



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 11:00 AM EDT

PDB ID : 5FU6 / pdb_00005fu6
Title : NOT module of the human CCR4-NOT complex (Crystallization mutant)
Authors : Raisch, T.; Bhandari, D.; Sabath, K.; Helms, S.; Valkov, E.; Weichenrieder, O.; Izaurralde, E.
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

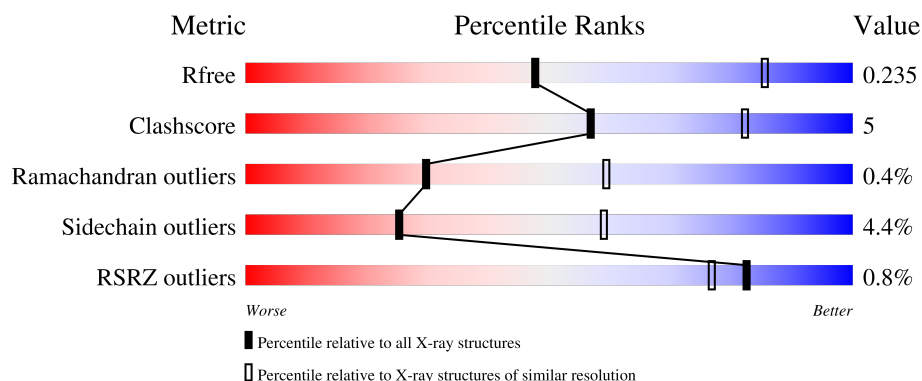
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	180053	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (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 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	D	535	
2	B	197	
2	E	197	
3	C	148	

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Mol	Chain	Length	Quality of chain
3	F	148	 86% 14%

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			

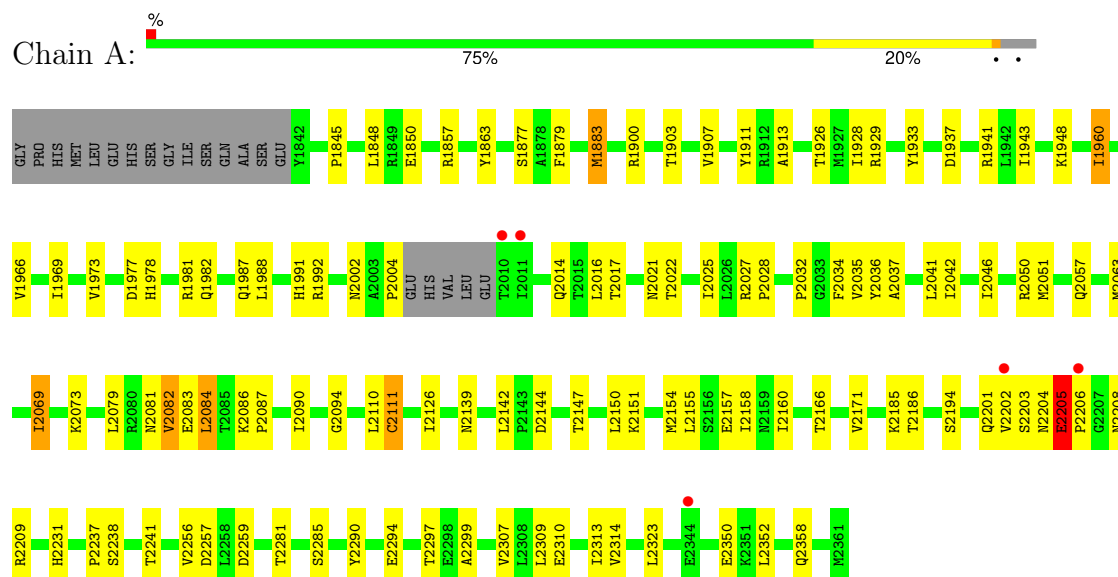
There are 12 discrepancies between the modelled and reference sequences:

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

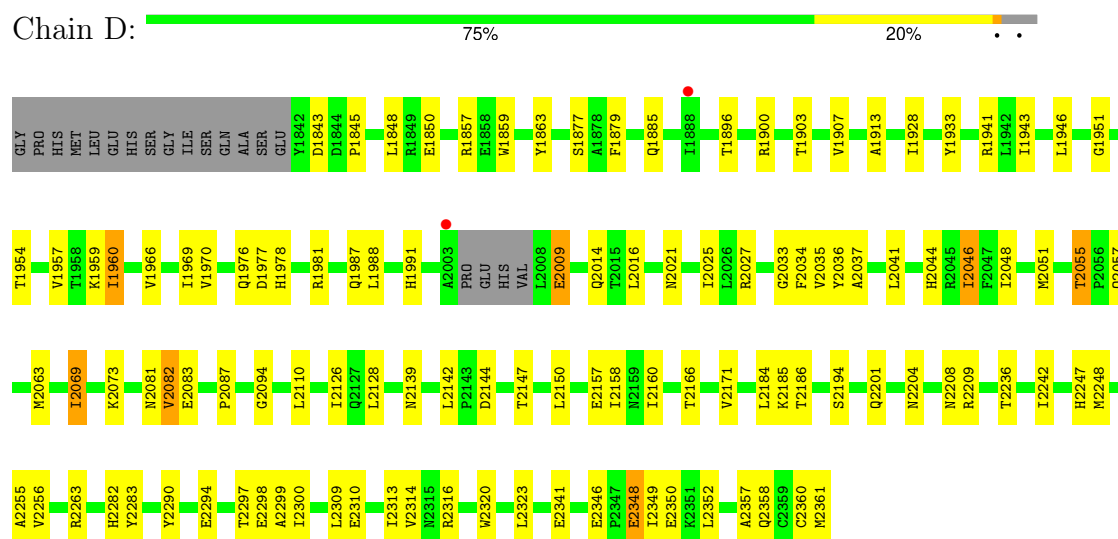
3 Residue-property plots

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.

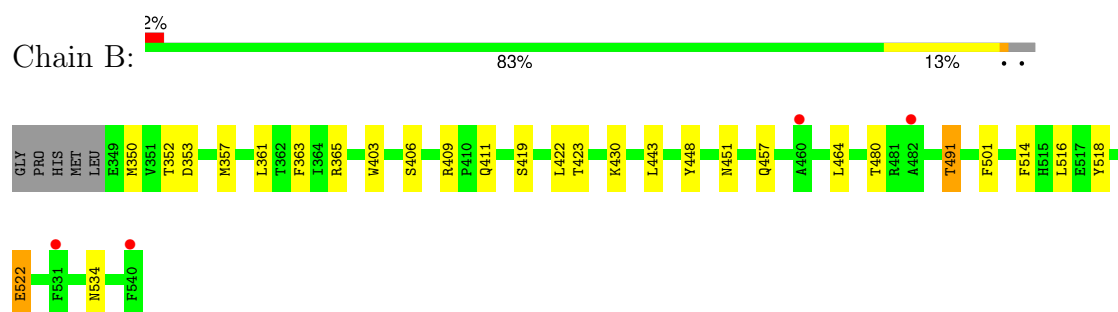
• Molecule 1: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1



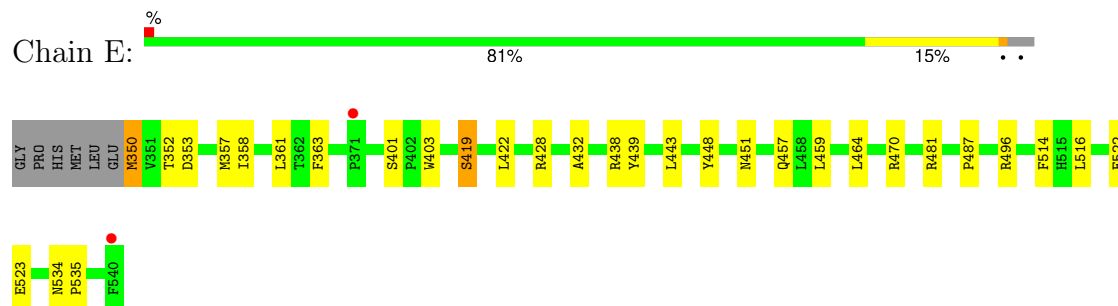
• Molecule 1: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 1



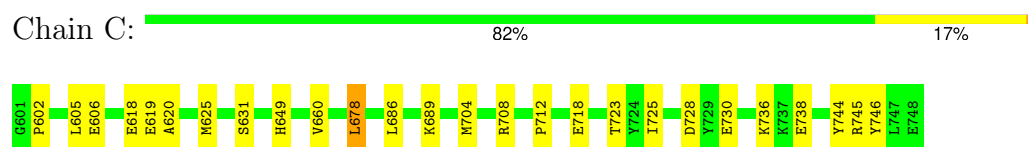
• Molecule 2: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2



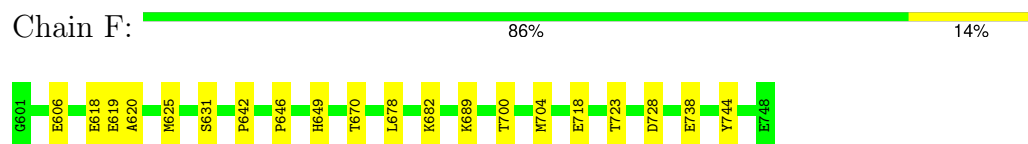
• Molecule 2: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 2



• Molecule 3: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 3



• Molecule 3: CCR4-NOT TRANSCRIPTION COMPLEX SUBUNIT 3



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) 99.5 (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)	0.32 , 77.3	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	0.91	2/4294 (0.0%)	1.47	26/5839 (0.4%)
1	D	0.91	1/4300 (0.0%)	1.48	39/5846 (0.7%)
2	B	0.86	0/1626	1.36	16/2211 (0.7%)
2	E	0.84	0/1613	1.33	12/2193 (0.5%)
3	C	0.81	0/1344	1.29	7/1819 (0.4%)
3	F	0.82	0/1344	1.29	9/1819 (0.5%)
All	All	0.88	3/14521 (0.0%)	1.41	109/19727 (0.6%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1883	MET	SD-CE	-5.50	1.65	1.79
1	D	1954	THR	CA-C	5.43	1.55	1.52
1	A	2205	GLU	CA-C	5.21	1.59	1.52

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	422	LEU	CA-C-N	8.34	131.28	120.44
2	B	422	LEU	C-N-CA	8.34	131.28	120.44
1	D	2204	ASN	N-CA-C	-7.15	104.71	113.50
1	A	2111	CYS	CA-C-N	6.92	129.55	120.28
1	A	2111	CYS	C-N-CA	6.92	129.55	120.28
1	D	1843	ASP	N-CA-C	-6.82	102.57	111.71
3	C	744	TYR	CA-C-N	6.75	130.24	120.38
3	C	744	TYR	C-N-CA	6.75	130.24	120.38
1	A	2202	VAL	CA-C-N	6.72	132.58	122.23
1	A	2202	VAL	C-N-CA	6.72	132.58	122.23
1	A	1850	GLU	CA-C-N	6.70	129.55	120.44
1	A	1850	GLU	C-N-CA	6.70	129.55	120.44
3	F	744	TYR	CA-C-N	6.66	130.11	120.38
3	F	744	TYR	C-N-CA	6.66	130.11	120.38
1	D	1850	GLU	CA-C-N	6.48	129.26	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1850	GLU	C-N-CA	6.48	129.26	120.44
1	A	2256	VAL	CA-C-N	6.20	129.21	120.28
1	A	2256	VAL	C-N-CA	6.20	129.21	120.28
2	E	363	PHE	CA-CB-CG	6.00	119.80	113.80
1	D	2110	LEU	CA-C-N	5.95	128.17	120.44
1	D	2110	LEU	C-N-CA	5.95	128.17	120.44
3	F	678	LEU	CA-C-N	5.93	129.26	120.90
3	F	678	LEU	C-N-CA	5.93	129.26	120.90
2	B	423	THR	CA-C-N	5.92	128.49	120.38
2	B	423	THR	C-N-CA	5.92	128.49	120.38
1	D	2055	THR	CB-CA-C	5.91	117.89	109.08
2	E	422	LEU	CA-C-N	5.91	128.12	120.44
2	E	422	LEU	C-N-CA	5.91	128.12	120.44
1	A	2057	GLN	CA-C-N	5.91	130.51	122.07
1	A	2057	GLN	C-N-CA	5.91	130.51	122.07
1	D	1843	ASP	CA-CB-CG	5.84	118.44	112.60
1	D	2358	GLN	CA-C-N	5.83	128.37	120.38
1	D	2358	GLN	C-N-CA	5.83	128.37	120.38
3	C	678	LEU	CA-C-N	5.83	129.11	120.90
3	C	678	LEU	C-N-CA	5.83	129.11	120.90
1	A	2110	LEU	CA-C-N	5.82	128.34	120.65
1	A	2110	LEU	C-N-CA	5.82	128.34	120.65
1	D	2057	GLN	CA-C-N	5.79	130.35	122.07
1	D	2057	GLN	C-N-CA	5.79	130.35	122.07
3	F	620	ALA	CA-C-N	5.76	128.57	120.28
3	F	620	ALA	C-N-CA	5.76	128.57	120.28
2	B	363	PHE	CA-CB-CG	5.72	119.52	113.80
1	A	2358	GLN	CA-C-N	5.70	128.71	120.38
1	A	2358	GLN	C-N-CA	5.70	128.71	120.38
1	D	2320	TRP	CA-C-N	5.69	126.40	120.03
1	D	2320	TRP	C-N-CA	5.69	126.40	120.03
3	F	718	GLU	CB-CG-CD	5.66	122.22	112.60
2	E	514	PHE	CA-C-N	5.60	130.22	122.77
2	E	514	PHE	C-N-CA	5.60	130.22	122.77
1	A	1911	TYR	CA-C-N	5.59	128.34	120.28
1	A	1911	TYR	C-N-CA	5.59	128.34	120.28
2	B	491	THR	CA-C-N	5.56	128.00	120.38
2	B	491	THR	C-N-CA	5.56	128.00	120.38
3	C	620	ALA	CA-C-N	5.56	128.29	120.28
3	C	620	ALA	C-N-CA	5.56	128.29	120.28
2	E	428	ARG	CA-C-N	5.55	127.65	120.44
2	E	428	ARG	C-N-CA	5.55	127.65	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2257	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	2208	ASN	CA-CB-CG	5.50	118.10	112.60
1	D	2016	LEU	CA-C-N	5.50	127.64	120.28
1	D	2016	LEU	C-N-CA	5.50	127.64	120.28
1	D	1857	ARG	CA-C-N	5.42	127.82	120.44
1	D	1857	ARG	C-N-CA	5.42	127.82	120.44
3	C	718	GLU	CB-CG-CD	5.42	121.82	112.60
2	E	352	THR	CA-C-N	5.41	131.87	121.54
2	E	352	THR	C-N-CA	5.41	131.87	121.54
2	B	518	TYR	CA-C-N	5.39	127.77	120.44
2	B	518	TYR	C-N-CA	5.39	127.77	120.44
2	E	464	LEU	CA-C-N	5.37	127.79	120.54
2	E	464	LEU	C-N-CA	5.37	127.79	120.54
1	D	2357	ALA	CA-C-N	5.34	127.90	120.63
1	D	2357	ALA	C-N-CA	5.34	127.90	120.63
2	B	522	GLU	CA-C-N	5.33	130.57	121.29
2	B	522	GLU	C-N-CA	5.33	130.57	121.29
1	D	2128	LEU	CA-C-N	5.33	127.42	120.28
1	D	2128	LEU	C-N-CA	5.33	127.42	120.28
1	D	1976	GLN	CA-C-N	5.31	127.66	120.65
1	D	1976	GLN	C-N-CA	5.31	127.66	120.65
1	D	2009	GLU	CA-C-N	5.30	127.38	120.28
1	D	2009	GLU	C-N-CA	5.30	127.38	120.28
1	A	2259	ASP	CA-CB-CG	5.28	117.88	112.60
1	A	2094	GLY	CA-C-N	5.24	127.31	120.28
1	A	2094	GLY	C-N-CA	5.24	127.31	120.28
1	D	2048	ILE	CA-C-N	5.24	128.07	120.79
1	D	2048	ILE	C-N-CA	5.24	128.07	120.79
2	B	534	ASN	CA-CB-CG	5.21	117.81	112.60
1	A	2139	ASN	CA-CB-CG	5.20	117.80	112.60
2	B	464	LEU	CA-C-N	5.20	127.24	120.28
2	B	464	LEU	C-N-CA	5.20	127.24	120.28
1	A	1857	ARG	CA-C-N	5.16	127.45	120.44
1	A	1857	ARG	C-N-CA	5.16	127.45	120.44
2	E	534	ASN	CA-CB-CG	5.15	117.75	112.60
1	D	2094	GLY	CA-C-N	5.15	127.18	120.28
1	D	2094	GLY	C-N-CA	5.15	127.18	120.28
2	B	352	THR	CA-C-N	5.14	131.37	121.54
2	B	352	THR	C-N-CA	5.14	131.37	121.54
1	D	2256	VAL	CA-C-N	5.11	127.13	120.28
1	D	2256	VAL	C-N-CA	5.11	127.13	120.28
1	D	2360	CYS	CA-C-N	5.07	130.82	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2360	CYS	C-N-CA	5.07	130.82	121.70
1	D	2348	GLU	CA-C-N	5.04	127.36	120.46
1	D	2348	GLU	C-N-CA	5.04	127.36	120.46
1	D	2034	PHE	CA-C-N	5.03	127.63	120.53
1	D	2034	PHE	C-N-CA	5.03	127.63	120.53
1	A	2034	PHE	CA-C-N	5.03	127.62	120.53
1	A	2034	PHE	C-N-CA	5.03	127.62	120.53
1	D	2341	GLU	CB-CG-CD	5.03	121.14	112.60
3	F	682	LYS	CA-C-N	5.02	126.96	120.44
3	F	682	LYS	C-N-CA	5.02	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	4186	0	4205	50	0
1	D	4193	0	4206	52	0
2	B	1578	0	1514	8	0
2	E	1566	0	1508	13	0
3	C	1293	0	1207	14	0
3	F	1293	0	1207	10	0
All	All	14109	0	13847	128	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 (128) 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:A:1879:PHE:HE2	1:A:1883:MET:HE3	1.51	0.75
1:D:2147:THR:HG23	1:D:2150:LEU:HB2	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:1879:PHE:CE2	1:A:1883:MET:HE3	2.27	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:2204:ASN:C	1:A:2206:PRO:HD3	2.24	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: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
3:F:704:MET:HE2	3:F:728:ASP:HA	1.87	0.56
1:D:2309:LEU:HD22	2:E:357:MET:HE1	1.89	0.55
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
3:C:704:MET:HE2	3:C:728:ASP:HA	1.89	0.53
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: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:D:2242:ILE:HG22	1:D:2248:MET:HE3	1.96	0.48
1:A:1926:THR:HG22	1:A:1929:ARG:HH22	1.79	0.47
1:A:2035:VAL:HG11	3:C:618:GLU:HG3	1.95	0.47
3:C:745:ARG:HD2	3:C:746:TYR:CZ	2.49	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:A:2087:PRO:HG2	3:C:619:GLU:CD	2.41	0.46
1:D:2087:PRO:HG2	3:F:619:GLU:CD	2.41	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:2151:LYS:HB2	1:A:2154:MET:HE2	1.97	0.45
1:A:1903:THR:O	1:A:1907:VAL:HG23	2.16	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:2051:MET:HE1	1:A:2063:MET:HB2	1.99	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:A:2017:THR:HG23	1:A:2063:MET:HE1	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:2051:MET:HE1	1:D:2063:MET:HE3	2.01	0.43
1:D:1863:TYR:CE1	1:D:1941:ARG:HD2	2.54	0.43
1:D:1913:ALA:HB1	1:D:1928:ILE:HG23	2.01	0.43
1:D:1903:THR:O	1:D:1907:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2037:ALA:O	1:D:2041:LEU:HG	2.18	0.43
1:D:2051:MET:HE1	1:D:2063:MET:HB2	2.01	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
1:A:2309:LEU:HD22	2:B:357:MET:HE1	2.01	0.43
1:A:2037:ALA:O	1:A:2041:LEU:HG	2.19	0.42
2:E:522:GLU:HG2	2:E:523:GLU:N	2.34	0.42
1:D:2242:ILE:CG2	1:D:2248:MET:HE3	2.49	0.42
1:A:2028:PRO:HB3	1:A:2035:VAL:HG23	2.01	0.42
1:A:2036:TYR:CG	3:C:625:MET:HE3	2.54	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
2:B:411:GLN:HB2	3:C:678:LEU:HD22	2.03	0.41
1:A:1982:GLN:HA	1:A:1982:GLN:HE21	1.85	0.41
1:D:2036:TYR:CG	3:F:625:MET:HE3	2.56	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:H	1:D:1885:GLN:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2281:THR:O	1:A:2285:SER:HB2	2.21	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 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%)	30	59
1	D	512/535 (96%)	493 (96%)	18 (4%)	1 (0%)	43	72
2	B	190/197 (96%)	180 (95%)	9 (5%)	1 (0%)	24	54
2	E	189/197 (96%)	178 (94%)	9 (5%)	2 (1%)	11	36
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%)	30	59

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 [i](#)

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%)	439 (95%)	23 (5%)	22	53
1	D	462/479 (96%)	440 (95%)	22 (5%)	23	55
2	B	167/172 (97%)	158 (95%)	9 (5%)	20	51
2	E	166/172 (96%)	157 (95%)	9 (5%)	20	51
3	C	136/136 (100%)	134 (98%)	2 (2%)	57	84
3	F	136/136 (100%)	133 (98%)	3 (2%)	45	77
All	All	1529/1574 (97%)	1461 (96%)	68 (4%)	25	59

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1877	SER
1	A	1900	ARG
1	A	1948	LYS
1	A	1960	ILE
1	A	2022	THR
1	A	2027	ARG
1	A	2042	ILE
1	A	2046	ILE
1	A	2069	ILE
1	A	2084	LEU
1	A	2111	CYS
1	A	2142	LEU
1	A	2166	THR
1	A	2171	VAL
1	A	2194	SER
1	A	2201	GLN
1	A	2203	SER
1	A	2209	ARG
1	A	2307	VAL
1	A	2310	GLU
1	A	2313	ILE
1	A	2323	LEU
1	A	2350	GLU
2	B	350	MET
2	B	361	LEU
2	B	403	TRP

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Mol	Chain	Res	Type
2	B	419	SER
2	B	443	LEU
2	B	480	THR
2	B	491	THR
2	B	516	LEU
2	B	522	GLU
3	C	631	SER
3	C	689	LYS
1	D	1877	SER
1	D	1900	ARG
1	D	1946	LEU
1	D	1957	VAL
1	D	1960	ILE
1	D	2009	GLU
1	D	2027	ARG
1	D	2046	ILE
1	D	2055	THR
1	D	2069	ILE
1	D	2139	ASN
1	D	2142	LEU
1	D	2166	THR
1	D	2171	VAL
1	D	2194	SER
1	D	2208	ASN
1	D	2236	THR
1	D	2310	GLU
1	D	2313	ILE
1	D	2323	LEU
1	D	2348	GLU
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	470	ARG
2	E	496	ARG
2	E	516	LEU
3	F	631	SER
3	F	689	LYS
3	F	700	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1884	HIS
1	A	1914	GLN
1	A	1919	HIS
1	A	1924	ASN
1	A	1935	ASN
1	A	1961	ASN
1	A	1964	ASN
1	A	1982	GLN
1	A	1987	GLN
1	A	2012	ASN
1	A	2081	ASN
1	A	2167	ASN
1	A	2175	GLN
1	A	2229	HIS
1	A	2232	ASN
1	A	2315	ASN
1	A	2332	ASN
1	A	2339	ASN
2	B	388	ASN
2	B	457	GLN
2	B	534	ASN
3	C	641	ASN
3	C	649	HIS
3	C	651	GLN
3	C	656	HIS
3	C	709	HIS
3	C	721	GLN
1	D	1884	HIS
1	D	1886	GLN
1	D	1919	HIS
1	D	1924	ASN
1	D	1964	ASN
1	D	1978	HIS
1	D	1982	GLN
1	D	1986	GLN
1	D	1987	GLN
1	D	2021	ASN
1	D	2044	HIS
1	D	2081	ASN
1	D	2167	ASN
1	D	2175	GLN

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Mol	Chain	Res	Type
1	D	2199	ASN
1	D	2201	GLN
1	D	2229	HIS
1	D	2247	HIS
1	D	2339	ASN
2	E	388	ASN
2	E	534	ASN
3	F	641	ASN
3	F	649	HIS
3	F	651	GLN
3	F	694	GLN
3	F	709	HIS
3	F	721	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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(Å ²)	Q<0.9
1	A	515/535 (96%)	-0.30	5 (0%) 79 73	40, 69, 121, 143	0
1	D	516/535 (96%)	-0.21	2 (0%) 88 85	39, 77, 130, 159	0
2	B	192/197 (97%)	0.15	4 (2%) 63 54	51, 96, 165, 179	0
2	E	191/197 (96%)	0.09	2 (1%) 79 73	47, 90, 146, 163	0
3	C	148/148 (100%)	-0.15	0 100 100	42, 84, 122, 140	0
3	F	148/148 (100%)	-0.31	0 100 100	47, 75, 108, 118	0
All	All	1710/1760 (97%)	-0.16	13 (0%) 82 77	39, 80, 133, 179	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	540	PHE	3.8
1	A	2202	VAL	3.4
2	B	540	PHE	3.3
1	A	2011	ILE	3.1
1	D	2003	ALA	2.4
1	D	1888	ILE	2.4
2	B	531	PHE	2.4
1	A	2206	PRO	2.4
2	B	460	ALA	2.3
2	E	371	PRO	2.2
1	A	2344	GLU	2.2
1	A	2010	THR	2.0
2	B	482	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.