



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:48 AM UTC

PDB ID : 5W0K / pdb_00005w0k
Title : Crystal structure of EBV gHgL/CL40/gp42 N-domain
Authors : Sathiyamoorthy, K.; Jardetzky, T.S.
Deposited on : 2017-05-31
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

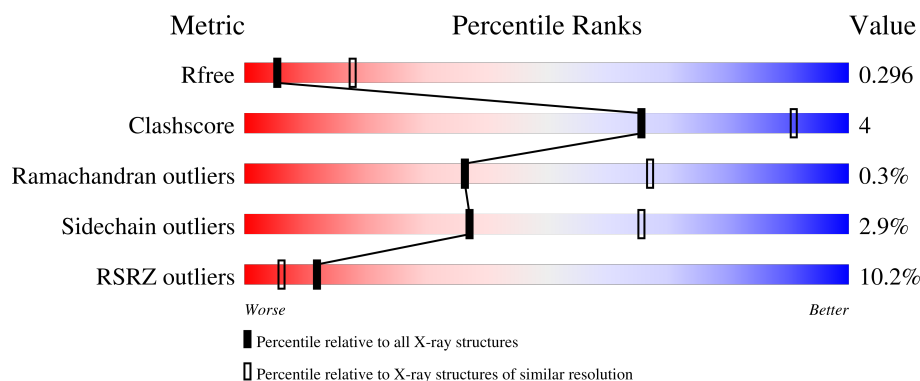
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	A	660	8% 89% 9% ..
1	C	660	21% 89% 10% ..
2	B	114	7% 75% 6% 18%
2	D	114	8% 71% 10% 19%
3	E	217	5% 91% 7% ..

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain	
3	H	217	2% 91% 7%	•
4	F	213	3% 89% 9%	•
4	L	213	2% 90% 8%	•
5	X	35	6% 66% 23% 9%	•
5	Y	35	9% 66% 20% 11%	•

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 37028 atoms, of which 18365 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	655	Total	C	H	N	O	S	0	0	0
			10212	3268	5115	842	956	31			
1	C	655	Total	C	H	N	O	S	0	0	0
			10212	3268	5115	842	956	31			

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	94	Total	C	H	N	O	S	0	0	0
			1422	454	704	120	140	4			
2	D	92	Total	C	H	N	O	S	0	0	0
			1391	442	690	118	137	4			

- Molecule 3 is a protein called CL40 IgG heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	H	213	Total	C	H	N	O	S	0	0	0
			3182	1024	1568	258	323	9			
3	E	214	Total	C	H	N	O	S	0	0	0
			3191	1026	1574	259	323	9			

- Molecule 4 is a protein called CL40 IgG light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	L	210	Total	C	H	N	O	S	0	0	0
			3185	1017	1555	272	334	7			
4	F	212	Total	C	H	N	O	S	0	0	0
			3223	1027	1574	278	337	7			

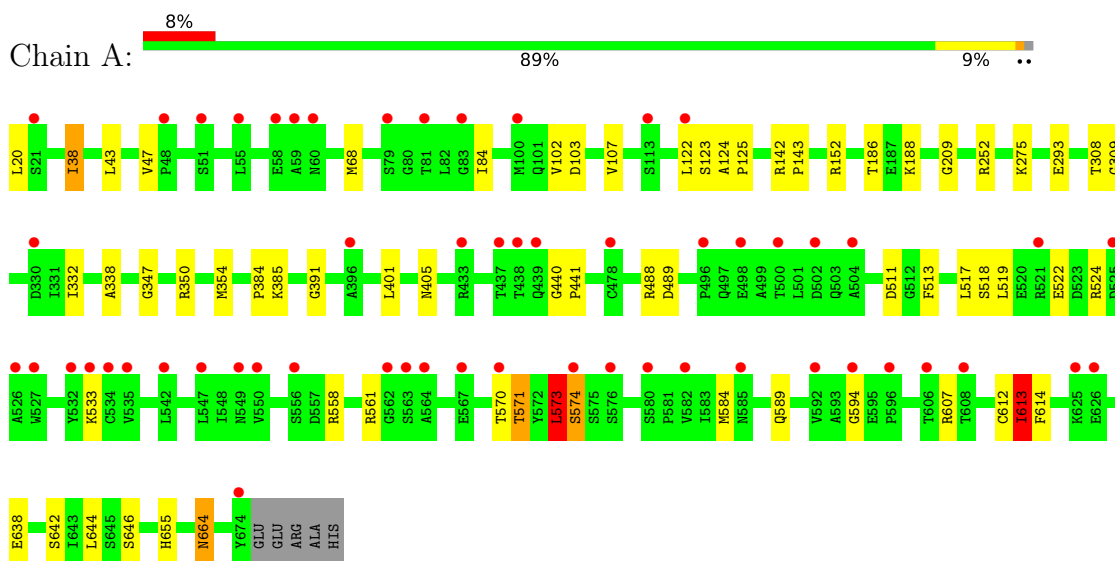
- Molecule 5 is a protein called Glycoprotein 42.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	34	Total	C	H	N	O	0	0	0
			543	184	262	45	52			
5	Y	31	Total	C	H	N	O	0	0	0
			467	170	208	41	48			

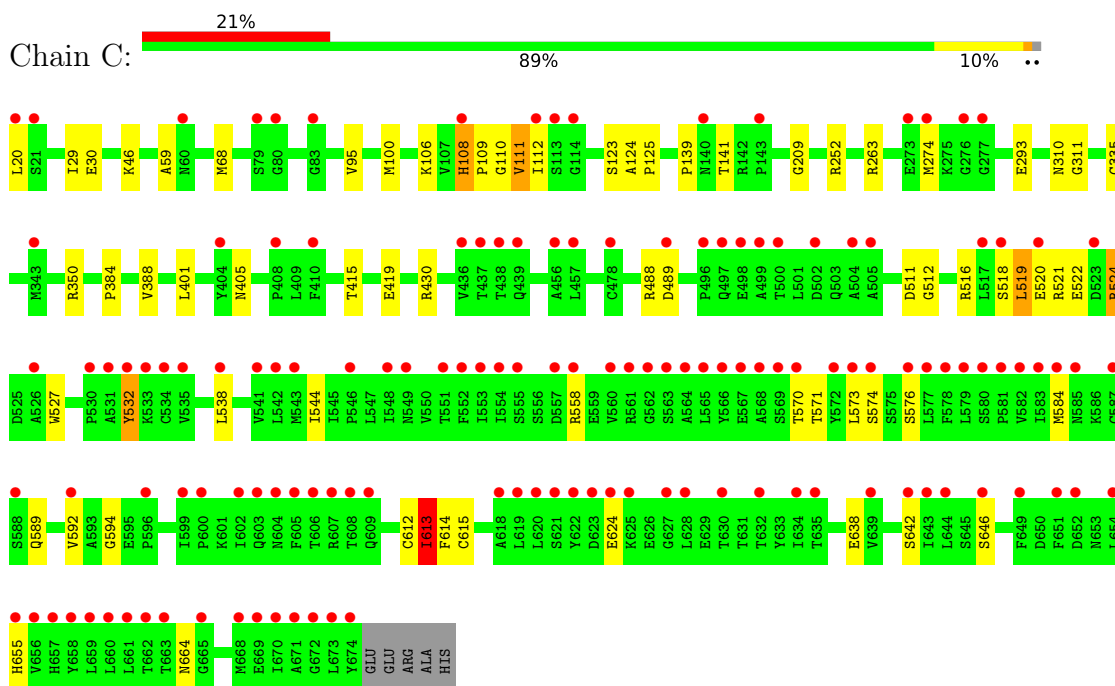
3 Residue-property plots [i](#)

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.

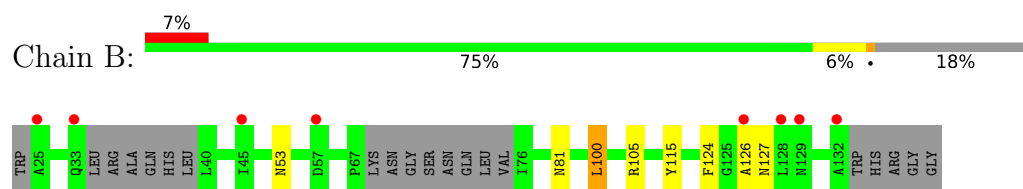
• Molecule 1: Envelope glycoprotein H



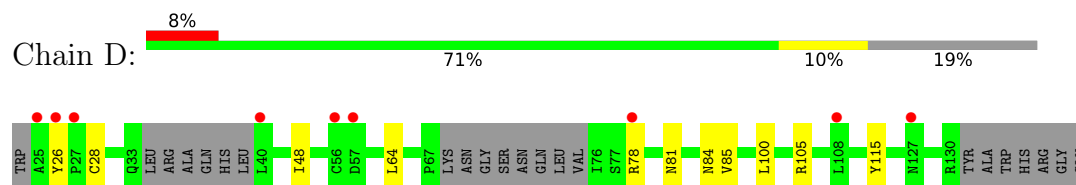
• Molecule 1: Envelope glycoprotein H



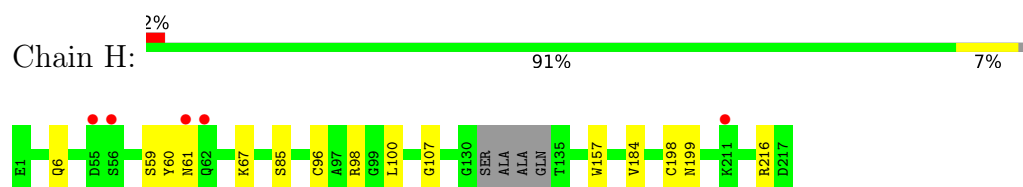
- Molecule 2: Envelope glycoprotein L



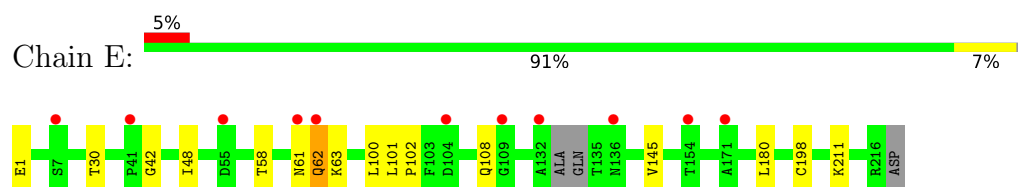
- Molecule 2: Envelope glycoprotein L



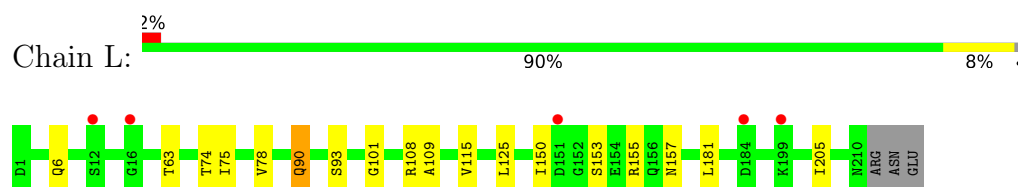
- Molecule 3: CL40 IgG heavy chain



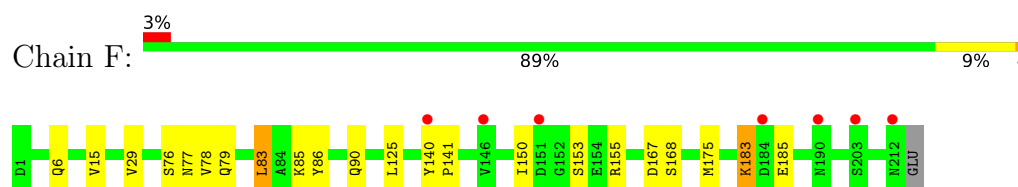
- Molecule 3: CL40 IgG heavy chain



- Molecule 4: CL40 IgG light chain

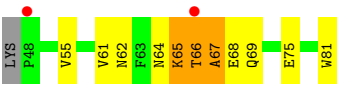


- Molecule 4: CL40 IgG light chain



- Molecule 5: Glycoprotein 42





● Molecule 5: Glycoprotein 42



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.38Å 133.13Å 254.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	22.76 – 3.10 22.76 – 3.10	Depositor EDS
% Data completeness (in resolution range)	90.5 (22.76-3.10) 90.4 (22.76-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.11.1 _2575	Depositor
R, R_{free}	0.242 , 0.299 0.241 , 0.296	Depositor DCC
R_{free} test set	2923 reflections (3.89%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	37028	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.55% 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	0.11	0/5206	0.32	0/7066
1	C	0.13	0/5206	0.33	0/7066
2	B	0.10	0/728	0.33	0/986
2	D	0.11	0/710	0.32	0/961
3	E	0.11	0/1660	0.33	0/2269
3	H	0.13	0/1657	0.34	0/2265
4	F	0.11	0/1686	0.33	0/2287
4	L	0.10	0/1667	0.30	0/2262
5	X	0.17	0/294	0.50	0/406
5	Y	0.20	0/271	0.54	0/374
All	All	0.12	0/19085	0.33	0/25942

There are no bond length outliers.

There are no bond angle outliers.

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	5097	5115	5115	42	0
1	C	5097	5115	5115	50	0
2	B	718	704	703	4	0
2	D	701	690	689	8	0
3	E	1617	1574	1574	4	0
3	H	1614	1568	1568	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1649	1574	1574	13	0
4	L	1630	1555	1555	9	0
5	X	281	262	262	9	0
5	Y	259	208	239	10	0
All	All	18663	18365	18394	140	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 4.

All (140) 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:A:612:CYS:O	1:A:614:PHE:N	1.99	0.95
1:A:488:ARG:NH1	1:A:511:ASP:OD1	2.10	0.84
2:B:100:LEU:O	2:B:105:ARG:NH1	2.12	0.82
1:C:516:ARG:O	1:C:524:ARG:NH2	2.14	0.81
3:E:48:ILE:O	3:E:62:GLN:NE2	2.15	0.80
1:A:123:SER:OG	1:A:309:GLY:O	1.98	0.79
4:L:63:THR:OG1	4:L:74:THR:OG1	1.99	0.79
1:C:488:ARG:NH1	1:C:511:ASP:OD1	2.16	0.79
4:F:155:ARG:NH2	4:F:185:GLU:OE2	2.18	0.76
1:A:152:ARG:NH2	5:X:75:GLU:OE2	2.17	0.76
5:X:66:THR:O	5:X:68:GLU:N	2.20	0.75
1:C:519:LEU:O	1:C:521:ARG:N	2.20	0.74
1:A:252:ARG:NH2	1:A:293:GLU:OE2	2.21	0.73
2:D:100:LEU:O	2:D:105:ARG:NH1	2.21	0.73
1:C:558:ARG:NH2	1:C:594:GLY:O	2.23	0.70
1:A:558:ARG:NH2	1:A:594:GLY:O	2.25	0.70
4:F:125:LEU:O	4:F:183:LYS:NZ	2.25	0.69
4:L:155:ARG:NH1	4:L:157:ASN:O	2.27	0.68
1:A:401:LEU:O	1:A:405:ASN:ND2	2.30	0.63
1:C:209:GLY:O	2:D:115:TYR:OH	2.16	0.63
1:A:589:GLN:OE1	1:A:589:GLN:N	2.32	0.62
1:C:123:SER:OG	1:C:311:GLY:N	2.31	0.62
1:C:612:CYS:O	1:C:613:ILE:C	2.42	0.62
1:C:589:GLN:N	1:C:589:GLN:OE1	2.31	0.61
1:A:209:GLY:O	2:B:115:TYR:OH	2.15	0.61
1:C:613:ILE:O	1:C:614:PHE:HB2	2.02	0.60
1:C:401:LEU:O	1:C:405:ASN:ND2	2.35	0.59
1:A:350:ARG:NH2	5:X:64:ASN:O	2.35	0.58
1:C:512:GLY:O	1:C:516:ARG:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:519:LEU:C	1:C:521:ARG:H	2.11	0.58
1:A:612:CYS:C	1:A:614:PHE:H	2.11	0.57
4:L:6:GLN:OE1	4:L:101:GLY:N	2.38	0.56
5:Y:65:LYS:O	5:Y:66:THR:HB	2.06	0.55
1:C:522:GLU:OE2	1:C:524:ARG:NH2	2.41	0.54
1:C:638:GLU:OE1	1:C:638:GLU:N	2.40	0.54
1:C:570:THR:HG22	1:C:571:THR:HG22	1.90	0.53
1:C:252:ARG:NH2	1:C:293:GLU:OE2	2.39	0.53
1:C:570:THR:HG21	1:C:576:SER:HA	1.90	0.53
3:H:67:LYS:NZ	3:H:85:SER:O	2.40	0.53
4:L:63:THR:O	4:L:74:THR:OG1	2.27	0.52
4:F:76:SER:O	4:F:77:ASN:C	2.52	0.52
5:Y:64:ASN:OD1	5:Y:64:ASN:C	2.52	0.52
1:A:613:ILE:HD12	1:A:613:ILE:O	2.10	0.52
3:H:59:SER:OG	3:H:61:ASN:OD1	2.26	0.51
1:A:68:MET:SD	2:B:81:ASN:ND2	2.79	0.51
1:C:100:MET:HB3	1:C:112:ILE:HG21	1.91	0.51
1:A:570:THR:OG1	1:A:571:THR:N	2.43	0.51
1:A:354:MET:HG2	5:X:61:VAL:HG11	1.93	0.50
4:L:150:ILE:N	4:L:153:SER:O	2.42	0.50
4:F:150:ILE:N	4:F:153:SER:O	2.40	0.50
4:L:90:GLN:NE2	4:L:93:SER:O	2.44	0.50
1:A:533:LYS:O	1:A:561:ARG:NH2	2.45	0.50
2:D:64:LEU:O	2:D:78:ARG:N	2.44	0.50
1:A:638:GLU:OE1	1:A:638:GLU:N	2.42	0.49
1:C:518:SER:C	1:C:519:LEU:O	2.54	0.49
1:A:102:VAL:O	1:A:122:LEU:HD22	2.11	0.49
1:A:522:GLU:HG3	1:A:524:ARG:HG2	1.94	0.49
1:C:527:TRP:CZ2	1:C:538:LEU:HG	2.48	0.48
1:C:108:HIS:O	1:C:111:VAL:HB	2.14	0.48
5:Y:64:ASN:O	5:Y:65:LYS:C	2.57	0.48
1:C:532:TYR:CE1	1:C:544:ILE:CD1	2.97	0.48
5:Y:68:GLU:OE1	5:Y:68:GLU:N	2.46	0.48
2:D:64:LEU:N	2:D:78:ARG:O	2.44	0.48
1:C:384:PRO:O	1:C:430:ARG:NH1	2.48	0.47
1:C:516:ARG:O	1:C:516:ARG:HD3	2.15	0.47
1:A:103:ASP:HA	1:A:122:LEU:HD22	1.96	0.47
1:C:570:THR:CG2	1:C:576:SER:HA	2.45	0.47
5:X:62:ASN:OD1	5:X:64:ASN:HB2	2.14	0.47
1:A:518:SER:O	1:A:522:GLU:HB2	2.16	0.46
1:A:573:LEU:O	1:A:574:SER:O	2.33	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:139:PRO:HG3	5:Y:81:TRP:CD2	2.51	0.46
4:F:15:VAL:O	4:F:78:VAL:O	2.33	0.46
1:A:122:LEU:O	1:A:122:LEU:HD23	2.15	0.46
3:H:157:TRP:CD2	3:H:184:VAL:HG21	2.51	0.46
1:C:29:ILE:HG23	1:C:30:GLU:H	1.80	0.46
5:Y:66:THR:HG21	5:Y:69:GLN:HG3	1.98	0.46
1:A:489:ASP:OD1	1:A:489:ASP:N	2.49	0.46
3:H:6:GLN:OE1	3:H:107:GLY:HA3	2.16	0.46
1:C:527:TRP:CZ3	1:C:532:TYR:CD1	3.04	0.46
1:C:642:SER:O	1:C:646:SER:OG	2.26	0.46
1:A:384:PRO:O	1:A:385:LYS:HG2	2.15	0.46
1:C:527:TRP:HA	1:C:532:TYR:CD2	2.51	0.46
1:A:642:SER:O	1:A:646:SER:OG	2.33	0.45
2:B:124:PHE:C	2:B:126:ALA:H	2.24	0.45
5:X:66:THR:O	5:X:67:ALA:C	2.59	0.45
5:Y:66:THR:CG2	5:Y:69:GLN:HG3	2.46	0.45
1:A:607:ARG:NH1	1:A:644:LEU:O	2.43	0.45
1:A:124:ALA:HB3	1:A:125:PRO:CD	2.46	0.45
4:F:167:ASP:OD1	4:F:168:SER:N	2.51	0.44
4:L:108:ARG:NH1	4:L:109:ALA:O	2.50	0.44
1:C:350:ARG:NH1	5:Y:64:ASN:H	2.16	0.44
1:A:332:ILE:HG22	1:A:338:ALA:HB3	1.99	0.44
4:F:6:GLN:NE2	4:F:86:TYR:O	2.45	0.44
1:C:612:CYS:O	1:C:612:CYS:SG	2.75	0.43
2:D:26:TYR:O	2:D:28:CYS:N	2.51	0.43
1:A:122:LEU:HD21	1:A:125:PRO:HG2	1.99	0.43
2:D:48:ILE:HD11	2:D:85:VAL:HG11	2.00	0.43
1:A:573:LEU:HB3	1:A:574:SER:H	1.74	0.43
1:C:571:THR:HG21	1:C:574:SER:CA	2.49	0.43
4:F:29:VAL:HG11	4:F:90:GLN:HB2	2.01	0.43
4:F:78:VAL:HG12	4:F:79:GLN:N	2.34	0.43
1:A:142:ARG:N	1:A:143:PRO:HD2	2.34	0.43
5:X:65:LYS:O	5:X:66:THR:C	2.60	0.43
1:C:68:MET:SD	2:D:81:ASN:ND2	2.86	0.43
1:C:123:SER:N	1:C:311:GLY:O	2.45	0.43
1:C:106:LYS:O	1:C:108:HIS:NE2	2.52	0.42
1:C:111:VAL:HG13	1:C:112:ILE:H	1.84	0.42
1:C:274:MET:HB2	1:C:512:GLY:HA2	2.01	0.42
4:F:140:TYR:HB3	4:F:141:PRO:HD3	2.00	0.42
1:A:664:ASN:O	1:A:664:ASN:ND2	2.51	0.42
1:C:489:ASP:OD1	1:C:489:ASP:N	2.50	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:100:LEU:O	3:E:102:PRO:O	2.37	0.42
1:A:186:THR:C	1:A:188:LYS:H	2.28	0.42
1:A:391:GLY:HA2	5:X:55:VAL:HG21	2.00	0.42
1:C:310:ASN:O	1:C:310:ASN:ND2	2.47	0.42
1:C:558:ARG:NH1	1:C:592:VAL:O	2.41	0.42
1:A:84:ILE:HD12	1:A:84:ILE:N	2.35	0.42
1:A:440:GLY:N	1:A:441:PRO:HD2	2.35	0.42
5:X:65:LYS:O	5:X:69:GLN:HB2	2.19	0.42
1:C:110:GLY:O	1:C:111:VAL:C	2.63	0.42
1:C:263:ARG:NH1	1:C:419:GLU:OE1	2.53	0.42
1:C:59:ALA:O	2:D:84:ASN:ND2	2.52	0.42
1:C:109:PRO:HG3	5:Y:63:PHE:CE1	2.54	0.42
3:E:145:VAL:O	3:E:180:LEU:N	2.47	0.42
1:C:571:THR:HG21	1:C:574:SER:N	2.35	0.41
1:C:571:THR:CG2	1:C:574:SER:H	2.34	0.41
4:F:83:LEU:HD13	4:F:83:LEU:O	2.20	0.41
1:C:124:ALA:HB3	1:C:125:PRO:HD3	2.02	0.41
4:F:29:VAL:O	4:F:29:VAL:HG12	2.19	0.41
1:A:47:VAL:O	1:A:47:VAL:HG23	2.20	0.41
1:A:107:VAL:HG21	1:A:347:GLY:HA2	2.03	0.41
1:A:613:ILE:O	1:A:613:ILE:CG1	2.68	0.41
1:C:571:THR:HA	1:C:624:GLU:O	2.21	0.41
3:E:42:GLY:O	4:F:85:LYS:NZ	2.54	0.41
5:Y:81:TRP:HA	5:Y:81:TRP:CE3	2.55	0.41
1:A:513:PHE:O	1:A:517:LEU:HD12	2.20	0.41
4:L:75:ILE:HG23	4:L:75:ILE:O	2.21	0.41
1:A:38:ILE:O	1:A:38:ILE:CG1	2.67	0.40
4:L:115:VAL:HG11	4:L:205:ILE:HG22	2.04	0.40
1:C:527:TRP:HA	1:C:532:TYR:CE2	2.56	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	653/660 (99%)	617 (94%)	32 (5%)	4 (1%)	21	52
1	C	653/660 (99%)	610 (93%)	41 (6%)	2 (0%)	36	67
2	B	88/114 (77%)	80 (91%)	8 (9%)	0	100	100
2	D	86/114 (75%)	81 (94%)	5 (6%)	0	100	100
3	E	210/217 (97%)	202 (96%)	8 (4%)	0	100	100
3	H	209/217 (96%)	194 (93%)	15 (7%)	0	100	100
4	F	210/213 (99%)	199 (95%)	11 (5%)	0	100	100
4	L	208/213 (98%)	199 (96%)	9 (4%)	0	100	100
5	X	32/35 (91%)	24 (75%)	6 (19%)	2 (6%)	1	6
5	Y	29/35 (83%)	22 (76%)	7 (24%)	0	100	100
All	All	2378/2478 (96%)	2228 (94%)	142 (6%)	8 (0%)	36	67

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	574	SER
1	A	613	ILE
5	X	67	ALA
1	C	520	GLU
1	A	573	LEU
1	A	571	THR
5	X	66	THR
1	C	613	ILE

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	561/565 (99%)	550 (98%)	11 (2%)	48	72
1	C	561/565 (99%)	543 (97%)	18 (3%)	34	64
2	B	82/98 (84%)	79 (96%)	3 (4%)	30	61
2	D	81/98 (83%)	81 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	185/187 (99%)	175 (95%)	10 (5%)	20	50
3	H	185/187 (99%)	178 (96%)	7 (4%)	29	60
4	F	188/189 (100%)	185 (98%)	3 (2%)	55	75
4	L	186/189 (98%)	182 (98%)	4 (2%)	45	71
5	X	32/33 (97%)	30 (94%)	2 (6%)	16	45
5	Y	29/33 (88%)	27 (93%)	2 (7%)	14	41
All	All	2090/2144 (98%)	2030 (97%)	60 (3%)	37	66

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	LEU
1	A	38	ILE
1	A	43	LEU
1	A	275	LYS
1	A	308	THR
1	A	519	LEU
1	A	573	LEU
1	A	584	MET
1	A	613	ILE
1	A	655	HIS
1	A	664	ASN
2	B	53	ASN
2	B	100	LEU
2	B	127	ASN
3	H	60	TYR
3	H	96	CYS
3	H	98	ARG
3	H	100	LEU
3	H	198	CYS
3	H	199	ASN
3	H	216	ARG
4	L	78	VAL
4	L	90	GLN
4	L	125	LEU
4	L	181	LEU
5	X	65	LYS
5	X	81	TRP
1	C	20	LEU
1	C	46	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	95	VAL
1	C	108	HIS
1	C	111	VAL
1	C	141	THR
1	C	335	CYS
1	C	388	VAL
1	C	415	THR
1	C	519	LEU
1	C	524	ARG
1	C	532	TYR
1	C	573	LEU
1	C	584	MET
1	C	613	ILE
1	C	615	CYS
1	C	655	HIS
1	C	664	ASN
3	E	1	GLU
3	E	30	THR
3	E	58	THR
3	E	61	ASN
3	E	62	GLN
3	E	63	LYS
3	E	101	LEU
3	E	108	GLN
3	E	198	CYS
3	E	211	LYS
4	F	83	LEU
4	F	175	MET
4	F	183	LYS
5	Y	61	VAL
5	Y	81	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	140	ASN
1	A	150	GLN
1	A	154	HIS
1	A	407	HIS
1	A	411	GLN
1	A	655	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	L	27	GLN
4	L	210	ASN
1	C	192	HIS
1	C	426	HIS
2	D	30	HIS
2	D	127	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](#)

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	655/660 (99%)	0.48	56 (8%) 16 9	21, 61, 127, 157	0
1	C	655/660 (99%)	0.94	139 (21%) 2 1	20, 67, 162, 192	0
2	B	94/114 (82%)	0.79	8 (8%) 16 9	34, 70, 110, 125	0
2	D	92/114 (80%)	0.52	9 (9%) 13 7	35, 66, 113, 127	0
3	E	214/217 (98%)	0.16	11 (5%) 33 18	22, 44, 77, 129	0
3	H	213/217 (98%)	0.16	5 (2%) 61 39	25, 45, 84, 108	0
4	F	212/213 (99%)	0.43	7 (3%) 49 29	23, 62, 110, 140	0
4	L	210/213 (98%)	0.35	5 (2%) 59 38	24, 65, 95, 113	0
5	X	34/35 (97%)	0.28	2 (5%) 28 15	43, 64, 92, 109	0
5	Y	31/35 (88%)	0.59	3 (9%) 13 7	41, 69, 93, 104	0
All	All	2410/2478 (97%)	0.55	245 (10%) 12 6	20, 60, 137, 192	0

All (245) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	567	GLU	7.0
1	A	625	LYS	6.7
1	C	553	ILE	6.5
1	C	671	ALA	6.0
1	C	624	GLU	5.8
1	C	580	SER	5.7
1	C	596	PRO	5.5
1	C	577	LEU	5.5
1	C	655	HIS	5.4
1	C	620	LEU	5.4
3	E	61	ASN	5.2
1	A	567	GLU	5.2
1	C	625	LYS	5.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	H	61	ASN	5.0
1	C	570	THR	5.0
1	C	554	ILE	5.0
1	A	500	THR	4.8
1	C	534	CYS	4.8
1	C	619	LEU	4.8
1	C	622	TYR	4.8
2	D	25	ALA	4.8
1	C	456	ALA	4.7
1	C	562	GLY	4.7
1	C	605	PHE	4.6
1	C	569	SER	4.6
1	C	438	THR	4.5
2	B	129	ASN	4.5
1	C	108	HIS	4.5
1	C	555	SER	4.5
1	C	574	SER	4.4
1	C	566	TYR	4.4
4	F	190	ASN	4.4
1	C	114	GLY	4.3
1	C	531	ALA	4.3
1	C	518	SER	4.3
1	C	564	ALA	4.2
2	D	26	TYR	4.2
1	C	599	ILE	4.1
1	C	587	CYS	4.0
1	C	496	PRO	3.9
1	C	579	LEU	3.9
1	C	669	GLU	3.9
3	H	55	ASP	3.9
1	C	502	ASP	3.8
1	C	565	LEU	3.8
1	C	582	VAL	3.7
1	C	672	GLY	3.7
1	C	504	ALA	3.7
2	D	127	ASN	3.7
1	A	592	VAL	3.6
1	C	439	GLN	3.6
1	A	60	ASN	3.6
1	A	496	PRO	3.6
1	C	592	VAL	3.6
1	C	573	LEU	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	437	THR	3.6
1	C	500	THR	3.6
1	A	437	THR	3.5
1	C	665	GLY	3.5
1	C	654	LEU	3.5
1	A	100	MET	3.5
1	A	527	TRP	3.5
1	C	478	CYS	3.4
1	A	574	SER	3.4
1	C	532	TYR	3.4
1	A	525	ASP	3.4
3	E	132	ALA	3.4
1	C	578	PHE	3.3
1	C	535	VAL	3.3
1	C	21	SER	3.3
1	C	113	SER	3.3
1	C	80	GLY	3.3
1	C	277	GLY	3.3
1	A	51	SER	3.3
1	C	560	VAL	3.3
1	A	502	ASP	3.2
1	C	498	GLU	3.2
3	E	109	GLY	3.2
1	C	656	VAL	3.2
1	C	643	ILE	3.2
1	C	561	ARG	3.2
1	C	552	PHE	3.2
1	C	576	SER	3.2
3	H	62	GLN	3.2
1	A	330	ASP	3.1
1	C	644	LEU	3.1
1	C	602	ILE	3.1
1	C	274	MET	3.1
1	A	79	SER	3.1
1	C	572	TYR	3.1
1	C	630	THR	3.1
1	A	596	PRO	3.0
1	A	674	TYR	3.0
1	C	658	TYR	3.0
1	A	564	ALA	3.0
1	C	632	THR	3.0
1	C	408	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	563	SER	3.0
1	C	635	THR	3.0
1	C	660	LEU	3.0
3	E	104	ASP	3.0
1	A	550	VAL	3.0
1	C	649	PHE	3.0
3	E	171	ALA	2.9
1	C	541	VAL	2.9
1	A	59	ALA	2.9
3	E	55	ASP	2.9
2	B	126	ALA	2.9
1	C	543	MET	2.9
3	E	62	GLN	2.9
1	C	600	PRO	2.9
1	A	585	ASN	2.9
4	F	212	ASN	2.9
1	C	652	ASP	2.8
1	C	581	PRO	2.8
1	C	673	LEU	2.8
1	A	526	ALA	2.8
1	C	657	HIS	2.8
1	A	439	GLN	2.8
1	C	621	SER	2.8
2	B	128	LEU	2.8
5	X	48	PRO	2.8
1	A	594	GLY	2.7
1	C	557	ASP	2.7
2	D	57	ASP	2.7
1	C	588	SER	2.7
4	L	12	SER	2.7
2	B	25	ALA	2.7
1	C	497	GLN	2.7
1	C	530	PRO	2.7
1	C	343	MET	2.7
1	C	608	THR	2.7
1	C	523	ASP	2.7
2	D	108	LEU	2.7
1	A	626	GLU	2.7
1	C	583	ILE	2.6
1	A	521	ARG	2.6
1	A	48	PRO	2.6
1	A	122	LEU	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	517	LEU	2.6
1	C	642	SER	2.6
1	C	659	LEU	2.6
5	Y	69	GLN	2.6
1	C	551	THR	2.6
1	C	607	ARG	2.5
1	C	639	VAL	2.5
4	F	184	ASP	2.5
1	C	674	TYR	2.5
2	B	33	GLN	2.5
2	B	132	ALA	2.5
1	C	670	ILE	2.5
1	A	478	CYS	2.5
1	C	520	GLU	2.5
1	C	662	THR	2.5
1	C	83	GLY	2.5
2	B	57	ASP	2.5
4	F	151	ASP	2.5
1	A	562	GLY	2.5
1	C	646	SER	2.4
1	A	433	ARG	2.4
1	A	549	ASN	2.4
1	A	81	THR	2.4
1	C	663	THR	2.4
1	C	79	SER	2.4
1	C	542	LEU	2.4
1	C	404	TYR	2.4
3	H	211	LYS	2.4
1	C	273	GLU	2.4
1	A	113	SER	2.4
1	A	576	SER	2.4
1	C	585	ASN	2.3
4	L	184	ASP	2.3
1	C	457	LEU	2.3
1	A	580	SER	2.3
3	E	136	ASN	2.3
4	F	140	TYR	2.3
1	A	55	LEU	2.3
1	A	438	THR	2.3
1	C	568	ALA	2.3
1	A	534	CYS	2.3
2	D	40	LEU	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	489	ASP	2.3
1	A	498	GLU	2.3
1	C	112	ILE	2.3
1	C	618	ALA	2.3
1	C	20	LEU	2.3
1	C	651	PHE	2.3
1	C	546	PRO	2.2
2	D	27	PRO	2.2
1	C	604	ASN	2.2
1	C	668	MET	2.2
1	C	563	SER	2.2
1	C	60	ASN	2.2
1	C	143	PRO	2.2
1	C	584	MET	2.2
3	E	41	PRO	2.2
1	A	532	TYR	2.2
1	C	609	GLN	2.2
1	C	634	ILE	2.2
2	B	45	ILE	2.2
1	C	623	ASP	2.2
5	Y	73	ASP	2.2
1	A	582	VAL	2.2
4	F	203	SER	2.2
1	C	276	GLY	2.2
4	L	16	GLY	2.2
1	C	499	ALA	2.1
1	A	570	THR	2.1
1	A	608	THR	2.1
1	C	661	LEU	2.1
1	C	603	GLN	2.1
1	C	505	ALA	2.1
1	A	21	SER	2.1
1	A	83	GLY	2.1
1	C	549	ASN	2.1
1	A	535	VAL	2.1
1	A	58	GLU	2.1
1	C	627	GLY	2.1
3	E	7	SER	2.1
1	C	436	VAL	2.1
4	F	146	VAL	2.1
1	C	533	LYS	2.1
1	C	538	LEU	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	526	ALA	2.1
1	A	556	SER	2.1
3	H	56	SER	2.1
2	D	78	ARG	2.1
1	C	606	THR	2.1
2	D	56	CYS	2.1
4	L	199	LYS	2.0
1	C	140	ASN	2.0
1	C	558	ARG	2.0
1	A	606	THR	2.0
3	E	154	THR	2.0
1	C	410	PHE	2.0
5	Y	72	GLY	2.0
1	A	533	LYS	2.0
1	C	548	ILE	2.0
1	A	396	ALA	2.0
1	A	504	ALA	2.0
5	X	66	THR	2.0
4	L	151	ASP	2.0
1	A	542	LEU	2.0
1	A	547	LEU	2.0
1	C	628	LEU	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.