

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2022 – 03:11 pm GMT

PDB ID	:	7PHW
Title	:	PfCyRPA bound to monoclonal antibody Cy.004 Fab fragment
Authors	:	Ragotte, R.J.; Higgins, M.K.
Deposited on	:	2021-08-18
Resolution	:	2.79 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
buster-report	:	1.1.7(2018)
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 2.79 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	3140 (2.80-2.80)
Clashscore	141614	3569(2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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							
1	Δ	949	5%							
	A	343	72%		18% • 8%					
			10%							
1	D	343	72%		17% • 9%					
			%							
2	В	321	62%	6% •	31%					
			7%			_				
2	E	321	62%	7% •	30%					
			%							
3	C	209	86%		12%	•				



Mol	Chain	Length	Quality of chain		
			5%		
3	F	209	84%	13%	••



2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11683 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	0	\mathbf{S}	0	0	0
1	A	517	2648	1708	424	503	13	0	0	0
1	Л	210	Total	С	Ν	0	S	0	0	0
	D	512	2599	1677	415	494	13	0	0	

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

Residue	Modelled	Actual	Comment	Reference
147	ALA	SER	conflict	UNP Q8IFM8
324	ALA	THR	conflict	UNP Q8IFM8
340	ALA	THR	conflict	UNP Q8IFM8
363	GLY	-	expression tag	UNP Q8IFM8
364	GLY	-	expression tag	UNP Q8IFM8
365	GLY	-	expression tag	UNP Q8IFM8
366	GLY	-	expression tag	UNP Q8IFM8
367	SER	-	expression tag	UNP Q8IFM8
368	GLU	-	expression tag	UNP Q8IFM8
369	PRO	-	expression tag	UNP Q8IFM8
370	GLU	-	expression tag	UNP Q8IFM8
371	ALA	-	expression tag	UNP Q8IFM8
147	ALA	SER	conflict	UNP Q8IFM8
324	ALA	THR	conflict	UNP Q8IFM8
340	ALA	THR	conflict	UNP Q8IFM8
363	GLY	-	expression tag	UNP Q8IFM8
364	GLY	-	expression tag	UNP Q8IFM8
365	GLY	-	expression tag	UNP Q8IFM8
366	GLY	-	expression tag	UNP Q8IFM8
367	SER	-	expression tag	UNP Q8IFM8
368	GLU	-	expression tag	UNP Q8IFM8
369	PRO	-	expression tag	UNP Q8IFM8
370	GLU	-	expression tag	UNP Q8IFM8
371	ALA	-	expression tag	UNP Q8IFM8
	Residue 147 324 340 363 364 365 366 367 368 369 370 371 147 324 340 363 369 370 371 147 324 340 363 363 364 365 366 367 368 369 361 362 363 364 365 366 367 368 369 370 370 371	Residue Modelled 147 ALA 324 ALA 340 ALA 363 GLY 364 GLY 365 GLY 366 GLY 367 SER 368 GLU 369 PRO 370 GLU 371 ALA 147 ALA 324 ALA 363 GLU 369 PRO 370 GLU 371 ALA 340 ALA 363 GLY 364 GLY 365 GLY 366 GLY 365 GLY 366 GLY 366 GLY 366 GLY 366 GLY 367 SER 368 GLU 369 PRO 370 GLU 3	Residue Modelled Actual 147 ALA SER 324 ALA THR 340 ALA THR 363 GLY - 363 GLY - 364 GLY - 365 GLY - 366 GLY - 367 SER - 368 GLU - 369 PRO - 370 GLU - 371 ALA SER 324 ALA THR 363 GLY - 364 GLY - 365 GLY - 366 GLY - 366 GLY - 367 SER - <td< td=""><td>ResidueModelledActualComment147ALASERconflict324ALATHRconflict340ALATHRconflict363GLY-expression tag364GLY-expression tag365GLY-expression tag366GLY-expression tag366GLY-expression tag366GLU-expression tag367SER-expression tag368GLU-expression tag369PRO-expression tag370GLU-expression tag371ALASERconflict340ALATHRconflict363GLY-expression tag364GLY-expression tag364GLY-expression tag366GLY-expression tag366GLY-expression tag366GLY-expression tag366GLY-expression tag368GLU-expression tag369PRO-expression tag369PRO-expression tag369PRO-expression tag369PRO-expression tag369PRO-expression tag369PRO-expression tag369</td></td<>	ResidueModelledActualComment 147 ALASERconflict 324 ALATHRconflict 340 ALATHRconflict 363 GLY-expression tag 364 GLY-expression tag 365 GLY-expression tag 366 GLY-expression tag 366 GLY-expression tag 366 GLU-expression tag 367 SER-expression tag 368 GLU-expression tag 369 PRO-expression tag 370 GLU-expression tag 371 ALASERconflict 340 ALATHRconflict 363 GLY-expression tag 364 GLY-expression tag 364 GLY-expression tag 366 GLY-expression tag 366 GLY-expression tag 366 GLY-expression tag 366 GLY-expression tag 368 GLU-expression tag 369 PRO-expression tag 369

There are 24 discrepancies between the modelled and reference sequences:



• Molecule 2 is a protein called Monoclonal antibody Cy.004 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
0	Р	202	Total	С	Ν	0	S	0	0	0
	D	220	1634	1023	277	329	5	0		0
0	F	226	Total	С	Ν	0	S	0	1	0
	Ľ	220	1655	1034	280	335	6			U

• Molecule 3 is a protein called Monoclonal antibody Cy.004 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	200	Total	С	Ν	0	S	0	0	0
0	U	209	1577	978	265	329	5	0		
2	Б	207	Total	С	Ν	0	S	0	0	0
0	Г	207	1566	972	263	327	4	0	0	0

• Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	А	1	Total Ca 1 1	0	0
4	В	1	Total Ca 1 1	0	0
4	D	1	Total Ca 1 1	0	0
4	Е	1	Total Ca 1 1	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









4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants	103.06Å 80.32 Å 114.91 Å	Deperitor
a, b, c, α , β , γ	90.00° 115.23° 90.00°	Depositor
$\mathbf{P}_{\text{assolution}}(\hat{\mathbf{A}})$	47.11 - 2.79	Depositor
Resolution (A)	47.11 - 2.79	EDS
% Data completeness	99.0 (47.11-2.79)	Depositor
(in resolution range)	99.0 (47.11-2.79)	EDS
R _{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) > 1$	$1.59 (at 2.81 \text{\AA})$	Xtriage
Refinement program	BUSTER 2.10.4 (24-FEB-2021)	Depositor
D D.	0.239 , 0.277	Depositor
Π, Π_{free}	0.225 , 0.266	DCC
R_{free} test set	2164 reflections $(5.15%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	61.1	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent $k_{sol}(e/A^3), B_{sol}(A^2)$	(Not available), (Not available)	EDS
L-test for twinning ²	$< L >=0.49, < L^2>=0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11683	wwPDB-VP
Average B, all atoms $(Å^2)$	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The analyses of the Patterson function reveals a significant off-origin peak that is 29.50 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.5323e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA

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).

Mal	Chain	Bond	lengths	Bond angles		
	Unam	RMSZ	# Z > 5	RMSZ	# Z > 5	
1	А	0.46	0/2708	0.66	0/3652	
1	D	0.42	0/2657	0.66	0/3585	
2	В	0.47	0/1670	0.63	0/2273	
2	Е	0.42	0/1695	0.64	0/2308	
3	С	0.42	0/1610	0.63	0/2192	
3	F	0.41	0/1599	0.63	0/2177	
All	All	0.44	0/11939	0.64	0/16187	

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	2548	35	0
1	D	2599	0	2494	59	0
2	В	1634	0	1582	11	0
2	Е	1655	0	1602	15	0
3	С	1577	0	1513	16	0
3	F	1566	0	1503	13	0
4	А	1	0	0	0	0



00.000	contract from proceeder pagem					
Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	В	1	0	0	0	0
4	D	1	0	0	0	0
4	Е	1	0	0	0	0
All	All	11683	0	11242	141	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 6.

All (141) 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)
1:D:83:VAL:HG21	1:D:88:ILE:CD1	1.66	1.23
2:E:127:ASP:HA	2:E:131:GLU:HG3	1.29	1.10
2:B:127:ASP:HA	2:B:131:GLU:HG3	1.29	1.10
1:D:83:VAL:HG21	1:D:88:ILE:HD12	1.11	1.09
3:C:40:ILE:HG21	3:C:119:THR:HG21	1.43	1.00
1:D:83:VAL:CG2	1:D:88:ILE:HD12	1.97	0.93
1:D:57:LYS:NZ	1:D:112:GLU:HG2	1.88	0.88
1:D:57:LYS:HZ1	1:D:112:GLU:HG2	1.37	0.87
1:D:81:LYS:NZ	1:D:142:LYS:HE2	1.89	0.87
1:A:42:ILE:HD13	1:A:353:ILE:HD12	1.55	0.85
1:D:83:VAL:CG2	1:D:88:ILE:CD1	2.53	0.84
1:A:316:LYS:O	1:A:319:LYS:HE2	1.77	0.83
1:D:83:VAL:HG12	1:D:84:LYS:H	1.43	0.81
1:D:81:LYS:HZ1	1:D:142:LYS:HE2	1.49	0.75
1:D:83:VAL:HG12	1:D:84:LYS:N	2.03	0.73
1:A:52:MET:HG2	1:A:165:VAL:HG23	1.70	0.73
3:F:125:ARG:HD2	3:F:157:TYR:CG	2.26	0.70
1:A:39:LEU:HD13	1:A:354:HIS:CE1	2.28	0.69
1:A:301:ALA:O	1:A:317:PRO:HD2	1.93	0.69
1:D:39:LEU:HD13	1:D:354:HIS:CE1	2.28	0.69
1:A:277:ASN:HD21	1:D:57:LYS:NZ	1.92	0.67
1:D:83:VAL:HG21	1:D:88:ILE:HD11	1.71	0.67
2:B:71:ARG:HG3	2:B:76:PHE:HB3	1.75	0.67
3:C:40:ILE:CG2	3:C:119:THR:HG21	2.21	0.66
1:D:52:MET:HG2	1:D:165:VAL:HG13	1.79	0.64
1:D:56:TYR:OH	1:D:139:ASN:O	2.16	0.63
2:E:71:ARG:HG3	2:E:76:PHE:HB3	1.81	0.63
1:A:170:LYS:HB2	1:A:235:ASN:HD21	1.64	0.62
1:D:81:LYS:HZ3	1:D:142:LYS:HE2	1.63	0.61
1:D:52:MET:HG2	1:D:165:VAL:CG1	2.30	0.61



	loub page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:D:179:ILE:HG23	1:D:199:MET:HG3	1.83	0.61
1:A:200:ALA:HB3	1:A:210:THR:HB	1.84	0.59
3:F:137:PRO:HD3	3:F:149:VAL:HG22	1.84	0.59
1:D:93:LEU:HD23	1:D:93:LEU:N	2.17	0.59
1:A:167:LEU:HB2	1:A:168:PRO:HD2	1.84	0.58
1:A:316:LYS:O	1:A:319:LYS:CE	2.49	0.57
2:E:127:ASP:CA	2:E:131:GLU:HG3	2.19	0.57
1:D:83:VAL:CG1	1:D:84:LYS:H	2.16	0.57
1:D:40:SER:HB3	1:D:353:ILE:HD11	1.87	0.56
1:D:81:LYS:NZ	1:D:142:LYS:CE	2.68	0.56
2:B:127:ASP:CA	2:B:131:GLU:HG3	2.20	0.56
2:E:110:THR:HG23	2:E:142:ILE:HA	1.88	0.56
1:D:140:ASP:OD1	1:D:143:GLU:N	2.36	0.54
2:B:110:THR:HG23	2:B:142:ILE:HA	1.90	0.54
1:A:124:PHE:HA	1:A:127:ARG:HD3	1.90	0.54
1:A:79:VAL:HG23	1:A:93:LEU:HD11	1.90	0.53
3:C:137:PRO:HD3	3:C:149:VAL:HG22	1.90	0.53
1:D:138:SER:HB2	1:D:143:GLU:O	2.09	0.52
2:E:113:TYR:CD1	2:E:141:VAL:HG13	2.44	0.52
2:E:182:VAL:HG12	2:E:232:HIS:CD2	2.44	0.52
1:D:37:THR:HG21	1:D:313:ILE:HD13	1.91	0.52
3:C:139:ASP:O	3:C:143:LYS:HG2	2.11	0.51
1:A:108:TYR:OH	1:A:179:ILE:HG13	2.10	0.51
1:D:219:TYR:CE2	1:D:220:LYS:NZ	2.73	0.51
2:E:227:ILE:HG12	2:E:242:LYS:HA	1.93	0.51
3:F:140:GLU:HA	3:F:143:LYS:NZ	2.26	0.50
1:A:77:ILE:HG22	1:A:93:LEU:HD12	1.93	0.50
2:B:227:ILE:HG12	2:B:242:LYS:HA	1.93	0.49
1:A:59:GLU:OE1	1:A:81:LYS:HE2	2.11	0.49
3:C:142:LEU:O	3:C:200:LYS:HD2	2.12	0.49
1:A:277:ASN:ND2	1:D:57:LYS:NZ	2.60	0.49
1:D:81:LYS:HZ1	1:D:142:LYS:CE	2.22	0.49
3:F:140:GLU:HA	3:F:143:LYS:HZ2	1.78	0.49
1:D:339:ARG:HD2	1:D:357:TYR:CE2	2.48	0.48
3:F:162:LYS:HB3	3:F:214:THR:HB	1.95	0.48
2:B:182:VAL:HG23	2:B:232:HIS:HD2	1.78	0.48
2:E:244:GLU:HG2	2:E:245:PRO:HD2	1.95	0.48
1:D:93:LEU:HD23	1:D:93:LEU:H	1.78	0.48
1:D:57:LYS:HZ3	1:D:112:GLU:HG2	1.75	0.47
1:D:319:LYS:HZ2	1:D:320:TYR:HE2	1.62	0.47
1:D:343:ILE:HG12	1:D:353:ILE:HG22	1.96	0.47



	ti a	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:D:138:SER:CB	1:D:143:GLU:O	2.62	0.47	
1:A:343:ILE:HG12	1:A:353:ILE:HG12	1.96	0.47	
2:B:174:VAL:HG11	2:B:182:VAL:HG11	1.95	0.47	
1:A:156:LEU:HG	1:A:199:MET:HG3	1.97	0.47	
3:C:119:THR:O	3:C:119:THR:HG23	2.14	0.47	
3:C:168:ASP:HA	3:C:208:VAL:HG13	1.97	0.47	
3:C:162:LYS:HB3	3:C:214:THR:HB	1.96	0.47	
1:D:83:VAL:CG1	1:D:84:LYS:N	2.72	0.47	
1:A:277:ASN:ND2	1:D:57:LYS:HZ1	2.12	0.46	
2:E:162:SER:OG	2:E:169:ALA:O	2.32	0.46	
1:D:79:VAL:HG23	1:D:93:LEU:HD21	1.98	0.46	
1:A:99:LEU:HD13	1:A:103:PRO:HB3	1.97	0.46	
1:A:108:TYR:OH	1:A:179:ILE:CG1	2.64	0.46	
1:D:156:LEU:HD13	1:D:161:LEU:HD11	1.98	0.46	
1:D:319:LYS:HG3	1:D:320:TYR:CD2	2.51	0.45	
2:E:159:SER:H	2:E:162:SER:HB3	1.81	0.45	
2:B:182:VAL:HG23	2:B:232:HIS:CD2	2.50	0.45	
1:D:140:ASP:OD2	1:D:142:LYS:HB2	2.17	0.45	
3:C:102:VAL:HA	3:C:120:THR:HA	1.99	0.45	
3:F:168:ASP:HA	3:F:208:VAL:HG13	1.97	0.45	
2:E:37:LEU:CD1	2:E:39:LEU:HD22	2.46	0.45	
1:A:108:TYR:HB3	1:A:177:PHE:CE1	2.53	0.44	
3:C:230:GLU:O	3:C:231:CYS:HB3	2.18	0.44	
1:D:83:VAL:CG2	1:D:88:ILE:CG1	2.95	0.44	
2:E:182:VAL:CG1	2:E:232:HIS:CD2	2.99	0.44	
1:A:228:LEU:HA	1:A:241:PHE:HB3	1.99	0.44	
1:D:42:ILE:HB	1:D:351:TYR:HB2	2.00	0.44	
1:A:54:PHE:HB3	1:A:165:VAL:HG11	2.00	0.44	
1:D:155:ILE:HD11	1:D:199:MET:HB3	2.00	0.44	
1:D:200:ALA:HB3	1:D:210:THR:HB	1.99	0.44	
1:A:94:PHE:CE2	3:C:111:ARG:NH2	2.86	0.44	
3:F:206:HIS:O	3:F:228:ARG:HD2	2.18	0.44	
1:D:219:TYR:HE2	1:D:220:LYS:NZ	2.15	0.44	
3:F:56:SER:O	3:F:59:SER:HB3	2.18	0.44	
1:A:342:PHE:HB3	1:A:354:HIS:HB2	1.99	0.43	
1:A:42:ILE:HG22	1:A:87:TRP:CD1	2.52	0.43	
1:D:228:LEU:HA	1:D:241:PHE:HB3	1.99	0.43	
3:F:178:GLU:HB2	3:F:192:LEU:HD21	2.01	0.43	
1:A:276:ASP:HB3	1:D:112:GLU:OE1	2.18	0.43	
1:D:138:SER:OG	1:D:139:ASN:N	2.52	0.43	
2:E:198:PHE:CD2	3:F:181:THR:HG23	2.54	0.43	



A + 1	A + 2	Interatomic	Clash
Atom-1	Atom-2	distance (\AA)	overlap (Å)
1:D:40:SER:HB3	1:D:353:ILE:CD1	2.48	0.43
3:C:56:SER:O	3:C:59:SER:HB3	2.19	0.42
1:D:246:ASN:HB2	1:D:247:ILE:HD12	2.01	0.42
3:C:26:GLN:NE2	3:C:119:THR:HG22	2.35	0.42
2:B:59:ALA:HB3	2:B:62:LYS:HB2	2.00	0.42
1:D:179:ILE:HG23	1:D:199:MET:CG	2.49	0.42
1:D:83:VAL:CG2	1:D:88:ILE:HG13	2.50	0.42
3:C:37:THR:HG23	3:C:93:THR:HG22	2.02	0.42
1:D:342:PHE:HB3	1:D:354:HIS:HB2	2.01	0.42
1:D:301:ALA:O	1:D:317:PRO:HD2	2.20	0.41
3:F:151:CYS:HB2	3:F:165:TRP:CZ2	2.55	0.41
1:D:339:ARG:HD2	1:D:357:TYR:HE2	1.84	0.41
1:A:277:ASN:HD21	1:D:57:LYS:CE	2.33	0.41
2:B:148:THR:HG22	2:B:235:SER:HB3	2.01	0.41
2:E:182:VAL:CG1	2:E:232:HIS:HD2	2.33	0.41
1:A:97:THR:HG21	1:A:118:LEU:HD12	2.01	0.41
1:D:93:LEU:N	1:D:93:LEU:CD2	2.82	0.41
1:D:174:ARG:HD2	1:D:176:TYR:OH	2.21	0.41
1:A:171:ILE:HG22	1:A:172:GLU:HG3	2.03	0.41
3:C:178:GLU:HB2	3:C:192:LEU:HD21	2.03	0.41
3:F:37:THR:HG23	3:F:93:THR:HG22	2.03	0.41
1:A:44:ASN:HB2	1:A:87:TRP:HD1	1.86	0.41
3:F:135:PHE:HB2	3:F:150:VAL:HB	2.02	0.41
1:A:170:LYS:HB2	1:A:235:ASN:ND2	2.33	0.40
2:E:182:VAL:HG12	2:E:232:HIS:HD2	1.86	0.40
1:A:239:PHE:HB2	1:A:256:ILE:HG12	2.04	0.40
2:B:203:GLN:OE1	2:B:209:SER:HB2	2.21	0.40
1:D:319:LYS:H	1:D:319:LYS:HG2	1.66	0.40
1:A:99:LEU:O	3:C:111:ARG:NH1	2.53	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	А	309/343~(90%)	288~(93%)	21 (7%)	0	100 100
1	D	302/343~(88%)	283~(94%)	19 (6%)	0	100 100
2	В	219/321~(68%)	210 (96%)	9~(4%)	0	100 100
2	Ε	225/321~(70%)	214 (95%)	11 (5%)	0	100 100
3	С	207/209~(99%)	200~(97%)	7 (3%)	0	100 100
3	F	205/209~(98%)	197~(96%)	8 (4%)	0	100 100
All	All	1467/1746~(84%)	1392 (95%)	75 (5%)	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 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	Perce	entiles
1	А	297/316~(94%)	268~(90%)	29 (10%)	8	24
1	D	292/316~(92%)	269~(92%)	23~(8%)	12	34
2	В	179/272~(66%)	169 (94%)	10 (6%)	21	51
2	Ε	183/272~(67%)	171 (93%)	12 (7%)	16	44
3	С	180/180~(100%)	170 (94%)	10 (6%)	21	51
3	F	179/180~(99%)	168 (94%)	11 (6%)	18	48
All	All	1310/1536~(85%)	1215 (93%)	95 (7%)	14	38

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	А	37	THR
1	А	68	LEU
1	А	72	GLU
1	А	82	LYS
1	А	93	LEU
1	А	110	ASP
1	А	127	ARG



Mol	Chain	\mathbf{Res}	Type
1	А	128	LYS
1	А	142	LYS
1	А	162	SER
1	А	167	LEU
1	А	182	VAL
1	А	183	SER
1	А	194	ASP
1	А	220	LYS
1	А	223	VAL
1	А	224	GLN
1	А	228	LEU
1	А	229	ARG
1	А	250	VAL
1	А	259	THR
1	А	263	ASP
1	А	270	ASN
1	А	276	ASP
1	А	297	ASP
1	А	315	ILE
1	А	319	LYS
1	А	320	TYR
1	А	362	GLU
2	В	71	ARG
2	В	84	LYS
2	В	120	ASP
2	В	131	GLU
2	В	142	ILE
2	В	149	LYS
2	В	182	VAL
2	В	218	SER
2	В	225	THR
2	В	246	LYS
3	С	46	THR
3	С	56	SER
3	С	102	VAL
3	С	120	THR
3	С	126	THR
3	С	164	GLN
3	С	171	LEU
3	С	196	LEU
3	С	207	LYS
3	С	231	CYS



Mol	Chain	Res	Type
1	D	45	ASN
1	D	82	LYS
1	D	85	ASP
1	D	93	LEU
1	D	109	VAL
1	D	128	LYS
1	D	162	SER
1	D	165	VAL
1	D	173	ASN
1	D	179	ILE
1	D	182	VAL
1	D	194	ASP
1	D	219	TYR
1	D	228	LEU
1	D	229	ARG
1	D	250	VAL
1	D	254	ASN
1	D	262	LYS
1	D	263	ASP
1	D	270	ASN
1	D	271	ARG
1	D	275	LYS
1	D	339	ARG
2	Е	22	THR
2	Е	39	LEU
2	Е	71	ARG
2	Е	86	ARG
2	Е	99	ARG
2	Е	103	ASN
2	Е	104	ASN
2	E	115	CYS
2	Е	131	GLU
2	Е	142	ILE
2	Ε	220	SER
2	Е	236	ASN
3	F	41	THR
3	F	46	THR
3	F	56	SER
3	F	102	VAL
3	F	125	ARG
3	F	142	LEU
3	F	164	GLN



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Mol	Chain	Res	Type
3	F	180	VAL
3	F	186	LYS
3	F	196	LEU
3	F	228	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	277	ASN
1	D	76	HIS
1	D	145	ASN
1	D	270	ASN
2	Е	104	ASN
2	Е	236	ASN

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)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.



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	<RSRZ $>$	#RSRZ>2	$OWAB(Å^2)$	Q<0.9
1	А	317/343~(92%)	0.77	18 (5%) 23 15	52, 84, 125, 146	0
1	D	312/343~(90%)	1.01	33 (10%) 6 3	66, 103, 143, 159	0
2	В	223/321~(69%)	0.56	4 (1%) 68 61	53, 79, 102, 109	0
2	Е	226/321~(70%)	0.84	24 (10%) 6 3	47, 89, 131, 138	0
3	С	209/209~(100%)	0.44	3 (1%) 75 70	58, 77, 107, 115	0
3	F	207/209~(99%)	0.61	11 (5%) 26 17	53, 81, 137, 151	0
All	All	1494/1746~(85%)	0.73	93 (6%) 20 13	47, 85, 132, 159	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	А	219	TYR	7.2
1	А	221	LEU	6.0
1	D	219	TYR	5.3
1	А	361	TYR	5.1
1	D	34	PHE	4.2
3	F	207	LYS	3.8
1	D	231	TYR	3.7
2	Е	83	VAL	3.7
3	F	226	PHE	3.6
1	D	32	HIS	3.6
2	Е	236	ASN	3.4
2	Е	191	LEU	3.3
2	Е	237	THR	3.2
3	F	165	TRP	3.2
3	F	196	LEU	3.2
1	А	360	ASN	3.1
1	А	320	TYR	3.1
3	F	163	VAL	2.9
2	Е	239	VAL	2.9



Mol	Chain	Res	Type	RSRZ
2	Е	209	SER	2.9
1	D	83	VAL	2.9
1	А	182	VAL	2.8
1	А	196	ILE	2.8
1	А	34	PHE	2.7
1	D	176	TYR	2.7
1	D	266	PHE	2.7
1	D	346	SER	2.7
2	Е	79	TYR	2.7
2	Е	156	LEU	2.6
1	D	214	ILE	2.6
2	Е	243	VAL	2.6
3	F	203	TYR	2.6
1	D	220	LYS	2.6
3	F	149	VAL	2.6
2	Е	220	SER	2.6
1	А	206	GLU	2.5
1	А	111	VAL	2.5
2	Е	63	GLY	2.5
1	D	58	ARG	2.5
1	D	348	GLN	2.5
1	D	109	VAL	2.5
1	D	342	PHE	2.5
1	D	261	GLU	2.4
1	А	71	GLU	2.4
3	F	164	GLN	2.4
1	D	321	GLY	2.4
1	А	231	TYR	2.4
1	D	328	TYR	2.4
1	D	237	LEU	2.4
2	Е	87	ALA	2.4
2	В	21	VAL	2.4
1	D	224	GLN	2.4
2	В	154	PHE	2.3
2	Е	223	THR	2.3
1	А	226	PHE	2.3
2	Е	233	LYS	2.3
1	А	218	ASN	2.3
3	F	143	LYS	2.3
1	D	169	LEU	2.3
1	D	114	ILE	2.3
1	А	158	ASP	2.3



Mol

2

2

3

D	311	ASN	2.3
Е	175	LYS	2.2
D	174	ARG	2.2
F	170	ALA	2.2
Ε	174	VAL	2.2
Ε	187	ASN	2.2
Ε	155	PRO	2.2
Е	202	LEU	2.2
D	55	ILE	2.1
D	171	ILE	2.1
Е	137	HIS	2.1
С	152	LEU	2.1
D	304	TYR	2.1
D	357	TYR	2.1
D	156	LEU	2.1
Е	173	LEU	2.1
Е	201	VAL	2.1
В	34	GLY	2.1
D	314	LEU	2.1
С	92	ILE	2.1
А	155	ILE	2.0
А	214	ILE	2.0
А	357	TYR	2.0

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 \mathbf{Res}

231

194

177

Type

ASN

GLY

 GLN

RSRZ

2.3

2.3

2.3

Chain

Е

Е

F

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

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

2.0

2.0

2.0

2.0

2.0

2.0

6.3 Carbohydrates (i)

D

D

 $\overline{\mathbf{C}}$

D

В

D

1

1

3

1

2

1

33

356

179

119

106

317

VAL

ILE

SER

 CYS

ARG

PRO

There are no monosaccharides in this entry.



6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	$B-factors(A^2)$	Q<0.9
4	CA	В	401	1/1	0.75	0.17	100,100,100,100	0
4	CA	А	401	1/1	0.90	0.20	63,63,63,63	0
4	CA	D	401	1/1	0.91	0.25	67,67,67,67	0
4	CA	Е	401	1/1	0.91	0.16	98,98,98,98	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

















6.5 Other polymers (i)

There are no such residues in this entry.

