



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2020 – 11:34 pm BST

PDB ID : 5XHV
Title : Crystal Structure Of Fab S40 In Complex With Influenza Hemagglutinin, HA1 subunit.
Authors : Lee, C.C.; Wang, A.H.J.; Yu, C.M.; Yang, A.S.
Deposited on : 2017-04-24
Resolution : 3.35 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 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

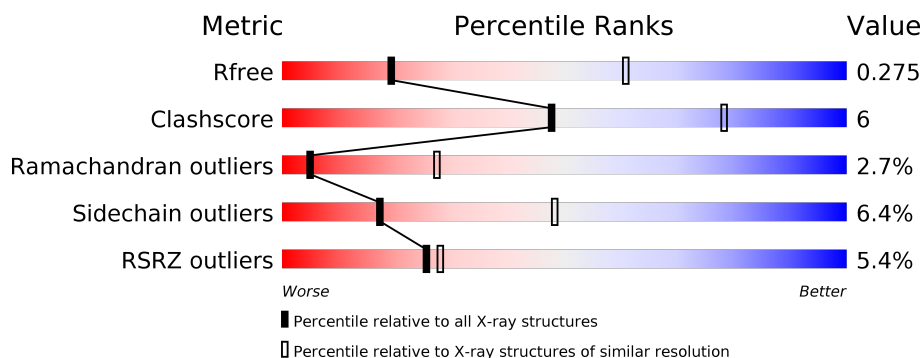
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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	A	324	<div> <div>2%</div> <div> <div></div> <div>64%</div> <div>21%</div> <div>•</div> <div>13%</div> </div> </div>
1	E	324	<div> <div>8%</div> <div> <div></div> <div>73%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>
2	H	229	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>21%</div> <div>• •</div> </div> </div>
2	P	229	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>25%</div> <div>• •</div> </div> </div>
3	L	214	<div> <div>4%</div> <div> <div></div> <div>86%</div> <div>14%</div> </div> </div>
3	Q	214	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>14%</div> <div>•</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11100 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 Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2225	1414	383	418	10			
1	E	283	Total	C	N	O	S	0	0	0
			2225	1414	383	418	10			

- Molecule 2 is a protein called S40 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	223	Total	C	N	O	S	0	0	0
			1663	1056	275	325	7			
2	P	223	Total	C	N	O	S	0	0	0
			1663	1056	275	325	7			

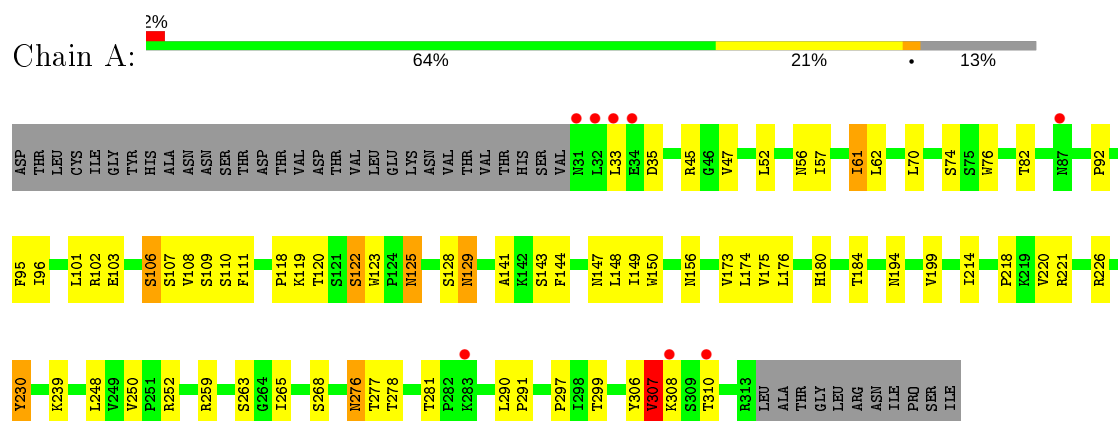
- Molecule 3 is a protein called S40 light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	214	Total	C	N	O	S	0	0	0
			1662	1048	273	335	6			
3	Q	214	Total	C	N	O	S	0	0	0
			1662	1048	273	335	6			

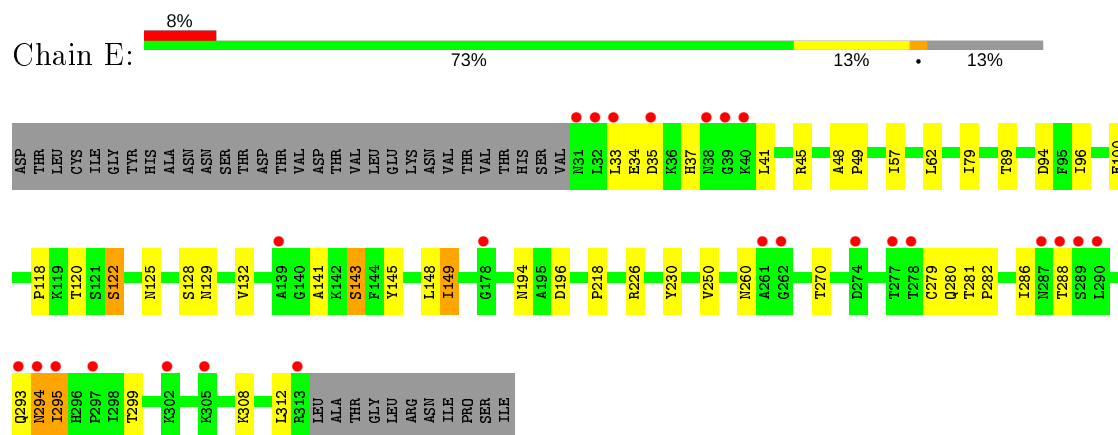
3 Residue-property plots [i](#)

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.

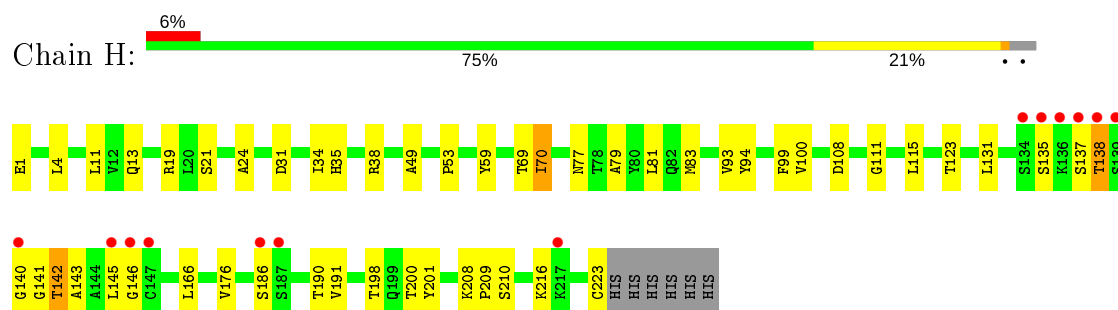
• Molecule 1: Hemagglutinin



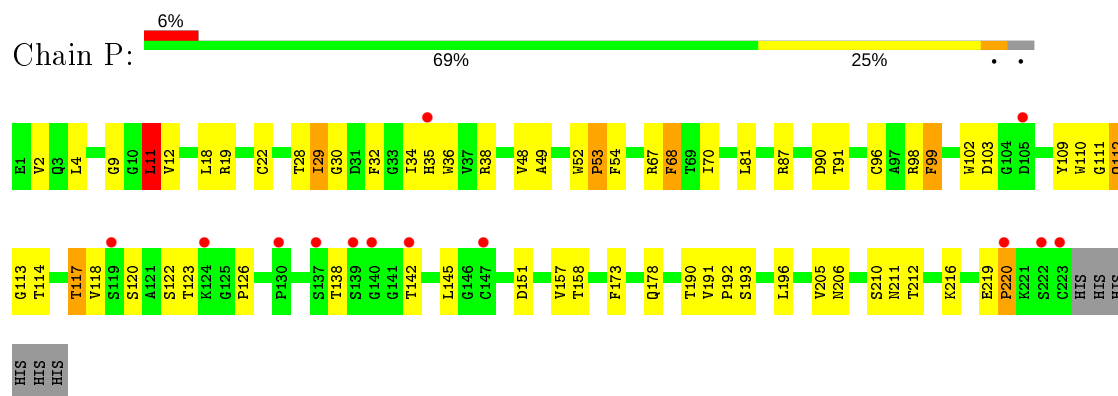
• Molecule 1: Hemagglutinin



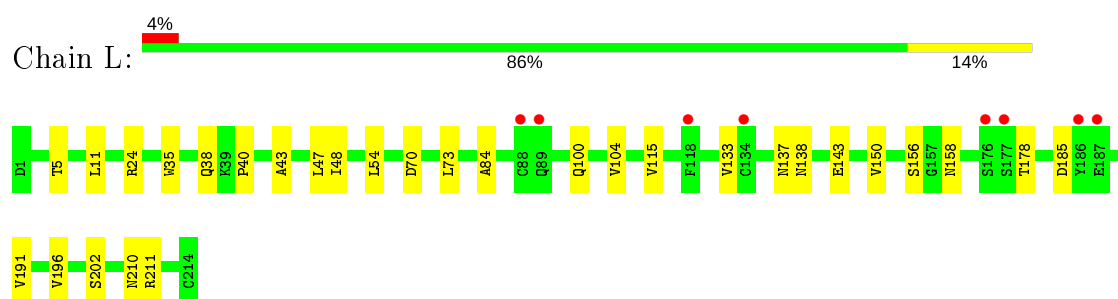
• Molecule 2: S40 heavy chain



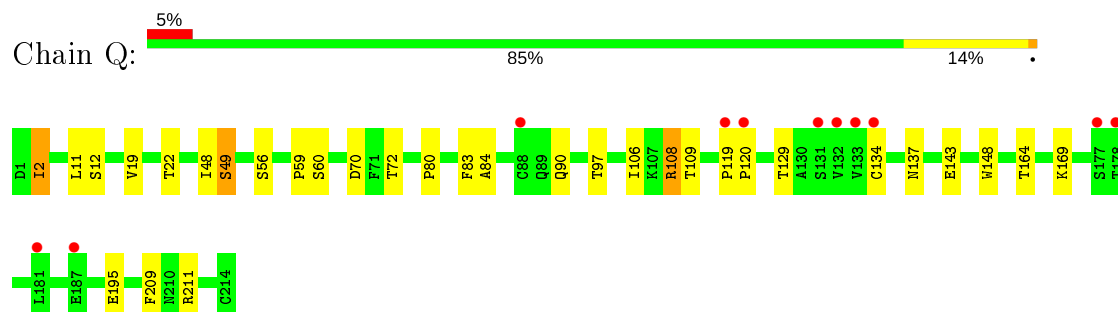
- Molecule 2: S40 heavy chain



- Molecule 3: S40 light chain



- Molecule 3: S40 light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	200.40Å 133.64Å 133.14Å 90.00° 110.47° 90.00°	Depositor
Resolution (Å)	25.00 – 3.35 24.88 – 3.34	Depositor EDS
% Data completeness (in resolution range)	76.6 (25.00-3.35) 76.4 (24.88-3.34)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.45 (at 3.30Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.230 , 0.275 0.233 , 0.275	Depositor DCC
R_{free} test set	1830 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	120.1	Xtriage
Anisotropy	0.821	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.21 , 95.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11100	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 4.08% 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 [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	A	0.55	0/2285	0.77	0/3100
1	E	0.52	0/2285	0.75	1/3100 (0.0%)
2	H	0.56	0/1708	0.71	0/2330
2	P	0.55	0/1708	0.72	1/2330 (0.0%)
3	L	0.50	0/1702	0.68	0/2313
3	Q	0.52	0/1702	0.70	0/2313
All	All	0.53	0/11390	0.73	2/15486 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	295	ILE	N-CA-C	7.42	131.02	111.00
2	P	11	LEU	CA-CB-CG	6.16	129.47	115.30

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	A	2225	0	2181	37	0
1	E	2225	0	2181	25	0
2	H	1663	0	1606	21	0
2	P	1663	0	1606	36	0
3	L	1662	0	1601	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	Q	1662	0	1601	11	0
All	All	11100	0	10776	133	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 (133) 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:P:49:ALA:HB1	2:P:70:ILE:HD11	1.47	0.94
3:L:115:VAL:HG21	3:L:196:VAL:HG21	1.60	0.84
2:P:29:ILE:HD11	2:P:34:ILE:HD11	1.59	0.84
1:E:293:GLN:HE22	1:E:299:THR:HG21	1.45	0.81
2:H:49:ALA:HB1	2:H:70:ILE:HD11	1.70	0.72
1:E:279:CYS:SG	1:E:280:GLN:N	2.65	0.69
3:Q:2:ILE:O	3:Q:97:THR:HG21	1.94	0.67
1:A:125:ASN:N	1:A:125:ASN:OD1	2.29	0.66
2:P:52:TRP:HB2	2:P:102:TRP:CD1	2.31	0.65
2:P:29:ILE:HD11	2:P:34:ILE:CD1	2.26	0.65
1:E:35:ASP:HB2	1:E:295:ILE:HD11	1.80	0.63
2:H:138:THR:CG2	2:H:142:THR:HG23	2.29	0.63
2:P:2:VAL:HG11	2:P:109:TYR:CD2	2.34	0.62
2:P:91:THR:HG23	2:P:117:THR:HA	1.80	0.62
1:E:294:ASN:ND2	1:E:294:ASN:O	2.33	0.62
2:H:81:LEU:HD22	2:H:83:MET:HE3	1.82	0.61
1:A:57:ILE:HG22	1:A:61:ILE:HD11	1.82	0.60
2:P:99:PHE:HZ	2:P:102:TRP:HA	1.66	0.60
2:H:191:VAL:HG21	2:H:201:TYR:CZ	2.36	0.60
2:H:24:ALA:HB3	2:H:77:ASN:HD21	1.65	0.60
3:L:47:LEU:C	3:L:48:ILE:HD12	2.23	0.59
1:E:128:SER:HB2	1:E:149:ILE:HD11	1.84	0.58
1:A:61:ILE:HD13	1:A:101:LEU:HD21	1.83	0.58
2:H:34:ILE:HG21	2:H:79:ALA:HB2	1.86	0.58
2:P:138:THR:HG22	2:P:142:THR:HG23	1.87	0.56
1:E:125:ASN:N	1:E:125:ASN:OD1	2.38	0.55
2:H:49:ALA:HB1	2:H:70:ILE:CD1	2.35	0.55
3:L:11:LEU:HD11	3:L:104:VAL:HG22	1.89	0.55
1:A:149:ILE:HG22	1:A:252:ARG:HB2	1.89	0.54
1:E:294:ASN:HA	1:E:308:LYS:HA	1.89	0.53
2:P:99:PHE:CZ	2:P:102:TRP:HA	2.43	0.53
1:A:107:SER:HB3	1:A:263:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:PRO:O	1:A:122:SER:OG	2.25	0.53
1:A:123:TRP:CE2	1:A:250:VAL:HG21	2.43	0.52
2:P:32:PHE:CD1	2:P:98:ARG:HD3	2.44	0.51
1:A:306:TYR:O	1:A:307:VAL:HG13	2.11	0.51
1:A:143:SER:OG	1:A:144:PHE:N	2.44	0.51
2:H:191:VAL:HG21	2:H:201:TYR:CE2	2.46	0.51
2:H:4:LEU:HD23	2:H:24:ALA:HA	1.93	0.51
1:A:281:THR:HG22	1:A:299:THR:HG22	1.92	0.51
2:P:87:ARG:O	2:P:118:VAL:HG13	2.10	0.50
3:Q:108:ARG:HD3	3:Q:109:THR:O	2.12	0.50
1:A:61:ILE:O	1:A:147:ASN:ND2	2.45	0.50
2:P:190:THR:HG21	3:Q:137:ASN:ND2	2.27	0.50
2:P:67:ARG:NH1	2:P:90:ASP:OD2	2.45	0.49
1:A:239:LYS:NZ	2:P:103:ASP:O	2.46	0.49
1:E:96:ILE:HG13	1:E:230:TYR:CE2	2.48	0.49
1:A:57:ILE:CG2	1:A:61:ILE:HD11	2.42	0.48
1:E:62:LEU:HB3	1:E:145:TYR:CD2	2.47	0.48
2:P:36:TRP:HB2	2:P:49:ALA:HB3	1.95	0.48
3:L:150:VAL:HG23	3:L:150:VAL:O	2.12	0.48
1:E:286:ILE:HG22	1:E:288:THR:HB	1.96	0.48
1:A:173:VAL:HG12	1:A:175:VAL:HG23	1.96	0.48
2:P:68:PHE:HB3	2:P:81:LEU:HD11	1.96	0.48
1:E:149:ILE:HG23	1:E:250:VAL:HG23	1.95	0.48
3:Q:134:CYS:HB2	3:Q:148:TRP:CZ2	2.49	0.48
3:Q:48:ILE:HG22	3:Q:49:SER:O	2.14	0.48
2:P:11:LEU:HD21	2:P:123:THR:CG2	2.44	0.48
1:A:149:ILE:HG23	1:A:250:VAL:HG23	1.95	0.47
1:A:199:VAL:HG11	1:A:248:LEU:HD13	1.96	0.47
1:A:33:LEU:N	1:A:290:LEU:HD13	2.29	0.47
2:P:112:GLN:NE2	2:P:113:GLY:O	2.47	0.47
2:P:110:TRP:N	2:P:110:TRP:CD1	2.82	0.47
1:E:118:PRO:O	1:E:122:SER:HB2	2.15	0.47
1:A:220:VAL:HG12	1:A:221:ARG:HG3	1.95	0.47
2:P:68:PHE:N	2:P:68:PHE:CD1	2.81	0.47
3:Q:11:LEU:HD23	3:Q:19:VAL:HG13	1.96	0.47
2:P:38:ARG:HD3	2:P:48:VAL:HG11	1.96	0.47
1:A:62:LEU:HD22	1:A:148:LEU:HD11	1.97	0.46
1:E:120:THR:HG22	2:P:54:PHE:CE2	2.50	0.46
1:E:141:ALA:HB2	2:P:19:ARG:NH1	2.31	0.46
1:E:62:LEU:HD22	1:E:148:LEU:HD11	1.97	0.45
2:P:30:GLY:HA2	2:P:53:PRO:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASP:HB3	1:A:310:THR:HG22	1.99	0.45
2:P:173:PHE:CD2	3:Q:164:THR:HG23	2.52	0.45
1:A:103:GLU:O	1:A:106:SER:OG	2.33	0.45
1:A:218:PRO:O	1:A:226:ARG:NH2	2.50	0.45
1:E:218:PRO:O	1:E:226:ARG:NH2	2.50	0.45
3:L:11:LEU:CD1	3:L:104:VAL:HG22	2.47	0.45
2:P:158:THR:HB	2:P:206:ASN:HB3	1.98	0.45
3:L:133:VAL:HG22	3:L:178:THR:HG22	1.98	0.44
2:P:11:LEU:O	2:P:12:VAL:HG13	2.18	0.44
1:A:141:ALA:HB2	2:H:19:ARG:NH2	2.33	0.44
2:H:38:ARG:HD3	2:H:94:TYR:CE2	2.52	0.44
1:A:92:PRO:HB3	1:A:220:VAL:HG11	2.00	0.44
1:E:132:VAL:HG13	1:E:143:SER:CA	2.46	0.44
1:A:96:ILE:HG13	1:A:230:TYR:CE2	2.53	0.44
2:P:22:CYS:HB2	2:P:36:TRP:CH2	2.52	0.44
2:H:208:LYS:N	2:H:209:PRO:CD	2.80	0.43
2:P:157:VAL:HG11	2:P:205:VAL:HG13	2.00	0.43
1:A:56:ASN:C	1:A:56:ASN:OD1	2.57	0.43
2:P:9:GLY:HA2	2:P:18:LEU:HD21	1.99	0.43
1:A:297:PRO:HA	1:A:306:TYR:HB2	2.01	0.43
2:P:35:HIS:O	2:P:96:CYS:HA	2.18	0.43
1:A:290:LEU:HB3	1:A:291:PRO:CD	2.49	0.43
2:P:4:LEU:O	2:P:111:GLY:HA3	2.19	0.43
1:A:102:ARG:HE	1:A:265:ILE:HD12	1.84	0.43
2:H:138:THR:HA	2:H:142:THR:HA	2.00	0.43
2:P:12:VAL:HG23	2:P:118:VAL:HB	2.00	0.43
1:E:34:GLU:HG2	1:E:288:THR:HA	2.01	0.43
2:P:210:SER:O	2:P:212:THR:N	2.52	0.43
2:P:219:GLU:HB2	2:P:220:PRO:HD2	2.00	0.43
1:A:45:ARG:O	1:A:47:VAL:HG23	2.19	0.43
2:H:24:ALA:HB3	2:H:77:ASN:ND2	2.31	0.43
3:L:38:GLN:O	3:L:84:ALA:HB1	2.18	0.43
1:A:119:LYS:HE3	1:A:128:SER:CB	2.50	0.42
3:Q:80:PRO:HA	3:Q:106:ILE:HD13	2.00	0.42
1:A:57:ILE:O	1:A:61:ILE:HG13	2.19	0.42
1:E:41:LEU:HG	1:E:270:THR:HG23	2.01	0.42
1:A:150:TRP:CZ2	1:A:180:HIS:CD2	3.07	0.42
3:Q:22:THR:HG22	3:Q:72:THR:HG23	2.01	0.42
2:H:123:THR:HG22	2:H:210:SER:HB3	2.01	0.42
2:H:131:LEU:HD12	2:H:146:GLY:HA3	2.00	0.42
1:A:52:LEU:HA	1:A:70:LEU:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:33:LEU:HD21	1:E:294:ASN:HB3	2.01	0.42
2:P:11:LEU:HD21	2:P:123:THR:HG22	2.01	0.42
2:H:111:GLY:O	3:L:43:ALA:HB2	2.20	0.41
1:A:276:ASN:HD22	1:A:277:THR:N	2.18	0.41
3:L:35:TRP:CG	3:L:73:LEU:HD13	2.55	0.41
1:A:76:TRP:O	1:A:108:VAL:O	2.38	0.41
2:H:143:ALA:O	2:H:190:THR:HA	2.20	0.41
3:Q:119:PRO:HB3	3:Q:209:PHE:CE2	2.55	0.41
3:Q:11:LEU:CD2	3:Q:19:VAL:HG13	2.50	0.41
1:E:294:ASN:C	1:E:295:ILE:HG13	2.40	0.41
2:H:35:HIS:CD2	2:H:99:PHE:CD1	3.09	0.41
2:H:81:LEU:HD23	2:H:81:LEU:C	2.41	0.41
2:H:93:VAL:HG22	2:H:115:LEU:HD11	2.03	0.41
1:E:132:VAL:HG13	1:E:143:SER:HA	2.02	0.41
1:E:281:THR:HB	1:E:282:PRO:HD2	2.02	0.41
1:E:48:ALA:HB1	1:E:49:PRO:HD2	2.01	0.41
1:E:57:ILE:HD11	1:E:79:ILE:HG21	2.03	0.41
3:L:191:VAL:HG13	3:L:210:ASN:OD1	2.20	0.41
1:A:101:LEU:HD11	1:A:174:LEU:HD21	2.04	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	A	281/324 (87%)	245 (87%)	30 (11%)	6 (2%)	7	32
1	E	281/324 (87%)	236 (84%)	40 (14%)	5 (2%)	8	35
2	H	221/229 (96%)	187 (85%)	27 (12%)	7 (3%)	4	24
2	P	221/229 (96%)	172 (78%)	39 (18%)	10 (4%)	2	17
3	L	212/214 (99%)	182 (86%)	25 (12%)	5 (2%)	6	30

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	Q	212/214 (99%)	184 (87%)	22 (10%)	6 (3%)	5	26
All	All	1428/1534 (93%)	1206 (84%)	183 (13%)	39 (3%)	5	27

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	307	VAL
2	H	108	ASP
2	P	112	GLN
2	P	211	ASN
1	A	109	SER
1	A	122	SER
1	E	37	HIS
1	E	122	SER
2	H	142	THR
3	L	158	ASN
3	L	211	ARG
2	P	28	THR
3	Q	143	GLU
3	Q	169	LYS
1	A	308	LYS
1	E	45	ARG
1	E	294	ASN
2	H	135	SER
3	L	143	GLU
2	P	29	ILE
3	Q	211	ARG
2	H	140	GLY
2	H	166	LEU
2	P	122	SER
2	P	151	ASP
1	A	106	SER
1	A	129	ASN
3	L	138	ASN
2	P	120	SER
2	H	141	GLY
3	Q	84	ALA
3	L	40	PRO
2	P	126	PRO
2	P	53	PRO
3	Q	120	PRO
2	H	53	PRO

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Mol	Chain	Res	Type
2	P	192	PRO
1	E	149	ILE
3	Q	59	PRO

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	247/284 (87%)	227 (92%)	20 (8%)	11	38
1	E	247/284 (87%)	238 (96%)	9 (4%)	35	64
2	H	181/187 (97%)	163 (90%)	18 (10%)	8	29
2	P	181/187 (97%)	169 (93%)	12 (7%)	16	47
3	L	189/189 (100%)	180 (95%)	9 (5%)	25	57
3	Q	189/189 (100%)	178 (94%)	11 (6%)	20	52
All	All	1234/1320 (94%)	1155 (94%)	79 (6%)	17	48

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	ILE
1	A	74	SER
1	A	82	THR
1	A	95	PHE
1	A	110	SER
1	A	111	PHE
1	A	120	THR
1	A	125	ASN
1	A	129	ASN
1	A	156	ASN
1	A	176	LEU
1	A	184	THR
1	A	194	ASN
1	A	214	ILE
1	A	230	TYR

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Mol	Chain	Res	Type
1	A	259	ARG
1	A	268	SER
1	A	276	ASN
1	A	278	THR
1	A	307	VAL
1	E	89	THR
1	E	94	ASP
1	E	100	GLU
1	E	129	ASN
1	E	143	SER
1	E	194	ASN
1	E	196	ASP
1	E	260	ASN
1	E	312	LEU
2	H	1	GLU
2	H	11	LEU
2	H	13	GLN
2	H	21	SER
2	H	31	ASP
2	H	59	TYR
2	H	69	THR
2	H	70	ILE
2	H	100	VAL
2	H	137	SER
2	H	138	THR
2	H	145	LEU
2	H	176	VAL
2	H	186	SER
2	H	198	THR
2	H	200	THR
2	H	216	LYS
2	H	223	CYS
3	L	5	THR
3	L	24	ARG
3	L	54	LEU
3	L	70	ASP
3	L	100	GLN
3	L	137	ASN
3	L	156	SER
3	L	185	ASP
3	L	202	SER
2	P	11	LEU

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Mol	Chain	Res	Type
2	P	68	PHE
2	P	99	PHE
2	P	114	THR
2	P	117	THR
2	P	145	LEU
2	P	178	GLN
2	P	191	VAL
2	P	193	SER
2	P	196	LEU
2	P	216	LYS
2	P	220	PRO
3	Q	2	ILE
3	Q	12	SER
3	Q	49	SER
3	Q	56	SER
3	Q	60	SER
3	Q	70	ASP
3	Q	83	PHE
3	Q	90	GLN
3	Q	108	ARG
3	Q	129	THR
3	Q	195	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	276	ASN
1	E	293	GLN
2	P	101	ASN
2	P	178	GLN
2	P	206	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](#)

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	283/324 (87%)	-0.12	8 (2%)	53	55	102, 150, 230, 342	0
1	E	283/324 (87%)	0.18	25 (8%)	10	11	127, 191, 274, 331	0
2	H	223/229 (97%)	-0.15	13 (5%)	23	25	106, 146, 237, 283	0
2	P	223/229 (97%)	0.18	13 (5%)	23	25	122, 194, 271, 316	0
3	L	214/214 (100%)	-0.07	8 (3%)	41	43	116, 167, 227, 255	0
3	Q	214/214 (100%)	-0.02	11 (5%)	28	30	119, 176, 245, 283	0
All	All	1440/1534 (93%)	0.00	78 (5%)	25	28	102, 171, 257, 342	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	33	LEU	11.3
1	E	31	ASN	8.9
1	E	289	SER	8.4
1	E	294	ASN	7.4
1	A	32	LEU	6.8
2	H	146	GLY	6.8
1	E	32	LEU	5.8
2	P	222	SER	5.3
1	E	38	ASN	5.2
1	A	310	THR	5.1
2	P	220	PRO	4.9
3	L	134	CYS	4.3
2	H	139	SER	4.2
1	E	33	LEU	4.2
1	A	31	ASN	4.1
1	E	302	LYS	4.1
3	Q	132	VAL	4.1
1	E	139	ALA	4.0
1	E	277	THR	4.0

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Mol	Chain	Res	Type	RSRZ
2	H	137	SER	3.9
1	E	297	PRO	3.8
3	Q	178	THR	3.8
2	H	135	SER	3.7
2	P	139	SER	3.6
2	P	142	THR	3.6
2	H	147	CYS	3.6
2	P	223	CYS	3.5
3	Q	133	VAL	3.5
3	Q	134	CYS	3.3
1	A	283	LYS	3.3
2	P	130	PRO	3.1
1	E	287	ASN	3.1
1	E	178	GLY	3.1
1	A	34	GLU	3.1
3	L	88	CYS	3.1
3	Q	119	PRO	3.1
3	Q	181	LEU	3.1
2	P	137	SER	3.0
2	P	124	LYS	3.0
1	E	295	ILE	3.0
2	P	119	SER	3.0
2	P	147	CYS	3.0
3	L	187	GLU	3.0
1	E	290	LEU	2.9
1	E	288	THR	2.9
1	A	87	ASN	2.8
2	H	138	THR	2.8
2	H	140	GLY	2.8
1	E	262	GLY	2.8
2	H	187	SER	2.7
2	H	186	SER	2.7
1	E	278	THR	2.6
3	L	89	GLN	2.5
1	E	40	LYS	2.5
3	Q	177	SER	2.5
1	E	274	ASP	2.5
1	A	308	LYS	2.4
3	L	186	TYR	2.4
2	H	134	SER	2.4
3	L	176	SER	2.4
3	Q	187	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
2	H	217	LYS	2.3
2	P	105	ASP	2.3
2	P	140	GLY	2.2
1	E	35	ASP	2.2
3	Q	120	PRO	2.2
1	E	305	LYS	2.2
1	E	313	ARG	2.2
1	E	293	GLN	2.1
3	L	177	SER	2.1
2	H	136	LYS	2.1
2	P	35	HIS	2.1
1	E	261	ALA	2.1
3	L	118	PHE	2.1
3	Q	88	CYS	2.0
3	Q	131	SER	2.0
2	H	145	LEU	2.0
1	E	39	GLY	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.