



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:22 AM UTC

PDB ID : 3TAD / pdb_00003tad
Title : Crystal Structure of the Liprin-alpha/Liprin-beta complex
Authors : Wei, Z.; Zheng, S.; Yu, C.; Zhang, M.
Deposited on : 2011-08-04
Resolution : 2.90 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

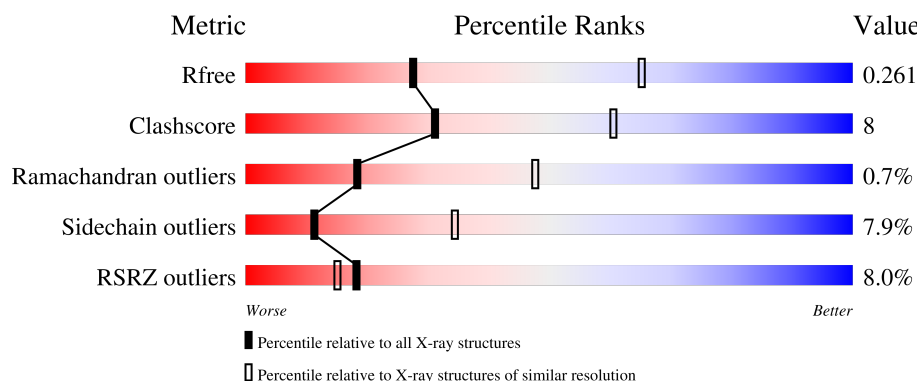
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	297	9% 69% 18% • 11%
1	B	297	9% 69% 17% • 12%
2	C	265	8% 74% 18% • 5%
2	D	265	3% 74% 19% • 5%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 8163 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 Liprin-alpha-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2087	1324	369	383	11			
1	B	261	Total	C	N	O	S	0	0	0
			2049	1301	363	374	11			

There are 86 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	860	GLY	-	expression tag	UNP O75334
A	861	PRO	-	expression tag	UNP O75334
A	862	GLY	-	expression tag	UNP O75334
A	863	SER	-	expression tag	UNP O75334
A	864	GLU	-	expression tag	UNP O75334
A	865	PHE	-	expression tag	UNP O75334
A	?	-	PRO	deletion	UNP O75334
A	?	-	SER	deletion	UNP O75334
A	?	-	GLY	deletion	UNP O75334
A	?	-	ASN	deletion	UNP O75334
A	?	-	VAL	deletion	UNP O75334
A	?	-	TRP	deletion	UNP O75334
A	?	-	VAL	deletion	UNP O75334
A	?	-	THR	deletion	UNP O75334
A	?	-	HIS	deletion	UNP O75334
A	?	-	GLU	deletion	UNP O75334
A	?	-	GLU	deletion	UNP O75334
A	?	-	MET	deletion	UNP O75334
A	?	-	GLU	deletion	UNP O75334
A	?	-	ASN	deletion	UNP O75334
A	?	-	LEU	deletion	UNP O75334
A	?	-	ALA	deletion	UNP O75334
A	?	-	ALA	deletion	UNP O75334
A	?	-	PRO	deletion	UNP O75334
A	?	-	ALA	deletion	UNP O75334

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP O75334
A	?	-	THR	deletion	UNP O75334
A	?	-	LYS	deletion	UNP O75334
A	?	-	GLU	deletion	UNP O75334
A	?	-	SER	deletion	UNP O75334
A	?	-	GLU	deletion	UNP O75334
A	?	-	GLU	deletion	UNP O75334
A	?	-	GLY	deletion	UNP O75334
A	?	-	SER	deletion	UNP O75334
A	?	-	TRP	deletion	UNP O75334
A	?	-	ALA	deletion	UNP O75334
A	?	-	GLN	deletion	UNP O75334
A	?	-	CYS	deletion	UNP O75334
A	?	-	PRO	deletion	UNP O75334
A	?	-	VAL	deletion	UNP O75334
A	?	-	PHE	deletion	UNP O75334
A	?	-	LEU	deletion	UNP O75334
A	?	-	GLN	deletion	UNP O75334
B	860	GLY	-	expression tag	UNP O75334
B	861	PRO	-	expression tag	UNP O75334
B	862	GLY	-	expression tag	UNP O75334
B	863	SER	-	expression tag	UNP O75334
B	864	GLU	-	expression tag	UNP O75334
B	865	PHE	-	expression tag	UNP O75334
B	?	-	PRO	deletion	UNP O75334
B	?	-	SER	deletion	UNP O75334
B	?	-	GLY	deletion	UNP O75334
B	?	-	ASN	deletion	UNP O75334
B	?	-	VAL	deletion	UNP O75334
B	?	-	TRP	deletion	UNP O75334
B	?	-	VAL	deletion	UNP O75334
B	?	-	THR	deletion	UNP O75334
B	?	-	HIS	deletion	UNP O75334
B	?	-	GLU	deletion	UNP O75334
B	?	-	GLU	deletion	UNP O75334
B	?	-	MET	deletion	UNP O75334
B	?	-	GLU	deletion	UNP O75334
B	?	-	ASN	deletion	UNP O75334
B	?	-	LEU	deletion	UNP O75334
B	?	-	ALA	deletion	UNP O75334
B	?	-	ALA	deletion	UNP O75334
B	?	-	PRO	deletion	UNP O75334

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Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ALA	deletion	UNP O75334
B	?	-	LYS	deletion	UNP O75334
B	?	-	THR	deletion	UNP O75334
B	?	-	LYS	deletion	UNP O75334
B	?	-	GLU	deletion	UNP O75334
B	?	-	SER	deletion	UNP O75334
B	?	-	GLU	deletion	UNP O75334
B	?	-	GLU	deletion	UNP O75334
B	?	-	GLY	deletion	UNP O75334
B	?	-	SER	deletion	UNP O75334
B	?	-	TRP	deletion	UNP O75334
B	?	-	ALA	deletion	UNP O75334
B	?	-	GLN	deletion	UNP O75334
B	?	-	CYS	deletion	UNP O75334
B	?	-	PRO	deletion	UNP O75334
B	?	-	VAL	deletion	UNP O75334
B	?	-	PHE	deletion	UNP O75334
B	?	-	LEU	deletion	UNP O75334
B	?	-	GLN	deletion	UNP O75334

- Molecule 2 is a protein called Liprin-beta-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	252	Total	C	N	O	S	0	1	0
			1968	1244	354	362	8			
2	D	253	Total	C	N	O	S	0	0	0
			2016	1278	361	369	8			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	589	GLY	-	expression tag	UNP Q8C8U0
C	590	PRO	-	expression tag	UNP Q8C8U0
C	591	GLY	-	expression tag	UNP Q8C8U0
C	592	SER	-	expression tag	UNP Q8C8U0
D	589	GLY	-	expression tag	UNP Q8C8U0
D	590	PRO	-	expression tag	UNP Q8C8U0
D	591	GLY	-	expression tag	UNP Q8C8U0
D	592	SER	-	expression tag	UNP Q8C8U0

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		

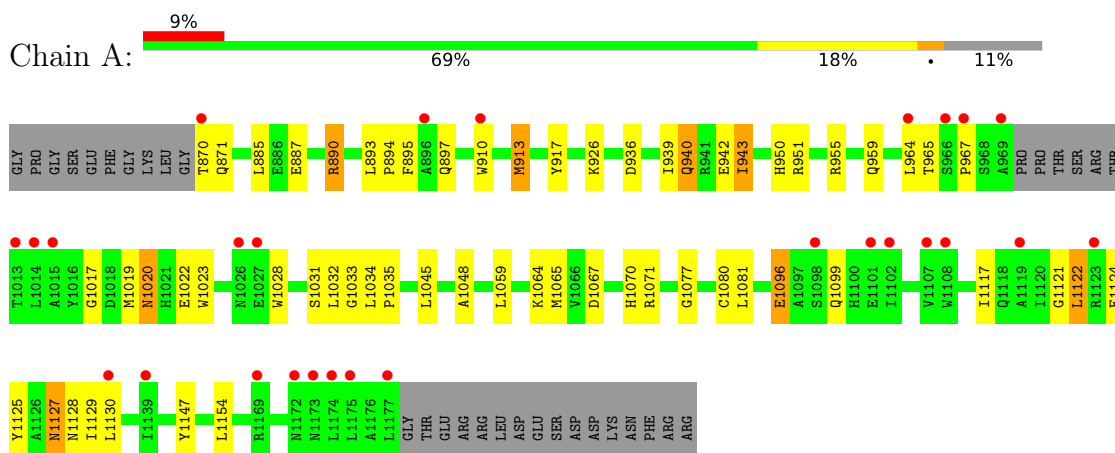
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		
4	C	4	Total	O	0	0
			4	4		
4	D	6	Total	O	0	0
			6	6		

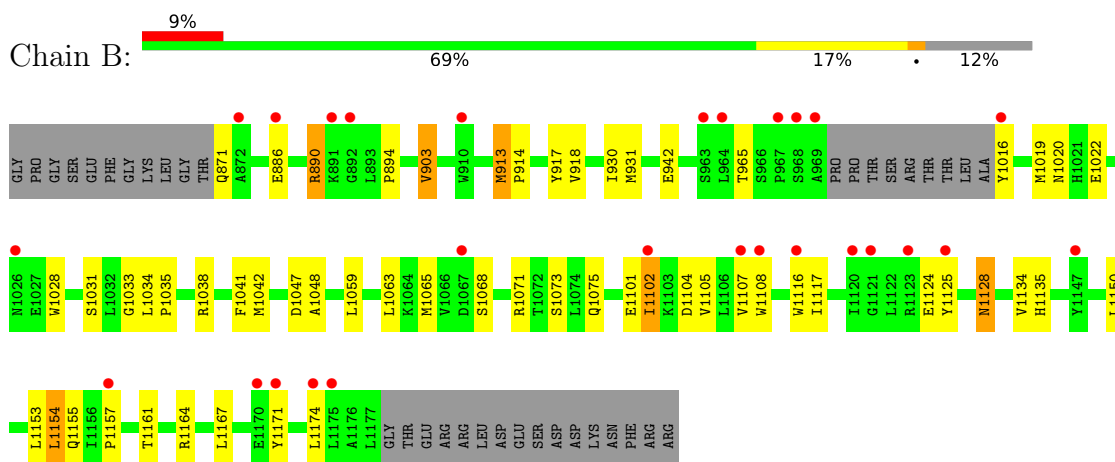
3 Residue-property plots [i](#)

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.

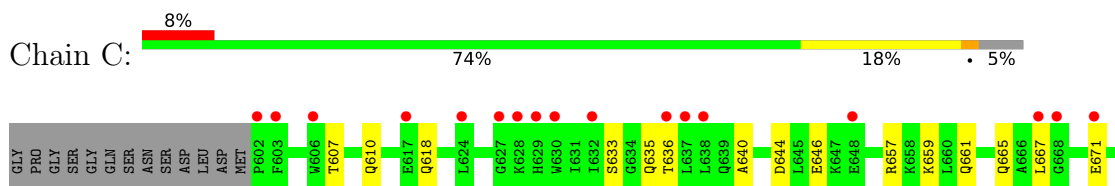
• Molecule 1: Liprin-alpha-2

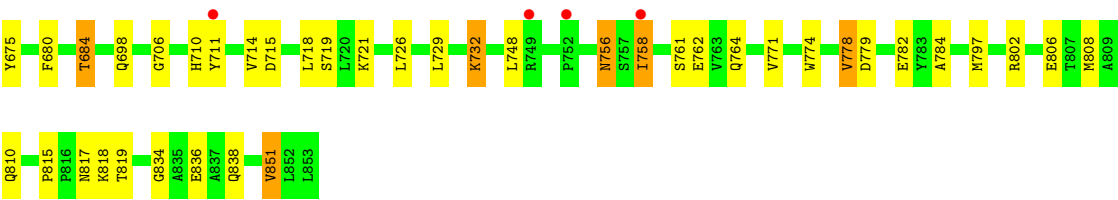


• Molecule 1: Liprin-alpha-2

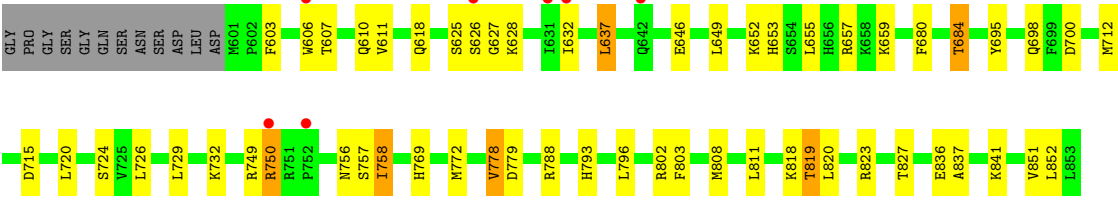


• Molecule 2: Liprin-beta-1





● Molecule 2: Liprin-beta-1



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	141.88Å 141.88Å 181.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	44.98 – 2.90 44.98 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.98-2.90) 98.5 (44.98-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.90 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.214 , 0.258 0.227 , 0.261	Depositor DCC
R_{free} test set	2263 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 68.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	8163	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% 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: GOL

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	0.50	0/2130	0.90	1/2893 (0.0%)
1	B	0.51	0/2091	0.86	0/2841
2	C	0.64	0/2012	1.00	2/2731 (0.1%)
2	D	0.66	0/2062	0.94	0/2798
All	All	0.58	0/8295	0.93	3/11263 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	784	ALA	CA-C-N	-8.50	111.03	119.87
2	C	784	ALA	C-N-CA	-8.50	111.03	119.87
1	A	893	LEU	N-CA-C	5.05	115.40	109.60

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	2087	0	2024	36	0
1	B	2049	0	1989	41	0
2	C	1968	0	1924	31	0
2	D	2016	0	1978	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	6	0	8	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	12	0	16	0	0
4	A	1	0	0	0	0
4	B	2	0	0	0	0
4	C	4	0	0	0	0
4	D	6	0	0	0	0
All	All	8163	0	7955	132	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 8.

All (132) 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:1128:ASN:HD22	1:B:1128:ASN:H	0.99	0.97
1:B:1105:VAL:HA	1:B:1108:TRP:CD1	2.07	0.90
1:B:1128:ASN:H	1:B:1128:ASN:ND2	1.69	0.88
2:D:603:PHE:HA	2:D:606:TRP:HD1	1.40	0.87
2:D:603:PHE:HA	2:D:606:TRP:CD1	2.10	0.86
2:D:803:PHE:CE2	2:D:808:MET:HE2	2.17	0.80
1:B:1104:ASP:O	1:B:1108:TRP:NE1	2.17	0.77
1:A:1125:TYR:O	1:A:1128:ASN:ND2	2.15	0.77
1:A:942:GLU:OE2	2:C:819:THR:HB	1.85	0.76
1:B:1128:ASN:HD22	1:B:1128:ASN:N	1.82	0.73
1:A:1121:GLY:C	1:A:1122:LEU:HD23	2.14	0.72
2:C:797:MET:HE3	2:C:808:MET:HE3	1.71	0.72
2:D:803:PHE:HE2	2:D:808:MET:HE2	1.55	0.71
2:C:797:MET:HE3	2:C:808:MET:CE	2.21	0.71
2:D:646:GLU:HG2	2:D:657:ARG:HG2	1.73	0.71
1:B:1128:ASN:ND2	1:B:1128:ASN:N	2.39	0.69
2:D:606:TRP:HE3	2:D:610:GLN:HB3	1.56	0.68
1:B:1065:MET:HE3	1:B:1071:ARG:HG2	1.74	0.67
2:C:815:PRO:HG2	2:C:818:LYS:HG3	1.77	0.67
1:B:942:GLU:OE2	2:D:819:THR:HB	1.94	0.67
2:D:627:GLY:HA3	2:D:649:LEU:HD23	1.77	0.65
2:D:769:HIS:HA	2:D:772:MET:HE3	1.81	0.63
2:D:695:TYR:HA	2:D:698:GLN:OE1	2.01	0.61
1:B:1101:GLU:O	1:B:1102:ILE:HB	1.99	0.61
1:B:1157:PRO:C	1:B:1164:ARG:HH21	2.07	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:606:TRP:CE3	2:D:610:GLN:HB3	2.35	0.61
2:C:714:VAL:O	2:C:718:LEU:HG	2.01	0.60
1:A:950:HIS:CD2	1:A:1045:LEU:HD12	2.36	0.60
1:B:913:MET:HE3	1:B:917:TYR:CE1	2.37	0.60
1:A:1019:MET:HE3	1:A:1023:TRP:CZ3	2.39	0.58
2:C:817:ASN:HA	2:D:652:LYS:HD3	1.85	0.57
1:A:1065:MET:HE3	1:A:1071:ARG:HG2	1.85	0.57
2:D:680:PHE:O	2:D:684:THR:HG22	2.04	0.57
2:D:653:HIS:HE1	2:D:655:LEU:HD12	1.71	0.56
2:D:750:ARG:HG3	2:D:750:ARG:HH11	1.71	0.56
1:A:1117:ILE:HD13	1:A:1154:LEU:HD21	1.88	0.56
1:A:1127:ASN:O	1:A:1130:LEU:HG	2.05	0.56
1:A:940:GLN:HG3	1:A:951:ARG:NH1	2.21	0.55
2:D:803:PHE:CZ	2:D:808:MET:HE2	2.41	0.55
1:B:1028:TRP:O	1:B:1031:SER:HB3	2.06	0.55
2:C:618:GLN:O	2:C:659:LYS:HE2	2.06	0.55
1:B:1153:LEU:C	1:B:1155:GLN:H	2.14	0.55
1:B:1059:LEU:HD23	1:B:1063:LEU:HD12	1.88	0.55
1:B:930:ILE:CD1	2:D:823:ARG:HG2	2.38	0.54
2:C:756:ASN:HD22	2:C:762:GLU:HG3	1.73	0.53
1:B:1041:PHE:CE1	1:B:1063:LEU:HD13	2.44	0.53
2:C:675:TYR:O	2:C:706:GLY:HA3	2.09	0.53
1:A:1019:MET:HE1	1:A:1081:LEU:HD13	1.90	0.52
2:C:698:GLN:H	2:C:698:GLN:NE2	2.08	0.52
2:D:778:VAL:CG1	2:D:778:VAL:O	2.59	0.51
1:A:890:ARG:O	1:A:890:ARG:HG2	2.09	0.51
2:C:607:THR:HG23	2:C:610:GLN:H	1.75	0.51
1:A:1028:TRP:HE1	1:A:1081:LEU:HD21	1.77	0.50
1:B:1059:LEU:HD22	1:B:1065:MET:HE2	1.93	0.50
1:A:1067:ASP:HB3	1:A:1070:HIS:ND1	2.27	0.50
1:B:1125:TYR:O	1:B:1128:ASN:ND2	2.44	0.50
2:D:611:VAL:HG11	2:D:637:LEU:HD11	1.93	0.49
1:A:1096:GLU:HA	1:A:1099:GLN:HG2	1.96	0.48
1:A:1124:GLU:HG3	1:A:1125:TYR:N	2.27	0.48
2:C:761:SER:O	2:C:764:GLN:HB2	2.13	0.48
1:B:1153:LEU:C	1:B:1155:GLN:N	2.70	0.48
1:B:1105:VAL:HG12	1:B:1108:TRP:CE2	2.49	0.47
1:B:903:VAL:HG11	1:B:931:MET:HE2	1.96	0.47
1:B:1034:LEU:N	1:B:1035:PRO:HD3	2.29	0.47
2:D:684:THR:HG21	2:D:700:ASP:OD2	2.14	0.47
1:A:1059:LEU:HD22	1:A:1065:MET:HE2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:894:PRO:HA	1:B:965:THR:HB	1.95	0.47
1:B:1102:ILE:CG2	1:B:1102:ILE:O	2.63	0.47
1:B:1117:ILE:HD13	1:B:1154:LEU:HD21	1.96	0.47
1:B:1041:PHE:CZ	1:B:1063:LEU:HD13	2.51	0.46
2:C:732:LYS:HD2	2:D:852:LEU:HD13	1.97	0.46
2:C:633:SER:HB3	2:C:636:THR:HG23	1.97	0.46
1:A:887:GLU:OE2	1:A:890:ARG:NH1	2.48	0.46
2:C:778:VAL:HG13	2:C:778:VAL:O	2.16	0.46
2:C:758:ILE:O	2:C:758:ILE:HG22	2.15	0.46
2:C:680:PHE:O	2:C:684:THR:HG22	2.16	0.46
1:A:1028:TRP:CZ2	1:A:1032:LEU:HD11	2.52	0.45
2:D:680:PHE:O	2:D:684:THR:CG2	2.64	0.45
2:C:646:GLU:HG2	2:C:657:ARG:HG2	1.98	0.45
2:C:710:HIS:HD2	2:C:711:TYR:CE2	2.33	0.45
2:C:815:PRO:HG2	2:C:818:LYS:CG	2.43	0.45
1:A:1019:MET:HE2	1:A:1048:ALA:HB2	1.98	0.45
2:C:640:ALA:HB1	2:C:644:ASP:HB2	1.99	0.45
2:D:618:GLN:O	2:D:659:LYS:HE2	2.17	0.45
1:A:936:ASP:OD1	1:A:955:ARG:NH1	2.49	0.45
1:B:1033:GLY:C	1:B:1035:PRO:HD3	2.42	0.45
1:A:939:ILE:HA	1:A:943:ILE:HG13	1.99	0.44
2:C:851:VAL:O	2:D:732:LYS:HD2	2.16	0.44
1:B:1108:TRP:HZ3	1:B:1116:TRP:HB2	1.83	0.44
1:A:870:THR:OG1	1:A:871:GLN:N	2.51	0.44
2:C:719:SER:C	2:C:721:LYS:H	2.25	0.44
2:D:749:ARG:O	2:D:750:ARG:C	2.58	0.44
1:B:1038:ARG:NH2	1:B:1042:MET:HE1	2.32	0.44
1:A:1064:LYS:HE3	1:A:1064:LYS:HB3	1.85	0.43
1:B:1020:ASN:HD22	1:B:1020:ASN:HA	1.66	0.43
2:D:750:ARG:HH11	2:D:750:ARG:CG	2.31	0.43
2:C:756:ASN:ND2	2:C:762:GLU:HG3	2.33	0.43
1:A:926:LYS:HD2	2:C:779:ASP:HB3	2.00	0.43
1:A:1096:GLU:HA	1:A:1099:GLN:HE21	1.82	0.43
1:A:894:PRO:HA	1:A:965:THR:HB	1.99	0.43
2:D:837:ALA:O	2:D:841:LYS:HG3	2.19	0.43
1:B:1105:VAL:C	1:B:1107:VAL:N	2.76	0.43
1:B:914:PRO:O	1:B:918:VAL:HG23	2.19	0.43
1:B:1153:LEU:O	1:B:1155:GLN:N	2.52	0.42
1:B:1073:SER:O	1:B:1135:HIS:HE1	2.01	0.42
1:A:1020:ASN:HD22	1:A:1020:ASN:HA	1.63	0.42
1:B:1047:ASP:OD2	1:B:1047:ASP:C	2.62	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1033:GLY:C	1:A:1035:PRO:HD3	2.45	0.42
2:C:797:MET:SD	2:C:808:MET:HE1	2.60	0.42
2:D:758:ILE:HD12	2:D:758:ILE:N	2.35	0.42
2:D:655:LEU:HD11	2:D:720:LEU:HG	2.01	0.42
1:B:1171:TYR:O	1:B:1174:LEU:HB3	2.19	0.41
2:C:778:VAL:O	2:C:778:VAL:CG1	2.67	0.41
1:B:1105:VAL:C	1:B:1107:VAL:H	2.28	0.41
2:C:756:ASN:O	2:C:762:GLU:HG3	2.20	0.41
1:A:1077:GLY:O	1:A:1080:CYS:HB3	2.21	0.41
1:A:885:LEU:HD13	1:A:910:TRP:CE2	2.55	0.41
1:A:940:GLN:HG3	1:A:951:ARG:CZ	2.50	0.41
2:D:778:VAL:O	2:D:778:VAL:HG13	2.21	0.41
2:D:793:HIS:CD2	2:D:796:LEU:H	2.39	0.41
2:D:811:LEU:HD23	2:D:811:LEU:HA	1.85	0.41
2:C:771:VAL:O	2:C:774:TRP:HB3	2.21	0.41
2:C:834:GLY:O	2:C:838:GLN:HB2	2.21	0.41
1:B:1019:MET:HE2	1:B:1048:ALA:CB	2.51	0.40
1:A:1017:GLY:HA2	1:A:1020:ASN:CG	2.46	0.40
1:B:1134:VAL:CG2	1:B:1153:LEU:HD13	2.51	0.40
1:B:886:GLU:O	1:B:890:ARG:HB3	2.22	0.40
1:A:913:MET:HE3	1:A:917:TYR:CE1	2.56	0.40
1:A:1034:LEU:N	1:A:1035:PRO:HD3	2.36	0.40
1:B:1150:LEU:HD23	1:B:1167:LEU:HD11	2.04	0.40
1:A:895:PHE:C	1:A:897:GLN:H	2.30	0.40
1:A:942:GLU:OE2	2:C:819:THR:CB	2.65	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	261/297 (88%)	244 (94%)	14 (5%)	3 (1%)	11 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	257/297 (86%)	244 (95%)	11 (4%)	2 (1%)	16	44
2	C	251/265 (95%)	237 (94%)	12 (5%)	2 (1%)	16	44
2	D	251/265 (95%)	243 (97%)	8 (3%)	0	100	100
All	All	1020/1124 (91%)	968 (95%)	45 (4%)	7 (1%)	18	48

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1102	ILE
1	B	1154	LEU
1	A	1127	ASN
2	C	756	ASN
1	A	967	PRO
2	C	758	ILE
1	A	1129	ILE

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	215/259 (83%)	203 (94%)	12 (6%)	19	50
1	B	211/259 (82%)	200 (95%)	11 (5%)	21	52
2	C	208/234 (89%)	190 (91%)	18 (9%)	9	30
2	D	216/234 (92%)	190 (88%)	26 (12%)	5	16
All	All	850/986 (86%)	783 (92%)	67 (8%)	11	34

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	890	ARG
1	A	913	MET
1	A	940	GLN
1	A	943	ILE

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Mol	Chain	Res	Type
1	A	959	GLN
1	A	964	LEU
1	A	1020	ASN
1	A	1022	GLU
1	A	1031	SER
1	A	1096	GLU
1	A	1122	LEU
1	A	1147	TYR
1	B	871	GLN
1	B	890	ARG
1	B	903	VAL
1	B	913	MET
1	B	1016	TYR
1	B	1022	GLU
1	B	1068	SER
1	B	1075	GLN
1	B	1124	GLU
1	B	1128	ASN
1	B	1161	THR
2	C	635	GLN
2	C	661	GLN
2	C	665	GLN
2	C	667	LEU
2	C	671	GLU
2	C	684	THR
2	C	715	ASP
2	C	726	LEU
2	C	729	LEU
2	C	732	LYS
2	C	748	LEU
2	C	778	VAL
2	C	782	GLU
2	C	802	ARG
2	C	806	GLU
2	C	810	GLN
2	C	836	GLU
2	C	851	VAL
2	D	607	THR
2	D	625	SER
2	D	626	SER
2	D	628	LYS
2	D	632	ILE

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Mol	Chain	Res	Type
2	D	637	LEU
2	D	684	THR
2	D	712	MET
2	D	715	ASP
2	D	724	SER
2	D	726	LEU
2	D	729	LEU
2	D	750	ARG
2	D	756	ASN
2	D	757	SER
2	D	758	ILE
2	D	778	VAL
2	D	779	ASP
2	D	788	ARG
2	D	802	ARG
2	D	818	LYS
2	D	819	THR
2	D	820	LEU
2	D	827	THR
2	D	836	GLU
2	D	851	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	950	HIS
1	A	1020	ASN
1	A	1026	ASN
1	A	1110	ASN
1	A	1135	HIS
1	A	1159	GLN
1	A	1162	GLN
1	B	871	GLN
1	B	924	ASN
1	B	959	GLN
1	B	1020	ASN
1	B	1062	HIS
1	B	1128	ASN
1	B	1135	HIS
1	B	1173	ASN
2	C	635	GLN
2	C	661	GLN

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Mol	Chain	Res	Type
2	C	698	GLN
2	C	710	HIS
2	C	756	ASN
2	C	793	HIS
2	C	810	GLN
2	C	828	HIS
2	D	639	GLN
2	D	653	HIS
2	D	741	ASN
2	D	765	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](#)

5 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	$\# Z > 2$
3	GOL	D	5	-	5,5,5	0.69	0	5,5,5	0.68	0
3	GOL	A	1	-	5,5,5	0.38	0	5,5,5	0.17	0
3	GOL	D	4	-	5,5,5	0.34	0	5,5,5	0.53	0
3	GOL	C	3	-	5,5,5	0.42	0	5,5,5	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	B	2	-	5,5,5	0.38	0	5,5,5	0.58	0

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
3	GOL	D	5	-	-	1/4/4/4	-
3	GOL	A	1	-	-	0/4/4/4	-
3	GOL	D	4	-	-	0/4/4/4	-
3	GOL	C	3	-	-	3/4/4/4	-
3	GOL	B	2	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	3	GOL	C1-C2-C3-O3
3	D	5	GOL	O1-C1-C2-O2
3	C	3	GOL	O1-C1-C2-O2
3	C	3	GOL	O2-C2-C3-O3
3	B	2	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	265/297 (89%)	0.84	27 (10%)	12 10	69, 116, 160, 173	0
1	B	261/297 (87%)	0.80	27 (10%)	12 10	64, 116, 182, 200	0
2	C	252/265 (95%)	0.34	21 (8%)	17 14	37, 76, 194, 215	1 (0%)
2	D	253/265 (95%)	-0.04	7 (2%)	55 46	48, 68, 138, 155	0
All	All	1031/1124 (91%)	0.49	82 (7%)	18 15	37, 98, 174, 215	1 (0%)

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1170	GLU	5.2
1	B	1175	LEU	4.5
1	A	969	ALA	4.3
2	C	603	PHE	4.3
2	C	632	ILE	4.3
2	C	630	TRP	3.9
1	A	1015	ALA	3.8
1	B	969	ALA	3.7
2	C	606	TRP	3.7
1	A	1107	VAL	3.7
2	C	648	GLU	3.6
2	C	758	ILE	3.6
2	D	606	TRP	3.6
2	C	636	THR	3.5
2	C	627	GLY	3.5
1	B	1125	TYR	3.4
1	A	1102	ILE	3.4
1	B	964	LEU	3.3
2	D	631	ILE	3.3
1	B	1174	LEU	3.2
2	C	749	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	1169	ARG	3.1
1	B	872	ALA	3.0
1	B	910	TRP	3.0
1	A	1174	LEU	3.0
2	C	671	GLU	2.9
2	C	628	LYS	2.9
1	A	1101	GLU	2.9
1	A	1172	ASN	2.9
1	A	1177	LEU	2.9
1	B	1120	ILE	2.9
2	C	624	LEU	2.9
2	D	752	PRO	2.8
2	D	750	ARG	2.8
1	B	1016	TYR	2.8
1	B	1102	ILE	2.8
1	A	1013	THR	2.8
1	B	892	GLY	2.8
1	B	1123	ARG	2.7
1	B	1107	VAL	2.7
2	C	629	HIS	2.6
1	A	1108	TRP	2.5
1	A	1173	ASN	2.5
1	B	1171	TYR	2.5
1	A	1014	LEU	2.4
2	C	667	LEU	2.4
2	C	602	PRO	2.4
2	C	752	PRO	2.4
2	D	632	ILE	2.4
1	A	1123	ARG	2.4
1	A	1098	SER	2.4
1	A	967	PRO	2.4
1	B	967	PRO	2.4
1	B	1121	GLY	2.3
2	C	668	GLY	2.3
1	B	886	GLU	2.3
2	C	637	LEU	2.3
1	B	1067	ASP	2.3
1	B	963	SER	2.3
1	A	1139	ILE	2.2
1	A	910	TRP	2.2
1	A	964	LEU	2.2
1	A	1026	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	1130	LEU	2.2
1	A	870	THR	2.2
2	C	711	TYR	2.2
1	B	968	SER	2.2
1	A	896	ALA	2.2
1	B	1157	PRO	2.1
1	B	1026	ASN	2.1
1	A	1119	ALA	2.1
2	C	638	LEU	2.1
1	B	1116	TRP	2.1
2	C	617	GLU	2.1
2	D	642	GLN	2.1
1	A	1175	LEU	2.1
1	B	1108	TRP	2.1
1	B	891	LYS	2.0
2	D	626	SER	2.0
1	B	1147	TYR	2.0
1	A	966	SER	2.0
1	A	1027	GLU	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
3	GOL	D	5	6/6	0.62	0.20	61,73,76,79	0
3	GOL	A	1	6/6	0.73	0.18	105,111,113,114	0
3	GOL	B	2	6/6	0.74	0.16	102,108,111,112	0
3	GOL	C	3	6/6	0.80	0.22	69,89,93,95	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	D	4	6/6	0.81	0.27	123,124,128,128	0

6.5 Other polymers [i](#)

There are no such residues in this entry.