



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:01 AM UTC

PDB ID : 6HJY / pdb_00006hgy
Title : X-ray structure of a pentameric ligand gated ion channel from *Erwinia chrysanthemi* (ELIC) Delta8 truncation mutant in complex with nanobody 72
Authors : Spurny, R.; Govaerts, C.; Evans, G.L.; Pardon, E.; Steyaert, J.; Ulens, C.
Deposited on : 2018-09-04
Resolution : 2.78 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

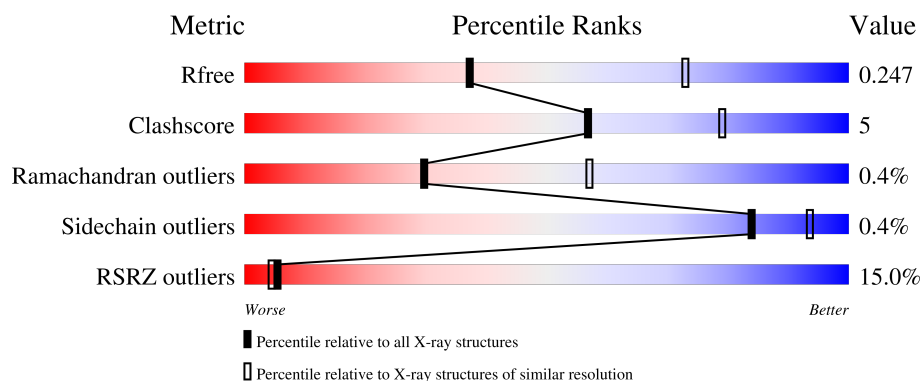
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.78 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	277	14% 90% 10%
2	B	280	10% 86% 13%
2	C	280	20% 88% 11%
3	D	276	16% 87% 11%
4	E	278	12% 89% 11%

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Mol	Chain	Length	Quality of chain
5	F	124	8% 89% 10%
5	J	124	35% 88% 12%
6	G	123	11% 90% 10%
6	H	123	12% 89% 10%
6	I	123	15% 88% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 16066 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 Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2274	1481	377	411	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	GLY	-	insertion	UNP P0C7B7
A	238	CYS	LEU	conflict	UNP P0C7B7

- Molecule 2 is a protein called Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	279	Total	C	N	O	S	0	0	0
			2289	1490	379	415	5			
2	C	279	Total	C	N	O	S	0	0	0
			2289	1490	379	415	5			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	6	PRO	-	expression tag	UNP P0C7B7
B	7	VAL	-	expression tag	UNP P0C7B7
B	164	GLY	-	insertion	UNP P0C7B7
B	238	CYS	LEU	conflict	UNP P0C7B7
C	6	PRO	-	expression tag	UNP P0C7B7
C	7	VAL	-	expression tag	UNP P0C7B7
C	164	GLY	-	insertion	UNP P0C7B7
C	238	CYS	LEU	conflict	UNP P0C7B7

- Molecule 3 is a protein called Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	276	Total	C	N	O	S	0	0	0
			2269	1478	376	410	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	164	GLY	-	insertion	UNP P0C7B7
D	238	CYS	LEU	conflict	UNP P0C7B7

- Molecule 4 is a protein called Cys-loop ligand-gated ion channel.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	278	Total	C	N	O	S	0	0	0
			2282	1485	378	414	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	164	GLY	-	insertion	UNP P0C7B7
E	238	CYS	LEU	conflict	UNP P0C7B7

- Molecule 5 is a protein called nanobody 72.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	124	Total	C	N	O	S	0	0	0
			938	584	170	179	5			
5	J	124	Total	C	N	O	S	0	0	0
			938	584	170	179	5			

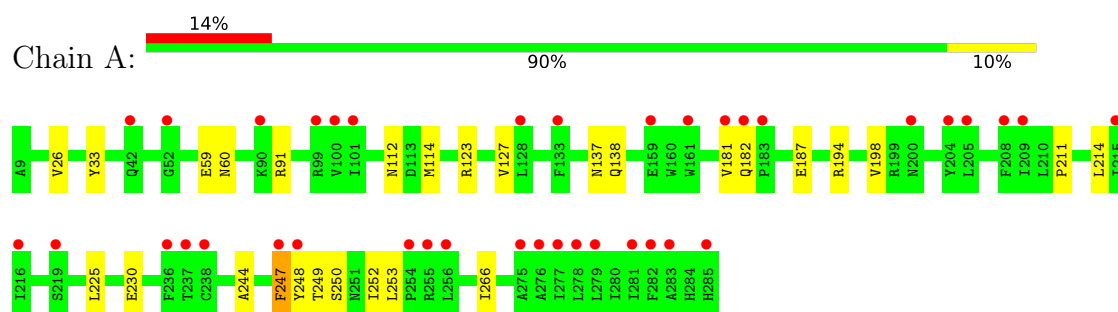
- Molecule 6 is a protein called nanobody 72.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	123	Total	C	N	O	S	0	0	0
			929	579	168	177	5			
6	H	123	Total	C	N	O	S	0	0	0
			929	579	168	177	5			
6	I	123	Total	C	N	O	S	0	0	0
			929	579	168	177	5			

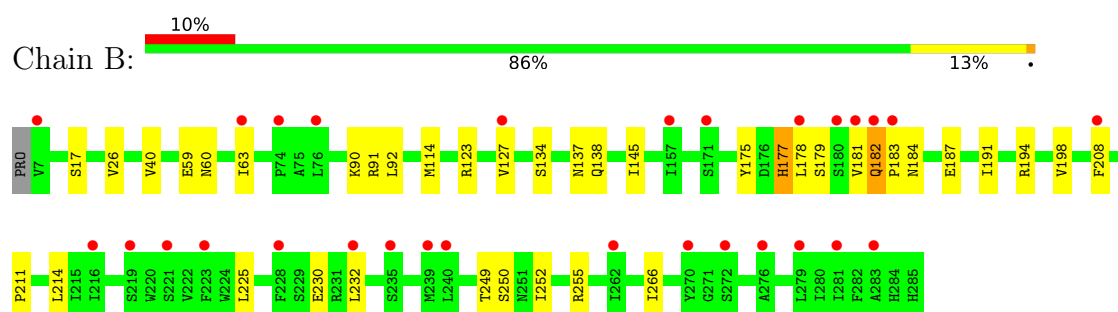
3 Residue-property plots [i](#)

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.

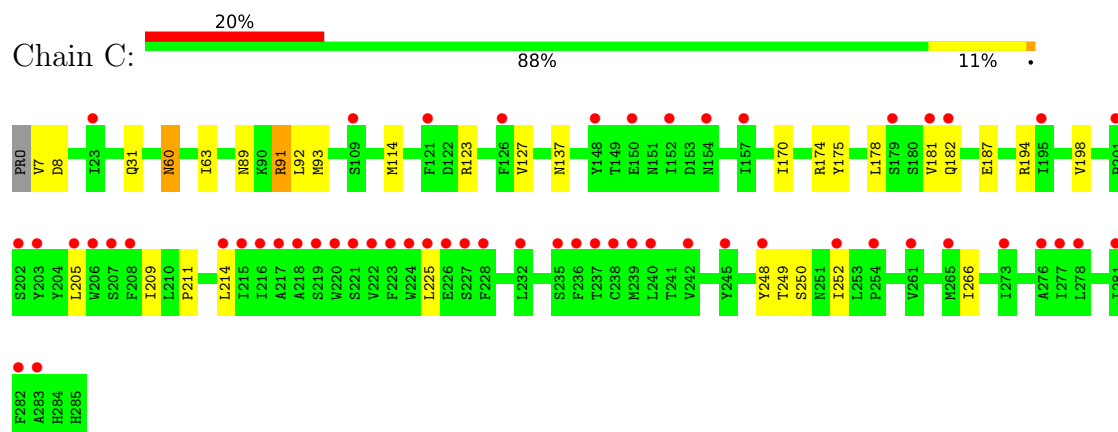
- Molecule 1: Cys-loop ligand-gated ion channel



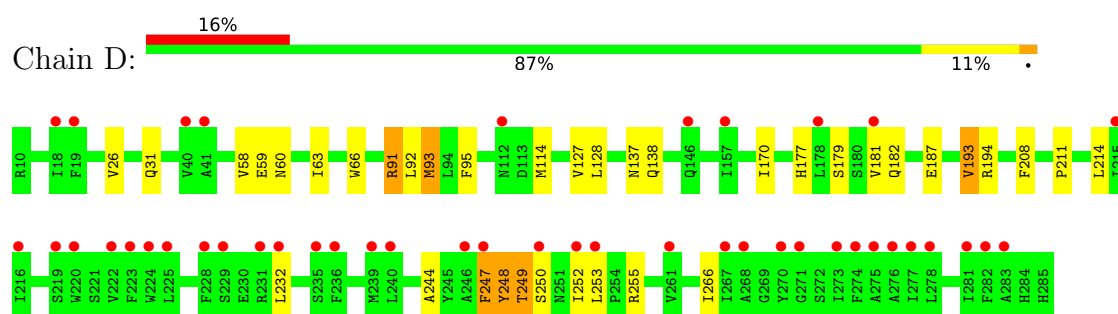
- Molecule 2: Cys-loop ligand-gated ion channel



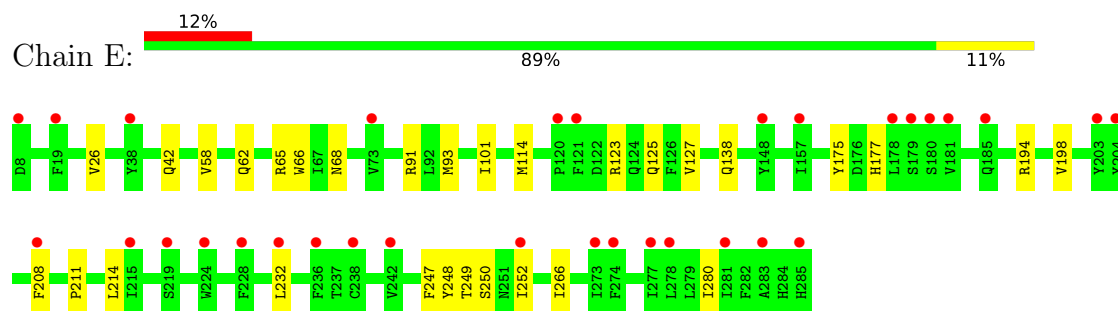
- Molecule 2: Cys-loop ligand-gated ion channel



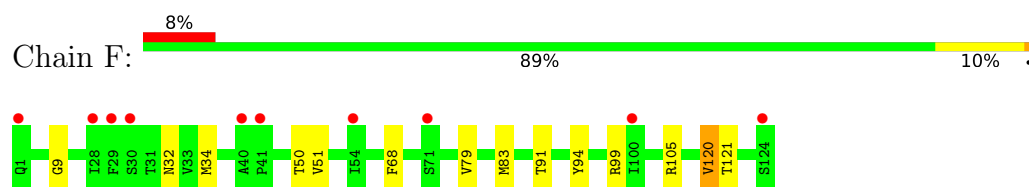
- Molecule 3: Cys-loop ligand-gated ion channel



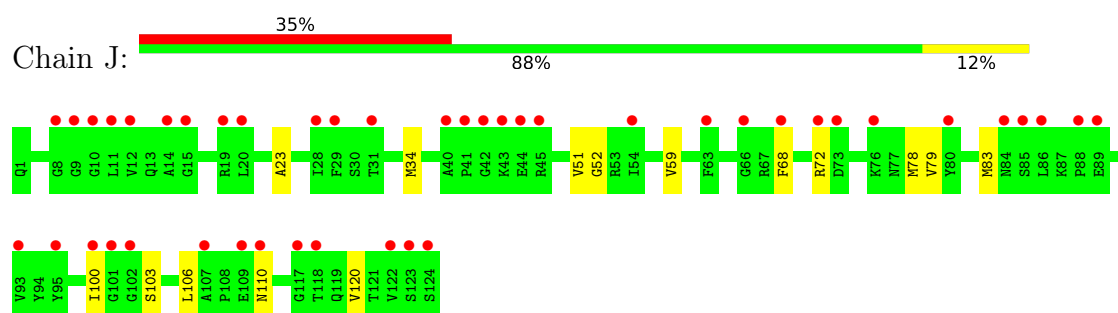
- Molecule 4: Cys-loop ligand-gated ion channel



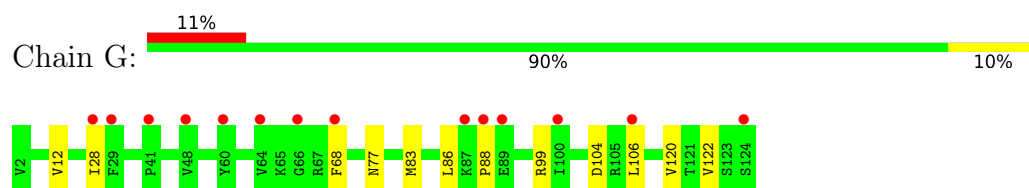
- Molecule 5: nanobody 72



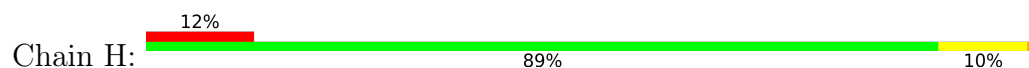
- Molecule 5: nanobody 72

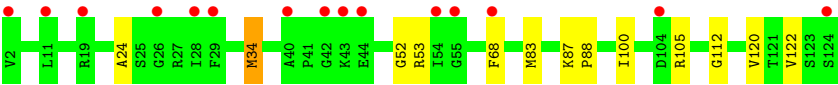


- Molecule 6: nanobody 72

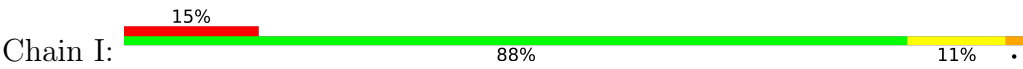


- Molecule 6: nanobody 72





● Molecule 6: nanobody 72



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	95.67Å 155.09Å 101.62Å 90.00° 103.08° 90.00°	Depositor
Resolution (Å)	49.49 – 2.78 49.49 – 2.78	Depositor EDS
% Data completeness (in resolution range)	99.0 (49.49-2.78) 99.2 (49.49-2.78)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.77Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.225 , 0.233 0.237 , 0.247	Depositor DCC
R_{free} test set	3602 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	76.5	Xtriage
Anisotropy	0.371	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 49.7	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	0.92	EDS
Total number of atoms	16066	wwPDB-VP
Average B, all atoms (Å ²)	101.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.31% 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	0.74	1/2339 (0.0%)	1.25	7/3190 (0.2%)
2	B	0.78	2/2354 (0.1%)	1.24	8/3211 (0.2%)
2	C	0.75	0/2354	1.22	3/3211 (0.1%)
3	D	0.75	0/2334	1.25	11/3183 (0.3%)
4	E	0.73	0/2347	1.22	2/3201 (0.1%)
5	F	0.66	0/955	1.18	4/1287 (0.3%)
5	J	0.74	0/955	1.22	1/1287 (0.1%)
6	G	0.65	0/946	1.17	3/1275 (0.2%)
6	H	0.70	1/946 (0.1%)	1.18	1/1275 (0.1%)
6	I	0.67	0/946	1.16	3/1275 (0.2%)
All	All	0.73	4/16476 (0.0%)	1.22	43/22395 (0.2%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	182	GLN	CA-C	6.51	1.61	1.52
6	H	34	MET	SD-CE	-6.00	1.64	1.79
2	B	183	PRO	CA-C	5.45	1.60	1.52
1	A	182	GLN	CA-C	5.19	1.57	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	247	PHE	CA-CB-CG	11.06	124.86	113.80
3	D	247	PHE	CA-CB-CG	10.72	124.52	113.80
1	A	181	VAL	N-CA-C	-8.40	105.06	112.12
3	D	177	HIS	N-CA-C	-8.09	99.63	110.55
2	B	179	SER	N-CA-C	-7.84	102.63	112.90
2	B	177	HIS	N-CA-C	-7.46	99.98	110.50
6	I	68	PHE	CA-CB-CG	6.64	120.44	113.80
5	F	68	PHE	CA-CB-CG	6.45	120.25	113.80
3	D	179	SER	N-CA-C	-6.35	104.58	112.90
6	G	68	PHE	CA-CB-CG	6.29	120.09	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	68	PHE	CA-CB-CG	6.21	120.01	113.80
6	H	68	PHE	CA-CB-CG	6.18	119.98	113.80
2	B	177	HIS	CA-C-O	-6.18	114.83	121.56
3	D	248	TYR	CA-C-N	6.08	128.68	120.65
3	D	248	TYR	C-N-CA	6.08	128.68	120.65
1	A	248	TYR	CA-C-N	6.06	128.65	120.65
1	A	248	TYR	C-N-CA	6.06	128.65	120.65
6	I	101	GLY	N-CA-C	-5.89	104.28	111.35
1	A	59	GLU	CA-C-N	5.69	132.41	121.54
1	A	59	GLU	C-N-CA	5.69	132.41	121.54
6	I	120	VAL	N-CA-CB	5.45	118.72	111.64
3	D	59	GLU	CA-C-N	5.43	131.91	121.54
3	D	59	GLU	C-N-CA	5.43	131.91	121.54
2	B	138	GLN	N-CA-C	-5.33	106.62	113.23
5	F	32	ASN	CA-C-N	5.31	129.00	120.30
5	F	32	ASN	C-N-CA	5.31	129.00	120.30
2	B	59	GLU	CA-C-N	5.29	131.65	121.54
2	B	59	GLU	C-N-CA	5.29	131.65	121.54
5	F	120	VAL	N-CA-CB	5.24	118.64	111.41
1	A	138	GLN	N-CA-C	-5.11	106.90	113.23
2	B	175	TYR	CA-C-N	5.11	127.54	120.29
2	B	175	TYR	C-N-CA	5.11	127.54	120.29
4	E	138	GLN	N-CA-C	-5.10	106.91	113.23
6	G	104	ASP	CA-C-N	5.09	127.62	120.28
6	G	104	ASP	C-N-CA	5.09	127.62	120.28
3	D	170	ILE	N-CA-CB	5.07	118.59	112.10
2	C	170	ILE	N-CA-CB	5.06	118.57	112.10
3	D	138	GLN	N-CA-C	-5.05	106.96	113.23
2	C	91	ARG	CA-C-N	5.04	130.89	122.73
2	C	91	ARG	C-N-CA	5.04	130.89	122.73
4	E	68	ASN	CA-CB-CG	5.01	117.61	112.60
3	D	249	THR	CA-C-N	5.01	127.24	120.38
3	D	249	THR	C-N-CA	5.01	127.24	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	2274	0	2229	18	0
2	B	2289	0	2242	23	0
2	C	2289	0	2242	21	0
3	D	2269	0	2224	27	0
4	E	2282	0	2233	25	0
5	F	938	0	914	6	0
5	J	938	0	914	17	0
6	G	929	0	903	4	0
6	H	929	0	903	11	0
6	I	929	0	903	7	0
All	All	16066	0	15707	145	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 (145) 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)
5:J:51:VAL:CG2	5:J:72:ARG:HH22	1.69	1.05
5:J:51:VAL:HB	5:J:72:ARG:NH2	1.86	0.90
5:J:72:ARG:O	5:J:78:MET:O	1.92	0.87
6:H:88:PRO:HA	6:H:122:VAL:HG13	1.56	0.84
6:H:24:ALA:HB2	6:H:34:MET:HE2	1.60	0.83
5:J:51:VAL:CG2	5:J:72:ARG:NH2	2.43	0.82
4:E:91:ARG:NH1	4:E:93:MET:HB2	1.96	0.80
5:J:51:VAL:HG21	5:J:72:ARG:HH22	1.45	0.80
5:J:51:VAL:CB	5:J:72:ARG:NH2	2.50	0.73
6:H:52:GLY:C	6:H:105:ARG:HH12	1.96	0.72
4:E:232:LEU:HD12	4:E:280:ILE:HG21	1.73	0.69
6:I:5:GLN:HG3	6:I:116:GLN:HE22	1.59	0.68
4:E:42:GLN:HG3	4:E:101:ILE:HG12	1.75	0.67
2:C:252:ILE:HD11	3:D:250:SER:HB2	1.78	0.66
4:E:91:ARG:HH12	4:E:93:MET:HB2	1.58	0.66
1:A:250:SER:HB2	4:E:252:ILE:HD11	1.79	0.65
2:C:225:LEU:HD21	3:D:232:LEU:HD22	1.79	0.65
5:J:51:VAL:HB	5:J:72:ARG:HH21	1.62	0.65
6:H:24:ALA:HB2	6:H:34:MET:CE	2.26	0.65
3:D:93:MET:HE3	3:D:95:PHE:CZ	2.32	0.64
1:A:137:ASN:HD21	1:A:187:GLU:HB3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:128:LEU:HB2	3:D:193:VAL:HG22	1.81	0.61
1:A:112:ASN:ND2	1:A:127:VAL:HG22	2.14	0.61
1:A:137:ASN:ND2	1:A:187:GLU:HB3	2.16	0.61
5:J:51:VAL:HG22	5:J:52:GLY:O	2.02	0.59
3:D:249:THR:HG23	3:D:253:LEU:HD13	1.85	0.59
3:D:208:PHE:HE2	3:D:249:THR:HA	1.69	0.58
2:C:60:ASN:O	2:C:63:ILE:HB	2.04	0.57
1:A:244:ALA:HA	1:A:247:PHE:CE2	2.38	0.57
1:A:249:THR:HG23	1:A:253:LEU:HD13	1.87	0.57
5:J:51:VAL:HG23	5:J:72:ARG:HH22	1.62	0.56
6:H:53:ARG:N	6:H:105:ARG:HH12	2.03	0.56
2:C:248:TYR:HE1	3:D:250:SER:HB3	1.70	0.56
4:E:232:LEU:CD1	4:E:280:ILE:HG21	2.34	0.56
4:E:123:ARG:HG2	4:E:198:VAL:HG22	1.88	0.56
1:A:225:LEU:HD22	1:A:230:GLU:HB3	1.88	0.56
3:D:181:VAL:O	3:D:182:GLN:HG3	2.06	0.56
2:C:60:ASN:HD21	2:C:89:ASN:HA	1.71	0.56
3:D:244:ALA:HA	3:D:247:PHE:CE2	2.41	0.55
1:A:252:ILE:HD11	2:B:250:SER:HB2	1.87	0.55
6:H:100:ILE:HD11	6:H:112:GLY:HA3	1.87	0.55
2:C:249:THR:HG21	2:C:266:ILE:HD11	1.89	0.55
2:C:123:ARG:HG2	2:C:198:VAL:HG22	1.89	0.54
2:C:137:ASN:HD21	2:C:187:GLU:HB3	1.73	0.54
2:B:137:ASN:HD21	2:B:187:GLU:HB3	1.71	0.53
2:B:177:HIS:O	2:B:178:LEU:HG	2.08	0.53
2:B:123:ARG:HG2	2:B:198:VAL:HG22	1.90	0.53
2:C:91:ARG:HH11	2:C:93:MET:HB2	1.74	0.53
2:B:181:VAL:O	2:B:182:GLN:HG3	2.07	0.53
3:D:255:ARG:HA	3:D:255:ARG:NE	2.23	0.53
2:B:252:ILE:HD11	2:C:250:SER:HB2	1.91	0.53
2:B:137:ASN:ND2	2:B:187:GLU:HB3	2.23	0.53
6:H:52:GLY:C	6:H:105:ARG:NH1	2.67	0.53
1:A:127:VAL:HG12	1:A:194:ARG:HG3	1.91	0.53
1:A:247:PHE:HB3	4:E:248:TYR:HB2	1.92	0.52
2:C:181:VAL:HG12	2:C:182:GLN:HG3	1.92	0.52
2:C:91:ARG:NH1	2:C:93:MET:HB2	2.24	0.52
3:D:93:MET:HE3	3:D:95:PHE:HZ	1.74	0.52
1:A:33:TYR:HE1	1:A:112:ASN:HB2	1.76	0.51
2:B:127:VAL:HG12	2:B:194:ARG:HG3	1.92	0.51
5:J:83:MET:HE1	5:J:120:VAL:HG21	1.94	0.50
2:C:137:ASN:ND2	2:C:187:GLU:HB3	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ARG:HG2	1:A:198:VAL:HG22	1.93	0.50
2:C:91:ARG:HG2	2:C:92:LEU:N	2.26	0.49
1:A:26:VAL:HG13	1:A:114:MET:HE1	1.94	0.49
5:J:51:VAL:HG22	5:J:52:GLY:N	2.27	0.49
2:B:225:LEU:HD22	2:B:230:GLU:HB3	1.95	0.49
3:D:127:VAL:HG12	3:D:194:ARG:HG3	1.95	0.49
2:B:145:ILE:HD13	2:B:191:ILE:HD13	1.94	0.49
2:C:7:VAL:HG12	2:C:8:ASP:N	2.27	0.49
5:J:51:VAL:HG23	5:J:72:ARG:NH2	2.25	0.49
6:H:100:ILE:CD1	6:H:112:GLY:HA3	2.42	0.48
4:E:26:VAL:HG13	4:E:114:MET:HE1	1.95	0.48
3:D:248:TYR:HA	4:E:247:PHE:HD1	1.77	0.48
3:D:249:THR:HG21	3:D:266:ILE:HD11	1.95	0.48
6:H:87:LYS:O	6:H:122:VAL:HG11	2.14	0.48
3:D:26:VAL:HG13	3:D:114:MET:HE1	1.96	0.48
5:F:50:THR:HG21	5:F:105:ARG:HB2	1.94	0.48
2:B:255:ARG:CZ	2:B:255:ARG:HA	2.44	0.47
6:G:28:ILE:CG2	6:G:77:ASN:HD21	2.28	0.47
5:J:34:MET:HE2	5:J:79:VAL:HG22	1.96	0.47
3:D:248:TYR:HD1	4:E:247:PHE:HA	1.79	0.47
6:H:53:ARG:N	6:H:105:ARG:NH1	2.63	0.47
6:I:34:MET:HE2	6:I:79:VAL:HG22	1.96	0.47
4:E:211:PRO:HA	4:E:214:LEU:HD12	1.98	0.46
4:E:127:VAL:HG12	4:E:194:ARG:HG3	1.98	0.46
5:F:91:THR:HG23	5:F:121:THR:HA	1.98	0.45
6:I:94:TYR:CE1	6:I:120:VAL:HG22	2.52	0.45
3:D:137:ASN:HD21	3:D:187:GLU:HB3	1.81	0.45
5:F:34:MET:HE2	5:F:79:VAL:HG22	1.98	0.45
4:E:208:PHE:CD2	4:E:249:THR:HG22	2.52	0.45
2:B:178:LEU:HA	2:B:181:VAL:HG23	1.98	0.45
4:E:125:GLN:HB2	5:J:103:SER:OG	2.16	0.45
2:B:26:VAL:HG13	2:B:114:MET:HE1	1.97	0.45
3:D:63:ILE:HD11	3:D:91:ARG:HA	1.98	0.44
4:E:232:LEU:CD1	4:E:280:ILE:CG2	2.94	0.44
2:B:208:PHE:HE1	2:B:249:THR:HA	1.83	0.44
4:E:62:GLN:OE1	4:E:65:ARG:HD3	2.17	0.44
4:E:232:LEU:HD11	4:E:280:ILE:HG22	2.00	0.44
1:A:91:ARG:HD2	2:B:134:SER:HB3	2.00	0.44
2:C:127:VAL:HG12	2:C:194:ARG:HG3	2.00	0.43
5:F:94:TYR:CE1	5:F:120:VAL:HG22	2.52	0.43
3:D:211:PRO:HA	3:D:214:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:249:THR:HG21	3:D:266:ILE:CD1	2.49	0.43
2:C:205:LEU:HA	2:C:209:ILE:HD12	1.99	0.43
3:D:63:ILE:HG23	3:D:92:LEU:HD11	2.00	0.43
4:E:232:LEU:HD11	4:E:280:ILE:CG2	2.49	0.43
6:G:83:MET:HE1	6:G:120:VAL:HG21	2.00	0.43
5:J:59:VAL:HG11	5:J:106:LEU:HD21	2.01	0.43
1:A:211:PRO:HA	1:A:214:LEU:HD12	2.01	0.43
2:C:175:TYR:HB2	2:C:178:LEU:HD12	2.00	0.43
4:E:58:VAL:HG11	4:E:66:TRP:CD1	2.54	0.43
4:E:208:PHE:HD2	4:E:249:THR:HG22	1.84	0.42
6:I:5:GLN:HG3	6:I:116:GLN:NE2	2.30	0.42
1:A:249:THR:HG21	1:A:266:ILE:HD11	2.00	0.42
6:I:88:PRO:HA	6:I:122:VAL:HB	2.01	0.42
4:E:175:TYR:HB3	4:E:177:HIS:CE1	2.54	0.42
6:G:88:PRO:HA	6:G:122:VAL:HB	2.02	0.42
2:B:17:SER:HB2	2:B:40:VAL:HB	2.02	0.42
4:E:249:THR:HG21	4:E:266:ILE:HD11	2.01	0.42
2:B:249:THR:HG21	2:B:266:ILE:HD11	2.01	0.42
1:A:33:TYR:CE1	1:A:112:ASN:HB2	2.54	0.42
1:A:225:LEU:HD21	2:B:232:LEU:HD23	2.01	0.42
2:C:211:PRO:HA	2:C:214:LEU:HD12	2.01	0.42
3:D:248:TYR:HB2	4:E:247:PHE:HB2	2.02	0.42
3:D:31:GLN:HG2	3:D:114:MET:HB2	2.02	0.42
3:D:252:ILE:HD11	4:E:250:SER:HB3	2.02	0.42
3:D:137:ASN:ND2	3:D:187:GLU:HB3	2.35	0.41
2:B:145:ILE:HD13	2:B:191:ILE:HG21	2.02	0.41
2:B:211:PRO:HA	2:B:214:LEU:HD12	2.02	0.41
5:F:83:MET:HE1	5:F:120:VAL:HG11	2.02	0.41
2:B:63:ILE:HD12	2:B:90:LYS:HG3	2.03	0.41
3:D:58:VAL:HG11	3:D:66:TRP:CD1	2.55	0.41
5:J:23:ALA:HA	5:J:78:MET:HG2	2.02	0.41
5:F:9:GLY:HA2	5:F:120:VAL:HG12	2.03	0.41
6:H:83:MET:HE1	6:H:120:VAL:HG21	2.02	0.41
5:J:100:ILE:HG22	5:J:110:ASN:O	2.21	0.41
2:C:174:ARG:HG3	2:C:187:GLU:HG3	2.04	0.40
3:D:244:ALA:HA	3:D:247:PHE:CZ	2.56	0.40
6:I:83:MET:HE1	6:I:120:VAL:HG11	2.03	0.40
2:B:91:ARG:HG2	2:B:92:LEU:N	2.36	0.40
2:B:208:PHE:CD1	2:B:249:THR:HG22	2.55	0.40
2:C:31:GLN:HG2	2:C:114:MET:HB2	2.03	0.40
6:I:99:ARG:C	6:I:101:GLY:H	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:G:12:VAL:HG11	6:G:86:LEU:HD13	2.02	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	275/277 (99%)	268 (98%)	6 (2%)	1 (0%)	30	57
2	B	277/280 (99%)	271 (98%)	4 (1%)	2 (1%)	18	44
2	C	277/280 (99%)	267 (96%)	9 (3%)	1 (0%)	30	57
3	D	274/276 (99%)	269 (98%)	4 (2%)	1 (0%)	30	57
4	E	276/278 (99%)	270 (98%)	6 (2%)	0	100	100
5	F	122/124 (98%)	118 (97%)	3 (2%)	1 (1%)	16	40
5	J	122/124 (98%)	114 (93%)	8 (7%)	0	100	100
6	G	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16	40
6	H	121/123 (98%)	116 (96%)	5 (4%)	0	100	100
6	I	121/123 (98%)	117 (97%)	3 (2%)	1 (1%)	16	40
All	All	1986/2008 (99%)	1927 (97%)	51 (3%)	8 (0%)	30	57

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ASN
6	I	100	ILE
2	B	60	ASN
3	D	60	ASN
6	G	99	ARG
2	B	184	ASN

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Mol	Chain	Res	Type
2	C	60	ASN
5	F	99	ARG

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	250/250 (100%)	250 (100%)	0	100	100
2	B	252/253 (100%)	252 (100%)	0	100	100
2	C	252/253 (100%)	252 (100%)	0	100	100
3	D	250/250 (100%)	247 (99%)	3 (1%)	63	84
4	E	251/251 (100%)	251 (100%)	0	100	100
5	F	96/96 (100%)	95 (99%)	1 (1%)	68	86
5	J	96/96 (100%)	96 (100%)	0	100	100
6	G	95/95 (100%)	94 (99%)	1 (1%)	65	85
6	H	95/95 (100%)	95 (100%)	0	100	100
6	I	95/95 (100%)	93 (98%)	2 (2%)	47	76
All	All	1732/1734 (100%)	1725 (100%)	7 (0%)	84	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	91	ARG
3	D	93	MET
3	D	193	VAL
5	F	51	VAL
6	G	106	LEU
6	I	51	VAL
6	I	106	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	ASN
1	A	139	GLN
1	A	146	GLN
1	A	154	ASN
1	A	184	ASN
2	B	103	ASN
2	B	146	GLN
2	B	154	ASN
2	B	285	HIS
2	C	60	ASN
2	C	137	ASN
2	C	146	GLN
2	C	151	ASN
2	C	154	ASN
3	D	103	ASN
3	D	137	ASN
3	D	139	GLN
3	D	151	ASN
3	D	154	ASN
3	D	177	HIS
3	D	251	ASN
3	D	264	GLN
3	D	285	HIS
4	E	62	GLN
4	E	112	ASN
4	E	137	ASN
4	E	139	GLN
4	E	146	GLN
4	E	154	ASN
4	E	251	ASN
4	E	284	HIS
6	G	77	ASN
6	G	82	GLN
6	G	84	ASN
6	H	77	ASN
6	I	110	ASN
5	J	110	ASN

5.3.3 RNA ⓘ

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

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	277/277 (100%)	0.88	38 (13%) 6 5	58, 80, 172, 216	0
2	B	279/280 (99%)	0.74	29 (10%) 11 9	56, 87, 191, 213	0
2	C	279/280 (99%)	1.02	56 (20%) 3 2	53, 88, 205, 230	0
3	D	276/276 (100%)	0.87	44 (15%) 5 4	53, 79, 200, 219	0
4	E	278/278 (100%)	0.84	32 (11%) 9 7	57, 88, 170, 220	0
5	F	124/124 (100%)	0.37	10 (8%) 18 14	60, 80, 118, 150	0
5	J	124/124 (100%)	1.60	44 (35%) 1 0	81, 119, 157, 186	0
6	G	123/123 (100%)	0.93	14 (11%) 10 8	72, 111, 144, 170	0
6	H	123/123 (100%)	1.09	15 (12%) 8 7	79, 117, 160, 183	0
6	I	123/123 (100%)	0.87	18 (14%) 6 5	58, 79, 120, 150	0
All	All	2006/2008 (99%)	0.90	300 (14%) 5 4	53, 91, 177, 230	0

All (300) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	181	VAL	7.0
3	D	277	ILE	6.1
1	A	181	VAL	6.0
4	E	252	ILE	5.9
3	D	222	VAL	5.7
3	D	232	LEU	5.7
2	C	215	ILE	5.6
2	C	214	LEU	5.1
2	C	232	LEU	5.0
3	D	235	SER	4.8
2	B	183	PRO	4.7
6	I	28	ILE	4.7
2	C	181	VAL	4.7

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Mol	Chain	Res	Type	RSRZ
1	A	204	TYR	4.5
2	C	242	VAL	4.5
2	C	218	ALA	4.4
4	E	181	VAL	4.4
5	J	88	PRO	4.3
2	B	270	TYR	4.3
6	H	44	GLU	4.3
6	I	101	GLY	4.3
1	A	281	ILE	4.3
6	I	27	ARG	4.2
3	D	219	SER	4.2
6	I	102	GLY	4.1
2	C	219	SER	4.1
6	I	100	ILE	4.1
4	E	208	PHE	4.1
2	C	23	ILE	4.0
6	H	40	ALA	4.0
4	E	232	LEU	3.9
4	E	278	LEU	3.9
1	A	282	PHE	3.9
2	C	148	TYR	3.9
4	E	283	ALA	3.9
3	D	229	SER	3.9
3	D	181	VAL	3.9
2	B	219	SER	3.8
6	I	103	SER	3.8
6	H	26	GLY	3.8
3	D	223	PHE	3.8
1	A	247	PHE	3.8
6	G	124	SER	3.7
6	H	42	GLY	3.7
5	J	109	GLU	3.7
1	A	277	ILE	3.7
6	H	124	SER	3.7
3	D	236	PHE	3.7
4	E	236	PHE	3.7
2	C	277	ILE	3.6
2	C	238	CYS	3.6
6	G	89	GLU	3.6
5	J	40	ALA	3.6
1	A	208	PHE	3.6
2	B	232	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
4	E	178	LEU	3.6
5	J	95	TYR	3.6
3	D	273	ILE	3.5
3	D	225	LEU	3.5
2	C	235	SER	3.5
6	I	29	PHE	3.5
2	B	178	LEU	3.4
2	C	228	PHE	3.4
6	I	55	GLY	3.4
2	C	207	SER	3.4
1	A	278	LEU	3.4
2	C	222	VAL	3.4
3	D	270	TYR	3.4
5	J	123	SER	3.4
2	C	225	LEU	3.4
2	C	245	TYR	3.3
1	A	133	PHE	3.3
3	D	19	PHE	3.3
4	E	274	PHE	3.3
2	C	157	ILE	3.3
1	A	255	ARG	3.3
1	A	215	ILE	3.3
5	J	19	ARG	3.3
1	A	182	GLN	3.3
6	I	110	ASN	3.3
4	E	224	TRP	3.2
1	A	42	GLN	3.2
5	J	45	ARG	3.2
5	J	11	LEU	3.2
3	D	224	TRP	3.2
6	I	13	GLN	3.2
2	B	182	GLN	3.2
2	C	182	GLN	3.2
2	C	283	ALA	3.2
3	D	220	TRP	3.1
5	J	14	ALA	3.1
6	H	104	ASP	3.1
3	D	275	ALA	3.1
5	F	28	ILE	3.1
2	C	221	SER	3.1
1	A	99	ARG	3.1
3	D	240	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
5	J	31	THR	3.1
2	C	236	PHE	3.1
3	D	228	PHE	3.1
2	C	179	SER	3.1
1	A	238	CYS	3.0
3	D	261	VAL	3.0
4	E	180	SER	3.0
5	J	124	SER	3.0
3	D	215	ILE	3.0
3	D	267	ILE	3.0
4	E	277	ILE	3.0
1	A	200	ASN	2.9
6	H	29	PHE	2.9
1	A	183	PRO	2.9
2	C	206	TRP	2.9
2	C	217	ALA	2.9
1	A	256	LEU	2.9
6	G	100	ILE	2.9
5	J	42	GLY	2.9
5	J	101	GLY	2.9
2	B	171	SER	2.9
2	B	235	SER	2.9
4	E	179	SER	2.9
6	H	54	ILE	2.9
3	D	178	LEU	2.9
3	D	253	LEU	2.9
6	H	43	LYS	2.8
2	B	223	PHE	2.8
3	D	239	MET	2.8
2	C	203	TYR	2.8
3	D	247	PHE	2.8
4	E	242	VAL	2.8
6	G	29	PHE	2.8
2	C	227	SER	2.8
6	H	55	GLY	2.8
4	E	204	TYR	2.8
5	F	54	ILE	2.8
5	F	30	SER	2.8
2	B	208	PHE	2.8
5	J	93	VAL	2.8
6	H	28	ILE	2.7
5	J	12	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
2	C	281	ILE	2.7
4	E	281	ILE	2.7
2	C	220	TRP	2.7
5	J	9	GLY	2.7
5	J	100	ILE	2.7
5	J	29	PHE	2.7
2	B	228	PHE	2.7
5	J	76	LYS	2.7
6	G	88	PRO	2.7
2	B	262	ILE	2.6
4	E	215	ILE	2.6
1	A	285	HIS	2.6
2	C	223	PHE	2.6
5	J	20	LEU	2.6
6	I	4	LEU	2.6
5	J	89	GLU	2.6
2	C	239	MET	2.6
2	B	283	ALA	2.6
4	E	120	PRO	2.6
6	I	124	SER	2.6
1	A	101	ILE	2.6
2	B	240	LEU	2.6
4	E	148	TYR	2.6
3	D	274	PHE	2.6
3	D	282	PHE	2.6
3	D	146	GLN	2.6
4	E	219	SER	2.5
4	E	273	ILE	2.5
6	I	54	ILE	2.5
5	J	72	ARG	2.5
5	J	102	GLY	2.5
6	G	66	GLY	2.5
2	C	201	PRO	2.5
5	J	122	VAL	2.5
1	A	161	TRP	2.5
3	D	252	ILE	2.5
5	J	54	ILE	2.5
5	J	8	GLY	2.5
1	A	254	PRO	2.5
5	F	41	PRO	2.5
2	C	126	PHE	2.5
3	D	157	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
6	I	76	LYS	2.5
5	J	80	TYR	2.5
2	B	239	MET	2.5
6	G	64	VAL	2.5
5	J	63	PHE	2.5
5	J	118	THR	2.5
2	C	216	ILE	2.5
5	F	40	ALA	2.5
3	D	250	SER	2.4
4	E	8	ASP	2.4
4	E	203	TYR	2.4
4	E	185	GLN	2.4
2	B	276	ALA	2.4
3	D	246	ALA	2.4
2	B	279	LEU	2.4
2	C	273	ILE	2.4
1	A	283	ALA	2.4
2	C	121	PHE	2.4
2	B	76	LEU	2.4
2	C	278	LEU	2.4
4	E	157	ILE	2.4
5	J	28	ILE	2.4
5	J	10	GLY	2.4
2	C	282	PHE	2.4
3	D	283	ALA	2.4
4	E	19	PHE	2.4
5	F	29	PHE	2.4
5	J	68	PHE	2.4
1	A	209	ILE	2.4
6	G	28	ILE	2.4
4	E	285	HIS	2.4
2	B	180	SER	2.4
5	F	124	SER	2.4
5	J	44	GLU	2.4
6	G	87	LYS	2.4
5	J	117	GLY	2.4
1	A	279	LEU	2.3
4	E	38	TYR	2.3
1	A	52	GLY	2.3
6	I	2	VAL	2.3
1	A	276	ALA	2.3
4	E	121	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
5	J	110	ASN	2.3
1	A	236	PHE	2.3
3	D	268	ALA	2.3
2	B	281	ILE	2.3
1	A	248	TYR	2.3
2	C	150	GLU	2.3
1	A	100	VAL	2.3
4	E	238	CYS	2.3
6	H	2	VAL	2.3
1	A	205	LEU	2.3
6	H	68	PHE	2.3
2	C	109	SER	2.3
5	F	71	SER	2.3
6	I	108	PRO	2.3
3	D	271	GLY	2.3
5	J	84	ASN	2.2
5	J	43	LYS	2.2
2	C	202	SER	2.2
2	C	240	LEU	2.2
2	B	7	VAL	2.2
2	B	216	ILE	2.2
1	A	90	LYS	2.2
5	J	15	GLY	2.2
5	J	66	GLY	2.2
2	C	265	MET	2.2
2	C	195	ILE	2.2
3	D	216	ILE	2.2
1	A	275	ALA	2.2
6	I	44	GLU	2.2
5	J	41	PRO	2.2
6	G	60	TYR	2.2
2	B	63	ILE	2.2
2	B	127	VAL	2.2
6	G	68	PHE	2.2
2	C	226	GLU	2.1
3	D	278	LEU	2.1
2	B	157	ILE	2.1
5	J	73	ASP	2.1
2	B	221	SER	2.1
4	E	228	PHE	2.1
2	C	224	TRP	2.1
2	C	205	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
3	D	112	ASN	2.1
2	C	152	ILE	2.1
2	C	252	ILE	2.1
3	D	281	ILE	2.1
1	A	219	SER	2.1
2	C	276	ALA	2.1
3	D	276	ALA	2.1
6	G	41	PRO	2.1
2	C	154	ASN	2.1
4	E	73	VAL	2.1
6	I	79	VAL	2.1
6	H	19	ARG	2.1
1	A	237	THR	2.1
2	C	237	THR	2.1
2	B	74	PRO	2.1
5	F	1	GLN	2.1
1	A	128	LEU	2.1
5	J	86	LEU	2.1
6	G	106	LEU	2.1
2	C	248	TYR	2.1
2	C	261	VAL	2.1
6	G	48	VAL	2.1
2	B	272	SER	2.0
3	D	41	ALA	2.0
5	J	85	SER	2.0
6	H	11	LEU	2.0
3	D	18	ILE	2.0
1	A	159	GLU	2.0
2	C	208	PHE	2.0
3	D	231	ARG	2.0
5	J	107	ALA	2.0
2	C	254	PRO	2.0
1	A	216	ILE	2.0
5	F	100	ILE	2.0
3	D	40	VAL	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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.