



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 11:39 am BST

PDB ID : 1XCQ
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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

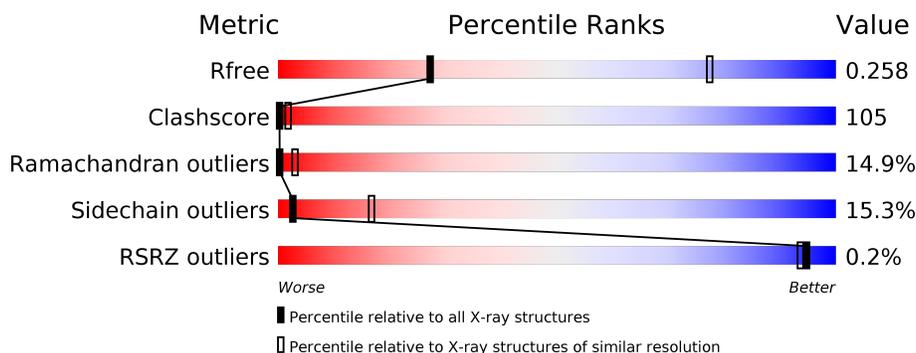
MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

1 Overall quality at a glance i

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 on 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	
1	Q	44	
1	S	44	
2	A	220	
2	C	220	
2	E	220	

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Mol	Chain	Length	Quality of chain
2	G	220	 5% 32% 46% 17%
3	B	218	 6% 22% 54% 17%
3	D	218	 • 25% 54% 17%
3	F	218	 5% 28% 50% 17%
3	H	218	 • 30% 52% 13%
4	L	80	 5% 28% 39% 11% 18%
4	M	80	 • 20% 36% 19% 23%
4	N	80	 • 21% 41% 15% 20%
4	O	80	 5% 18% 48% 8% 23%

2 Entry composition [i](#)

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
			Total	C	N	O			
1	P	24	167	106	33	28	0	0	0
1	Q	44	346	213	75	58	0	0	0
1	S	44	346	213	75	58	0	0	0

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

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

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

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

- 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 [i](#)

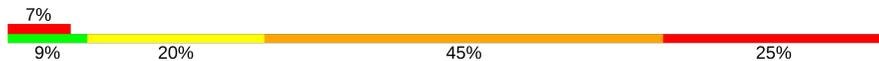
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: 

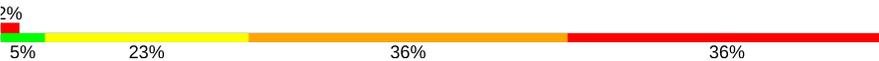


- Molecule 1: Capsid protein C

Chain Q: 



- Molecule 1: Capsid protein C

Chain S: 



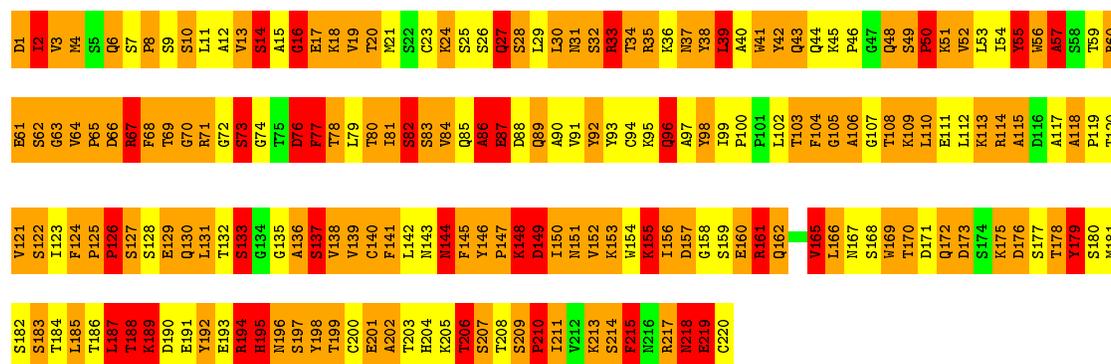
- Molecule 2: Monoclonal antibody 19D9D6 Light chain

Chain A: 



- Molecule 2: Monoclonal antibody 19D9D6 Light chain

Chain C: 6% 30% 48% 17%



D62	D63	F64	K65	G66	F68	A69	F70	S71	L72	E73	T74	S75	A76	S77	A78	A79	Y80	L81	Q82	I83	N84	S85	L86	K87	N88	E89	D90	T91	F92	A93	T94	F95	C96	A97	R98	F99	L100	L101	R102	Q103	Q104	Y105	F106	D107	W108	G109	A110	G111	T112	T113	V114	T115	V116	S117	S118	A119	K120	T121
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T122	P123	P124	S125	V126	Y127	P128	L129	A130	P131	G132	S133	E134	A135	Q136	T137	N138	S139	M140	V141	L142	L143	G144	H145	C146	V147	K148	G149	Y150	F151	P152	E153	P154	V155	T156	V157	T158	M159	M160	S161	G162	S163	L164	S165	S166	G167	V168	H169	T170	F171	P172	A173	V174	L175	Q176	S177	D178	L179	Y180	T181
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L182	S183	S184	S185	V186	T187	V188	P189	S190	S191	T192	W193	P194	S195	E196	T197	V198	T199	C200	M201	V202	A203	H204	P205	A206	S207	S208	T209	K210	V211	D212	K213	K214	I215	V216	P217	R218
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● Molecule 3: Monoclonal antibody 19D9D6 Heavy chain



Q1	I2	Q3	L4	V5	Q6	S7	G8	P9	E10	L11	K12	K13	P14	G15	E16	T17	V18	K19	L20	S21	C22	K23	A24	G26	Y27	E28	T29	F29	T30	D31	F32	S33	M34	H35	W36	V37	N38	Q39	A40	P41	G42	K43	G44	L45	M46	W47	M48	G49	H50	V51	M52	T53	E54	T55	G56	E57	P58	L59	T59	Y60
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A61	D62	D63	F64	K65	G66	R67	F68	A69	S70	F71	L72	E73	T74	G75	A76	S77	V78	A79	Y80	L81	Q82	I83	N84	S85	L86	K87	E89	D90	T91	F92	A93	T94	F95	C96	A97	R98	F99	L100	L101	R102	Q103	Q104	Y105	F106	D107	W108	G109	A110	G111	T112	T113	V114	T115	V116	S117	S118	A119	K120	T121
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T122	P123	P124	S125	V126	Y127	P128	L129	A130	P131	G132	S133	E134	A135	Q136	T137	N138	S139	M140	V141	L142	L143	G144	H145	C146	V147	K148	G149	Y150	F151	P152	E153	P154	V155	T156	V157	T158	M159	M160	S161	G162	S163	L164	S165	S166	G167	V168	H169	T170	F171	P172	A173	V174	L175	Q176	S177	D178	L179	Y180	T181
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L182	S183	S184	S185	V186	T187	V188	P189	S190	S191	T192	W193	P194	S195	E196	T197	V198	T199	C200	M201	V202	A203	H204	P205	A206	S207	S208	T209	K210	V211	D212	K213	K214	I215	V216	P217	R218
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● Molecule 3: Monoclonal antibody 19D9D6 Heavy chain



Q1	I2	Q3	L4	V5	Q6	S7	G8	P9	E10	L11	K12	K13	P14	G15	E16	T17	V18	K19	L20	S21	C22	K23	A24	G26	Y27	E28	T29	F29	T30	D31	F32	S33	M34	H35	W36	V37	N38	Q39	A40	P41	G42	K43	G44	L45	M46	W47	M48	G49	H50	V51	M52	T53	E54	T55	G56	E57	P58	L59	T59	Y60
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A61	D62	D63	F64	K65	G66	R67	F68	A69	S70	F71	L72	E73	T74	G75	A76	S77	V78	A79	Y80	L81	Q82	I83	N84	S85	L86	K87	E89	D90	T91	F92	A93	T94	F95	C96	A97	R98	F99	L100	L101	R102	Q103	Q104	Y105	F106	D107	W108	G109	A110	G111	T112	T113	V114	T115	V116	S117	S118	A119	K120
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T121	P123	P124	S125	V126	Y127	P128	L129	A130	P131	G132	S133	E134	A135	Q136	T137	N138	S139	M140	V141	L142	L143	G144	H145	C146	V147	K148	G149	Y150	F151	P152	E153	P154	V155	T156	V157	T158	M159	M160	S161	G162	S163	L164	S165	S166	G167	V168	H169	T170	F171	P172	A173	V174	L175	Q176	S177	D178	L179	Y180	T181
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L182	S183	S184	S185	V186	T187	V188	P189	S190	S191	T192	W193	P194	S195	E196	T197	V198	T199	C200	M201	V202	A203	H204	P205	A206	S207	S208	T209	K210	V211	D212	K213	K214	I215	V216	P217	R218
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● Molecule 3: Monoclonal antibody 19D9D6 Heavy chain



Q1	I2	Q3	L4	V5	Q6	S7	G8	P9	E10	L11	K12	K13	P14	G15	E16	T17	V18	K19	L20	S21	C22	K23	A24	G26	Y27	E28	T28	F29	T30	D31	F32	S33	M34	H35	W36	V37	N38	Q39	A40	P41	G42	K43	G44	L45	M46	W47	M48	G49	H50	V51	M52	T53	E54	T55	G56	E57	P58	L59	T59	Y60
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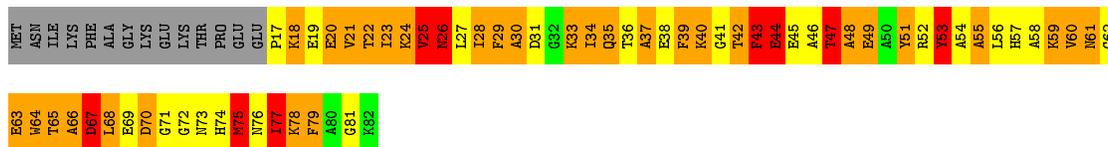
A61	D62	D63	F64	K65	G66	R67	F68	A69	S70	F71	L72	E73	T74	G75	A76	S77	V78	A79	Y80	L81	Q82	I83	N84	S85	L86	K87	E89	D90	T91	F92	A93	T94	F95	C96	A97	R98	F99	L100	L101	R102	Q103	Q104	Y105	F106	D107	W108	G109	A110	G111	T112	T113	V114	T115	V116	S117	S118	A119	K120
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T121	T122	P123	P124	S125	V126	Y127	P128	L129	A130	P131	G132	S133	A134	A135	Q136	T137	N138	S139	M140	V141	L142	L143	G144	H145	C146	L146	V147	K148	G149	Y150	F151	P152	E153	P154	V155	T156	V157	T158	M159	M160	S161	G162	S163	L164	S165	S166	G167	V168	H169	H169	G169	A110	F171	P172	A173	V174	L175	Q176	S177	D178	L179	Y180
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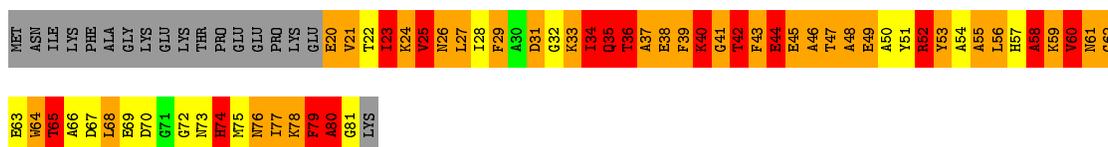
- Molecule 4: Protein L

Chain L: 5% 28% 39% 11% 18%



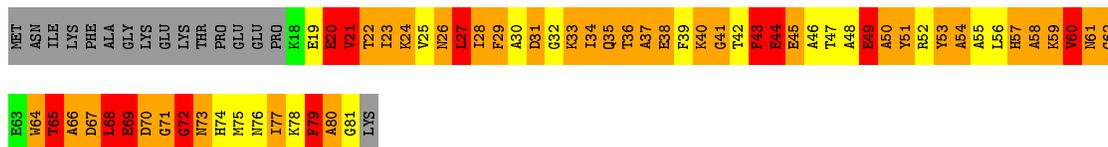
- Molecule 4: Protein L

Chain M: 20% 36% 19% 23%



- Molecule 4: Protein L

Chain N: 21% 41% 15% 20%



- Molecule 4: Protein L

Chain O: 5% 18% 48% 8% 23%



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 21.60 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.4 (21.62-3.50) 99.4 (21.60-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 3.53Å)	Xtrriage
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	Xtrriage
Anisotropy	0.156	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 114.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.24$	Xtrriage
Estimated twinning fraction	0.116 for h,-k,-l	Xtrriage
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

Xtrriage'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.*

¹ Intensities estimated from amplitudes.

² 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.

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	
		RMSZ	# Z >5	RMSZ	# Z >5
1	P	2.91	16/170 (9.4%)	2.24	7/229 (3.1%)
1	Q	3.71	60/353 (17.0%)	2.35	15/472 (3.2%)
1	S	3.33	39/353 (11.0%)	2.12	14/472 (3.0%)
2	A	3.90	300/1745 (17.2%)	2.20	77/2366 (3.3%)
2	C	3.73	280/1745 (16.0%)	2.19	57/2366 (2.4%)
2	E	4.10	328/1745 (18.8%)	2.40	95/2366 (4.0%)
2	G	3.78	269/1738 (15.5%)	2.22	73/2358 (3.1%)
3	B	4.01	330/1707 (19.3%)	2.24	84/2335 (3.6%)
3	D	3.78	293/1707 (17.2%)	2.12	67/2335 (2.9%)
3	F	3.95	312/1707 (18.3%)	2.22	79/2335 (3.4%)
3	H	3.82	282/1707 (16.5%)	2.18	65/2335 (2.8%)
4	L	4.08	98/517 (19.0%)	2.34	23/695 (3.3%)
4	M	4.13	94/489 (19.2%)	2.35	29/659 (4.4%)
4	N	4.05	96/499 (19.2%)	2.07	15/673 (2.2%)
4	O	3.83	95/489 (19.4%)	2.15	17/659 (2.6%)
All	All	3.88	2892/16671 (17.3%)	2.22	717/22655 (3.2%)

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 2892 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	93	TYR	CG-CD1	-22.17	1.10	1.39
3	H	89	GLU	CG-CD	20.91	1.83	1.51
3	D	127	TYR	CE1-CZ	-20.53	1.11	1.38
1	S	31	VAL	CB-CG1	20.39	1.95	1.52
2	G	193	GLU	CD-OE1	20.15	1.47	1.25

The worst 5 of 717 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	60	ARG	NE-CZ-NH1	18.43	129.51	120.30
1	Q	40	ARG	NE-CZ-NH1	17.41	129.01	120.30
3	F	178	ASP	CB-CG-OD2	16.47	133.12	118.30
2	C	161	ARG	NE-CZ-NH2	-15.38	112.61	120.30
1	Q	13	ARG	NE-CZ-NH1	-15.12	112.74	120.30

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	39	0
1	Q	346	0	366	101	2
1	S	346	0	366	95	1
2	A	1708	0	1656	371	0
2	C	1708	0	1657	364	2
2	E	1708	0	1658	359	0
2	G	1701	0	1652	435	0
3	B	1660	0	1614	332	0
3	D	1660	0	1614	351	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	1660	0	1614	290	0
3	H	1660	0	1614	431	0
4	L	507	0	482	91	0
4	M	480	0	457	95	0
4	N	490	0	461	110	0
4	O	480	0	457	127	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	15830	3384	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 105.

The worst 5 of 3384 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:CB	1:Q:22:VAL:CA	1.75	1.65
1:S:3:THR:CG2	1:S:3:THR:CB	1.74	1.65
2:C:189:LYS:CA	2:C:189:LYS:CB	1.75	1.64
2:E:153:LYS:CG	2:E:153:LYS:CB	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	7
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	8
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	3
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	4
3	H	216/218 (99%)	138 (64%)	51 (24%)	27 (12%)	0	5
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	4
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	5
All	All	2087/2204 (95%)	1373 (66%)	403 (19%)	311 (15%)	0	3

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 [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	Percentiles	
1	P	15/37 (40%)	13 (87%)	2 (13%)	4	21
1	Q	37/37 (100%)	29 (78%)	8 (22%)	1	5
1	S	37/37 (100%)	25 (68%)	12 (32%)	0	2
2	A	195/195 (100%)	171 (88%)	24 (12%)	4	23
2	C	195/195 (100%)	167 (86%)	28 (14%)	3	18
2	E	195/195 (100%)	161 (83%)	34 (17%)	2	11
2	G	194/195 (100%)	165 (85%)	29 (15%)	3	17
3	B	187/187 (100%)	156 (83%)	31 (17%)	2	13
3	D	187/187 (100%)	165 (88%)	22 (12%)	5	25
3	F	187/187 (100%)	155 (83%)	32 (17%)	2	12
3	H	187/187 (100%)	161 (86%)	26 (14%)	3	20
4	L	48/62 (77%)	41 (85%)	7 (15%)	3	18
4	M	46/62 (74%)	37 (80%)	9 (20%)	1	7
4	N	46/62 (74%)	38 (83%)	8 (17%)	2	11
4	O	46/62 (74%)	42 (91%)	4 (9%)	10	38
All	All	1802/1887 (96%)	1526 (85%)	276 (15%)	2	17

5 of 276 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	M	34	ILE
2	E	179	TYR

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Mol	Chain	Res	Type
3	H	62	ASP
4	M	65	THR
2	E	59	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	82	GLN
2	E	31	ASN
2	G	204	HIS
3	D	138	ASN
1	Q	14	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 carbohydrates 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 [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	P	24/44 (54%)	-0.45	0 100 100	88, 139, 163, 172	0
1	Q	44/44 (100%)	-0.11	3 (6%) 17 16	63, 126, 196, 211	0
1	S	44/44 (100%)	-0.11	1 (2%) 60 54	69, 131, 193, 203	0
2	A	220/220 (100%)	-1.12	0 100 100	29, 41, 78, 152	0
2	C	220/220 (100%)	-1.01	0 100 100	29, 53, 109, 182	0
2	E	220/220 (100%)	-1.13	0 100 100	27, 40, 81, 135	0
2	G	219/220 (99%)	-1.04	0 100 100	28, 54, 107, 158	0
3	B	218/218 (100%)	-1.05	0 100 100	27, 40, 85, 180	0
3	D	218/218 (100%)	-1.08	0 100 100	26, 47, 115, 165	0
3	F	218/218 (100%)	-1.11	0 100 100	26, 39, 78, 143	0
3	H	218/218 (100%)	-0.97	0 100 100	27, 48, 111, 164	0
4	L	66/80 (82%)	-1.04	0 100 100	27, 49, 99, 163	0
4	M	62/80 (77%)	-1.08	0 100 100	29, 46, 84, 115	0
4	N	64/80 (80%)	-0.96	0 100 100	27, 50, 110, 151	0
4	O	62/80 (77%)	-1.14	0 100 100	30, 47, 81, 103	0
All	All	2117/2204 (96%)	-1.02	4 (0%) 95 93	26, 47, 126, 211	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	Q	38	PRO	3.3
1	Q	21	ASP	2.4
1	S	39	ARG	2.1
1	Q	5	PRO	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 carbohydrates 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.