

# Full wwPDB X-ray Structure Validation Report (i)

#### Feb 1, 2022 – 03:12 pm GMT

PDB ID	:	7PI7
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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity		4 02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.26
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber $(2001)$
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.26

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY\;DIFFRACTION$ 

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
$R_{free}$	130704	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622(2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (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 <=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	
			4%	
1	А	343	77%	15% • 8%
			9%	
1	D	343	78%	13% • 8%
			27%	
2	В	221	76%	21% ••
			23%	
2	Ε	221	78%	20% ••
			17%	
3	С	217	83%	14% •



Mol	Chain	Length	Quality of chain	
			15%	
3	F	217	88%	11%



## 2 Entry composition (i)

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.

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
1	Λ	217	Total	С	Ν	Ο	$\mathbf{S}$	0	0	0
1	Л	517	2648	1707	428	500	13	0	0	0
1	Л	317	Total	С	Ν	0	S	0	0	0
1	I D		2651	1707	428	503	13	0	0	0

• Molecule 1 is a protein called Cysteine-rich protective antigen.

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

There are 24 discrepancies between the modelled and reference sequences:



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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	В	216	Total	С	Ν	0	$\mathbf{S}$	186	0	0
	D	210	1617	1019	266	327	5	100	0	0
0	F	210	Total	С	Ν	0	S	372	0	0
		219	1637	1031	270	331	5		0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	216	Total	С	Ν	0	S	0	0	0
J		210	1657	1027	284	341	5	0	0	0
2	Б	216	Total	С	Ν	0	S	220	0	0
J	3 F		1657	1027	284	341	5	329	0	0

• Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	20	TotalO2020	0	0
4	В	9	Total O 9 9	0	0
4	С	19	Total O 19 19	0	0
4	D	20	TotalO2020	0	0
4	Е	3	Total O 3 3	0	0
4	F	5	$\begin{array}{cc} \text{Total} & \text{O} \\ 5 & 5 \end{array}$	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



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• Molecule 2: Monoclonal antibody Cy.002 heavy chain







• Molecule 2: Monoclonal antibody Cy.002 heavy chain





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants	205.05Å 80.69Å 117.36Å	Dopositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $108.73^{\circ}$ $90.00^{\circ}$	Depositor
Bosolution(A)	37.92 - 2.72	Depositor
Resolution (A)	37.92 - 2.72	EDS
% Data completeness	99.8 (37.92-2.72)	Depositor
(in resolution range)	99.8 (37.92-2.72)	EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.79 (at 2.72 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.4 (20-APR-2021)	Depositor
B B.	0.273 , $0.300$	Depositor
II, II, <i>free</i>	0.260 , $0.285$	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 $k_{sol}(e/A^3)$ , $B_{sol}(A^2)$	(Not available), (Not available)	EDS
L-test for $twinning^2$	$ < L >=0.51, < L^2>=0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	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.

<sup>&</sup>lt;sup>2</sup>Theoretical 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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 5 Model quality (i)

## 5.1 Standard geometry (i)

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		
	Ullaill	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.47	0/2708	0.67	0/3654	
1	D	0.47	0/2711	0.68	0/3657	
2	В	0.45	0/1654	0.67	0/2257	
2	Е	0.43	0/1675	0.68	0/2287	
3	С	0.42	0/1690	0.61	0/2294	
3	F	0.38	0/1690	0.60	0/2294	
All	All	0.44	0/12128	0.66	0/16443	

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts (i)

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	А	2648	0	2551	40	0
1	D	2651	0	2545	30	0
2	В	1617	0	1581	37	0
2	Е	1637	0	1604	30	0
3	С	1657	0	1595	20	0
3	F	1657	0	1595	18	0
4	А	20	0	0	1	0
4	В	9	0	0	0	0
4	С	19	0	0	0	0
4	D	20	0	0	0	0



Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	Е	3	0	0	1	0
4	F	5	0	0	0	0
All	All	11943	0	11471	171	0

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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 (171) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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
1:A:348:GLN:HG3	1:A:349:GLY:N	1.79	0.97
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: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
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



Interatomic Clash				
Atom-1	Atom-2	distance (Å)	overlap (Å)	
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	
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: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	
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:A:154:TYR:HB2	1:A:199:MET:HE1	1.87	0.56	
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: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:D:82:LYS:HZ1	1:D:84:LYS:HZ2	1.54	0.54	
1:A:42:ILE:HG22	1:A:87:TRP:CD1	2.43	0.54	
2:B:30:LEU:HD23	2:B:224:PRO:C	2.26	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	



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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:B:21:VAL:C	2:B:22:GLN:HG3	2.32	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
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



	to as pagem	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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
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
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:30:LEU:HD12	2:B:30:LEU:C	2.38	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



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (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	Perce	entiles
1	А	309/343~(90%)	291 (94%)	18 (6%)	0	100	100
1	D	309/343~(90%)	286~(93%)	23 (7%)	0	100	100
2	В	212/221~(96%)	184 (87%)	28 (13%)	0	100	100
2	Ε	217/221~(98%)	194 (89%)	23 (11%)	0	100	100
3	С	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 (i)

In the following table, the Percentiles column shows the percent side chain 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	Perce	ntiles
1	А	298/316~(94%)	288~(97%)	10 (3%)	37	65
1	D	298/316~(94%)	280 (94%)	18 (6%)	19	40
2	В	185/189~(98%)	175~(95%)	10 (5%)	22	45
2	Ε	187/189~(99%)	174 (93%)	13 (7%)	15	34
3	С	188/189~(100%)	180 (96%)	8 (4%)	29	55
3	F	188/189 (100%)	186 (99%)	2(1%)	73	89
All	All	1344/1388~(97%)	1283 (96%)	61 (4%)	27	53

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	202	HIS
1	А	224	GLN
1	А	249	ASN
1	А	257	GLU
1	А	258	CYS
1	А	268	CYS
1	A	270	ASN
1	А	311	ASN
1	А	346	SER
1	А	361	TYR
2	В	24	GLN
2	В	25	GLN
2	В	69	ARG
2	В	96	ASN
2	В	100	LEU
2	В	117	ARG
2	В	137	SER
2	В	168	PHE
2	В	219	ASN



Mol	Chain	Res	Type
2	В	231	LYS
3	С	31	LEU
3	C	44	ARG
3	C	105	ASP
3	C	113	GLN
3	C	131	ARG
3	C	188	GLU
3	С	231	SER
3	С	234	ARG
1	D	31	ARG
1	D	32	HIS
1	D	50	ARG
1	D	67	ASP
1	D	91	ASN
1	D	94	PHE
1	D	95	LYS
1	D	127	ARG
1	D	138	SER
1	D	169	LEU
1	D	174	ARG
1	D	193	LYS
1	D	249	ASN
1	D	257	GLU
1	D	263	ASP
1	D	270	ASN
1	D	278	LYS
1	D	361	TYR
2	Е	22	GLN
2	Е	25	GLN
2	Е	39	LEU
2	Е	40	SER
2	Е	59	ARG
2	Е	69	ARG
2	Е	96	ASN
2	Е	105	LEU
2	Е	117	ARG
2	Е	170	GLU
2	Е	172	VAL
2	Е	173	THR
2	Е	231	LYS
3	F	31	LEU
3	F	131	ARG

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Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	146	ASN
1	А	191	ASN
1	А	281	GLN
1	А	287	ASN
1	А	338	ASN
1	А	348	GLN
1	А	352	ASN
2	В	24	GLN
2	В	222	HIS
2	В	226	ASN
3	С	100	ASN
3	С	113	GLN
3	С	170	GLN
1	D	173	ASN
1	D	224	GLN

#### 5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

#### 5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

There are no ligands in this entry.

#### 5.7 Other polymers (i)

There are no such residues in this entry.



## 5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.



## 6 Fit of model and data (i)

### 6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median,  $95^{th}$  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	< <b>RSRZ</b> >	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	317/343~(92%)	0.50	15 (4%) 31 30	44, 72, 108, 134	0
1	D	317/343~(92%)	0.78	31 (9%) 7 6	44, 81, 132, 155	0
2	В	188/221 (85%)	1.82	60 (31%) 0 0	52, 120, 149, 158	0
2	Е	$165/221 \ (74\%)$	1.64	50 (30%) 0 0	55, 117, 182, 207	0
3	С	216/217~(99%)	0.85	36 (16%) 1 1	46, 82, 172, 224	0
3	F	174/217~(80%)	0.87	33 (18%) 1 1	47, 77, 174, 219	0
All	All	1377/1562~(88%)	0.98	225 (16%) 1 1	44, 85, 158, 224	0

All (225) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	159	ALA	10.6
2	В	168	PHE	8.8
2	В	181	LEU	8.4
3	F	217	CYS	7.3
2	В	36	SER	7.3
2	Е	185	VAL	7.3
2	В	160	LEU	6.9
2	В	169	PRO	6.8
3	F	219	VAL	6.8
3	F	202	LEU	6.7
3	С	150	SER	6.6
2	В	216	TYR	6.6
2	В	84	GLN	6.6
2	Е	175	SER	6.4
2	В	204	VAL	6.2
2	В	182	THR	6.0
3	F	232	PHE	5.8
3	С	159	LEU	5.6
1	D	191	ASN	5.5



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Mol	Chain	Res	Type	RSRZ
3	F	204	LEU	5.5
2	Е	136	ALA	5.4
1	А	191	ASN	5.4
2	Е	220	VAL	5.3
2	Е	168	PHE	5.2
2	Е	163	LEU	5.2
3	F	216	ALA	5.1
2	Е	164	VAL	5.1
2	В	166	ASP	5.1
2	Е	229	VAL	5.1
3	F	231	SER	4.9
3	С	143	PRO	4.8
1	А	361	TYR	4.8
3	С	211	LYS	4.8
1	А	31	ARG	4.7
2	В	192	LEU	4.7
2	Е	134	SER	4.7
1	D	75	THR	4.6
2	Е	105	LEU	4.6
2	Е	225	SER	4.6
2	Е	174	VAL	4.5
2	Е	166	ASP	4.5
3	F	138	VAL	4.4
2	Е	170	GLU	4.4
2	В	205	THR	4.3
2	Е	192	LEU	4.3
2	В	233	VAL	4.3
2	В	197	LEU	4.3
2	Е	137	SER	4.2
2	В	141	PRO	4.1
1	D	192	LYS	4.1
2	В	235	PRO	4.1
2	Е	195	SER	4.1
2	В	179	GLY	4.1
3	С	151	GLY	4.1
3	С	205	SER	4.0
2	В	170	GLU	4.0
2	В	143	VAL	3.9
2	В	234	GLU	3.9
3	С	148	LEU	3.8
3	F	169	VAL	3.7
2	Е	230	ASP	3.7



Mol	Chain	Res	Type	RSRZ
2	В	203	VAL	3.7
2	Е	203	VAL	3.7
2	В	83	PHE	3.7
2	Е	84	GLN	3.7
2	В	21	VAL	3.6
1	D	78	TYR	3.6
3	F	135	ALA	3.6
2	В	142	SER	3.6
2	В	105	LEU	3.6
2	Е	198	TYR	3.6
2	Е	197	LEU	3.5
2	Е	96	ASN	3.5
3	С	142	PRO	3.5
2	В	178	SER	3.5
3	С	204	LEU	3.5
3	F	175	ASN	3.5
1	А	41	PHE	3.5
2	Е	36	SER	3.5
3	F	171	TRP	3.4
1	D	173	ASN	3.4
2	В	167	TYR	3.4
3	F	228	VAL	3.4
3	С	215	TYR	3.4
1	D	361	TYR	3.3
2	В	174	VAL	3.3
2	Е	165	LYS	3.3
3	F	229	THR	3.3
2	Е	169	PRO	3.3
2	Е	224	PRO	3.3
2	В	132	THR	3.3
3	F	177	LEU	3.2
1	А	324	ALA	3.2
3	С	137	SER	3.2
2	В	103	SER	3.2
3	С	171	TRP	3.2
3	С	157	CYS	3.2
3	F	230	LYS	3.1
3	C	158	LEU	3.1
1	A	348	GLN	3.1
3	С	152	THR	3.0
3	F	200	SER	3.0
3	F	170	GLN	3.0



Mol	Chain	Res	Type	RSRZ
3	С	177	LEU	3.0
1	D	122	GLU	3.0
2	В	162	CYS	3.0
1	А	142	LYS	3.0
3	F	201	THR	3.0
3	С	138	VAL	2.9
2	Е	228	LYS	2.9
3	F	225	SER	2.9
1	D	144	TYR	2.9
2	В	20	GLU	2.9
2	Ε	219	ASN	2.9
1	А	34	PHE	2.9
2	Ε	173	THR	2.9
2	Е	231	LYS	2.9
2	В	229	VAL	2.9
2	Ε	70	ILE	2.8
3	С	210	GLU	2.8
3	С	65	GLY	2.8
2	В	37	VAL	2.8
2	Е	44	SER	2.8
2	Ε	20	GLU	2.8
1	D	66	ASP	2.8
2	Ε	101	GLN	2.7
2	В	194	SER	2.7
1	D	76	HIS	2.7
2	В	130	THR	2.7
2	В	131	VAL	2.7
1	D	229	ARG	2.7
2	В	134	SER	2.7
3	С	134	ALA	2.7
3	С	149	LYS	2.7
3	С	141	PHE	2.7
2	В	30	LEU	2.6
3	F	226	SER	2.6
2	В	133	VAL	2.6
1	A	120	GLU	2.6
1	D	316	LYS	2.6
3	F	218	GLU	2.6
3	F	165	ARG	2.6
3	F	220	THR	2.6
2	В	102	LEU	2.6
2	В	185	VAL	2.6



Mol	Chain	Res	Type	RSRZ
3	F	173	VAL	2.6
1	А	325	ALA	2.5
2	В	96	ASN	2.5
1	D	346	SER	2.5
3	F	167	ALA	2.5
2	В	89	ILE	2.5
3	С	221	HIS	2.5
1	А	122	GLU	2.5
3	С	217	CYS	2.5
3	С	200	SER	2.5
3	С	219	VAL	2.5
2	В	171	PRO	2.4
1	D	95	LYS	2.4
3	F	186	VAL	2.4
3	F	172	LYS	2.4
3	С	235	GLY	2.4
3	F	67	PRO	2.4
3	F	44	ARG	2.4
1	D	83	VAL	2.4
2	Е	133	VAL	2.4
2	В	224	PRO	2.4
2	Е	93	THR	2.4
2	Е	31	VAL	2.4
2	Е	171	PRO	2.4
2	В	175	SER	2.4
1	D	41	PHE	2.4
2	Е	34	GLY	2.3
2	Е	226	ASN	2.3
1	D	348	GLN	2.3
2	Е	30	LEU	2.3
2	Е	48	ILE	2.3
1	D	193	LYS	2.3
1	D	102	ARG	2.3
1	D	228	LEU	2.3
3	С	144	SER	2.3
2	В	93	THR	2.3
1	А	289	GLU	2.3
1	D	146	ASN	2.2
1	D	42	ILE	2.2
3	С	175	ASN	2.2
3	С	135	ALA	2.2
2	Е	24	GLN	2.2



Mol	Chain	Res	Type	RSRZ
2	Е	90	LYS	2.2
2	В	63	GLY	2.2
1	D	91	ASN	2.2
2	Е	191	VAL	2.2
2	В	232	LYS	2.2
2	В	172	VAL	2.1
2	Е	107	SER	2.1
1	D	116	ILE	2.1
2	В	34	GLY	2.1
3	С	160	ASN	2.1
1	А	350	ILE	2.1
3	F	198	LEU	2.1
2	В	81	PRO	2.1
1	D	136	PHE	2.1
1	D	85	ASP	2.1
1	D	88	ILE	2.1
3	С	230	LYS	2.1
3	F	205	SER	2.1
1	А	174	ARG	2.1
1	D	96	GLU	2.1
1	D	302	GLU	2.1
3	F	203	THR	2.1
3	С	198	LEU	2.1
2	В	217	ILE	2.1
2	Е	43	ALA	2.1
1	D	165	VAL	2.1
2	В	220	VAL	2.0
2	Е	37	VAL	2.0
3	С	236	GLU	2.0
2	В	231	LYS	2.0
2	В	22	GLN	2.0
2	Е	33	PRO	2.0
3	С	206	LYS	2.0
2	В	23	LEU	2.0
1	А	88	ILE	2.0
1	D	345	SER	2.0
2	В	86	LYS	2.0
3	С	155	VAL	2.0

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## 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 monosaccharides 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.

