



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:33 PM UTC

PDB ID : 7PHV / pdb_00007phv
Title : PfCyRPA bound to monoclonal antibody Cy.007 Fab fragment
Authors : Ragotte, R.J.; Higgins, M.K.
Deposited on : 2021-08-18
Resolution : 3.09 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

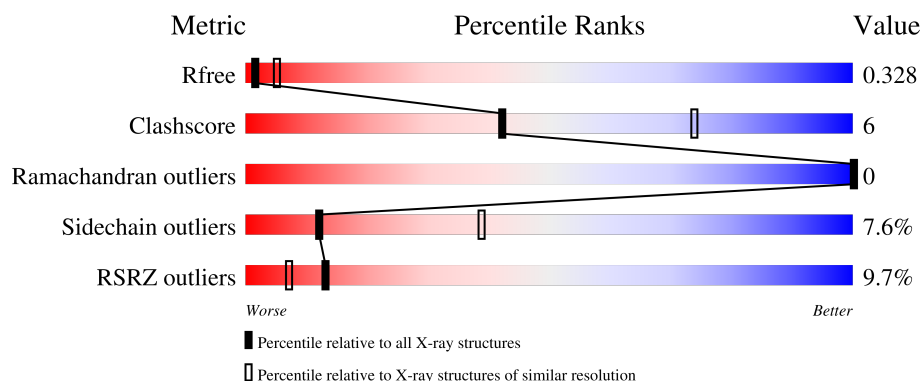
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.09 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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% 66% 22% • 8%
1	D	343	10% 68% 19% • 11%
2	B	233	4% 81% 13% • 5%
2	E	233	4% 80% 13% • 6%
3	C	209	6% 91% 7% •

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	F	209	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NH4	B	301	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11521 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	316	Total	C	N	O	S	0	0	0
			2633	1697	420	503	13			
1	D	305	Total	C	N	O	S	0	0	0
			2539	1640	404	483	12			

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

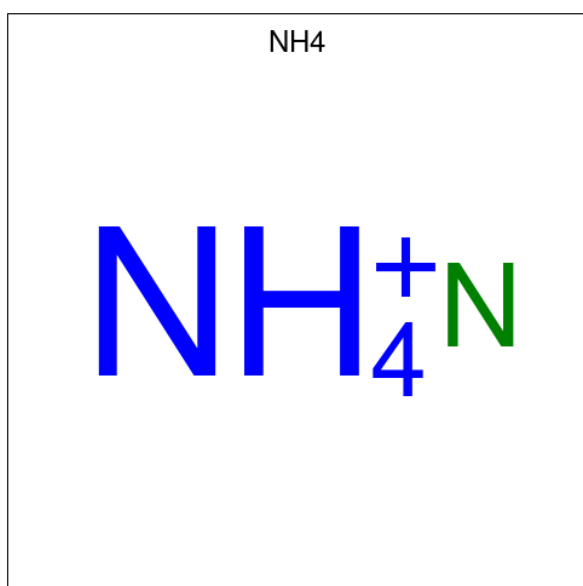
- Molecule 2 is a protein called Monoclonal antibody Cy.007 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	221	Total	C	N	O	S	518	0	0
			1619	1013	272	327	7			
2	E	220	Total	C	N	O	S	646	0	0
			1614	1010	271	326	7			

- Molecule 3 is a protein called Monoclonal antibody Cy.007 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	207	Total	C	N	O	S	549	0	0
			1557	965	265	323	4			
3	F	207	Total	C	N	O	S	489	0	0
			1557	965	265	323	4			

- Molecule 4 is AMMONIUM ION (CCD ID: NH4) (formula: H₄N).

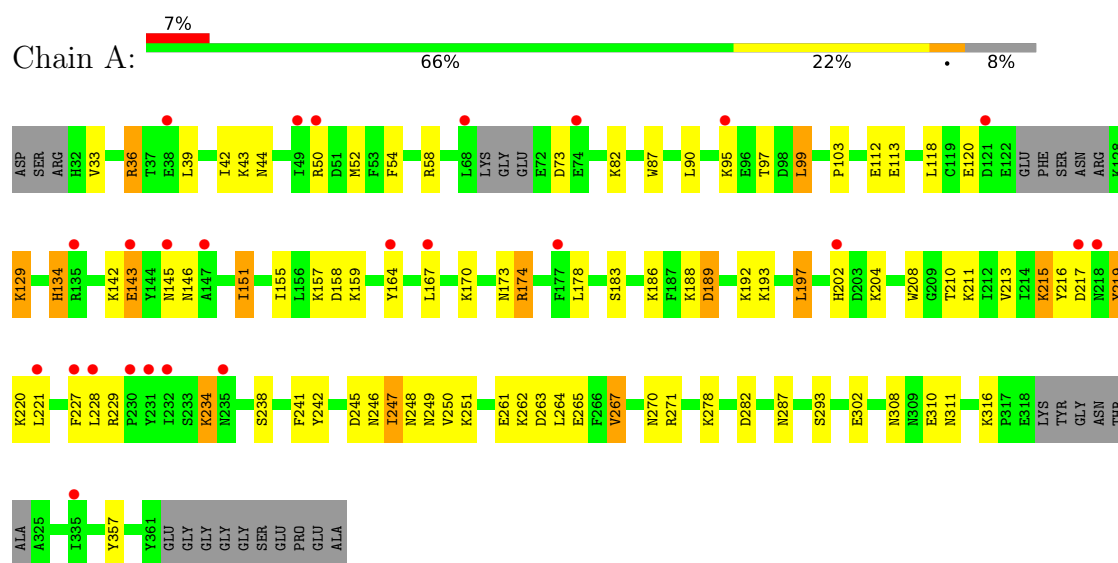


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	N	0	0
			1	1		
4	E	1	Total	N	0	0
			1	1		

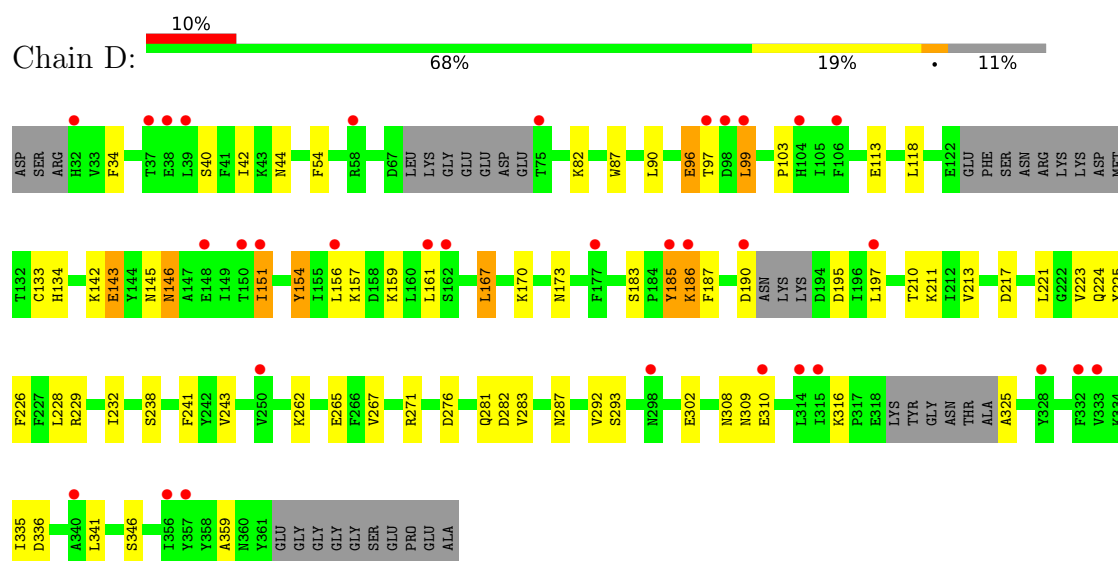
3 Residue-property plots [i](#)

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

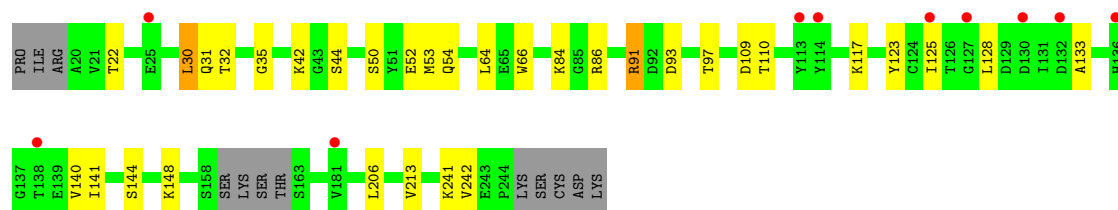


- Molecule 1: Cysteine-rich protective antigen



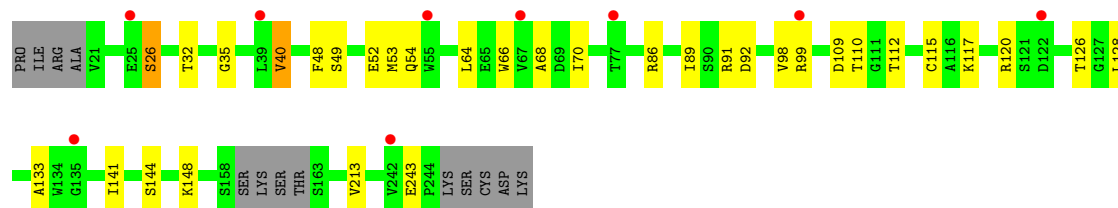
- Molecule 2: Monoclonal antibody Cy.007 heavy chain

Chain B: 

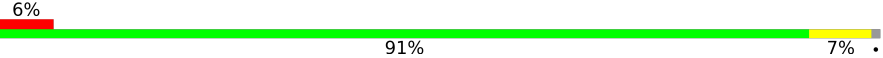


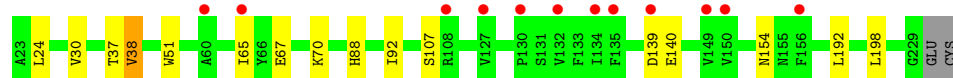
- Molecule 2: Monoclonal antibody Cy.007 heavy chain

Chain E: 



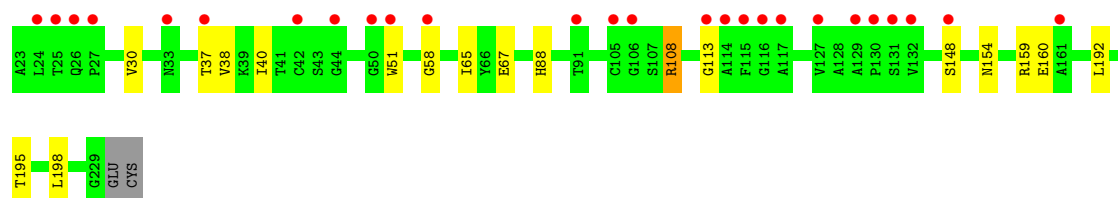
- Molecule 3: Monoclonal antibody Cy.007 light chain

Chain C: 



- Molecule 3: Monoclonal antibody Cy.007 light chain

Chain F: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	74.10Å 87.00Å 342.77Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.24 – 3.09 45.24 – 3.09	Depositor EDS
% Data completeness (in resolution range)	100.0 (45.24-3.09) 99.9 (45.24-3.09)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 3.06Å)	Xtriage
Refinement program	BUSTER 2.10.4 (20-OCT-2021)	Depositor
R, R_{free}	0.287 , 0.332 0.290 , 0.328	Depositor DCC
R_{free} test set	2060 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	109.4	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 137.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	11521	wwPDB-VP
Average B, all atoms (Å ²)	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NH4

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	0.85	0/2692	1.15	11/3634 (0.3%)
1	D	0.78	0/2597	1.07	4/3509 (0.1%)
2	B	0.60	0/1654	0.89	2/2254 (0.1%)
2	E	0.58	0/1649	0.90	0/2247
3	C	0.57	0/1590	0.88	0/2163
3	F	0.58	0/1590	0.86	0/2163
All	All	0.70	0/11772	0.99	17/15970 (0.1%)

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	LEU	N-CA-C	7.65	121.60	110.28
1	D	287	ASN	CA-CB-CG	6.68	119.28	112.60
1	A	220	LYS	CA-C-N	6.66	130.32	120.87
1	A	220	LYS	C-N-CA	6.66	130.32	120.87
1	A	287	ASN	CA-CB-CG	6.51	119.11	112.60
1	A	219	TYR	CA-C-N	6.43	130.69	121.50
1	A	219	TYR	C-N-CA	6.43	130.69	121.50
1	A	263	ASP	CA-CB-CG	5.80	118.40	112.60
1	A	73	ASP	CA-CB-CG	5.41	118.01	112.60
2	B	31	GLN	CA-C-N	5.33	127.80	120.39
2	B	31	GLN	C-N-CA	5.33	127.80	120.39
1	D	54	PHE	CA-CB-CG	5.23	119.03	113.80
1	D	336	ASP	N-CA-CB	-5.15	103.53	111.46
1	A	216	TYR	CA-C-N	5.05	133.35	121.52
1	A	216	TYR	C-N-CA	5.05	133.35	121.52
1	A	54	PHE	CA-CB-CG	5.03	118.83	113.80
1	D	276	ASP	CA-CB-CG	5.02	117.62	112.60

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	2633	0	2528	40	0
1	D	2539	0	2429	36	0
2	B	1619	0	1570	13	0
2	E	1614	0	1565	17	0
3	C	1557	0	1493	5	0
3	F	1557	0	1493	7	0
4	B	1	0	0	1	0
4	E	1	0	0	1	0
All	All	11521	0	11078	115	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 (115) 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:D:325:ALA:HB1	1:D:346:SER:HB2	1.63	0.81
1:A:134:HIS:CE1	1:A:146:ASN:HD22	2.02	0.77
2:B:52:GLU:OE1	4:B:301:NH4:N	2.19	0.75
3:F:108:ARG:HA	3:F:113:GLY:HA2	1.71	0.73
2:E:92:ASP:HB2	2:E:99:ARG:HH12	1.53	0.72
2:E:40:VAL:HG23	2:E:99:ARG:HG2	1.75	0.67
2:B:30:LEU:H	2:B:30:LEU:HD13	1.60	0.66
2:B:91:ARG:HD3	2:B:93:ASP:OD1	1.95	0.65
1:D:156:LEU:HD13	1:D:161:LEU:HD21	1.78	0.64
3:C:51:TRP:HE1	3:C:88:HIS:CE1	2.17	0.63
2:B:117:LYS:HB3	2:B:133:ALA:HB3	1.82	0.62
3:F:51:TRP:HE1	3:F:88:HIS:CE1	2.18	0.62
2:E:68:ALA:HB3	2:E:89:ILE:HD11	1.82	0.62
2:E:117:LYS:HB3	2:E:133:ALA:HB3	1.82	0.61
2:B:66:TRP:HB2	2:B:128:LEU:HD11	1.82	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:HIS:HE1	1:A:146:ASN:HD22	1.49	0.61
1:A:192:LYS:HD2	1:A:193:LYS:HG2	1.83	0.60
1:D:186:LYS:NZ	1:D:190:ASP:O	2.36	0.59
2:E:112:THR:HG21	3:F:58:GLY:HA2	1.85	0.58
2:B:86:ARG:NH2	2:B:109:ASP:OD2	2.37	0.58
2:E:66:TRP:HB2	2:E:128:LEU:HD11	1.85	0.58
2:E:52:GLU:OE1	4:E:301:NH4:N	2.37	0.57
2:E:86:ARG:NH2	2:E:109:ASP:OD2	2.37	0.57
1:A:183:SER:O	1:A:219:TYR:OH	2.23	0.57
1:A:215:LYS:NZ	1:A:267:VAL:HB	2.20	0.56
3:F:30:VAL:HG21	3:F:40:ILE:HG12	1.86	0.56
1:A:308:ASN:C	1:A:310:GLU:H	2.15	0.56
1:D:133:CYS:SG	1:D:151:ILE:HD11	2.47	0.56
1:D:308:ASN:C	1:D:310:GLU:H	2.14	0.55
1:A:44:ASN:HB2	1:A:87:TRP:HD1	1.71	0.55
1:D:167:LEU:HD13	1:D:232:ILE:HB	1.89	0.54
1:A:134:HIS:HE1	1:A:146:ASN:ND2	2.06	0.54
1:D:159:LYS:NZ	1:D:183:SER:HB2	2.23	0.54
1:D:44:ASN:HB2	1:D:87:TRP:HD1	1.73	0.53
2:B:42:LYS:HG2	2:B:97:THR:HG22	1.90	0.53
1:D:282:ASP:H	1:D:293:SER:HB3	1.74	0.53
1:D:302:GLU:HG2	1:D:316:LYS:HG3	1.91	0.53
1:A:97:THR:CG2	1:A:99:LEU:HG	2.39	0.53
1:A:151:ILE:HD12	1:A:208:TRP:CD1	2.44	0.53
1:A:282:ASP:H	1:A:293:SER:HB3	1.73	0.52
1:D:34:PHE:HB3	1:D:359:ALA:HB3	1.91	0.52
1:D:143:GLU:OE2	1:D:145:ASN:ND2	2.42	0.52
1:D:97:THR:CG2	1:D:99:LEU:HG	2.39	0.52
2:E:26:SER:HB3	2:E:40:VAL:HG12	1.92	0.52
1:A:302:GLU:HG2	1:A:316:LYS:HG3	1.91	0.51
1:D:308:ASN:C	1:D:310:GLU:N	2.68	0.51
1:A:42:ILE:CD1	1:A:82:LYS:HG3	2.40	0.51
1:A:215:LYS:HZ3	1:A:267:VAL:HB	1.76	0.51
1:D:213:VAL:HB	1:D:265:GLU:HG3	1.92	0.50
1:D:42:ILE:CD1	1:D:82:LYS:HG3	2.41	0.50
1:D:170:LYS:HE3	1:D:173:ASN:HA	1.93	0.50
1:A:143:GLU:OE2	1:A:145:ASN:ND2	2.44	0.50
1:D:281:GLN:OE1	1:D:293:SER:OG	2.22	0.50
1:A:227:PHE:CZ	1:A:247:ILE:HG13	2.46	0.50
3:C:51:TRP:NE1	3:C:88:HIS:CE1	2.79	0.50
2:B:123:TYR:CZ	2:B:125:ILE:HG12	2.47	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:VAL:HG12	3:C:92:ILE:HB	1.94	0.49
3:C:67:GLU:HB3	3:C:70:LYS:CG	2.43	0.49
2:E:120:ARG:NH1	3:F:67:GLU:OE2	2.46	0.49
2:E:53:MET:HG3	2:E:98:VAL:HG21	1.95	0.49
1:A:42:ILE:HD13	1:A:82:LYS:HG3	1.95	0.48
1:A:213:VAL:HB	1:A:265:GLU:HG3	1.94	0.48
1:D:142:LYS:HE2	2:E:126:THR:HG23	1.94	0.48
2:B:110:THR:HG23	2:B:141:ILE:HA	1.96	0.48
1:D:159:LYS:HZ1	1:D:183:SER:HB2	1.79	0.48
1:A:186:LYS:HE2	1:A:189:ASP:HA	1.96	0.48
2:E:110:THR:HG23	2:E:141:ILE:HA	1.95	0.48
1:A:170:LYS:HE2	1:A:173:ASN:HA	1.96	0.48
1:A:211:LYS:HE3	1:A:213:VAL:HG22	1.96	0.48
1:D:283:VAL:HG22	1:D:292:VAL:HG13	1.96	0.48
1:A:36:ARG:HG2	1:A:357:TYR:CD1	2.50	0.47
1:A:245:ASP:H	1:A:250:VAL:HB	1.80	0.47
1:D:170:LYS:CE	1:D:173:ASN:HA	2.45	0.47
1:A:246:ASN:HB3	1:A:249:ASN:CG	2.40	0.46
1:A:242:TYR:CE2	1:A:251:LYS:HB3	2.50	0.46
1:A:103:PRO:HG2	1:A:118:LEU:HD22	1.97	0.46
2:E:32:THR:HG23	2:E:35:GLY:HA3	1.98	0.46
2:B:22:THR:OG1	2:B:44:SER:OG	2.33	0.46
1:A:170:LYS:CE	1:A:173:ASN:HA	2.45	0.46
2:E:70:ILE:HG12	2:E:91:ARG:HG2	1.98	0.45
1:D:335:ILE:HD11	1:D:341:LEU:HG	1.98	0.45
1:D:103:PRO:HG2	1:D:118:LEU:HD22	1.98	0.45
1:D:42:ILE:HD13	1:D:82:LYS:HG3	1.97	0.45
1:D:146:ASN:HD22	1:D:146:ASN:C	2.23	0.45
1:A:151:ILE:CD1	1:A:208:TRP:CD1	3.00	0.45
1:A:308:ASN:C	1:A:310:GLU:N	2.74	0.45
1:D:211:LYS:HE3	1:D:213:VAL:HG22	1.99	0.45
1:D:185:TYR:HD2	1:D:224:GLN:HE21	1.65	0.45
1:D:223:VAL:HG13	1:D:225:TYR:HE1	1.82	0.44
1:A:174:ARG:HH21	1:A:202:HIS:CE1	2.36	0.43
1:D:223:VAL:HG22	1:D:243:VAL:HG22	1.98	0.43
1:A:248:ASN:HA	1:A:251:LYS:NZ	2.33	0.43
1:D:90:LEU:HB3	1:D:142:LYS:HG3	2.01	0.43
1:A:90:LEU:HB3	1:A:142:LYS:HG3	2.00	0.43
2:B:32:THR:HG23	2:B:35:GLY:HA3	2.01	0.43
1:D:228:LEU:HD12	1:D:241:PHE:HB3	2.01	0.43
2:E:48:PHE:HZ	2:E:98:VAL:HG23	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:LYS:HE3	1:A:197:LEU:HD23	2.00	0.43
1:A:157:LYS:O	1:A:158:ASP:HB2	2.19	0.42
1:A:52:MET:HE3	1:A:52:MET:HB2	1.96	0.42
3:F:148:SER:HB3	3:F:195:THR:HG23	2.01	0.42
1:A:129:LYS:HB3	1:A:129:LYS:HE3	1.61	0.42
1:A:234:LYS:HB3	1:A:234:LYS:HE3	1.79	0.42
1:A:228:LEU:HD12	1:A:241:PHE:HB3	2.03	0.41
2:B:53:MET:HE1	2:B:117:LYS:HG3	2.02	0.41
3:F:51:TRP:NE1	3:F:88:HIS:CE1	2.85	0.41
2:E:53:MET:HE1	2:E:117:LYS:HG3	2.03	0.41
1:A:151:ILE:HG23	1:A:208:TRP:HB2	2.03	0.41
1:A:164:TYR:OH	1:A:178:LEU:O	2.31	0.41
2:B:148:LYS:HG3	2:B:206:LEU:HD21	2.02	0.40
1:D:154:TYR:CZ	1:D:157:LYS:HA	2.56	0.40
1:D:187:PHE:HA	1:D:221:LEU:HD22	2.02	0.40
1:D:96:GLU:H	1:D:96:GLU:HG2	1.74	0.40
3:C:24:LEU:HD21	3:C:107:SER:HB3	2.04	0.40
1:D:42:ILE:HG22	1:D:87:TRP:CD1	2.57	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	308/343 (90%)	289 (94%)	19 (6%)	0	100	100
1	D	295/343 (86%)	270 (92%)	25 (8%)	0	100	100
2	B	217/233 (93%)	207 (95%)	10 (5%)	0	100	100
2	E	216/233 (93%)	204 (94%)	12 (6%)	0	100	100
3	C	205/209 (98%)	193 (94%)	12 (6%)	0	100	100
3	F	205/209 (98%)	189 (92%)	16 (8%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1446/1570 (92%)	1352 (94%)	94 (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	297/316 (94%)	260 (88%)	37 (12%)	4	19
1	D	286/316 (90%)	263 (92%)	23 (8%)	11	37
2	B	179/191 (94%)	168 (94%)	11 (6%)	17	46
2	E	179/191 (94%)	169 (94%)	10 (6%)	19	49
3	C	177/179 (99%)	168 (95%)	9 (5%)	21	52
3	F	177/179 (99%)	168 (95%)	9 (5%)	21	52
All	All	1295/1372 (94%)	1196 (92%)	99 (8%)	12	39

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	VAL
1	A	36	ARG
1	A	39	LEU
1	A	43	LYS
1	A	50	ARG
1	A	58	ARG
1	A	95	LYS
1	A	99	LEU
1	A	112	GLU
1	A	113	GLU
1	A	120	GLU
1	A	129	LYS
1	A	134	HIS
1	A	143	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	151	ILE
1	A	155	ILE
1	A	167	LEU
1	A	174	ARG
1	A	188	LYS
1	A	189	ASP
1	A	197	LEU
1	A	204	LYS
1	A	210	THR
1	A	215	LYS
1	A	217	ASP
1	A	229	ARG
1	A	234	LYS
1	A	238	SER
1	A	247	ILE
1	A	261	GLU
1	A	262	LYS
1	A	264	LEU
1	A	267	VAL
1	A	270	ASN
1	A	271	ARG
1	A	278	LYS
1	A	311	ASN
2	B	30	LEU
2	B	50	SER
2	B	54	GLN
2	B	64	LEU
2	B	84	LYS
2	B	91	ARG
2	B	140	VAL
2	B	144	SER
2	B	213	VAL
2	B	241	LYS
2	B	242	VAL
3	C	30	VAL
3	C	37	THR
3	C	38	VAL
3	C	65	ILE
3	C	139	ASP
3	C	140	GLU
3	C	154	ASN
3	C	192	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	198	LEU
1	D	40	SER
1	D	96	GLU
1	D	99	LEU
1	D	113	GLU
1	D	134	HIS
1	D	143	GLU
1	D	146	ASN
1	D	151	ILE
1	D	154	TYR
1	D	167	LEU
1	D	185	TYR
1	D	186	LYS
1	D	195	ASP
1	D	197	LEU
1	D	210	THR
1	D	217	ASP
1	D	226	PHE
1	D	229	ARG
1	D	238	SER
1	D	262	LYS
1	D	267	VAL
1	D	271	ARG
1	D	309	ASN
2	E	26	SER
2	E	40	VAL
2	E	49	SER
2	E	54	GLN
2	E	64	LEU
2	E	115	CYS
2	E	144	SER
2	E	148	LYS
2	E	213	VAL
2	E	243	GLU
3	F	37	THR
3	F	38	VAL
3	F	65	ILE
3	F	108	ARG
3	F	154	ASN
3	F	159	ARG
3	F	160	GLU
3	F	192	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	198	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	91	ASN
1	A	134	HIS
1	A	145	ASN
1	A	218	ASN
1	A	254	ASN
1	A	308	ASN
1	A	311	ASN
1	A	352	ASN
2	B	202	GLN
1	D	91	ASN
1	D	145	ASN
1	D	218	ASN
1	D	224	GLN
1	D	254	ASN
1	D	277	ASN
1	D	352	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are modelled with single atom - 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

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	316/343 (92%)	0.56	25 (7%) 18 10	82, 109, 149, 160	0
1	D	305/343 (88%)	0.66	33 (10%) 11 6	83, 136, 180, 216	0
2	B	148/233 (63%)	0.55	10 (6%) 23 12	74, 145, 193, 200	1 (0%)
2	E	132/233 (56%)	0.51	9 (6%) 23 12	88, 181, 215, 226	1 (0%)
3	C	136/209 (65%)	0.61	12 (8%) 15 9	159, 187, 240, 246	0
3	F	145/209 (69%)	1.12	26 (17%) 3 1	187, 211, 239, 245	0
All	All	1182/1570 (75%)	0.65	115 (9%) 13 7	74, 149, 222, 246	2 (0%)

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	116	GLY	6.5
3	F	114	ALA	6.2
3	F	106	GLY	6.2
3	F	105	CYS	5.4
3	F	117	ALA	5.2
3	F	115	PHE	5.1
1	A	147	ALA	5.1
1	D	356	ILE	4.7
1	A	145	ASN	4.6
3	C	132	VAL	4.6
3	C	150	VAL	4.4
3	F	51	TRP	4.3
3	F	24	LEU	4.2
2	B	127	GLY	4.2
3	F	127	VAL	4.1
3	F	26	GLN	3.9
3	F	25	THR	3.9
3	F	132	VAL	3.8
2	B	132	ASP	3.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	55	TRP	3.8
1	D	151	ILE	3.8
3	C	130	PRO	3.7
1	A	221	LEU	3.6
1	D	314	LEU	3.6
1	A	218	ASN	3.6
1	D	99	LEU	3.6
1	D	162	SER	3.5
2	B	130	ASP	3.4
2	E	135	GLY	3.3
3	C	127	VAL	3.3
1	D	148	GLU	3.3
3	C	60	ALA	3.2
1	D	332	PHE	3.2
1	D	39	LEU	3.2
3	F	130	PRO	3.2
3	F	50	GLY	3.1
1	A	68	LEU	3.1
1	D	340	ALA	3.1
1	D	161	LEU	3.0
1	D	250	VAL	3.0
3	F	148	SER	3.0
1	A	49	ILE	3.0
1	D	98	ASP	3.0
1	A	232	ILE	3.0
1	A	231	TYR	2.9
1	A	167	LEU	2.9
1	D	328	TYR	2.9
2	B	136	HIS	2.8
1	D	190	ASP	2.8
1	A	143	GLU	2.8
3	F	42	CYS	2.8
1	A	74	GLU	2.8
2	B	114	TYR	2.8
3	F	129	ALA	2.8
1	D	38	GLU	2.8
2	B	113	TYR	2.7
1	D	185	TYR	2.7
2	B	181	VAL	2.6
1	D	357	TYR	2.6
1	A	95	LYS	2.6
1	A	121	ASP	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	75	THR	2.6
2	E	242	VAL	2.6
3	C	134	ILE	2.5
1	A	228	LEU	2.5
2	E	122	ASP	2.5
1	D	106	PHE	2.4
1	D	186	LYS	2.4
1	D	97	THR	2.4
3	F	91	THR	2.4
1	A	230	PRO	2.4
2	B	125	ILE	2.4
1	D	156	LEU	2.4
2	B	138	THR	2.4
1	D	32	HIS	2.4
2	E	39	LEU	2.4
1	A	50	ARG	2.3
2	E	99	ARG	2.3
2	B	25	GLU	2.3
1	D	37	THR	2.3
1	A	335	ILE	2.3
3	F	44	GLY	2.3
1	D	298	ASN	2.3
1	A	38	GLU	2.3
1	A	227	PHE	2.3
1	D	315	ILE	2.2
3	C	65	ILE	2.2
1	D	177	PHE	2.2
1	A	217	ASP	2.2
1	D	197	LEU	2.2
3	F	58	GLY	2.2
1	A	177	PHE	2.2
3	F	37	THR	2.2
1	A	164	TYR	2.2
1	D	333	VAL	2.1
3	F	161	ALA	2.1
2	E	77	THR	2.1
1	A	135	ARG	2.1
3	C	108	ARG	2.1
3	F	33	ASN	2.1
1	D	104	HIS	2.1
1	D	150	THR	2.1
3	F	131	SER	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	C	149	VAL	2.1
1	A	235	ASN	2.1
3	F	113	GLY	2.1
1	D	310	GLU	2.1
1	D	58	ARG	2.0
3	C	135	PHE	2.0
3	F	27	PRO	2.0
1	A	202	HIS	2.0
3	C	139	ASP	2.0
3	C	156	PHE	2.0
2	E	25	GLU	2.0
2	E	67	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](#)

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, 95th 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(Å ²)	Q<0.9
4	NH4	E	301	1/1	0.46	0.36	118,118,118,118	0
4	NH4	B	301	1/1	0.63	0.53	72,72,72,72	0

6.5 Other polymers [i](#)

There are no such residues in this entry.