



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 11:42 AM UTC

PDB ID : 7PI2 / pdb_00007pi2
Title : PfCyRPA bound to monoclonal antibody Cy.003 Fab fragment
Authors : Ragotte, R.J.; Higgins, M.K.
Deposited on : 2021-08-19
Resolution : 3.14 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:

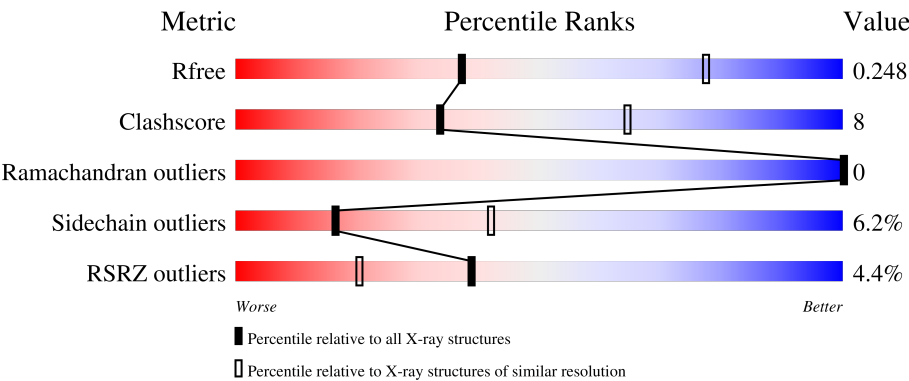
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)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

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.14 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	2351 (3.18-3.10)
Clashscore	190562	2452 (3.18-3.10)
Ramachandran outliers	187476	2324 (3.18-3.10)
Sidechain outliers	187428	2324 (3.18-3.10)
RSRZ outliers	180081	2351 (3.18-3.10)

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	343	7% 72%20%6%
1	D	343	3% 73%19%5%
1	G	343	5% 65%22%10%
1	J	343	5% 71%19%7%
2	B	231	2% 86%10%

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Mol	Chain	Length	Quality of chain
2	E	231	
2	H	231	
2	K	231	
3	C	210	
3	F	210	
3	I	210	
3	L	210	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 23353 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 Cysteine-rich protective antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	0	0
			2674	1719	431	511	13			
1	D	327	Total	C	N	O	S	0	0	0
			2725	1752	440	520	13			
1	G	310	Total	C	N	O	S	0	0	0
			2580	1663	413	491	13			
1	J	319	Total	C	N	O	S	0	0	0
			2646	1702	426	505	13			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	147	ALA	SER	conflict	UNP Q8IFM8
A	324	ALA	THR	conflict	UNP Q8IFM8
A	340	ALA	THR	conflict	UNP Q8IFM8
A	363	GLY	-	expression tag	UNP Q8IFM8
A	364	GLY	-	expression tag	UNP Q8IFM8
A	365	GLY	-	expression tag	UNP Q8IFM8
A	366	GLY	-	expression tag	UNP Q8IFM8
A	367	SER	-	expression tag	UNP Q8IFM8
A	368	GLU	-	expression tag	UNP Q8IFM8
A	369	PRO	-	expression tag	UNP Q8IFM8
A	370	GLU	-	expression tag	UNP Q8IFM8
A	371	ALA	-	expression tag	UNP Q8IFM8
D	147	ALA	SER	conflict	UNP Q8IFM8
D	324	ALA	THR	conflict	UNP Q8IFM8
D	340	ALA	THR	conflict	UNP Q8IFM8
D	363	GLY	-	expression tag	UNP Q8IFM8
D	364	GLY	-	expression tag	UNP Q8IFM8
D	365	GLY	-	expression tag	UNP Q8IFM8
D	366	GLY	-	expression tag	UNP Q8IFM8
D	367	SER	-	expression tag	UNP Q8IFM8
D	368	GLU	-	expression tag	UNP Q8IFM8

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Chain	Residue	Modelled	Actual	Comment	Reference
D	369	PRO	-	expression tag	UNP Q8IFM8
D	370	GLU	-	expression tag	UNP Q8IFM8
D	371	ALA	-	expression tag	UNP Q8IFM8
G	147	ALA	SER	conflict	UNP Q8IFM8
G	324	ALA	THR	conflict	UNP Q8IFM8
G	340	ALA	THR	conflict	UNP Q8IFM8
G	363	GLY	-	expression tag	UNP Q8IFM8
G	364	GLY	-	expression tag	UNP Q8IFM8
G	365	GLY	-	expression tag	UNP Q8IFM8
G	366	GLY	-	expression tag	UNP Q8IFM8
G	367	SER	-	expression tag	UNP Q8IFM8
G	368	GLU	-	expression tag	UNP Q8IFM8
G	369	PRO	-	expression tag	UNP Q8IFM8
G	370	GLU	-	expression tag	UNP Q8IFM8
G	371	ALA	-	expression tag	UNP Q8IFM8
J	147	ALA	SER	conflict	UNP Q8IFM8
J	324	ALA	THR	conflict	UNP Q8IFM8
J	340	ALA	THR	conflict	UNP Q8IFM8
J	363	GLY	-	expression tag	UNP Q8IFM8
J	364	GLY	-	expression tag	UNP Q8IFM8
J	365	GLY	-	expression tag	UNP Q8IFM8
J	366	GLY	-	expression tag	UNP Q8IFM8
J	367	SER	-	expression tag	UNP Q8IFM8
J	368	GLU	-	expression tag	UNP Q8IFM8
J	369	PRO	-	expression tag	UNP Q8IFM8
J	370	GLU	-	expression tag	UNP Q8IFM8
J	371	ALA	-	expression tag	UNP Q8IFM8

- Molecule 2 is a protein called Monoclonal antibody Cy.003 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	222	Total	C	N	O	S	0	0	0
			1616	1012	277	320	7			
2	E	223	Total	C	N	O	S	0	0	0
			1622	1015	278	322	7			
2	H	225	Total	C	N	O	S	0	0	0
			1637	1024	281	325	7			
2	K	225	Total	C	N	O	S	0	0	0
			1637	1024	281	325	7			

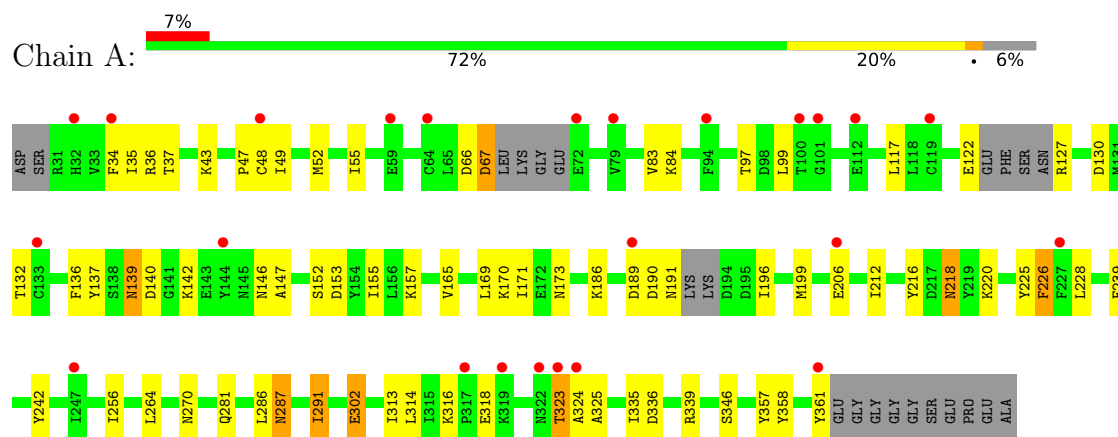
- Molecule 3 is a protein called Monoclonal antibody Cy.003 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	208	Total 1556	C 965	N 264	O 323	S 4	0	0	0
3	F	207	Total 1552	C 963	N 263	O 322	S 4	0	0	0
3	I	208	Total 1556	C 965	N 264	O 323	S 4	0	0	0
3	L	207	Total 1552	C 963	N 263	O 322	S 4	0	0	0

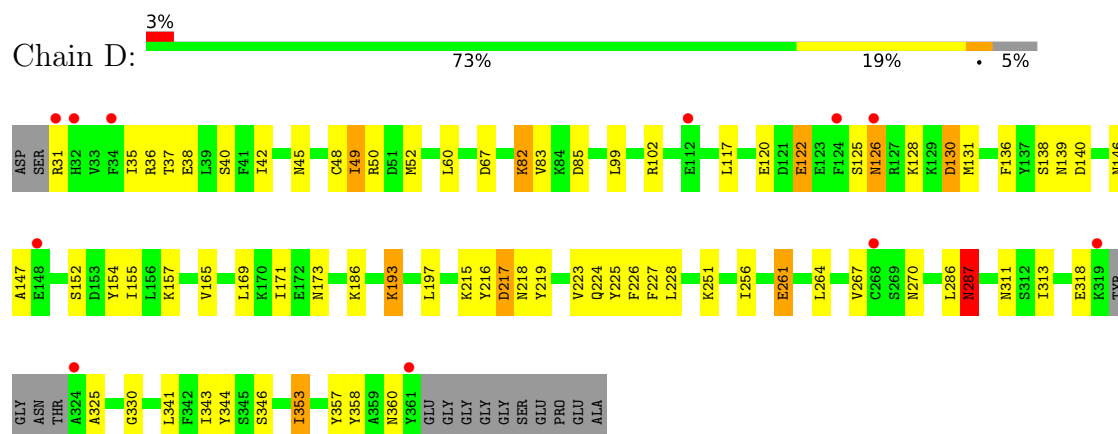
3 Residue-property plots [i](#)

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.

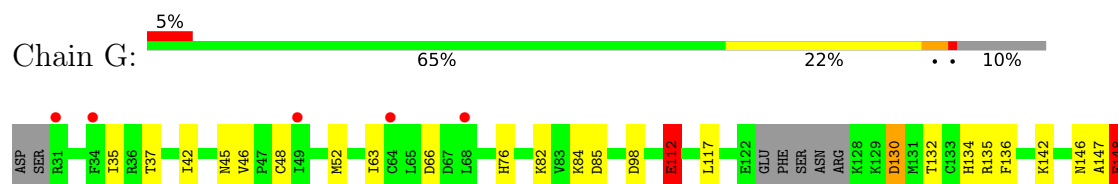
• Molecule 1: Cysteine-rich protective antigen

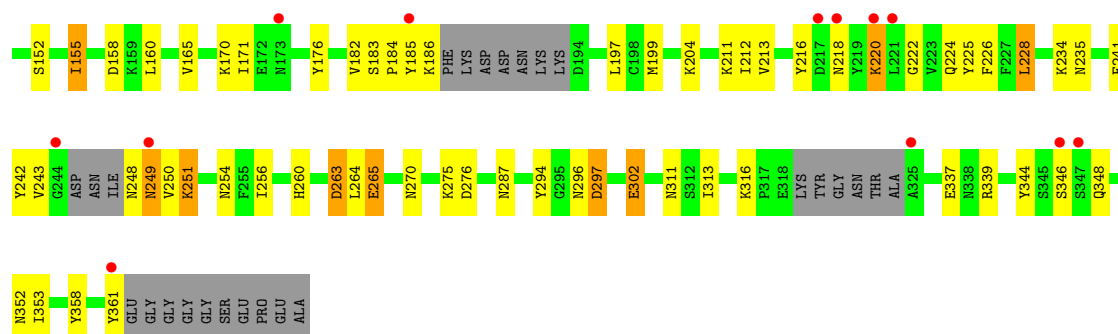


• Molecule 1: Cysteine-rich protective antigen

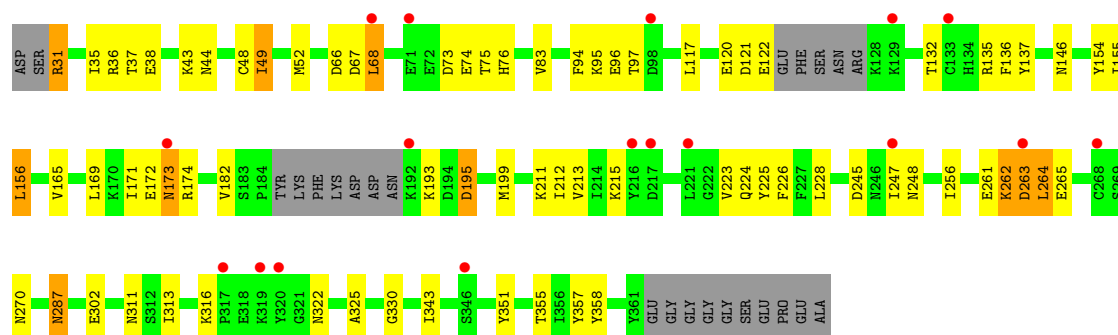


• Molecule 1: Cysteine-rich protective antigen

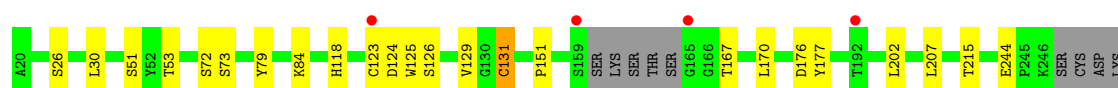
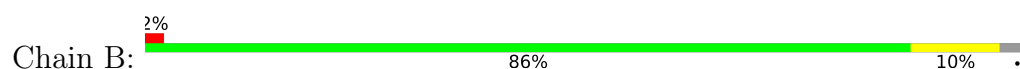




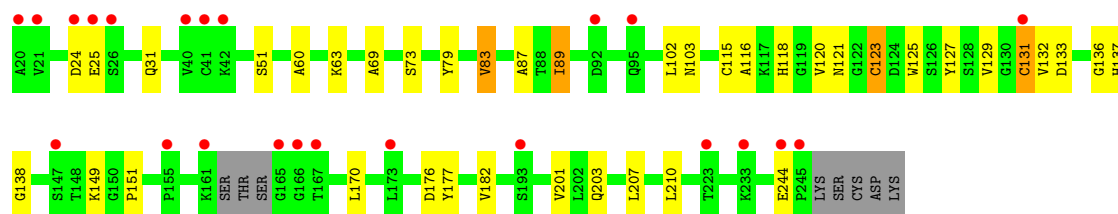
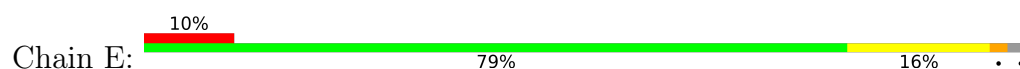
• Molecule 1: Cysteine-rich protective antigen



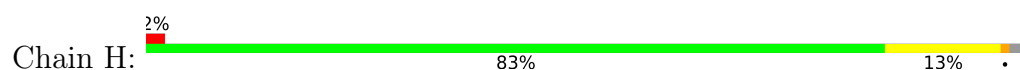
• Molecule 2: Monoclonal antibody Cy.003 heavy chain



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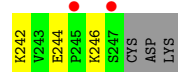
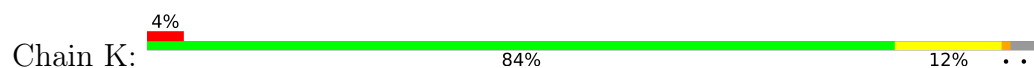


• Molecule 2: Monoclonal antibody Cy.003 heavy chain

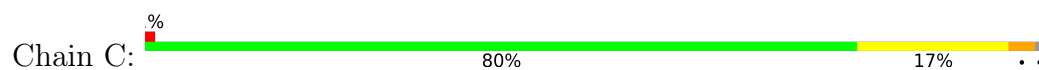




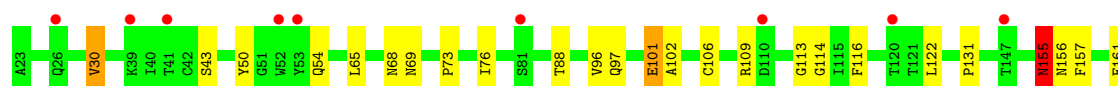
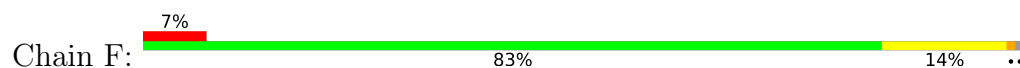
- Molecule 2: Monoclonal antibody Cy.003 heavy chain



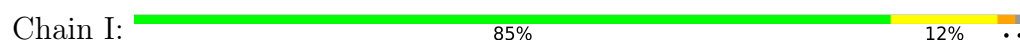
- Molecule 3: Monoclonal antibody Cy.003 light chain



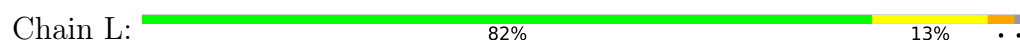
- Molecule 3: Monoclonal antibody Cy.003 light chain

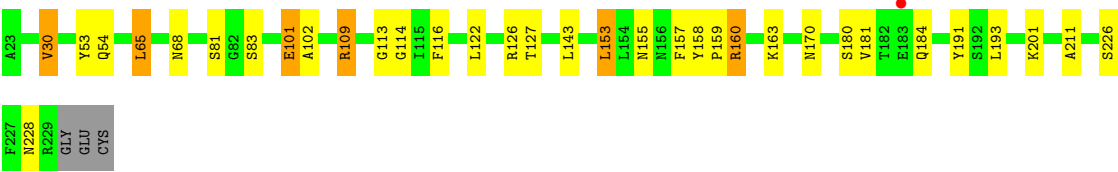


- Molecule 3: Monoclonal antibody Cy.003 light chain



- Molecule 3: Monoclonal antibody Cy.003 light chain





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	354.30Å 71.05Å 164.79Å 90.00° 91.16° 90.00°	Depositor
Resolution (Å)	88.56 – 3.14 88.56 – 3.14	Depositor EDS
% Data completeness (in resolution range)	99.8 (88.56-3.14) 99.8 (88.56-3.14)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 3.13Å)	Xtriage
Refinement program	BUSTER 2.10.3 (19-MAR-2020)	Depositor
R, R_{free}	0.219 , 0.239 0.226 , 0.248	Depositor DCC
R_{free} test set	3461 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	59.8	Xtriage
Anisotropy	0.791	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 80.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	23353	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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	0.73	1/2734 (0.0%)	1.05	9/3691 (0.2%)
1	D	0.68	0/2787	1.04	6/3761 (0.2%)
1	G	0.77	0/2637	1.07	8/3558 (0.2%)
1	J	0.74	0/2705	1.06	9/3652 (0.2%)
2	B	0.67	0/1653	0.97	0/2250
2	E	0.73	0/1659	1.04	3/2258 (0.1%)
2	H	0.74	0/1674	1.04	3/2277 (0.1%)
2	K	0.77	1/1674 (0.1%)	1.05	1/2277 (0.0%)
3	C	0.72	0/1588	1.01	4/2158 (0.2%)
3	F	0.65	0/1584	0.96	1/2153 (0.0%)
3	I	0.77	1/1588 (0.1%)	1.00	3/2158 (0.1%)
3	L	0.70	0/1584	0.99	1/2153 (0.0%)
All	All	0.72	3/23867 (0.0%)	1.03	48/32346 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	229	ARG	CA-C	6.15	1.61	1.52
2	K	130	GLY	C-O	-6.02	1.20	1.24
1	A	281	GLN	CA-C	5.87	1.55	1.52

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	323	THR	N-CA-C	9.22	122.17	111.11
1	A	287	ASN	CA-CB-CG	7.93	120.53	112.60
1	G	98	ASP	CA-CB-CG	7.49	120.09	112.60
1	G	346	SER	N-CA-C	7.30	120.30	111.40
3	C	155	ASN	N-CA-C	7.23	121.03	109.24
2	E	123	CYS	N-CA-C	6.86	117.54	108.07
1	D	287	ASN	CA-CB-CG	6.85	119.45	112.60
1	A	34	PHE	CA-CB-CG	6.67	120.47	113.80
1	J	154	TYR	CA-C-N	6.62	129.86	120.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	154	TYR	C-N-CA	6.62	129.86	120.53
3	C	156	ASN	N-CA-C	6.58	120.32	111.24
1	D	226	PHE	N-CA-C	6.39	120.89	112.13
1	A	218	ASN	CA-CB-CG	6.36	118.96	112.60
1	J	83	VAL	N-CA-CB	6.26	119.35	111.46
3	F	155	ASN	N-CA-C	6.20	119.58	109.59
1	A	318	GLU	CA-C-N	6.12	129.40	120.71
1	A	318	GLU	C-N-CA	6.12	129.40	120.71
1	G	287	ASN	CA-CB-CG	6.03	118.63	112.60
1	D	318	GLU	N-CA-C	5.86	119.53	112.38
3	I	95	GLY	CA-C-N	5.86	128.57	120.49
3	I	95	GLY	C-N-CA	5.86	128.57	120.49
1	J	195	ASP	N-CA-C	-5.86	104.81	111.14
2	E	83	VAL	N-CA-CB	-5.82	105.40	112.33
1	G	148	GLU	CB-CG-CD	5.81	122.48	112.60
1	D	217	ASP	CA-CB-CG	5.78	118.38	112.60
1	G	84	LYS	N-CA-C	5.72	119.01	111.28
1	J	226	PHE	N-CA-C	5.71	119.77	112.12
1	A	226	PHE	N-CA-C	5.65	119.76	111.34
1	A	189	ASP	N-CA-C	5.59	117.75	108.20
3	I	126	ARG	N-CA-CB	-5.58	102.73	111.56
1	J	263	ASP	N-CA-C	5.55	120.47	111.37
2	H	124	ASP	CA-CB-CG	5.45	118.05	112.60
1	G	249	ASN	N-CA-C	5.38	122.26	110.80
3	L	65	LEU	N-CA-C	-5.37	106.41	113.12
2	E	149	LYS	N-CA-C	5.37	120.19	113.43
1	G	297	ASP	CA-CB-CG	-5.37	107.23	112.60
1	D	139	ASN	CA-C-N	5.37	131.38	121.94
1	D	139	ASN	C-N-CA	5.37	131.38	121.94
1	G	112	GLU	CB-CG-CD	5.32	121.65	112.60
1	J	287	ASN	CA-CB-CG	5.29	117.89	112.60
1	J	49	ILE	N-CA-C	-5.27	106.55	111.45
1	A	140	ASP	CA-CB-CG	5.21	117.81	112.60
2	K	123	CYS	N-CA-C	5.15	115.34	108.23
3	C	95	GLY	CA-C-N	5.12	127.56	120.49
3	C	95	GLY	C-N-CA	5.12	127.56	120.49
1	J	49	ILE	CB-CG1-CD1	5.08	124.48	113.80
2	H	160	SER	CA-C-N	5.01	130.72	121.70
2	H	160	SER	C-N-CA	5.01	130.72	121.70

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	2674	0	2560	50	0
1	D	2725	0	2622	44	0
1	G	2580	0	2479	51	0
1	J	2646	0	2549	40	0
2	B	1616	0	1566	15	0
2	E	1622	0	1571	34	0
2	H	1637	0	1589	34	0
2	K	1637	0	1589	30	0
3	C	1556	0	1502	26	0
3	F	1552	0	1499	21	0
3	I	1556	0	1502	23	0
3	L	1552	0	1499	36	0
All	All	23353	0	22527	354	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 8.

All (354) 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:A:55:ILE:HG13	1:A:335:ILE:HG22	1.26	1.18
1:G:186:LYS:HB2	1:G:222:GLY:O	1.43	1.16
2:K:132:VAL:HG12	3:L:53:TYR:OH	1.59	1.03
3:F:163:LYS:HG3	3:F:215:THR:HB	1.41	1.02
3:L:160:ARG:HB3	3:L:191:TYR:CD2	1.98	0.98
1:G:213:VAL:HB	1:G:265:GLU:HG3	1.43	0.96
1:D:227:PHE:HE2	1:D:251:LYS:HZ2	1.11	0.95
2:B:79:TYR:O	2:B:84:LYS:HE3	1.66	0.95
1:J:68:LEU:HD23	1:J:68:LEU:H	1.31	0.93
1:J:247:ILE:HG13	1:J:248:ASN:N	1.82	0.93
1:J:68:LEU:HG	1:J:73:ASP:HB3	1.51	0.92
1:A:314:LEU:HD21	1:A:316:LYS:HE3	1.53	0.90
1:J:263:ASP:O	1:J:264:LEU:HD23	1.72	0.87
1:D:130:ASP:HB3	1:D:152:SER:HA	1.56	0.85
1:A:139:ASN:HD22	1:A:139:ASN:H	1.20	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:148:THR:HG22	2:H:179:PRO:HD3	1.60	0.84
1:A:302:GLU:OE1	1:A:316:LYS:HG2	1.76	0.83
1:A:302:GLU:OE1	1:A:316:LYS:HE2	1.78	0.83
2:H:125:TRP:CD1	3:I:109:ARG:HH11	1.97	0.82
1:A:122:GLU:HB3	1:A:127:ARG:HG3	1.63	0.81
2:K:129:VAL:HG11	3:L:116:PHE:CZ	2.16	0.81
2:K:132:VAL:CG1	3:L:53:TYR:OH	2.27	0.81
2:H:129:VAL:HG11	3:I:116:PHE:CZ	2.16	0.80
2:E:129:VAL:HG11	3:F:116:PHE:CZ	2.17	0.80
1:J:247:ILE:HG13	1:J:248:ASN:H	1.46	0.80
2:H:125:TRP:CD1	3:I:109:ARG:HD2	2.17	0.79
3:L:54:GLN:HB2	3:L:65:LEU:HD11	1.64	0.79
1:G:130:ASP:HB3	1:G:152:SER:HA	1.62	0.79
1:J:212:ILE:HD13	1:J:264:LEU:HD13	1.64	0.79
3:C:228:ASN:O	3:C:229:ARG:HD3	1.83	0.78
1:G:186:LYS:CB	1:G:222:GLY:O	2.28	0.78
2:K:132:VAL:HG13	3:L:53:TYR:CE1	2.17	0.77
2:H:30:LEU:HD12	2:H:148:THR:HG23	1.64	0.77
1:J:182:VAL:HG21	1:J:225:TYR:HB2	1.65	0.77
1:G:148:GLU:CD	1:G:148:GLU:H	1.92	0.77
1:A:55:ILE:CG1	1:A:335:ILE:HG22	2.12	0.76
2:E:69:ALA:HB1	2:E:89:ILE:HG12	1.66	0.76
2:B:79:TYR:O	2:B:84:LYS:CE	2.34	0.76
1:D:155:ILE:HG22	1:D:197:LEU:HD21	1.68	0.76
2:K:132:VAL:CG1	3:L:53:TYR:CZ	2.69	0.76
1:A:314:LEU:CD2	1:A:316:LYS:HE3	2.16	0.76
1:G:220:LYS:O	1:G:220:LYS:HG2	1.84	0.75
1:D:341:LEU:HD13	1:D:353:ILE:HD11	1.70	0.74
2:K:128:SER:HB2	3:L:109:ARG:HB3	1.70	0.73
2:H:28:GLY:HA3	2:H:139:THR:CG2	2.18	0.73
1:D:122:GLU:OE1	1:D:128:LYS:HD3	1.89	0.73
1:A:170:LYS:HE2	1:A:173:ASN:HA	1.71	0.72
2:B:124:ASP:OD1	2:B:125:TRP:N	2.22	0.72
1:J:322:ASN:HB3	1:J:325:ALA:HB2	1.70	0.72
3:L:160:ARG:HB3	3:L:191:TYR:CE2	2.25	0.72
1:A:55:ILE:HG13	1:A:335:ILE:CG2	2.13	0.72
2:K:132:VAL:CG1	3:L:53:TYR:CE1	2.72	0.72
3:C:228:ASN:O	3:C:228:ASN:OD1	2.08	0.71
1:D:325:ALA:HB1	1:D:346:SER:HB2	1.73	0.71
3:F:30:VAL:HG12	3:F:122:LEU:HD12	1.74	0.70
1:G:234:LYS:CE	1:G:337:GLU:OE2	2.40	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:30:VAL:HG12	3:C:122:LEU:HD12	1.75	0.69
1:D:155:ILE:CG2	1:D:197:LEU:HD21	2.22	0.69
3:F:163:LYS:CG	3:F:215:THR:HB	2.21	0.69
2:H:129:VAL:HG23	3:I:114:GLY:HA3	1.72	0.69
2:B:79:TYR:HB2	2:B:84:LYS:HG2	1.73	0.69
1:A:147:ALA:HB3	2:B:125:TRP:CH2	2.27	0.69
1:A:335:ILE:HD11	1:A:339:ARG:HB3	1.74	0.68
3:F:155:ASN:ND2	3:F:156:ASN:OD1	2.26	0.68
1:A:130:ASP:HB3	1:A:152:SER:HA	1.76	0.68
2:E:116:ALA:HB1	2:E:132:VAL:HG11	1.75	0.68
2:H:129:VAL:HG11	3:I:116:PHE:CE2	2.28	0.68
3:I:30:VAL:HG12	3:I:122:LEU:HD12	1.76	0.68
3:L:30:VAL:HG12	3:L:122:LEU:HD12	1.76	0.68
3:C:154:LEU:HD22	3:C:193:LEU:HD22	1.76	0.67
1:G:135:ARG:NH1	1:G:204:LYS:O	2.27	0.67
2:H:30:LEU:HD12	2:H:148:THR:CG2	2.23	0.67
1:J:44:ASN:HB2	1:J:351:TYR:HE2	1.60	0.67
1:A:139:ASN:H	1:A:139:ASN:ND2	1.91	0.67
2:H:129:VAL:CG1	3:I:116:PHE:CZ	2.78	0.66
1:J:173:ASN:C	1:J:173:ASN:HD22	2.02	0.66
1:D:343:ILE:HB	1:D:353:ILE:HD12	1.76	0.66
1:G:135:ARG:NH2	2:H:124:ASP:O	2.29	0.66
1:D:40:SER:O	1:D:353:ILE:HG22	1.96	0.65
3:F:131:PRO:HB3	3:F:157:PHE:CD2	2.31	0.65
3:C:97:GLN:OE1	1:D:173:ASN:ND2	2.30	0.65
2:H:60:ALA:HB3	2:H:63:LYS:HB2	1.80	0.64
2:K:129:VAL:CG1	3:L:116:PHE:CZ	2.80	0.64
3:C:165:GLN:HG3	3:C:172:LEU:CD1	2.28	0.64
2:E:25:GLU:OE2	2:E:136:GLY:HA3	1.98	0.64
1:D:120:GLU:OE1	1:D:128:LYS:NZ	2.31	0.64
3:C:208:LYS:HD2	3:C:209:VAL:HG23	1.81	0.63
1:A:212:ILE:HD13	1:A:264:LEU:HG	1.80	0.63
1:A:286:LEU:O	1:A:287:ASN:HB2	1.99	0.63
1:G:218:ASN:OD1	1:G:220:LYS:HB3	1.97	0.63
1:A:216:TYR:OH	1:A:218:ASN:ND2	2.32	0.63
1:G:242:TYR:HB3	1:G:251:LYS:HB3	1.81	0.63
2:E:25:GLU:HG3	2:E:115:CYS:HB2	1.80	0.63
2:K:79:TYR:HB2	2:K:84:LYS:HG2	1.80	0.62
2:K:132:VAL:HG13	3:L:53:TYR:HE1	1.63	0.62
1:G:155:ILE:HG12	1:G:199:MET:HB3	1.81	0.62
1:J:302:GLU:HG2	1:J:316:LYS:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:131:CYS:HB3	3:C:68:ASN:OD1	2.00	0.61
1:D:131:MET:HE2	1:D:154:TYR:CE2	2.35	0.61
2:K:129:VAL:HG23	3:L:114:GLY:HA3	1.81	0.61
2:E:129:VAL:CG1	3:F:116:PHE:CZ	2.84	0.60
1:D:286:LEU:O	1:D:287:ASN:HB2	1.99	0.60
2:H:127:TYR:CD1	3:I:113:GLY:HA2	2.35	0.60
1:G:171:ILE:HD12	1:G:176:TYR:CE2	2.36	0.60
3:C:165:GLN:HG3	3:C:172:LEU:HD13	1.83	0.60
1:G:170:LYS:O	1:G:235:ASN:HB2	2.01	0.60
1:G:248:ASN:HD22	1:G:249:ASN:H	1.48	0.60
2:H:28:GLY:HA3	2:H:139:THR:HG22	1.83	0.60
1:J:173:ASN:O	1:J:173:ASN:ND2	2.30	0.60
2:H:79:TYR:HB2	2:H:84:LYS:HG2	1.81	0.60
2:B:129:VAL:HG22	3:C:108:SER:O	2.02	0.60
1:J:263:ASP:C	1:J:264:LEU:HD23	2.26	0.60
2:K:131:CYS:HB3	3:L:68:ASN:OD1	2.02	0.59
1:J:68:LEU:H	1:J:68:LEU:CD2	2.08	0.59
2:E:25:GLU:OE1	2:E:25:GLU:N	2.26	0.59
2:E:83:VAL:HG12	2:E:87:ALA:HB2	1.85	0.59
1:D:122:GLU:HB3	1:D:126:ASN:HB3	1.84	0.59
1:A:122:GLU:HB3	1:A:127:ARG:CG	2.31	0.59
3:L:160:ARG:HB3	3:L:191:TYR:CG	2.37	0.58
1:D:67:ASP:OD2	1:D:102:ARG:HD2	2.02	0.58
1:D:343:ILE:HD12	1:D:353:ILE:HD12	1.85	0.58
2:E:129:VAL:HG23	3:F:114:GLY:HA3	1.85	0.58
2:E:69:ALA:CB	2:E:89:ILE:HG12	2.33	0.57
1:J:213:VAL:HB	1:J:265:GLU:HG2	1.85	0.57
2:K:60:ALA:HB3	2:K:63:LYS:HG3	1.85	0.57
1:G:224:GLN:HG3	1:G:226:PHE:CZ	2.40	0.57
1:A:49:ILE:HG13	1:A:67:ASP:HB2	1.87	0.57
1:D:353:ILE:HG23	1:D:353:ILE:O	2.05	0.57
1:A:130:ASP:CB	1:A:152:SER:HA	2.34	0.56
2:B:129:VAL:HG13	3:C:114:GLY:HA3	1.87	0.56
2:E:83:VAL:CG1	2:E:87:ALA:HB2	2.36	0.56
1:G:213:VAL:CB	1:G:265:GLU:HG3	2.27	0.56
2:H:122:GLY:O	2:H:123:CYS:HB3	2.05	0.56
2:K:128:SER:CB	3:L:109:ARG:HB3	2.35	0.56
1:A:314:LEU:HD21	1:A:316:LYS:CE	2.29	0.56
2:E:79:TYR:CE2	2:E:89:ILE:HG13	2.40	0.56
3:I:54:GLN:HB2	3:I:65:LEU:HD11	1.88	0.56
3:I:154:LEU:HD11	3:I:214:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ILE:HG12	1:A:199:MET:HB3	1.88	0.56
1:J:31:ARG:HE	1:J:31:ARG:HA	1.70	0.56
1:D:60:LEU:HB3	1:D:82:LYS:HG2	1.88	0.56
3:C:211:ALA:HB2	3:C:226:SER:HB3	1.88	0.55
2:K:176:ASP:HB3	2:K:207:LEU:HD23	1.89	0.55
1:A:302:GLU:OE1	1:A:316:LYS:CG	2.50	0.55
2:B:176:ASP:HB3	2:B:207:LEU:HD13	1.88	0.55
3:F:43:SER:HB3	3:F:88:THR:HG22	1.88	0.55
1:G:248:ASN:HB3	1:G:251:LYS:HE3	1.89	0.55
2:K:129:VAL:HG11	3:L:116:PHE:CE2	2.42	0.55
1:A:302:GLU:CG	1:A:316:LYS:HG2	2.37	0.55
1:D:155:ILE:HG22	1:D:197:LEU:CD2	2.36	0.55
2:H:176:ASP:HB3	2:H:207:LEU:HD13	1.89	0.55
1:J:193:LYS:HD3	1:J:215:LYS:NZ	2.21	0.54
3:C:141:GLU:HA	3:C:144:LYS:HD2	1.90	0.54
3:I:131:PRO:HD3	3:I:216:HIS:CD2	2.43	0.54
3:F:161:GLU:H	3:F:161:GLU:CD	2.16	0.54
3:L:158:TYR:CD1	3:L:159:PRO:HA	2.43	0.54
2:E:151:PRO:HB3	2:E:177:TYR:HB3	1.88	0.54
1:G:45:ASN:OD1	1:G:46:VAL:HG23	2.08	0.54
2:H:28:GLY:HA3	2:H:139:THR:HG21	1.88	0.53
3:C:54:GLN:HB2	3:C:65:LEU:HD11	1.91	0.53
2:E:129:VAL:HG11	3:F:116:PHE:CE2	2.43	0.53
1:D:138:SER:OG	1:D:140:ASP:O	2.21	0.53
3:F:54:GLN:HB2	3:F:65:LEU:HD11	1.91	0.53
1:A:302:GLU:OE1	1:A:316:LYS:CE	2.51	0.53
1:A:286:LEU:HB2	1:A:291:ILE:HD13	1.90	0.53
2:H:107:ALA:HB3	3:L:170:ASN:ND2	2.23	0.53
3:I:154:LEU:HD11	3:I:214:VAL:CG1	2.38	0.53
1:G:216:TYR:CZ	1:G:218:ASN:HB3	2.45	0.52
1:D:147:ALA:HB3	2:E:125:TRP:CH2	2.45	0.52
3:F:50:TYR:H	3:F:69:ASN:ND2	2.06	0.52
1:G:155:ILE:CD1	1:G:211:LYS:HG3	2.39	0.52
2:H:151:PRO:HB3	2:H:177:TYR:HB3	1.91	0.52
1:A:170:LYS:CE	1:A:173:ASN:HA	2.38	0.52
1:G:197:LEU:HD11	1:G:211:LYS:HE3	1.91	0.52
1:J:137:TYR:CD2	2:K:124:ASP:HB3	2.45	0.52
1:G:348:GLN:O	1:G:348:GLN:HG3	2.09	0.52
3:C:161:GLU:CD	3:C:161:GLU:H	2.17	0.52
2:H:30:LEU:CD1	2:H:148:THR:HG23	2.35	0.52
3:I:181:VAL:HG22	3:I:193:LEU:HD12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:PRO:HB3	2:B:177:TYR:HB3	1.91	0.51
2:E:120:VAL:HG13	2:E:121:ASN:N	2.25	0.51
2:E:176:ASP:HB3	2:E:207:LEU:HD23	1.92	0.51
2:E:24:ASP:OD1	2:E:137:HIS:NE2	2.35	0.51
2:K:151:PRO:HB3	2:K:177:TYR:HB3	1.91	0.51
2:K:125:TRP:CD1	3:L:109:ARG:HD3	2.46	0.51
1:J:67:ASP:HB2	1:J:75:THR:HG23	1.93	0.51
1:A:52:MET:HG2	1:A:165:VAL:HG23	1.93	0.51
2:E:25:GLU:CG	2:E:115:CYS:HB2	2.41	0.51
2:K:132:VAL:HG13	2:K:132:VAL:O	2.11	0.51
1:D:42:ILE:HD11	1:D:82:LYS:HD2	1.94	0.50
2:H:51:SER:HA	2:H:73:SER:HB2	1.94	0.50
2:H:125:TRP:CD1	3:I:109:ARG:NH1	2.75	0.50
1:A:302:GLU:CD	1:A:316:LYS:HG2	2.37	0.50
2:E:83:VAL:HG13	2:E:102:LEU:HD13	1.92	0.50
1:D:40:SER:HB3	1:D:353:ILE:CG2	2.42	0.50
3:F:43:SER:CB	3:F:88:THR:HG22	2.41	0.50
1:G:234:LYS:HE2	1:G:337:GLU:OE2	2.12	0.50
2:B:118:HIS:CE1	2:B:123:CYS:SG	3.05	0.49
1:D:193:LYS:HB3	1:D:215:LYS:HG2	1.92	0.49
1:G:37:THR:HG21	1:G:313:ILE:HD13	1.94	0.49
1:J:68:LEU:HD23	1:J:68:LEU:N	2.14	0.49
1:D:49:ILE:HG22	1:D:50:ARG:HG2	1.95	0.49
1:A:137:TYR:CD1	2:B:124:ASP:HB3	2.48	0.49
1:G:186:LYS:HB2	1:G:222:GLY:C	2.30	0.49
3:C:131:PRO:HD3	3:C:216:HIS:ND1	2.27	0.49
2:E:83:VAL:HG12	2:E:87:ALA:CB	2.42	0.49
2:B:51:SER:HA	2:B:73:SER:HB2	1.95	0.49
1:A:302:GLU:HG2	1:A:316:LYS:HG2	1.95	0.48
3:L:101:GLU:O	3:L:102:ALA:HB2	2.13	0.48
1:G:224:GLN:NE2	1:G:248:ASN:OD1	2.46	0.48
2:K:213:VAL:HG21	3:L:153:LEU:HD11	1.94	0.48
3:C:160:ARG:CZ	3:C:181:VAL:HG21	2.43	0.48
1:G:52:MET:HE2	1:G:63:ILE:HD12	1.96	0.48
2:E:51:SER:HA	2:E:73:SER:HB2	1.96	0.48
1:G:148:GLU:CD	1:G:148:GLU:N	2.68	0.48
1:J:52:MET:HG2	1:J:165:VAL:HG23	1.95	0.48
1:A:335:ILE:HG13	1:A:339:ARG:HB2	1.96	0.48
1:D:227:PHE:CE2	1:D:251:LYS:NZ	2.74	0.48
2:H:125:TRP:NE1	3:I:109:ARG:NH1	2.61	0.48
1:D:155:ILE:HG22	1:D:155:ILE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:203:GLN:HG2	2:E:207:LEU:O	2.14	0.48
3:I:211:ALA:HB2	3:I:226:SER:HB3	1.95	0.48
1:G:260:HIS:HE2	1:G:263:ASP:C	2.21	0.47
3:C:47:SER:HB2	3:C:109:ARG:HB3	1.97	0.47
1:A:139:ASN:HD22	1:A:139:ASN:N	1.88	0.47
1:J:256:ILE:HG22	1:J:270:ASN:HA	1.95	0.47
3:F:176:ASN:HD22	3:F:199:LEU:HD21	1.78	0.47
1:G:35:ILE:HG12	1:G:358:TYR:HD1	1.80	0.47
2:K:51:SER:HA	2:K:73:SER:HB2	1.97	0.47
3:L:158:TYR:HA	3:L:159:PRO:C	2.39	0.47
3:C:181:VAL:HG22	3:C:193:LEU:HD12	1.96	0.47
1:D:52:MET:HG2	1:D:165:VAL:HG23	1.96	0.47
1:G:66:ASP:HB3	1:G:76:HIS:HB2	1.96	0.47
1:A:190:ASP:O	1:A:191:ASN:HB2	2.15	0.47
1:G:52:MET:HG2	1:G:165:VAL:HG23	1.97	0.47
1:D:343:ILE:HD12	1:D:353:ILE:CD1	2.44	0.47
2:K:225:THR:HG23	2:K:242:LYS:HZ3	1.80	0.47
1:A:47:PRO:HG2	1:A:66:ASP:OD1	2.14	0.47
1:A:302:GLU:OE1	1:A:316:LYS:CD	2.62	0.47
3:C:211:ALA:CB	3:C:226:SER:HB3	2.45	0.47
1:J:35:ILE:HG12	1:J:358:TYR:HD1	1.80	0.47
2:E:131:CYS:HB3	3:F:68:ASN:OD1	2.15	0.47
1:J:74:GLU:HG2	1:J:75:THR:H	1.79	0.47
3:L:160:ARG:O	3:L:160:ARG:NH1	2.48	0.47
3:L:181:VAL:HG22	3:L:193:LEU:HD12	1.97	0.47
1:D:225:TYR:N	1:D:225:TYR:CD1	2.83	0.46
3:F:101:GLU:O	3:F:102:ALA:HB2	2.16	0.46
2:E:127:TYR:CD1	3:F:113:GLY:HA2	2.50	0.46
1:G:42:ILE:HD11	1:G:82:LYS:HD2	1.97	0.46
3:C:101:GLU:O	3:C:102:ALA:HB2	2.16	0.46
1:D:35:ILE:HG12	1:D:358:TYR:HD1	1.81	0.46
1:G:212:ILE:HD13	1:G:264:LEU:HG	1.97	0.46
1:J:74:GLU:HG2	1:J:75:THR:N	2.31	0.46
1:J:37:THR:HG21	1:J:313:ILE:HD13	1.98	0.46
1:A:228:LEU:HD11	1:A:239:PHE:HB3	1.96	0.46
1:G:296:ASN:HB3	1:G:302:GLU:HG3	1.97	0.46
2:H:125:TRP:CG	3:I:109:ARG:HH11	2.33	0.46
1:A:35:ILE:HG12	1:A:358:TYR:HD1	1.81	0.46
1:G:225:TYR:HD1	1:G:243:VAL:HG12	1.81	0.46
1:D:136:PHE:CD2	1:D:146:ASN:HB3	2.51	0.46
2:K:127:TYR:CD1	3:L:113:GLY:HA2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:129:VAL:HG12	2:K:129:VAL:O	2.17	0.45
1:D:36:ARG:HB3	1:D:357:TYR:HB3	1.99	0.45
2:H:123:CYS:HB2	3:I:49:TYR:CD2	2.51	0.45
1:D:261:GLU:HG2	1:D:267:VAL:HG12	1.97	0.45
1:J:136:PHE:CD2	1:J:146:ASN:HB3	2.51	0.45
1:J:262:LYS:HA	1:J:262:LYS:HD3	1.65	0.45
2:E:25:GLU:OE2	2:E:136:GLY:C	2.59	0.45
2:E:25:GLU:OE2	2:E:136:GLY:CA	2.64	0.45
3:I:101:GLU:O	3:I:102:ALA:HB2	2.16	0.45
1:J:156:LEU:HD22	1:J:199:MET:HG2	1.98	0.45
1:D:42:ILE:HD13	1:D:85:ASP:HA	1.99	0.45
1:D:154:TYR:O	1:D:157:LYS:HG3	2.17	0.45
1:J:94:PHE:O	1:J:97:THR:HG22	2.17	0.45
1:A:323:THR:HG23	1:A:324:ALA:N	2.32	0.45
1:G:130:ASP:CB	1:G:152:SER:HA	2.38	0.45
1:G:228:LEU:HA	1:G:241:PHE:HB3	1.99	0.45
2:E:118:HIS:HD2	2:E:132:VAL:HG22	1.82	0.45
1:A:97:THR:HG21	1:A:99:LEU:HD12	1.98	0.45
3:C:126:ARG:HH22	3:C:129:ALA:HB2	1.82	0.45
2:E:60:ALA:HB3	2:E:63:LYS:HG3	1.99	0.44
1:D:31:ARG:HG2	1:D:360:ASN:HD21	1.82	0.44
2:H:125:TRP:NE1	3:I:109:ARG:HH11	2.15	0.44
1:J:135:ARG:NH1	2:K:125:TRP:CZ3	2.85	0.44
3:L:101:GLU:HG3	3:L:184:GLN:HB3	2.00	0.44
1:A:169:LEU:HD23	1:A:171:ILE:HD11	2.00	0.43
2:E:69:ALA:HB1	2:E:89:ILE:CG1	2.41	0.43
1:G:248:ASN:ND2	1:G:249:ASN:H	2.15	0.43
1:D:37:THR:HG21	1:D:313:ILE:HD13	2.00	0.43
1:D:256:ILE:HG22	1:D:270:ASN:HA	1.99	0.43
1:A:136:PHE:CD2	1:A:146:ASN:HB3	2.54	0.43
2:H:129:VAL:HG12	2:H:129:VAL:O	2.19	0.43
2:H:107:ALA:CB	3:L:170:ASN:HD22	2.32	0.43
1:J:66:ASP:HB3	1:J:76:HIS:HB2	2.00	0.43
1:J:121:ASP:O	1:J:122:GLU:HG2	2.19	0.43
1:A:83:VAL:HG13	1:A:84:LYS:H	1.84	0.43
1:D:186:LYS:HB2	1:D:219:TYR:HE1	1.83	0.43
1:D:169:LEU:HD23	1:D:171:ILE:HD11	2.00	0.43
3:F:211:ALA:HB2	3:F:226:SER:HB3	1.99	0.43
2:E:118:HIS:CE1	2:E:123:CYS:SG	3.12	0.42
2:H:128:SER:CB	3:I:109:ARG:HB2	2.49	0.42
2:H:231:ASN:HD22	2:H:238:LYS:HG3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:95:LYS:HE3	1:J:96:GLU:OE2	2.19	0.42
1:A:256:ILE:HG22	1:A:270:ASN:HA	2.00	0.42
1:J:212:ILE:CD1	1:J:264:LEU:HD13	2.43	0.42
3:F:101:GLU:HG3	3:F:184:GLN:HB3	2.01	0.42
1:G:256:ILE:HG22	1:G:270:ASN:HA	2.00	0.42
1:J:169:LEU:HD23	1:J:171:ILE:HD11	2.00	0.42
3:C:136:PHE:HA	3:C:137:PRO:HD3	1.94	0.42
1:D:216:TYR:CE1	1:D:218:ASN:HB3	2.55	0.42
1:G:225:TYR:CD1	1:G:243:VAL:HG12	2.54	0.42
1:A:130:ASP:HB3	1:A:153:ASP:H	1.85	0.42
1:G:155:ILE:HD12	1:G:211:LYS:HG3	2.01	0.42
2:K:124:ASP:OD1	2:K:124:ASP:N	2.51	0.42
1:D:330:GLY:HA2	1:D:344:TYR:HB3	2.00	0.42
1:G:183:SER:HA	1:G:184:PRO:HD3	1.91	0.42
1:J:36:ARG:HB3	1:J:357:TYR:HB3	2.02	0.42
3:L:211:ALA:HB2	3:L:226:SER:HB3	2.00	0.42
1:A:36:ARG:HB3	1:A:357:TYR:HB3	2.02	0.42
1:G:136:PHE:CD2	1:G:146:ASN:HB3	2.54	0.42
1:J:330:GLY:HA2	1:J:343:ILE:O	2.19	0.42
2:K:129:VAL:CG2	3:L:114:GLY:HA3	2.49	0.42
1:G:234:LYS:HE3	1:G:337:GLU:OE2	2.19	0.42
3:L:160:ARG:CB	3:L:191:TYR:CD2	2.87	0.42
1:G:344:TYR:CE2	1:G:352:ASN:HB2	2.55	0.41
2:E:25:GLU:CD	2:E:138:GLY:H	2.26	0.41
1:A:225:TYR:CD1	1:A:225:TYR:N	2.87	0.41
1:J:155:ILE:HD13	1:J:211:LYS:HB2	2.01	0.41
3:L:126:ARG:HG2	3:L:127:THR:N	2.36	0.41
2:E:129:VAL:O	2:E:129:VAL:HG12	2.20	0.41
2:B:53:THR:HG22	2:B:72:SER:HA	2.02	0.41
2:B:167:THR:CG2	2:B:215:THR:OG1	2.69	0.41
3:F:73:PRO:HG2	3:F:76:ILE:HG13	2.02	0.41
3:L:143:LEU:O	3:L:201:LYS:CD	2.69	0.41
1:G:112:GLU:CD	1:G:112:GLU:H	2.27	0.41
3:C:126:ARG:NH2	3:C:129:ALA:HB2	2.35	0.41
3:C:207:HIS:O	3:C:230:GLY:C	2.64	0.41
1:G:147:ALA:HB3	2:H:125:TRP:CH2	2.56	0.41
2:H:125:TRP:HD1	3:I:109:ARG:HD2	1.81	0.41
2:H:173:LEU:HG	2:H:175:LYS:HG2	2.01	0.41
1:J:171:ILE:HG22	1:J:172:GLU:HG2	2.02	0.41
3:L:158:TYR:CG	3:L:159:PRO:HA	2.56	0.41
2:K:246:LYS:HD2	2:K:246:LYS:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:157:PHE:CE2	3:L:160:ARG:HA	2.56	0.41
1:A:37:THR:HG21	1:A:313:ILE:HD13	2.03	0.40
1:A:325:ALA:HB1	1:A:346:SER:HB2	2.02	0.40
1:G:275:LYS:HD2	1:G:294:TYR:CZ	2.57	0.40
2:K:125:TRP:C	2:K:127:TYR:N	2.76	0.40
1:A:226:PHE:HB2	1:A:242:TYR:HB2	2.03	0.40
3:C:165:GLN:HG3	3:C:172:LEU:HD11	2.02	0.40
2:E:25:GLU:OE2	2:E:138:GLY:N	2.48	0.40
1:G:316:LYS:HB3	1:G:316:LYS:HE3	1.94	0.40
3:I:101:GLU:HG3	3:I:184:GLN:HB3	2.03	0.40
1:D:52:MET:HE3	1:D:52:MET:HB2	1.95	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	313/343 (91%)	292 (93%)	21 (7%)	0	100	100
1	D	323/343 (94%)	302 (94%)	21 (6%)	0	100	100
1	G	300/343 (88%)	271 (90%)	29 (10%)	0	100	100
1	J	313/343 (91%)	286 (91%)	27 (9%)	0	100	100
2	B	218/231 (94%)	211 (97%)	7 (3%)	0	100	100
2	E	219/231 (95%)	212 (97%)	7 (3%)	0	100	100
2	H	221/231 (96%)	212 (96%)	9 (4%)	0	100	100
2	K	221/231 (96%)	211 (96%)	10 (4%)	0	100	100
3	C	206/210 (98%)	194 (94%)	12 (6%)	0	100	100
3	F	205/210 (98%)	194 (95%)	11 (5%)	0	100	100
3	I	206/210 (98%)	194 (94%)	12 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	L	205/210 (98%)	196 (96%)	9 (4%)	0	100	100
All	All	2950/3136 (94%)	2775 (94%)	175 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	300/316 (95%)	284 (95%)	16 (5%)	20	47
1	D	306/316 (97%)	284 (93%)	22 (7%)	13	37
1	G	290/316 (92%)	262 (90%)	28 (10%)	8	27
1	J	297/316 (94%)	274 (92%)	23 (8%)	12	34
2	B	177/186 (95%)	170 (96%)	7 (4%)	28	55
2	E	178/186 (96%)	168 (94%)	10 (6%)	19	45
2	H	180/186 (97%)	173 (96%)	7 (4%)	28	56
2	K	180/186 (97%)	170 (94%)	10 (6%)	19	45
3	C	177/179 (99%)	168 (95%)	9 (5%)	21	48
3	F	177/179 (99%)	169 (96%)	8 (4%)	24	52
3	I	177/179 (99%)	166 (94%)	11 (6%)	16	42
3	L	177/179 (99%)	166 (94%)	11 (6%)	16	42
All	All	2616/2724 (96%)	2454 (94%)	162 (6%)	16	42

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	LYS
1	A	48	CYS
1	A	67	ASP
1	A	117	LEU
1	A	132	THR

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Mol	Chain	Res	Type
1	A	139	ASN
1	A	142	LYS
1	A	157	LYS
1	A	186	LYS
1	A	196	ILE
1	A	206	GLU
1	A	220	LYS
1	A	291	ILE
1	A	302	GLU
1	A	336	ASP
1	A	361	TYR
2	B	26	SER
2	B	30	LEU
2	B	126	SER
2	B	131	CYS
2	B	170	LEU
2	B	202	LEU
2	B	244	GLU
3	C	30	VAL
3	C	101	GLU
3	C	106	CYS
3	C	143	LEU
3	C	160	ARG
3	C	165	GLN
3	C	201	LYS
3	C	209	VAL
3	C	229	ARG
1	D	38	GLU
1	D	45	ASN
1	D	48	CYS
1	D	49	ILE
1	D	82	LYS
1	D	83	VAL
1	D	99	LEU
1	D	117	LEU
1	D	122	GLU
1	D	125	SER
1	D	126	ASN
1	D	130	ASP
1	D	193	LYS
1	D	217	ASP
1	D	223	VAL

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Mol	Chain	Res	Type
1	D	224	GLN
1	D	228	LEU
1	D	261	GLU
1	D	264	LEU
1	D	287	ASN
1	D	311	ASN
1	D	353	ILE
2	E	31	GLN
2	E	89	ILE
2	E	103	ASN
2	E	131	CYS
2	E	133	ASP
2	E	170	LEU
2	E	182	VAL
2	E	201	VAL
2	E	210	LEU
2	E	244	GLU
3	F	30	VAL
3	F	96	VAL
3	F	97	GLN
3	F	101	GLU
3	F	106	CYS
3	F	109	ARG
3	F	155	ASN
3	F	203	ASP
1	G	48	CYS
1	G	85	ASP
1	G	112	GLU
1	G	117	LEU
1	G	130	ASP
1	G	132	THR
1	G	134	HIS
1	G	142	LYS
1	G	148	GLU
1	G	155	ILE
1	G	158	ASP
1	G	160	LEU
1	G	182	VAL
1	G	185	TYR
1	G	220	LYS
1	G	228	LEU
1	G	250	VAL

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Mol	Chain	Res	Type
1	G	251	LYS
1	G	254	ASN
1	G	263	ASP
1	G	265	GLU
1	G	276	ASP
1	G	297	ASP
1	G	302	GLU
1	G	311	ASN
1	G	339	ARG
1	G	353	ILE
1	G	361	TYR
2	H	31	GLN
2	H	84	LYS
2	H	170	LEU
2	H	175	LYS
2	H	241	LYS
2	H	244	GLU
2	H	246	LYS
3	I	30	VAL
3	I	81	SER
3	I	88	THR
3	I	101	GLU
3	I	106	CYS
3	I	109	ARG
3	I	111	ASN
3	I	126	ARG
3	I	143	LEU
3	I	167	LYS
3	I	170	ASN
1	J	31	ARG
1	J	38	GLU
1	J	43	LYS
1	J	48	CYS
1	J	49	ILE
1	J	68	LEU
1	J	117	LEU
1	J	120	GLU
1	J	132	THR
1	J	156	LEU
1	J	173	ASN
1	J	174	ARG
1	J	195	ASP

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Mol	Chain	Res	Type
1	J	223	VAL
1	J	224	GLN
1	J	228	LEU
1	J	245	ASP
1	J	261	GLU
1	J	262	LYS
1	J	264	LEU
1	J	287	ASN
1	J	311	ASN
1	J	355	THR
2	K	26	SER
2	K	31	GLN
2	K	84	LYS
2	K	104	ASN
2	K	131	CYS
2	K	170	LEU
2	K	182	VAL
2	K	202	LEU
2	K	207	LEU
2	K	244	GLU
3	L	30	VAL
3	L	81	SER
3	L	83	SER
3	L	101	GLU
3	L	109	ARG
3	L	153	LEU
3	L	155	ASN
3	L	160	ARG
3	L	163	LYS
3	L	180	SER
3	L	228	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	139	ASN
1	A	173	ASN
1	A	218	ASN
1	A	224	GLN
1	A	277	ASN
1	A	322	ASN

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Mol	Chain	Res	Type
3	C	155	ASN
3	C	156	ASN
3	C	170	ASN
3	C	228	ASN
1	D	91	ASN
1	D	173	ASN
1	D	218	ASN
1	D	246	ASN
1	D	277	ASN
2	E	31	GLN
2	E	95	GLN
2	E	121	ASN
2	E	187	ASN
3	F	69	ASN
3	F	155	ASN
1	G	91	ASN
1	G	104	HIS
1	G	173	ASN
1	G	224	GLN
1	G	248	ASN
1	G	277	ASN
1	G	287	ASN
1	G	338	ASN
1	G	352	ASN
2	H	31	GLN
2	H	101	GLN
2	H	231	ASN
3	I	216	HIS
1	J	91	ASN
1	J	104	HIS
1	J	202	HIS
1	J	352	ASN
2	K	31	GLN
2	K	95	GLN
2	K	101	GLN
2	K	196	HIS
3	L	207	HIS
3	L	217	GLN

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	321/343 (93%)	0.75	24 (7%)	20	10	53, 95, 155, 222	0
1	D	327/343 (95%)	0.52	11 (3%)	48	27	55, 92, 155, 186	0
1	G	310/343 (90%)	0.57	17 (5%)	30	16	54, 90, 133, 182	0
1	J	319/343 (93%)	0.67	17 (5%)	32	16	49, 95, 156, 187	0
2	B	222/231 (96%)	0.29	4 (1%)	67	46	50, 74, 101, 112	0
2	E	223/231 (96%)	1.04	23 (10%)	12	6	36, 110, 150, 160	0
2	H	225/231 (97%)	0.23	5 (2%)	62	41	41, 68, 89, 118	0
2	K	225/231 (97%)	0.50	10 (4%)	39	20	42, 73, 133, 160	0
3	C	208/210 (99%)	0.26	3 (1%)	73	53	47, 76, 104, 114	0
3	F	207/210 (98%)	0.96	15 (7%)	21	11	50, 104, 200, 211	0
3	I	208/210 (99%)	0.08	1 (0%)	87	73	40, 66, 85, 103	0
3	L	207/210 (98%)	0.24	1 (0%)	87	73	40, 79, 117, 122	0
All	All	3002/3136 (95%)	0.53	131 (4%)	39	20	36, 82, 150, 222	0

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	24	ASP	4.6
1	J	217	ASP	4.4
1	D	126	ASN	4.3
1	A	94	PHE	4.1
2	E	25	GLU	3.8
2	B	165	GLY	3.8
1	J	221	LEU	3.7
1	G	221	LEU	3.5
2	H	247	SER	3.5
1	A	324	ALA	3.4
1	A	119	CYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	J	319	LYS	3.2
1	A	133	CYS	3.2
1	A	227	PHE	3.2
2	H	161	LYS	3.1
1	G	346	SER	3.1
2	H	24	ASP	3.1
2	E	41	CYS	3.1
3	C	45	GLY	3.0
1	J	71	GLU	3.0
1	J	192	LYS	3.0
1	A	319	LYS	2.9
2	E	21	VAL	2.9
1	A	101	GLY	2.9
3	I	230	GLY	2.9
1	J	173	ASN	2.9
1	J	133	CYS	2.8
1	G	244	GLY	2.8
1	J	346	SER	2.8
1	A	34	PHE	2.8
1	G	325	ALA	2.8
1	G	34	PHE	2.8
1	G	31	ARG	2.8
1	J	129	LYS	2.8
3	F	41	THR	2.8
2	E	26	SER	2.7
1	G	217	ASP	2.7
1	D	324	ALA	2.7
2	E	40	VAL	2.7
2	K	161	LYS	2.7
1	J	320	TYR	2.7
2	E	95	GLN	2.7
1	G	173	ASN	2.6
2	K	26	SER	2.6
2	E	20	ALA	2.6
1	A	112	GLU	2.6
3	F	39	LYS	2.6
2	E	167	THR	2.5
2	K	92	ASP	2.5
2	K	108	GLU	2.5
1	A	323	THR	2.5
3	F	198	THR	2.5
1	G	361	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	166	GLY	2.5
2	K	24	ASP	2.5
3	F	229	ARG	2.5
2	E	155	PRO	2.5
2	H	93	ASN	2.4
3	F	26	GLN	2.4
2	E	42	LYS	2.4
1	G	185	TYR	2.4
1	J	247	ILE	2.4
2	E	92	ASP	2.4
3	L	183	GLU	2.4
1	G	64	CYS	2.4
2	E	131	CYS	2.4
1	D	32	HIS	2.3
1	G	220	LYS	2.3
1	A	189	ASP	2.3
1	D	31	ARG	2.3
1	A	100	THR	2.3
3	F	204	TYR	2.3
3	F	110	ASP	2.3
1	G	249	ASN	2.3
3	F	169	ASP	2.3
1	D	34	PHE	2.2
2	B	192	THR	2.2
3	F	81	SER	2.2
2	K	245	PRO	2.2
3	F	120	THR	2.2
3	F	207	HIS	2.2
1	J	216	TYR	2.2
2	E	147	SER	2.2
2	E	165	GLY	2.2
2	E	233	LYS	2.2
1	A	32	HIS	2.2
3	F	210	TYR	2.2
1	G	218	ASN	2.2
2	E	244	GLU	2.2
2	B	123	CYS	2.2
2	K	20	ALA	2.2
1	J	98	ASP	2.2
1	J	68	LEU	2.2
1	A	317	PRO	2.2
2	E	161	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
2	E	245	PRO	2.2
2	K	165	GLY	2.2
1	A	59	GLU	2.1
1	A	322	ASN	2.1
1	D	361	TYR	2.1
3	F	53	TYR	2.1
1	D	124	PHE	2.1
1	J	317	PRO	2.1
1	D	319	LYS	2.1
1	G	49	ILE	2.1
1	J	263	ASP	2.1
3	F	52	TRP	2.1
3	F	147	THR	2.1
1	A	206	GLU	2.1
1	D	148	GLU	2.1
1	G	347	SER	2.1
2	B	159	SER	2.1
1	G	68	LEU	2.1
2	E	173	LEU	2.1
1	A	144	TYR	2.1
1	A	361	TYR	2.1
1	D	268	CYS	2.1
2	K	131	CYS	2.1
1	A	72	GLU	2.1
2	K	247	SER	2.0
1	A	247	ILE	2.0
3	C	24	LEU	2.0
2	E	223	THR	2.0
2	H	165	GLY	2.0
1	A	79	VAL	2.0
2	E	193	SER	2.0
3	C	110	ASP	2.0
1	A	48	CYS	2.0
1	A	64	CYS	2.0
1	J	268	CYS	2.0
1	D	112	GLU	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.