



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 02:05 AM UTC

PDB ID : 8XX7 / pdb_00008xx7
EMDB ID : EMD-38748
Title : Structure of CXCR2 bound to CXCL5 (CXCR2-CXCL5-Go Full map)
Authors : Sano, F.K.; Saha, S.; Sharma, S.; Ganguly, M.; Shihoya, W.; Nureki, O.;
Shukla, A.K.; Banerjee, R.
Deposited on : 2024-01-17
Resolution : 3.32 Å(reported)
Based on initial model : .

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : **NOT EXECUTED**
MapQ : **FAILED**
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

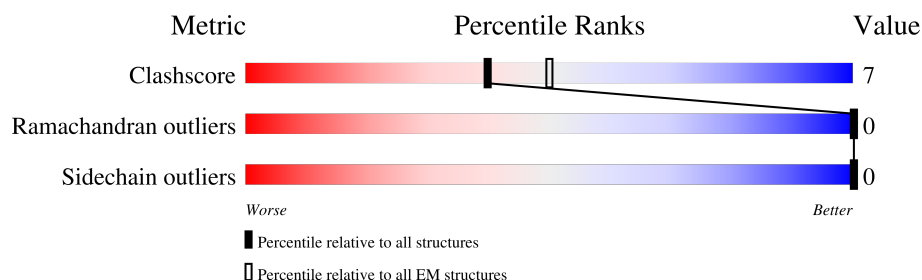
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.32 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)	EM structures (#Entries)
Clashscore	229148	23984
Ramachandran outliers	224038	23583
Sidechain outliers	223484	23102

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	B	78	73% 10% 17%
1	D	78	73% 10% 17%
2	C	416	65% 7% 28%
2	R	416	66% 6% 28%
3	A	240	77% 12% 10%
3	F	240	78% 12% 10%
4	E	350	77% 19% .
4	H	350	75% 21% .
5	G	71	70% . 25%

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Mol	Chain	Length	Quality of chain
5	I	71	69% 6% 25%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 15054 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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-X-C motif chemokine 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	D	65	Total	C	N	O	S	0	0
			483	308	83	87	5		
1	B	65	Total	C	N	O	S	0	0
			483	308	83	87	5		

- Molecule 2 is a protein called C-X-C chemokine receptor type 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	R	300	Total	C	N	O	S	0	0
			2337	1553	386	382	16		
2	C	300	Total	C	N	O	S	0	0
			2353	1564	390	383	16		

There are 114 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-55	MET	-	initiating methionine	UNP P25025
R	-54	GLY	-	expression tag	UNP P25025
R	-53	LYS	-	expression tag	UNP P25025
R	-52	THR	-	expression tag	UNP P25025
R	-51	ILE	-	expression tag	UNP P25025
R	-50	ILE	-	expression tag	UNP P25025
R	-49	ALA	-	expression tag	UNP P25025
R	-48	LEU	-	expression tag	UNP P25025
R	-47	SER	-	expression tag	UNP P25025
R	-46	TYR	-	expression tag	UNP P25025
R	-45	ILE	-	expression tag	UNP P25025
R	-44	PHE	-	expression tag	UNP P25025
R	-43	CYS	-	expression tag	UNP P25025
R	-42	LEU	-	expression tag	UNP P25025
R	-41	VAL	-	expression tag	UNP P25025
R	-40	PHE	-	expression tag	UNP P25025
R	-39	ALA	-	expression tag	UNP P25025

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-38	ASP	-	expression tag	UNP P25025
R	-37	TYR	-	expression tag	UNP P25025
R	-36	LYS	-	expression tag	UNP P25025
R	-35	ASP	-	expression tag	UNP P25025
R	-34	ASP	-	expression tag	UNP P25025
R	-33	ASP	-	expression tag	UNP P25025
R	-32	ASP	-	expression tag	UNP P25025
R	-31	ALA	-	expression tag	UNP P25025
R	-30	ALA	-	expression tag	UNP P25025
R	-29	ASN	-	expression tag	UNP P25025
R	-28	PHE	-	expression tag	UNP P25025
R	-27	THR	-	expression tag	UNP P25025
R	-26	PRO	-	expression tag	UNP P25025
R	-25	VAL	-	expression tag	UNP P25025
R	-24	ASN	-	expression tag	UNP P25025
R	-23	GLY	-	expression tag	UNP P25025
R	-22	SER	-	expression tag	UNP P25025
R	-21	SER	-	expression tag	UNP P25025
R	-20	GLY	-	expression tag	UNP P25025
R	-19	ASN	-	expression tag	UNP P25025
R	-18	GLN	-	expression tag	UNP P25025
R	-17	SER	-	expression tag	UNP P25025
R	-16	VAL	-	expression tag	UNP P25025
R	-15	ARG	-	expression tag	UNP P25025
R	-14	LEU	-	expression tag	UNP P25025
R	-13	VAL	-	expression tag	UNP P25025
R	-12	THR	-	expression tag	UNP P25025
R	-11	SER	-	expression tag	UNP P25025
R	-10	SER	-	expression tag	UNP P25025
R	-9	SER	-	expression tag	UNP P25025
R	-8	LEU	-	expression tag	UNP P25025
R	-7	GLU	-	expression tag	UNP P25025
R	-6	VAL	-	expression tag	UNP P25025
R	-5	LEU	-	expression tag	UNP P25025
R	-4	PHE	-	expression tag	UNP P25025
R	-3	GLN	-	expression tag	UNP P25025
R	-2	GLY	-	expression tag	UNP P25025
R	-1	PRO	-	expression tag	UNP P25025
R	0	GLY	-	expression tag	UNP P25025
R	1	SER	-	expression tag	UNP P25025
C	-55	MET	-	initiating methionine	UNP P25025
C	-54	GLY	-	expression tag	UNP P25025

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-53	LYS	-	expression tag	UNP P25025
C	-52	THR	-	expression tag	UNP P25025
C	-51	ILE	-	expression tag	UNP P25025
C	-50	ILE	-	expression tag	UNP P25025
C	-49	ALA	-	expression tag	UNP P25025
C	-48	LEU	-	expression tag	UNP P25025
C	-47	SER	-	expression tag	UNP P25025
C	-46	TYR	-	expression tag	UNP P25025
C	-45	ILE	-	expression tag	UNP P25025
C	-44	PHE	-	expression tag	UNP P25025
C	-43	CYS	-	expression tag	UNP P25025
C	-42	LEU	-	expression tag	UNP P25025
C	-41	VAL	-	expression tag	UNP P25025
C	-40	PHE	-	expression tag	UNP P25025
C	-39	ALA	-	expression tag	UNP P25025
C	-38	ASP	-	expression tag	UNP P25025
C	-37	TYR	-	expression tag	UNP P25025
C	-36	LYS	-	expression tag	UNP P25025
C	-35	ASP	-	expression tag	UNP P25025
C	-34	ASP	-	expression tag	UNP P25025
C	-33	ASP	-	expression tag	UNP P25025
C	-32	ASP	-	expression tag	UNP P25025
C	-31	ALA	-	expression tag	UNP P25025
C	-30	ALA	-	expression tag	UNP P25025
C	-29	ASN	-	expression tag	UNP P25025
C	-28	PHE	-	expression tag	UNP P25025
C	-27	THR	-	expression tag	UNP P25025
C	-26	PRO	-	expression tag	UNP P25025
C	-25	VAL	-	expression tag	UNP P25025
C	-24	ASN	-	expression tag	UNP P25025
C	-23	GLY	-	expression tag	UNP P25025
C	-22	SER	-	expression tag	UNP P25025
C	-21	SER	-	expression tag	UNP P25025
C	-20	GLY	-	expression tag	UNP P25025
C	-19	ASN	-	expression tag	UNP P25025
C	-18	GLN	-	expression tag	UNP P25025
C	-17	SER	-	expression tag	UNP P25025
C	-16	VAL	-	expression tag	UNP P25025
C	-15	ARG	-	expression tag	UNP P25025
C	-14	LEU	-	expression tag	UNP P25025
C	-13	VAL	-	expression tag	UNP P25025
C	-12	THR	-	expression tag	UNP P25025

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	SER	-	expression tag	UNP P25025
C	-10	SER	-	expression tag	UNP P25025
C	-9	SER	-	expression tag	UNP P25025
C	-8	LEU	-	expression tag	UNP P25025
C	-7	GLU	-	expression tag	UNP P25025
C	-6	VAL	-	expression tag	UNP P25025
C	-5	LEU	-	expression tag	UNP P25025
C	-4	PHE	-	expression tag	UNP P25025
C	-3	GLN	-	expression tag	UNP P25025
C	-2	GLY	-	expression tag	UNP P25025
C	-1	PRO	-	expression tag	UNP P25025
C	0	GLY	-	expression tag	UNP P25025
C	1	SER	-	expression tag	UNP P25025

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(o) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	215	Total	C	N	O	S	0	0
			1711	1088	288	324	11		
3	F	215	Total	C	N	O	S	0	0
			1711	1088	288	324	11		

There are 78 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	initiating methionine	UNP P09471
A	-10	GLY	-	expression tag	UNP P09471
A	-9	HIS	-	expression tag	UNP P09471
A	-8	HIS	-	expression tag	UNP P09471
A	-7	HIS	-	expression tag	UNP P09471
A	-6	HIS	-	expression tag	UNP P09471
A	-5	HIS	-	expression tag	UNP P09471
A	-4	HIS	-	expression tag	UNP P09471
A	-3	GLU	-	expression tag	UNP P09471
A	-2	ASN	-	expression tag	UNP P09471
A	-1	LEU	-	expression tag	UNP P09471
A	0	TYR	-	expression tag	UNP P09471
A	1	PHE	-	expression tag	UNP P09471
A	2	GLN	-	expression tag	UNP P09471
A	3	GLY	-	expression tag	UNP P09471
A	42	ASP	GLY	engineered mutation	UNP P09471
A	43	ASN	GLU	engineered mutation	UNP P09471

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Chain	Residue	Modelled	Actual	Comment	Reference
A	174	GLY	-	linker	UNP P09471
A	175	GLY	-	linker	UNP P09471
A	176	SER	-	linker	UNP P09471
A	177	GLY	-	linker	UNP P09471
A	178	GLY	-	linker	UNP P09471
A	179	SER	-	linker	UNP P09471
A	180	GLY	-	linker	UNP P09471
A	181	GLY	-	linker	UNP P09471
A	227	ASP	ALA	engineered mutation	UNP P09471
A	230	ASP	GLY	engineered mutation	UNP P09471
A	?	-	ASP	deletion	UNP P09471
A	?	-	GLN	deletion	UNP P09471
A	?	-	VAL	deletion	UNP P09471
A	?	-	LEU	deletion	UNP P09471
A	?	-	HIS	deletion	UNP P09471
A	?	-	GLU	deletion	UNP P09471
A	?	-	ASP	deletion	UNP P09471
A	?	-	GLU	deletion	UNP P09471
A	?	-	THR	deletion	UNP P09471
A	?	-	THR	deletion	UNP P09471
A	332	ALA	ILE	engineered mutation	UNP P09471
A	335	ILE	VAL	engineered mutation	UNP P09471
F	-11	MET	-	initiating methionine	UNP P09471
F	-10	GLY	-	expression tag	UNP P09471
F	-9	HIS	-	expression tag	UNP P09471
F	-8	HIS	-	expression tag	UNP P09471
F	-7	HIS	-	expression tag	UNP P09471
F	-6	HIS	-	expression tag	UNP P09471
F	-5	HIS	-	expression tag	UNP P09471
F	-4	HIS	-	expression tag	UNP P09471
F	-3	GLU	-	expression tag	UNP P09471
F	-2	ASN	-	expression tag	UNP P09471
F	-1	LEU	-	expression tag	UNP P09471
F	0	TYR	-	expression tag	UNP P09471
F	1	PHE	-	expression tag	UNP P09471
F	2	GLN	-	expression tag	UNP P09471
F	3	GLY	-	expression tag	UNP P09471
F	42	ASP	GLY	engineered mutation	UNP P09471
F	43	ASN	GLU	engineered mutation	UNP P09471
F	174	GLY	-	linker	UNP P09471
F	175	GLY	-	linker	UNP P09471
F	176	SER	-	linker	UNP P09471

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Chain	Residue	Modelled	Actual	Comment	Reference
F	177	GLY	-	linker	UNP P09471
F	178	GLY	-	linker	UNP P09471
F	179	SER	-	linker	UNP P09471
F	180	GLY	-	linker	UNP P09471
F	181	GLY	-	linker	UNP P09471
F	227	ASP	ALA	engineered mutation	UNP P09471
F	230	ASP	GLY	engineered mutation	UNP P09471
F	?	-	ASP	deletion	UNP P09471
F	?	-	GLN	deletion	UNP P09471
F	?	-	VAL	deletion	UNP P09471
F	?	-	LEU	deletion	UNP P09471
F	?	-	HIS	deletion	UNP P09471
F	?	-	GLU	deletion	UNP P09471
F	?	-	ASP	deletion	UNP P09471
F	?	-	GLU	deletion	UNP P09471
F	?	-	THR	deletion	UNP P09471
F	?	-	THR	deletion	UNP P09471
F	332	ALA	ILE	engineered mutation	UNP P09471
F	335	ILE	VAL	engineered mutation	UNP P09471

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	336	Total	C	N	O	S	0	0
			2581	1592	464	504	21		
4	H	336	Total	C	N	O	S	0	0
			2581	1592	464	504	21		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	MET	-	initiating methionine	UNP P62873
E	-8	HIS	-	expression tag	UNP P62873
E	-7	HIS	-	expression tag	UNP P62873
E	-6	HIS	-	expression tag	UNP P62873
E	-5	HIS	-	expression tag	UNP P62873
E	-4	HIS	-	expression tag	UNP P62873
E	-3	HIS	-	expression tag	UNP P62873
E	-2	GLY	-	expression tag	UNP P62873
E	-1	SER	-	expression tag	UNP P62873
E	0	SER	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP P62873
E	2	SER	-	expression tag	UNP P62873
H	-9	MET	-	initiating methionine	UNP P62873
H	-8	HIS	-	expression tag	UNP P62873
H	-7	HIS	-	expression tag	UNP P62873
H	-6	HIS	-	expression tag	UNP P62873
H	-5	HIS	-	expression tag	UNP P62873
H	-4	HIS	-	expression tag	UNP P62873
H	-3	HIS	-	expression tag	UNP P62873
H	-2	GLY	-	expression tag	UNP P62873
H	-1	SER	-	expression tag	UNP P62873
H	0	SER	-	expression tag	UNP P62873
H	1	GLY	-	expression tag	UNP P62873
H	2	SER	-	expression tag	UNP P62873

- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	53	Total	C	N	O	S	0	0
			407	257	70	77	3		
5	I	53	Total	C	N	O	S	0	0
			407	257	70	77	3		

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. 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. 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-X-C motif chemokine 5

Chain D: 



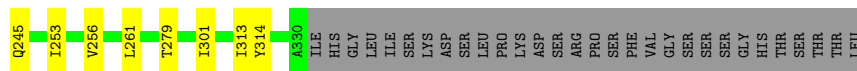
- Molecule 1: C-X-C motif chemokine 5

Chain B: 



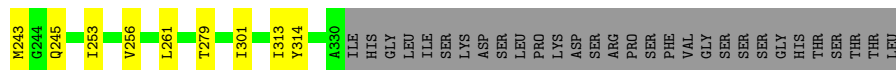
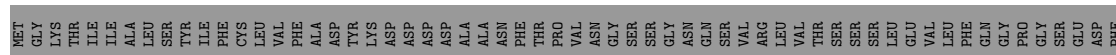
- Molecule 2: C-X-C chemokine receptor type 2

Chain R: 



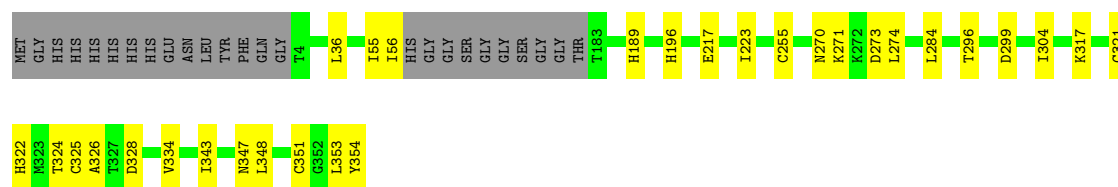
- Molecule 2: C-X-C chemokine receptor type 2

Chain C: 



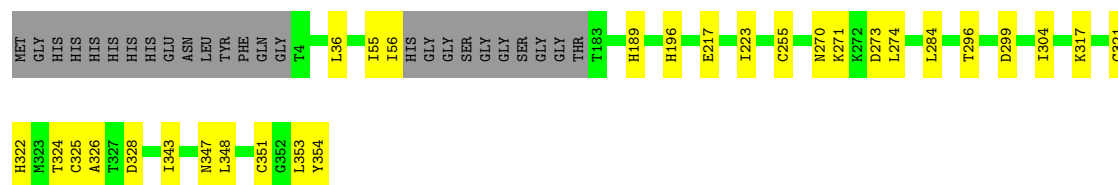
- Molecule 3: Guanine nucleotide-binding protein G(o) subunit alpha

Chain A:  77% 12% 10%



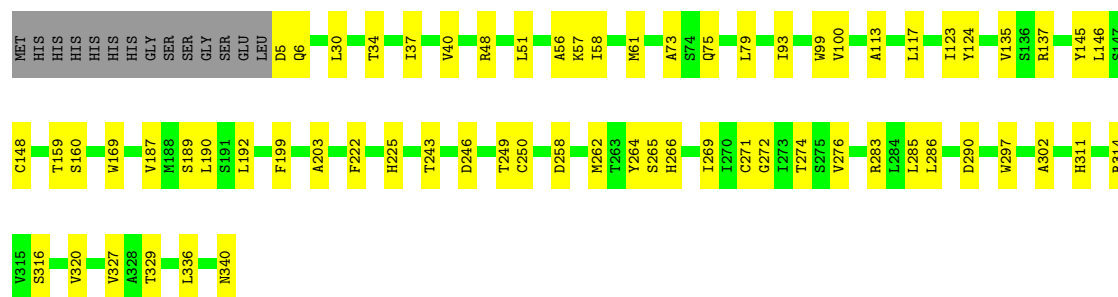
- Molecule 3: Guanine nucleotide-binding protein G(o) subunit alpha

Chain F:  78% 12% 10%



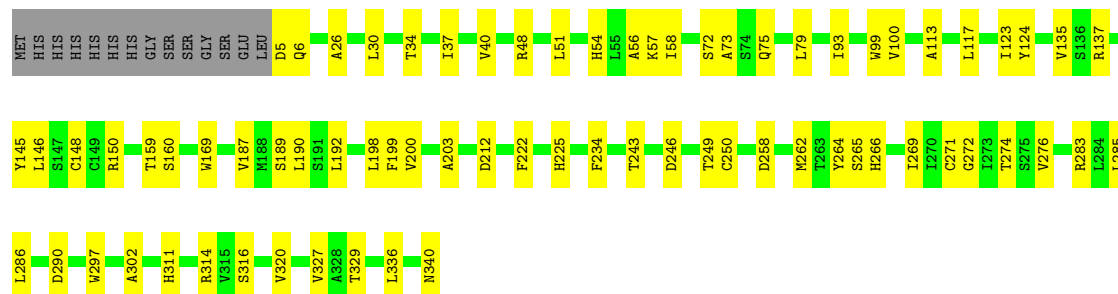
- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain E:  77% 19% .



- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain H:  75% 21% .



- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain G:  70% . 25%



● Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131780	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.2	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	B	0.24	0/489	0.33	0/660
1	D	0.24	0/489	0.33	0/660
2	C	0.22	0/2405	0.32	0/3276
2	R	0.22	0/2389	0.32	0/3259
3	A	0.08	0/1740	0.22	0/2340
3	F	0.08	0/1740	0.22	0/2340
4	E	0.11	0/2628	0.31	0/3562
4	H	0.11	0/2628	0.31	0/3562
5	G	0.08	0/413	0.21	0/558
5	I	0.08	0/413	0.21	0/558
All	All	0.16	0/15334	0.29	0/20775

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	B	483	0	504	6	0
1	D	483	0	504	6	0
2	C	2353	0	2475	40	0
2	R	2337	0	2436	42	0
3	A	1711	0	1711	47	0
3	F	1711	0	1711	48	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	2581	0	2482	39	0
4	H	2581	0	2482	43	0
5	G	407	0	418	3	0
5	I	407	0	418	4	0
All	All	15054	0	15141	213	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 (213) 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:R:243:MET:HE1	3:F:348:LEU:HD11	1.38	1.05
2:C:243:MET:HE1	3:A:348:LEU:CD1	1.90	1.01
2:C:243:MET:HE1	3:A:348:LEU:HD11	1.39	1.01
2:R:243:MET:HE1	3:F:348:LEU:CD1	1.90	1.00
2:C:245:GLN:HB3	3:A:354:TYR:CD1	2.07	0.90
2:C:253:ILE:HG13	3:A:353:LEU:HD22	1.53	0.89
2:R:245:GLN:HB3	3:F:354:TYR:CD1	2.07	0.88
2:R:253:ILE:HG13	3:F:353:LEU:HD22	1.52	0.88
2:R:144:ARG:HG2	3:F:351:CYS:HB3	1.57	0.87
2:C:144:ARG:HG2	3:A:351:CYS:HB3	1.57	0.85
2:R:253:ILE:HD11	3:F:353:LEU:HD11	1.60	0.84
2:R:253:ILE:HD11	3:F:353:LEU:CD1	2.08	0.83
2:C:253:ILE:HD11	3:A:353:LEU:CD1	2.09	0.82
2:C:253:ILE:HD11	3:A:353:LEU:HD11	1.61	0.81
2:R:243:MET:CE	3:F:348:LEU:CD1	2.60	0.79
2:R:253:ILE:HG13	3:F:353:LEU:CD2	2.11	0.78
2:C:243:MET:CE	3:A:348:LEU:CD1	2.61	0.78
2:C:253:ILE:HG13	3:A:353:LEU:CD2	2.13	0.78
2:R:144:ARG:HA	3:F:351:CYS:SG	2.25	0.76
2:C:144:ARG:HA	3:A:351:CYS:SG	2.26	0.76
2:C:245:GLN:HG2	3:A:354:TYR:CZ	2.23	0.74
2:C:245:GLN:HB3	3:A:354:TYR:CE1	2.24	0.73
2:R:245:GLN:HG2	3:F:354:TYR:CZ	2.23	0.73
2:R:245:GLN:HB3	3:F:354:TYR:CE1	2.24	0.72
4:E:160:SER:HB2	4:E:190:LEU:HD23	1.71	0.72
4:H:160:SER:HB2	4:H:190:LEU:HD23	1.71	0.72
2:R:243:MET:HE1	3:F:348:LEU:HD12	1.74	0.70
3:F:343:ILE:O	3:F:347:ASN:ND2	2.24	0.70
3:A:343:ILE:O	3:A:347:ASN:ND2	2.24	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:51:LEU:HB2	4:H:336:LEU:HB2	1.76	0.68
2:R:144:ARG:HG2	3:F:351:CYS:CB	2.23	0.67
2:R:243:MET:CE	3:F:348:LEU:HD12	2.25	0.67
2:C:144:ARG:HG2	3:A:351:CYS:CB	2.23	0.67
4:E:79:LEU:HB3	4:E:93:ILE:HB	1.77	0.66
4:H:79:LEU:HB3	4:H:93:ILE:HB	1.77	0.65
4:E:51:LEU:HB2	4:E:336:LEU:HB2	1.76	0.65
2:C:243:MET:HE1	3:A:348:LEU:HD12	1.75	0.65
2:C:151:ALA:HB1	3:A:343:ILE:CG2	2.27	0.65
2:C:243:MET:CE	3:A:348:LEU:HD12	2.26	0.65
2:R:151:ALA:HB1	3:F:343:ILE:CG2	2.27	0.64
2:C:243:MET:CE	3:A:348:LEU:HD11	2.22	0.64
3:A:343:ILE:CG2	3:A:347:ASN:HD21	2.14	0.61
4:E:250:CYS:HB2	4:E:264:TYR:HB2	1.83	0.60
3:F:343:ILE:CG2	3:F:347:ASN:HD21	2.14	0.60
3:A:343:ILE:HG23	3:A:347:ASN:HD21	1.67	0.59
3:A:271:LYS:HD3	3:A:274:LEU:HD12	1.84	0.59
2:R:243:MET:CE	3:F:348:LEU:HD11	2.22	0.59
3:F:271:LYS:HD3	3:F:274:LEU:HD12	1.84	0.59
4:H:250:CYS:HB2	4:H:264:TYR:HB2	1.83	0.59
2:R:253:ILE:CG1	3:F:353:LEU:CD2	2.81	0.58
3:F:343:ILE:HG23	3:F:347:ASN:HD21	1.67	0.58
3:A:325:CYS:SG	3:A:326:ALA:N	2.76	0.58
3:F:325:CYS:SG	3:F:326:ALA:N	2.76	0.58
2:R:253:ILE:HD11	3:F:353:LEU:HD13	1.85	0.57
3:A:343:ILE:HG22	3:A:347:ASN:ND2	2.20	0.57
2:C:253:ILE:HD11	3:A:353:LEU:HD13	1.85	0.56
2:R:144:ARG:HG2	3:F:351:CYS:SG	2.45	0.56
4:H:271:CYS:HB2	4:H:290:ASP:HB2	1.87	0.56
2:C:256:VAL:HG22	2:C:313:ILE:CG2	2.36	0.56
4:E:320:VAL:HG22	4:E:327:VAL:HG22	1.88	0.56
3:F:343:ILE:CG2	3:F:347:ASN:ND2	2.69	0.56
4:H:37:ILE:HG21	4:H:283:ARG:HH12	1.71	0.56
4:E:146:LEU:HD11	4:E:159:THR:HB	1.88	0.56
4:H:266:HIS:HB2	4:H:297:TRP:HH2	1.70	0.56
4:E:266:HIS:HB2	4:E:297:TRP:HH2	1.70	0.55
4:E:187:VAL:HA	4:E:203:ALA:HA	1.88	0.55
3:F:343:ILE:HG22	3:F:347:ASN:ND2	2.20	0.55
4:H:320:VAL:HG22	4:H:327:VAL:HG22	1.88	0.55
3:A:343:ILE:CG2	3:A:347:ASN:ND2	2.69	0.55
4:H:187:VAL:HA	4:H:203:ALA:HA	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:37:ILE:HG21	4:E:283:ARG:HH12	1.71	0.55
2:C:144:ARG:HG2	3:A:351:CYS:SG	2.46	0.55
4:E:271:CYS:HB2	4:E:290:ASP:HB2	1.87	0.55
2:R:238:LEU:CD2	3:F:348:LEU:HD11	2.37	0.54
2:R:253:ILE:CG1	3:F:353:LEU:HD21	2.37	0.54
2:C:253:ILE:CG1	3:A:353:LEU:CD2	2.82	0.54
2:R:256:VAL:HG22	2:R:313:ILE:CG2	2.36	0.54
4:H:146:LEU:HD11	4:H:159:THR:HB	1.88	0.54
2:R:238:LEU:HD21	3:F:348:LEU:HD21	1.89	0.54
2:R:245:GLN:HG2	3:F:354:TYR:CE2	2.43	0.54
2:C:238:LEU:CD2	3:A:348:LEU:HD11	2.38	0.53
2:C:253:ILE:CG1	3:A:353:LEU:HD21	2.38	0.53
3:F:255:CYS:O	3:F:317:LYS:NZ	2.41	0.53
2:C:238:LEU:HD21	3:A:348:LEU:HD21	1.89	0.53
1:B:44:VAL:HG11	1:B:63:LEU:HD21	1.91	0.53
3:A:255:CYS:O	3:A:317:LYS:NZ	2.41	0.53
2:C:201:GLY:O	2:C:204:THR:OG1	2.24	0.52
2:R:238:LEU:HD22	3:F:348:LEU:HD11	1.91	0.52
2:C:245:GLN:HG2	3:A:354:TYR:CE2	2.44	0.52
2:R:112:TRP:NE1	2:R:115:GLY:O	2.40	0.51
4:E:274:THR:HG21	4:E:316:SER:HA	1.92	0.51
4:H:222:PHE:HE1	4:H:258:ASP:HA	1.75	0.51
3:F:321:CYS:SG	3:F:322:HIS:N	2.84	0.51
4:E:99:TRP:HB3	4:E:117:LEU:HD12	1.92	0.51
4:E:222:PHE:HE1	4:E:258:ASP:HA	1.76	0.51
2:R:137:LEU:HD22	2:R:314:TYR:CZ	2.46	0.51
3:A:284:LEU:HD21	3:A:304:ILE:HD11	1.93	0.51
4:H:99:TRP:HB3	4:H:117:LEU:HD12	1.92	0.51
1:D:44:VAL:HG11	1:D:63:LEU:HD21	1.91	0.50
4:H:274:THR:HG21	4:H:316:SER:HA	1.92	0.50
2:C:238:LEU:HD22	3:A:348:LEU:HD11	1.92	0.50
2:R:279:THR:HG22	2:R:279:THR:O	2.10	0.50
2:C:279:THR:HG22	2:C:279:THR:O	2.10	0.50
4:E:48:ARG:HE	4:E:340:ASN:HB3	1.76	0.50
2:C:112:TRP:NE1	2:C:115:GLY:O	2.40	0.50
3:F:284:LEU:HD21	3:F:304:ILE:HD11	1.93	0.50
4:H:48:ARG:HE	4:H:340:ASN:HB3	1.76	0.50
3:A:321:CYS:SG	3:A:322:HIS:N	2.84	0.50
2:R:151:ALA:HB1	3:F:343:ILE:HG21	1.95	0.49
2:C:137:LEU:HD22	2:C:314:TYR:CZ	2.46	0.49
4:H:266:HIS:HB3	4:H:269:ILE:HG12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:58:ILE:O	4:H:316:SER:OG	2.23	0.49
2:C:151:ALA:HB1	3:A:343:ILE:HG21	1.95	0.48
3:F:270:ASN:OD1	3:F:324:THR:OG1	2.32	0.48
4:H:249:THR:HG22	4:H:265:SER:HB3	1.96	0.48
4:H:262:MET:HE2	4:H:302:ALA:HB2	1.96	0.48
4:E:266:HIS:HB3	4:E:269:ILE:HG12	1.95	0.48
4:E:262:MET:HE2	4:E:302:ALA:HB2	1.96	0.48
3:F:325:CYS:N	3:F:328:ASP:OD2	2.42	0.47
4:H:5:ASP:OD1	4:H:6:GLN:N	2.47	0.47
4:H:159:THR:OG1	4:H:169:TRP:NE1	2.46	0.47
4:E:225:HIS:NE2	4:E:243:THR:OG1	2.42	0.47
1:B:32:VAL:HG22	1:B:44:VAL:HG12	1.97	0.47
3:A:270:ASN:OD1	3:A:324:THR:OG1	2.32	0.47
3:F:36:LEU:HD13	3:F:223:ILE:HD11	1.97	0.47
2:R:201:GLY:O	2:R:204:THR:OG1	2.24	0.47
4:E:249:THR:HG22	4:E:265:SER:HB3	1.96	0.47
4:E:113:ALA:HB2	4:E:123:ILE:HG12	1.97	0.47
3:A:36:LEU:HD13	3:A:223:ILE:HD11	1.97	0.46
4:H:290:ASP:HA	4:H:314:ARG:HG3	1.97	0.46
4:H:192:LEU:HD23	4:H:199:PHE:HB3	1.97	0.46
1:D:62:PHE:O	1:D:66:VAL:HG23	2.16	0.46
3:A:189:HIS:HB2	3:A:196:HIS:NE2	2.30	0.46
2:C:224:LEU:HD11	2:C:261:LEU:HD21	1.97	0.46
2:C:245:GLN:CG	3:A:354:TYR:CZ	2.97	0.46
4:E:290:ASP:HA	4:E:314:ARG:HG3	1.97	0.46
2:R:224:LEU:HD11	2:R:261:LEU:HD21	1.97	0.46
3:F:189:HIS:HB2	3:F:196:HIS:NE2	2.30	0.46
1:D:54:ILE:HG22	1:D:55:CYS:N	2.30	0.46
4:E:159:THR:OG1	4:E:169:TRP:NE1	2.46	0.46
4:E:192:LEU:HD23	4:E:199:PHE:HB3	1.97	0.46
1:B:54:ILE:HG22	1:B:55:CYS:N	2.30	0.45
4:E:5:ASP:OD1	4:E:6:GLN:N	2.47	0.45
1:B:62:PHE:O	1:B:66:VAL:HG23	2.16	0.45
3:F:55:ILE:HG23	3:F:56:ILE:H	1.81	0.45
4:H:113:ALA:HB2	4:H:123:ILE:HG12	1.97	0.45
1:D:32:VAL:HG22	1:D:44:VAL:HG12	1.97	0.45
2:R:192:VAL:HG12	2:R:193:SER:N	2.31	0.45
4:E:311:HIS:NE2	4:E:329:THR:OG1	2.44	0.45
3:A:55:ILE:HG23	3:A:56:ILE:H	1.81	0.45
3:A:217:GLU:OE1	4:E:57:LYS:NZ	2.49	0.45
3:F:217:GLU:OE1	4:H:57:LYS:NZ	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:192:VAL:HG12	2:C:193:SER:N	2.31	0.44
2:R:113:ILE:HG22	2:R:113:ILE:O	2.18	0.44
2:C:178:LEU:N	2:C:179:PRO:CD	2.81	0.44
3:A:296:THR:HG23	3:A:299:ASP:H	1.82	0.44
4:E:124:TYR:CE2	4:E:135:VAL:HG22	2.53	0.44
2:R:245:GLN:CG	3:F:354:TYR:CZ	2.96	0.44
4:H:124:TYR:CE2	4:H:135:VAL:HG22	2.53	0.44
2:C:222:VAL:HB	2:C:223:PRO:HD3	1.99	0.43
3:F:296:THR:HG23	3:F:299:ASP:H	1.82	0.43
2:C:113:ILE:O	2:C:113:ILE:HG22	2.18	0.43
4:H:137:ARG:HD2	4:H:137:ARG:HA	1.83	0.43
4:E:117:LEU:HD23	4:E:145:TYR:HB3	2.01	0.43
2:R:222:VAL:HB	2:R:223:PRO:HD3	1.99	0.43
2:R:178:LEU:N	2:R:179:PRO:CD	2.81	0.43
4:E:148:CYS:SG	4:E:189:SER:HA	2.58	0.43
4:H:54:HIS:NE2	4:H:72:SER:OG	2.42	0.43
5:I:26:ASP:OD1	5:I:26:ASP:N	2.52	0.43
4:H:311:HIS:NE2	4:H:329:THR:OG1	2.44	0.43
4:H:148:CYS:SG	4:H:189:SER:HA	2.58	0.43
4:E:137:ARG:HD2	4:E:137:ARG:HA	1.83	0.42
1:D:62:PHE:CZ	1:D:66:VAL:HG21	2.54	0.42
4:H:117:LEU:HD23	4:H:145:TYR:HB3	2.01	0.42
4:H:276:VAL:HG13	4:H:285:LEU:HD11	2.00	0.42
3:A:325:CYS:N	3:A:328:ASP:OD2	2.42	0.42
4:E:34:THR:HB	5:G:38:MET:HE2	2.02	0.42
1:B:44:VAL:HG23	1:B:56:LEU:HB2	2.01	0.42
5:G:26:ASP:OD1	5:G:26:ASP:N	2.52	0.42
4:H:34:THR:HB	5:I:38:MET:HE2	2.02	0.42
4:E:40:VAL:HG11	5:G:51:LEU:HD11	2.02	0.42
4:E:246:ASP:HA	4:E:272:GLY:HA3	2.01	0.42
4:E:61:MET:HE3	4:E:61:MET:HB3	1.94	0.42
4:H:150:ARG:HD3	4:H:150:ARG:HA	1.95	0.42
4:E:276:VAL:HG13	4:E:285:LEU:HD11	2.00	0.42
2:R:151:ALA:HB1	3:F:343:ILE:HG22	2.01	0.41
2:R:51:VAL:HG22	2:R:301:ILE:HD11	2.03	0.41
4:H:246:ASP:HA	4:H:272:GLY:HA3	2.01	0.41
1:B:62:PHE:CZ	1:B:66:VAL:HG21	2.54	0.41
4:H:225:HIS:NE2	4:H:243:THR:OG1	2.42	0.41
4:E:56:ALA:HB1	4:E:75:GLN:HB2	2.03	0.41
3:F:273:ASP:OD1	3:F:274:LEU:N	2.53	0.41
1:D:44:VAL:HG23	1:D:56:LEU:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:58:ILE:O	4:E:316:SER:OG	2.23	0.41
4:H:30:LEU:O	4:H:34:THR:HG22	2.21	0.41
2:R:152:THR:O	2:R:152:THR:HG22	2.21	0.41
2:R:238:LEU:CD2	3:F:348:LEU:HD21	2.51	0.41
4:E:286:LEU:HD22	4:E:327:VAL:HG11	2.03	0.41
4:H:40:VAL:HG11	5:I:51:LEU:HD11	2.02	0.41
4:H:73:ALA:HB1	4:H:100:VAL:HG11	2.03	0.41
4:H:286:LEU:HD22	4:H:327:VAL:HG11	2.03	0.41
2:R:253:ILE:HG12	3:F:353:LEU:HD21	2.02	0.40
3:A:273:ASP:OD1	3:A:274:LEU:N	2.53	0.40
3:A:322:HIS:CE1	3:A:334:VAL:HG21	2.57	0.40
4:E:30:LEU:O	4:E:34:THR:HG22	2.21	0.40
4:H:56:ALA:HB1	4:H:75:GLN:HB2	2.03	0.40
2:C:245:GLN:CB	3:A:354:TYR:CE1	3.01	0.40
2:C:51:VAL:HG22	2:C:301:ILE:HD11	2.03	0.40
4:E:73:ALA:HB1	4:E:100:VAL:HG11	2.03	0.40
4:H:198:LEU:HD23	4:H:212:ASP:HA	2.03	0.40
4:H:26:ALA:HA	5:I:30:VAL:HG22	2.04	0.40
4:H:200:VAL:HG22	4:H:234:PHE:CZ	2.56	0.40
2:C:107:SER:O	2:C:111:GLY:N	2.50	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 PDB entries followed by that with respect to all EM entries.

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	B	63/78 (81%)	63 (100%)	0	0	100	100
1	D	63/78 (81%)	63 (100%)	0	0	100	100
2	C	298/416 (72%)	293 (98%)	5 (2%)	0	100	100
2	R	298/416 (72%)	293 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
3	F	211/240 (88%)	201 (95%)	10 (5%)	0	100	100
4	E	334/350 (95%)	318 (95%)	16 (5%)	0	100	100
4	H	334/350 (95%)	318 (95%)	16 (5%)	0	100	100
5	G	51/71 (72%)	51 (100%)	0	0	100	100
5	I	51/71 (72%)	51 (100%)	0	0	100	100
All	All	1914/2310 (83%)	1852 (97%)	62 (3%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	B	55/65 (85%)	55 (100%)	0	100	100
1	D	55/65 (85%)	55 (100%)	0	100	100
2	C	255/368 (69%)	255 (100%)	0	100	100
2	R	251/368 (68%)	251 (100%)	0	100	100
3	A	189/206 (92%)	189 (100%)	0	100	100
3	F	189/206 (92%)	189 (100%)	0	100	100
4	E	278/291 (96%)	278 (100%)	0	100	100
4	H	278/291 (96%)	278 (100%)	0	100	100
5	G	43/58 (74%)	43 (100%)	0	100	100
5	I	43/58 (74%)	43 (100%)	0	100	100
All	All	1636/1976 (83%)	1636 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	R	89	ASN
2	R	323	HIS
2	C	89	ASN
2	C	323	HIS
3	A	256	ASN
3	A	333	GLN
3	A	347	ASN
4	E	91	HIS
4	E	125	ASN
4	E	156	GLN
3	F	205	GLN
3	F	256	ASN
3	F	333	GLN
3	F	346	ASN
3	F	347	ASN
4	H	91	HIS
4	H	125	ASN
4	H	156	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 ⓘ

There are no chain breaks in this entry.

6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38748. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

This section was not generated.

6.2 Central slices

This section was not generated.

6.3 Largest variance slices

This section was not generated.

6.4 Orthogonal standard-deviation projections (False-color)

This section was not generated.

6.5 Orthogonal surface views

This section was not generated.

6.6 Mask visualisation

This section was not generated. No masks/segmentation were deposited.

7 Map analysis ⓘ

This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ

This section was not generated.

7.2 Volume estimate versus contour level ⓘ

This section was not generated.

7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.

8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit

This section was not generated.