



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 18, 2026 – 03:23 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 wwPDB X-ray Structure Validation Summary 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

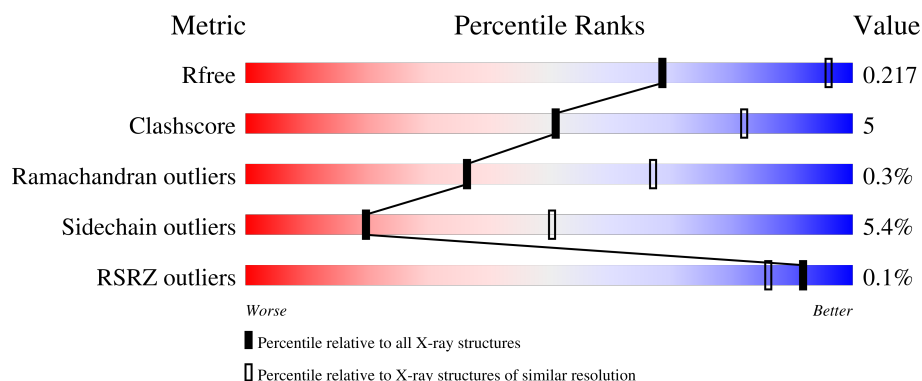
1 Overall quality at a glance

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	 75% 20% . .
1	E	535	 75% 19% . .
2	B	197	 79% 18% .
2	F	197	 83% 13% . . .
3	C	148	 79% 20% .

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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			

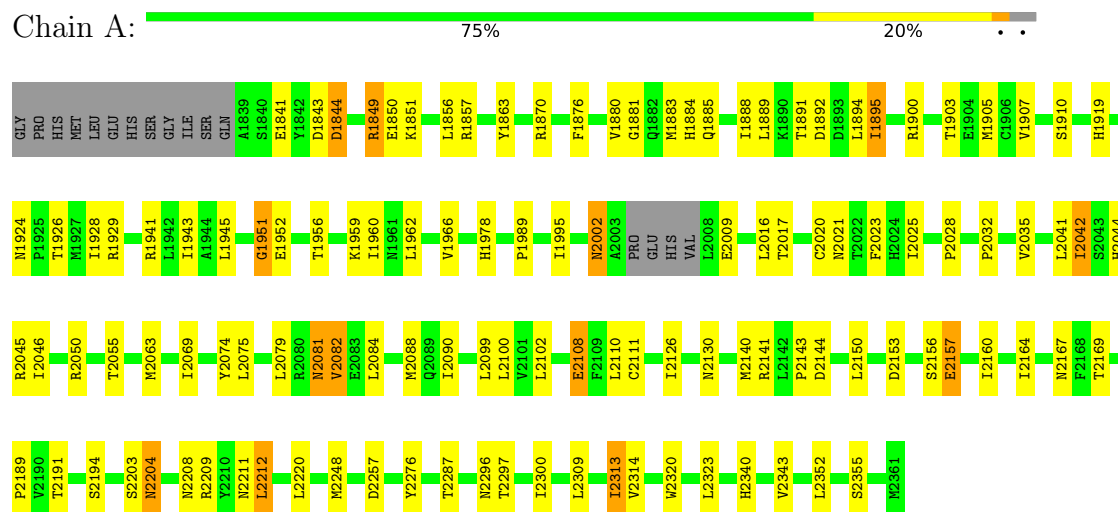
There are 12 discrepancies between the modelled and reference sequences:

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

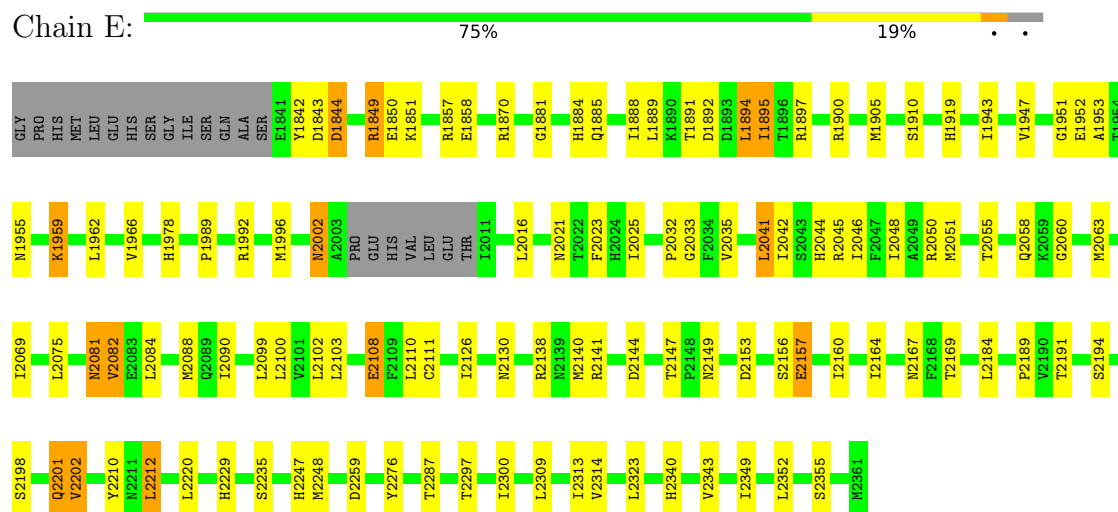
3 Residue-property plots

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.

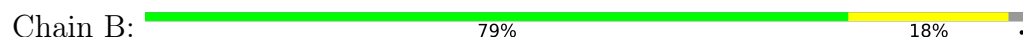
• Molecule 1: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1

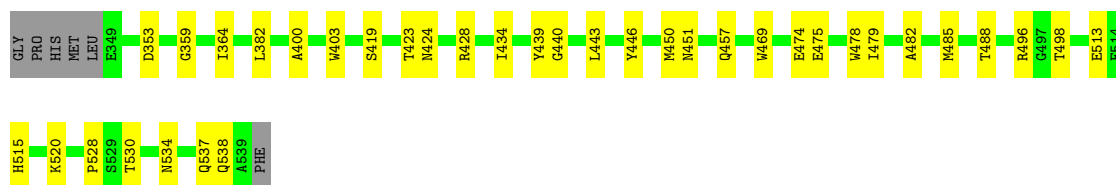


• Molecule 1: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1

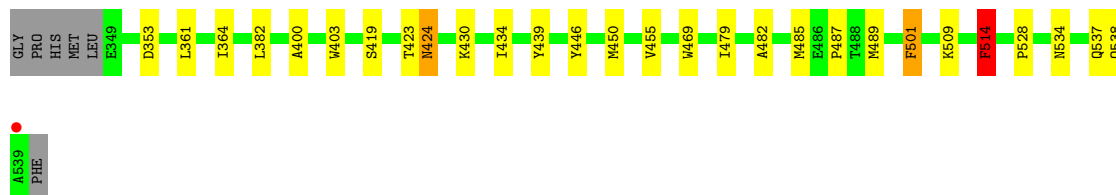
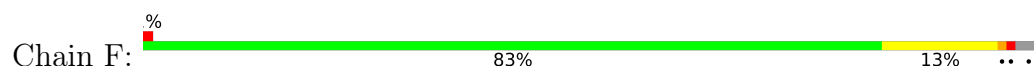


• Molecule 2: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2

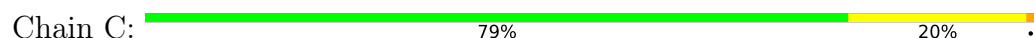




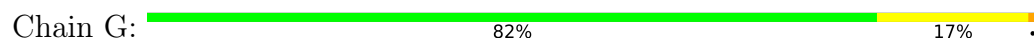
• Molecule 2: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2



• Molecule 3: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 3



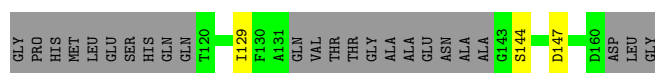
• Molecule 3: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 3



• 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

The worst 5 of 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

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.

The worst 5 of 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

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	515/535 (96%)	499 (97%)	15 (3%)	1 (0%)	43 73
1	E	510/535 (95%)	488 (96%)	20 (4%)	2 (0%)	30 61

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	428	ARG
2	F	400	ALA
2	B	400	ALA
1	E	2202	VAL
1	A	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

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	2084	LEU
1	E	2340	HIS
1	E	2108	GLU
1	E	2198	SER
2	F	424	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1982	GLN
1	E	2199	ASN
1	E	1987	GLN
1	E	2044	HIS
1	E	2225	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 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.