



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:13 AM UTC

PDB ID : 7WVL / pdb_00007wvl
Title : Structure of P4A2 Fab in complex with Spike-RBD from SARS-CoV-2
Authors : Narayanan, N.; Nair, D.T.
Deposited on : 2022-02-10
Resolution : 3.00 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

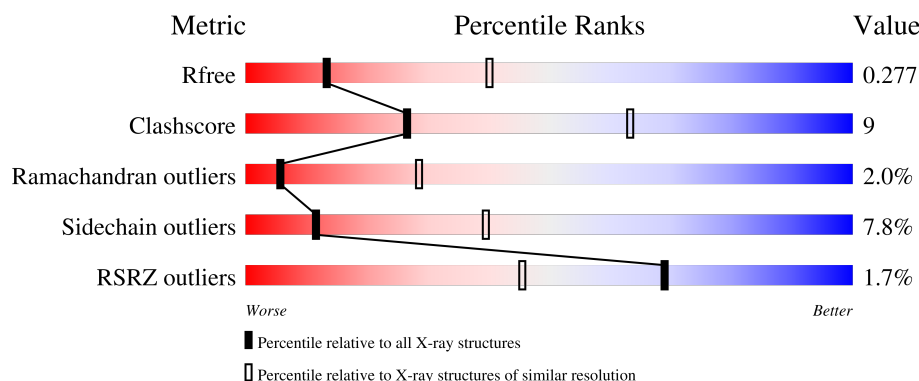
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	L	218	 74% 23% ..
2	H	212	 % 70% 25% .
3	F	223	 3% 58% 19% . 21%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4627 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 P4A2 Fab Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	216	Total	C	N	O	S	0	0	0
			1660	1034	288	331	7			

- Molecule 2 is a protein called P4A2 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	212	Total	C	N	O	S	0	0	0
			1566	984	253	321	8			

- Molecule 3 is a protein called Spike protein S1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	177	Total	C	N	O	S	0	0	0
			1341	847	230	259	5			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	533	GLY	-	expression tag	UNP P0DTC2
F	534	SER	-	expression tag	UNP P0DTC2
F	535	LEU	-	expression tag	UNP P0DTC2
F	536	GLU	-	expression tag	UNP P0DTC2
F	537	VAL	-	expression tag	UNP P0DTC2
F	538	LEU	-	expression tag	UNP P0DTC2
F	539	PHE	-	expression tag	UNP P0DTC2
F	540	GLN	-	expression tag	UNP P0DTC2
F	541	GLY	-	expression tag	UNP P0DTC2
F	542	PRO	-	expression tag	UNP P0DTC2
F	543	GLY	-	expression tag	UNP P0DTC2
F	544	SER	-	expression tag	UNP P0DTC2
F	545	HIS	-	expression tag	UNP P0DTC2
F	546	HIS	-	expression tag	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
F	547	HIS	-	expression tag	UNP P0DTC2
F	548	HIS	-	expression tag	UNP P0DTC2
F	549	HIS	-	expression tag	UNP P0DTC2
F	550	HIS	-	expression tag	UNP P0DTC2
F	551	HIS	-	expression tag	UNP P0DTC2
F	552	HIS	-	expression tag	UNP P0DTC2
F	553	HIS	-	expression tag	UNP P0DTC2
F	554	HIS	-	expression tag	UNP P0DTC2

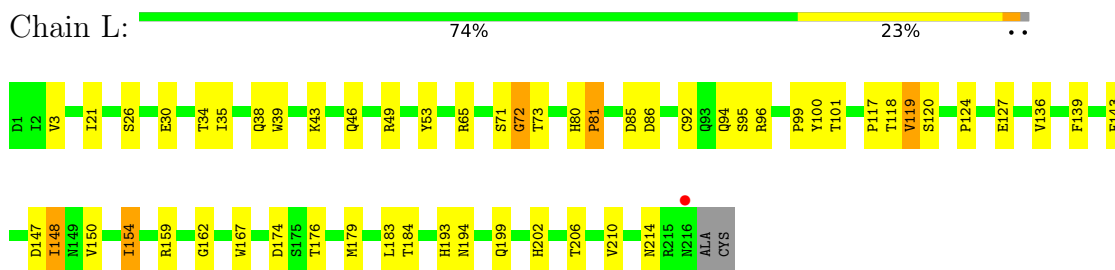
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	L	23	Total O 23 23	0	0
4	H	25	Total O 25 25	0	0
4	F	12	Total O 12 12	0	0

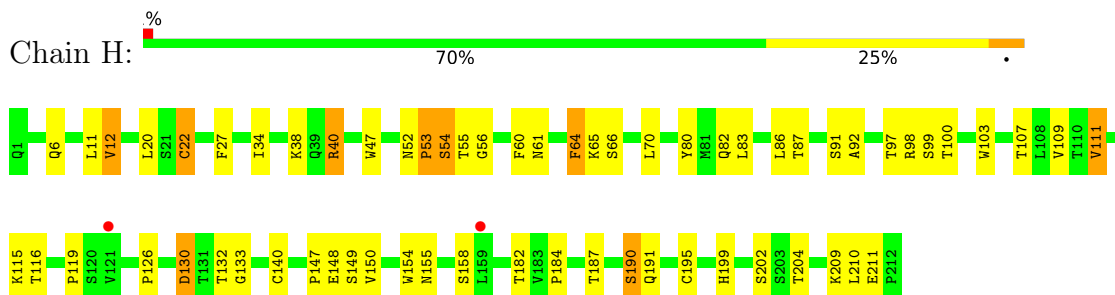
3 Residue-property plots [i](#)

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.

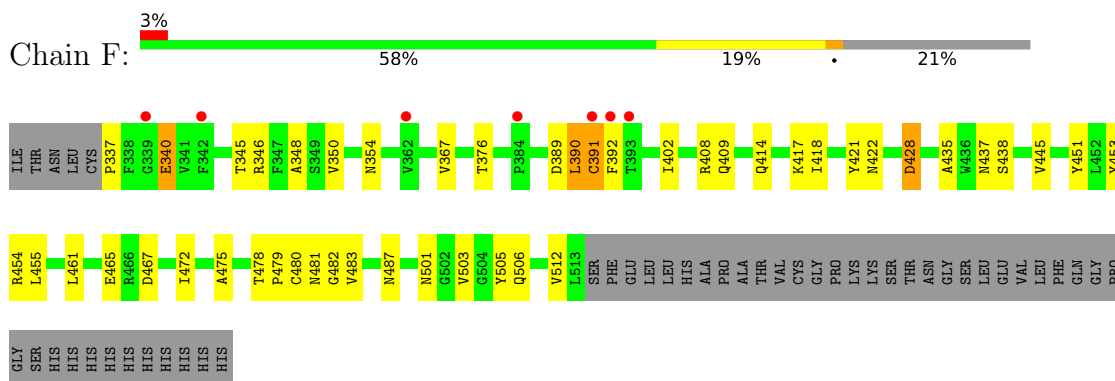
• Molecule 1: P4A2 Fab Light Chain



• Molecule 2: P4A2 Fab heavy chain



• Molecule 3: Spike protein S1



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	85.31Å 85.31Å 205.19Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	73.88 – 3.00 73.88 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.4 (73.88-3.00) 99.6 (73.88-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.233 , 0.279 0.232 , 0.277	Depositor DCC
R_{free} test set	1379 reflections (7.65%)	wwPDB-VP
Wilson B-factor (Å ²)	93.1	Xtriage
Anisotropy	0.096	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 72.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for -h,-k,l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	4627	wwPDB-VP
Average B, all atoms (Å ²)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.02% 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	L	0.14	0/1697	0.35	0/2305
2	H	0.14	0/1605	0.40	0/2197
3	F	0.24	0/1375	0.43	2/1875 (0.1%)
All	All	0.18	0/4677	0.39	2/6377 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	F	337	PRO	N-CA-CB	6.65	110.31	103.00
3	F	391	CYS	N-CA-C	5.54	122.61	110.80

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	L	1660	0	1603	27	0
2	H	1566	0	1507	32	0
3	F	1341	0	1192	25	0
4	F	12	0	0	1	0
4	H	25	0	0	3	0
4	L	23	0	0	1	0
All	All	4627	0	4302	82	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 9.

All (82) 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:H:91:SER:HB3	2:H:111:VAL:HG12	1.65	0.78
1:L:124:PRO:HD3	1:L:136:VAL:HG22	1.69	0.75
1:L:3:VAL:HG22	1:L:26:SER:HB3	1.67	0.75
2:H:52:ASN:O	2:H:54:SER:N	2.24	0.70
1:L:150:VAL:HG21	1:L:179:MET:HE1	1.78	0.66
1:L:167:TRP:CD1	1:L:179:MET:HG3	2.32	0.65
1:L:80:HIS:HB3	1:L:81:PRO:HD3	1.78	0.64
3:F:461:LEU:HD22	3:F:465:GLU:HB3	1.78	0.64
1:L:199:GLN:HG2	1:L:210:VAL:HG22	1.79	0.64
2:H:190:SER:OG	2:H:191:GLN:N	2.26	0.64
2:H:97:THR:HG1	2:H:103:TRP:CD1	2.17	0.63
2:H:12:VAL:HG21	2:H:86:LEU:HD12	1.80	0.62
2:H:20:LEU:HD22	2:H:107:THR:HG21	1.82	0.62
1:L:95:SER:HA	1:L:100:TYR:HD1	1.65	0.61
2:H:184:PRO:O	2:H:187:THR:OG1	2.19	0.61
3:F:451:TYR:HA	4:F:609:HOH:O	2.01	0.59
3:F:472:ILE:HD13	3:F:482:GLY:HA2	1.84	0.59
3:F:428:ASP:OD1	3:F:428:ASP:N	2.36	0.59
3:F:348:ALA:HB2	3:F:354:ASN:HB2	1.85	0.59
2:H:83:LEU:HB3	2:H:86:LEU:HD21	1.85	0.58
3:F:422:ASN:HD21	3:F:454:ARG:H	1.52	0.58
3:F:453:TYR:HE2	3:F:455:LEU:HD13	1.69	0.58
1:L:71:SER:O	1:L:73:THR:N	2.39	0.56
1:L:65:ARG:HB3	1:L:81:PRO:HD2	1.87	0.56
1:L:127:GLU:N	1:L:127:GLU:OE1	2.39	0.55
3:F:376:THR:HB	3:F:435:ALA:HB3	1.88	0.55
1:L:38:GLN:HG3	1:L:53:TYR:HA	1.88	0.55
2:H:40:ARG:HG3	2:H:92:ALA:HB2	1.89	0.54
1:L:65:ARG:HG2	1:L:81:PRO:HG2	1.89	0.54
2:H:132:THR:OG1	2:H:133:GLY:N	2.42	0.53
1:L:117:PRO:HB3	1:L:143:PHE:HB3	1.90	0.53
2:H:27:PHE:CZ	2:H:98:ARG:HD2	2.45	0.52
3:F:475:ALA:HB3	3:F:487:ASN:HB3	1.92	0.51
2:H:70:LEU:O	4:H:301:HOH:O	2.19	0.51
3:F:437:ASN:OD1	3:F:438:SER:N	2.44	0.51
2:H:119:PRO:HD3	2:H:199:HIS:CD2	2.46	0.51
3:F:479:PRO:O	3:F:481:ASN:N	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:61:ASN:HA	2:H:64:PHE:HB2	1.93	0.50
2:H:70:LEU:HG	2:H:80:TYR:HB2	1.92	0.50
1:L:174:ASP:HB3	1:L:176:THR:HG23	1.92	0.50
1:L:99:PRO:HG3	2:H:60:PHE:CZ	2.48	0.49
1:L:154:ILE:HD11	1:L:193:HIS:CG	2.48	0.49
3:F:454:ARG:NH2	3:F:467:ASP:O	2.43	0.49
1:L:194:ASN:OD1	1:L:214:ASN:ND2	2.46	0.48
3:F:478:THR:HG22	3:F:480:CYS:H	1.78	0.48
3:F:409:GLN:OE1	3:F:418:ILE:N	2.46	0.48
3:F:472:ILE:H	3:F:472:ILE:HD12	1.78	0.48
1:L:39:TRP:CZ3	1:L:92:CYS:HB3	2.49	0.47
1:L:95:SER:HA	1:L:100:TYR:CD1	2.48	0.47
3:F:501:ASN:HB3	3:F:505:TYR:HB2	1.96	0.47
2:H:91:SER:HA	2:H:109:VAL:HG23	1.96	0.47
1:L:65:ARG:NH2	1:L:86:ASP:OD1	2.49	0.46
1:L:43:LYS:NZ	1:L:85:ASP:OD2	2.44	0.46
2:H:155:ASN:HB3	2:H:158:SER:HB3	1.97	0.45
3:F:350:VAL:HG11	3:F:418:ILE:HG13	1.98	0.45
1:L:46:GLN:HG2	4:L:320:HOH:O	2.15	0.45
2:H:38:LYS:HE2	2:H:40:ARG:HE	1.81	0.45
3:F:417:LYS:O	3:F:421:TYR:HB2	2.16	0.45
3:F:350:VAL:HB	3:F:422:ASN:HD22	1.82	0.45
2:H:126:PRO:HB2	2:H:130:ASP:CG	2.42	0.44
3:F:408:ARG:H	3:F:408:ARG:HG2	1.49	0.44
2:H:66:SER:O	2:H:83:LEU:HA	2.17	0.44
2:H:87:THR:O	2:H:111:VAL:HG11	2.17	0.44
1:L:148:ILE:HD12	1:L:202:HIS:HB2	1.99	0.44
2:H:6:GLN:HG2	2:H:22:CYS:HB2	1.99	0.44
3:F:340:GLU:H	3:F:340:GLU:HG3	1.57	0.44
2:H:154:TRP:HZ3	2:H:210:LEU:HD11	1.82	0.44
2:H:56:GLY:HA2	4:H:322:HOH:O	2.18	0.43
2:H:202:SER:O	2:H:204:THR:HG23	2.18	0.43
1:L:119:VAL:HA	1:L:139:PHE:O	2.18	0.43
3:F:345:THR:HG23	3:F:346:ARG:HD2	1.99	0.43
3:F:503:VAL:O	3:F:506:GLN:HB2	2.18	0.43
1:L:159:ARG:HE	1:L:159:ARG:HA	1.84	0.42
1:L:35:ILE:HD13	1:L:72:GLY:H	1.84	0.42
2:H:11:LEU:HB2	2:H:147:PRO:HG3	2.02	0.42
2:H:12:VAL:O	2:H:111:VAL:HA	2.18	0.42
2:H:52:ASN:OD1	3:F:483:VAL:HG21	2.20	0.42
2:H:53:PRO:O	2:H:54:SER:OG	2.36	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:389:ASP:O	3:F:390:LEU:HB3	2.20	0.41
2:H:80:TYR:N	4:H:301:HOH:O	2.53	0.41
2:H:209:LYS:HZ2	2:H:211:GLU:HG2	1.86	0.41
1:L:162:GLY:O	1:L:183:LEU:HA	2.22	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	L	214/218 (98%)	200 (94%)	12 (6%)	2 (1%)	14	48
2	H	210/212 (99%)	185 (88%)	19 (9%)	6 (3%)	3	20
3	F	175/223 (78%)	143 (82%)	28 (16%)	4 (2%)	5	25
All	All	599/653 (92%)	528 (88%)	59 (10%)	12 (2%)	6	28

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	72	GLY
2	H	54	SER
2	H	149	SER
3	F	391	CYS
3	F	392	PHE
1	L	81	PRO
2	H	55	THR
3	F	390	LEU
2	H	47	TRP
2	H	65	LYS
2	H	53	PRO
3	F	512	VAL

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	L	187/190 (98%)	172 (92%)	15 (8%)	11	38
2	H	179/183 (98%)	161 (90%)	18 (10%)	7	29
3	F	133/193 (69%)	127 (96%)	6 (4%)	24	59
All	All	499/566 (88%)	460 (92%)	39 (8%)	11	39

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	21	ILE
1	L	30	GLU
1	L	34	THR
1	L	49	ARG
1	L	94	GLN
1	L	96	ARG
1	L	101	THR
1	L	118	THR
1	L	119	VAL
1	L	120	SER
1	L	147	ASP
1	L	148	ILE
1	L	154	ILE
1	L	184	THR
1	L	206	THR
2	H	12	VAL
2	H	22	CYS
2	H	34	ILE
2	H	40	ARG
2	H	64	PHE
2	H	82	GLN
2	H	99	SER
2	H	100	THR
2	H	111	VAL
2	H	115	LYS
2	H	116	THR

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Mol	Chain	Res	Type
2	H	130	ASP
2	H	140	CYS
2	H	148	GLU
2	H	150	VAL
2	H	182	THR
2	H	190	SER
2	H	195	CYS
3	F	340	GLU
3	F	367	VAL
3	F	402	ILE
3	F	414	GLN
3	F	428	ASP
3	F	445	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	17	GLN
1	L	93	GLN
1	L	94	GLN
1	L	141	ASN
2	H	199	HIS
3	F	422	ASN
3	F	439	ASN
3	F	487	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	L	216/218 (99%)	-0.24	1 (0%) 87 72	52, 76, 115, 135	0
2	H	212/212 (100%)	-0.06	2 (0%) 81 61	52, 79, 125, 141	0
3	F	177/223 (79%)	0.36	7 (3%) 42 23	72, 114, 185, 206	0
All	All	605/653 (92%)	-0.00	10 (1%) 69 45	52, 85, 155, 206	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	391	CYS	3.3
3	F	393	THR	2.9
3	F	362	VAL	2.6
3	F	392	PHE	2.4
1	L	216	ASN	2.3
3	F	384	PRO	2.2
3	F	342	PHE	2.2
2	H	159	LEU	2.2
3	F	339	GLY	2.1
2	H	121	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.