



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 06:05 AM UTC

PDB ID : 1XCQ / pdb_00001xcq
Title : Complex HCV core-Fab 19D9D6-Protein L mutant (D55A,L57H,Y64W) in space group P21
Authors : Menez, R.; Housden, N.G.; Harrison, S.; Jolivet-Reynaud, C.; Gore, M.G.; Stura, E.A.
Deposited on : 2004-09-03
Resolution : 3.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

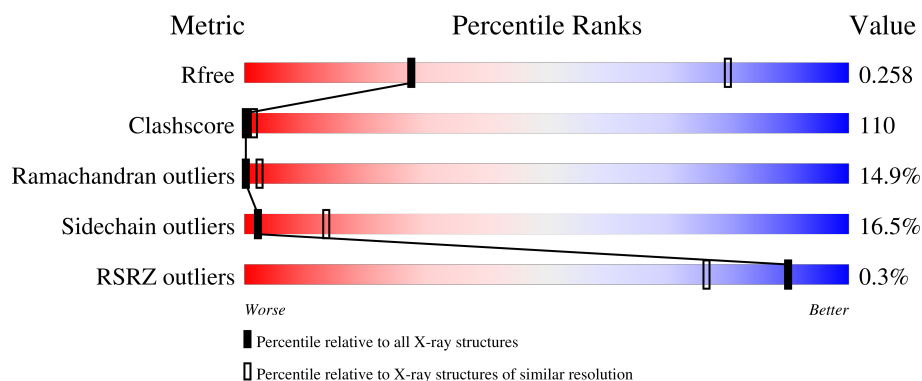
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	P	44	5% 5% 25% 20% 45%
1	Q	44	5% 25% 41% 30%
1	S	44	2% 7% 25% 32% 36%
2	A	220	• 10% 70% 16%
2	C	220	• 19% 56% 24%

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Mol	Chain	Length	Quality of chain
2	E	220	
2	G	220	
3	B	218	
3	D	218	
3	F	218	
3	H	218	
4	L	80	
4	M	80	
4	N	80	
4	O	80	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16467 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 Capsid protein C.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	P	24	Total	C	N	O	0	0	0
			167	106	33	28			
1	Q	44	Total	C	N	O	0	0	0
			346	213	75	58			
1	S	44	Total	C	N	O	0	0	0
			346	213	75	58			

- Molecule 2 is a protein called Monoclonal antibody 19D9D6 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			
2	C	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			
2	E	220	Total	C	N	O	S	0	0	0
			1708	1063	291	346	8			
2	G	219	Total	C	N	O	S	0	0	0
			1701	1060	290	344	7			

- Molecule 3 is a protein called Monoclonal antibody 19D9D6 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			
3	D	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			
3	F	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			
3	H	218	Total	C	N	O	S	0	0	0
			1660	1058	270	325	7			

- Molecule 4 is a protein called Protein L.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	L	66	Total	C	N	O	S	0	0	0
			507	322	85	99	1			
4	M	62	Total	C	N	O	S	0	0	0
			480	305	80	94	1			
4	N	64	Total	C	N	O	S	0	0	0
			490	311	82	96	1			
4	O	62	Total	C	N	O	S	0	0	0
			480	305	80	94	1			

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	P	1	Total	O	0	0
			1	1		
5	A	29	Total	O	0	0
			29	29		
5	B	31	Total	O	0	0
			31	31		
5	L	9	Total	O	0	0
			9	9		
5	C	13	Total	O	0	0
			13	13		
5	D	10	Total	O	0	0
			10	10		
5	Q	6	Total	O	0	0
			6	6		
5	M	3	Total	O	0	0
			3	3		
5	E	17	Total	O	0	0
			17	17		
5	F	34	Total	O	0	0
			34	34		
5	N	7	Total	O	0	0
			7	7		
5	S	3	Total	O	0	0
			3	3		
5	G	11	Total	O	0	0
			11	11		
5	H	9	Total	O	0	0
			9	9		
5	O	3	Total	O	0	0
			3	3		

3 Residue-property plots

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: Capsid protein C

Chain P: 5% 5% 25% 20% 45%



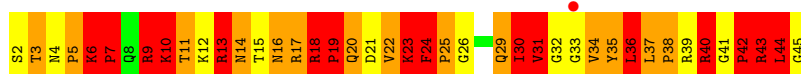
- Molecule 1: Capsid protein C

Chain Q: 5% 25% 41% 30%



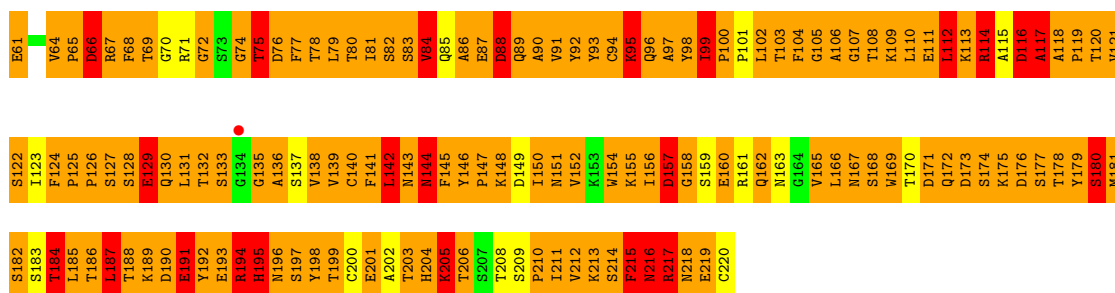
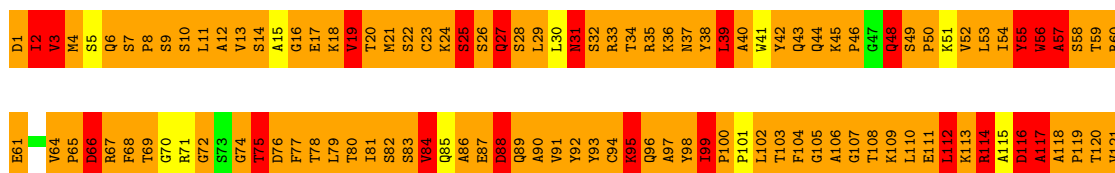
- Molecule 1: Capsid protein C

Chain S: 2% 7% 25% 32% 36%

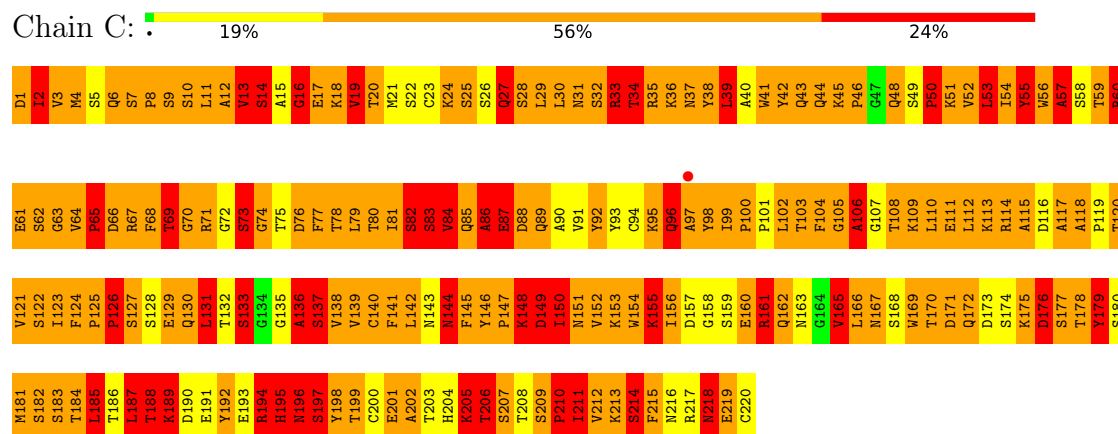


- Molecule 2: Monoclonal antibody 19D9D6 Light chain

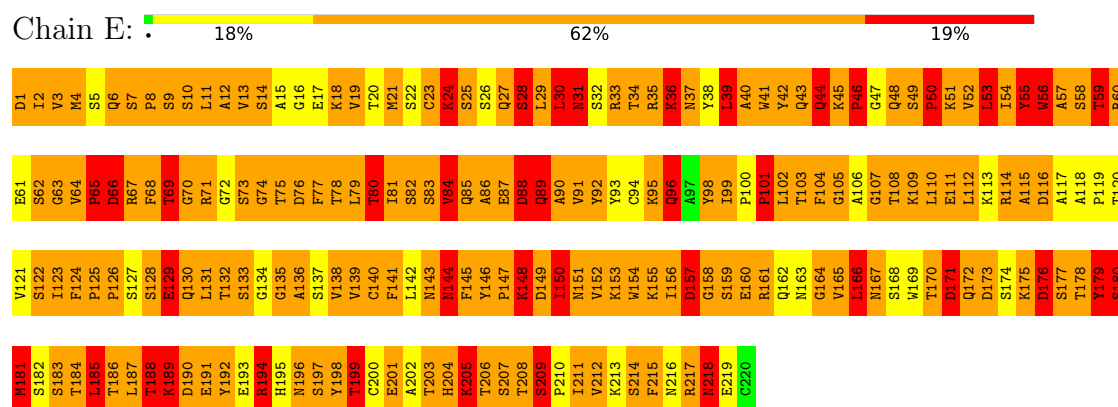
Chain A: 10% 70% 16%



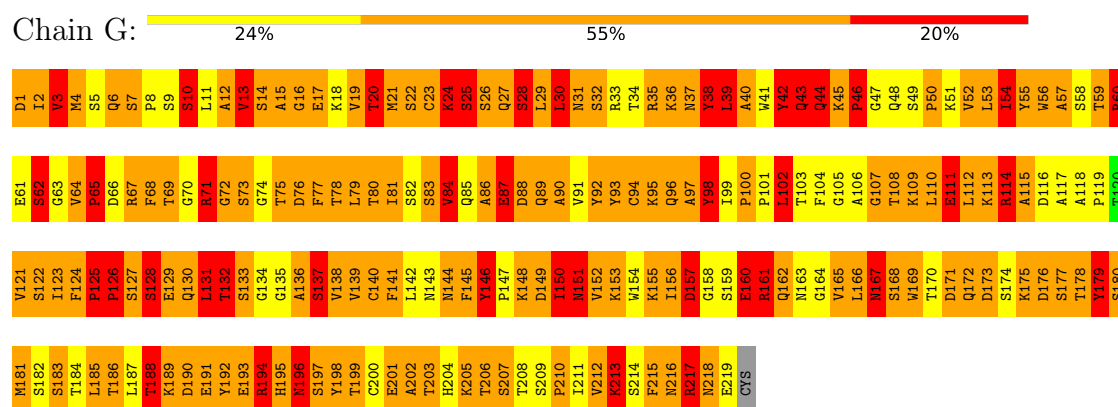
- Molecule 2: Monoclonal antibody 19D9D6 Light chain



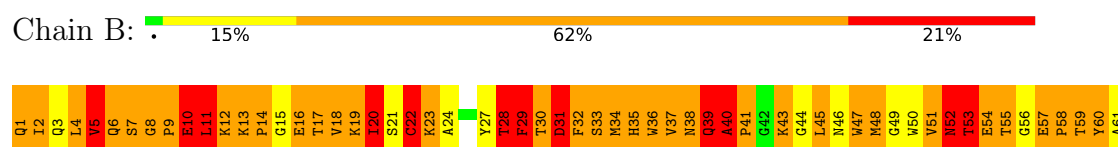
• Molecule 2: Monoclonal antibody 19D9D6 Light chain

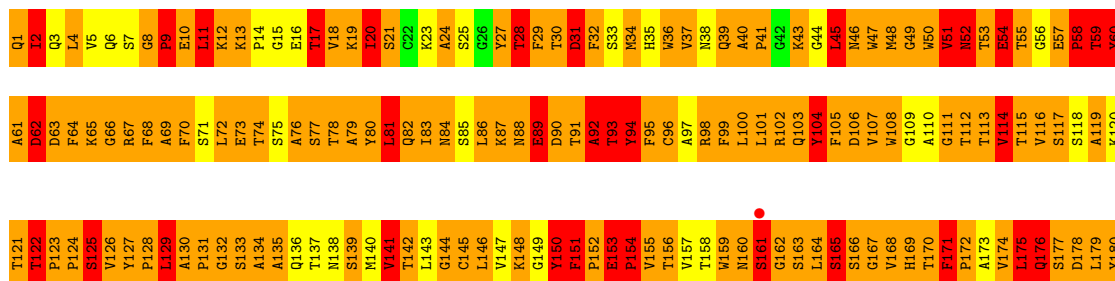


• Molecule 2: Monoclonal antibody 19D9D6 Light chain



• Molecule 3: Monoclonal antibody 19D9D6 Heavy chain





T181 L182 S183 S184 S185 V186 V187 V188 P189 S190 S191 T192 V193 P194 S195 E196 T197 V198 T199 C200 N201 V202 A203 H204 P205 A206 S207 S208 T209 K210 V211 D212 K213 K214 I215 V216 P217 R218

• Molecule 4: Protein L

Chain L: 14% 55% 14% 18%

MET ASN ILE LYS PHE D67 L68 E69 D70 G71 G72 N73 H74 H75 N76 P17 K18 K78 E19 F79 E20 V25 N26 L27 L28 F29 A30 D31 G32 K33 I34 Q35 T36 A37 E38 F39 K40 G41 T42 F43 E44 E45 A46 T47 A48 E49 A50 Y51 R52 Y53 A54 A55 L56 H57 A58 K59 V60 N61 G62

E63 W64 T65 A66 D67 L68 E69 D70 G71 G72 N73 H74 H75 N76 I77 K78 F79 A80 G81 K82

• Molecule 4: Protein L

Chain M: 12% 48% 16% 22%

MET ASN ILE LYS PHE D67 L68 E69 D70 G71 G72 N73 H74 H75 N76 P17 K18 K78 E19 F79 E20 V25 N26 L27 L28 F29 A30 D31 G32 K33 I34 Q35 T36 A37 E38 F39 K40 G41 T42 F43 E44 E45 A46 T47 A48 E49 A50 Y51 R52 Y53 A54 A55 L56 H57 A58 K59 V60 N61 G62

E63 W64 T65 A66 D67 L68 E69 D70 G71 G72 N73 H74 H75 N76 I77 K78 F79 A80 G81 LYS

• Molecule 4: Protein L

Chain N: 12% 48% 19% 20%

MET ASN ILE LYS PHE D67 L68 E69 D70 G71 G72 N73 H74 H75 N76 P17 K18 K78 E19 F79 E20 V25 N26 L27 L28 F29 A30 D31 G32 K33 I34 Q35 T36 A37 E38 F39 K40 G41 T42 F43 E44 E45 A46 T47 A48 E49 A50 Y51 R52 Y53 A54 A55 L56 H57 A58 K59 V60 N61 G62

E63 W64 T65 A66 D67 L68 E69 D70 G71 G72 N73 H74 H75 N76 I77 K78 F79 A80 G81 LYS

• Molecule 4: Protein L

Chain O: 14% 48% 12% 22%

MET ASN ILE LYS PHE D67 L68 E69 D70 G71 G72 N73 H74 H75 N76 P17 K18 K78 E19 F79 E20 V25 N26 L27 L28 F29 A30 D31 G32 K33 I34 Q35 T36 A37 E38 F39 K40 G41 T42 F43 E44 E45 A46 T47 A48 E49 A50 Y51 R52 Y53 A54 A55 L56 H57 A58 K59 V60 N61 G62

E63 W64 T65 A66 D67 L68 E69 D70 G71 G72 N73 H74 H75 N76 I77 K78 F79 A80 G81 LYS

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	43.60Å 230.52Å 123.64Å 90.00° 91.67° 90.00°	Depositor
Resolution (Å)	21.62 – 3.50 21.62 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (21.62-3.50) 99.0 (21.62-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.53Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.192 , 0.264 0.196 , 0.258	Depositor DCC
R_{free} test set	1535 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	72.1	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 204.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.116 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16467	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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	P	3.59	27/170 (15.9%)	2.25	8/229 (3.5%)
1	Q	4.54	79/353 (22.4%)	2.45	23/472 (4.9%)
1	S	3.84	65/353 (18.4%)	2.52	17/472 (3.6%)
2	A	4.93	477/1745 (27.3%)	2.58	135/2366 (5.7%)
2	C	4.54	393/1745 (22.5%)	2.53	124/2366 (5.2%)
2	E	4.88	475/1745 (27.2%)	2.70	139/2366 (5.9%)
2	G	4.45	407/1738 (23.4%)	2.53	125/2358 (5.3%)
3	B	4.93	452/1707 (26.5%)	2.63	141/2335 (6.0%)
3	D	4.78	428/1707 (25.1%)	2.55	144/2335 (6.2%)
3	F	4.85	477/1707 (27.9%)	2.58	138/2335 (5.9%)
3	H	4.69	413/1707 (24.2%)	2.64	134/2335 (5.7%)
4	L	4.88	147/517 (28.4%)	2.67	46/695 (6.6%)
4	M	4.75	130/489 (26.6%)	2.51	34/659 (5.2%)
4	N	4.84	149/499 (29.9%)	2.42	32/673 (4.8%)
4	O	4.83	118/489 (24.1%)	2.65	41/659 (6.2%)
All	All	4.74	4237/16671 (25.4%)	2.58	1281/22655 (5.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	1
2	E	0	3
2	G	0	2
3	D	0	1
3	F	0	1
3	H	0	1
4	L	0	1
All	All	0	10

The worst 5 of 4237 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	121	VAL	CA-CB	-27.29	1.21	1.54
2	A	192	TYR	CA-C	-25.61	1.27	1.52
3	H	9	PRO	CA-C	-24.04	1.26	1.52
2	A	106	ALA	CA-C	-23.69	1.21	1.52
1	Q	11	THR	CA-CB	23.64	1.75	1.54

The worst 5 of 1281 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	6	LYS	CA-C-N	18.32	142.74	119.84
1	S	6	LYS	C-N-CA	18.32	142.74	119.84
2	A	100	PRO	N-CA-C	-14.24	93.33	110.70
3	B	90	ASP	N-CA-C	-13.31	97.01	113.38
2	G	66	ASP	N-CA-C	-13.11	97.29	113.02

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	179	TYR	Sidechain
3	D	127	TYR	Sidechain
2	E	28	SER	Mainchain
2	E	55	TYR	Sidechain
4	L	53	TYR	Sidechain

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	P	167	0	162	40	0
1	Q	346	0	366	103	2
1	S	346	0	366	98	1
2	A	1708	0	1658	388	0
2	C	1708	0	1658	380	2
2	E	1708	0	1658	372	0
2	G	1701	0	1653	456	0
3	B	1660	0	1615	339	0
3	D	1660	0	1615	366	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1660	0	1615	304	0
3	H	1660	0	1615	437	0
4	L	507	0	482	93	0
4	M	480	0	457	105	0
4	N	490	0	461	114	0
4	O	480	0	457	135	1
5	A	29	0	0	0	0
5	B	31	0	0	0	0
5	C	13	0	0	0	0
5	D	10	0	0	2	0
5	E	17	0	0	4	0
5	F	34	0	0	5	0
5	G	11	0	0	4	0
5	H	9	0	0	4	0
5	L	9	0	0	1	0
5	M	3	0	0	1	0
5	N	7	0	0	0	0
5	O	3	0	0	0	0
5	P	1	0	0	1	0
5	Q	6	0	0	1	0
5	S	3	0	0	0	0
All	All	16467	0	15838	3518	3

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 110.

The worst 5 of 3518 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:Q:22:VAL:CA	1:Q:22:VAL:CB	1.75	1.65
1:S:3:THR:CB	1:S:3:THR:CG2	1.74	1.65
2:C:189:LYS:CA	2:C:189:LYS:CB	1.75	1.64
2:E:153:LYS:CB	2:E:153:LYS:CG	1.75	1.63
2:G:156:ILE:CB	2:G:156:ILE:CG2	1.77	1.63

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:149:ASP:OD1	1:Q:10:LYS:O[1_455]	2.02	0.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:171:ASP:OD1	1:Q:18:ARG:NH1[1_455]	2.11	0.09
1:S:21:ASP:OD2	4:O:22:THR:OG1[1_655]	2.12	0.08

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	P	22/44 (50%)	5 (23%)	4 (18%)	13 (59%)	0	0
1	Q	42/44 (96%)	14 (33%)	15 (36%)	13 (31%)	0	0
1	S	42/44 (96%)	10 (24%)	14 (33%)	18 (43%)	0	0
2	A	218/220 (99%)	158 (72%)	38 (17%)	22 (10%)	0	6
2	C	218/220 (99%)	147 (67%)	35 (16%)	36 (16%)	0	2
2	E	218/220 (99%)	163 (75%)	34 (16%)	21 (10%)	0	6
2	G	217/220 (99%)	147 (68%)	38 (18%)	32 (15%)	0	3
3	B	216/218 (99%)	144 (67%)	39 (18%)	33 (15%)	0	2
3	D	216/218 (99%)	142 (66%)	40 (18%)	34 (16%)	0	2
3	F	216/218 (99%)	149 (69%)	39 (18%)	28 (13%)	0	3
3	H	216/218 (99%)	138 (64%)	51 (24%)	27 (12%)	0	4
4	L	64/80 (80%)	47 (73%)	8 (12%)	9 (14%)	0	3
4	M	60/80 (75%)	33 (55%)	19 (32%)	8 (13%)	0	3
4	N	62/80 (78%)	39 (63%)	13 (21%)	10 (16%)	0	2
4	O	60/80 (75%)	37 (62%)	16 (27%)	7 (12%)	0	4
All	All	2087/2204 (95%)	1373 (66%)	403 (19%)	311 (15%)	0	2

5 of 311 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	20	GLN

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Mol	Chain	Res	Type
1	P	25	PRO
1	P	34	VAL
1	P	35	TYR
1	P	37	LEU

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	P	15/37 (40%)	13 (87%)	2 (13%)	4	20
1	Q	37/37 (100%)	28 (76%)	9 (24%)	1	4
1	S	37/37 (100%)	26 (70%)	11 (30%)	0	2
2	A	195/195 (100%)	169 (87%)	26 (13%)	4	20
2	C	195/195 (100%)	158 (81%)	37 (19%)	1	8
2	E	195/195 (100%)	161 (83%)	34 (17%)	2	11
2	G	194/195 (100%)	168 (87%)	26 (13%)	4	20
3	B	187/187 (100%)	154 (82%)	33 (18%)	2	11
3	D	187/187 (100%)	159 (85%)	28 (15%)	3	17
3	F	187/187 (100%)	152 (81%)	35 (19%)	1	9
3	H	187/187 (100%)	160 (86%)	27 (14%)	3	18
4	L	48/62 (77%)	40 (83%)	8 (17%)	2	13
4	M	46/62 (74%)	38 (83%)	8 (17%)	2	11
4	N	46/62 (74%)	37 (80%)	9 (20%)	1	8
4	O	46/62 (74%)	42 (91%)	4 (9%)	9	33
All	All	1802/1887 (96%)	1505 (84%)	297 (16%)	2	13

5 of 297 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	S	13	ARG
3	H	154	PRO

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Mol	Chain	Res	Type
1	S	31	VAL
2	G	160	GLU
2	C	176	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 76 such sidechains are listed below:

Mol	Chain	Res	Type
4	N	35	GLN
2	G	216	ASN
1	S	29	GLN
2	G	130	GLN
4	O	76	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](#)

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
3	F	3
2	G	2
3	B	1
2	A	1
3	D	1

The worst 5 of 8 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	212:ASP	C	213:LYS	N	1.19
1	F	113:THR	C	114:VAL	N	1.19
1	F	131:PRO	C	132:GLY	N	1.19
1	F	193:TRP	C	194:PRO	N	1.19
1	A	171:ASP	C	172:GLN	N	1.17

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	P	24/44 (54%)	-0.03	0 100 100	88, 139, 163, 172	0
1	Q	44/44 (100%)	-0.02	0 100 100	63, 126, 196, 211	0
1	S	44/44 (100%)	0.15	1 (2%) 61 37	69, 131, 193, 203	0
2	A	220/220 (100%)	-0.53	1 (0%) 87 68	29, 41, 78, 152	0
2	C	220/220 (100%)	-0.40	1 (0%) 87 68	29, 53, 109, 182	0
2	E	220/220 (100%)	-0.53	0 100 100	27, 40, 81, 135	0
2	G	219/220 (99%)	-0.42	0 100 100	28, 54, 107, 158	0
3	B	218/218 (100%)	-0.52	0 100 100	27, 40, 85, 180	0
3	D	218/218 (100%)	-0.52	2 (0%) 81 58	26, 47, 115, 165	0
3	F	218/218 (100%)	-0.57	0 100 100	26, 39, 78, 143	0
3	H	218/218 (100%)	-0.43	1 (0%) 87 68	27, 48, 111, 164	0
4	L	66/80 (82%)	-0.47	0 100 100	27, 49, 99, 163	0
4	M	62/80 (77%)	-0.36	0 100 100	28, 46, 84, 115	0
4	N	64/80 (80%)	-0.46	0 100 100	27, 50, 110, 151	0
4	O	62/80 (77%)	-0.47	0 100 100	30, 47, 81, 103	0
All	All	2117/2204 (96%)	-0.46	6 (0%) 90 76	26, 47, 126, 211	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	49	GLY	2.8
1	S	33	GLY	2.4
2	C	97	ALA	2.3
2	A	134	GLY	2.3
3	D	163	SER	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.