



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:19 PM UTC

PDB ID : 4AK8 / pdb_00004ak8
Title : Structure of F241L mutant of langerin carbohydrate recognition domain.
Authors : Chabrol, E.; Thepaut, M.; Dezutter-Dambuyant, C.; Vives, C.; Marcoux, J.; Kahn, R.; Valadeau-Guilemond, J.; Vachette, P.; Durand, D.; Fieschi, F.
Deposited on : 2012-02-22
Resolution : 1.40 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
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

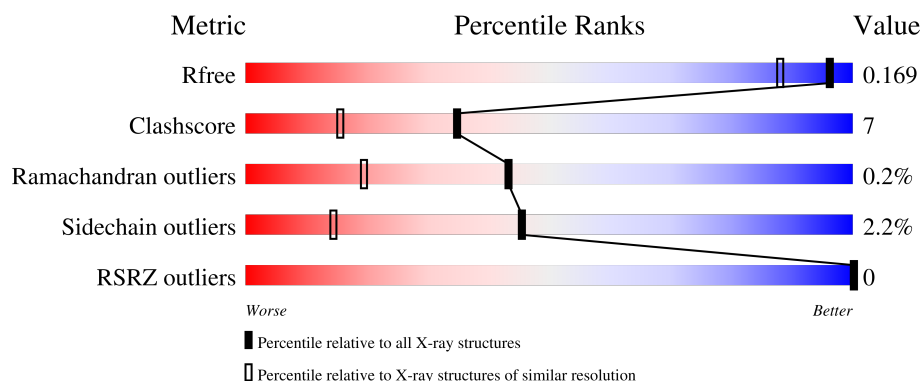
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	155	48% 32% 5% 16%
1	B	155	50% 30% • 17%
1	C	155	44% 36% • • 16%
1	D	155	57% 25% • 14%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5148 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 C-TYPE LECTIN DOMAIN FAMILY 4 MEMBER K.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	130	Total	C	N	O	S	0	2	0
			1069	692	175	197	5			
1	B	128	Total	C	N	O	S	0	6	0
			1075	703	176	191	5			
1	C	130	Total	C	N	O	S	0	5	0
			1083	705	176	197	5			
1	D	133	Total	C	N	O	S	0	5	0
			1105	718	179	203	5			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	174	MET	-	expression tag	UNP Q9UJ71
A	175	TRP	-	expression tag	UNP Q9UJ71
A	176	SER	-	expression tag	UNP Q9UJ71
A	177	HIS	-	expression tag	UNP Q9UJ71
A	178	PRO	-	expression tag	UNP Q9UJ71
A	179	GLN	-	expression tag	UNP Q9UJ71
A	180	PHE	-	expression tag	UNP Q9UJ71
A	181	GLU	-	expression tag	UNP Q9UJ71
A	182	LYS	-	expression tag	UNP Q9UJ71
A	183	ILE	-	expression tag	UNP Q9UJ71
A	184	GLU	-	expression tag	UNP Q9UJ71
A	185	GLY	-	expression tag	UNP Q9UJ71
A	186	ARG	-	expression tag	UNP Q9UJ71
A	187	MET	-	expression tag	UNP Q9UJ71
A	241	LEU	PHE	engineered mutation	UNP Q9UJ71
A	278	ALA	VAL	variant	UNP Q9UJ71
B	174	MET	-	expression tag	UNP Q9UJ71
B	175	TRP	-	expression tag	UNP Q9UJ71
B	176	SER	-	expression tag	UNP Q9UJ71
B	177	HIS	-	expression tag	UNP Q9UJ71
B	178	PRO	-	expression tag	UNP Q9UJ71

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	179	GLN	-	expression tag	UNP Q9UJ71
B	180	PHE	-	expression tag	UNP Q9UJ71
B	181	GLU	-	expression tag	UNP Q9UJ71
B	182	LYS	-	expression tag	UNP Q9UJ71
B	183	ILE	-	expression tag	UNP Q9UJ71
B	184	GLU	-	expression tag	UNP Q9UJ71
B	185	GLY	-	expression tag	UNP Q9UJ71
B	186	ARG	-	expression tag	UNP Q9UJ71
B	187	MET	-	expression tag	UNP Q9UJ71
B	241	LEU	PHE	engineered mutation	UNP Q9UJ71
B	278	ALA	VAL	variant	UNP Q9UJ71
C	174	MET	-	expression tag	UNP Q9UJ71
C	175	TRP	-	expression tag	UNP Q9UJ71
C	176	SER	-	expression tag	UNP Q9UJ71
C	177	HIS	-	expression tag	UNP Q9UJ71
C	178	PRO	-	expression tag	UNP Q9UJ71
C	179	GLN	-	expression tag	UNP Q9UJ71
C	180	PHE	-	expression tag	UNP Q9UJ71
C	181	GLU	-	expression tag	UNP Q9UJ71
C	182	LYS	-	expression tag	UNP Q9UJ71
C	183	ILE	-	expression tag	UNP Q9UJ71
C	184	GLU	-	expression tag	UNP Q9UJ71
C	185	GLY	-	expression tag	UNP Q9UJ71
C	186	ARG	-	expression tag	UNP Q9UJ71
C	187	MET	-	expression tag	UNP Q9UJ71
C	241	LEU	PHE	engineered mutation	UNP Q9UJ71
C	278	ALA	VAL	variant	UNP Q9UJ71
D	174	MET	-	expression tag	UNP Q9UJ71
D	175	TRP	-	expression tag	UNP Q9UJ71
D	176	SER	-	expression tag	UNP Q9UJ71
D	177	HIS	-	expression tag	UNP Q9UJ71
D	178	PRO	-	expression tag	UNP Q9UJ71
D	179	GLN	-	expression tag	UNP Q9UJ71
D	180	PHE	-	expression tag	UNP Q9UJ71
D	181	GLU	-	expression tag	UNP Q9UJ71
D	182	LYS	-	expression tag	UNP Q9UJ71
D	183	ILE	-	expression tag	UNP Q9UJ71
D	184	GLU	-	expression tag	UNP Q9UJ71
D	185	GLY	-	expression tag	UNP Q9UJ71
D	186	ARG	-	expression tag	UNP Q9UJ71
D	187	MET	-	expression tag	UNP Q9UJ71
D	241	LEU	PHE	engineered mutation	UNP Q9UJ71

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	278	ALA	VAL	variant	UNP Q9UJ71

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ca 1 1	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0
2	D	1	Total Ca 1 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	D	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	225	Total O 225 225	0	0
5	B	209	Total O 209 209	0	0
5	C	174	Total O 174 174	0	0

Continued on next page...

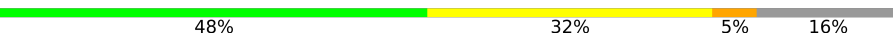
Continued from previous page...

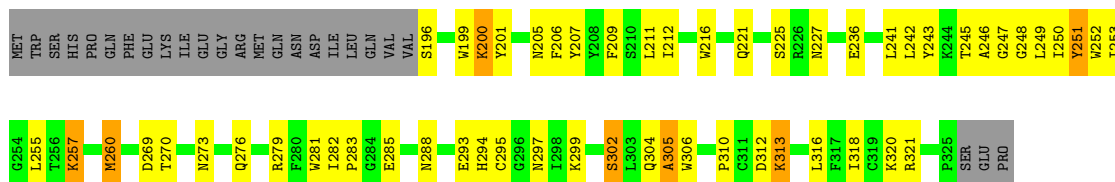
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	199	Total 199	O 199	0	0

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.

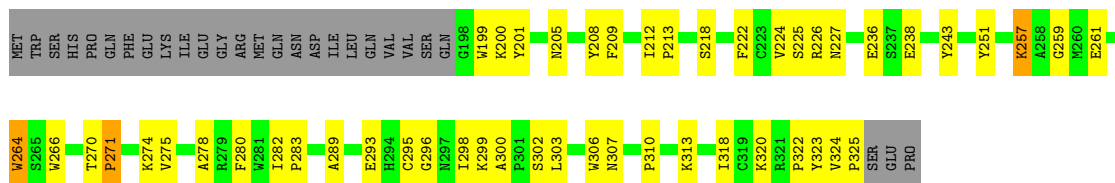
• Molecule 1: C-TYPE LECTIN DOMAIN FAMILY 4 MEMBER K

Chain A: 

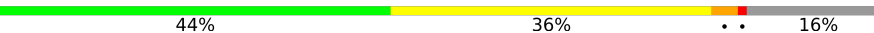


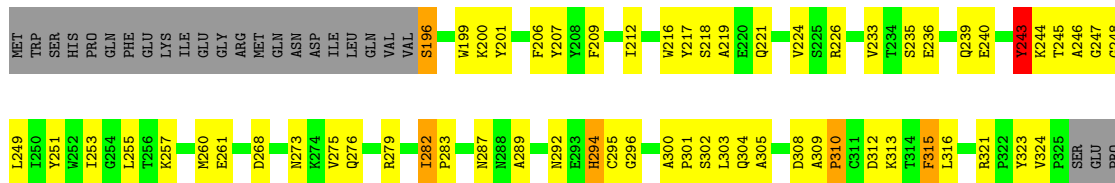
• Molecule 1: C-TYPE LECTIN DOMAIN FAMILY 4 MEMBER K

Chain B: 



• Molecule 1: C-TYPE LECTIN DOMAIN FAMILY 4 MEMBER K

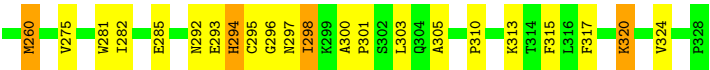
Chain C: 



• Molecule 1: C-TYPE LECTIN DOMAIN FAMILY 4 MEMBER K

Chain D: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 42	Depositor
Cell constants a, b, c, α , β , γ	79.96Å 79.96Å 90.42Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.52 – 1.40 19.52 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.2 (19.52-1.40) 99.3 (19.52-1.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.65 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.175 , 0.219 0.177 , 0.169	Depositor DCC
R_{free} test set	5599 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	13.6	Xtriage
Anisotropy	0.009	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.104 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5148	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.14% 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: CL, MG, CA

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	2.36	45/1110 (4.1%)	1.89	19/1511 (1.3%)
1	B	2.23	43/1128 (3.8%)	1.73	15/1534 (1.0%)
1	C	2.31	43/1136 (3.8%)	1.91	29/1545 (1.9%)
1	D	2.13	35/1159 (3.0%)	1.69	5/1575 (0.3%)
All	All	2.26	166/4533 (3.7%)	1.81	68/6165 (1.1%)

All (166) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	212	ILE	CA-C	12.93	1.61	1.52
1	B	212	ILE	CA-CB	10.59	1.62	1.54
1	A	282	ILE	CA-CB	-9.49	1.41	1.54
1	B	296	GLY	CA-C	-9.48	1.43	1.52
1	D	275	VAL	CA-CB	9.48	1.65	1.54
1	D	247	GLY	N-CA	9.26	1.58	1.45
1	A	255	LEU	CA-C	-9.16	1.40	1.52
1	B	266	TRP	C-O	9.08	1.35	1.24
1	C	249	LEU	CA-C	8.97	1.65	1.53
1	C	209	PHE	C-O	8.87	1.34	1.24
1	A	295	CYS	N-CA	8.72	1.57	1.45
1	D	295	CYS	N-CA	8.13	1.56	1.45
1	A	250	ILE	N-CA	8.13	1.56	1.46
1	A	221	GLN	C-O	8.07	1.33	1.24
1	C	219	ALA	CA-CB	-8.01	1.41	1.53
1	C	310	PRO	N-CA	-7.78	1.37	1.47
1	C	244	LYS	N-CA	7.63	1.55	1.46
1	A	200	LYS	N-CA	-7.62	1.36	1.46
1	C	295	CYS	CA-C	-7.61	1.43	1.52
1	C	212	ILE	CA-CB	-7.60	1.48	1.54
1	D	217	TYR	N-CA	-7.60	1.37	1.46
1	A	245	THR	CA-CB	7.58	1.65	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	323	TYR	N-CA	7.49	1.55	1.46
1	A	207	TYR	C-O	7.47	1.33	1.23
1	B	282	ILE	C-N	7.39	1.42	1.33
1	B	280	PHE	C-O	7.31	1.34	1.23
1	A	205	ASN	CG-ND2	-7.27	1.18	1.33
1	B	275	VAL	CA-CB	7.20	1.63	1.54
1	D	206	PHE	CD1-CE1	7.16	1.60	1.38
1	B	295	CYS	C-O	7.11	1.32	1.23
1	C	233	VAL	CA-C	-7.10	1.44	1.52
1	A	246	ALA	CA-C	7.04	1.62	1.52
1	D	217	TYR	CA-CB	6.96	1.64	1.53
1	D	197	GLN	C-O	6.89	1.33	1.23
1	A	293	GLU	N-CA	6.88	1.56	1.46
1	A	243	TYR	CG-CD1	6.86	1.53	1.39
1	B	213	PRO	C-O	6.84	1.31	1.23
1	C	224	VAL	CA-C	6.80	1.61	1.52
1	A	225	SER	C-O	6.79	1.32	1.24
1	C	282	ILE	CA-CB	-6.79	1.45	1.54
1	C	255	LEU	CA-C	-6.78	1.44	1.52
1	D	310	PRO	CA-CB	6.78	1.62	1.53
1	A	313	LYS	N-CA	6.78	1.54	1.46
1	D	224	VAL	N-CA	6.74	1.54	1.46
1	D	281	TRP	CA-C	6.73	1.61	1.52
1	B	224	VAL	CA-CB	-6.68	1.46	1.54
1	C	218	SER	CA-C	6.66	1.61	1.52
1	B	257	LYS	CA-C	6.65	1.62	1.53
1	C	273	ASN	CA-CB	-6.63	1.44	1.53
1	C	247	GLY	N-CA	6.62	1.54	1.45
1	B	278	ALA	C-O	6.58	1.32	1.24
1	C	289	ALA	N-CA	6.58	1.54	1.46
1	A	246	ALA	CA-CB	6.57	1.64	1.53
1	B	325	PRO	N-CA	6.56	1.56	1.47
1	A	253	ILE	CA-CB	-6.55	1.45	1.54
1	D	218	SER	CA-C	6.52	1.61	1.52
1	B	300	ALA	C-O	6.50	1.32	1.23
1	B	306	TRP	C-O	6.49	1.31	1.23
1	A	281	TRP	CA-C	6.45	1.61	1.52
1	A	312	ASP	CA-C	6.44	1.61	1.52
1	D	324	VAL	CA-C	6.43	1.59	1.52
1	B	282	ILE	C-O	-6.42	1.16	1.24
1	B	199	TRP	C-O	6.40	1.31	1.23
1	C	287	ASN	N-CA	6.37	1.54	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	201	TYR	CA-C	-6.31	1.45	1.52
1	C	308	ASP	CA-CB	6.25	1.62	1.53
1	C	305	ALA	N-CA	-6.23	1.38	1.46
1	C	246	ALA	CA-C	6.23	1.61	1.52
1	C	309	ALA	CA-C	-6.20	1.45	1.52
1	A	299	LYS	N-CA	6.18	1.53	1.46
1	A	302	SER	CA-CB	6.15	1.64	1.53
1	D	297	ASN	N-CA	6.11	1.53	1.45
1	D	221	GLN	CA-C	6.09	1.60	1.52
1	D	300	ALA	CA-CB	-6.04	1.44	1.53
1	B	205	ASN	C-O	6.02	1.31	1.23
1	B	302	SER	C-O	6.02	1.31	1.23
1	D	242	LEU	C-O	-5.98	1.17	1.24
1	A	206	PHE	C-O	5.97	1.31	1.23
1	D	213	PRO	CA-CB	-5.95	1.47	1.54
1	C	246	ALA	C-O	-5.95	1.16	1.24
1	B	300	ALA	CA-CB	-5.94	1.44	1.53
1	B	282	ILE	N-CA	5.93	1.53	1.46
1	B	222	PHE	C-O	5.91	1.30	1.24
1	A	282	ILE	N-CA	5.91	1.53	1.47
1	D	219	ALA	CA-CB	-5.90	1.44	1.53
1	D	282	ILE	N-CA	5.87	1.53	1.46
1	A	283	PRO	C-O	-5.87	1.16	1.23
1	C	282	ILE	C-O	-5.84	1.17	1.25
1	C	302	SER	N-CA	-5.83	1.38	1.45
1	D	296	GLY	N-CA	5.79	1.51	1.45
1	D	317	PHE	N-CA	5.79	1.53	1.45
1	B	324	VAL	N-CA	5.76	1.53	1.46
1	C	268	ASP	N-CA	5.71	1.53	1.46
1	C	273	ASN	CA-C	5.71	1.60	1.53
1	A	299	LYS	CA-C	-5.71	1.46	1.52
1	A	250	ILE	CA-CB	-5.70	1.47	1.54
1	B	274	LYS	N-CA	5.70	1.53	1.46
1	C	302	SER	CA-C	5.70	1.59	1.52
1	C	321	ARG	CA-CB	5.70	1.65	1.54
1	D	229	HIS	CA-CB	5.68	1.64	1.54
1	C	255	LEU	CB-CG	-5.64	1.42	1.53
1	A	306	TRP	CA-CB	5.61	1.61	1.53
1	A	299	LYS	C-O	5.60	1.31	1.24
1	A	321	ARG	CA-CB	-5.60	1.44	1.53
1	B	282	ILE	CA-C	5.59	1.58	1.52
1	A	273	ASN	C-O	5.56	1.30	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	247	GLY	CA-C	5.54	1.57	1.51
1	B	264	TRP	CA-CB	-5.53	1.44	1.53
1	B	271	PRO	N-CD	5.52	1.55	1.47
1	B	275	VAL	CA-C	-5.51	1.45	1.52
1	D	293	GLU	N-CA	5.50	1.54	1.46
1	D	300	ALA	N-CA	5.48	1.54	1.45
1	D	224	VAL	CA-CB	5.48	1.61	1.54
1	A	201	TYR	C-O	5.48	1.30	1.24
1	A	209	PHE	CA-C	-5.46	1.46	1.52
1	B	293	GLU	N-CA	5.39	1.54	1.46
1	B	283	PRO	CG-CD	5.38	1.69	1.50
1	B	209	PHE	N-CA	-5.36	1.39	1.46
1	A	269	ASP	N-CA	5.34	1.53	1.46
1	A	252	TRP	N-CA	5.34	1.52	1.46
1	A	283	PRO	N-CA	5.33	1.53	1.47
1	B	271	PRO	C-O	5.33	1.29	1.23
1	C	216	TRP	CA-C	-5.33	1.45	1.52
1	D	231	THR	CA-CB	5.32	1.62	1.53
1	A	270	THR	CA-CB	5.31	1.61	1.53
1	B	303	LEU	CA-CB	5.31	1.62	1.53
1	C	275	VAL	CB-CG1	5.30	1.70	1.52
1	D	300	ALA	CA-C	-5.28	1.46	1.52
1	D	285	GLU	CA-C	5.26	1.59	1.52
1	B	280	PHE	CE1-CZ	5.26	1.54	1.38
1	D	301	PRO	N-CA	-5.26	1.40	1.47
1	A	250	ILE	CA-C	5.25	1.59	1.52
1	D	249	LEU	C-O	-5.25	1.17	1.23
1	C	301	PRO	CA-CB	-5.25	1.47	1.53
1	A	285	GLU	C-O	-5.23	1.18	1.24
1	D	317	PHE	CA-C	-5.22	1.46	1.52
1	C	226	ARG	CG-CD	-5.22	1.36	1.52
1	C	217	TYR	CA-CB	5.22	1.61	1.53
1	A	257	LYS	N-CA	5.20	1.52	1.46
1	A	225	SER	N-CA	5.20	1.53	1.46
1	B	199	TRP	N-CA	5.20	1.52	1.46
1	D	212	ILE	CA-CB	-5.19	1.47	1.54
1	B	300	ALA	N-CA	5.19	1.54	1.45
1	C	296	GLY	CA-C	5.18	1.56	1.51
1	B	218	SER	CB-OG	5.18	1.52	1.42
1	D	224	VAL	CA-C	5.17	1.59	1.52
1	B	320	LYS	CD-CE	-5.16	1.36	1.52
1	A	297	ASN	C-N	5.14	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	233	VAL	CA-CB	5.14	1.61	1.54
1	C	216	TRP	N-CA	5.14	1.52	1.46
1	A	216	TRP	C-O	5.11	1.29	1.24
1	D	294	HIS	N-CA	5.11	1.52	1.46
1	B	225	SER	N-CA	5.11	1.53	1.46
1	C	309	ALA	CA-CB	5.08	1.60	1.53
1	D	234	THR	CB-OG1	-5.08	1.35	1.43
1	B	307	ASN	N-CA	-5.08	1.39	1.45
1	A	288	ASN	CB-CG	-5.05	1.39	1.52
1	C	248	GLY	C-N	5.05	1.40	1.33
1	A	242	LEU	CA-CB	5.04	1.61	1.53
1	A	318	ILE	CB-CG1	5.04	1.63	1.53
1	C	316	LEU	N-CA	5.03	1.52	1.45
1	B	310	PRO	N-CA	-5.03	1.41	1.47
1	C	207	TYR	N-CA	5.02	1.52	1.46
1	C	275	VAL	CA-CB	-5.02	1.48	1.54
1	B	295	CYS	N-CA	5.02	1.52	1.45
1	B	270	THR	CA-CB	5.01	1.60	1.53

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	246	ALA	O-C-N	10.71	134.75	122.22
1	A	205	ASN	CA-C-O	-10.13	109.25	121.11
1	C	305	ALA	N-CA-C	9.09	125.06	113.88
1	C	239	GLN	O-C-N	7.64	130.22	122.12
1	A	251	TYR	O-C-N	7.58	132.18	123.31
1	C	309	ALA	O-C-N	-7.16	116.42	121.65
1	A	205	ASN	OD1-CG-ND2	6.92	129.51	122.60
1	A	246	ALA	O-C-N	6.85	130.23	122.22
1	A	248	GLY	O-C-N	-6.80	113.76	122.39
1	A	248	GLY	CA-C-O	6.78	126.55	119.02
1	A	276	GLN	N-CA-C	-6.76	105.03	113.28
1	B	278	ALA	CA-C-O	-6.44	112.82	120.10
1	D	208	TYR	O-C-N	-6.33	115.81	123.27
1	B	295	CYS	CA-C-N	6.32	126.54	122.18
1	B	295	CYS	C-N-CA	6.32	126.54	122.18
1	B	226	ARG	N-CA-C	-6.21	105.01	112.59
1	B	322	PRO	CB-CA-C	-6.21	102.96	111.21
1	C	245	THR	N-CA-C	6.14	117.97	111.28
1	C	244	LYS	N-CA-C	-6.11	104.54	111.14
1	A	305	ALA	CA-C-O	6.11	126.69	119.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	SER	CA-C-O	6.10	127.98	121.45
1	B	201	TYR	O-C-N	-6.09	115.48	123.21
1	A	297	ASN	CA-C-O	6.07	128.62	121.58
1	C	315	PHE	O-C-N	6.01	130.44	123.17
1	B	238	GLU	CA-C-O	-5.96	114.10	120.42
1	B	271	PRO	CB-CA-C	-5.96	103.77	111.46
1	B	323	TYR	CE1-CZ-CE2	5.92	132.13	120.30
1	C	243	TYR	O-C-N	5.86	129.48	122.27
1	A	205	ASN	N-CA-C	5.85	118.75	109.50
1	D	320	LYS	CD-CE-NZ	-5.75	93.51	111.90
1	C	292	ASN	CA-C-O	-5.70	114.50	120.32
1	A	312	ASP	O-C-N	5.70	130.23	122.37
1	A	297	ASN	O-C-N	-5.59	115.28	122.94
1	C	239	GLN	N-CA-C	5.58	117.37	111.28
1	C	219	ALA	N-CA-C	-5.57	105.11	111.07
1	A	260	MET	CB-CG-SD	-5.53	96.12	112.70
1	D	224	VAL	O-C-N	5.51	127.21	121.87
1	A	299	LYS	CA-C-O	-5.46	113.42	119.81
1	C	302	SER	CA-C-O	-5.43	115.47	121.33
1	C	255	LEU	O-C-N	-5.43	116.69	123.04
1	C	295	CYS	O-C-N	-5.42	116.61	123.17
1	C	305	ALA	CA-C-O	5.33	125.26	119.24
1	B	266	TRP	CA-C-O	-5.32	114.58	120.38
1	C	247	GLY	N-CA-C	-5.28	105.72	114.48
1	A	306	TRP	CA-C-O	-5.27	115.04	121.05
1	C	251	TYR	O-C-N	5.26	129.46	123.31
1	A	251	TYR	CA-C-N	-5.25	113.25	120.71
1	A	251	TYR	C-N-CA	-5.25	113.25	120.71
1	C	312	ASP	CA-C-O	-5.24	113.09	119.43
1	C	200	LYS	O-C-N	-5.22	117.12	123.29
1	B	226	ARG	CA-C-O	-5.22	113.79	119.95
1	A	249	LEU	O-C-N	5.21	129.10	123.10
1	A	255	LEU	CA-C-O	5.20	126.79	120.81
1	C	236	GLU	N-CA-C	5.20	116.94	111.28
1	B	289	ALA	N-CA-C	5.18	117.60	110.35
1	C	249	LEU	CA-C-O	-5.17	115.62	121.72
1	C	300	ALA	N-CA-C	-5.17	103.01	110.40
1	B	236	GLU	O-C-N	-5.14	116.68	122.12
1	D	201	TYR	N-CA-C	5.12	117.86	110.28
1	C	245	THR	CA-C-O	5.12	125.98	120.55
1	C	218	SER	CA-CB-OG	-5.11	100.87	111.10
1	C	273	ASN	CA-C-O	-5.10	115.33	120.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	278	ALA	N-CA-C	-5.10	105.84	111.71
1	C	236	GLU	N-CA-CB	-5.10	102.62	110.12
1	B	275	VAL	O-C-N	-5.09	116.59	121.83
1	C	294	HIS	O-C-N	5.06	128.27	122.25
1	C	253	ILE	O-C-N	-5.03	116.29	122.57
1	D	315	PHE	O-C-N	-5.02	117.53	123.25

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	1069	0	997	20	0
1	B	1075	0	1036	16	0
1	C	1083	0	1030	23	0
1	D	1105	0	1051	13	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	D	1	0	0	0	0
5	A	225	0	0	5	0
5	B	209	0	0	6	0
5	C	174	0	0	1	0
5	D	199	0	0	3	0
All	All	5148	0	4114	63	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 (63) 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:A:227:ASN:HB2	1:C:260:MET:CE	1.68	1.22
1:A:227:ASN:CB	1:C:260:MET:HE3	1.81	1.10
1:A:227:ASN:HB2	1:C:260:MET:HE3	1.12	1.09
1:B:227:ASN:HB2	1:D:260:MET:SD	2.02	0.99
1:B:251:TYR:HB2	1:B:298[B]:ILE:HD11	1.52	0.92
1:C:276:GLN:O	1:C:279:ARG:NH1	2.07	0.86
1:B:200[B]:LYS:HD2	5:B:2007:HOH:O	1.82	0.80
1:A:236[A]:GLU:HG3	1:A:279:ARG:NH1	1.98	0.79
1:A:227:ASN:HB2	1:C:260:MET:HE2	1.64	0.78
1:C:196:SER:HB3	1:C:199:TRP:HE1	1.52	0.74
1:A:196:SER:HB2	5:A:2002:HOH:O	1.87	0.73
1:A:227:ASN:CG	1:C:260:MET:HE3	2.13	0.73
1:D:240[A]:GLU:HG3	1:D:303:LEU:HD21	1.76	0.68
1:B:227:ASN:CB	1:D:260:MET:SD	2.82	0.67
1:D:313[A]:LYS:HE2	5:D:2181:HOH:O	1.95	0.66
1:B:298[B]:ILE:HD13	1:B:298[B]:ILE:H	1.61	0.65
1:D:298[B]:ILE:HG13	1:D:305:ALA:HB1	1.80	0.61
1:D:320:LYS:HE2	5:D:2187:HOH:O	1.99	0.61
1:C:257:LYS:NZ	1:C:294:HIS:HD2	1.99	0.61
1:D:257:LYS:NZ	1:D:294:HIS:HD2	1.98	0.61
1:B:251:TYR:O	1:B:298[B]:ILE:HD13	2.00	0.60
1:A:227:ASN:CB	1:C:260:MET:CE	2.56	0.60
1:B:298[A]:ILE:CG2	5:B:2185:HOH:O	2.50	0.59
1:D:257:LYS:HZ2	1:D:294:HIS:HD2	1.50	0.58
1:D:298[B]:ILE:HG13	1:D:305:ALA:CB	2.34	0.57
1:A:320:LYS:HE2	5:A:2218:HOH:O	2.03	0.57
1:C:261:GLU:N	1:C:261:GLU:OE1	2.40	0.55
1:B:298[A]:ILE:HG23	5:B:2185:HOH:O	2.05	0.54
1:C:240[B]:GLU:HG3	1:C:303:LEU:HD21	1.89	0.53
1:C:310:PRO:HG2	1:C:313[B]:LYS:HE3	1.90	0.53
1:C:310:PRO:HD2	1:C:313[B]:LYS:HD2	1.89	0.53
1:B:299[B]:LYS:HE2	5:B:2181:HOH:O	2.09	0.52
1:C:294:HIS:HE1	5:C:2141:HOH:O	1.93	0.52
1:D:292[B]:ASN:OD1	5:D:2146:HOH:O	2.19	0.51
1:A:196:SER:HB3	1:A:199:TRP:HE1	1.76	0.50
1:A:294:HIS:HE1	5:A:2172:HOH:O	1.93	0.50
1:B:200[B]:LYS:CD	5:B:2007:HOH:O	2.53	0.49
1:B:257:LYS:HE3	1:B:264:TRP:CZ2	2.48	0.48
1:A:257:LYS:NZ	1:A:294:HIS:HD2	2.12	0.48
1:A:211:LEU:O	1:A:212:ILE:HD13	2.14	0.46
1:A:200:LYS:NZ	5:A:2009:HOH:O	2.49	0.46
1:A:313:LYS:HE3	1:A:313:LYS:HB3	1.51	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:TYR:HB2	5:B:2185:HOH:O	2.16	0.45
1:C:324:VAL:O	1:C:324:VAL:HG23	2.16	0.45
1:C:206:PHE:CE2	1:C:323:TYR:HD2	2.35	0.44
1:B:208:TYR:O	1:B:318:ILE:HA	2.17	0.44
1:D:200:LYS:HE2	1:D:200:LYS:HB3	1.67	0.43
1:C:243:TYR:C	1:C:243:TYR:CD1	2.96	0.43
1:C:313[A]:LYS:HD3	1:C:315:PHE:CZ	2.54	0.43
1:B:313:LYS:HE3	1:B:313:LYS:HB3	1.60	0.43
1:C:257:LYS:NZ	1:C:294:HIS:CD2	2.85	0.42
1:C:282:ILE:HA	1:C:304[A]:GLN:HB3	2.01	0.42
1:A:302:SER:O	1:A:305:ALA:HB2	2.20	0.42
1:A:304[B]:GLN:NE2	5:A:2206:HOH:O	2.39	0.42
1:A:294:HIS:HB2	1:C:221[B]:GLN:OE1	2.20	0.41
1:D:243:TYR:CD1	1:D:243:TYR:C	2.98	0.41
1:C:257:LYS:HZ2	1:C:294:HIS:CD2	2.39	0.41
1:D:222:PHE:C	1:D:222:PHE:CD1	2.98	0.41
1:A:310:PRO:HD2	1:A:313:LYS:HG3	2.03	0.41
1:A:251:TYR:HA	1:A:316:LEU:O	2.20	0.41
1:B:251:TYR:HB2	1:B:298[B]:ILE:CD1	2.36	0.41
1:C:310:PRO:HD2	1:C:313[B]:LYS:CD	2.50	0.41

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	130/155 (84%)	128 (98%)	2 (2%)	0	100	100
1	B	132/155 (85%)	125 (95%)	6 (4%)	1 (1%)	16	3
1	C	133/155 (86%)	132 (99%)	1 (1%)	0	100	100
1	D	136/155 (88%)	131 (96%)	5 (4%)	0	100	100
All	All	531/620 (86%)	516 (97%)	14 (3%)	1 (0%)	43	19

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	259	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/136 (84%)	112 (98%)	2 (2%)	51	20
1	B	116/136 (85%)	114 (98%)	2 (2%)	53	21
1	C	117/136 (86%)	114 (97%)	3 (3%)	40	11
1	D	120/136 (88%)	116 (97%)	4 (3%)	33	7
All	All	467/544 (86%)	456 (98%)	11 (2%)	45	12

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	LEU
1	A	260	MET
1	B	261	GLU
1	B	271	PRO
1	C	196	SER
1	C	243	TYR
1	C	283	PRO
1	D	243	TYR
1	D	260	MET
1	D	298[A]	ILE
1	D	298[B]	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	291	ASN
1	A	294	HIS
1	B	294	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	294	HIS
1	D	221	GLN
1	D	294	HIS

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 ⓘ

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

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 ⓘ

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	130/155 (83%)	-1.36	0 100 100	9, 13, 26, 50	2 (1%)
1	B	128/155 (82%)	-1.31	0 100 100	6, 14, 30, 42	6 (4%)
1	C	130/155 (83%)	-1.32	0 100 100	8, 15, 29, 44	5 (3%)
1	D	133/155 (85%)	-1.34	0 100 100	7, 14, 27, 43	5 (3%)
All	All	521/620 (84%)	-1.33	0 100 100	6, 14, 29, 50	18 (3%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	CA	A	1326	1/1	1.00	0.00	16,16,16,16	0
2	CA	B	1326	1/1	1.00	0.01	19,19,19,19	0
2	CA	C	1326	1/1	1.00	0.01	19,19,19,19	0
2	CA	D	1330	1/1	1.00	0.01	16,16,16,16	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	A	1327	1/1	1.00	0.03	20,20,20,20	0
3	MG	B	1327	1/1	1.00	0.02	20,20,20,20	0
3	MG	C	1327	1/1	1.00	0.03	21,21,21,21	0
3	MG	D	1331	1/1	1.00	0.02	13,13,13,13	0
4	CL	D	1329	1/1	1.00	0.03	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.