



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:24 AM UTC

PDB ID : 5FU7 / pdb_00005fu7
Title : drosophila nanos NBR peptide bound to the NOT module of the human CCR4-NOT complex
Authors : Raisch, T.; Bhandari, D.; Sabath, K.; Helms, S.; Valkov, E.; Weichenrieder, O.; Izaurralde, E.
Deposited on : 2016-01-21
Resolution : 3.10 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

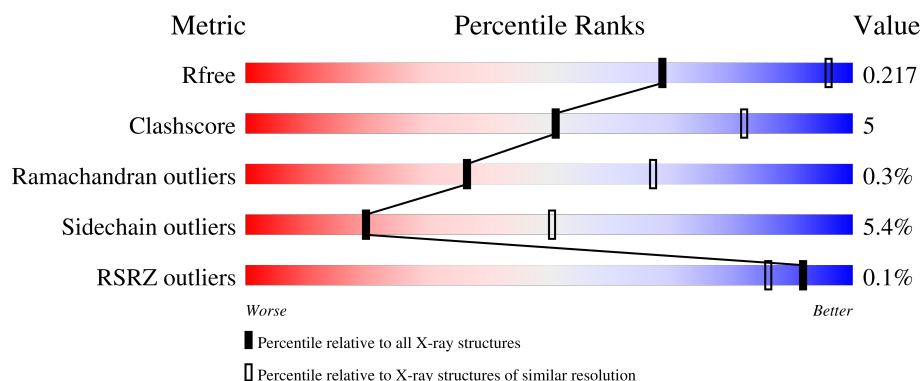
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

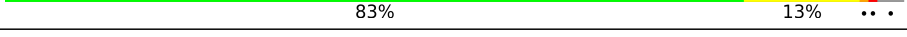
The reported resolution of this entry is 3.10 Å.

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.



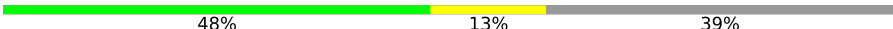
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	535	
1	E	535	
2	B	197	
2	F	197	
3	C	148	

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Mol	Chain	Length	Quality of chain
3	G	148	 82% 17% .
4	D	54	 48% 13% 39%
4	H	54	 50% 6% 44%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14548 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 CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	519	Total	C	N	O	S	0	0	0
			4213	2724	722	744	23			
1	E	514	Total	C	N	O	S	0	0	0
			4178	2703	717	735	23			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1827	GLY	-	expression tag	UNP A5YKK6
A	1828	PRO	-	expression tag	UNP A5YKK6
A	1829	HIS	-	expression tag	UNP A5YKK6
A	1830	MET	-	expression tag	UNP A5YKK6
A	1831	LEU	-	expression tag	UNP A5YKK6
A	1832	GLU	-	expression tag	UNP A5YKK6
A	2344	GLU	HIS	engineered mutation	UNP A5YKK6
A	2345	GLU	CYS	engineered mutation	UNP A5YKK6
A	2346	GLU	ALA	engineered mutation	UNP A5YKK6
E	1827	GLY	-	expression tag	UNP A5YKK6
E	1828	PRO	-	expression tag	UNP A5YKK6
E	1829	HIS	-	expression tag	UNP A5YKK6
E	1830	MET	-	expression tag	UNP A5YKK6
E	1831	LEU	-	expression tag	UNP A5YKK6
E	1832	GLU	-	expression tag	UNP A5YKK6
E	2344	GLU	HIS	engineered mutation	UNP A5YKK6
E	2345	GLU	CYS	engineered mutation	UNP A5YKK6
E	2346	GLU	ALA	engineered mutation	UNP A5YKK6

- Molecule 2 is a protein called CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	191	Total	C	N	O	S	0	0	0
			1570	1012	263	287	8			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	191	Total	C	N	O	S	0	0	0
			1570	1012	263	287	8			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	344	GLY	-	expression tag	UNP Q9NZN8
B	345	PRO	-	expression tag	UNP Q9NZN8
B	346	HIS	-	expression tag	UNP Q9NZN8
B	347	MET	-	expression tag	UNP Q9NZN8
B	348	LEU	-	expression tag	UNP Q9NZN8
B	349	GLU	-	expression tag	UNP Q9NZN8
F	344	GLY	-	expression tag	UNP Q9NZN8
F	345	PRO	-	expression tag	UNP Q9NZN8
F	346	HIS	-	expression tag	UNP Q9NZN8
F	347	MET	-	expression tag	UNP Q9NZN8
F	348	LEU	-	expression tag	UNP Q9NZN8
F	349	GLU	-	expression tag	UNP Q9NZN8

- Molecule 3 is a protein called CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	148	Total	C	N	O	S	0	0	0
			1292	840	216	229	7			
3	G	148	Total	C	N	O	S	0	0	0
			1293	840	216	230	7			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	601	GLY	-	expression tag	UNP O75175
C	602	PRO	-	expression tag	UNP O75175
C	603	HIS	-	expression tag	UNP O75175
C	604	MET	-	expression tag	UNP O75175
C	605	LEU	-	expression tag	UNP O75175
C	606	GLU	-	expression tag	UNP O75175
G	601	GLY	-	expression tag	UNP O75175
G	602	PRO	-	expression tag	UNP O75175
G	603	HIS	-	expression tag	UNP O75175
G	604	MET	-	expression tag	UNP O75175
G	605	LEU	-	expression tag	UNP O75175
G	606	GLU	-	expression tag	UNP O75175

- Molecule 4 is a protein called NANOS, ISOFORM B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	33	Total	C	N	O	S	0	0	0
			238	148	35	53	2			
4	H	30	Total	C	N	O	S	0	0	0
			194	120	31	42	1			

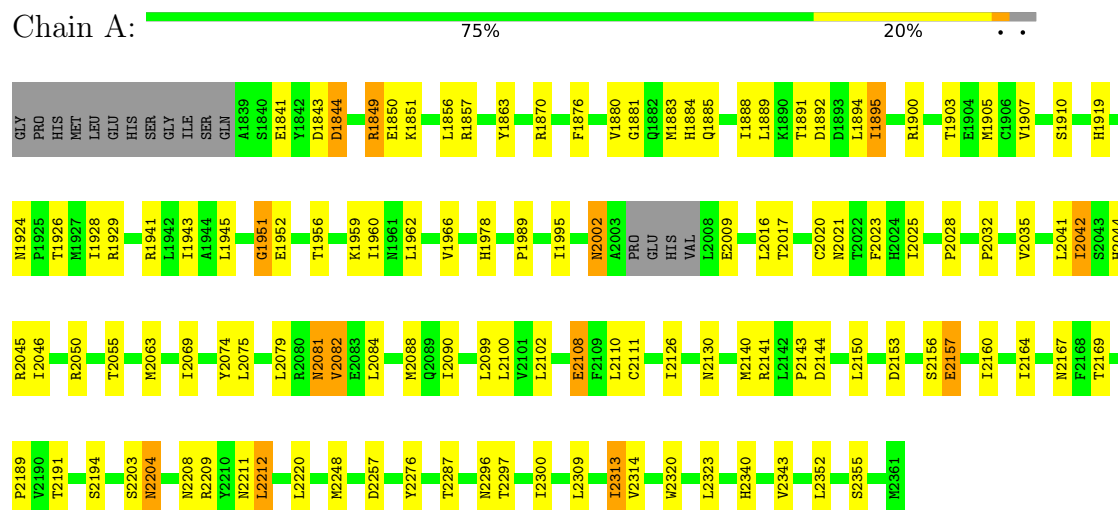
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	110	GLY	-	expression tag	UNP A0A0B4KGY
D	111	PRO	-	expression tag	UNP A0A0B4KGY
D	112	HIS	-	expression tag	UNP A0A0B4KGY
D	113	MET	-	expression tag	UNP A0A0B4KGY
D	114	LEU	-	expression tag	UNP A0A0B4KGY
D	115	GLU	-	expression tag	UNP A0A0B4KGY
H	110	GLY	-	expression tag	UNP A0A0B4KGY
H	111	PRO	-	expression tag	UNP A0A0B4KGY
H	112	HIS	-	expression tag	UNP A0A0B4KGY
H	113	MET	-	expression tag	UNP A0A0B4KGY
H	114	LEU	-	expression tag	UNP A0A0B4KGY
H	115	GLU	-	expression tag	UNP A0A0B4KGY

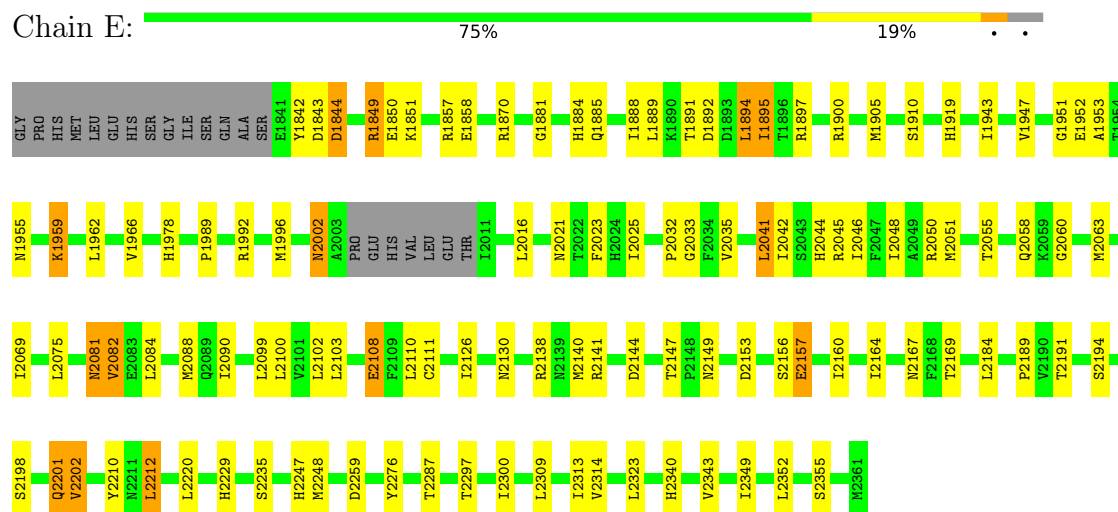
3 Residue-property plots

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.

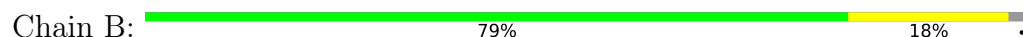
• Molecule 1: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1

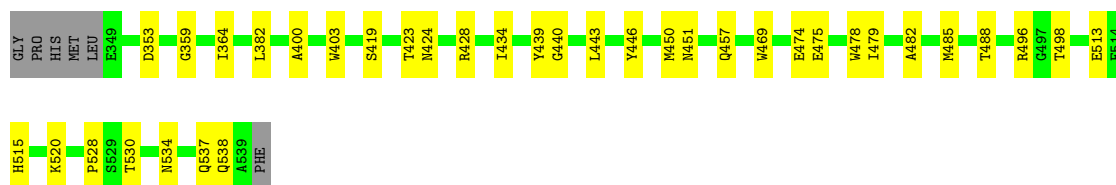


• Molecule 1: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1

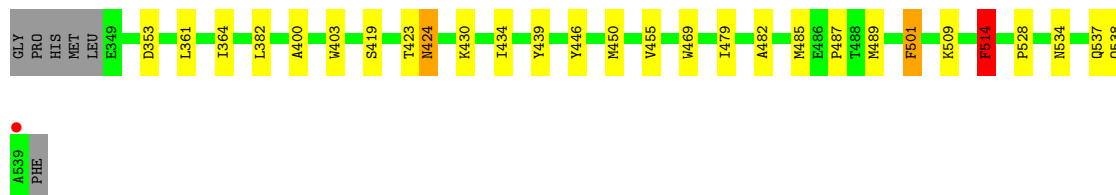
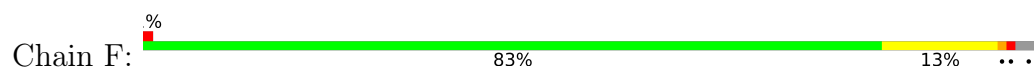


• Molecule 2: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2

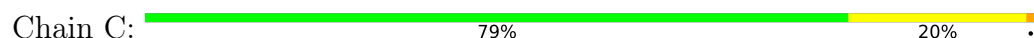




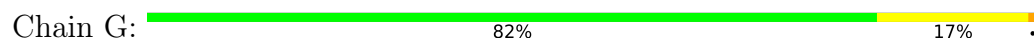
• Molecule 2: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2



• Molecule 3: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 3



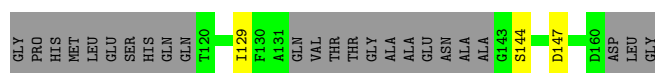
• Molecule 3: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 3



• Molecule 4: NANOS, ISOFORM B



• Molecule 4: NANOS, ISOFORM B



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.95Å 135.67Å 104.97Å 90.00° 107.98° 90.00°	Depositor
Resolution (Å)	48.58 – 3.10 48.58 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.58-3.10) 99.7 (48.58-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 3.12Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.165 , 0.227 (Not available) , 0.217	Depositor DCC
R_{free} test set	1892 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å ²)	82.0	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 81.9	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	0.96	EDS
Total number of atoms	14548	wwPDB-VP
Average B, all atoms (Å ²)	99.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.31% 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	0.91	1/4320 (0.0%)	1.48	38/5874 (0.6%)
1	E	0.91	1/4285 (0.0%)	1.49	26/5826 (0.4%)
2	B	0.83	0/1617	1.36	9/2198 (0.4%)
2	F	0.83	0/1617	1.36	9/2198 (0.4%)
3	C	0.81	0/1343	1.27	5/1819 (0.3%)
3	G	0.81	0/1344	1.31	5/1819 (0.3%)
4	D	0.92	0/239	1.60	2/322 (0.6%)
4	H	0.90	0/194	1.61	0/262
All	All	0.88	2/14959 (0.0%)	1.43	94/20318 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	2082	VAL	CA-C	5.51	1.59	1.52
1	A	2082	VAL	CA-C	5.05	1.59	1.52

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	514	PHE	CA-CB-CG	8.48	122.28	113.80
1	A	2257	ASP	CA-CB-CG	8.44	121.04	112.60
3	G	630	ASP	CA-CB-CG	8.02	120.62	112.60
1	E	1892	ASP	CA-CB-CG	7.52	120.12	112.60
1	A	2167	ASN	CA-C-N	7.37	131.13	120.38
1	A	2167	ASN	C-N-CA	7.37	131.13	120.38
3	C	630	ASP	CA-CB-CG	7.35	119.95	112.60
1	E	2167	ASN	CA-C-N	7.12	130.54	120.28
1	E	2167	ASN	C-N-CA	7.12	130.54	120.28
2	B	419	SER	CA-C-N	6.74	129.61	120.38
2	B	419	SER	C-N-CA	6.74	129.61	120.38
1	E	2169	THR	CA-C-N	6.66	127.37	119.98
1	E	2169	THR	C-N-CA	6.66	127.37	119.98
1	A	2169	THR	CA-C-N	6.59	127.30	119.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2169	THR	C-N-CA	6.59	127.30	119.98
1	E	2130	ASN	CA-CB-CG	6.55	119.15	112.60
1	A	2130	ASN	CA-CB-CG	6.45	119.05	112.60
2	F	419	SER	CA-C-N	6.32	129.61	120.38
2	F	419	SER	C-N-CA	6.32	129.61	120.38
3	C	711	GLU	N-CA-C	-6.28	102.16	110.07
1	A	1951	GLY	CA-C-N	6.21	130.21	121.02
1	A	1951	GLY	C-N-CA	6.21	130.21	121.02
1	E	1843	ASP	CA-C-N	6.03	129.64	121.20
1	E	1843	ASP	C-N-CA	6.03	129.64	121.20
2	B	359	GLY	CA-C-N	5.97	128.56	120.44
2	B	359	GLY	C-N-CA	5.97	128.56	120.44
1	A	2204	ASN	CA-CB-CG	5.96	118.56	112.60
1	E	1989	PRO	CA-C-N	5.95	128.26	120.28
1	E	1989	PRO	C-N-CA	5.95	128.26	120.28
1	A	2110	LEU	CA-C-N	5.86	128.41	120.44
1	A	2110	LEU	C-N-CA	5.86	128.41	120.44
3	G	711	GLU	N-CA-C	-5.84	102.70	110.07
2	F	424	ASN	N-CA-C	5.84	117.32	111.07
1	E	2212	LEU	CA-C-N	5.82	128.08	120.28
1	E	2212	LEU	C-N-CA	5.82	128.08	120.28
1	A	2153	ASP	CA-C-N	5.82	128.40	120.54
1	A	2153	ASP	C-N-CA	5.82	128.40	120.54
1	A	2203	SER	CA-C-N	5.78	128.49	120.63
1	A	2203	SER	C-N-CA	5.78	128.49	120.63
1	E	2153	ASP	CA-C-N	5.76	128.31	120.54
1	E	2153	ASP	C-N-CA	5.76	128.31	120.54
1	E	1849	ARG	CA-C-N	5.67	127.81	120.44
1	E	1849	ARG	C-N-CA	5.67	127.81	120.44
1	E	2259	ASP	CA-CB-CG	5.67	118.27	112.60
1	A	1849	ARG	CA-C-N	5.66	127.79	120.44
1	A	1849	ARG	C-N-CA	5.66	127.79	120.44
3	C	606	GLU	N-CA-C	-5.62	105.30	111.82
1	A	1989	PRO	CA-C-N	5.61	127.80	120.28
1	A	1989	PRO	C-N-CA	5.61	127.80	120.28
3	G	606	GLU	N-CA-C	-5.55	105.38	111.82
3	G	699	HIS	CA-C-N	5.51	127.92	120.38
3	G	699	HIS	C-N-CA	5.51	127.92	120.38
2	B	440	GLY	CA-C-N	5.48	127.62	120.28
2	B	440	GLY	C-N-CA	5.48	127.62	120.28
1	A	2212	LEU	CA-C-N	5.47	127.61	120.28
1	A	2212	LEU	C-N-CA	5.47	127.61	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1919	HIS	CA-C-N	5.38	127.81	122.00
1	A	1919	HIS	C-N-CA	5.38	127.81	122.00
1	E	2149	ASN	CA-CB-CG	5.36	117.96	112.60
1	A	1843	ASP	CA-C-N	5.35	128.69	121.20
1	A	1843	ASP	C-N-CA	5.35	128.69	121.20
1	A	1850	GLU	CA-C-N	5.34	127.38	120.44
1	A	1850	GLU	C-N-CA	5.34	127.38	120.44
3	C	747	LEU	CA-C-N	5.30	131.24	121.70
3	C	747	LEU	C-N-CA	5.30	131.24	121.70
1	E	1850	GLU	CA-C-N	5.29	127.31	120.44
1	E	1850	GLU	C-N-CA	5.29	127.31	120.44
1	E	1843	ASP	CA-CB-CG	5.26	117.86	112.60
1	E	2041	LEU	CA-C-N	5.25	127.94	120.53
1	E	2041	LEU	C-N-CA	5.25	127.94	120.53
1	E	1919	HIS	CA-C-N	5.24	127.65	122.00
1	E	1919	HIS	C-N-CA	5.24	127.65	122.00
1	A	2041	LEU	CA-C-N	5.23	127.90	120.53
1	A	2041	LEU	C-N-CA	5.23	127.90	120.53
2	B	353	ASP	CA-C-N	5.22	128.96	120.60
2	B	353	ASP	C-N-CA	5.22	128.96	120.60
1	E	1843	ASP	N-CA-C	-5.20	104.32	111.81
1	A	2313	ILE	CA-C-N	5.15	128.47	120.34
1	A	2313	ILE	C-N-CA	5.15	128.47	120.34
2	F	353	ASP	CA-C-N	5.14	128.82	120.60
2	F	353	ASP	C-N-CA	5.14	128.82	120.60
2	F	501	PHE	CA-CB-CG	5.14	118.94	113.80
2	B	475	GLU	CB-CG-CD	5.13	121.33	112.60
1	A	2296	ASN	CA-CB-CG	5.12	117.72	112.60
1	A	2320	TRP	CA-C-N	5.11	125.65	119.98
1	A	2320	TRP	C-N-CA	5.11	125.65	119.98
1	A	2211	ASN	CA-C-N	5.10	127.42	120.54
1	A	2211	ASN	C-N-CA	5.10	127.42	120.54
2	F	487	PRO	CA-C-N	5.04	126.99	120.44
2	F	487	PRO	C-N-CA	5.04	126.99	120.44
1	A	2009	GLU	CA-C-N	5.03	129.11	120.71
1	A	2009	GLU	C-N-CA	5.03	129.11	120.71
4	D	121	ASP	CA-C-N	5.01	126.96	120.44
4	D	121	ASP	C-N-CA	5.01	126.96	120.44

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	4213	0	4224	55	0
1	E	4178	0	4190	52	0
2	B	1570	0	1512	14	0
2	F	1570	0	1512	13	0
3	C	1292	0	1207	16	0
3	G	1293	0	1207	13	0
4	D	238	0	208	5	0
4	H	194	0	158	4	0
All	All	14548	0	14218	150	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 5.

All (150) 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:E:2184:LEU:HD22	1:E:2247:HIS:HD2	1.35	0.92
1:A:1857:ARG:HG3	1:A:1905:MET:HE1	1.63	0.80
1:E:1978:HIS:HE1	1:E:2033:GLY:H	1.31	0.79
1:E:1857:ARG:HG3	1:E:1905:MET:HE1	1.67	0.77
1:A:1952:GLU:HB2	4:H:129:ILE:HG12	1.72	0.71
2:B:498:THR:HG22	2:B:513:GLU:HB3	1.72	0.71
1:E:2021:ASN:O	1:E:2025:ILE:HG12	1.91	0.71
3:G:638:LEU:HD12	3:G:678:LEU:HD21	1.74	0.70
1:A:2021:ASN:O	1:A:2025:ILE:HG12	1.89	0.70
1:E:2184:LEU:HD22	1:E:2247:HIS:CD2	2.23	0.70
3:C:638:LEU:HD12	3:C:678:LEU:HD21	1.72	0.70
1:A:1884:HIS:HB2	1:A:1889:LEU:HD12	1.76	0.68
1:E:1884:HIS:HB2	1:E:1889:LEU:HD12	1.76	0.67
1:A:1903:THR:O	1:A:1907:VAL:HG23	1.97	0.65
2:F:528:PRO:HG2	3:G:643:CYS:HB2	1.79	0.63
1:A:2081:ASN:HD21	3:C:606:GLU:HB2	1.66	0.60
1:E:2051:MET:HE1	1:E:2063:MET:HE3	1.84	0.59
4:D:129:ILE:HG12	1:E:1952:GLU:HB2	1.84	0.58
2:B:451:ASN:O	2:B:457:GLN:HB2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:2023:PHE:HB3	1:E:2042:ILE:HD11	1.85	0.58
1:E:1881:GLY:O	1:E:1885:GLN:HG2	2.03	0.58
2:B:423:THR:HG22	3:C:703:MET:HG2	1.85	0.57
1:A:1943:ILE:HG21	1:A:1966:VAL:HG11	1.86	0.57
1:A:1952:GLU:CB	4:H:129:ILE:HG12	2.35	0.57
1:A:1943:ILE:CG2	1:A:1966:VAL:HG11	2.34	0.56
1:A:2189:PRO:HB2	1:A:2191:THR:HG22	1.86	0.56
1:A:1926:THR:HG22	1:A:1929:ARG:HH22	1.70	0.56
1:E:2081:ASN:HD21	3:G:606:GLU:HB2	1.71	0.56
1:E:1943:ILE:HG21	1:E:1966:VAL:HG11	1.86	0.56
1:A:2309:LEU:HD21	1:A:2352:LEU:HB3	1.88	0.56
3:C:708:ARG:HD3	3:C:712:PRO:HD3	1.87	0.56
1:A:2157:GLU:HA	1:A:2160:ILE:HD12	1.87	0.56
2:F:455:VAL:HG12	3:G:641:ASN:HB3	1.88	0.56
1:A:1881:GLY:O	1:A:1885:GLN:HG2	2.05	0.56
1:A:1863:TYR:HE1	1:A:1941:ARG:HD2	1.71	0.55
1:E:2144:ASP:HB3	1:E:2147:THR:HG23	1.87	0.55
1:E:2189:PRO:HB2	1:E:2191:THR:HG22	1.87	0.55
3:G:708:ARG:HD3	3:G:712:PRO:HD3	1.88	0.54
1:E:1943:ILE:CG2	1:E:1966:VAL:HG11	2.37	0.54
1:A:2017:THR:HG23	1:A:2063:MET:HE1	1.89	0.54
1:E:2002:ASN:HD21	1:E:2050:ARG:HH11	1.55	0.54
2:F:534:ASN:HB3	2:F:537:GLN:HG3	1.89	0.54
1:A:2002:ASN:HD21	1:A:2050:ARG:HH11	1.56	0.53
1:A:1880:VAL:HG11	4:D:130:PHE:HD2	1.73	0.53
3:C:704:MET:HE2	3:C:728:ASP:HA	1.90	0.53
1:E:2309:LEU:HD21	1:E:2352:LEU:HB3	1.89	0.53
2:B:534:ASN:HB3	2:B:537:GLN:HG3	1.90	0.53
1:E:2157:GLU:HA	1:E:2160:ILE:HD12	1.90	0.53
3:C:723:THR:HG22	3:C:738:GLU:HA	1.90	0.53
1:A:2044:HIS:HD2	1:A:2046:ILE:HB	1.75	0.51
1:A:2100:LEU:HD21	2:B:382:LEU:HD13	1.91	0.51
1:E:1951:GLY:HA3	1:E:1959:LYS:HE3	1.91	0.51
1:A:2023:PHE:HB3	1:A:2042:ILE:HD11	1.92	0.51
1:E:2100:LEU:HD21	2:F:382:LEU:HD13	1.92	0.51
3:G:723:THR:HG22	3:G:738:GLU:HA	1.93	0.50
1:A:1844:ASP:CG	1:A:1900:ARG:HH22	2.19	0.50
1:A:2297:THR:HB	1:A:2300:ILE:HG13	1.94	0.50
1:A:1962:LEU:HD13	4:D:123:ILE:HG21	1.94	0.49
1:E:2099:LEU:HD23	1:E:2102:LEU:HD12	1.94	0.49
2:B:528:PRO:HG2	3:C:643:CYS:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2075:LEU:CD2	1:A:2088:MET:HE1	2.43	0.49
3:C:646:PRO:HG2	3:C:649:HIS:HD2	1.77	0.49
1:A:2099:LEU:HD23	1:A:2102:LEU:HD12	1.94	0.49
1:A:2313:ILE:HD11	1:A:2355:SER:HB2	1.95	0.49
2:B:482:ALA:HB3	2:B:485:MET:HB2	1.94	0.49
3:G:646:PRO:HG2	3:G:649:HIS:HD2	1.78	0.48
1:E:2044:HIS:CD2	1:E:2046:ILE:H	2.31	0.48
1:E:2055:THR:HG23	1:E:2058:GLN:HA	1.95	0.48
1:A:2164:ILE:HD13	1:A:2220:LEU:HD21	1.95	0.48
1:E:2313:ILE:HD11	1:E:2355:SER:HB2	1.95	0.48
2:F:469:TRP:CZ2	2:F:509:LYS:HE3	2.49	0.48
1:A:1978:HIS:CE1	1:A:2032:PRO:HD2	2.49	0.47
1:E:2108:GLU:CD	1:E:2108:GLU:H	2.22	0.47
1:E:2164:ILE:HD13	1:E:2220:LEU:HD21	1.96	0.47
2:F:430:LYS:O	3:G:730:GLU:HB3	2.15	0.46
1:A:1889:LEU:HA	1:A:1895:ILE:HD11	1.97	0.46
1:A:1951:GLY:HA3	1:A:1959:LYS:NZ	2.30	0.46
1:A:1995:ILE:HG21	3:C:631:SER:HA	1.96	0.46
2:F:482:ALA:HB3	2:F:485:MET:HB2	1.96	0.46
3:C:672:PHE:CE1	3:C:705:TRP:HB2	2.50	0.46
1:A:1884:HIS:NE2	1:E:1953:ALA:HB1	2.31	0.46
1:A:2016:LEU:HD11	1:A:2050:ARG:HB3	1.98	0.46
1:E:1889:LEU:HA	1:E:1895:ILE:HD11	1.96	0.46
1:E:2044:HIS:HD2	1:E:2046:ILE:HB	1.79	0.46
1:E:2103:LEU:HA	1:E:2110:LEU:HD12	1.97	0.46
1:E:2108:GLU:OE2	1:E:2138:ARG:HG2	2.15	0.46
1:E:2016:LEU:HD11	1:E:2050:ARG:HB3	1.96	0.45
1:E:1844:ASP:CG	1:E:1900:ARG:HH22	2.25	0.45
3:G:747:LEU:O	3:G:748:GLU:HG2	2.16	0.45
1:E:2229:HIS:CD2	1:E:2247:HIS:HE1	2.33	0.45
1:A:2079:LEU:HD23	1:A:2084:LEU:HD11	1.97	0.45
2:F:446:TYR:CE2	2:F:450:MET:HG3	2.52	0.45
3:G:621:ALA:HA	3:G:624:HIS:CE1	2.51	0.45
3:C:718:GLU:HG2	4:H:147:ASP:HA	1.99	0.45
2:B:496:ARG:HG2	2:B:515:HIS:HB2	1.99	0.45
1:E:2349:ILE:HD13	2:F:361:LEU:HD13	1.98	0.45
1:A:1891:THR:HG23	1:A:1894:LEU:HB2	2.00	0.44
2:B:446:TYR:CE2	2:B:450:MET:HG3	2.52	0.44
1:E:2201:GLN:HA	1:E:2210:TYR:HA	2.00	0.44
2:F:423:THR:HA	3:G:703:MET:HE2	2.00	0.44
1:A:1892:ASP:OD2	4:D:123:ILE:HD12	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1992:ARG:NH1	1:E:1996:MET:HE2	2.32	0.44
1:E:2297:THR:HB	1:E:2300:ILE:HG13	1.99	0.44
1:A:2143:PRO:HB2	1:A:2150:LEU:HD11	2.00	0.44
1:E:2075:LEU:CD2	1:E:2088:MET:HE1	2.48	0.44
2:F:469:TRP:HZ2	2:F:509:LYS:HE3	1.83	0.44
2:F:501:PHE:HB3	2:F:514:PHE:HZ	1.82	0.44
4:D:144:SER:HB2	4:D:147:ASP:OD2	2.18	0.44
1:E:1947:VAL:HA	1:E:1962:LEU:HD23	2.00	0.44
1:E:1891:THR:HG23	1:E:1894:LEU:HB2	2.01	0.43
1:E:2248:MET:HE1	1:E:2287:THR:HG23	2.00	0.43
3:C:621:ALA:HA	3:C:624:HIS:CE1	2.52	0.43
1:E:1842:TYR:C	1:E:1844:ASP:H	2.26	0.43
1:E:1951:GLY:HA3	1:E:1959:LYS:CE	2.49	0.43
1:E:1952:GLU:HG3	1:E:1955:ASN:HD22	1.83	0.43
1:A:1863:TYR:CE1	1:A:1941:ARG:HD2	2.54	0.42
2:B:474:GLU:HB2	2:B:520:LYS:HD2	2.01	0.42
4:H:144:SER:HB3	4:H:147:ASP:OD2	2.18	0.42
1:A:1876:PHE:HB2	1:A:1945:LEU:HD13	2.01	0.42
1:A:2108:GLU:CD	1:A:2108:GLU:H	2.26	0.42
1:E:2060:GLY:HA2	1:E:2063:MET:HE2	2.01	0.42
1:E:2126:ILE:HG21	1:E:2314:VAL:HG21	2.01	0.42
1:A:2208:ASN:O	1:A:2209:ARG:HG2	2.19	0.42
3:C:743:GLU:HB2	3:C:746:TYR:CD2	2.55	0.42
3:C:646:PRO:HG2	3:C:649:HIS:CD2	2.54	0.41
2:B:439:TYR:HB3	2:B:443:LEU:HD23	2.02	0.41
1:E:2023:PHE:CE1	1:E:2041:LEU:HD13	2.55	0.41
2:B:434:ILE:HA	2:B:439:TYR:OH	2.19	0.41
3:G:661:GLU:HA	3:G:664:GLN:HE21	1.84	0.41
1:A:2126:ILE:HG21	1:A:2314:VAL:HG21	2.02	0.41
1:A:1951:GLY:HA3	1:A:1959:LYS:HD3	2.03	0.41
2:F:434:ILE:HA	2:F:439:TYR:OH	2.20	0.41
1:A:2075:LEU:HD22	1:A:2088:MET:HE1	2.02	0.41
1:E:2140:MET:HE1	1:E:2276:TYR:HD2	1.86	0.41
1:A:2044:HIS:CD2	1:A:2046:ILE:HB	2.54	0.41
1:A:1856:LEU:HD23	1:A:1905:MET:SD	2.61	0.41
1:A:1891:THR:HG23	1:A:1894:LEU:H	1.86	0.41
1:A:1924:ASN:O	1:A:1928:ILE:HG12	2.21	0.41
1:A:2140:MET:HE1	1:A:2276:TYR:HD2	1.86	0.41
1:E:1978:HIS:CE1	1:E:2032:PRO:HD2	2.56	0.41
1:E:2035:VAL:HG11	3:G:618:GLU:HG3	2.02	0.41
1:A:2035:VAL:HG11	3:C:618:GLU:HG3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:528:PRO:C	2:B:530:THR:H	2.28	0.41
3:C:721:GLN:HA	3:C:740:PHE:O	2.21	0.41
1:E:1897:ARG:HG2	1:E:1900:ARG:HH21	1.86	0.41
1:A:2002:ASN:HD21	1:A:2050:ARG:HD2	1.86	0.40
1:A:2028:PRO:HB2	1:A:2074:TYR:CD1	2.56	0.40
2:B:469:TRP:HB3	2:B:478:TRP:CE3	2.56	0.40
1:A:1880:VAL:HA	1:A:1883:MET:HE3	2.03	0.40
1:A:2248:MET:HE1	1:A:2287:THR:HG23	2.02	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	515/535 (96%)	499 (97%)	15 (3%)	1 (0%)	43	73
1	E	510/535 (95%)	488 (96%)	20 (4%)	2 (0%)	30	61
2	B	189/197 (96%)	174 (92%)	13 (7%)	2 (1%)	11	39
2	F	189/197 (96%)	175 (93%)	13 (7%)	1 (0%)	24	57
3	C	146/148 (99%)	138 (94%)	8 (6%)	0	100	100
3	G	146/148 (99%)	139 (95%)	7 (5%)	0	100	100
4	D	29/54 (54%)	29 (100%)	0	0	100	100
4	H	26/54 (48%)	25 (96%)	1 (4%)	0	100	100
All	All	1750/1868 (94%)	1667 (95%)	77 (4%)	6 (0%)	36	67

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	428	ARG
2	F	400	ALA

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Mol	Chain	Res	Type
2	B	400	ALA
1	E	2202	VAL
1	A	2082	VAL
1	E	2082	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	464/479 (97%)	434 (94%)	30 (6%)	15	44
1	E	460/479 (96%)	429 (93%)	31 (7%)	15	43
2	B	167/172 (97%)	161 (96%)	6 (4%)	31	62
2	F	167/172 (97%)	160 (96%)	7 (4%)	26	58
3	C	136/136 (100%)	131 (96%)	5 (4%)	30	61
3	G	136/136 (100%)	131 (96%)	5 (4%)	30	61
4	D	24/41 (58%)	23 (96%)	1 (4%)	26	58
4	H	16/41 (39%)	16 (100%)	0	100	100
All	All	1570/1656 (95%)	1485 (95%)	85 (5%)	20	50

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1841	GLU
1	A	1844	ASP
1	A	1849	ARG
1	A	1851	LYS
1	A	1870	ARG
1	A	1888	ILE
1	A	1895	ILE
1	A	1910	SER
1	A	1956	THR
1	A	1960	ILE
1	A	2002	ASN

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Mol	Chain	Res	Type
1	A	2020	CYS
1	A	2042	ILE
1	A	2045	ARG
1	A	2055	THR
1	A	2069	ILE
1	A	2081	ASN
1	A	2090	ILE
1	A	2108	GLU
1	A	2111	CYS
1	A	2141	ARG
1	A	2144	ASP
1	A	2156	SER
1	A	2157	GLU
1	A	2194	SER
1	A	2204	ASN
1	A	2212	LEU
1	A	2323	LEU
1	A	2340	HIS
1	A	2343	VAL
2	B	364	ILE
2	B	403	TRP
2	B	424	ASN
2	B	479	ILE
2	B	488	THR
2	B	538	GLN
3	C	610	GLU
3	C	694	GLN
3	C	697	ARG
3	C	703	MET
3	C	748	GLU
4	D	122	GLU
1	E	1844	ASP
1	E	1849	ARG
1	E	1851	LYS
1	E	1858	GLU
1	E	1870	ARG
1	E	1888	ILE
1	E	1894	LEU
1	E	1895	ILE
1	E	1910	SER
1	E	1959	LYS
1	E	2002	ASN

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Mol	Chain	Res	Type
1	E	2045	ARG
1	E	2048	ILE
1	E	2069	ILE
1	E	2081	ASN
1	E	2084	LEU
1	E	2090	ILE
1	E	2108	GLU
1	E	2111	CYS
1	E	2141	ARG
1	E	2156	SER
1	E	2157	GLU
1	E	2194	SER
1	E	2198	SER
1	E	2201	GLN
1	E	2202	VAL
1	E	2212	LEU
1	E	2235	SER
1	E	2323	LEU
1	E	2340	HIS
1	E	2343	VAL
2	F	364	ILE
2	F	403	TRP
2	F	424	ASN
2	F	479	ILE
2	F	489	MET
2	F	514	PHE
2	F	538	GLN
3	G	610	GLU
3	G	665	ARG
3	G	694	GLN
3	G	703	MET
3	G	734	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1885	GLN
1	A	1886	GLN
1	A	1919	HIS
1	A	1976	GLN
1	A	1987	GLN
1	A	2002	ASN

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Mol	Chain	Res	Type
1	A	2012	ASN
1	A	2044	HIS
1	A	2081	ASN
1	A	2159	ASN
1	A	2225	GLN
1	A	2280	HIS
1	A	2315	ASN
2	B	424	ASN
2	B	426	HIS
2	B	492	ASN
2	B	515	HIS
2	B	526	HIS
3	C	641	ASN
3	C	651	GLN
3	C	664	GLN
3	C	699	HIS
3	C	707	GLN
1	E	1885	GLN
1	E	1886	GLN
1	E	1961	ASN
1	E	1964	ASN
1	E	1978	HIS
1	E	1982	GLN
1	E	1987	GLN
1	E	2002	ASN
1	E	2012	ASN
1	E	2044	HIS
1	E	2057	GLN
1	E	2081	ASN
1	E	2199	ASN
1	E	2201	GLN
1	E	2225	GLN
1	E	2229	HIS
1	E	2247	HIS
1	E	2253	ASN
2	F	424	ASN
2	F	492	ASN
3	G	624	HIS
3	G	651	GLN
3	G	664	GLN
3	G	694	GLN
3	G	699	HIS

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Mol	Chain	Res	Type
3	G	709	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no 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 [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(Å²)	Q<0.9	
1	A	519/535 (97%)	-0.67	0	100	100	49, 81, 137, 163	0
1	E	514/535 (96%)	-0.63	0	100	100	55, 92, 142, 185	0
2	B	191/197 (96%)	-0.52	0	100	100	67, 109, 205, 217	0
2	F	191/197 (96%)	-0.48	1 (0%)	87	73	73, 102, 174, 190	0
3	C	148/148 (100%)	-0.54	0	100	100	50, 101, 133, 157	0
3	G	148/148 (100%)	-0.64	0	100	100	51, 89, 123, 136	0
4	D	33/54 (61%)	-0.23	0	100	100	109, 137, 158, 164	0
4	H	30/54 (55%)	-0.03	0	100	100	120, 136, 165, 181	0
All	All	1774/1868 (94%)	-0.59	1 (0%)	92	86	49, 95, 157, 217	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	539	ALA	2.2

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.