	0.59
1:B:68:ALA:HA	1:B:244:ASN:ND2	2.16	0.59
1:B:223:ASN:C	1:B:223:ASN:HD22	2.10	0.59
1:A:92:LYS:HB2	1:A:92:LYS:HZ3	1.64	0.59
1:C:132:ARG:HH21	1:C:181:ARG:HH22	1.50	0.59
1:C:169:LYS:HD3	1:C:169:LYS:N	2.18	0.59
1:A:86:PHE:CD1	1:A:88:PHE:HE1	2.20	0.58
1:C:3:LEU:HD12	1:C:32:ARG:HB2	1.85	0.58
1:C:45:ILE:HG12	1:C:67:LEU:HD11	1.85	0.58
1:B:190:LEU:O	1:B:191:LEU:HG	2.04	0.57
1:C:131:ASP:C	1:C:132:ARG:HD2	2.29	0.57
1:A:156:ALA:H	1:A:186:ASN:HD21	1.51	0.57
1:B:59:ARG:HG2	1:B:59:ARG:NH1	2.19	0.57
1:A:64:ASN:N	1:A:64:ASN:HD22	2.02	0.57
1:A:256:ASP:HA	1:A:264:VAL:O	2.06	0.56
1:C:253:HIS:HB2	1:C:268:PHE:O	2.05	0.56
1:A:134:VAL:C	1:A:153:LEU:HD12	2.31	0.56
1:B:216:GLU:OE1	1:B:216:GLU:HA	2.04	0.56
1:A:109:ASN:HA	1:A:113:VAL:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:LEU:HB3	1:A:306:MSE:HG3	1.87	0.55
1:C:142:THR:HG22	1:C:143:LYS:H	1.70	0.55
1:C:92:LYS:HE2	1:C:143:LYS:O	2.07	0.55
1:B:138:ALA:HB1	2:B:338:LPA:O2	2.06	0.55
1:B:83:ASN:ND2	1:B:151:THR:HG21	2.13	0.55
1:A:92:LYS:NZ	1:A:92:LYS:CB	2.64	0.54
1:B:290:LEU:N	1:B:290:LEU:HD12	2.23	0.54
1:A:28:PRO:C	1:A:30:THR:H	2.14	0.54
1:A:225:THR:HG22	1:A:226:PRO:O	2.08	0.54
1:C:264:VAL:HG21	1:C:290:LEU:HD21	1.89	0.54
1:C:216:GLU:HA	1:C:216:GLU:OE1	2.08	0.54
1:C:135:SER:HB2	1:C:152:LEU:HD23	1.89	0.54
1:B:124:VAL:HG12	1:B:133:LYS:HA	1.88	0.53
1:C:294:ALA:O	1:C:298:GLN:NE2	2.39	0.53
1:C:113:VAL:HG23	1:C:191:LEU:HD23	1.91	0.53
1:C:142:THR:CG2	1:C:143:LYS:N	2.70	0.53
1:C:168:ASP:HB3	1:C:171:LYS:HG3	1.89	0.53
1:B:9:ASP:HB2	1:B:219:ILE:HG22	1.91	0.53
1:B:90:ALA:HB3	1:B:95:TYR:CG	2.44	0.53
1:C:90:ALA:HB3	1:C:95:TYR:CG	2.43	0.53
1:A:50:ASN:C	1:A:50:ASN:OD1	2.51	0.53
1:A:132:ARG:NH1	1:A:185:THR:OG1	2.41	0.52
1:B:69:ARG:N	1:B:244:ASN:HD22	1.97	0.52
1:C:109:ASN:O	1:C:111:LEU:N	2.43	0.52
1:C:135:SER:HB2	1:C:152:LEU:CD2	2.40	0.52
1:B:34:LEU:HD13	1:B:88:PHE:CE1	2.44	0.52
1:B:73:GLY:HA3	1:B:287:PRO:HD3	1.92	0.51
1:B:133:LYS:HB3	1:B:184:VAL:HG22	1.93	0.51
1:A:99:ILE:O	1:A:103:ILE:HD12	2.10	0.51
1:A:142:THR:HG22	1:A:143:LYS:N	2.20	0.51
1:C:109:ASN:C	1:C:111:LEU:H	2.19	0.51
1:C:169:LYS:H	1:C:169:LYS:CD	2.23	0.51
1:C:204:THR:O	1:C:207:PHE:HB3	2.11	0.51
1:B:290:LEU:HD12	1:B:290:LEU:H	1.74	0.50
1:C:117:ALA:O	1:C:118:SER:C	2.52	0.50
1:A:122:ASP:OD1	1:A:122:ASP:N	2.39	0.50
1:A:220:ILE:HG21	1:A:226:PRO:HB3	1.93	0.50
1:C:5:LEU:HD23	1:C:217:ALA:HB2	1.93	0.50
1:C:143:LYS:H	1:C:143:LYS:HD3	1.76	0.50
1:A:290:LEU:CD2	1:A:328:LEU:HD11	2.42	0.50
1:B:60:MSE:HE3	1:B:65:VAL:HG12	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ASP:O	1:C:132:ARG:HD2	2.12	0.50
1:A:220:ILE:CG2	1:A:226:PRO:HB3	2.42	0.50
1:B:187:LEU:HB3	1:B:194:ILE:CD1	2.42	0.49
1:B:83:ASN:HB3	1:B:151:THR:HG23	1.94	0.49
1:C:126:LYS:HG3	1:C:130:GLY:O	2.11	0.49
1:A:156:ALA:H	1:A:186:ASN:ND2	2.10	0.49
1:C:120:ARG:HB3	1:C:120:ARG:HH11	1.74	0.49
1:A:195:THR:OG1	1:A:198:GLN:HB2	2.13	0.49
1:C:132:ARG:NH2	1:C:181:ARG:HH22	2.10	0.49
1:A:10:SER:HB2	1:A:222:PRO:HD3	1.93	0.49
1:A:142:THR:CG2	1:A:144:ASP:OD1	2.61	0.49
1:B:211:TYR:O	1:B:213:GLU:N	2.46	0.49
1:A:64:ASN:HB3	1:B:64:ASN:HB2	1.95	0.49
1:A:308:GLN:CD	1:A:333:ALA:HB2	2.38	0.48
1:C:195:THR:OG1	1:C:198:GLN:HG3	2.13	0.48
1:A:132:ARG:HH11	1:A:132:ARG:CB	2.20	0.48
1:A:96:ASP:C	1:A:96:ASP:OD1	2.56	0.48
1:C:90:ALA:HB3	1:C:95:TYR:CB	2.41	0.48
1:A:183:ARG:CZ	1:A:183:ARG:HB3	2.43	0.48
1:B:22:CYS:HA	1:B:26:GLN:HG2	1.95	0.48
1:B:108:LEU:O	1:B:109:ASN:C	2.57	0.48
1:C:24:PHE:HD1	1:C:147:PHE:CD1	2.31	0.48
1:A:142:THR:HG21	1:A:144:ASP:OD1	2.14	0.48
1:A:259:PHE:O	1:A:260:THR:C	2.56	0.48
1:A:311:CYS:HB2	1:A:332:MSE:HE1	1.95	0.48
1:C:142:THR:CG2	1:C:143:LYS:H	2.26	0.48
1:C:132:ARG:HH21	1:C:181:ARG:NH2	2.12	0.47
1:A:44:VAL:HA	1:A:68:ALA:O	2.13	0.47
1:A:274:HIS:NE2	1:C:242:GLU:OE2	2.43	0.47
1:B:50:ASN:HB2	1:B:281:PHE:CD1	2.48	0.47
1:C:188:THR:O	1:C:192:PRO:HA	2.13	0.47
1:A:86:PHE:O	1:A:149:HIS:HA	2.14	0.47
1:A:282:THR:HG21	1:A:290:LEU:CD1	2.27	0.47
1:A:86:PHE:CD1	1:A:88:PHE:CE1	3.02	0.47
1:B:211:TYR:C	1:B:213:GLU:H	2.22	0.47
1:A:194:ILE:HA	1:A:198:GLN:OE1	2.15	0.47
1:A:277:ARG:HB3	1:C:277:ARG:HB3	1.97	0.47
1:C:67:LEU:HD12	1:C:68:ALA:N	2.29	0.47
1:C:114:SER:O	1:C:125:VAL:HG12	2.15	0.47
1:C:235:PHE:O	1:C:236:ALA:C	2.58	0.47
1:C:86:PHE:O	1:C:149:HIS:HA	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:ASN:N	1:C:166:ASN:ND2	2.61	0.46
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.63	0.46
1:B:314:LEU:O	1:B:315:LEU:C	2.58	0.46
1:A:92:LYS:HG2	1:A:93:PRO:HA	1.98	0.46
1:C:126:LYS:HA	1:C:130:GLY:HA2	1.98	0.46
1:A:92:LYS:NZ	1:A:143:LYS:O	2.47	0.46
1:A:67:LEU:HG	1:A:68:ALA:N	2.31	0.46
1:B:194:ILE:H	1:B:194:ILE:HG12	1.57	0.46
1:B:132:ARG:HB3	1:B:185:THR:HB	1.98	0.46
1:A:1:SER:OG	1:A:213:GLU:OE2	2.31	0.45
1:C:166:ASN:N	1:C:166:ASN:HD22	2.14	0.45
1:B:332:MSE:O	1:B:333:ALA:C	2.59	0.45
1:C:330:ALA:O	1:C:333:ALA:HB3	2.16	0.45
1:A:183:ARG:HG2	1:A:183:ARG:O	2.17	0.45
1:B:6:LEU:O	1:B:35:PHE:HA	2.16	0.45
1:C:190:LEU:H	1:C:190:LEU:HG	1.27	0.45
1:B:59:ARG:CG	1:B:59:ARG:NH1	2.74	0.45
1:A:336:VAL:HG12	1:A:337:ARG:N	2.30	0.45
1:C:267:HIS:O	1:C:278:ALA:HA	2.17	0.45
1:C:84:THR:HG23	1:C:196:HIS:CE1	2.52	0.45
1:C:170:LYS:HE3	1:C:256:ASP:OD1	2.17	0.45
1:C:264:VAL:CG2	1:C:290:LEU:CD2	2.95	0.45
1:C:233:GLU:OE1	1:C:237:ARG:NE	2.43	0.44
1:B:19:VAL:O	1:B:20:GLU:C	2.60	0.44
1:C:95:TYR:HD2	1:C:146:GLY:HA3	1.82	0.44
1:C:311:CYS:CB	1:C:332:MSE:HE1	2.47	0.44
1:C:264:VAL:HG22	1:C:290:LEU:CD2	2.48	0.44
1:A:59:ARG:HG2	1:A:164:TYR:CE1	2.53	0.44
1:C:160:ARG:O	1:C:161:LEU:C	2.61	0.44
1:C:264:VAL:HG22	1:C:290:LEU:HD22	1.98	0.44
1:A:27:MSE:HE2	1:A:27:MSE:HB3	1.60	0.44
1:C:90:ALA:CB	1:C:95:TYR:HB2	2.46	0.44
1:A:12:ASP:C	1:A:12:ASP:OD1	2.61	0.44
1:B:38:ARG:NH1	1:B:81:LEU:O	2.47	0.44
1:A:292:ALA:HB2	1:C:292:ALA:HB2	2.00	0.43
1:B:47:ARG:NH2	1:B:287:PRO:HG2	2.33	0.43
1:C:154:LEU:HD13	1:C:194:ILE:HG22	1.99	0.43
1:C:186:ASN:HB3	1:C:187:LEU:H	1.52	0.43
1:A:260:THR:HG23	3:A:341:HOH:O	2.17	0.43
1:C:47:ARG:HA	1:C:69:ARG:HD3	2.00	0.43
1:C:134:VAL:O	1:C:153:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:208:PHE:CE2	1:A:214:ARG:HB3	2.54	0.43
1:A:251:PHE:CD1	1:A:251:PHE:N	2.87	0.43
1:A:287:PRO:O	1:A:288:ALA:C	2.61	0.43
1:C:109:ASN:C	1:C:111:LEU:N	2.77	0.43
1:B:213:GLU:CG	1:B:214:ARG:N	2.80	0.43
1:B:223:ASN:C	1:B:223:ASN:ND2	2.77	0.43
1:C:297:LEU:HD23	1:C:297:LEU:HA	1.86	0.43
1:C:332:MSE:O	1:C:333:ALA:C	2.62	0.43
1:A:223:ASN:HB3	1:B:52:TRP:CH2	2.53	0.42
1:C:35:PHE:HB3	1:C:87:THR:HB	2.00	0.42
1:C:259:PHE:O	1:C:260:THR:C	2.60	0.42
1:A:74:GLY:HA2	1:A:283:ASP:O	2.19	0.42
1:B:102:SER:HA	1:B:105:LEU:HB2	2.01	0.42
1:A:223:ASN:HB3	1:B:52:TRP:CZ3	2.55	0.42
1:B:315:LEU:HD22	1:B:325:LEU:HD12	2.01	0.42
1:A:30:THR:HG22	1:A:31:GLN:HG2	2.02	0.42
1:C:105:LEU:O	1:C:108:LEU:HB2	2.19	0.42
1:A:6:LEU:O	1:A:35:PHE:HA	2.19	0.42
1:C:127:THR:N	1:C:130:GLY:HA2	2.30	0.42
1:C:169:LYS:N	1:C:169:LYS:CD	2.81	0.42
1:B:12:ASP:OD1	1:B:12:ASP:C	2.62	0.42
1:A:9:ASP:HB2	1:A:219:ILE:CG2	2.50	0.42
1:C:143:LYS:HE3	1:C:143:LYS:HB2	1.86	0.42
1:C:132:ARG:HG3	1:C:185:THR:OG1	2.20	0.42
1:A:142:THR:HG22	1:A:145:ARG:H	1.84	0.42
1:A:308:GLN:NE2	1:A:333:ALA:HB2	2.35	0.42
1:B:168:ASP:O	1:B:172:LEU:HG	2.19	0.42
1:C:66:ARG:HA	1:C:66:ARG:HD3	1.44	0.42
1:A:291:GLU:OE2	1:C:296:ARG:HD2	2.20	0.41
1:A:296:ARG:HD2	1:C:291:GLU:OE2	2.20	0.41
1:A:268:PHE:N	1:A:268:PHE:CD1	2.88	0.41
1:A:326:ARG:HH12	1:C:25:ARG:HB2	1.85	0.41
1:B:90:ALA:HB3	1:B:95:TYR:CD2	2.54	0.41
1:A:92:LYS:CG	1:A:93:PRO:HA	2.50	0.41
1:A:285:LEU:HD23	1:A:285:LEU:HA	1.91	0.41
1:A:332:MSE:O	1:A:333:ALA:C	2.64	0.41
1:B:308:GLN:O	1:B:309:GLN:C	2.63	0.41
1:C:73:GLY:HA3	1:C:287:PRO:HD3	2.03	0.41
1:C:81:LEU:C	1:C:83:ASN:H	2.28	0.41
1:B:13:PRO:HA	1:B:39:ASN:OD1	2.20	0.41
1:C:257:GLU:HB2	1:C:331:TRP:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:GLU:OE1	1:B:310:GLU:HA	2.21	0.41
1:C:42:THR:HA	1:C:66:ARG:O	2.20	0.41
1:A:45:ILE:HG13	1:A:69:ARG:HA	2.01	0.41
1:A:312:GLU:OE2	1:A:329:SER:OG	2.30	0.41
1:B:263:GLY:O	1:B:282:THR:HA	2.21	0.41
1:C:14:TRP:CH2	1:C:66:ARG:HD2	2.55	0.41
1:A:13:PRO:HB3	1:A:39:ASN:HB3	2.02	0.41
1:B:315:LEU:HD22	1:B:315:LEU:HA	1.87	0.41
1:C:2:THR:HG23	1:C:3:LEU:HD13	2.03	0.41
1:C:92:LYS:HA	1:C:93:PRO:C	2.45	0.41
1:A:254:LEU:O	1:A:255:LEU:HD23	2.21	0.41
1:A:323:LYS:O	1:A:324:GLU:C	2.63	0.40
1:C:166:ASN:O	1:C:167:PRO:C	2.64	0.40
1:A:134:VAL:O	1:A:153:LEU:HD12	2.21	0.40
1:A:303:ARG:O	1:A:304:ALA:C	2.63	0.40
1:B:297:LEU:HD23	1:B:297:LEU:HA	1.92	0.40
1:C:142:THR:HG21	1:C:144:ASP:OD1	2.21	0.40
1:A:280:VAL:HG11	1:A:290:LEU:HB3	2.02	0.40
1:A:296:ARG:NH1	1:C:291:GLU:OE2	2.51	0.40
1:B:14:TRP:CH2	1:B:66:ARG:HB3	2.56	0.40
1:A:64:ASN:N	1:A:64:ASN:ND2	2.69	0.40
1:A:318:PHE:C	3:A:339:HOH:O	2.64	0.40
1:C:99:ILE:O	1:C:103:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	326/337 (97%)	301 (92%)	20 (6%)	5 (2%)	8 27
1	B	326/337 (97%)	305 (94%)	16 (5%)	5 (2%)	8 27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	335/337 (99%)	297 (89%)	31 (9%)	7 (2%)	5	20
All	All	987/1011 (98%)	903 (92%)	67 (7%)	17 (2%)	7	24

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	188	THR
1	B	81	LEU
1	B	212	GLY
1	B	246	GLY
1	C	94	GLU
1	C	157	ASP
1	C	186	ASN
1	C	187	LEU
1	B	29	ALA
1	C	110	ALA
1	C	183	ARG
1	A	29	ALA
1	A	167	PRO
1	A	260	THR
1	C	189	GLU
1	A	173	ALA
1	B	192	PRO

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	276/277 (100%)	235 (85%)	41 (15%)	3	9
1	B	276/277 (100%)	239 (87%)	37 (13%)	4	12
1	C	282/277 (102%)	243 (86%)	39 (14%)	3	11
All	All	834/831 (100%)	717 (86%)	117 (14%)	3	11

All (117) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	THR
1	A	17	LEU
1	A	30	THR
1	A	31	GLN
1	A	32	ARG
1	A	55	CYS
1	A	64	ASN
1	A	66	ARG
1	A	92	LYS
1	A	99	ILE
1	A	103	ILE
1	A	122	ASP
1	A	124	VAL
1	A	127	THR
1	A	132	ARG
1	A	133	LYS
1	A	140	ARG
1	A	142	THR
1	A	158	LEU
1	A	163	ASN
1	A	184	VAL
1	A	188	THR
1	A	190	LEU
1	A	201	GLU
1	A	215	VAL
1	A	220	ILE
1	A	224	LYS
1	A	227	ASP
1	A	247	GLN
1	A	254	LEU
1	A	265	GLU
1	A	280	VAL
1	A	284	SER
1	A	297	LEU
1	A	315	LEU
1	A	316	VAL
1	A	320	GLU
1	A	322	GLU
1	A	326	ARG
1	A	336	VAL
1	A	337	ARG
1	B	4	ARG
1	B	17	LEU

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Mol	Chain	Res	Type
1	B	59	ARG
1	B	64	ASN
1	B	99	ILE
1	B	103	ILE
1	B	114	SER
1	B	116	GLU
1	B	120	ARG
1	B	128	VAL
1	B	133	LYS
1	B	143	LYS
1	B	144	ASP
1	B	154	LEU
1	B	158	LEU
1	B	169	LYS
1	B	172	LEU
1	B	183	ARG
1	B	184	VAL
1	B	185	THR
1	B	191	LEU
1	B	194	ILE
1	B	195	THR
1	B	198	GLN
1	B	201	GLU
1	B	214	ARG
1	B	219	ILE
1	B	223	ASN
1	B	224	LYS
1	B	265	GLU
1	B	315	LEU
1	B	316	VAL
1	B	320	GLU
1	B	322	GLU
1	B	323	LYS
1	B	336	VAL
1	B	337	ARG
1	C	3	LEU
1	C	17	LEU
1	C	25	ARG
1	C	54	GLU
1	C	66	ARG
1	C	92	LYS
1	C	99	ILE

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Mol	Chain	Res	Type
1	C	114	SER
1	C	121	ASN
1	C	124	VAL
1	C	126	LYS
1	C	128	VAL
1	C	129	GLU
1	C	132	ARG
1	C	141	GLU
1	C	143	LYS
1	C	151	THR
1	C	154	LEU
1	C	163	ASN
1	C	169	LYS
1	C	172	LEU
1	C	180	VAL
1	C	184	VAL
1	C	189	GLU
1	C	190	LEU
1	C	191	LEU
1	C	194	ILE
1	C	205	GLU
1	C	220	ILE
1	C	265	GLU
1	C	272	LYS
1	C	290	LEU
1	C	307	LEU
1	C	316	VAL
1	C	320	GLU
1	C	322	GLU
1	C	326	ARG
1	C	327	GLU
1	C	337	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	ASN
1	A	155	ASN
1	A	166	ASN
1	A	186	ASN
1	A	230	ASN
1	A	238	GLN

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Mol	Chain	Res	Type
1	A	267	HIS
1	A	279	GLN
1	B	64	ASN
1	B	83	ASN
1	B	210	HIS
1	B	244	ASN
1	B	247	GLN
1	B	298	GLN
1	C	50	ASN
1	C	64	ASN
1	C	166	ASN
1	C	198	GLN
1	C	247	GLN
1	C	253	HIS

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](#)

2 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	LPA	B	338	-	12,12,12	0.93	0	14,14,14	1.78	4 (28%)
2	LPA	A	338	-	12,12,12	0.76	0	14,14,14	1.44	1 (7%)

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	LPA	B	338	-	-	5/7/14/14	0/1/1/1
2	LPA	A	338	-	-	1/7/14/14	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	338	LPA	C3-C2-C1	-4.38	103.07	114.51
2	A	338	LPA	C6-S6-S8	3.38	106.28	95.19
2	B	338	LPA	O2-C1-C2	-2.31	115.77	123.09
2	B	338	LPA	C4-C3-C2	-2.24	104.90	113.13
2	B	338	LPA	O1-C1-C2	2.21	120.98	114.00

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	338	LPA	C3-C4-C5-C6
2	B	338	LPA	C1-C2-C3-C4
2	B	338	LPA	C3-C4-C5-C6
2	B	338	LPA	C2-C3-C4-C5
2	B	338	LPA	O2-C1-C2-C3
2	B	338	LPA	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	338	LPA	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	325/337 (96%)	-0.42	2 (0%) 85 81	16, 34, 53, 80	0
1	B	325/337 (96%)	-0.39	1 (0%) 90 87	19, 33, 63, 83	0
1	C	332/337 (98%)	-0.20	2 (0%) 85 81	23, 41, 73, 79	0
All	All	982/1011 (97%)	-0.34	5 (0%) 87 83	16, 35, 67, 83	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	128	VAL	2.5
1	A	175	LYS	2.2
1	C	194	ILE	2.1
1	A	158	LEU	2.0
1	C	193	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($\text{\AA}^2$)	Q<0.9
2	LPA	A	338	12/12	0.88	0.22	74,78,82,84	0
2	LPA	B	338	12/12	0.93	0.15	74,76,79,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.