



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:13 PM GMT

PDB ID : 3TAD
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

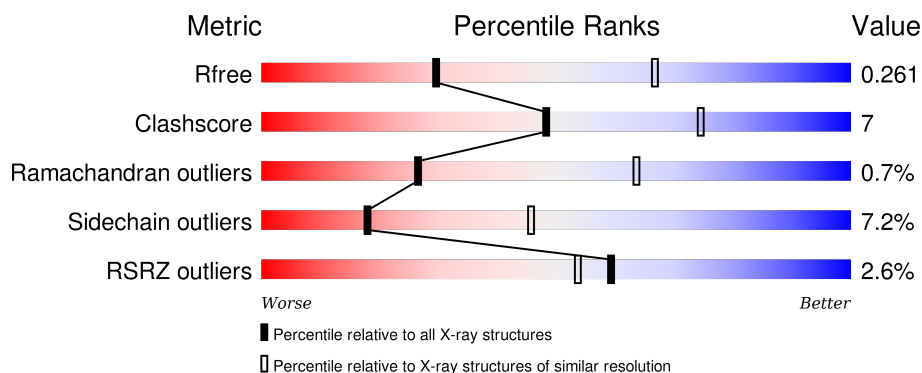
1 Overall quality at a glance

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}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	 2% 72% 16% • 11%
1	B	297	 2% 70% 17% • 12%
2	C	265	 5% 76% 17% • 5%
2	D	265	 75% 18% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	GOL	C	3	-	-	-	X
3	GOL	D	4	-	-	-	X

2 Entry composition

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 (three-letter code: 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		

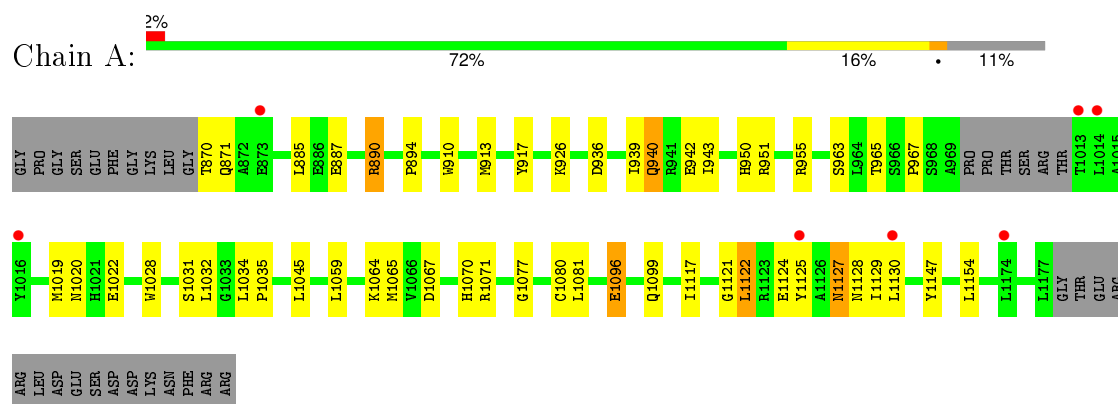
- Molecule 4 is water.

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		

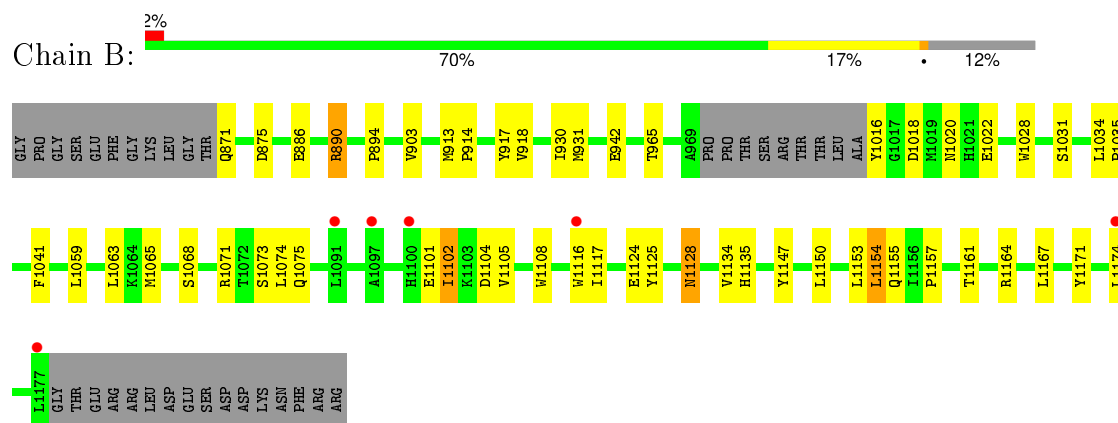
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

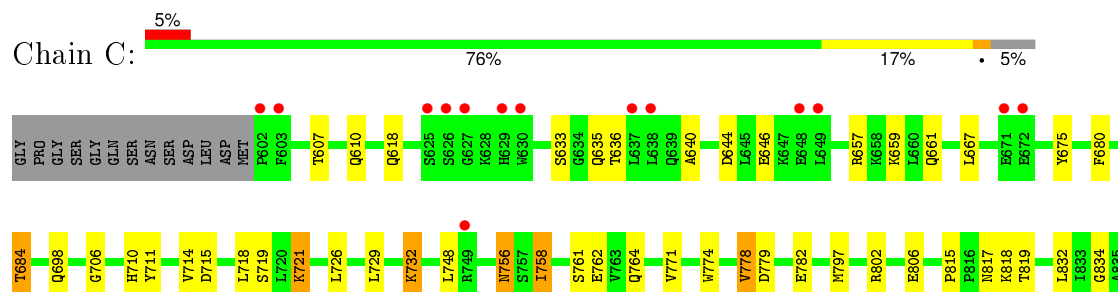
- Molecule 1: Liprin-alpha-2

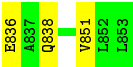


- Molecule 1: Liprin-alpha-2

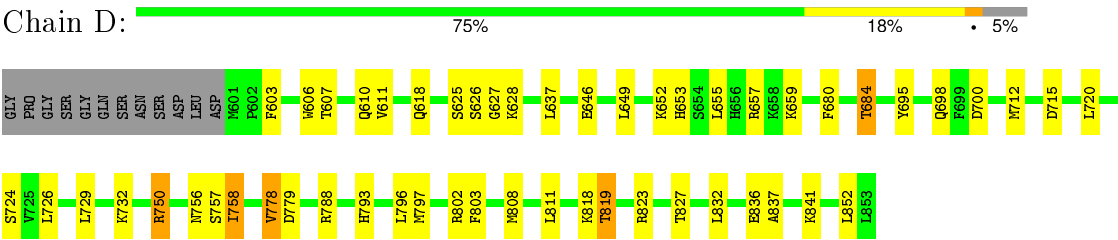


- Molecule 2: Liprin-beta-1





● 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 43.05 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (44.98-2.90) 98.5 (43.05-2.90)	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 (5.29%)	DCC
Wilson B-factor (Å ²)	82.5	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 70.9	EDS
Estimated twinning fraction	0.021 for h,-h-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	1 of 45029 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.94	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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	0.40	0/2130	0.57	0/2893
1	B	0.40	0/2091	0.54	0/2841
2	C	0.48	0/2012	0.66	0/2731
2	D	0.50	0/2062	0.69	0/2798
All	All	0.45	0/8295	0.62	0/11263

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	2087	0	2024	30	0
1	B	2049	0	1989	34	0
2	C	1968	0	1924	29	0
2	D	2016	0	1978	33	0
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	118	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 7.

All (118) 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
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
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
2:D:803:PHE:HE2	2:D:808:MET:HE2	1.59	0.68
1:A:1121:GLY:C	1:A:1122:LEU:HD23	2.14	0.68
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:803:PHE:CE2	2:D:808:MET:HE2	2.32	0.64
1:B:1101:GLU:O	1:B:1102:ILE:HB	1.99	0.61
2:D:695:TYR:HA	2:D:698:GLN:OE1	2.01	0.61
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
2:C:817:ASN:HA	2:D:652:LYS:HD3	1.85	0.57
2:D:680:PHE:O	2:D:684:THR:HG22	2.04	0.57
1:B:903:VAL:HG11	1:B:931:MET:HE2	1.87	0.57
1:B:1157:PRO:C	1:B:1164:ARG:HH21	2.07	0.56
2:D:653:HIS:HE1	2:D:655:LEU:HD12	1.71	0.56
1:A:1065:MET:HE3	1:A:1071:ARG:HG2	1.86	0.56
2:D:750:ARG:HG3	2:D:750:ARG:HH11	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:1065:MET:HE3	1:B:1071:ARG:HA	1.88	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: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
2:C:698:GLN:H	2:C:698:GLN:NE2	2.08	0.52
2:D:778:VAL:O	2:D:778:VAL:CG1	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:A:1067:ASP:HB3	1:A:1070:HIS:ND1	2.27	0.50
1:B:1153:LEU:C	1:B:1155:GLN:H	2.14	0.50
1:B:1125:TYR:O	1:B:1128:ASN:ND2	2.44	0.50
1:A:1019:MET:HE3	1:A:1081:LEU:HD13	1.94	0.49
2:D:611:VAL:HG11	2:D:637:LEU:HD11	1.93	0.49
1:A:1124:GLU:HG3	1:A:1125:TYR:N	2.27	0.48
2:D:797:MET:HE2	2:D:832:LEU:HD23	1.95	0.48
1:A:1096:GLU:HA	1:A:1099:GLN:HG2	1.96	0.48
2:C:761:SER:O	2:C:764:GLN:HB2	2.13	0.48
1:B:1105:VAL:HG12	1:B:1108:TRP:CE2	2.49	0.47
2:D:684:THR:HG21	2:D:700:ASP:OD2	2.14	0.47
1:B:1034:LEU:N	1:B:1035:PRO:HD3	2.29	0.47
1:B:1102:ILE:O	1:B:1102:ILE:CG2	2.63	0.47
1:B:894:PRO:HA	1:B:965:THR:HB	1.95	0.47
1:B:1117:ILE:HD13	1:B:1154:LEU:HD21	1.96	0.47
1:B:1065:MET:HE1	1:B:1074:LEU:HD22	1.98	0.46
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
2:D:680:PHE:O	2:D:684:THR:CG2	2.64	0.45
1:A:1028:TRP:CZ2	1:A:1032:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:803:PHE:CE2	2:D:808:MET:CE	2.99	0.45
2:C:815:PRO:HG2	2:C:818:LYS:CG	2.43	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: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: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:1059:LEU:HD22	1:A:1065:MET:HE2	2.00	0.44
1:A:870:THR:OG1	1:A:871:GLN:N	2.51	0.44
2:D:750:ARG:CG	2:D:750:ARG:HH11	2.31	0.43
1:B:1020:ASN:HD22	1:B:1020:ASN:HA	1.66	0.43
1:A:1064:LYS:HE3	1:A:1064:LYS:HB3	1.85	0.43
2:C:756:ASN:ND2	2:C:762:GLU:HG3	2.33	0.43
1:A:1096:GLU:HA	1:A:1099:GLN:HE21	1.82	0.43
1:A:926:LYS:HD2	2:C:779:ASP:HB3	2.00	0.43
1:B:1153:LEU:C	1:B:1155:GLN:N	2.70	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
2:D:808:MET:HE2	2:D:808:MET:HB2	1.82	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
2:D:803:PHE:HE2	2:D:808:MET:CE	2.28	0.42
1:A:1020:ASN:HD22	1:A:1020:ASN:HA	1.63	0.42
2:C:797:MET:HE2	2:C:832:LEU:HD23	2.01	0.42
2:D:758:ILE:N	2:D:758:ILE:HD12	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
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: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
1:A:885:LEU:HD13	1:A:910:TRP:CE2	2.55	0.41
2:D:793:HIS:CD2	2:D:796:LEU:H	2.39	0.41
2:D:811:LEU:HA	2:D:811:LEU:HD23	1.85	0.41
2:C:834:GLY:O	2:C:838:GLN:HB2	2.21	0.41
2:C:771:VAL:O	2:C:774:TRP:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:719:SER:C	2:C:721:LYS:H	2.25	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:942:GLU:OE2	2:C:819:THR:CB	2.65	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	261/297 (88%)	244 (94%)	14 (5%)	3 (1%)	17	51
1	B	257/297 (86%)	244 (95%)	11 (4%)	2 (1%)	24	60
2	C	251/265 (95%)	237 (94%)	12 (5%)	2 (1%)	24	60
2	D	251/265 (95%)	243 (97%)	8 (3%)	0	100	100
All	All	1020/1124 (91%)	968 (95%)	45 (4%)	7 (1%)	26	63

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%)	205 (95%)	10 (5%)	32	68
1	B	211/259 (82%)	197 (93%)	14 (7%)	21	51
2	C	208/234 (89%)	193 (93%)	15 (7%)	18	46
2	D	216/234 (92%)	194 (90%)	22 (10%)	9	27
All	All	850/986 (86%)	789 (93%)	61 (7%)	18	46

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

Mol	Chain	Res	Type
1	A	890	ARG
1	A	913	MET
1	A	917	TYR
1	A	940	GLN
1	A	963	SER
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	875	ASP
1	B	890	ARG
1	B	913	MET
1	B	917	TYR
1	B	1016	TYR
1	B	1018	ASP
1	B	1022	GLU
1	B	1068	SER
1	B	1075	GLN
1	B	1124	GLU
1	B	1128	ASN
1	B	1147	TYR
1	B	1161	THR

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Mol	Chain	Res	Type
2	C	635	GLN
2	C	661	GLN
2	C	667	LEU
2	C	684	THR
2	C	715	ASP
2	C	721	LYS
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	836	GLU
2	D	607	THR
2	D	625	SER
2	D	626	SER
2	D	628	LYS
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	827	THR
2	D	836	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	950	HIS

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Mol	Chain	Res	Type
1	A	1020	ASN
1	A	1135	HIS
1	A	1162	GLN
1	B	871	GLN
1	B	1020	ASN
1	B	1128	ASN
1	B	1135	HIS
2	C	661	GLN
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	643	GLN
2	D	653	HIS
2	D	710	HIS
2	D	741	ASN
2	D	756	ASN
2	D	765	GLN
2	D	793	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 carbohydrates 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	A	1	-	5,5,5	0.33	0	5,5,5	0.23	0
3	GOL	B	2	-	5,5,5	0.31	0	5,5,5	0.57	0
3	GOL	C	3	-	5,5,5	0.39	0	5,5,5	0.65	0
3	GOL	D	4	-	5,5,5	0.30	0	5,5,5	0.50	0
3	GOL	D	5	-	5,5,5	0.61	0	5,5,5	0.63	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	A	1	-	-	0/4/4/4	0/0/0/0
3	GOL	B	2	-	-	0/4/4/4	0/0/0/0
3	GOL	C	3	-	-	0/4/4/4	0/0/0/0
3	GOL	D	4	-	-	0/4/4/4	0/0/0/0
3	GOL	D	5	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [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%)	0.03	7 (2%) 59 54	69, 116, 160, 173	0
1	B	261/297 (87%)	0.00	6 (2%) 64 59	64, 116, 182, 200	0
2	C	252/265 (95%)	0.16	14 (5%) 28 21	48, 76, 194, 215	0
2	D	253/265 (95%)	-0.21	0 100 100	48, 68, 138, 155	0
All	All	1031/1124 (91%)	-0.00	27 (2%) 59 54	48, 98, 174, 215	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	637	LEU	6.7
2	C	627	GLY	3.8
2	C	638	LEU	3.7
2	C	626	SER	3.6
1	B	1177	LEU	3.5
1	B	1174	LEU	3.0
2	C	671	GLU	3.0
2	C	649	LEU	2.9
2	C	602	PRO	2.8
2	C	629	HIS	2.7
1	A	1014	LEU	2.6
2	C	625	SER	2.5
1	A	873	GLU	2.4
1	A	1130	LEU	2.4
1	B	1100	HIS	2.4
2	C	749	ARG	2.3
2	C	630	TRP	2.3
1	B	1091	LEU	2.3
1	A	1174	LEU	2.3
1	A	1016	TYR	2.2
2	C	603	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
2	C	648	GLU	2.2
2	C	672	GLU	2.1
1	B	1116	TRP	2.1
1	A	1125	TYR	2.1
1	B	1097	ALA	2.0
1	A	1013	THR	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
3	GOL	D	4	6/6	0.64	0.35	4.08	123,124,128,128	0
3	GOL	C	3	6/6	0.84	0.29	2.78	69,89,93,95	0
3	GOL	B	2	6/6	0.70	0.14	-1.53	102,108,111,112	0
3	GOL	A	1	6/6	0.59	0.14	-	105,111,113,114	0
3	GOL	D	5	6/6	0.82	0.18	-	61,73,76,79	0

6.5 Other polymers [i](#)

There are no such residues in this entry.