



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 03:18 am BST

PDB ID : 5FU6
Title : NOT module of the human CCR4-NOT complex (Crystallization mutant)
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Deposited on : 2016-01-21
Resolution : 2.90 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

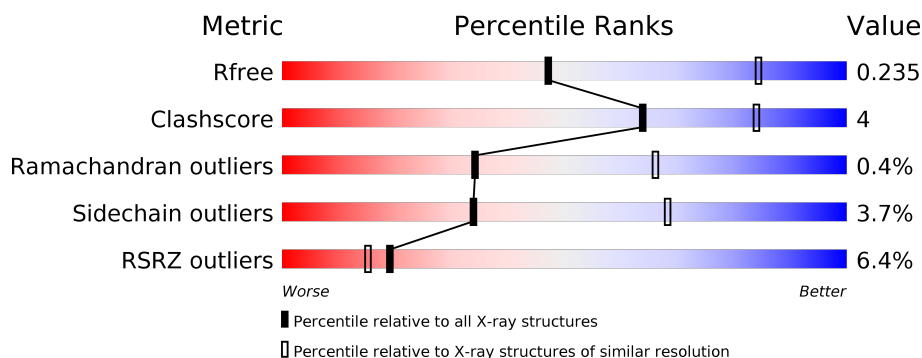
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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	<div> <div>5%</div> <div> <div></div> <div>79%</div> <div>16%</div> <div>• •</div> </div> </div>
1	D	535	<div> <div>5%</div> <div> <div></div> <div>80%</div> <div>16%</div> <div>•</div> </div> </div>
2	B	197	<div> <div>17%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>•</div> </div> </div>
2	E	197	<div> <div>8%</div> <div> <div></div> <div>85%</div> <div>11%</div> <div>• •</div> </div> </div>
3	C	148	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
3	F	148	<div> <div>3%</div> <div> <div></div> <div>93%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14109 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	515	Total	C	N	O	S	0	0	0
			4186	2709	718	735	24			
1	D	516	Total	C	N	O	S	0	0	0
			4193	2712	719	738	24			

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
D	1827	GLY	-	expression tag	UNP A5YKK6
D	1828	PRO	-	expression tag	UNP A5YKK6
D	1829	HIS	-	expression tag	UNP A5YKK6
D	1830	MET	-	expression tag	UNP A5YKK6
D	1831	LEU	-	expression tag	UNP A5YKK6
D	1832	GLU	-	expression tag	UNP A5YKK6
D	2344	GLU	HIS	engineered mutation	UNP A5YKK6
D	2345	GLU	CYS	engineered mutation	UNP A5YKK6
D	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	192	Total	C	N	O	S	0	0	0
			1578	1019	264	288	7			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	191	Total	C	N	O	S	0	0	0
			1566	1010	263	285	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
E	344	GLY	-	expression tag	UNP Q9NZN8
E	345	PRO	-	expression tag	UNP Q9NZN8
E	346	HIS	-	expression tag	UNP Q9NZN8
E	347	MET	-	expression tag	UNP Q9NZN8
E	348	LEU	-	expression tag	UNP Q9NZN8
E	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
			1293	840	216	230	7			
3	F	148	Total	C	N	O	S	0	0	0
			1293	840	216	230	7			

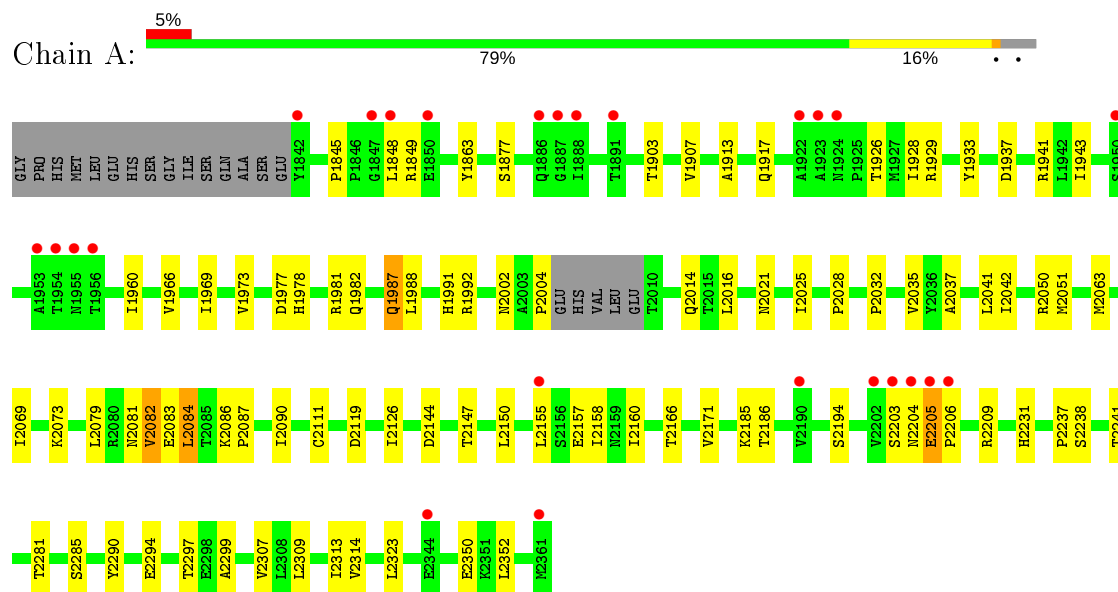
There are 12 discrepancies between the modelled and reference sequences:

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
F	601	GLY	-	expression tag	UNP O75175
F	602	PRO	-	expression tag	UNP O75175
F	603	HIS	-	expression tag	UNP O75175
F	604	MET	-	expression tag	UNP O75175
F	605	LEU	-	expression tag	UNP O75175
F	606	GLU	-	expression tag	UNP O75175

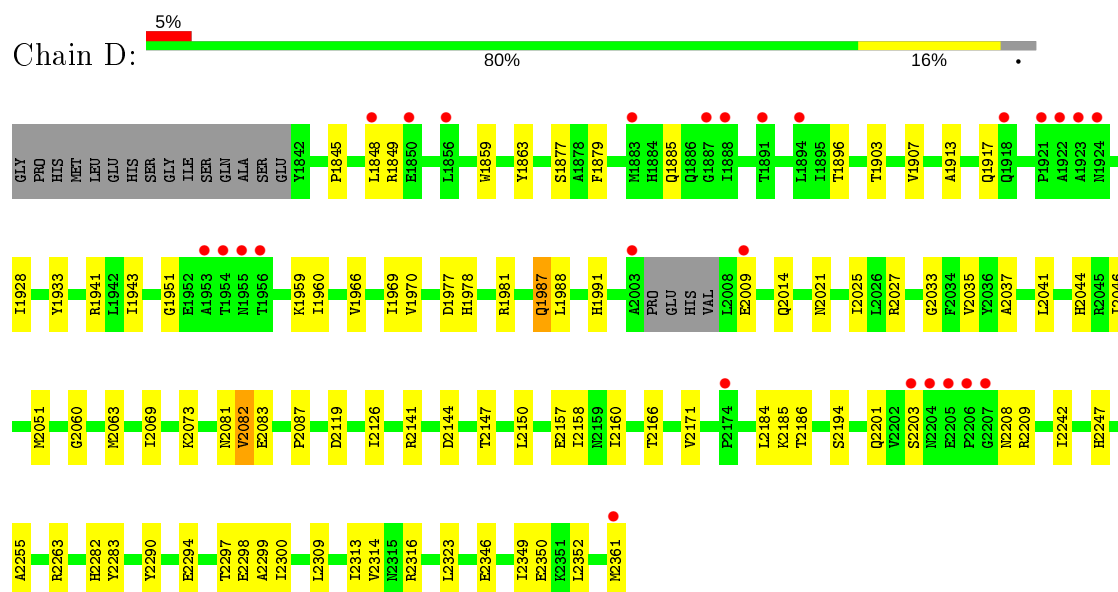
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

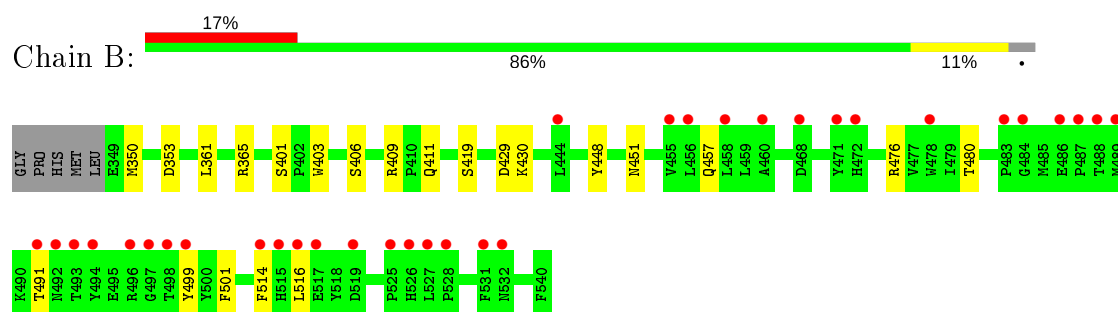
• Molecule 1: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1



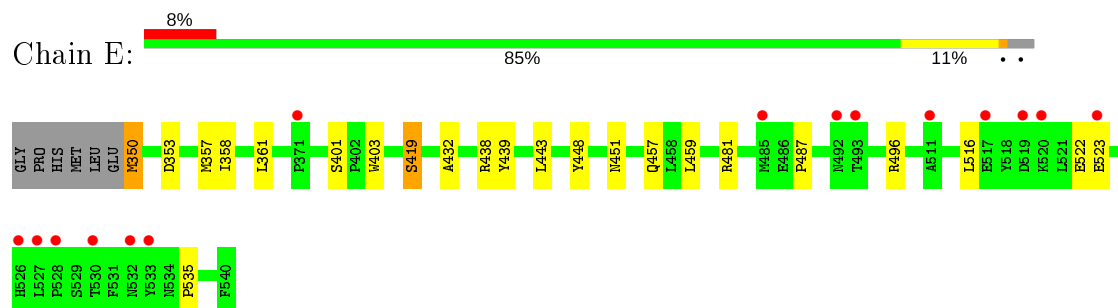
• Molecule 1: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1



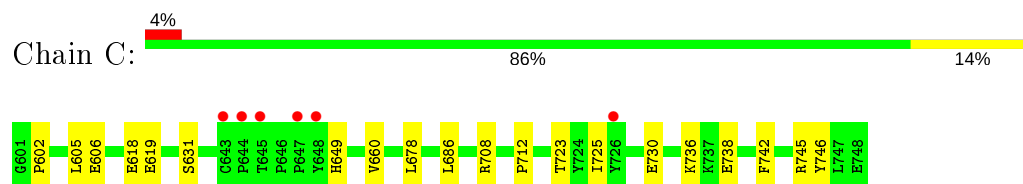
• Molecule 2: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2



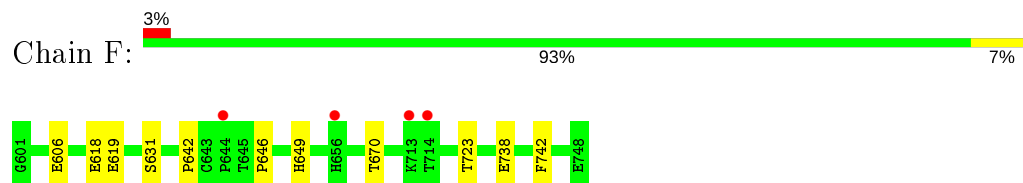
- Molecule 2: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2



- Molecule 3: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 3



- Molecule 3: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.98Å 135.32Å 101.33Å 90.00° 107.67° 90.00°	Depositor
Resolution (Å)	48.24 – 2.90 48.24 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (48.24-2.90) 99.6 (48.24-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.91Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.181 , 0.221 0.192 , 0.235	Depositor DCC
R_{free} test set	2200 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	68.9	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 70.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14109	wwPDB-VP
Average B, all atoms (Å ²)	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.23% 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	0.53	0/4294	0.70	0/5839
1	D	0.52	0/4300	0.69	0/5846
2	B	0.50	0/1626	0.71	0/2211
2	E	0.49	0/1613	0.70	0/2193
3	C	0.48	0/1344	0.65	0/1819
3	F	0.48	0/1344	0.65	0/1819
All	All	0.51	0/14521	0.69	0/19727

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

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	4186	0	4205	44	0
1	D	4193	0	4206	48	0
2	B	1578	0	1514	7	0
2	E	1566	0	1508	12	0
3	C	1293	0	1207	12	0
3	F	1293	0	1207	8	0
All	All	14109	0	13847	116	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 4.

All (116) 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:D:2184:LEU:HD22	1:D:2247:HIS:HD2	1.35	0.91
3:C:602:PRO:HB2	3:C:605:LEU:HD23	1.51	0.90
1:D:2147:THR:HG23	1:D:2150:LEU:HB2	1.71	0.73
1:A:2147:THR:HG23	1:A:2150:LEU:HB2	1.71	0.72
2:B:501:PHE:CD1	2:B:514:PHE:HZ	2.10	0.69
1:D:2144:ASP:O	1:D:2147:THR:HG22	1.94	0.68
1:A:2144:ASP:O	1:A:2147:THR:HG22	1.95	0.67
1:A:1969:ILE:O	1:A:1973:VAL:HG23	1.95	0.67
1:D:2184:LEU:HD22	1:D:2247:HIS:CD2	2.25	0.67
1:D:1978:HIS:HE1	1:D:2033:GLY:H	1.42	0.67
3:C:708:ARG:HD3	3:C:712:PRO:HD3	1.77	0.67
1:A:2082:VAL:HG13	1:A:2083:GLU:H	1.60	0.66
1:D:2082:VAL:HG13	1:D:2083:GLU:H	1.61	0.66
3:C:660:VAL:HG22	3:C:686:LEU:HD23	1.78	0.66
2:B:430:LYS:HB3	3:C:730:GLU:HG2	1.80	0.64
2:B:451:ASN:O	2:B:457:GLN:HB2	2.00	0.62
1:A:1987:GLN:HG3	1:A:2037:ALA:HB2	1.82	0.61
1:A:2185:LYS:HG3	1:A:2186:THR:HG23	1.82	0.61
1:D:1987:GLN:HG3	1:D:2037:ALA:HB2	1.82	0.61
1:D:2309:LEU:HD21	1:D:2352:LEU:HB3	1.83	0.61
1:A:2309:LEU:HD21	1:A:2352:LEU:HB3	1.82	0.59
1:D:2021:ASN:O	1:D:2025:ILE:HG12	2.04	0.58
1:D:2185:LYS:HG3	1:D:2186:THR:HG23	1.86	0.58
1:A:2204:ASN:C	1:A:2206:PRO:HD3	2.24	0.58
1:A:2021:ASN:O	1:A:2025:ILE:HG12	2.04	0.57
3:C:725:ILE:HG22	3:C:736:LYS:HG3	1.87	0.57
1:A:1913:ALA:HB1	1:A:1928:ILE:HG23	1.88	0.55
1:D:2297:THR:HB	1:D:2300:ILE:HD12	1.88	0.54
1:A:2002:ASN:HD21	1:A:2050:ARG:HG3	1.74	0.53
3:C:723:THR:HG22	3:C:738:GLU:HA	1.91	0.52
1:D:1977:ASP:OD1	1:D:1981:ARG:HG3	2.08	0.52
1:D:2044:HIS:CD2	1:D:2046:ILE:H	2.28	0.52
1:A:2004:PRO:HB3	1:A:2050:ARG:HH12	1.74	0.52
1:D:1863:TYR:HE1	1:D:1941:ARG:HD2	1.74	0.52
3:F:723:THR:HG22	3:F:738:GLU:HA	1.91	0.52
1:D:2158:ILE:HD12	1:D:2282:HIS:HB2	1.92	0.52
1:A:1845:PRO:HD2	1:A:1848:LEU:HD22	1.92	0.52
1:D:1845:PRO:HD2	1:D:1848:LEU:HD22	1.93	0.51
2:E:448:TYR:OH	3:F:649:HIS:HD2	1.94	0.50
1:A:1863:TYR:HE1	1:A:1941:ARG:HD2	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:451:ASN:O	2:E:457:GLN:HB2	2.12	0.49
1:D:2060:GLY:HA2	1:D:2063:MET:HE2	1.94	0.49
1:D:1966:VAL:O	1:D:1970:VAL:HG23	2.13	0.49
1:D:2201:GLN:HE21	1:D:2209:ARG:HH12	1.59	0.49
1:D:2035:VAL:HG11	3:F:618:GLU:HG3	1.95	0.49
1:A:2081:ASN:HD21	3:C:606:GLU:HB2	1.77	0.48
1:A:1926:THR:HG22	1:A:1929:ARG:HH22	1.79	0.47
3:C:745:ARG:HD2	3:C:746:TYR:CZ	2.49	0.47
1:A:2035:VAL:HG11	3:C:618:GLU:HG3	1.95	0.47
1:D:2081:ASN:HD21	3:F:606:GLU:HB2	1.79	0.47
2:E:481:ARG:HD2	2:E:487:PRO:HD3	1.97	0.47
1:D:1859:TRP:HB2	1:D:1879:PHE:CZ	2.50	0.46
2:E:439:TYR:HB3	2:E:443:LEU:HD23	1.96	0.46
1:D:2158:ILE:HG23	1:D:2282:HIS:CG	2.50	0.46
1:A:1978:HIS:CE1	1:A:2032:PRO:HD2	2.51	0.46
1:D:1933:TYR:HE1	1:D:1988:LEU:HD11	1.81	0.45
1:A:1903:THR:O	1:A:1907:VAL:HG23	2.16	0.45
1:A:2051:MET:HE1	1:A:2063:MET:HB2	1.99	0.45
2:E:432:ALA:HB1	2:E:438:ARG:HH12	1.82	0.45
1:A:2016:LEU:HD11	1:A:2050:ARG:HB3	1.99	0.45
1:D:2255:ALA:O	1:D:2263:ARG:NH1	2.49	0.45
1:A:2079:LEU:HD23	1:A:2084:LEU:HD11	1.97	0.45
1:A:2155:LEU:O	1:A:2158:ILE:HG12	2.16	0.45
1:D:1943:ILE:HG21	1:D:1966:VAL:HG11	1.98	0.45
1:D:1991:HIS:HB2	1:D:2037:ALA:HB1	1.99	0.45
1:A:1991:HIS:HB2	1:A:2037:ALA:HB1	1.99	0.44
1:D:2290:TYR:CZ	1:D:2294:GLU:HG3	2.53	0.44
1:D:1960:ILE:HG13	1:D:2014:GLN:HB3	2.00	0.44
1:D:1951:GLY:HA2	1:D:1959:LYS:HB2	1.98	0.44
2:B:406:SER:HB3	2:B:409:ARG:HH12	1.83	0.44
1:A:2205:GLU:N	1:A:2206:PRO:HD3	2.33	0.44
1:A:2290:TYR:CZ	1:A:2294:GLU:HG3	2.52	0.44
1:A:1933:TYR:HE1	1:A:1988:LEU:HD11	1.82	0.43
1:D:1913:ALA:HB1	1:D:1928:ILE:HG23	2.01	0.43
1:D:1863:TYR:CE1	1:D:1941:ARG:HD2	2.54	0.43
1:D:1903:THR:O	1:D:1907:VAL:HG23	2.18	0.43
1:D:2037:ALA:O	1:D:2041:LEU:HG	2.18	0.43
1:D:2126:ILE:HG22	1:D:2314:VAL:HG11	2.01	0.43
1:D:2157:GLU:HA	1:D:2160:ILE:HD12	2.01	0.43
1:A:1960:ILE:HG13	1:A:2014:GLN:HB3	2.01	0.43
1:A:2297:THR:HG22	1:A:2299:ALA:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2037:ALA:O	1:A:2041:LEU:HG	2.19	0.42
1:D:2051:MET:HE1	1:D:2063:MET:HB2	2.00	0.42
2:E:522:GLU:HG2	2:E:523:GLU:N	2.34	0.42
1:A:2028:PRO:HB3	1:A:2035:VAL:HG23	2.01	0.42
1:D:2297:THR:HG22	1:D:2299:ALA:H	1.84	0.42
1:A:1937:ASP:OD1	1:A:1992:ARG:HD3	2.19	0.42
1:A:2126:ILE:HG22	1:A:2314:VAL:HG11	2.02	0.42
1:D:2298:GLU:OE1	2:E:350:MET:HA	2.20	0.42
1:A:1943:ILE:HG21	1:A:1966:VAL:HG11	2.00	0.42
1:D:2349:ILE:HD12	2:E:357:MET:HB3	2.02	0.42
2:E:443:LEU:HD13	3:F:670:THR:HA	2.02	0.42
1:A:2157:GLU:HA	1:A:2160:ILE:HD12	2.00	0.42
2:E:439:TYR:CG	2:E:443:LEU:HD23	2.55	0.42
2:E:535:PRO:HD3	3:F:642:PRO:HB2	2.02	0.42
2:B:448:TYR:OH	3:C:649:HIS:HD2	2.03	0.41
1:A:1977:ASP:OD1	1:A:1981:ARG:HG3	2.21	0.41
1:A:2087:PRO:HG2	3:C:619:GLU:CD	2.41	0.41
2:B:411:GLN:HB2	3:C:678:LEU:HD22	2.03	0.41
1:A:1982:GLN:HE21	1:A:1982:GLN:HA	1.85	0.41
1:D:2087:PRO:HG2	3:F:619:GLU:CD	2.41	0.41
1:D:2346:GLU:HG3	2:E:358:ILE:HD11	2.01	0.41
1:A:2069:ILE:HG22	1:A:2073:LYS:HE2	2.03	0.41
1:A:2231:HIS:CE1	1:A:2237:PRO:HD3	2.55	0.41
1:A:2238:SER:OG	1:A:2241:THR:HG23	2.21	0.41
1:D:1896:THR:HG23	1:D:1969:ILE:HD11	2.03	0.41
1:D:1943:ILE:CG2	1:D:1966:VAL:HG11	2.51	0.41
1:D:2069:ILE:HG22	1:D:2073:LYS:HE2	2.02	0.41
1:A:2086:LYS:O	1:A:2090:ILE:HD12	2.21	0.41
1:D:1885:GLN:HG2	1:D:1885:GLN:H	1.73	0.41
1:A:1987:GLN:CG	1:A:2037:ALA:HB2	2.49	0.40
1:D:2242:ILE:HG12	1:D:2283:TYR:CE1	2.56	0.40
2:B:365:ARG:HA	2:B:365:ARG:HD3	1.93	0.40
1:D:2316:ARG:HG2	1:D:2361:MET:HG2	2.03	0.40
3:F:646:PRO:HG2	3:F:649:HIS:ND1	2.37	0.40
1:A:2281:THR:O	1:A:2285:SER:HB2	2.21	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	511/535 (96%)	490 (96%)	19 (4%)	2 (0%)	34	66
1	D	512/535 (96%)	493 (96%)	18 (4%)	1 (0%)	47	78
2	B	190/197 (96%)	180 (95%)	9 (5%)	1 (0%)	29	61
2	E	189/197 (96%)	178 (94%)	9 (5%)	2 (1%)	14	42
3	C	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
3	F	146/148 (99%)	141 (97%)	5 (3%)	0	100	100
All	All	1694/1760 (96%)	1623 (96%)	65 (4%)	6 (0%)	34	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2082	VAL
1	A	2205	GLU
2	B	353	ASP
1	D	2082	VAL
2	E	353	ASP
2	E	419	SER

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	462/479 (96%)	445 (96%)	17 (4%)	34	68
1	D	462/479 (96%)	446 (96%)	16 (4%)	36	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	167/172 (97%)	156 (93%)	11 (7%)	16	44
2	E	166/172 (96%)	158 (95%)	8 (5%)	25	58
3	C	136/136 (100%)	134 (98%)	2 (2%)	65	87
3	F	136/136 (100%)	134 (98%)	2 (2%)	65	87
All	All	1529/1574 (97%)	1473 (96%)	56 (4%)	34	68

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1849	ARG
1	A	1877	SER
1	A	1917	GLN
1	A	1987	GLN
1	A	2042	ILE
1	A	2084	LEU
1	A	2111	CYS
1	A	2119	ASP
1	A	2166	THR
1	A	2171	VAL
1	A	2194	SER
1	A	2203	SER
1	A	2209	ARG
1	A	2307	VAL
1	A	2313	ILE
1	A	2323	LEU
1	A	2350	GLU
2	B	350	MET
2	B	361	LEU
2	B	401	SER
2	B	403	TRP
2	B	419	SER
2	B	429	ASP
2	B	476	ARG
2	B	480	THR
2	B	491	THR
2	B	499	TYR
2	B	516	LEU
3	C	631	SER
3	C	742	PHE
1	D	1849	ARG
1	D	1877	SER

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Mol	Chain	Res	Type
1	D	1917	GLN
1	D	1987	GLN
1	D	2009	GLU
1	D	2027	ARG
1	D	2119	ASP
1	D	2141	ARG
1	D	2166	THR
1	D	2171	VAL
1	D	2194	SER
1	D	2203	SER
1	D	2208	ASN
1	D	2313	ILE
1	D	2323	LEU
1	D	2350	GLU
2	E	350	MET
2	E	361	LEU
2	E	401	SER
2	E	403	TRP
2	E	419	SER
2	E	459	LEU
2	E	496	ARG
2	E	516	LEU
3	F	631	SER
3	F	742	PHE

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

Mol	Chain	Res	Type
1	A	1882	GLN
1	A	1919	HIS
1	A	1982	GLN
1	A	2081	ASN
1	A	2159	ASN
1	A	2175	GLN
3	C	649	HIS
1	D	1886	GLN
1	D	1919	HIS
1	D	1978	HIS
1	D	1982	GLN
1	D	2044	HIS
1	D	2081	ASN
1	D	2175	GLN

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Mol	Chain	Res	Type
1	D	2201	GLN
1	D	2229	HIS
1	D	2247	HIS
3	F	649	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 carbohydrates 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	515/535 (96%)	0.10	25 (4%) 29 26	40, 69, 121, 143	0
1	D	516/535 (96%)	0.21	26 (5%) 28 25	39, 77, 130, 159	0
2	B	192/197 (97%)	0.81	34 (17%) 1 1	51, 96, 165, 179	0
2	E	191/197 (96%)	0.40	15 (7%) 12 10	47, 90, 146, 163	0
3	C	148/148 (100%)	0.17	6 (4%) 37 32	42, 84, 122, 140	0
3	F	148/148 (100%)	0.16	4 (2%) 54 50	47, 75, 108, 118	0
All	All	1710/1760 (97%)	0.26	110 (6%) 19 15	39, 80, 133, 179	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	492	ASN	7.4
1	D	2204	ASN	7.3
2	B	516	LEU	7.2
2	B	493	THR	7.1
1	D	1887	GLY	7.1
2	B	494	TYR	6.5
2	E	527	LEU	6.2
1	A	2204	ASN	5.9
1	D	1956	THR	5.8
1	D	1888	ILE	5.5
1	A	2206	PRO	5.2
1	D	1922	ALA	5.1
2	B	499	TYR	5.1
1	A	2344	GLU	4.8
2	B	488	THR	4.8
1	D	2203	SER	4.6
2	B	489	MET	4.6
2	E	519	ASP	4.6
2	B	497	GLY	4.5

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Mol	Chain	Res	Type	RSRZ
1	D	1921	PRO	4.5
1	D	1954	THR	4.5
1	A	1955	ASN	4.5
1	A	1956	THR	4.4
2	B	515	HIS	4.2
1	A	2361	MET	4.1
3	C	644	PRO	4.1
1	D	1894	LEU	4.0
1	A	1953	ALA	3.9
1	A	1887	GLY	3.9
1	A	2203	SER	3.9
1	D	2361	MET	3.9
3	C	726	TYR	3.9
1	D	2206	PRO	3.9
2	B	531	PHE	3.8
2	B	514	PHE	3.8
1	A	2205	GLU	3.7
1	D	1883	MET	3.7
1	A	1888	ILE	3.7
3	C	645	THR	3.6
1	D	2003	ALA	3.6
2	B	460	ALA	3.5
2	B	486	GLU	3.5
2	E	526	HIS	3.4
1	A	2202	VAL	3.4
2	E	493	THR	3.4
1	D	2009	GLU	3.3
1	A	1954	THR	3.3
2	B	468	ASP	3.3
1	A	1950	SER	3.3
3	C	648	TYR	3.3
1	D	1953	ALA	3.3
2	E	371	PRO	3.2
2	E	523	GLU	3.2
1	D	1955	ASN	3.2
1	D	2207	GLY	3.2
2	B	455	VAL	3.2
1	D	1891	THR	3.1
2	B	519	ASP	3.1
2	E	532	ASN	3.0
3	C	647	PRO	3.0
2	B	517	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	E	485	MET	3.0
2	E	520	LYS	2.9
1	D	2174	PRO	2.9
2	B	487	PRO	2.9
1	A	1848	LEU	2.9
2	B	471	TYR	2.9
1	D	1848	LEU	2.9
1	A	1891	THR	2.9
2	B	498	THR	2.9
3	F	644	PRO	2.8
1	A	1842	TYR	2.8
2	B	484	GLY	2.7
2	B	528	PRO	2.7
1	D	1850	GLU	2.6
2	E	530	THR	2.6
2	B	496	ARG	2.6
1	A	1886	GLN	2.5
2	B	472	HIS	2.5
2	B	526	HIS	2.5
2	B	525	PRO	2.4
3	F	656	HIS	2.4
3	C	643	CYS	2.4
1	A	1923	ALA	2.4
2	B	527	LEU	2.4
1	D	1923	ALA	2.4
1	D	2205	GLU	2.3
1	A	1850	GLU	2.3
1	D	1856	LEU	2.2
1	A	1924	ASN	2.2
1	D	1918	GLN	2.2
2	E	533	TYR	2.2
2	E	511	ALA	2.2
2	E	517	GLU	2.2
2	E	492	ASN	2.2
3	F	714	THR	2.2
1	A	1922	ALA	2.1
2	B	478	TRP	2.1
1	A	1847	GLY	2.1
2	B	458	LEU	2.1
2	B	491	THR	2.1
1	D	1924	ASN	2.1
2	B	483	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	444	LEU	2.1
2	B	532	ASN	2.1
1	A	2155	LEU	2.0
2	B	456	LEU	2.0
1	A	2190	VAL	2.0
2	E	528	PRO	2.0
3	F	713	LYS	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 carbohydrates 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.