



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:12 AM UTC

PDB ID : 6KR4 / pdb_00006kr4
Title : Crystal structure of the liprin-alpha3_SAM123/LAR_D1D2 complex
Authors : Xie, X.; Liang, M.; Luo, L.; Wei, Z.
Deposited on : 2019-08-20
Resolution : 2.85 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

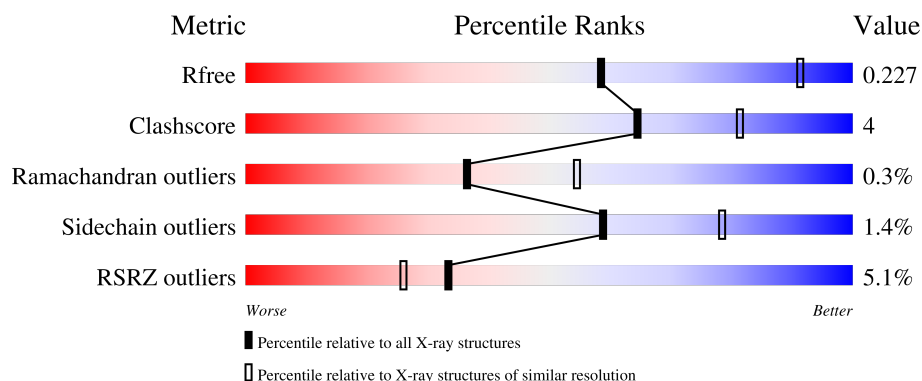
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.85 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	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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	580	90% 9% .
1	B	580	2% 88% 10% .
1	C	580	2% 88% 11% ..
1	D	580	6% 86% 12% .
2	E	325	7% 70% 11% 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	325	7% 67% 14% 19%
2	G	325	2% 95%
2	H	325	13% 61% 10% 29%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24833 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 Receptor-type tyrosine-protein phosphatase F.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	575	Total	C	N	O	S	0	6	0
			4669	2956	818	861	34			
1	B	571	Total	C	N	O	S	0	2	0
			4597	2910	799	855	33			
1	C	575	Total	C	N	O	S	0	4	0
			4638	2933	812	859	34			
1	D	568	Total	C	N	O	S	0	3	0
			4566	2896	791	846	33			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1328	HIS	-	expression tag	UNP P10586
A	1329	MET	-	expression tag	UNP P10586
A	1330	GLY	-	expression tag	UNP P10586
A	1331	SER	-	expression tag	UNP P10586
B	1328	HIS	-	expression tag	UNP P10586
B	1329	MET	-	expression tag	UNP P10586
B	1330	GLY	-	expression tag	UNP P10586
B	1331	SER	-	expression tag	UNP P10586
C	1328	HIS	-	expression tag	UNP P10586
C	1329	MET	-	expression tag	UNP P10586
C	1330	GLY	-	expression tag	UNP P10586
C	1331	SER	-	expression tag	UNP P10586
D	1328	HIS	-	expression tag	UNP P10586
D	1329	MET	-	expression tag	UNP P10586
D	1330	GLY	-	expression tag	UNP P10586
D	1331	SER	-	expression tag	UNP P10586

- Molecule 2 is a protein called Liprin-alpha-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	266	Total	C	N	O	S	0	0	0
			2111	1332	380	386	13			
2	F	264	Total	C	N	O	S	0	0	0
			2091	1315	372	391	13			
2	H	231	Total	C	N	O	S	0	0	0
			1789	1135	317	325	12			
2	G	15	Total	C	N	O	S	0	0	0
			108	71	18	18	1			

There are 16 discrepancies between the modelled and reference sequences:

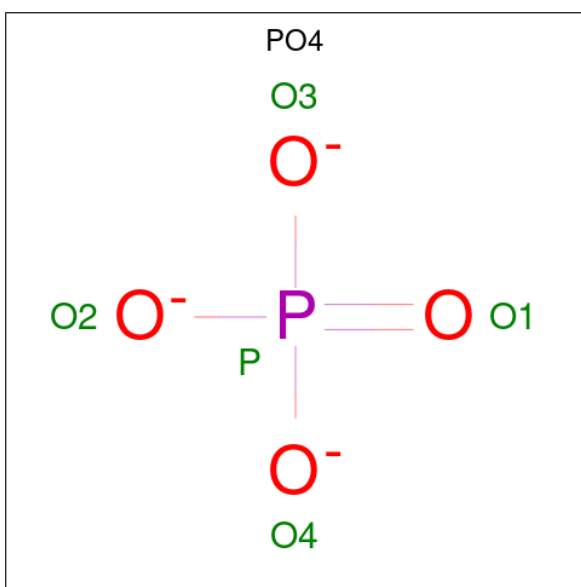
Chain	Residue	Modelled	Actual	Comment	Reference
E	802	GLY	-	expression tag	UNP P60469
E	803	PRO	-	expression tag	UNP P60469
E	804	GLY	-	expression tag	UNP P60469
E	805	SER	-	expression tag	UNP P60469
F	802	GLY	-	expression tag	UNP P60469
F	803	PRO	-	expression tag	UNP P60469
F	804	GLY	-	expression tag	UNP P60469
F	805	SER	-	expression tag	UNP P60469
H	802	GLY	-	expression tag	UNP P60469
H	803	PRO	-	expression tag	UNP P60469
H	804	GLY	-	expression tag	UNP P60469
H	805	SER	-	expression tag	UNP P60469
G	802	GLY	-	expression tag	UNP P60469
G	803	PRO	-	expression tag	UNP P60469
G	804	GLY	-	expression tag	UNP P60469
G	805	SER	-	expression tag	UNP P60469

- Molecule 3 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: C₈H₁₈O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	8	5		
3	B	1	Total	C	O	0	0
			13	8	5		
3	C	1	Total	C	O	0	0
			13	8	5		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



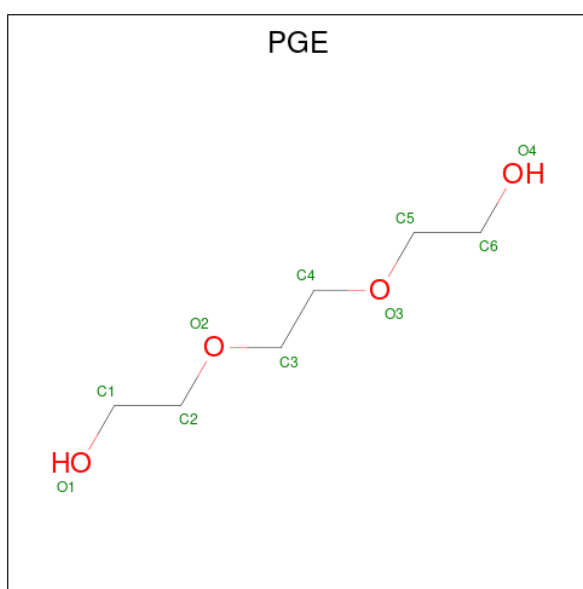
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

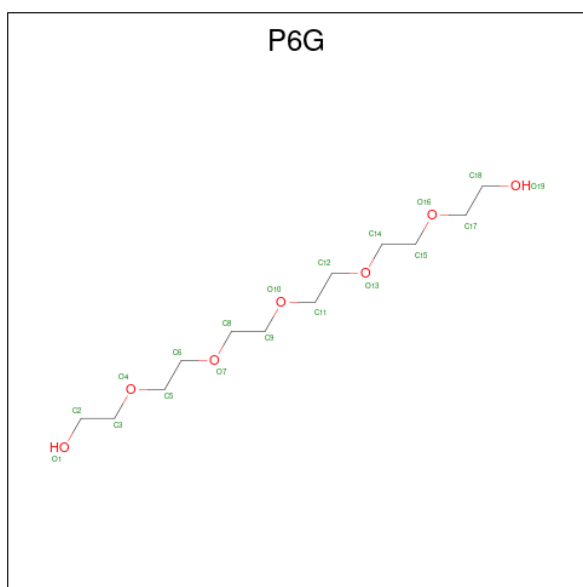
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			10	6	4		
5	D	1	Total	C	O	0	0
			10	6	4		

- Molecule 6 is HEXAETHYLENE GLYCOL (CCD ID: P6G) (formula: $C_{12}H_{26}O_7$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total	C	O	0	0
			19	12	7		

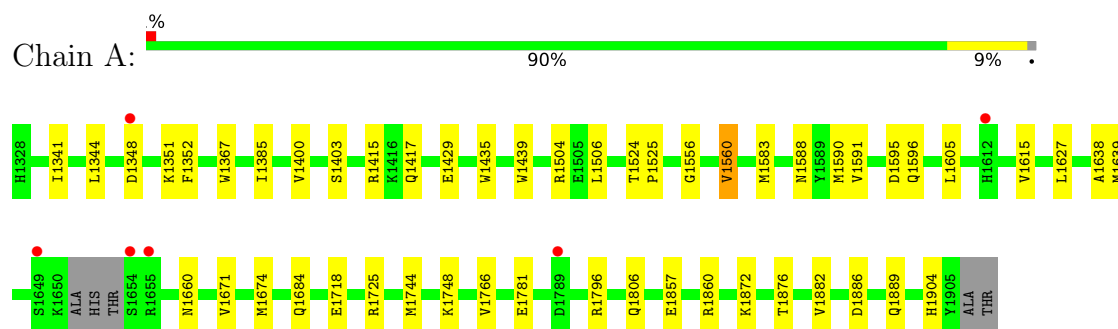
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	94	Total O 94 94	0	0
7	B	4	Total O 4 4	0	0
7	C	43	Total O 43 43	0	0
7	D	16	Total O 16 16	0	0
7	E	3	Total O 3 3	0	0
7	F	1	Total O 1 1	0	0

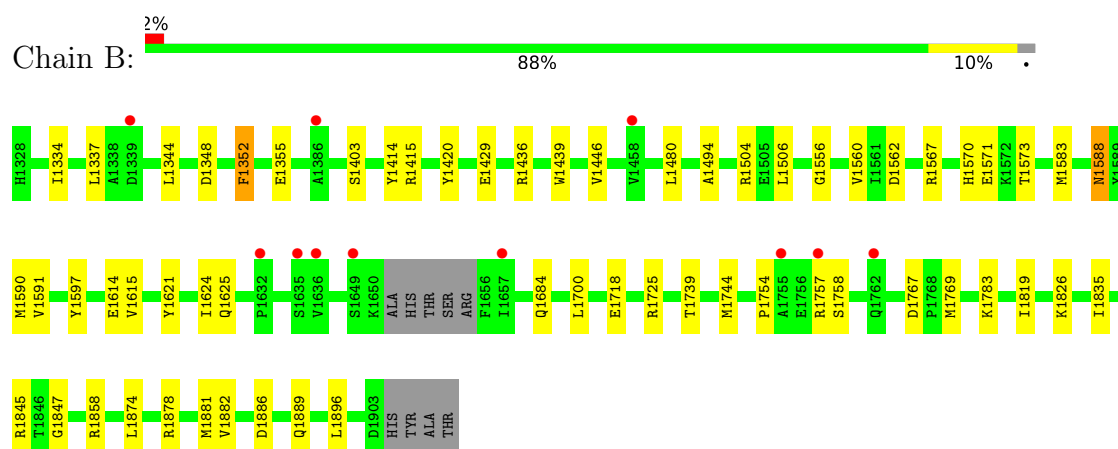
3 Residue-property plots

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.

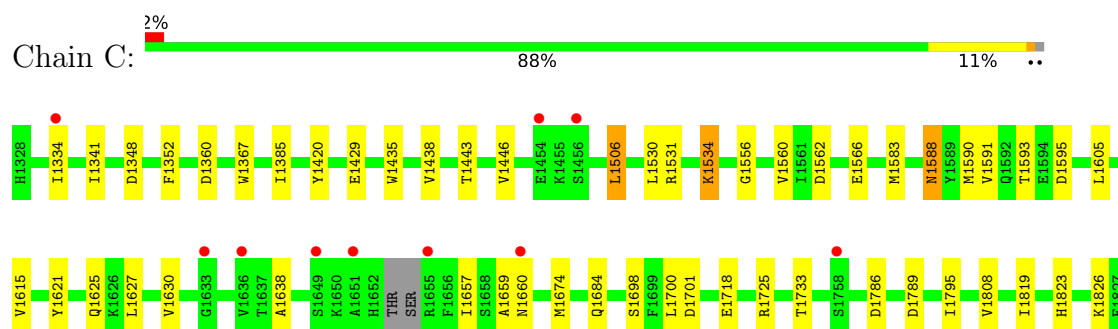
- Molecule 1: Receptor-type tyrosine-protein phosphatase F

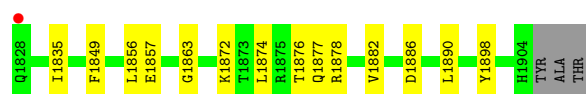


- Molecule 1: Receptor-type tyrosine-protein phosphatase F

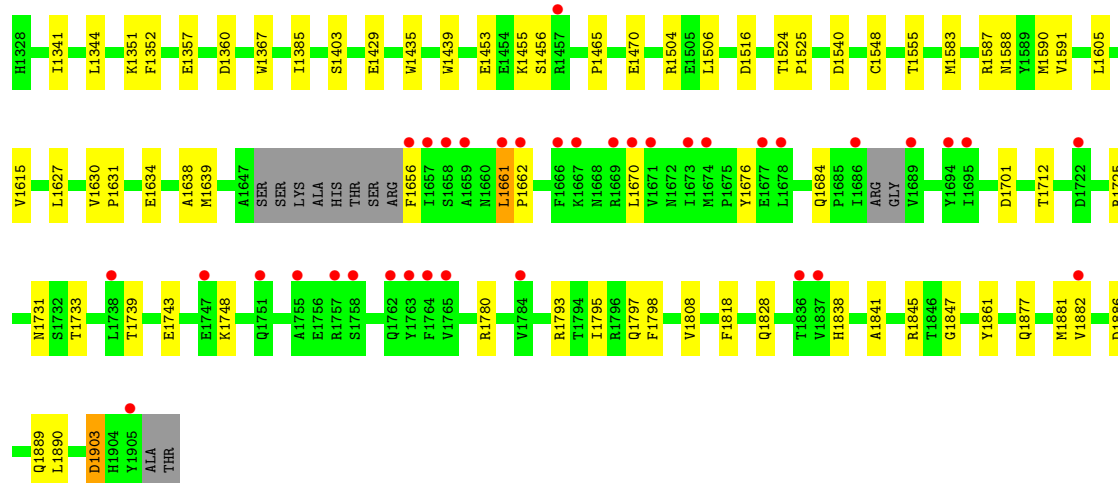
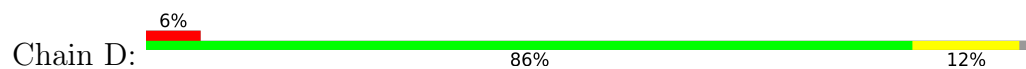


- Molecule 1: Receptor-type tyrosine-protein phosphatase F

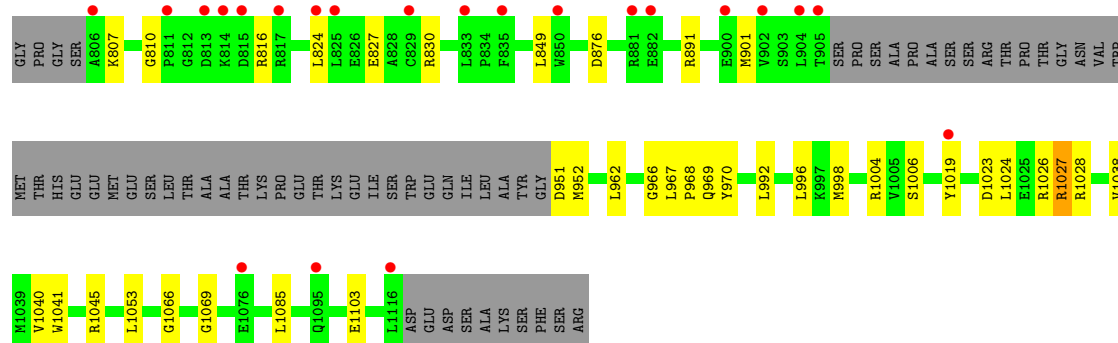




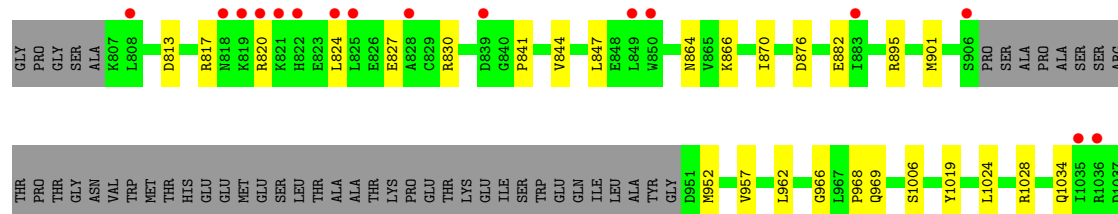
• Molecule 1: Receptor-type tyrosine-protein phosphatase F

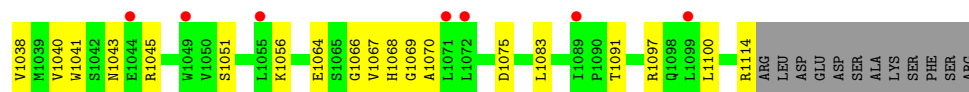


• Molecule 2: Liprin-alpha-3

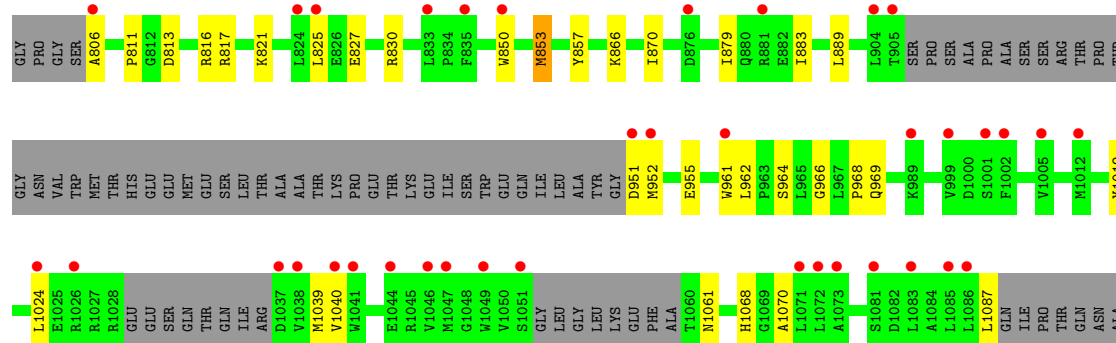


• Molecule 2: Liprin-alpha-3

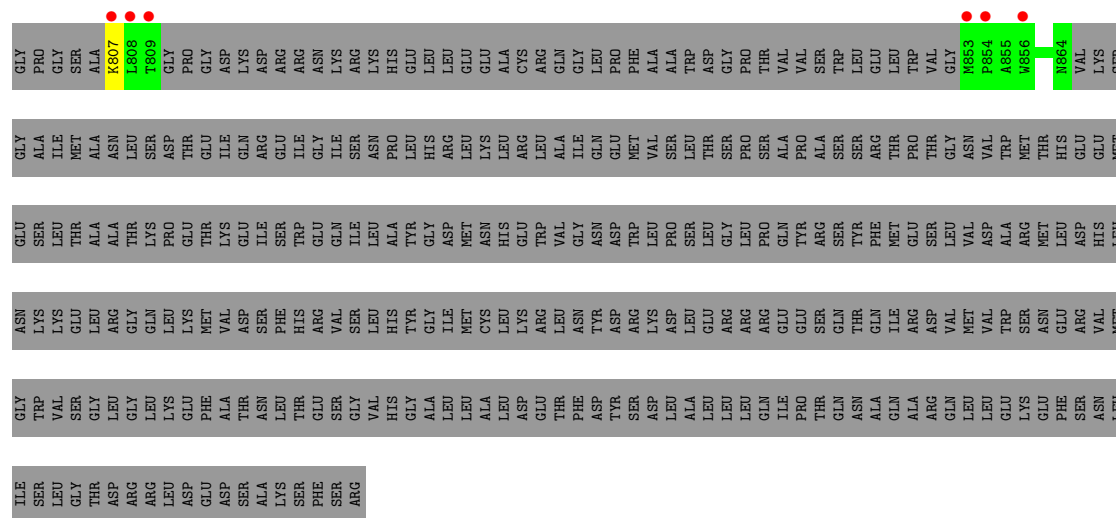




• Molecule 2: Liprin-alpha-3



• Molecule 2: Liprin-alpha-3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	250.38Å 147.68Å 143.97Å 90.00° 103.85° 90.00°	Depositor
Resolution (Å)	42.17 – 2.85 42.17 – 2.85	Depositor EDS
% Data completeness (in resolution range)	98.7 (42.17-2.85) 91.5 (42.17-2.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.192 , 0.230 0.194 , 0.227	Depositor DCC
R_{free} test set	2000 reflections (1.69%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.312	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	24833	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% 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: PGE, PG4, P6G, PO4

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	0.67	0/4795	0.83	2/6494 (0.0%)
1	B	0.44	0/4709	0.76	0/6383
1	C	0.56	0/4756	0.79	4/6444 (0.1%)
1	D	0.47	0/4680	0.79	5/6345 (0.1%)
2	E	0.44	0/2151	0.78	0/2908
2	F	0.37	0/2132	0.75	0/2886
2	G	0.30	0/110	0.56	0/150
2	H	0.36	0/1821	0.76	0/2463
All	All	0.51	0/25154	0.78	11/34073 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1630	VAL	CA-C-N	7.46	125.10	119.66
1	D	1630	VAL	C-N-CA	7.46	125.10	119.66
1	D	1903	ASP	N-CA-C	6.60	118.35	111.03
1	D	1661	LEU	CA-C-N	6.28	126.48	119.32
1	D	1661	LEU	C-N-CA	6.28	126.48	119.32
1	C	1360	ASP	CA-C-N	6.17	125.86	119.56
1	C	1360	ASP	C-N-CA	6.17	125.86	119.56
1	C	1630	VAL	CA-C-N	6.00	124.04	119.66
1	C	1630	VAL	C-N-CA	6.00	124.04	119.66
1	A	1748	LYS	N-CA-C	-5.98	106.12	113.41
1	A	1766	VAL	N-CA-C	5.06	115.05	107.51

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	4669	0	4572	23	0
1	B	4597	0	4475	32	0
1	C	4638	0	4526	33	0
1	D	4566	0	4441	37	0
2	E	2111	0	2091	23	0
2	F	2091	0	2038	26	0
2	G	108	0	99	1	0
2	H	1789	0	1747	23	0
3	A	13	0	18	1	0
3	B	13	0	18	1	0
3	C	13	0	18	2	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	1	0
5	C	10	0	14	0	0
5	D	10	0	14	1	0
6	D	19	0	26	0	0
7	A	94	0	0	0	0
7	B	4	0	0	0	0
7	C	43	0	0	1	0
7	D	16	0	0	0	0
7	E	3	0	0	0	0
7	F	1	0	0	0	0
All	All	24833	0	24097	191	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 4.

All (191) 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)
2:E:998:MET:HE3	2:E:1004:ARG:HG2	1.59	0.84
1:B:1769:MET:HE3	1:B:1783:LYS:HB2	1.64	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1540:ASP:HB2	5:D:2002:PGE:H62	1.62	0.79
2:E:1027:ARG:HG2	2:E:1040:VAL:HG21	1.66	0.76
2:F:1028:ARG:HG3	2:F:1040:VAL:HG12	1.67	0.75
2:E:1028:ARG:HG3	2:E:1040:VAL:HG12	1.69	0.74
2:F:827:GLU:OE2	2:F:830:ARG:NH2	2.21	0.73
1:C:1826:LYS:HD2	1:C:1835:ILE:HD11	1.69	0.73
2:E:952:MET:HE1	2:E:1019:TYR:HB3	1.69	0.72
2:F:952:MET:HE1	2:F:1019:TYR:HB3	1.74	0.68
1:D:1439:TRP:O	1:D:1504:ARG:NH1	2.26	0.68
1:B:1754:PRO:HB2	1:B:1757:ARG:O	1.94	0.68
2:F:876:ASP:OD1	2:F:895:ARG:NH2	2.27	0.68
1:C:1367:TRP:HB3	1:C:1385:ILE:HD13	1.77	0.65
1:A:1344:LEU:HD23	1:A:1351:LYS:HB3	1.79	0.65
1:A:1857:GLU:HB2	3:A:2001:PG4:H51	1.78	0.65
2:H:952:MET:HE1	2:H:1019:TYR:HB3	1.79	0.65
1:A:1556:GLY:O	1:A:1560:VAL:HG12	1.96	0.64
1:A:1744:MET:HE3	1:A:1806:GLN:HG3	1.80	0.64
2:F:864:ASN:ND2	2:F:882:GLU:O	2.28	0.64
1:A:1439:TRP:O	1:A:1504:ARG:NH1	2.31	0.64
2:E:992:LEU:HD22	2:E:998:MET:HE2	1.79	0.64
1:A:1684:GLN:O	1:A:1725:ARG:NH2	2.31	0.63
1:B:1439:TRP:O	1:B:1504:ARG:NH1	2.33	0.61
2:H:827:GLU:OE1	2:H:830:ARG:NH2	2.35	0.60
2:E:1038:VAL:HA	2:E:1041:TRP:CD1	2.37	0.59
2:F:1024:LEU:HD12	2:F:1040:VAL:HG13	1.84	0.59
1:C:1657:ILE:HG22	1:C:1659:ALA:H	1.68	0.58
1:C:1886:ASP:OD1	1:C:1886:ASP:N	2.36	0.58
1:A:1671:VAL:O	1:A:1674:MET:HE3	2.04	0.58
1:B:1718:GLU:N	1:B:1718:GLU:OE1	2.36	0.58
2:H:811:PRO:HA	2:H:816:ARG:HG2	1.84	0.58
2:H:879:ILE:HG23	2:H:883:ILE:HD12	1.85	0.57
1:A:1718:GLU:OE1	1:A:1718:GLU:N	2.36	0.57
1:B:1826:LYS:HD2	1:B:1835:ILE:HD11	1.84	0.57
1:D:1627:LEU:HA	1:D:1638:ALA:HB3	1.85	0.56
1:D:1583:MET:HE2	1:D:1590:MET:HB3	1.87	0.56
2:E:827:GLU:OE1	2:E:830:ARG:NH2	2.40	0.55
1:C:1872:LYS:O	1:C:1876:THR:HG23	2.07	0.55
1:A:1886:ASP:N	1:A:1886:ASP:OD1	2.40	0.55
2:E:970:TYR:CE1	2:E:998:MET:HG2	2.42	0.55
2:E:1024:LEU:HD12	2:E:1040:VAL:HG13	1.88	0.55
2:H:1024:LEU:HD12	2:H:1040:VAL:HG13	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1593:THR:OG1	1:C:1595:ASP:OD1	2.23	0.55
1:C:1556:GLY:O	1:C:1560:VAL:HG12	2.07	0.54
1:D:1712:THR:HG23	1:D:1838:HIS:HB3	1.89	0.54
1:C:1435:TRP:HZ3	1:C:1506:LEU:HD22	1.73	0.54
2:H:1061:ASN:ND2	2:H:1087:LEU:O	2.31	0.54
2:F:1091:THR:HA	2:F:1097:ARG:HE	1.72	0.53
1:C:1660:ASN:ND2	1:C:1674:MET:HE1	2.23	0.53
1:B:1556:GLY:O	1:B:1560:VAL:HG12	2.09	0.53
1:B:1403:SER:O	1:B:1436:ARG:NH2	2.42	0.53
1:D:1847:GLY:HA2	1:D:1881:MET:HE3	1.91	0.53
1:B:1446:VAL:HG23	1:B:1506:LEU:HD11	1.90	0.53
1:B:1415:ARG:NH2	1:D:1360:ASP:OD2	2.42	0.53
1:D:1341:ILE:HD12	1:D:1605:LEU:HD22	1.92	0.52
1:A:1781:GLU:HG2	1:A:1796[B]:ARG:HG2	1.90	0.52
2:F:820:ARG:O	2:F:824:LEU:HD13	2.10	0.51
2:E:824:LEU:HD12	2:E:849:LEU:HD22	1.91	0.51
2:F:1068:HIS:CE1	2:F:1070:ALA:HB3	2.46	0.51
1:D:1587:ARG:O	1:D:1590:MET:HG2	2.11	0.51
2:H:866:LYS:H	2:H:870:ILE:HD12	1.76	0.51
1:B:1355:GLU:OE2	1:B:1597:TYR:OH	2.26	0.51
1:C:1700:LEU:HD23	1:C:1874:LEU:HD22	1.92	0.51
1:A:1639:MET:HE3	1:A:1889:GLN:NE2	2.27	0.50
1:C:1534:LYS:NZ	1:C:1566:GLU:OE2	2.30	0.50
1:B:1583:MET:HE2	1:B:1590:MET:HB3	1.93	0.50
1:D:1435:TRP:HZ3	1:D:1506:LEU:HD22	1.76	0.50
1:D:1639:MET:HE3	1:D:1889:GLN:HG2	1.91	0.50
2:F:1075:ASP:O	2:F:1114:ARG:NH2	2.43	0.50
2:H:813:ASP:O	2:H:817:ARG:HG3	2.12	0.50
1:C:1857:GLU:HB2	3:C:2001:PG4:H51	1.92	0.50
1:C:1718:GLU:N	1:C:1718:GLU:OE1	2.44	0.50
1:D:1465:PRO:HB3	1:D:1470:GLU:HG3	1.94	0.49
2:F:901:MET:HE2	2:F:901:MET:HA	1.93	0.49
1:B:1758:SER:OG	1:B:1767:ASP:OD1	2.24	0.49
1:C:1367:TRP:CB	1:C:1385:ILE:HD13	2.43	0.48
1:D:1903:ASP:OD2	2:H:816:ARG:NH2	2.45	0.48
1:C:1583:MET:HE2	1:C:1590:MET:HB3	1.95	0.48
2:H:1068:HIS:CE1	2:H:1070:ALA:HB3	2.48	0.48
1:A:1435:TRP:HZ3	1:A:1506:LEU:HD22	1.79	0.48
1:B:1624:ILE:HD12	1:B:1896:LEU:HD22	1.94	0.48
1:B:1700:LEU:HD23	1:B:1874:LEU:HD22	1.95	0.48
1:C:1627:LEU:HA	1:C:1638:ALA:HB3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1808:VAL:HB	1:D:1890:LEU:HD22	1.94	0.48
1:B:1886:ASP:OD1	1:B:1886:ASP:N	2.47	0.48
2:F:866:LYS:H	2:F:870:ILE:HD12	1.78	0.48
1:A:1660:ASN:OD1	1:A:1674:MET:HE1	2.14	0.47
1:C:1733:THR:HA	1:C:1795:ILE:HG13	1.96	0.47
1:C:1863:GLY:HA3	2:G:807:LYS:HD3	1.96	0.47
1:C:1446:VAL:HG23	1:C:1506:LEU:HD11	1.96	0.47
2:E:901:MET:HA	2:E:901:MET:HE2	1.97	0.47
1:B:1420:TYR:OH	1:B:1562:ASP:OD2	2.29	0.47
2:E:951:ASP:OD1	2:E:952:MET:N	2.43	0.47
1:B:1684:GLN:O	1:B:1725:ARG:NH2	2.47	0.47
1:D:1798:PHE:HB3	1:D:1818:PHE:CE1	2.49	0.47
2:F:968:PRO:HD2	2:F:1064:GLU:HG2	1.97	0.46
1:D:1684:GLN:O	1:D:1725:ARG:NH2	2.48	0.46
1:B:1588:ASN:C	1:B:1588:ASN:HD22	2.21	0.46
1:D:1524:THR:HB	1:D:1525:PRO:HD3	1.97	0.46
1:A:1595:ASP:OD1	1:A:1596:GLN:N	2.49	0.46
1:C:1341:ILE:HD12	1:C:1605:LEU:HD22	1.97	0.46
1:A:1341:ILE:HD12	1:A:1605:LEU:HD22	1.98	0.46
2:E:1023:ASP:OD1	2:E:1026:ARG:NH1	2.49	0.46
2:E:1045:ARG:NH1	4:E:1201:PO4:O3	2.49	0.46
1:B:1567:ARG:HG2	1:B:1573:THR:O	2.16	0.45
1:C:1684:GLN:O	1:C:1725:ARG:NH2	2.45	0.45
2:F:1043:ASN:ND2	2:F:1067:VAL:O	2.37	0.45
1:B:1480:LEU:HD11	1:B:1494:ALA:HB2	1.98	0.45
1:D:1455:LYS:HG3	1:D:1516:ASP:OD2	2.16	0.45
2:E:876:ASP:OD1	2:E:891:ARG:NE	2.49	0.45
1:B:1847:GLY:HA2	1:B:1881:MET:HE3	1.99	0.45
1:C:1438:VAL:HG13	1:C:1443:THR:HB	1.99	0.45
2:F:841:PRO:HA	2:F:844:VAL:HG22	1.99	0.45
1:A:1524:THR:HB	1:A:1525:PRO:HD3	1.98	0.44
1:A:1400:VAL:O	1:A:1403:SER:OG	2.28	0.44
1:D:1903:ASP:CG	2:H:816:ARG:HH12	2.25	0.44
2:F:1051:SER:HB2	2:F:1056:LYS:HG2	1.99	0.44
2:F:1091:THR:HA	2:F:1097:ARG:NE	2.31	0.44
1:A:1367:TRP:HB3	1:A:1385:ILE:HD13	1.98	0.44
1:D:1344:LEU:HD23	1:D:1351:LYS:HB3	1.98	0.44
2:E:1041:TRP:HB2	2:E:1069:GLY:HA3	1.98	0.44
1:D:1701:ASP:CG	1:D:1877:GLN:HE22	2.25	0.44
1:B:1739:THR:HG22	1:B:1845:ARG:NH1	2.32	0.44
1:C:1588:ASN:HD22	1:C:1588:ASN:C	2.23	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1733:THR:HA	1:D:1795:ILE:HG13	1.98	0.44
1:D:1453:GLU:OE2	1:D:1456:SER:HA	2.18	0.44
1:D:1656:PHE:HE1	1:D:1676:TYR:CD1	2.35	0.44
1:C:1420:TYR:OH	1:C:1562:ASP:OD2	2.26	0.43
2:H:951:ASP:OD1	2:H:952:MET:N	2.48	0.43
2:F:1038:VAL:HA	2:F:1041:TRP:CD1	2.53	0.43
2:H:889:LEU:HD23	2:H:889:LEU:HA	1.84	0.43
2:E:1006:SER:OG	2:E:1066:GLY:O	2.28	0.43
1:B:1878:ARG:O	1:B:1881:MET:HG2	2.18	0.43
2:H:825:LEU:HD23	2:H:825:LEU:HA	1.76	0.43
1:D:1661:LEU:HA	1:D:1662:PRO:HD3	1.86	0.43
1:C:1823:HIS:HB3	3:C:2001:PG4:H72	2.00	0.43
1:B:1414:TYR:OH	1:B:1571:GLU:OE2	2.22	0.42
1:A:1872:LYS:O	1:A:1876:THR:HG23	2.20	0.42
1:A:1904:HIS:C	1:A:1904:HIS:HD1	2.28	0.42
1:B:1334:ILE:HA	1:B:1337:LEU:HB2	2.02	0.42
1:A:1583:MET:HE2	1:A:1590:MET:HB3	2.02	0.42
1:C:1786:ASP:HB3	1:C:1789:ASP:OD1	2.20	0.42
1:D:1731:ASN:HA	1:D:1793:ARG:NH1	2.35	0.42
2:F:1041:TRP:HB2	2:F:1069:GLY:HA3	2.01	0.42
2:H:853:MET:HG3	2:H:857:TYR:HD2	1.85	0.42
1:B:1621:TYR:O	1:B:1625:GLN:HG2	2.20	0.42
1:B:1819:ILE:HG22	3:B:2001:PG4:H61	2.01	0.42
1:D:1367:TRP:HB3	1:D:1385:ILE:HD13	2.02	0.42
1:D:1631:PRO:HB2	1:D:1634:GLU:HG3	2.00	0.42
2:E:1053:LEU:HD22	2:E:1103:GLU:HG3	2.01	0.42
1:A:1344:LEU:HA	1:A:1351:LYS:HB3	2.02	0.42
1:B:1614:GLU:OE1	1:B:1858:ARG:NH2	2.47	0.42
1:C:1698:SER:HB2	1:C:1878:ARG:HD2	2.01	0.42
1:C:1701:ASP:CG	1:C:1877:GLN:HE22	2.28	0.42
1:D:1886:ASP:N	1:D:1886:ASP:OD1	2.44	0.42
2:F:847:LEU:HD23	2:F:847:LEU:HA	1.85	0.41
1:A:1627:LEU:HA	1:A:1638:ALA:HB3	2.01	0.41
1:B:1570[A]:HIS:ND1	1:D:1357:GLU:O	2.53	0.41
2:E:966:GLY:C	2:E:968:PRO:HD3	2.45	0.41
2:F:1034:GLN:O	2:F:1045:ARG:NH2	2.53	0.41
1:C:1621:TYR:O	1:C:1625:GLN:HG2	2.19	0.41
1:D:1861:TYR:HA	2:H:806:ALA:HA	2.02	0.41
2:F:1006:SER:OG	2:F:1066:GLY:O	2.24	0.41
2:H:961:TRP:O	2:H:964:SER:OG	2.32	0.41
2:H:966:GLY:C	2:H:968:PRO:HD3	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1819:ILE:HG12	1:C:1849:PHE:CE1	2.55	0.41
2:E:992:LEU:HD23	2:E:996:LEU:HD12	2.01	0.41
2:H:962:LEU:HD12	2:H:962:LEU:HA	1.86	0.41
2:H:1039:MET:HE2	2:H:1039:MET:HB3	1.97	0.41
1:B:1414:TYR:OH	1:B:1570[A]:HIS:HD2	2.04	0.41
1:C:1808:VAL:HB	1:C:1890:LEU:HD22	2.03	0.41
1:D:1828:GLN:NE2	2:H:955:GLU:OE2	2.54	0.41
2:E:810:GLY:O	2:E:816:ARG:HG3	2.21	0.41
2:F:957:VAL:O	2:F:962:LEU:HB2	2.20	0.41
2:H:821:LYS:HG3	2:H:850:TRP:HD1	1.86	0.41
1:B:1886:ASP:HA	1:B:1889:GLN:HB2	2.03	0.41
2:E:967:LEU:N	2:E:968:PRO:HD3	2.35	0.41
2:F:813:ASP:O	2:F:817:ARG:HG3	2.21	0.41
2:F:966:GLY:C	2:F:968:PRO:HD3	2.46	0.41
2:F:1083:LEU:HD23	2:F:1100:LEU:HD11	2.03	0.41
1:D:1743:GLU:HB2	1:D:1748:LYS:HG3	2.02	0.40
1:C:1856:LEU:HD22	1:C:1898:TYR:CD2	2.55	0.40
1:D:1780:ARG:HD2	1:D:1797:GLN:OE1	2.21	0.40
1:C:1334:ILE:HD12	7:C:2121:HOH:O	2.20	0.40
1:D:1739:THR:HG22	1:D:1845:ARG:NH1	2.36	0.40
2:H:952:MET:HE3	2:H:952:MET:HB2	1.91	0.40
1:D:1548:CYS:SG	1:D:1555:THR:OG1	2.69	0.40
1:B:1344:LEU:HB3	1:B:1352:PHE:CG	2.55	0.40
1:D:1670:LEU:HD12	1:D:1841:ALA:HB2	2.03	0.40
2:E:962:LEU:HD12	2:E:962:LEU:HA	1.94	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	577/580 (100%)	558 (97%)	17 (3%)	2 (0%)	36 54

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	569/580 (98%)	553 (97%)	14 (2%)	2 (0%)	30	48
1	C	575/580 (99%)	558 (97%)	15 (3%)	2 (0%)	36	54
1	D	565/580 (97%)	550 (97%)	13 (2%)	2 (0%)	30	48
2	E	262/325 (81%)	254 (97%)	8 (3%)	0	100	100
2	F	260/325 (80%)	250 (96%)	10 (4%)	0	100	100
2	G	11/325 (3%)	11 (100%)	0	0	100	100
2	H	221/325 (68%)	215 (97%)	6 (3%)	0	100	100
All	All	3040/3620 (84%)	2949 (97%)	83 (3%)	8 (0%)	36	54

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1882	VAL
1	C	1882	VAL
1	D	1882	VAL
1	A	1591	VAL
1	A	1882	VAL
1	B	1591	VAL
1	C	1591	VAL
1	D	1591	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/504 (100%)	496 (98%)	9 (2%)	51	73
1	B	495/504 (98%)	489 (99%)	6 (1%)	63	80
1	C	499/504 (99%)	488 (98%)	11 (2%)	45	69
1	D	489/504 (97%)	484 (99%)	5 (1%)	68	83
2	E	223/280 (80%)	219 (98%)	4 (2%)	51	73
2	F	222/280 (79%)	221 (100%)	1 (0%)	81	90

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	9/280 (3%)	9 (100%)	0	100	100
2	H	186/280 (66%)	184 (99%)	2 (1%)	65	81
All	All	2628/3136 (84%)	2590 (99%)	38 (1%)	59	78

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1348	ASP
1	A	1352	PHE
1	A	1415	ARG
1	A	1417	GLN
1	A	1429	GLU
1	A	1560	VAL
1	A	1588	ASN
1	A	1615	VAL
1	A	1860	ARG
1	B	1348	ASP
1	B	1352	PHE
1	B	1429	GLU
1	B	1588	ASN
1	B	1615	VAL
1	B	1744	MET
1	C	1348	ASP
1	C	1352	PHE
1	C	1429[A]	GLU
1	C	1429[B]	GLU
1	C	1506	LEU
1	C	1530	LEU
1	C	1531[A]	ARG
1	C	1531[B]	ARG
1	C	1534	LYS
1	C	1588	ASN
1	C	1615	VAL
1	D	1352	PHE
1	D	1403	SER
1	D	1429	GLU
1	D	1588	ASN
1	D	1615	VAL
2	E	807	LYS
2	E	969	GLN
2	E	1027	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	1085	LEU
2	F	969	GLN
2	H	853	MET
2	H	969	GLN

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	1517	HIS
1	A	1596	GLN
1	B	1369	ASN
1	B	1418	ASN
1	B	1496	HIS
1	B	1664	ASN
1	C	1418	ASN
1	C	1441	GLN
1	C	1537	ASN
1	C	1579	HIS
1	C	1596	GLN
1	C	1664	ASN
1	C	1750	HIS
1	D	1369	ASN
1	D	1619	ASN
1	D	1750	HIS
1	D	1821	GLN
1	D	1869	GLN
2	E	954	HIS
2	F	1098	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

11 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	$\# Z > 2$
4	PO4	E	1201	-	4,4,4	1.01	0	6,6,6	0.42	0
5	PGE	D	2002	-	9,9,9	0.17	0	8,8,8	0.22	0
4	PO4	D	2003	-	4,4,4	0.98	0	6,6,6	0.47	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
5	PGE	D	2002	-	-	1/7/7/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	D	2002	PGE	O3-C5-C6-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	1201	PO4	1	0
5	D	2002	PGE	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	575/580 (99%)	-0.35	6 (1%)	79 74	20, 42, 75, 159	6 (1%)
1	B	571/580 (98%)	0.24	11 (1%)	66 59	34, 77, 125, 155	2 (0%)
1	C	575/580 (99%)	-0.13	11 (1%)	66 59	24, 58, 103, 196	4 (0%)
1	D	568/580 (97%)	0.35	36 (6%)	26 19	24, 80, 169, 212	3 (0%)
2	E	266/325 (81%)	0.49	22 (8%)	17 13	48, 85, 161, 236	0
2	F	264/325 (81%)	0.72	23 (8%)	16 12	61, 118, 198, 267	0
2	G	15/325 (4%)	1.76	6 (40%)	1 0	145, 168, 208, 212	0
2	H	231/325 (71%)	1.24	41 (17%)	4 3	85, 135, 224, 283	0
All	All	3065/3620 (84%)	0.23	156 (5%)	33 26	20, 72, 169, 283	15 (0%)

All (156) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	824	LEU	6.5
1	B	1635	SER	5.9
1	D	1673	ILE	4.7
2	H	1072	LEU	4.7
2	H	1107	LEU	4.5
2	F	824	LEU	4.4
1	D	1686	ILE	4.3
1	D	1657	ILE	4.2
2	H	1086	LEU	4.1
2	F	825	LEU	4.1
2	H	1100	LEU	4.0
2	F	850	TRP	4.0
1	D	1755	ALA	3.9
2	H	1037	ASP	3.8
2	H	904	LEU	3.7
2	H	1073	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1656	PHE	3.6
1	D	1662	PRO	3.5
2	H	961	TRP	3.5
1	D	1762	GLN	3.5
2	H	1071	LEU	3.5
1	B	1755	ALA	3.5
1	D	1671	VAL	3.4
2	H	1049	TRP	3.4
2	F	1036	ARG	3.4
2	H	989	LYS	3.4
1	D	1659	ALA	3.3
1	D	1695	ILE	3.3
2	H	952	MET	3.3
2	H	1108	ILE	3.3
2	E	815	ASP	3.3
2	H	1024	LEU	3.3
2	H	1046	VAL	3.2
2	E	811	PRO	3.2
2	G	807	LYS	3.2
1	A	1649	SER	3.2
2	E	1116	LEU	3.1
1	B	1649	SER	3.1
2	G	808	LEU	3.1
1	D	1758	SER	3.0
2	H	1038	VAL	3.0
1	D	1670	LEU	3.0
2	E	806	ALA	3.0
2	H	1040	VAL	3.0
2	H	1085	LEU	2.9
2	H	1051	SER	2.9
2	F	819	LYS	2.9
2	H	876	ASP	2.9
1	D	1666	PHE	2.9
2	E	817	ARG	2.9
1	B	1386	ALA	2.8
1	C	1660	ASN	2.8
2	E	825	LEU	2.8
2	F	818	ASN	2.8
2	H	833	LEU	2.8
1	C	1636	VAL	2.7
2	E	835	PHE	2.7
2	H	825	LEU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	1454	GLU	2.7
1	D	1747	GLU	2.7
2	H	1005	VAL	2.7
2	H	1047	MET	2.7
2	H	1083	LEU	2.7
1	D	1765	VAL	2.7
1	D	1882	VAL	2.6
1	C	1651	ALA	2.6
1	D	1738	LEU	2.6
2	H	824	LEU	2.6
2	H	1012	MET	2.6
1	B	1339	ASP	2.6
1	B	1762	GLN	2.6
2	E	881	ARG	2.5
2	F	820	ARG	2.5
1	D	1694	TYR	2.5
2	E	829	CYS	2.5
1	D	1751	GLN	2.5
1	D	1764	PHE	2.5
2	H	951	ASP	2.5
1	D	1905	TYR	2.5
2	H	1099	LEU	2.5
1	D	1669	ARG	2.5
2	F	822	HIS	2.5
2	F	1099	LEU	2.4
1	D	1677	GLU	2.4
2	H	999	VAL	2.4
1	C	1758	SER	2.4
2	H	835	PHE	2.4
2	F	849	LEU	2.4
2	F	1035	ILE	2.4
1	C	1649	SER	2.4
2	F	906	SER	2.4
2	G	853	MET	2.4
1	C	1633	GLY	2.4
1	D	1722	ASP	2.4
2	H	1002	PHE	2.4
1	A	1654	SER	2.4
2	E	902	VAL	2.3
1	A	1789	ASP	2.3
1	A	1612[A]	HIS	2.3
1	C	1334	ILE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	1763	TYR	2.3
2	F	821	LYS	2.3
1	C	1828	GLN	2.3
2	H	1081	SER	2.3
1	D	1784	VAL	2.3
2	G	854	PRO	2.3
1	A	1348	ASP	2.3
2	E	813	ASP	2.3
2	G	809	THR	2.3
2	E	904	LEU	2.2
2	F	808	LEU	2.2
2	E	1095	GLN	2.2
1	B	1657	ILE	2.2
1	D	1836	THR	2.2
1	B	1458	VAL	2.2
1	D	1689	VAL	2.2
1	D	1757	ARG	2.2
1	D	1658	SER	2.2
2	H	1001	SER	2.2
2	E	814	LYS	2.2
2	H	1044	GLU	2.2
2	H	1026	ARG	2.2
2	E	905	THR	2.2
2	H	850	TRP	2.2
2	E	1019	TYR	2.2
1	C	1456	SER	2.2
2	F	1071	LEU	2.2
1	C	1655	ARG	2.1
2	H	881	ARG	2.1
1	B	1636	VAL	2.1
2	E	833	LEU	2.1
2	F	1055	LEU	2.1
1	D	1837	VAL	2.1
2	E	850	TRP	2.1
2	F	828	ALA	2.1
2	E	1076	GLU	2.1
2	F	883	ILE	2.1
2	F	1044	GLU	2.1
1	D	1678	LEU	2.1
2	H	905	THR	2.1
1	A	1655	ARG	2.1
2	H	1041	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	882	GLU	2.1
1	D	1667	LYS	2.0
2	F	1072	LEU	2.0
1	D	1457	ARG	2.0
2	F	1089	ILE	2.0
2	H	806	ALA	2.0
2	E	900	GLU	2.0
1	B	1632	PRO	2.0
1	D	1661	LEU	2.0
1	B	1757	ARG	2.0
2	F	839	ASP	2.0
1	D	1674	MET	2.0
2	F	1049	TRP	2.0
2	G	856	TRP	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
4	PO4	C	2003	5/5	0.50	0.20	156,159,161,164	0
4	PO4	B	2002	5/5	0.55	0.19	195,195,196,196	0
4	PO4	A	2002	5/5	0.56	0.17	207,207,209,210	0
4	PO4	D	2003	5/5	0.69	0.17	172,172,174,175	0
4	PO4	E	1201	5/5	0.78	0.15	157,157,158,159	0
6	P6G	D	2001	19/19	0.87	0.13	51,69,87,87	0
3	PG4	C	2001	13/13	0.88	0.14	60,67,73,77	0
5	PGE	D	2002	10/10	0.90	0.16	78,80,87,90	0
3	PG4	B	2001	13/13	0.91	0.11	53,59,72,72	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	PGE	C	2002	10/10	0.92	0.16	66,86,94,94	0
3	PG4	A	2001	13/13	0.97	0.08	29,40,45,57	0

6.5 Other polymers [i](#)

There are no such residues in this entry.