



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:40 AM UTC

PDB ID : 6EY0 / pdb_00006ey0
Title : N-terminal part (residues 30-212) of PorM with the llama nanobody nb01
Authors : Leone, P.; Roche, J.; Cambillau, C.; Roussel, A.
Deposited on : 2017-11-10
Resolution : 2.40 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

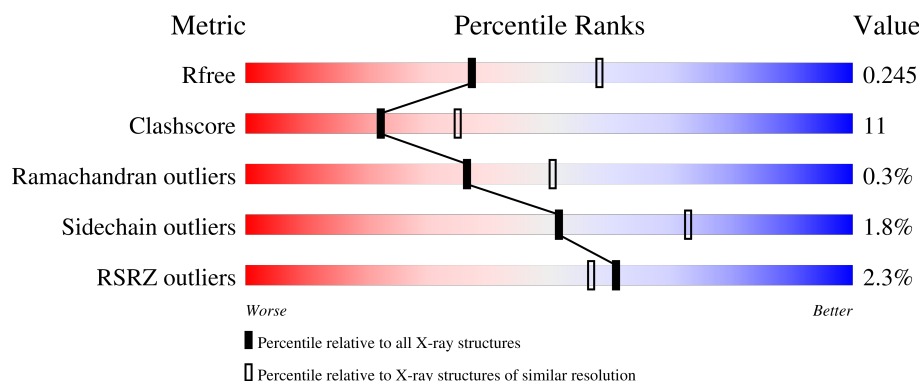
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	197	2% 55% 16% • 25%
1	B	197	% 58% 15% •• 25%
1	C	197	% 61% 13% •• 25%
1	D	197	4% 55% 16% • 27%
2	E	134	3% 69% 23% • 7%

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Mol	Chain	Length	Quality of chain	
2	G	134	3% 80% 16%	•
2	H	134	1% 74% 19% 7%	
3	F	136	1% 86% 10%	•

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8729 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 T9SS component cytoplasmic membrane protein PorM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	147	Total	C	N	O	S	0	0	0
			1150	722	198	226	4			
1	B	148	Total	C	N	O	S	0	0	0
			1157	726	199	228	4			
1	C	147	Total	C	N	O	S	0	0	0
			1150	722	198	226	4			
1	D	144	Total	C	N	O	S	0	0	0
			1126	708	194	220	4			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	MET	-	initiating methionine	UNP A0A1R4DSC1
A	22	GLY	-	expression tag	UNP A0A1R4DSC1
A	23	HIS	-	expression tag	UNP A0A1R4DSC1
A	24	HIS	-	expression tag	UNP A0A1R4DSC1
A	25	HIS	-	expression tag	UNP A0A1R4DSC1
A	26	HIS	-	expression tag	UNP A0A1R4DSC1
A	27	HIS	-	expression tag	UNP A0A1R4DSC1
A	28	HIS	-	expression tag	UNP A0A1R4DSC1
A	29	SER	-	expression tag	UNP A0A1R4DSC1
A	30	SER	-	expression tag	UNP A0A1R4DSC1
A	31	GLY	-	expression tag	UNP A0A1R4DSC1
A	32	VAL	-	expression tag	UNP A0A1R4DSC1
A	33	ASP	-	expression tag	UNP A0A1R4DSC1
A	34	LEU	-	expression tag	UNP A0A1R4DSC1
A	35	GLY	-	expression tag	UNP A0A1R4DSC1
A	36	THR	-	expression tag	UNP A0A1R4DSC1
A	37	GLU	-	expression tag	UNP A0A1R4DSC1
A	38	ASN	-	expression tag	UNP A0A1R4DSC1
A	39	LEU	-	expression tag	UNP A0A1R4DSC1
A	40	TYR	-	expression tag	UNP A0A1R4DSC1
A	41	PHE	-	expression tag	UNP A0A1R4DSC1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	42	GLN	-	expression tag	UNP A0A1R4DSC1
A	43	SER	-	expression tag	UNP A0A1R4DSC1
B	21	MET	-	initiating methionine	UNP A0A1R4DSC1
B	22	GLY	-	expression tag	UNP A0A1R4DSC1
B	23	HIS	-	expression tag	UNP A0A1R4DSC1
B	24	HIS	-	expression tag	UNP A0A1R4DSC1
B	25	HIS	-	expression tag	UNP A0A1R4DSC1
B	26	HIS	-	expression tag	UNP A0A1R4DSC1
B	27	HIS	-	expression tag	UNP A0A1R4DSC1
B	28	HIS	-	expression tag	UNP A0A1R4DSC1
B	29	SER	-	expression tag	UNP A0A1R4DSC1
B	30	SER	-	expression tag	UNP A0A1R4DSC1
B	31	GLY	-	expression tag	UNP A0A1R4DSC1
B	32	VAL	-	expression tag	UNP A0A1R4DSC1
B	33	ASP	-	expression tag	UNP A0A1R4DSC1
B	34	LEU	-	expression tag	UNP A0A1R4DSC1
B	35	GLY	-	expression tag	UNP A0A1R4DSC1
B	36	THR	-	expression tag	UNP A0A1R4DSC1
B	37	GLU	-	expression tag	UNP A0A1R4DSC1
B	38	ASN	-	expression tag	UNP A0A1R4DSC1
B	39	LEU	-	expression tag	UNP A0A1R4DSC1
B	40	TYR	-	expression tag	UNP A0A1R4DSC1
B	41	PHE	-	expression tag	UNP A0A1R4DSC1
B	42	GLN	-	expression tag	UNP A0A1R4DSC1
B	43	SER	-	expression tag	UNP A0A1R4DSC1
C	21	MET	-	initiating methionine	UNP A0A1R4DSC1
C	22	GLY	-	expression tag	UNP A0A1R4DSC1
C	23	HIS	-	expression tag	UNP A0A1R4DSC1
C	24	HIS	-	expression tag	UNP A0A1R4DSC1
C	25	HIS	-	expression tag	UNP A0A1R4DSC1
C	26	HIS	-	expression tag	UNP A0A1R4DSC1
C	27	HIS	-	expression tag	UNP A0A1R4DSC1
C	28	HIS	-	expression tag	UNP A0A1R4DSC1
C	29	SER	-	expression tag	UNP A0A1R4DSC1
C	30	SER	-	expression tag	UNP A0A1R4DSC1
C	31	GLY	-	expression tag	UNP A0A1R4DSC1
C	32	VAL	-	expression tag	UNP A0A1R4DSC1
C	33	ASP	-	expression tag	UNP A0A1R4DSC1
C	34	LEU	-	expression tag	UNP A0A1R4DSC1
C	35	GLY	-	expression tag	UNP A0A1R4DSC1
C	36	THR	-	expression tag	UNP A0A1R4DSC1
C	37	GLU	-	expression tag	UNP A0A1R4DSC1

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Chain	Residue	Modelled	Actual	Comment	Reference
C	38	ASN	-	expression tag	UNP A0A1R4DSC1
C	39	LEU	-	expression tag	UNP A0A1R4DSC1
C	40	TYR	-	expression tag	UNP A0A1R4DSC1
C	41	PHE	-	expression tag	UNP A0A1R4DSC1
C	42	GLN	-	expression tag	UNP A0A1R4DSC1
C	43	SER	-	expression tag	UNP A0A1R4DSC1
D	21	MET	-	initiating methionine	UNP A0A1R4DSC1
D	22	GLY	-	expression tag	UNP A0A1R4DSC1
D	23	HIS	-	expression tag	UNP A0A1R4DSC1
D	24	HIS	-	expression tag	UNP A0A1R4DSC1
D	25	HIS	-	expression tag	UNP A0A1R4DSC1
D	26	HIS	-	expression tag	UNP A0A1R4DSC1
D	27	HIS	-	expression tag	UNP A0A1R4DSC1
D	28	HIS	-	expression tag	UNP A0A1R4DSC1
D	29	SER	-	expression tag	UNP A0A1R4DSC1
D	30	SER	-	expression tag	UNP A0A1R4DSC1
D	31	GLY	-	expression tag	UNP A0A1R4DSC1
D	32	VAL	-	expression tag	UNP A0A1R4DSC1
D	33	ASP	-	expression tag	UNP A0A1R4DSC1
D	34	LEU	-	expression tag	UNP A0A1R4DSC1
D	35	GLY	-	expression tag	UNP A0A1R4DSC1
D	36	THR	-	expression tag	UNP A0A1R4DSC1
D	37	GLU	-	expression tag	UNP A0A1R4DSC1
D	38	ASN	-	expression tag	UNP A0A1R4DSC1
D	39	LEU	-	expression tag	UNP A0A1R4DSC1
D	40	TYR	-	expression tag	UNP A0A1R4DSC1
D	41	PHE	-	expression tag	UNP A0A1R4DSC1
D	42	GLN	-	expression tag	UNP A0A1R4DSC1
D	43	SER	-	expression tag	UNP A0A1R4DSC1

- Molecule 2 is a protein called llama nanobody nb01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	125	Total 976	C 609	N 170	O 193	S 4	0	0	0
2	G	129	Total 1012	C 630	N 180	O 198	S 4	0	0	0
2	H	124	Total 968	C 605	N 169	O 190	S 4	0	0	0

- Molecule 3 is a protein called llama nanobody nb01.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	131	Total	C	N	O	S	0	0	0
			1032	642	186	200	4			

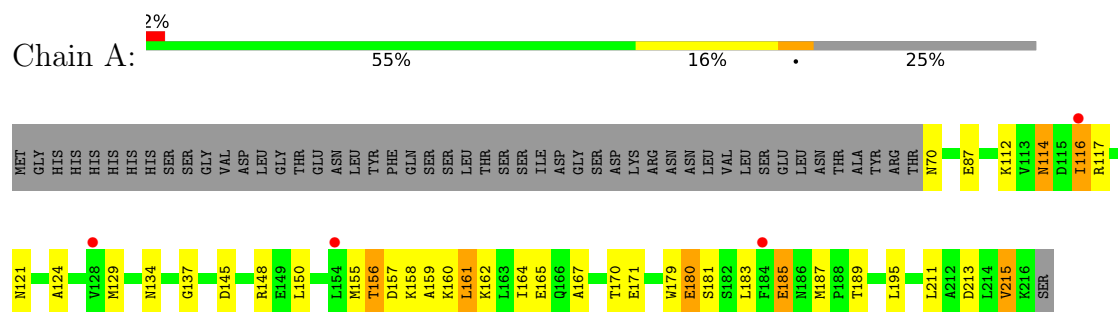
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	23	Total	O	0	0
			23	23		
4	B	14	Total	O	0	0
			14	14		
4	C	24	Total	O	0	0
			24	24		
4	D	28	Total	O	0	0
			28	28		
4	E	5	Total	O	0	0
			5	5		
4	F	31	Total	O	0	0
			31	31		
4	G	25	Total	O	0	0
			25	25		
4	H	8	Total	O	0	0
			8	8		

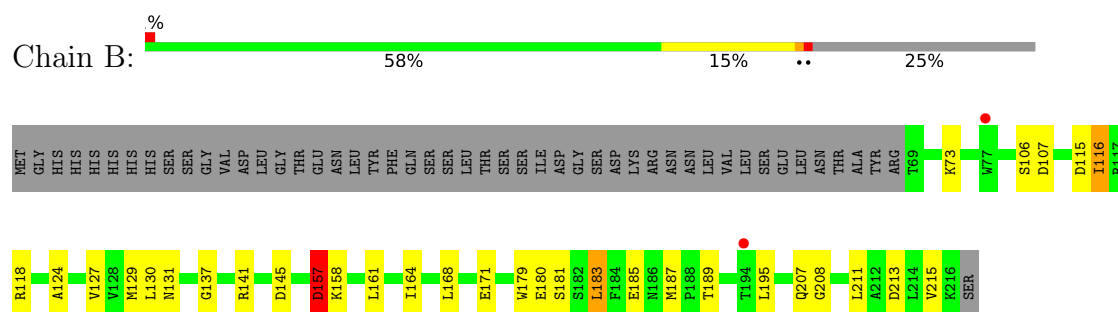
3 Residue-property plots [i](#)

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.

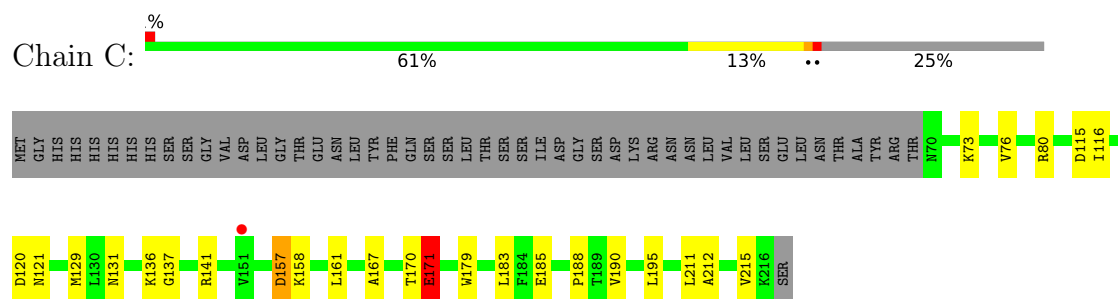
- Molecule 1: T9SS component cytoplasmic membrane protein PorM



- Molecule 1: T9SS component cytoplasmic membrane protein PorM



- Molecule 1: T9SS component cytoplasmic membrane protein PorM



- Molecule 1: T9SS component cytoplasmic membrane protein PorM



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.28Å 99.92Å 80.29Å 90.00° 93.83° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 40.00 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.5 (40.00-2.40) 98.5 (40.00-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.213 , 0.242 0.223 , 0.245	Depositor DCC
R_{free} test set	3023 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	58.3	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for l,-k,h	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8729	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.68% 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 ⓘ

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	0.84	0/1161	1.48	4/1562 (0.3%)
1	B	0.84	1/1168 (0.1%)	1.52	10/1572 (0.6%)
1	C	0.81	1/1161 (0.1%)	1.53	12/1562 (0.8%)
1	D	0.84	0/1136	1.50	2/1527 (0.1%)
2	E	0.75	0/997	1.19	4/1348 (0.3%)
2	G	0.76	0/1036	1.13	4/1401 (0.3%)
2	H	0.69	0/989	1.13	3/1337 (0.2%)
3	F	0.72	0/1058	1.13	1/1431 (0.1%)
All	All	0.79	2/8706 (0.0%)	1.35	40/11740 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	129	MET	SD-CE	-7.90	1.59	1.79
1	C	171	GLU	CA-C	6.35	1.61	1.53

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	ASP	CA-C-N	8.36	131.83	120.54
1	C	157	ASP	C-N-CA	8.36	131.83	120.54
1	C	157	ASP	N-CA-C	-7.04	100.90	110.68
1	D	115	ASP	CA-CB-CG	6.51	119.11	112.60
2	E	90	TYR	CA-C-N	6.17	131.84	122.65
2	E	90	TYR	C-N-CA	6.17	131.84	122.65
1	A	134	ASN	CA-CB-CG	6.05	118.65	112.60
1	C	158	LYS	N-CA-C	5.96	118.27	111.11
2	E	92	CYS	CA-C-N	-5.86	112.62	122.29
2	E	92	CYS	C-N-CA	-5.86	112.62	122.29
2	G	113	SER	CA-C-N	5.72	129.23	120.82
2	G	113	SER	C-N-CA	5.72	129.23	120.82
1	A	159	ALA	N-CA-C	-5.72	104.95	111.07
2	G	100(H)	GLU	CB-CG-CD	5.69	122.28	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	157	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	215	VAL	CA-C-N	5.62	131.81	121.70
1	A	215	VAL	C-N-CA	5.62	131.81	121.70
2	H	76	ASN	CA-CB-CG	5.51	118.11	112.60
1	C	120	ASP	N-CA-C	5.51	118.21	111.82
1	B	73	LYS	CA-C-N	5.32	127.75	120.46
1	B	73	LYS	C-N-CA	5.32	127.75	120.46
2	H	104	GLY	CA-C-N	5.30	127.64	120.44
2	H	104	GLY	C-N-CA	5.30	127.64	120.44
1	B	115	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	157	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	207	GLN	CA-C-N	5.20	125.86	119.99
1	B	207	GLN	C-N-CA	5.20	125.86	119.99
1	B	208	GLY	CA-C-N	5.14	127.17	120.28
1	B	208	GLY	C-N-CA	5.14	127.17	120.28
1	D	117	ARG	N-CA-C	-5.13	100.72	108.67
1	C	212	ALA	CA-C-N	5.10	127.12	120.28
1	C	212	ALA	C-N-CA	5.10	127.12	120.28
3	F	100(H)	GLU	CB-CG-CD	5.10	121.28	112.60
1	C	115	ASP	CA-C-N	5.07	128.66	121.66
1	C	115	ASP	C-N-CA	5.07	128.66	121.66
2	G	114	HIS	N-CA-C	5.07	116.83	110.24
1	B	116	ILE	CA-C-N	5.01	126.95	120.44
1	B	116	ILE	C-N-CA	5.01	126.95	120.44
1	C	136	LYS	CA-C-N	5.01	125.50	119.94
1	C	136	LYS	C-N-CA	5.01	125.50	119.94

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	1150	0	1196	28	0
1	B	1157	0	1203	28	0
1	C	1150	0	1196	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1126	0	1177	22	0
2	E	976	0	928	43	0
2	G	1012	0	954	15	0
2	H	968	0	921	19	0
3	F	1032	0	968	8	0
4	A	23	0	0	0	0
4	B	14	0	0	0	0
4	C	24	0	0	1	0
4	D	28	0	0	0	0
4	E	5	0	0	2	0
4	F	31	0	0	0	0
4	G	25	0	0	0	0
4	H	8	0	0	0	0
All	All	8729	0	8543	181	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 11.

All (181) 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:183:LEU:CD2	1:B:195:LEU:HD21	1.74	1.16
1:B:183:LEU:HD23	1:B:195:LEU:HD21	1.20	1.11
1:D:117:ARG:HH21	1:D:193:ILE:HG21	1.14	1.10
1:A:145:ASP:OD1	1:A:171:GLU:HG3	1.49	1.09
2:H:63:VAL:HB	2:H:67:PHE:HD2	1.15	1.07
1:B:141:ARG:HB2	1:B:180:GLU:OE1	1.55	1.05
1:D:117:ARG:NH2	1:D:193:ILE:HG21	1.71	1.04
2:H:63:VAL:HB	2:H:67:PHE:CD2	1.95	1.00
2:E:22:CYS:HB2	2:E:36:TRP:CZ2	2.07	0.90
2:E:5:VAL:HB	2:E:23:ALA:HB3	1.52	0.89
2:H:67:PHE:HD1	2:H:82:MET:HA	1.42	0.84
2:E:24:ALA:CB	2:E:29:PHE:CE1	2.62	0.83
2:E:24:ALA:HB2	2:E:29:PHE:HE1	1.41	0.83
2:E:24:ALA:CB	2:E:29:PHE:HE1	1.91	0.83
2:E:22:CYS:HB2	2:E:36:TRP:HZ2	1.42	0.82
1:A:116:ILE:HG22	1:A:117:ARG:HH21	1.46	0.80
2:H:67:PHE:CD1	2:H:82:MET:HA	2.16	0.80
1:B:181:SER:O	1:B:185:GLU:HB2	1.82	0.80
2:E:4:LEU:HD21	2:E:34:MET:HE1	1.65	0.79
3:F:22:CYS:HB3	3:F:78:VAL:HG22	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:141:ARG:CB	1:B:180:GLU:OE1	2.33	0.77
1:B:183:LEU:HD22	1:B:195:LEU:HD21	1.67	0.77
2:E:51:ILE:CD1	2:E:71:ARG:HB2	2.15	0.76
1:A:114:ASN:O	1:A:117:ARG:HG2	1.85	0.76
1:B:181:SER:O	1:B:185:GLU:CB	2.33	0.76
1:C:141:ARG:HG2	1:C:171:GLU:CG	2.17	0.75
2:E:52:SER:O	2:E:55:ASN:HA	1.89	0.73
1:C:141:ARG:HG2	1:C:171:GLU:OE2	1.90	0.72
2:E:106:GLY:HA2	4:E:201:HOH:O	1.89	0.71
1:A:155:MET:HB3	1:A:162:LYS:HE2	1.73	0.71
1:A:155:MET:CE	1:A:165:GLU:OE1	2.39	0.71
2:E:6:GLU:OE1	2:E:104:GLY:HA3	1.91	0.71
2:G:29:PHE:HE1	2:G:78:VAL:HG23	1.54	0.70
1:C:157:ASP:HB3	1:C:161:LEU:HD13	1.74	0.70
1:D:145:ASP:OD1	1:D:171:GLU:HG3	1.91	0.70
2:E:36:TRP:HE3	2:E:91:TYR:O	1.75	0.69
1:B:158:LYS:HB3	1:B:161:LEU:HD13	1.73	0.69
1:B:145:ASP:OD1	1:B:171:GLU:HG3	1.93	0.69
2:E:51:ILE:HD13	2:E:71:ARG:HB2	1.76	0.68
1:D:113:VAL:O	1:D:117:ARG:CZ	2.42	0.68
2:E:36:TRP:CE3	2:E:91:TYR:O	2.46	0.68
3:F:22:CYS:HB3	3:F:78:VAL:CG2	2.23	0.67
2:E:2:VAL:HG13	2:E:28:THR:HG21	1.75	0.67
1:B:183:LEU:HD23	1:B:195:LEU:CD2	2.14	0.67
2:E:36:TRP:CH2	2:E:92:CYS:HB2	2.30	0.67
1:B:137:GLY:C	1:B:180:GLU:HG2	2.21	0.66
2:E:36:TRP:CZ3	2:E:91:TYR:C	2.74	0.65
2:E:4:LEU:HD23	2:E:92:CYS:SG	2.36	0.65
1:C:171:GLU:HA	1:C:179:TRP:CD1	2.31	0.64
2:H:2:VAL:HG13	2:H:28:THR:HG21	1.79	0.64
1:A:156:THR:CG2	1:A:213:ASP:OD1	2.46	0.64
1:D:181:SER:O	1:D:185:GLU:HB2	1.98	0.63
2:G:26:GLY:HA2	2:G:76:ASN:CG	2.24	0.62
2:E:24:ALA:HB3	2:E:29:PHE:CE1	2.34	0.62
1:A:137:GLY:C	1:A:180:GLU:HG2	2.25	0.61
1:A:116:ILE:HG22	1:A:117:ARG:NH2	2.14	0.61
1:A:148:ARG:HH21	1:A:171:GLU:HG2	1.65	0.61
2:H:25:SER:O	2:H:28:THR:HG23	2.01	0.61
2:E:36:TRP:CZ3	2:E:92:CYS:CA	2.83	0.60
1:A:121:ASN:O	1:A:189:THR:HG23	2.02	0.60
1:A:156:THR:HG23	1:A:213:ASP:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ASP:HB2	1:B:213:ASP:OD2	2.01	0.59
1:D:137:GLY:C	1:D:180:GLU:HG2	2.27	0.59
1:C:167:ALA:HA	1:C:170:THR:HG23	1.85	0.58
1:A:158:LYS:HD3	1:A:161:LEU:HD22	1.85	0.58
2:G:24:ALA:HB3	2:G:29:PHE:CZ	2.38	0.58
1:D:129:MET:HE3	1:D:137:GLY:HA2	1.86	0.57
1:B:130:LEU:HD11	1:B:185:GLU:HA	1.86	0.57
2:E:36:TRP:CZ3	2:E:92:CYS:N	2.73	0.57
2:E:6:GLU:HG2	4:E:201:HOH:O	2.05	0.56
1:A:124:ALA:HB3	1:A:189:THR:HG22	1.88	0.56
1:B:130:LEU:CD1	1:B:185:GLU:HA	2.36	0.56
2:E:36:TRP:HZ3	2:E:91:TYR:C	2.12	0.56
1:B:164:ILE:O	1:B:168:LEU:HD13	2.06	0.56
1:D:127:VAL:O	1:D:131:ASN:OD1	2.25	0.55
1:D:117:ARG:NH2	1:D:193:ILE:CG2	2.57	0.55
2:H:89:VAL:HG22	2:H:108:GLN:HG2	1.88	0.55
1:D:187:MET:HE1	1:D:195:LEU:HD22	1.89	0.55
1:B:106:SER:OG	1:B:189:THR:HG21	2.07	0.54
2:E:52(A):ARG:HD3	2:E:52(A):ARG:H	1.72	0.54
2:E:36:TRP:CZ3	2:E:92:CYS:HA	2.42	0.54
1:C:141:ARG:HG2	1:C:171:GLU:CD	2.33	0.54
1:D:156:THR:HG22	1:D:213:ASP:OD2	2.08	0.54
2:E:52(A):ARG:HH11	2:E:52(A):ARG:HG3	1.72	0.54
1:B:107:ASP:OD1	1:B:118:ARG:HB2	2.08	0.53
3:F:2:VAL:HG13	3:F:28:THR:HG21	1.89	0.53
2:E:37:PHE:HE1	2:E:93:ALA:HB3	1.74	0.53
1:C:116:ILE:HD13	1:C:190:VAL:HG12	1.90	0.52
2:H:11:LEU:HA	2:H:110:THR:O	2.09	0.52
1:B:179:TRP:CE2	1:B:183:LEU:HD13	2.44	0.52
2:G:24:ALA:HB3	2:G:29:PHE:CE2	2.45	0.52
2:G:25:SER:HB2	2:G:28:THR:HG23	1.92	0.52
1:A:155:MET:CB	1:A:162:LYS:HE2	2.39	0.51
1:D:131:ASN:HD21	1:D:134:ASN:HB2	1.75	0.51
2:H:10:GLY:H	2:H:18:LEU:HD21	1.76	0.51
2:H:67:PHE:CE1	2:H:82:MET:HB3	2.45	0.51
1:A:155:MET:HB3	1:A:162:LYS:CE	2.39	0.51
1:C:121:ASN:O	1:C:188:PRO:HA	2.11	0.51
1:B:179:TRP:CE2	1:B:183:LEU:CD1	2.94	0.50
1:C:141:ARG:CD	1:C:171:GLU:OE2	2.58	0.50
2:G:45:ARG:HD2	2:G:91:TYR:CD2	2.47	0.50
1:A:160:LYS:O	1:A:164:ILE:HG13	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:SER:O	1:A:185:GLU:HB3	2.11	0.50
2:G:29:PHE:CE1	2:G:78:VAL:HG23	2.42	0.50
1:A:167:ALA:O	1:A:170:THR:HG23	2.12	0.50
2:H:36:TRP:HD1	2:H:69:ILE:HD12	1.76	0.49
1:C:171:GLU:HA	1:C:179:TRP:NE1	2.26	0.49
1:C:129:MET:HE3	1:C:137:GLY:HA2	1.95	0.49
1:A:116:ILE:CG2	1:A:117:ARG:NH2	2.75	0.49
2:E:36:TRP:CE3	2:E:91:TYR:C	2.90	0.49
1:C:76:VAL:HG12	1:C:80:ARG:HD2	1.94	0.49
3:F:36:TRP:HD1	3:F:69:ILE:HD12	1.78	0.49
2:E:51:ILE:HD11	2:E:71:ARG:HB2	1.93	0.49
2:G:87:THR:HG23	2:G:110:THR:HA	1.94	0.49
1:C:141:ARG:HG2	1:C:171:GLU:HG3	1.91	0.48
1:C:73:LYS:HE3	4:C:302:HOH:O	2.12	0.48
1:A:183:LEU:HD13	1:A:195:LEU:HD21	1.95	0.48
1:B:107:ASP:CG	1:B:118:ARG:HB2	2.37	0.48
1:D:159:ALA:O	1:D:163:LEU:HB2	2.13	0.48
3:F:24:ALA:HB3	3:F:29:PHE:CE1	2.49	0.48
2:H:58:TYR:CE1	2:H:100:ARG:HB3	2.49	0.48
1:C:141:ARG:CG	1:C:171:GLU:OE2	2.59	0.48
2:E:36:TRP:CE3	2:E:92:CYS:HA	2.48	0.48
2:H:11:LEU:HB2	2:H:110:THR:HB	1.95	0.48
1:D:117:ARG:HE	1:D:193:ILE:HD13	1.79	0.47
2:E:36:TRP:CH2	2:E:92:CYS:CB	2.97	0.47
2:E:36:TRP:HZ3	2:E:92:CYS:N	2.12	0.47
1:B:107:ASP:OD1	1:B:118:ARG:CB	2.62	0.47
1:B:179:TRP:NE1	1:B:183:LEU:HD11	2.29	0.47
2:G:34:MET:HG3	2:G:78:VAL:HG21	1.96	0.47
2:H:87:THR:HG23	2:H:110:THR:HA	1.96	0.47
2:H:2:VAL:HG22	2:H:28:THR:HG22	1.96	0.47
1:A:171:GLU:O	1:A:179:TRP:HB2	2.15	0.47
2:E:5:VAL:HB	2:E:23:ALA:CB	2.34	0.47
2:E:37:PHE:CE1	2:E:93:ALA:HB3	2.50	0.47
2:E:58:TYR:CE1	2:E:100:ARG:HB3	2.50	0.46
3:F:87:THR:HG23	3:F:110:THR:HA	1.97	0.46
1:A:129:MET:HE3	1:A:137:GLY:HA2	1.98	0.46
1:B:179:TRP:NE1	1:B:183:LEU:CD1	2.79	0.46
2:E:92:CYS:O	2:E:103:TRP:HA	2.16	0.46
2:E:87:THR:HG23	2:E:110:THR:HA	1.98	0.46
1:D:100:LEU:HA	1:D:113:VAL:CG2	2.46	0.46
1:C:116:ILE:HD12	1:C:116:ILE:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:22:CYS:HB3	2:H:78:VAL:HG12	1.98	0.45
2:G:29:PHE:HE2	2:G:76:ASN:HB3	1.81	0.45
1:B:116:ILE:HG22	1:B:118:ARG:HG2	1.98	0.45
2:E:36:TRP:CZ3	2:E:92:CYS:HB2	2.52	0.45
3:F:40:ALA:HB3	3:F:43:LYS:HD3	1.99	0.45
1:A:211:LEU:O	1:A:215:VAL:HG23	2.18	0.44
1:C:183:LEU:HB3	1:C:195:LEU:HD21	1.99	0.44
2:E:34:MET:HB2	2:E:51:ILE:CG2	2.48	0.44
1:A:158:LYS:HB3	1:A:161:LEU:HB2	2.01	0.43
1:B:181:SER:O	1:B:185:GLU:N	2.45	0.43
1:C:211:LEU:O	1:C:215:VAL:HG23	2.17	0.43
2:E:36:TRP:CZ3	2:E:92:CYS:CB	3.02	0.43
1:D:200:GLN:O	1:D:204:ARG:HG2	2.19	0.43
2:E:21:SER:HB3	2:E:79:TYR:CE1	2.54	0.42
1:A:87:GLU:HG3	1:A:150:LEU:HD22	2.00	0.42
1:D:140:LEU:O	1:D:144:VAL:HG23	2.18	0.42
1:D:211:LEU:O	1:D:215:VAL:HG23	2.19	0.42
2:G:58:TYR:CE1	2:G:100:ARG:HB3	2.54	0.42
1:D:158:LYS:HB3	1:D:161:LEU:HB2	2.00	0.42
2:G:66:ARG:HB3	2:G:82(A):ASN:O	2.20	0.42
3:F:25:SER:O	3:F:28:THR:HG23	2.20	0.42
2:H:24:ALA:HB1	2:H:28:THR:OG1	2.19	0.42
1:B:127:VAL:O	1:B:131:ASN:HB2	2.19	0.42
2:H:67:PHE:HE1	2:H:82:MET:HB3	1.82	0.42
1:D:87:GLU:HG3	1:D:150:LEU:HD22	2.02	0.41
1:A:112:LYS:O	1:A:117:ARG:HG3	2.20	0.41
1:A:112:LYS:HB2	1:A:117:ARG:HD2	2.02	0.41
1:D:107:ASP:OD1	1:D:119:LYS:HB2	2.21	0.41
1:D:148:ARG:HD3	1:D:166:GLN:HG3	2.02	0.41
1:A:156:THR:HG23	1:A:213:ASP:CG	2.45	0.41
1:B:124:ALA:HB3	1:B:189:THR:HG22	2.02	0.41
2:E:13:GLN:HA	2:E:112:SER:C	2.46	0.41
2:E:34:MET:O	2:E:51:ILE:HG22	2.20	0.41
2:G:36:TRP:HD1	2:G:69:ILE:HD12	1.86	0.41
2:G:29:PHE:CE2	2:G:76:ASN:HB3	2.56	0.40
2:H:21:SER:HB3	2:H:79:TYR:CD1	2.56	0.40
1:B:211:LEU:O	1:B:215:VAL:HG23	2.22	0.40
2:G:115:HIS:ND1	2:G:115:HIS:C	2.79	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	145/197 (74%)	136 (94%)	7 (5%)	2 (1%)	9	13
1	B	146/197 (74%)	136 (93%)	10 (7%)	0	100	100
1	C	145/197 (74%)	141 (97%)	4 (3%)	0	100	100
1	D	142/197 (72%)	135 (95%)	6 (4%)	1 (1%)	18	28
2	E	123/134 (92%)	122 (99%)	1 (1%)	0	100	100
2	G	127/134 (95%)	123 (97%)	4 (3%)	0	100	100
2	H	122/134 (91%)	119 (98%)	3 (2%)	0	100	100
3	F	129/136 (95%)	126 (98%)	3 (2%)	0	100	100
All	All	1079/1326 (81%)	1038 (96%)	38 (4%)	3 (0%)	36	50

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	114	ASN
1	A	156	THR
1	D	116	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	129/174 (74%)	122 (95%)	7 (5%)	20	35
1	B	130/174 (75%)	127 (98%)	3 (2%)	44	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	129/174 (74%)	126 (98%)	3 (2%)	44	66
1	D	126/174 (72%)	123 (98%)	3 (2%)	43	65
2	E	102/110 (93%)	102 (100%)	0	100	100
2	G	106/110 (96%)	106 (100%)	0	100	100
2	H	101/110 (92%)	100 (99%)	1 (1%)	68	84
3	F	108/112 (96%)	108 (100%)	0	100	100
All	All	931/1138 (82%)	914 (98%)	17 (2%)	51	73

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	70	ASN
1	A	116	ILE
1	A	157	ASP
1	A	161	LEU
1	A	180	GLU
1	A	185	GLU
1	A	187	MET
1	B	157	ASP
1	B	183	LEU
1	B	187	MET
1	C	131	ASN
1	C	171	GLU
1	C	185	GLU
1	D	116	ILE
1	D	180	GLU
1	D	181	SER
2	H	53	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	C	131	ASN
1	C	186	ASN
1	D	131	ASN
1	D	169	ASN
3	F	76	ASN
3	F	81	GLN

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Mol	Chain	Res	Type
3	F	118	HIS
2	H	81	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](#)

There are no ligands in this entry.

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	147/197 (74%)	0.22	4 (2%) 56 52	87, 104, 139, 178	0
1	B	148/197 (75%)	0.21	2 (1%) 73 69	84, 107, 161, 186	0
1	C	147/197 (74%)	0.12	1 (0%) 84 81	80, 100, 130, 157	0
1	D	144/197 (73%)	0.16	7 (4%) 35 31	83, 100, 134, 174	0
2	E	125/134 (93%)	0.22	4 (3%) 50 46	126, 168, 237, 255	0
2	G	129/134 (96%)	-0.01	4 (3%) 51 47	75, 89, 126, 188	0
2	H	124/134 (92%)	0.15	1 (0%) 82 80	116, 152, 234, 262	0
3	F	131/136 (96%)	-0.07	2 (1%) 72 68	82, 96, 143, 181	0
All	All	1095/1326 (82%)	0.13	25 (2%) 61 57	75, 107, 201, 262	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	G	116	HIS	4.1
1	A	128	VAL	3.6
2	E	15	GLY	2.6
1	D	154	LEU	2.6
1	D	116	ILE	2.5
1	A	154	LEU	2.4
2	E	48	VAL	2.4
2	G	113	SER	2.4
2	H	36	TRP	2.4
2	E	26	GLY	2.3
1	A	184	PHE	2.3
1	D	77	TRP	2.3
3	F	118	HIS	2.3
3	F	78	VAL	2.3
1	D	74	VAL	2.2
1	D	165	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	G	28	THR	2.1
1	D	123	ASP	2.1
2	E	14	ALA	2.0
1	C	151	VAL	2.0
1	D	184	PHE	2.0
2	G	8	GLY	2.0
1	A	116	ILE	2.0
1	B	194	THR	2.0
1	B	77	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.