



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:00 PM UTC

PDB ID : 7PI7 / pdb_00007pi7
Title : PfCyRPA bound to monoclonal antibody Cy.002 Fab fragment
Authors : Ragotte, R.J.; Higgins, M.K.
Deposited on : 2021-08-19
Resolution : 2.72 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:

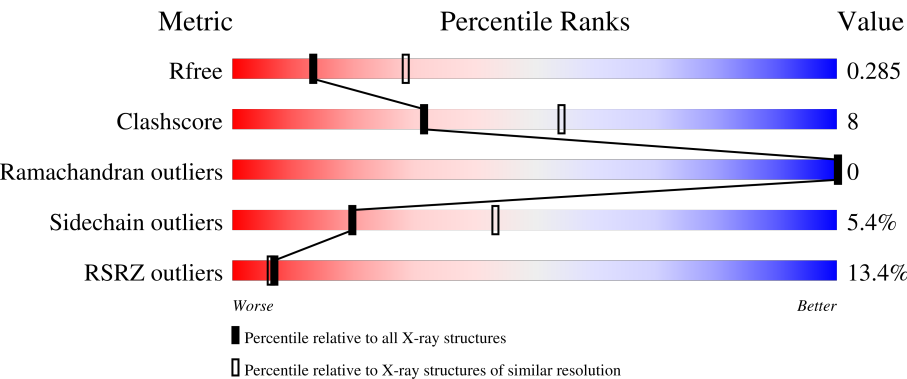
MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
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 2.72 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	
1	D	343	
2	B	221	
2	E	221	
3	C	217	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
			6%	13%
3	F	217		

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11943 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	317	Total	C	N	O	S	0	0	0
			2648	1707	428	500	13			
1	D	317	Total	C	N	O	S	0	0	0
			2651	1707	428	503	13			

There are 24 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
D	369	PRO	-	expression tag	UNP Q8IFM8
D	370	GLU	-	expression tag	UNP Q8IFM8
D	371	ALA	-	expression tag	UNP Q8IFM8

- Molecule 2 is a protein called Monoclonal antibody Cy.002 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	216	Total	C	N	O	S	186	0	0
			1617	1019	266	327	5			
2	E	219	Total	C	N	O	S	372	0	0
			1637	1031	270	331	5			

- Molecule 3 is a protein called Monoclonal antibody Cy.002 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	216	Total	C	N	O	S	0	0	0
			1657	1027	284	341	5			
3	F	216	Total	C	N	O	S	329	0	0
			1657	1027	284	341	5			

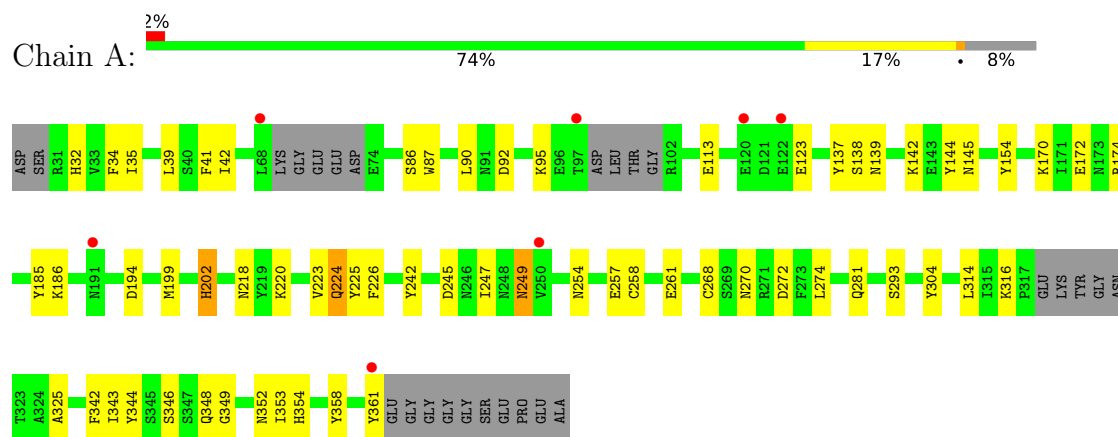
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	20	Total	O	0	0
			20	20		
4	B	9	Total	O	0	0
			9	9		
4	C	19	Total	O	0	0
			19	19		
4	D	20	Total	O	0	0
			20	20		
4	E	3	Total	O	0	0
			3	3		
4	F	5	Total	O	0	0
			5	5		

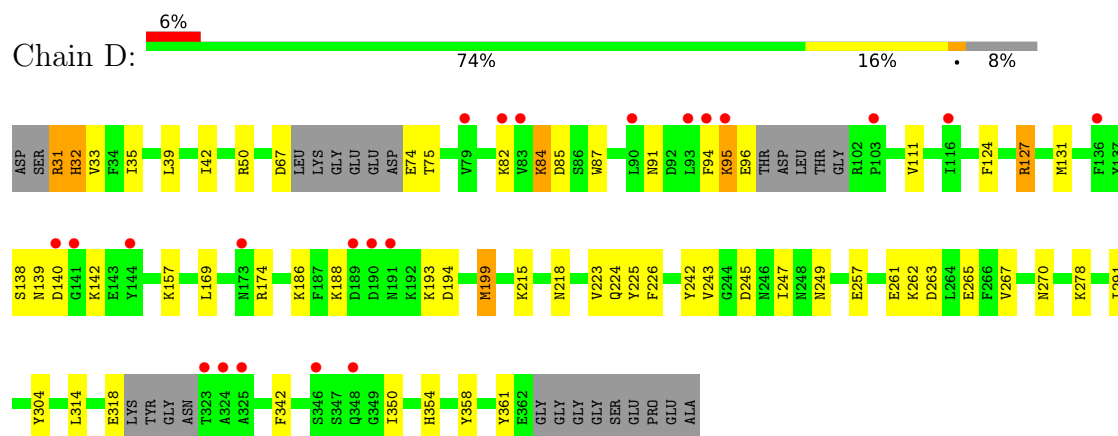
3 Residue-property plots [i](#)

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.

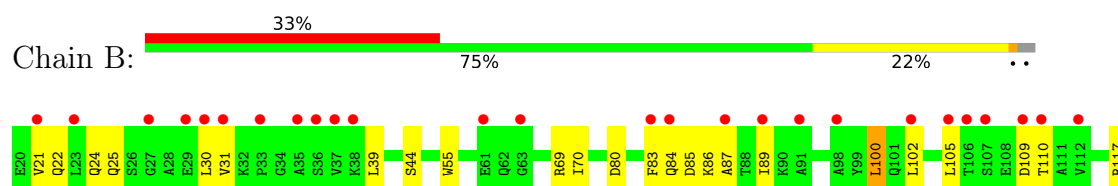
• Molecule 1: Cysteine-rich protective antigen

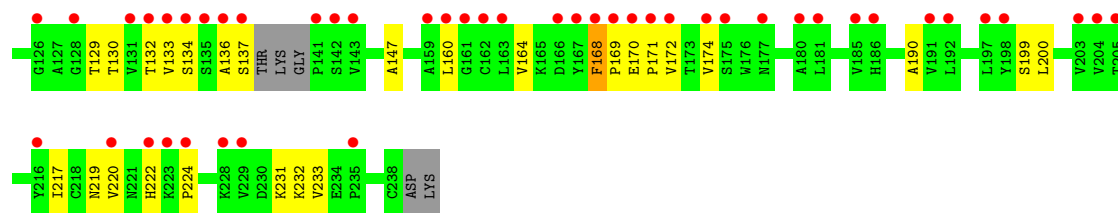


• Molecule 1: Cysteine-rich protective antigen

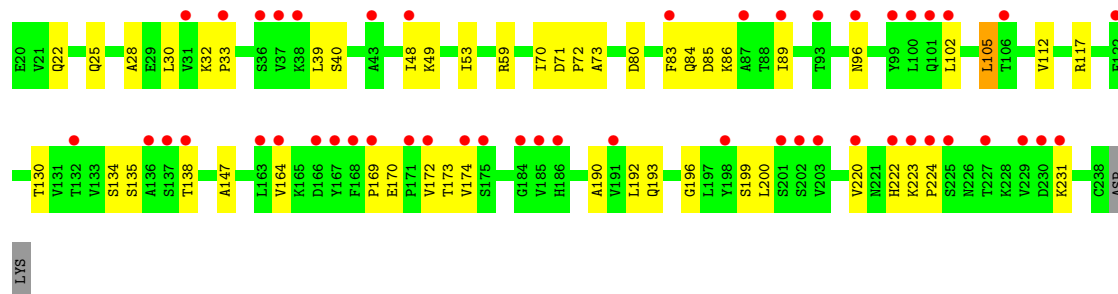
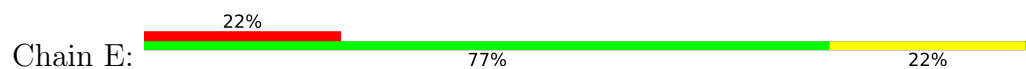


• Molecule 2: Monoclonal antibody Cy.002 heavy chain

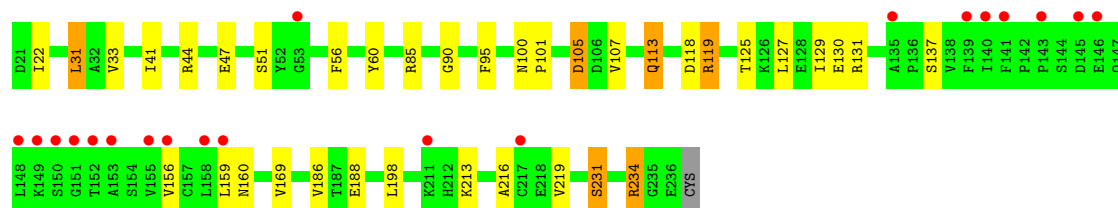
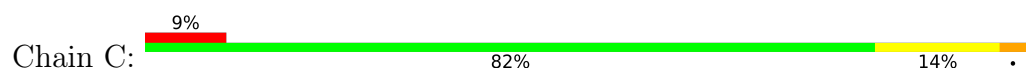




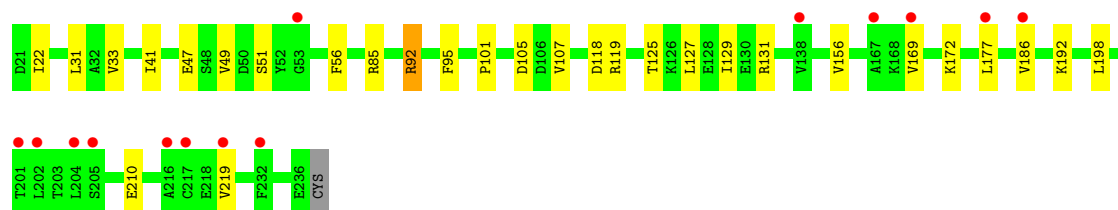
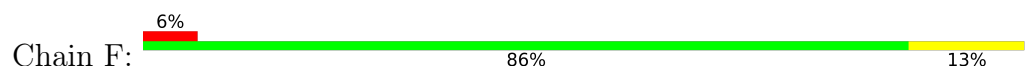
• Molecule 2: Monoclonal antibody Cy.002 heavy chain



• Molecule 3: Monoclonal antibody Cy.002 light chain



• Molecule 3: Monoclonal antibody Cy.002 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	205.05Å 80.69Å 117.36Å 90.00° 108.73° 90.00°	Depositor
Resolution (Å)	37.92 – 2.72 37.92 – 2.72	Depositor EDS
% Data completeness (in resolution range)	99.8 (37.92-2.72) 99.7 (37.92-2.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.72Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-APR-2021)	Depositor
R, R_{free}	0.273 , 0.300 0.259 , 0.285	Depositor DCC
R_{free} test set	2096 reflections (4.28%)	wwPDB-VP
Wilson B-factor (Å ²)	68.2	Xtriage
Anisotropy	0.718	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 84.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11943	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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	0.80	2/2708 (0.1%)	1.08	11/3654 (0.3%)
1	D	0.79	1/2711 (0.0%)	1.08	7/3657 (0.2%)
2	B	0.79	0/1654	1.13	3/2257 (0.1%)
2	E	0.77	0/1675	1.12	5/2287 (0.2%)
3	C	0.75	0/1690	1.01	2/2294 (0.1%)
3	F	0.71	0/1690	1.00	3/2294 (0.1%)
All	All	0.77	3/12128 (0.0%)	1.07	31/16443 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	GLU	CA-C	5.62	1.58	1.52
1	A	325	ALA	CA-C	5.49	1.59	1.52
1	D	199	MET	SD-CE	-5.39	1.66	1.79

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	33	VAL	N-CA-C	6.92	118.56	108.53
1	D	194	ASP	CA-C-N	6.73	129.59	120.38
1	D	194	ASP	C-N-CA	6.73	129.59	120.38
1	A	194	ASP	CA-C-N	6.58	129.39	120.38
1	A	194	ASP	C-N-CA	6.58	129.39	120.38
1	D	85	ASP	CA-CB-CG	6.15	118.75	112.60
2	E	102	LEU	CD1-CG-CD2	6.13	124.29	110.80
1	D	139	ASN	N-CA-C	-6.09	105.89	113.38
1	D	140	ASP	N-CA-C	-6.06	99.75	108.60
3	C	105	ASP	CA-CB-CG	5.95	118.55	112.60
1	A	145	ASN	CA-CB-CG	5.43	118.03	112.60
1	A	34	PHE	CA-CB-CG	5.43	119.23	113.80
3	F	49	VAL	N-CA-CB	-5.39	105.11	112.28
2	B	85	ASP	CA-C-N	5.36	130.80	122.49
2	B	85	ASP	C-N-CA	5.36	130.80	122.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	156	VAL	N-CA-C	5.33	115.53	107.80
1	A	139	ASN	CA-C-N	5.28	129.13	122.16
1	A	139	ASN	C-N-CA	5.28	129.13	122.16
2	E	85	ASP	CA-C-N	5.22	130.58	122.49
2	E	85	ASP	C-N-CA	5.22	130.58	122.49
2	B	147	ALA	N-CA-C	5.21	116.26	109.64
1	A	261	GLU	CA-C-N	5.18	130.87	122.53
1	A	261	GLU	C-N-CA	5.18	130.87	122.53
3	C	156	VAL	N-CA-C	5.18	115.31	107.80
1	A	86	SER	N-CA-C	5.17	117.04	109.24
2	E	71	ASP	N-CA-C	-5.14	98.51	108.59
2	E	147	ALA	N-CA-C	5.11	116.12	109.64
1	D	291	ILE	N-CA-CB	5.08	118.31	111.90
3	F	105	ASP	CA-CB-CG	5.03	117.63	112.60
1	A	249	ASN	CA-C-N	5.01	127.30	120.63
1	A	249	ASN	C-N-CA	5.01	127.30	120.63

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	2648	0	2551	40	0
1	D	2651	0	2545	33	0
2	B	1617	0	1581	37	0
2	E	1637	0	1604	30	0
3	C	1657	0	1595	20	0
3	F	1657	0	1595	18	0
4	A	20	0	0	1	0
4	B	9	0	0	0	0
4	C	19	0	0	0	0
4	D	20	0	0	0	0
4	E	3	0	0	1	0
4	F	5	0	0	0	0
All	All	11943	0	11471	174	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 (174) 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)
2:E:30:LEU:HD13	2:E:169:PRO:HG3	1.27	1.13
2:B:30:LEU:HD23	2:B:224:PRO:O	1.54	1.07
2:B:102:LEU:HB3	2:B:105:LEU:HD21	1.44	0.96
1:A:220:LYS:HB2	1:A:223:VAL:HG11	1.44	0.95
1:A:348:GLN:HG3	1:A:349:GLY:N	1.79	0.94
1:D:261:GLU:HG3	1:D:267:VAL:HG12	1.53	0.89
1:A:92:ASP:O	1:A:95:LYS:HG3	1.73	0.88
1:A:348:GLN:HG3	1:A:349:GLY:H	1.38	0.85
1:A:220:LYS:HB2	1:A:223:VAL:CG1	2.07	0.85
1:A:348:GLN:CG	1:A:349:GLY:H	1.92	0.82
1:A:220:LYS:CB	1:A:223:VAL:CG1	2.58	0.82
1:A:154:TYR:HB2	1:A:199:MET:HE1	1.62	0.82
2:B:164:VAL:HG11	2:B:172:VAL:HG21	1.62	0.81
2:E:30:LEU:HB2	2:E:224:PRO:HB3	1.62	0.81
2:B:132:THR:HG21	2:B:171:PRO:HD3	1.64	0.80
1:A:348:GLN:CG	1:A:349:GLY:N	2.45	0.80
1:D:82:LYS:NZ	1:D:84:LYS:HZ2	1.79	0.80
2:B:70:ILE:HB	2:B:89:ILE:HG22	1.65	0.79
2:B:55:TRP:CD1	2:B:89:ILE:HD12	2.22	0.73
1:A:41:PHE:HE1	1:A:352:ASN:OD1	1.73	0.71
2:B:70:ILE:HB	2:B:89:ILE:CG2	2.20	0.71
2:B:21:VAL:O	2:B:22:GLN:HG3	1.90	0.71
2:E:48:ILE:HG12	2:E:72:PRO:HG2	1.74	0.69
2:E:49:LYS:HG3	2:E:73:ALA:HA	1.74	0.69
3:C:216:ALA:HB2	3:C:231:SER:HB3	1.75	0.69
1:A:314:LEU:HD21	1:A:316:LYS:HE3	1.76	0.68
2:E:84:GLN:HB2	2:E:86:LYS:NZ	2.09	0.68
3:F:172:LYS:HE3	3:F:177:LEU:HD21	1.77	0.67
2:B:84:GLN:HB2	2:B:86:LYS:NZ	2.10	0.67
1:D:82:LYS:NZ	1:D:84:LYS:NZ	2.42	0.67
2:E:70:ILE:HB	2:E:89:ILE:HG22	1.77	0.67
2:B:217:ILE:HG12	2:B:232:LYS:HA	1.78	0.66
1:A:344:TYR:CE2	1:A:352:ASN:ND2	2.65	0.65
1:D:261:GLU:HG3	1:D:267:VAL:CG1	2.25	0.65
1:A:220:LYS:HB3	1:A:223:VAL:CG1	2.26	0.64
2:B:39:LEU:HD22	2:B:129:THR:HG21	1.81	0.63
1:A:220:LYS:CB	1:A:223:VAL:HG11	2.19	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:192:LEU:HD21	2:E:196:GLY:HA2	1.80	0.62
3:F:92:ARG:O	3:F:95:PHE:CE1	2.53	0.62
3:C:213:LYS:HA	3:C:234:ARG:HG2	1.82	0.62
2:B:22:GLN:HB2	2:B:44:SER:HB2	1.82	0.62
1:D:131:MET:CE	1:D:199:MET:HE1	2.30	0.60
1:A:281:GLN:NE2	1:A:293:SER:OG	2.33	0.60
1:D:31:ARG:HE	1:D:32:HIS:H	1.49	0.59
1:D:142:LYS:O	1:D:142:LYS:HG2	2.02	0.59
1:D:124:PHE:HA	1:D:127:ARG:HD2	1.84	0.59
1:A:218:ASN:HB2	1:A:225:TYR:OH	2.02	0.59
1:D:218:ASN:HB2	1:D:225:TYR:OH	2.03	0.59
2:B:30:LEU:HD23	2:B:224:PRO:C	2.26	0.58
1:D:74:GLU:HA	1:D:96:GLU:HG3	1.84	0.58
1:A:245:ASP:O	3:C:119:ARG:NH2	2.36	0.58
2:E:112:VAL:HG22	2:E:130:THR:OG1	2.03	0.58
3:F:107:VAL:HG22	3:F:129:ILE:HG12	1.86	0.57
1:D:262:LYS:HB2	1:D:265:GLU:HB3	1.86	0.57
1:A:226:PHE:HB2	1:A:242:TYR:HB2	1.86	0.57
2:E:192:LEU:HD23	2:E:193:GLN:O	2.05	0.57
1:D:223:VAL:HG22	1:D:224:GLN:O	2.04	0.57
1:D:226:PHE:HB2	1:D:242:TYR:HB2	1.86	0.56
3:C:107:VAL:HG22	3:C:129:ILE:HG12	1.87	0.56
2:B:21:VAL:C	2:B:22:GLN:HG3	2.32	0.54
2:E:30:LEU:HB2	2:E:224:PRO:CB	2.36	0.54
2:B:84:GLN:HB2	2:B:86:LYS:HZ2	1.70	0.54
2:B:80:ASP:O	2:B:83:PHE:O	2.26	0.54
1:D:42:ILE:HG22	1:D:87:TRP:CD1	2.43	0.54
1:A:42:ILE:HG22	1:A:87:TRP:CD1	2.43	0.54
3:F:85:ARG:HD2	3:F:101:PRO:O	2.08	0.53
3:F:172:LYS:CG	3:F:177:LEU:HD23	2.39	0.53
3:C:60:TYR:OH	3:C:113:GLN:NE2	2.41	0.53
2:E:80:ASP:O	2:E:83:PHE:O	2.26	0.53
3:C:137:SER:HB2	3:C:160:ASN:HB3	1.91	0.53
2:B:21:VAL:O	2:B:22:GLN:CG	2.54	0.53
3:C:85:ARG:HD2	3:C:101:PRO:O	2.09	0.53
2:B:169:PRO:HD2	2:B:222:HIS:HE1	1.73	0.52
2:E:84:GLN:HB2	2:E:86:LYS:HZ2	1.73	0.52
3:F:92:ARG:O	3:F:95:PHE:HE1	1.91	0.52
3:F:172:LYS:CE	3:F:177:LEU:HD21	2.39	0.52
3:C:169:VAL:HG22	3:C:219:VAL:HG22	1.92	0.52
2:B:169:PRO:HD2	2:B:222:HIS:CE1	2.45	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LYS:HZ3	1:D:84:LYS:HZ2	1.57	0.52
2:E:30:LEU:CD2	2:E:138:THR:HG23	2.40	0.52
1:A:174:ARG:HD3	1:A:202:HIS:HD2	1.75	0.51
1:D:261:GLU:CG	1:D:267:VAL:HG12	2.34	0.51
1:D:245:ASP:O	3:F:119:ARG:NH2	2.44	0.51
1:D:42:ILE:CG2	1:D:87:TRP:CD1	2.94	0.51
2:B:160:LEU:HB2	2:B:233:VAL:HG11	1.92	0.51
2:E:32:LYS:HE3	2:E:135:SER:O	2.11	0.51
3:F:172:LYS:CE	3:F:177:LEU:CD2	2.88	0.51
1:A:224:GLN:HG2	1:A:226:PHE:CZ	2.47	0.50
1:A:343:ILE:HG12	1:A:353:ILE:HG13	1.94	0.50
2:E:33:PRO:HD3	2:E:134:SER:O	2.11	0.50
1:A:42:ILE:CG2	1:A:87:TRP:CD1	2.94	0.49
2:B:130:THR:CG2	2:B:171:PRO:HG3	2.42	0.49
3:F:169:VAL:HG22	3:F:219:VAL:HG22	1.93	0.49
2:E:28:ALA:HB3	2:E:223:LYS:HB2	1.93	0.49
2:E:70:ILE:HB	2:E:89:ILE:CG2	2.42	0.49
1:A:123:GLU:HB3	4:A:413:HOH:O	2.13	0.49
2:B:171:PRO:O	2:B:222:HIS:HD2	1.95	0.48
2:E:190:ALA:HB2	2:E:200:LEU:HD23	1.95	0.48
2:E:84:GLN:HB2	2:E:86:LYS:HZ3	1.77	0.48
1:A:224:GLN:HG3	1:A:225:TYR:N	2.28	0.48
1:A:220:LYS:HB3	1:A:223:VAL:HG13	1.93	0.47
2:B:171:PRO:HD2	2:B:224:PRO:HG2	1.96	0.47
3:F:41:ILE:HG12	3:F:125:THR:HG21	1.96	0.47
2:B:30:LEU:HD12	2:B:30:LEU:C	2.38	0.47
1:D:75:THR:HB	1:D:96:GLU:HA	1.97	0.47
2:B:31:VAL:O	2:B:31:VAL:HG23	2.15	0.47
1:D:31:ARG:NE	1:D:32:HIS:H	2.12	0.47
1:A:32:HIS:HB2	1:A:361:TYR:CD2	2.50	0.46
2:B:31:VAL:O	2:B:133:VAL:HA	2.14	0.46
2:B:190:ALA:HB2	2:B:200:LEU:HD23	1.96	0.46
2:E:164:VAL:O	2:E:199:SER:HA	2.16	0.46
3:F:172:LYS:HE2	3:F:177:LEU:CD2	2.46	0.46
3:C:159:LEU:HD11	3:C:219:VAL:CG2	2.46	0.45
1:A:185:TYR:CE1	1:A:224:GLN:HB2	2.52	0.45
1:D:247:ILE:HD13	3:F:118:ASP:HA	1.99	0.45
2:E:105:LEU:H	2:E:105:LEU:HD22	1.82	0.45
3:C:41:ILE:HG12	3:C:125:THR:HG21	1.98	0.45
1:A:138:SER:HB2	1:A:144:TYR:CD2	2.52	0.45
2:B:174:VAL:HG13	2:B:220:VAL:HG22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:LYS:CB	1:A:223:VAL:HG13	2.41	0.44
2:B:164:VAL:O	2:B:199:SER:HA	2.17	0.44
1:A:247:ILE:HD13	3:C:118:ASP:HA	2.00	0.44
1:D:223:VAL:HG21	1:D:243:VAL:HB	2.00	0.44
1:A:39:LEU:HD13	1:A:354:HIS:CE1	2.52	0.44
3:C:22:ILE:HG12	3:C:47:GLU:HB2	1.99	0.44
1:D:31:ARG:HE	1:D:32:HIS:N	2.13	0.44
1:D:304:TYR:CE2	1:D:314:LEU:HD13	2.53	0.44
2:E:84:GLN:H	2:E:86:LYS:NZ	2.16	0.44
2:B:84:GLN:H	2:B:86:LYS:NZ	2.16	0.43
1:D:39:LEU:HD13	1:D:354:HIS:CE1	2.53	0.43
1:D:82:LYS:HZ1	1:D:84:LYS:HZ2	1.60	0.43
2:B:87:ALA:HB1	2:B:100:LEU:HD21	2.00	0.43
1:A:304:TYR:CE2	1:A:314:LEU:HD13	2.53	0.43
1:D:223:VAL:HG22	1:D:224:GLN:N	2.34	0.43
2:E:190:ALA:HA	2:E:200:LEU:HB3	2.01	0.43
1:A:342:PHE:HB3	1:A:354:HIS:HB2	2.01	0.43
1:D:95:LYS:HD2	1:D:95:LYS:HA	1.56	0.43
2:E:48:ILE:HG22	2:E:96:ASN:OD1	2.19	0.43
3:F:22:ILE:HG12	3:F:47:GLU:HB2	1.99	0.43
2:B:134:SER:HB3	2:B:169:PRO:HG3	2.01	0.43
3:C:159:LEU:HD11	3:C:219:VAL:HG22	2.01	0.43
1:D:188:LYS:HE2	4:E:301:HOH:O	2.19	0.43
3:C:33:VAL:HG22	3:C:127:LEU:HD11	2.01	0.43
2:E:174:VAL:HG22	2:E:220:VAL:HG22	2.01	0.43
3:F:107:VAL:CG2	3:F:129:ILE:HG12	2.48	0.43
1:A:90:LEU:HD22	1:A:142:LYS:HG2	2.00	0.43
2:B:105:LEU:HD22	2:B:109:ASP:HB3	2.00	0.42
3:C:186:VAL:HG22	3:C:198:LEU:HD12	2.00	0.42
2:B:190:ALA:HA	2:B:200:LEU:HB3	2.01	0.42
1:A:35:ILE:HG12	1:A:358:TYR:HD1	1.85	0.42
3:F:51:SER:HB3	3:F:56:PHE:HE2	1.85	0.42
3:C:31:LEU:HD22	3:C:33:VAL:HG13	2.02	0.42
3:F:186:VAL:HG22	3:F:198:LEU:HD12	2.01	0.42
3:C:100:ASN:HA	3:C:101:PRO:HA	1.90	0.42
2:E:28:ALA:H	2:E:223:LYS:HD2	1.84	0.42
2:B:84:GLN:HB2	2:B:86:LYS:HZ3	1.81	0.42
1:D:82:LYS:HZ1	1:D:84:LYS:NZ	2.18	0.42
1:A:41:PHE:CE1	1:A:352:ASN:OD1	2.64	0.41
1:D:35:ILE:HG12	1:D:358:TYR:HD1	1.85	0.41
3:F:33:VAL:HG22	3:F:127:LEU:HD11	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:48:ILE:CD1	2:E:53:ILE:HG13	2.51	0.41
2:E:48:ILE:HD11	2:E:53:ILE:HG13	2.02	0.41
2:B:55:TRP:HD1	2:B:89:ILE:HD12	1.81	0.41
3:C:107:VAL:CG2	3:C:129:ILE:HG12	2.49	0.41
3:C:90:GLY:HA3	3:C:95:PHE:CD2	2.56	0.41
1:D:342:PHE:HB3	1:D:354:HIS:HB2	2.02	0.41
2:E:49:LYS:HG3	2:E:73:ALA:CA	2.48	0.41
1:A:272:ASP:OD2	1:A:274:LEU:HD12	2.21	0.40
1:A:174:ARG:NH2	1:A:202:HIS:NE2	2.69	0.40
1:D:127:ARG:NH1	1:D:157:LYS:O	2.51	0.40
2:E:169:PRO:HG2	2:E:222:HIS:NE2	2.36	0.40
2:B:136:ALA:HB3	2:B:168:PHE:CD1	2.56	0.40
1:A:113:GLU:HG2	1:A:137:TYR:OH	2.21	0.40
3:C:51:SER:HB3	3:C:56:PHE:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	309/343 (90%)	291 (94%)	18 (6%)	0	100	100
1	D	309/343 (90%)	286 (93%)	23 (7%)	0	100	100
2	B	212/221 (96%)	184 (87%)	28 (13%)	0	100	100
2	E	217/221 (98%)	194 (89%)	23 (11%)	0	100	100
3	C	214/217 (99%)	210 (98%)	4 (2%)	0	100	100
3	F	214/217 (99%)	209 (98%)	5 (2%)	0	100	100
All	All	1475/1562 (94%)	1374 (93%)	101 (7%)	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	298/316 (94%)	287 (96%)	11 (4%)	30	57
1	D	298/316 (94%)	274 (92%)	24 (8%)	11	26
2	B	185/189 (98%)	174 (94%)	11 (6%)	18	40
2	E	187/189 (99%)	176 (94%)	11 (6%)	18	40
3	C	188/189 (100%)	178 (95%)	10 (5%)	20	44
3	F	188/189 (100%)	183 (97%)	5 (3%)	39	68
All	All	1344/1388 (97%)	1272 (95%)	72 (5%)	20	43

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	170	LYS
1	A	186	LYS
1	A	202	HIS
1	A	224	GLN
1	A	249	ASN
1	A	254	ASN
1	A	257	GLU
1	A	258	CYS
1	A	268	CYS
1	A	270	ASN
1	A	346	SER
2	B	24	GLN
2	B	25	GLN
2	B	69	ARG
2	B	100	LEU
2	B	110	THR
2	B	117	ARG
2	B	137	SER
2	B	168	PHE
2	B	170	GLU
2	B	219	ASN
2	B	231	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	31	LEU
3	C	44	ARG
3	C	105	ASP
3	C	113	GLN
3	C	119	ARG
3	C	130	GLU
3	C	131	ARG
3	C	188	GLU
3	C	231	SER
3	C	234	ARG
1	D	31	ARG
1	D	32	HIS
1	D	50	ARG
1	D	67	ASP
1	D	84	LYS
1	D	91	ASN
1	D	94	PHE
1	D	95	LYS
1	D	111	VAL
1	D	127	ARG
1	D	138	SER
1	D	169	LEU
1	D	174	ARG
1	D	186	LYS
1	D	193	LYS
1	D	215	LYS
1	D	249	ASN
1	D	257	GLU
1	D	263	ASP
1	D	270	ASN
1	D	278	LYS
1	D	318	GLU
1	D	350	ILE
1	D	361	TYR
2	E	22	GLN
2	E	25	GLN
2	E	39	LEU
2	E	40	SER
2	E	59	ARG
2	E	105	LEU
2	E	117	ARG
2	E	170	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	172	VAL
2	E	173	THR
2	E	231	LYS
3	F	31	LEU
3	F	92	ARG
3	F	131	ARG
3	F	192	LYS
3	F	210	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	ASN
1	A	191	ASN
1	A	224	GLN
1	A	281	GLN
1	A	311	ASN
1	A	348	GLN
1	A	352	ASN
2	B	193	GLN
2	B	222	HIS
2	B	226	ASN
3	C	113	GLN
3	C	147	GLN
3	C	170	GLN
1	D	62	ASN
1	D	91	ASN
1	D	139	ASN
1	D	146	ASN
1	D	173	ASN
1	D	224	GLN
1	D	254	ASN
1	D	270	ASN
2	E	193	GLN
2	E	221	ASN
3	F	62	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	317/343 (92%)	0.40	7 (2%) 62 59	44, 72, 108, 134	0
1	D	317/343 (92%)	0.67	22 (6%) 23 20	44, 81, 132, 155	0
2	B	188/221 (85%)	1.81	72 (38%) 1 0	52, 120, 149, 158	0
2	E	165/221 (74%)	1.65	49 (29%) 1 1	55, 117, 182, 207	0
3	C	216/217 (99%)	0.59	20 (9%) 14 12	46, 82, 172, 224	0
3	F	174/217 (80%)	0.62	14 (8%) 18 16	47, 77, 174, 219	0
All	All	1377/1562 (88%)	0.86	184 (13%) 7 6	44, 85, 158, 224	0

All (184) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	169	PRO	6.1
2	E	203	VAL	6.1
2	E	220	VAL	5.3
2	B	36	SER	5.2
2	B	168	PHE	5.2
2	B	159	ALA	5.0
2	E	185	VAL	4.8
2	E	164	VAL	4.8
2	E	174	VAL	4.7
2	E	171	PRO	4.6
2	E	168	PHE	4.5
2	E	229	VAL	4.5
2	B	143	VAL	4.5
2	E	163	LEU	4.4
2	B	181	LEU	4.2
2	E	169	PRO	4.1
1	D	191	ASN	4.1
2	B	204	VAL	4.1
1	D	141	GLY	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	166	ASP	4.0
2	B	160	LEU	3.9
3	F	202	LEU	3.9
2	B	37	VAL	3.9
2	B	141	PRO	3.9
2	B	216	TYR	3.8
2	E	231	LYS	3.8
2	E	137	SER	3.8
2	E	225	SER	3.8
2	B	133	VAL	3.8
2	B	170	GLU	3.7
2	B	203	VAL	3.7
1	D	144	TYR	3.6
2	B	126	GLY	3.5
2	B	137	SER	3.5
2	B	162	CYS	3.5
2	E	101	GLN	3.5
1	D	93	LEU	3.5
2	B	142	SER	3.4
3	F	232	PHE	3.4
2	E	36	SER	3.4
2	E	201	SER	3.4
2	E	184	GLY	3.3
2	B	229	VAL	3.3
2	E	202	SER	3.3
2	B	161	GLY	3.3
1	A	97	THR	3.3
2	B	135	SER	3.3
2	B	205	THR	3.3
2	B	102	LEU	3.2
2	E	138	THR	3.2
2	B	132	THR	3.1
3	C	152	THR	3.1
2	E	37	VAL	3.1
1	D	95	LYS	3.1
2	B	105	LEU	3.1
3	F	138	VAL	3.1
2	B	131	VAL	3.1
3	C	158	LEU	3.1
2	B	167	TYR	3.0
2	B	180	ALA	3.0
1	D	346	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	89	ILE	3.0
2	E	31	VAL	3.0
1	A	68	LEU	2.9
2	B	192	LEU	2.9
2	B	222	HIS	2.9
2	E	167	TYR	2.9
1	D	324	ALA	2.9
2	E	102	LEU	2.9
2	B	185	VAL	2.9
3	C	150	SER	2.9
2	E	136	ALA	2.9
3	F	204	LEU	2.9
2	B	171	PRO	2.8
2	B	89	ILE	2.8
2	B	220	VAL	2.8
3	F	219	VAL	2.8
2	B	106	THR	2.8
2	E	224	PRO	2.7
2	B	163	LEU	2.7
2	B	29	GLU	2.7
2	B	174	VAL	2.7
1	A	122	GLU	2.7
1	D	83	VAL	2.7
2	E	83	PHE	2.7
3	C	145	ASP	2.7
2	B	87	ALA	2.7
2	B	191	VAL	2.7
1	D	190	ASP	2.7
2	B	134	SER	2.7
3	F	205	SER	2.7
2	B	91	ALA	2.7
2	E	87	ALA	2.7
3	C	143	PRO	2.7
2	B	84	GLN	2.6
3	C	141	PHE	2.6
2	E	222	HIS	2.6
2	B	83	PHE	2.6
2	E	33	PRO	2.6
2	B	31	VAL	2.6
2	B	136	ALA	2.6
2	E	93	THR	2.6
2	E	227	THR	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	230	ASP	2.6
2	E	100	LEU	2.6
1	D	94	PHE	2.6
2	B	30	LEU	2.5
2	B	197	LEU	2.5
2	E	198	TYR	2.5
2	E	48	ILE	2.5
3	C	159	LEU	2.5
1	D	116	ILE	2.5
3	C	140	ILE	2.5
2	B	224	PRO	2.5
2	B	109	ASP	2.4
1	A	250	VAL	2.4
2	E	172	VAL	2.4
3	F	216	ALA	2.4
2	E	186	HIS	2.4
1	D	189	ASP	2.4
3	C	146	GLU	2.4
1	A	361	TYR	2.3
2	B	186	HIS	2.3
2	E	38	LYS	2.3
1	D	323	THR	2.3
2	B	175	SER	2.3
1	D	103	PRO	2.3
1	D	79	VAL	2.3
2	B	21	VAL	2.3
3	C	155	VAL	2.3
1	D	136	PHE	2.3
3	F	177	LEU	2.3
2	B	110	THR	2.3
2	B	198	TYR	2.3
3	C	151	GLY	2.3
2	B	172	VAL	2.3
2	B	23	LEU	2.3
2	E	106	THR	2.3
2	B	235	PRO	2.3
2	E	175	SER	2.3
2	B	112	VAL	2.3
3	F	217	CYS	2.2
2	E	223	LYS	2.2
2	B	177	ASN	2.2
3	C	148	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	82	LYS	2.2
2	E	191	VAL	2.2
2	B	61	GLU	2.2
2	E	99	TYR	2.2
2	B	228	LYS	2.2
2	E	166	ASP	2.2
3	F	53	GLY	2.2
3	F	169	VAL	2.2
1	D	325	ALA	2.1
2	B	98	ALA	2.1
1	A	120	GLU	2.1
1	D	173	ASN	2.1
2	B	128	GLY	2.1
3	C	135	ALA	2.1
3	C	211	LYS	2.1
1	D	140	ASP	2.1
3	C	156	VAL	2.1
2	E	122	PHE	2.1
3	C	153	ALA	2.1
3	F	201	THR	2.1
1	A	191	ASN	2.1
2	B	35	ALA	2.1
2	E	43	ALA	2.1
3	F	167	ALA	2.1
3	C	149	LYS	2.1
2	E	132	THR	2.1
2	B	33	PRO	2.1
3	C	139	PHE	2.1
2	B	38	LYS	2.0
2	B	223	LYS	2.0
2	E	96	ASN	2.0
3	C	217	CYS	2.0
2	B	107	SER	2.0
1	D	90	LEU	2.0
1	D	348	GLN	2.0
2	B	27	GLY	2.0
2	B	63	GLY	2.0
3	C	53	GLY	2.0
3	F	186	VAL	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.