



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 04:40 PM EDT

PDB ID : 6II4
Title : Crystal structure of H7 hemagglutinin from A/Anhui/1/2013 in complex with a human neutralizing antibody L4A-14
Authors : Jiang, H.H.; Shi, Y.; Qi, J.; Gao, G.F.
Deposited on : 2018-10-03
Resolution : 3.30 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	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)	:	2.37.1

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X-RAY DIFFRACTION

A.



Similar resolution
 (#Entries, resolution range(Å))

Quality of chain

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Mol	Chain	Length	Quality of chain
3	H	225	<div><div></div><div>17%</div><div>66%</div><div>30%</div><div></div><div></div></div>
4	F	212	<div><div></div><div>15%</div><div>77%</div><div>22%</div><div></div><div></div></div>
4	L	212	<div><div></div><div>10%</div><div>76%</div><div>21%</div><div></div><div></div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14016 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	317	Total	C	N	O	S	0	0	1
			2413	1498	437	463	15			
1	C	317	Total	C	N	O	S	0	0	1
			2413	1498	437	463	15			

- Molecule 2 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1352	832	237	276	7			
2	D	166	Total	C	N	O	S	0	0	0
			1352	832	237	276	7			

- Molecule 3 is a protein called Heavy chain of L4A-14 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	220	Total	C	N	O	S	0	0	0
			1645	1038	279	323	5			
3	H	220	Total	C	N	O	S	0	0	0
			1645	1038	279	323	5			

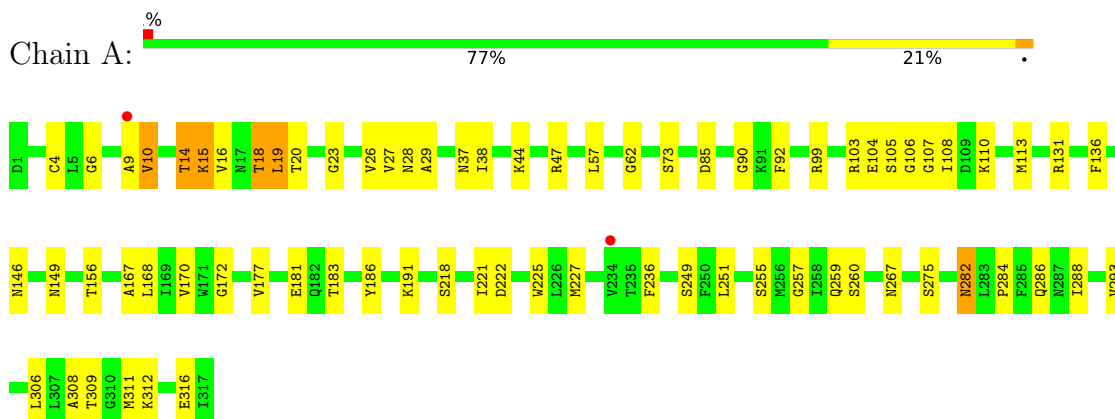
- Molecule 4 is a protein called Light chain of L4A-14 Fab.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	212	Total	C	N	O	S	0	0	0
			1598	992	269	332	5			
4	L	212	Total	C	N	O	S	0	0	0
			1598	992	269	332	5			

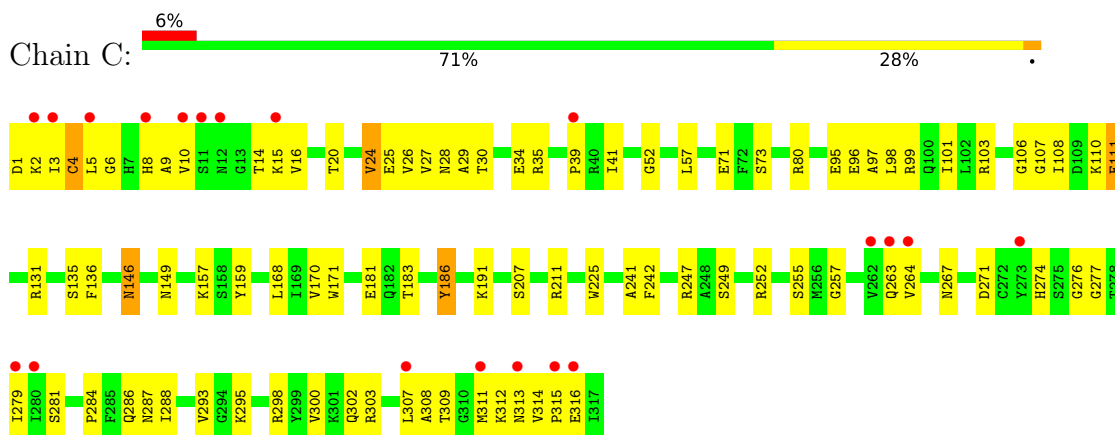
3 Residue-property plots [i](#)

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.

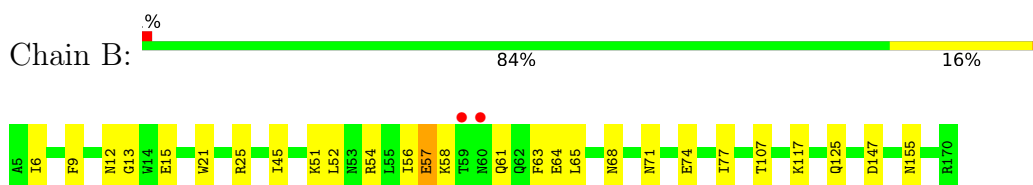
• Molecule 1: Hemagglutinin



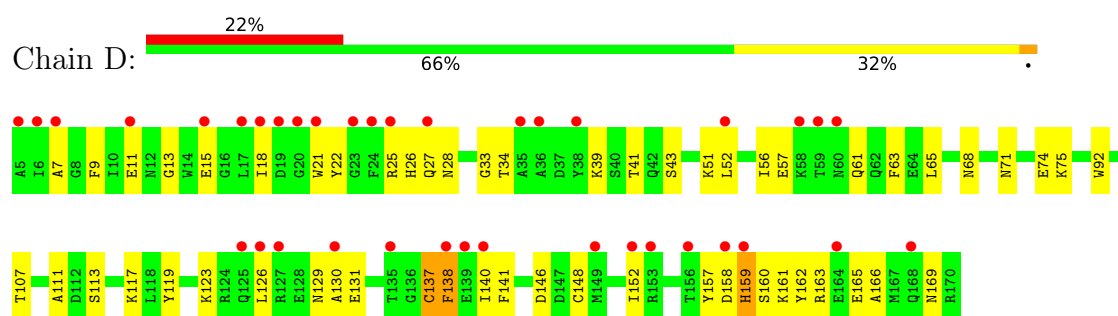
• Molecule 1: Hemagglutinin



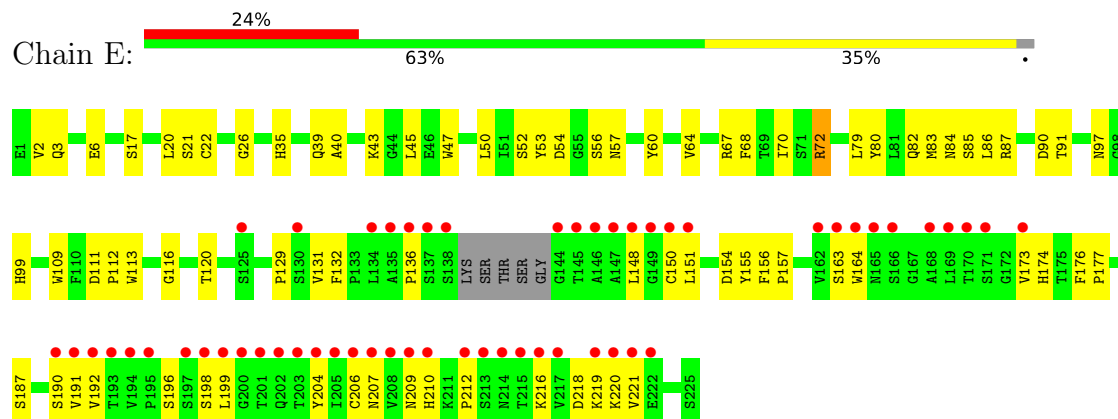
• Molecule 2: Hemagglutinin



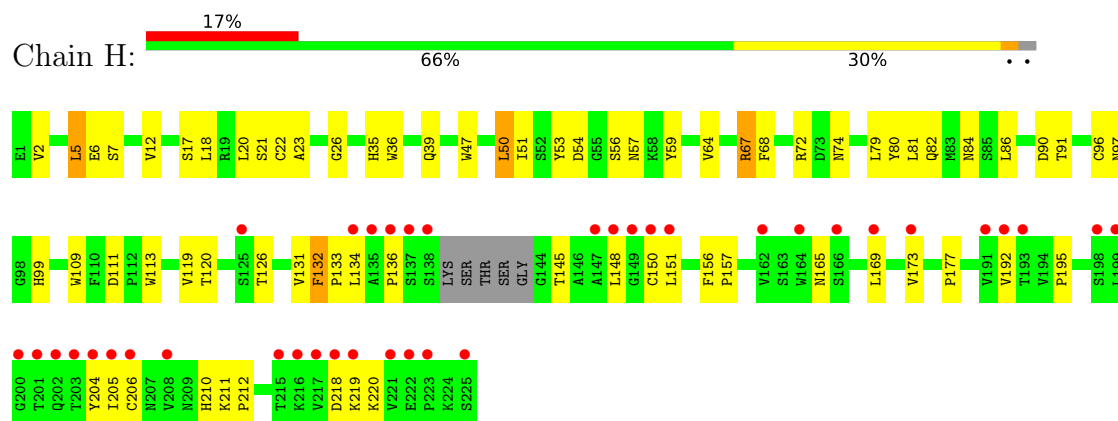
• Molecule 2: Hemagglutinin



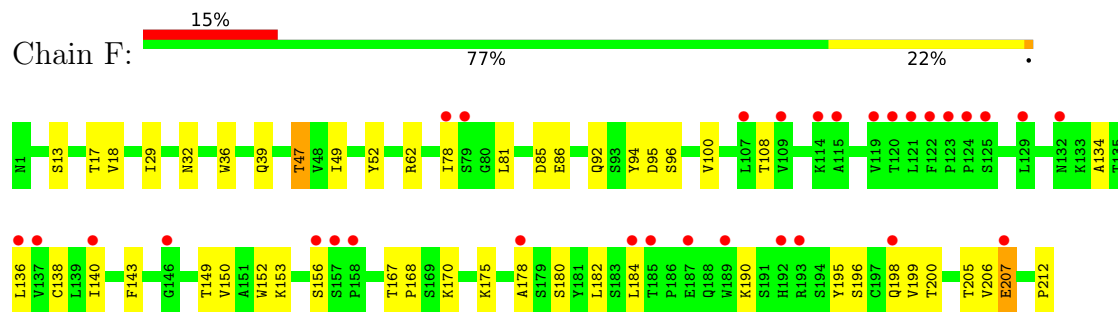
• Molecule 3: Heavy chain of L4A-14 Fab



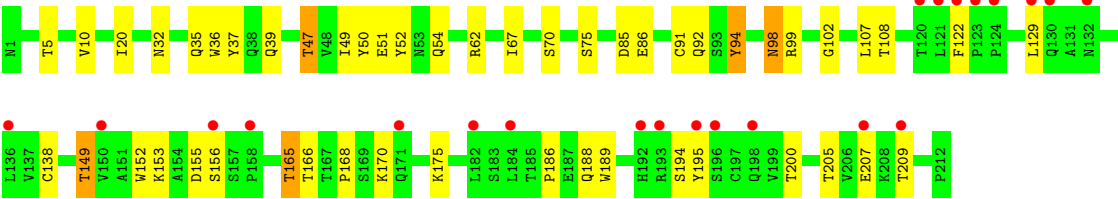
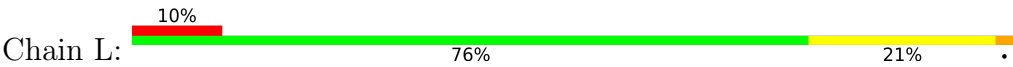
• Molecule 3: Heavy chain of L4A-14 Fab



• Molecule 4: Light chain of L4A-14 Fab



• Molecule 4: Light chain of L4A-14 Fab



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	127.48Å 127.48Å 429.65Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.04 – 3.30 41.04 – 3.29	Depositor EDS
% Data completeness (in resolution range)	99.8 (41.04-3.30) 99.8 (41.04-3.29)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 3.32Å)	Xtriage
Refinement program	PHENIX (1.11.1-2575_1692: ???)	Depositor
R, R_{free}	0.227 , 0.276 0.227 , 0.276	Depositor DCC
R_{free} test set	1981 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	91.3	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 69.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h-k,k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	14016	wwPDB-VP
Average B, all atoms (Å ²)	128.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% 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	A	0.25	0/2459	0.48	0/3324
1	C	0.25	0/2459	0.48	0/3324
2	B	0.25	0/1375	0.44	0/1853
2	D	0.24	0/1375	0.41	0/1853
3	E	0.25	0/1686	0.48	0/2296
3	H	0.25	0/1686	0.47	0/2296
4	F	0.25	0/1637	0.46	0/2232
4	L	0.25	0/1637	0.47	0/2232
All	All	0.25	0/14314	0.47	0/19410

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
1	A	0	1
4	F	0	1
4	L	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	15	LYS	Peptide
4	F	94	TYR	Peptide
4	L	94	TYR	Peptide

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	2413	0	2374	47	0
1	C	2413	0	2374	65	0
2	B	1352	0	1252	23	0
2	D	1352	0	1252	38	0
3	E	1645	0	1597	48	0
3	H	1645	0	1597	46	0
4	F	1598	0	1525	29	0
4	L	1598	0	1525	33	0
All	All	14016	0	13496	294	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 11.

All (294) 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)
3:H:206:CYS:O	3:H:218:ASP:HA	1.53	1.08
3:E:206:CYS:O	3:E:218:ASP:HA	1.68	0.94
4:F:153:LYS:HB2	4:F:196:SER:HB3	1.56	0.88
2:D:159:HIS:O	2:D:163:ARG:HB2	1.73	0.87
1:C:15:LYS:HB2	1:C:16:VAL:HA	1.57	0.85
3:H:204:TYR:O	3:H:220:LYS:HA	1.80	0.81
1:A:259:GLN:HE22	2:B:68:ASN:HB2	1.49	0.76
3:E:21:SER:HA	3:E:79:LEU:O	1.86	0.76
4:L:36:TRP:HB2	4:L:49:ILE:HB	1.68	0.75
3:E:131:VAL:HA	3:E:151:LEU:O	1.87	0.74
4:F:36:TRP:HB2	4:F:49:ILE:HB	1.72	0.72
4:L:153:LYS:HD3	4:L:156:SER:HA	1.71	0.72
2:D:7:ALA:HB1	2:D:11:GLU:HG3	1.71	0.71
2:B:125:GLN:HE22	2:B:155:ASN:HA	1.56	0.71
2:D:165:GLU:O	2:D:169:ASN:ND2	2.23	0.70
3:H:173:VAL:HG22	3:H:192:VAL:HG23	1.75	0.69
1:C:35:ARG:NH1	1:C:303:ARG:O	2.25	0.68
3:E:109:TRP:HE1	4:F:47:THR:HG21	1.59	0.68
1:A:308:ALA:HB3	1:A:309:THR:HA	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:THR:H	1:C:25:GLU:HB2	1.59	0.67
4:F:199:VAL:HB	4:F:206:VAL:O	1.94	0.67
3:E:91:THR:HG23	3:E:120:THR:HA	1.77	0.67
3:H:21:SER:HA	3:H:79:LEU:O	1.95	0.67
3:H:91:THR:HG23	3:H:120:THR:HA	1.77	0.67
3:H:205:ILE:HG23	3:H:218:ASP:HB3	1.78	0.66
4:L:86:GLU:HG3	4:L:108:THR:HA	1.77	0.66
4:F:150:VAL:HA	4:F:198:GLN:O	1.96	0.65
1:C:28:ASN:O	1:C:309:THR:N	2.30	0.65
1:C:41:ILE:HB	1:C:264:VAL:HA	1.79	0.65
4:F:32:ASN:O	4:F:52:TYR:OH	2.14	0.65
3:E:20:LEU:O	3:E:80:TYR:HA	1.98	0.63
3:H:111:ASP:OD1	3:H:113:TRP:NE1	2.31	0.63
3:H:109:TRP:HE1	4:L:47:THR:HG21	1.65	0.62
3:E:52:SER:O	3:E:72:ARG:NH2	2.32	0.62
1:C:293:VAL:HG11	2:D:65:LEU:HG	1.82	0.61
1:A:29:ALA:HA	1:A:309:THR:HG23	1.82	0.61
3:H:97:ASN:OD1	4:L:99:ARG:NH2	2.34	0.61
1:A:177:VAL:HG13	1:A:218:SER:HB2	1.83	0.60
2:B:51:LYS:HZ2	2:B:107:THR:HG1	1.47	0.60
1:C:286:GLN:OE1	1:C:288:ILE:N	2.33	0.60
1:A:18:THR:OG1	1:A:19:LEU:N	2.35	0.60
2:B:52:LEU:O	2:B:56:ILE:HG13	2.02	0.60
1:C:103:ARG:HB3	1:C:257:GLY:HA3	1.84	0.60
3:E:22:CYS:HB3	3:E:79:LEU:HB3	1.84	0.60
1:A:9:ALA:HB2	2:B:13:GLY:HA3	1.83	0.60
3:H:131:VAL:HA	3:H:151:LEU:O	2.01	0.60
3:E:67:ARG:NH2	3:E:90:ASP:OD2	2.34	0.59
1:C:39:PRO:HA	1:C:277:GLY:HA3	1.85	0.59
3:E:64:VAL:HG13	3:E:68:PHE:HB2	1.85	0.59
1:C:287:ASN:ND2	1:C:300:VAL:O	2.34	0.59
2:B:52:LEU:HG	2:B:56:ILE:HD11	1.84	0.59
3:H:68:PHE:HA	3:H:82:GLN:O	2.03	0.59
1:C:110:LYS:HB3	1:C:247:ARG:HD3	1.83	0.59
1:C:10:VAL:N	1:C:313:ASN:OD1	2.36	0.59
3:H:99:HIS:NE2	4:L:94:TYR:OH	2.35	0.58
2:B:68:ASN:ND2	2:B:71:ASN:O	2.29	0.58
3:E:17:SER:HA	3:E:84:ASN:HA	1.86	0.58
3:H:99:HIS:ND1	3:H:111:ASP:OD2	2.33	0.58
1:C:96:GLU:OE2	1:C:103:ARG:NH2	2.37	0.58
4:L:35:GLN:HE21	4:L:51:GLU:H	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ILE:HG23	2:D:138:PHE:HB2	1.86	0.57
3:E:177:PRO:HG2	4:F:168:PRO:HG3	1.86	0.57
2:D:68:ASN:ND2	2:D:71:ASN:O	2.34	0.57
1:A:167:ALA:O	1:A:227:MET:HA	2.04	0.57
3:E:129:PRO:HB3	3:E:155:TYR:HB3	1.86	0.57
2:D:52:LEU:HG	2:D:56:ILE:HD11	1.86	0.57
4:L:32:ASN:O	4:L:52:TYR:OH	2.22	0.57
2:B:57:GLU:O	2:B:61:GLN:NE2	2.37	0.56
3:E:163:SER:OG	3:E:207:ASN:O	2.20	0.56
1:A:37:ASN:OD1	1:A:38:ILE:N	2.38	0.56
2:D:28:ASN:ND2	2:D:146:ASP:OD1	2.37	0.56
1:C:73:SER:HA	1:C:107:GLY:HA3	1.86	0.56
2:D:57:GLU:O	2:D:61:GLN:NE2	2.38	0.56
1:A:286:GLN:OE1	1:A:288:ILE:N	2.39	0.56
1:C:10:VAL:HG11	1:C:27:VAL:HA	1.87	0.55
3:E:2:VAL:HA	3:E:26:GLY:HA3	1.87	0.55
2:D:52:LEU:O	2:D:56:ILE:HG13	2.06	0.55
1:A:308:ALA:HB1	2:B:107:THR:HG21	1.89	0.55
3:E:6:GLU:OE1	3:E:116:GLY:N	2.36	0.55
3:H:67:ARG:NH2	3:H:90:ASP:OD2	2.40	0.55
4:F:170:LYS:N	4:F:175:LYS:O	2.40	0.55
1:C:263:GLN:OE1	1:C:264:VAL:N	2.39	0.54
1:A:251:LEU:HD12	1:A:251:LEU:H	1.72	0.54
3:E:97:ASN:ND2	3:E:112:PRO:O	2.32	0.54
4:F:153:LYS:HD3	4:F:156:SER:HA	1.90	0.54
4:L:186:PRO:HA	4:L:189:TRP:HB3	1.89	0.54
1:A:10:VAL:HB	1:A:27:VAL:HG23	1.90	0.54
1:C:5:LEU:HD12	2:D:119:TYR:HD1	1.73	0.54
2:D:162:TYR:O	2:D:166:ALA:HB2	2.08	0.54
4:L:129:LEU:HD22	4:L:186:PRO:HB3	1.90	0.54
1:C:308:ALA:HB3	1:C:309:THR:HA	1.89	0.54
4:L:10:VAL:HG13	4:L:107:LEU:HD23	1.87	0.54
3:H:17:SER:HA	3:H:84:ASN:HA	1.90	0.54
4:L:155:ASP:OD1	4:L:194:SER:OG	2.18	0.54
4:L:170:LYS:N	4:L:175:LYS:O	2.40	0.54
1:A:259:GLN:NE2	2:B:68:ASN:HB2	2.22	0.53
1:A:293:VAL:HG11	2:B:65:LEU:HG	1.89	0.53
1:C:279:ILE:HD11	1:C:288:ILE:HB	1.90	0.53
3:E:40:ALA:HB3	3:E:43:LYS:HB2	1.90	0.53
1:C:24:VAL:HG21	1:C:312:LYS:HD3	1.90	0.53
1:C:96:GLU:OE1	1:C:99:ARG:NH1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LYS:HD3	1:A:16:VAL:HA	1.91	0.53
3:E:198:SER:O	3:E:204:TYR:OH	2.26	0.53
1:C:106:GLY:HA2	1:C:255:SER:HB3	1.91	0.52
4:F:167:THR:HG22	4:F:178:ALA:HB2	1.90	0.52
4:F:190:LYS:HG2	4:F:212:PRO:HB3	1.90	0.52
1:C:131:ARG:NH1	1:C:136:PHE:O	2.38	0.52
3:E:67:ARG:NH1	3:E:87:ARG:HG3	2.25	0.52
2:D:25:ARG:HA	2:D:34:THR:HA	1.92	0.52
3:E:67:ARG:HH12	3:E:87:ARG:HG3	1.75	0.52
1:C:271:ASP:HB3	1:C:295:LYS:HB2	1.92	0.52
4:L:62:ARG:NH2	4:L:85:ASP:OD1	2.43	0.52
1:A:28:ASN:O	1:A:309:THR:N	2.43	0.52
1:C:15:LYS:HB2	1:C:16:VAL:CA	2.37	0.52
4:F:62:ARG:NH2	4:F:85:ASP:OD1	2.39	0.52
4:F:200:THR:HA	4:F:205:THR:HA	1.91	0.52
3:H:210:HIS:CD2	3:H:212:PRO:HD2	2.44	0.52
1:A:168:LEU:HB3	1:A:249:SER:HB2	1.93	0.51
4:F:152:TRP:CE2	4:F:182:LEU:HB2	2.45	0.51
1:A:44:LYS:HD3	1:A:267:ASN:HA	1.92	0.51
3:E:176:PHE:HE2	3:E:191:VAL:HG12	1.74	0.51
3:H:126:THR:HA	3:H:156:PHE:HD1	1.75	0.51
1:A:6:GLY:HA2	2:B:9:PHE:HB3	1.91	0.51
4:L:35:GLN:NE2	4:L:51:GLU:H	2.08	0.51
1:C:9:ALA:HB2	2:D:13:GLY:HA3	1.93	0.51
2:D:51:LYS:NZ	2:D:107:THR:OG1	2.40	0.51
2:D:130:ALA:HB2	2:D:140:ILE:HG12	1.93	0.51
2:D:158:ASP:OD1	2:D:160:SER:OG	2.27	0.51
3:E:67:ARG:NH1	3:E:85:SER:O	2.43	0.51
3:E:154:ASP:H	3:E:187:SER:HG	1.58	0.50
1:C:34:GLU:HG2	1:C:281:SER:HB2	1.93	0.50
2:D:158:ASP:HB3	2:D:161:LYS:HG3	1.93	0.50
2:D:26:HIS:N	2:D:33:GLY:O	2.41	0.50
1:A:316:GLU:HG3	2:B:13:GLY:O	2.11	0.50
1:A:47:ARG:NH1	1:A:73:SER:OG	2.44	0.50
1:A:146:ASN:OD1	3:H:57:ASN:ND2	2.44	0.50
1:C:4:CYS:HA	2:D:137:CYS:HA	1.93	0.50
3:H:53:TYR:O	3:H:72:ARG:NH1	2.45	0.50
1:C:52:GLY:HA2	1:C:80:ARG:HG3	1.94	0.50
3:H:7:SER:OG	3:H:21:SER:OG	2.29	0.50
1:A:26:VAL:HG21	1:A:308:ALA:O	2.12	0.50
4:F:134:ALA:O	4:F:184:LEU:N	2.35	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:ASN:OD1	3:E:57:ASN:ND2	2.45	0.49
1:A:15:LYS:HD2	1:A:306:LEU:HD12	1.95	0.49
3:H:54:ASP:OD1	3:H:56:SER:OG	2.24	0.49
1:C:95:GLU:OE2	2:D:71:ASN:ND2	2.44	0.49
1:C:6:GLY:HA2	2:D:9:PHE:HB3	1.94	0.49
3:E:47:TRP:CZ2	3:E:50:LEU:HD23	2.48	0.49
1:A:105:SER:HB3	1:A:251:LEU:HD23	1.95	0.48
1:A:73:SER:HA	1:A:107:GLY:HA3	1.95	0.48
3:H:177:PRO:HG2	4:L:168:PRO:HG3	1.95	0.48
3:H:133:PRO:HD3	3:H:219:LYS:HE2	1.94	0.48
1:A:108:ILE:HD12	1:A:110:LYS:HE3	1.96	0.48
1:C:186:TYR:HB2	1:C:191:LYS:HE3	1.96	0.48
3:E:111:ASP:OD1	3:E:113:TRP:NE1	2.44	0.48
3:E:35:HIS:CD2	3:E:99:HIS:HB3	2.48	0.48
3:E:132:PHE:HB2	3:E:151:LEU:HB3	1.96	0.48
2:B:6:ILE:HD11	2:B:25:ARG:HG2	1.96	0.48
1:A:131:ARG:NH1	1:A:136:PHE:O	2.46	0.48
3:H:39:GLN:NE2	4:L:39:GLN:OE1	2.35	0.48
4:L:200:THR:HA	4:L:205:THR:HA	1.95	0.48
4:F:18:VAL:HG12	4:F:81:LEU:HD21	1.96	0.48
4:L:188:GLN:O	4:L:195:TYR:OH	2.30	0.48
1:A:14:THR:HG21	1:A:29:ALA:HB3	1.96	0.47
3:H:20:LEU:O	3:H:80:TYR:HA	2.14	0.47
1:A:284:PRO:HG3	2:B:56:ILE:HG12	1.97	0.47
4:F:136:LEU:N	4:F:182:LEU:O	2.41	0.47
2:B:117:LYS:HA	2:B:117:LYS:HD3	1.69	0.47
1:C:311:MET:HG3	2:D:111:ALA:HB1	1.97	0.47
3:E:209:ASN:HA	3:E:216:LYS:HG2	1.95	0.47
3:H:12:VAL:HG21	3:H:86:LEU:HD13	1.97	0.47
1:A:9:ALA:O	2:B:15:GLU:HG2	2.15	0.47
3:E:39:GLN:OE1	4:F:39:GLN:NE2	2.40	0.47
3:H:22:CYS:HB3	3:H:79:LEU:HB3	1.95	0.47
4:L:50:TYR:CE1	4:L:54:GLN:HB3	2.50	0.47
1:C:35:ARG:HD2	1:C:303:ARG:NH2	2.30	0.47
3:E:136:PRO:HD3	3:E:148:LEU:HB3	1.97	0.47
2:D:131:GLU:HG3	2:D:141:PHE:HE1	1.80	0.47
1:A:57:LEU:HD21	1:A:99:ARG:HG2	1.97	0.46
1:A:260:SER:OG	1:A:275:SER:O	2.22	0.46
1:C:170:VAL:HG22	1:C:225:TRP:HB3	1.96	0.46
3:E:68:PHE:HA	3:E:82:GLN:O	2.16	0.46
3:H:2:VAL:HA	3:H:26:GLY:HA3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:170:LYS:HD2	4:L:175:LYS:HB2	1.96	0.46
1:C:9:ALA:O	2:D:15:GLU:HG2	2.15	0.46
1:A:62:GLY:O	1:A:131:ARG:NH2	2.49	0.46
1:A:106:GLY:HA2	1:A:255:SER:HB3	1.98	0.46
1:C:207:SER:O	1:C:211:ARG:NH1	2.42	0.46
3:E:196:SER:HA	3:E:199:LEU:HD13	1.98	0.46
3:H:47:TRP:CZ2	3:H:50:LEU:HD23	2.50	0.46
3:E:204:TYR:O	3:E:220:LYS:HA	2.16	0.46
3:E:219:LYS:HD2	3:E:219:LYS:HA	1.71	0.46
4:L:20:ILE:O	4:L:75:SER:HA	2.16	0.46
4:F:29:ILE:O	4:F:52:TYR:OH	2.32	0.46
2:D:113:SER:O	2:D:117:LYS:HG2	2.16	0.45
1:C:99:ARG:O	1:C:103:ARG:HG3	2.16	0.45
2:D:21:TRP:CD1	2:D:41:THR:HG23	2.52	0.45
1:C:302:GLN:OE1	1:C:302:GLN:N	2.43	0.45
3:H:145:THR:HG22	3:H:195:PRO:HA	1.99	0.45
4:L:50:TYR:CZ	4:L:54:GLN:HB3	2.51	0.45
1:C:149:ASN:HA	1:C:183:THR:O	2.17	0.45
4:F:86:GLU:HG3	4:F:108:THR:HA	1.99	0.45
2:D:129:ASN:ND2	2:D:157:TYR:OH	2.43	0.45
4:F:95:ASP:OD1	4:F:96:SER:N	2.47	0.45
4:F:152:TRP:CG	4:F:182:LEU:HD13	2.52	0.45
3:E:47:TRP:HZ2	3:E:50:LEU:HD23	1.81	0.44
4:L:52:TYR:CD1	4:L:67:ILE:HD11	2.52	0.44
1:C:111:GLU:OE2	1:C:159:TYR:OH	2.21	0.44
1:C:274:HIS:CE1	1:C:276:GLY:H	2.36	0.44
2:D:123:LYS:O	2:D:126:LEU:C	2.56	0.44
1:C:57:LEU:HD22	1:C:98:LEU:HD23	2.00	0.44
3:H:6:GLU:HG3	3:H:96:CYS:SG	2.58	0.44
4:L:138:CYS:HB2	4:L:152:TRP:CH2	2.53	0.44
1:A:156:THR:HA	1:A:236:PHE:O	2.18	0.44
1:C:2:LYS:HB3	2:D:27:GLN:HB3	1.98	0.44
1:C:108:ILE:O	1:C:252:ARG:NH2	2.51	0.44
2:D:18:ILE:H	2:D:18:ILE:HG13	1.75	0.44
3:H:136:PRO:HD3	3:H:148:LEU:HB3	1.99	0.43
1:C:298:ARG:HD2	2:D:92:TRP:CD1	2.53	0.43
3:H:6:GLU:OE2	3:H:6:GLU:N	2.50	0.43
2:B:125:GLN:NE2	2:B:155:ASN:HA	2.29	0.43
3:H:165:ASN:HD22	3:H:169:LEU:HD22	1.84	0.43
1:A:18:THR:CG2	1:A:23:GLY:HA3	2.48	0.43
1:C:97:ALA:O	1:C:101:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:198:GLN:HA	4:F:207:GLU:HB2	2.01	0.43
4:L:37:TYR:CE1	4:L:47:THR:HG22	2.52	0.43
3:H:5:LEU:HB2	3:H:23:ALA:HB3	2.01	0.43
3:H:36:TRP:NE1	3:H:81:LEU:HB2	2.34	0.43
1:C:168:LEU:HB3	1:C:249:SER:HB2	2.01	0.43
2:D:123:LYS:HZ2	2:D:138:PHE:HE1	1.66	0.43
4:F:95:ASP:O	4:F:96:SER:C	2.57	0.43
2:B:58:LYS:HA	2:B:61:GLN:HG3	2.01	0.43
1:C:284:PRO:HG3	2:D:56:ILE:HG12	2.00	0.43
3:E:148:LEU:HD13	3:E:221:VAL:HG11	2.00	0.43
1:A:104:GLU:HB3	2:B:64:GLU:OE2	2.19	0.43
1:C:135:SER:OG	1:C:136:PHE:N	2.51	0.43
1:A:149:ASN:HA	1:A:183:THR:O	2.18	0.42
1:C:29:ALA:HA	1:C:309:THR:HG23	2.00	0.42
1:C:30:THR:HG22	1:C:309:THR:HG21	2.00	0.42
3:H:134:LEU:HD22	4:L:122:PHE:HB3	2.00	0.42
4:L:149:THR:OG1	4:L:200:THR:HB	2.19	0.42
1:C:34:GLU:OE1	1:C:35:ARG:N	2.52	0.42
3:H:51:ILE:HD13	3:H:72:ARG:HG2	2.01	0.42
4:F:92:GLN:HA	4:F:100:VAL:O	2.19	0.42
4:L:92:GLN:OE1	4:L:99:ARG:NH1	2.52	0.42
2:B:74:GLU:HB3	2:B:77:ILE:HG22	2.01	0.42
3:E:54:ASP:OD1	3:E:56:SER:OG	2.31	0.42
3:H:72:ARG:NH1	3:H:74:ASN:OD1	2.49	0.42
4:L:165:THR:OG1	4:L:166:THR:O	2.38	0.42
2:D:74:GLU:OE1	2:D:75:LYS:N	2.53	0.42
3:E:39:GLN:HB2	3:E:45:LEU:HD23	2.02	0.42
3:E:173:VAL:HG22	3:E:192:VAL:HG23	2.02	0.42
4:F:17:THR:HA	4:F:78:ILE:O	2.20	0.42
3:E:83:MET:HB3	3:E:86:LEU:HD21	2.02	0.42
1:A:172:GLY:HA2	1:A:222:ASP:O	2.19	0.42
2:B:21:TRP:NE1	2:B:45:ILE:HD11	2.35	0.42
1:C:108:ILE:HD12	1:C:110:LYS:HE3	2.02	0.42
4:F:149:THR:OG1	4:F:200:THR:HB	2.19	0.42
3:H:211:LYS:HB2	3:H:212:PRO:HD3	2.01	0.42
1:A:316:GLU:O	2:B:12:ASN:ND2	2.52	0.41
1:C:5:LEU:O	2:D:9:PHE:N	2.53	0.41
1:C:307:LEU:HD12	1:C:307:LEU:HA	1.82	0.41
3:H:132:PHE:HB2	3:H:151:LEU:HB3	2.02	0.41
4:L:91:CYS:O	4:L:102:GLY:N	2.49	0.41
1:C:171:TRP:HB2	1:C:242:PHE:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:VAL:HA	1:C:315:PRO:HD3	1.94	0.41
2:D:39:LYS:O	2:D:43:SER:CB	2.68	0.41
3:E:174:HIS:O	3:E:190:SER:HA	2.20	0.41
4:L:98:ASN:N	4:L:98:ASN:OD1	2.54	0.41
1:A:170:VAL:HG22	1:A:225:TRP:HB3	2.02	0.41
1:C:271:ASP:HB3	1:C:295:LYS:HD2	2.03	0.41
1:A:103:ARG:HB3	1:A:257:GLY:HA3	2.02	0.41
1:C:71:GLU:O	1:C:252:ARG:NH2	2.54	0.41
1:C:157:LYS:HA	1:C:157:LYS:HD3	1.82	0.41
4:F:138:CYS:HB3	4:F:180:SER:HB3	2.01	0.41
1:A:282:ASN:N	1:A:282:ASN:OD1	2.54	0.41
1:C:186:TYR:CZ	1:C:241:ALA:HA	2.56	0.41
3:H:219:LYS:HD2	3:H:219:LYS:HA	1.92	0.41
1:C:26:VAL:HG12	1:C:312:LYS:HA	2.03	0.41
3:H:35:HIS:CD2	3:H:99:HIS:HB3	2.56	0.41
1:A:186:TYR:O	1:A:191:LYS:NZ	2.32	0.40
3:E:60:TYR:HE2	3:E:70:ILE:H	1.69	0.40
3:E:164:TRP:CD1	3:E:173:VAL:HG11	2.56	0.40
3:H:156:PHE:HA	3:H:157:PRO:HA	1.86	0.40
1:A:90:GLY:HA3	1:A:221:ILE:O	2.21	0.40
3:H:50:LEU:HG	3:H:59:TYR:HB2	2.03	0.40
2:D:148:CYS:O	2:D:152:ILE:HG13	2.22	0.40
3:E:132:PHE:HD2	3:E:151:LEU:HD23	1.86	0.40
3:E:210:HIS:CD2	3:E:212:PRO:HD2	2.55	0.40
4:F:140:ILE:HG22	4:F:143:PHE:CE2	2.56	0.40
4:L:67:ILE:HD13	4:L:67:ILE:HA	1.90	0.40
1:A:311:MET:HG2	1:A:312:LYS:N	2.36	0.40
3:E:156:PHE:HA	3:E:157:PRO:HA	1.91	0.40
3:H:91:THR:HA	3:H:119:VAL:O	2.22	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	315/317 (99%)	291 (92%)	24 (8%)	0	100	100
1	C	315/317 (99%)	287 (91%)	27 (9%)	1 (0%)	41	71
2	B	164/166 (99%)	153 (93%)	11 (7%)	0	100	100
2	D	164/166 (99%)	158 (96%)	6 (4%)	0	100	100
3	E	216/225 (96%)	201 (93%)	15 (7%)	0	100	100
3	H	216/225 (96%)	202 (94%)	14 (6%)	0	100	100
4	F	210/212 (99%)	199 (95%)	11 (5%)	0	100	100
4	L	210/212 (99%)	197 (94%)	13 (6%)	0	100	100
All	All	1810/1840 (98%)	1688 (93%)	121 (7%)	1 (0%)	51	81

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	316	GLU

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	265/266 (100%)	254 (96%)	11 (4%)	30	60
1	C	265/266 (100%)	255 (96%)	10 (4%)	33	62
2	B	143/143 (100%)	139 (97%)	4 (3%)	43	70
2	D	143/143 (100%)	138 (96%)	5 (4%)	36	64
3	E	183/187 (98%)	179 (98%)	4 (2%)	52	74
3	H	183/187 (98%)	176 (96%)	7 (4%)	33	62
4	F	184/184 (100%)	180 (98%)	4 (2%)	52	74
4	L	184/184 (100%)	176 (96%)	8 (4%)	29	59
All	All	1550/1560 (99%)	1497 (97%)	53 (3%)	37	65

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	CYS
1	A	10	VAL
1	A	14	THR
1	A	18	THR
1	A	19	LEU
1	A	20	THR
1	A	85	ASP
1	A	92	PHE
1	A	113	MET
1	A	181	GLU
1	A	282	ASN
2	B	54	ARG
2	B	57	GLU
2	B	63	PHE
2	B	147	ASP
1	C	1	ASP
1	C	4	CYS
1	C	8	HIS
1	C	20	THR
1	C	24	VAL
1	C	111	GLU
1	C	146	ASN
1	C	181	GLU
1	C	186	TYR
1	C	267	ASN
2	D	22	TYR
2	D	63	PHE
2	D	137	CYS
2	D	138	PHE
2	D	159	HIS
3	E	3	GLN
3	E	53	TYR
3	E	72	ARG
3	E	150	CYS
4	F	13	SER
4	F	47	THR
4	F	195	TYR
4	F	207	GLU
3	H	5	LEU
3	H	18	LEU
3	H	50	LEU
3	H	64	VAL
3	H	67	ARG

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Mol	Chain	Res	Type
3	H	132	PHE
3	H	150	CYS
4	L	5	THR
4	L	47	THR
4	L	70	SER
4	L	98	ASN
4	L	149	THR
4	L	165	THR
4	L	207	GLU
4	L	209	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	125	GLN
4	L	35	GLN

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 monosaccharides 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 ⓘ

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	317/317 (100%)	-0.01	2 (0%) 89 90	40, 81, 129, 176	0
1	C	317/317 (100%)	0.29	20 (6%) 20 20	58, 114, 232, 296	0
2	B	166/166 (100%)	0.25	2 (1%) 79 78	38, 87, 116, 212	0
2	D	166/166 (100%)	1.18	37 (22%) 0 1	91, 218, 288, 323	0
3	E	220/225 (97%)	1.18	55 (25%) 0 0	54, 115, 308, 410	0
3	H	220/225 (97%)	0.86	38 (17%) 1 1	52, 113, 261, 367	0
4	F	212/212 (100%)	0.74	31 (14%) 2 2	53, 126, 299, 337	0
4	L	212/212 (100%)	0.34	22 (10%) 6 6	34, 100, 234, 300	0
All	All	1830/1840 (99%)	0.55	207 (11%) 5 5	34, 106, 265, 410	0

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	123	PRO	13.0
3	E	169	LEU	10.4
3	H	203	THR	10.4
3	E	206	CYS	9.9
3	E	200	GLY	9.8
3	H	201	THR	9.1
3	E	203	THR	8.4
2	D	59	THR	8.3
3	H	204	TYR	8.2
3	H	223	PRO	7.5
2	D	7	ALA	7.5
3	E	198	SER	7.5
3	E	208	VAL	7.4
3	H	135	ALA	7.4
3	E	201	THR	7.3
4	F	156	SER	7.0

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Mol	Chain	Res	Type	RSRZ
3	E	197	SER	6.8
3	E	164	TRP	6.7
3	E	202	GLN	6.6
2	D	19	ASP	6.4
3	H	200	GLY	6.4
2	D	5	ALA	6.3
4	L	196	SER	6.3
4	F	184	LEU	6.2
4	F	125	SER	6.2
3	E	204	TYR	6.2
3	E	217	VAL	6.0
3	H	217	VAL	6.0
3	E	150	CYS	5.8
4	F	129	LEU	5.8
3	E	209	ASN	5.7
3	H	221	VAL	5.7
2	D	25	ARG	5.7
3	E	149	GLY	5.7
4	F	132	ASN	5.6
1	C	2	LYS	5.5
3	E	215	THR	5.4
3	H	199	LEU	5.4
4	F	109	VAL	5.4
2	D	21	TRP	5.4
1	C	315	PRO	5.3
4	L	136	LEU	5.3
2	D	23	GLY	5.2
4	F	157	SER	5.1
3	E	134	LEU	5.1
3	H	136	PRO	5.0
4	L	123	PRO	4.9
2	D	6	ILE	4.9
2	B	60	ASN	4.9
2	D	38	TYR	4.9
3	H	169	LEU	4.8
2	D	139	GLU	4.8
3	E	221	VAL	4.7
3	E	193	THR	4.6
3	H	138	SER	4.6
3	E	205	ILE	4.6
3	E	171	SER	4.6
4	F	137	VAL	4.5

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Mol	Chain	Res	Type	RSRZ
3	H	206	CYS	4.5
2	D	20	GLY	4.5
3	H	208	VAL	4.4
3	E	147	ALA	4.4
2	D	164	GLU	4.4
3	H	198	SER	4.4
3	H	193	THR	4.3
3	E	166	SER	4.3
1	C	8	HIS	4.3
3	E	192	VAL	4.2
3	E	165	ASN	4.2
4	F	124	PRO	4.2
4	L	129	LEU	4.1
4	F	119	VAL	4.1
3	E	136	PRO	4.1
3	E	207	ASN	4.1
3	E	195	PRO	4.1
3	H	147	ALA	4.1
2	B	59	THR	4.1
4	L	195	TYR	4.0
3	E	168	ALA	4.0
3	H	191	VAL	4.0
4	L	122	PHE	3.8
4	L	209	THR	3.8
3	H	164	TRP	3.8
1	C	273	TYR	3.8
3	E	191	VAL	3.8
3	H	137	SER	3.8
3	H	149	GLY	3.6
4	F	198	GLN	3.6
4	L	124	PRO	3.6
3	E	137	SER	3.6
1	C	279	ILE	3.6
3	E	199	LEU	3.6
4	L	156	SER	3.6
1	C	15	LYS	3.5
2	D	130	ALA	3.5
4	F	121	LEU	3.4
3	E	170	THR	3.4
4	L	184	LEU	3.4
3	H	219	LYS	3.3
2	D	149	MET	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	11	SER	3.3
3	E	130	SER	3.3
3	E	216	LYS	3.3
3	E	145	THR	3.3
4	F	136	LEU	3.3
4	L	182	LEU	3.3
1	C	3	ILE	3.2
3	E	144	GLY	3.2
3	E	135	ALA	3.2
4	L	193	ARG	3.2
3	H	216	LYS	3.2
3	H	150	CYS	3.1
2	D	36	ALA	3.1
3	E	148	LEU	3.1
2	D	159	HIS	3.1
2	D	126	LEU	3.0
2	D	153	ARG	3.0
3	E	220	LYS	3.0
1	C	262	VAL	3.0
2	D	18	ILE	3.0
4	L	192	HIS	3.0
2	D	152	ILE	3.0
3	E	194	VAL	3.0
3	H	215	THR	3.0
1	A	9	ALA	2.9
2	D	60	ASN	2.9
3	H	192	VAL	2.9
4	F	120	THR	2.9
2	D	138	PHE	2.9
4	L	121	LEU	2.8
4	F	158	PRO	2.8
2	D	15	GLU	2.8
1	C	280	ILE	2.8
2	D	17	LEU	2.7
1	C	12	ASN	2.7
2	D	135	THR	2.7
3	E	213	SER	2.7
4	F	193	ARG	2.7
2	D	27	GLN	2.7
4	F	78	ILE	2.7
3	H	125	SER	2.6
4	F	187	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	307	LEU	2.6
3	H	173	VAL	2.6
4	F	140	ILE	2.6
3	H	205	ILE	2.6
4	F	115	ALA	2.6
3	E	219	LYS	2.6
3	H	162	VAL	2.6
3	H	218	ASP	2.6
3	E	151	LEU	2.6
2	D	125	GLN	2.6
3	E	173	VAL	2.6
3	E	212	PRO	2.6
3	H	222	GLU	2.5
2	D	140	ILE	2.5
1	C	313	ASN	2.5
4	L	207	GLU	2.5
4	F	189	TRP	2.4
4	L	171	GLN	2.4
3	E	125	SER	2.4
1	C	264	VAL	2.4
3	E	222	GLU	2.4
1	C	311	MET	2.4
3	H	151	LEU	2.4
4	L	198	GLN	2.4
4	F	146	GLY	2.4
4	L	130	GLN	2.4
3	H	166	SER	2.3
4	F	122	PHE	2.3
2	D	24	PHE	2.3
2	D	11	GLU	2.3
3	H	148	LEU	2.3
2	D	58	LYS	2.3
3	E	146	ALA	2.3
3	E	190	SER	2.3
4	F	185	THR	2.3
2	D	35	ALA	2.3
1	C	5	LEU	2.3
2	D	127	ARG	2.2
2	D	158	ASP	2.2
4	L	158	PRO	2.2
4	F	192	HIS	2.2
3	E	210	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	162	VAL	2.2
2	D	52	LEU	2.2
1	C	39	PRO	2.2
4	L	132	ASN	2.2
1	C	316	GLU	2.2
4	F	207	GLU	2.2
2	D	168	GLN	2.2
4	L	150	VAL	2.1
4	F	178	ALA	2.1
4	L	120	THR	2.1
4	F	79	SER	2.1
3	H	225	SER	2.1
1	C	10	VAL	2.1
3	H	134	LEU	2.1
1	A	234	VAL	2.1
4	F	114	LYS	2.0
1	C	263	GLN	2.0
4	F	107	LEU	2.0
3	E	138	SER	2.0
3	H	202	GLN	2.0
3	E	214	ASN	2.0
3	E	163	SER	2.0
2	D	156	THR	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 monosaccharides 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.