



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 25, 2023 – 02:50 AM EDT

PDB ID : 5W0K
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 : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35.1
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) : 2.35.1

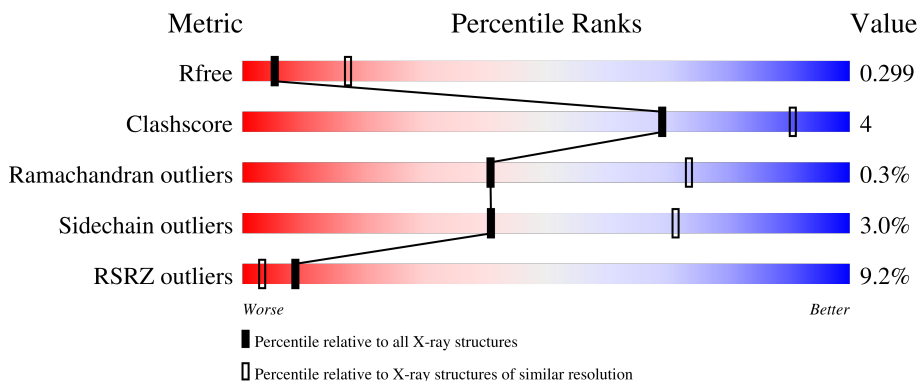
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (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% 90% 8% ..
1	C	660	 17% 89% 9% ..
2	B	114	 6% 75% 6% • 18%
2	D	114	 6% 70% 11% 19%
3	E	217	 3% 91% 7% •

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Mol	Chain	Length	Quality of chain
3	H	217	<p>91% 7%</p>
4	F	213	<p>89% 9%</p>
4	L	213	<p>91% 7%</p>
5	X	35	<p>66% 23% 9%</p>
5	Y	35	<p>66% 20% 11%</p>

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
			Total	C	H	N	O	S			
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
			Total	C	H	N	O	S			
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
			Total	C	H	N	O	S			
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
			Total	C	H	N	O	S			
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			

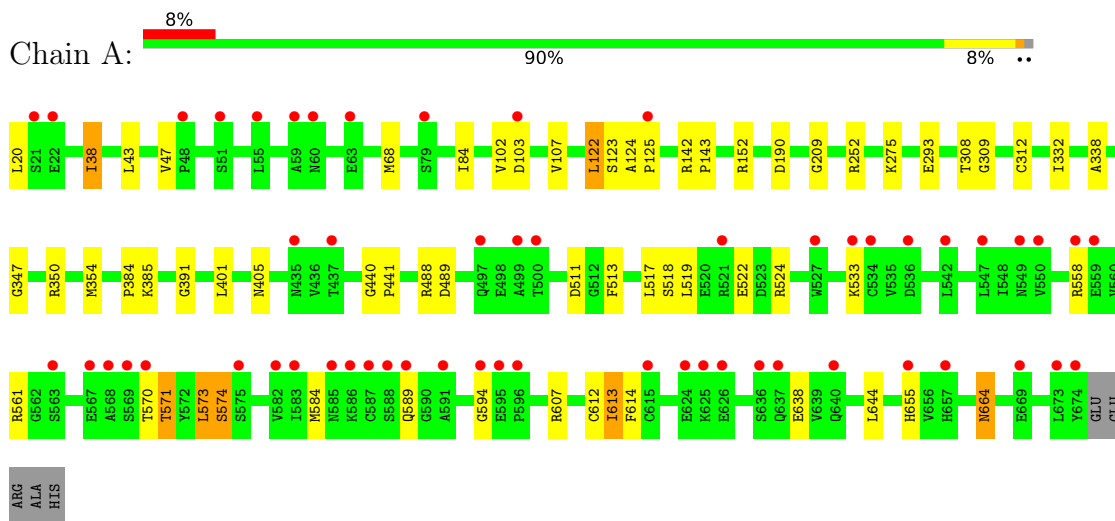
- Molecule 5 is a protein called Glycoprotein 42.

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

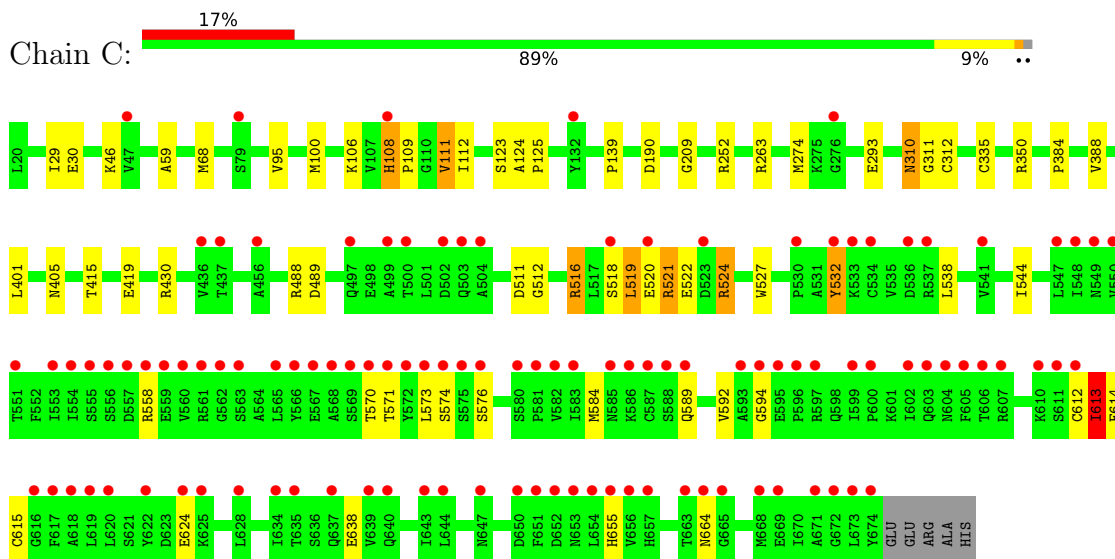
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

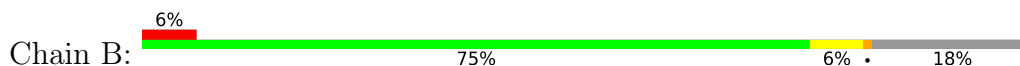
- Molecule 1: Envelope glycoprotein H



- Molecule 1: Envelope glycoprotein H

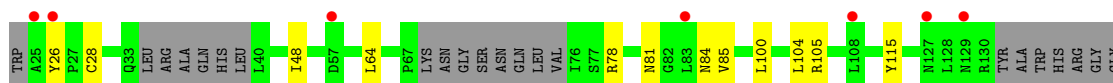


- Molecule 2: Envelope glycoprotein L

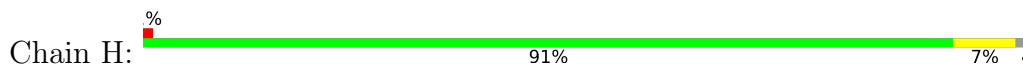




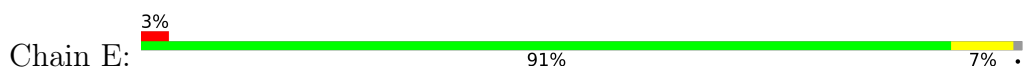
- Molecule 2: Envelope glycoprotein L



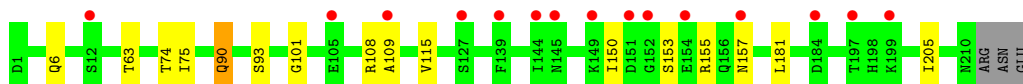
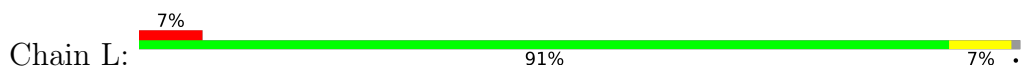
- Molecule 3: CL40 IgG heavy chain



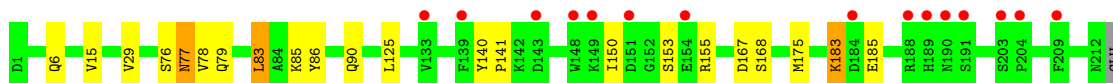
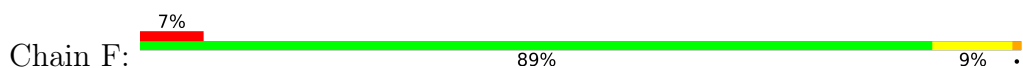
- Molecule 3: CL40 IgG heavy chain



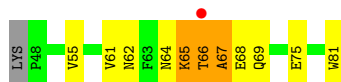
- Molecule 4: CL40 IgG light chain



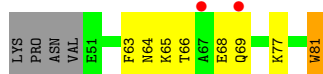
- Molecule 4: CL40 IgG light chain



- 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 49.28 – 2.88	Depositor EDS
% Data completeness (in resolution range)	90.5 (22.76-3.10) 78.0 (49.28-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 2.86Å)	Xtrriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.242 , 0.299 0.243 , 0.299	Depositor DCC
R_{free} test set	2923 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	59.5	Xtrriage
Anisotropy	0.061	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	37028	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtrriage'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	0.25	0/5206	0.44	0/7066
1	C	0.25	0/5206	0.46	0/7066
2	B	0.24	0/728	0.43	0/986
2	D	0.25	0/710	0.46	0/961
3	E	0.25	0/1660	0.48	0/2269
3	H	0.26	0/1657	0.47	0/2265
4	F	0.26	0/1686	0.48	0/2287
4	L	0.25	0/1667	0.46	0/2262
5	X	0.27	0/294	0.51	0/406
5	Y	0.31	0/271	0.51	0/374
All	All	0.25	0/19085	0.46	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	39	0
1	C	5097	5115	5115	48	0
2	B	718	704	703	4	0
2	D	701	690	689	8	0
3	E	1617	1574	1574	5	0
3	H	1614	1568	1568	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1649	1574	1574	13	0
4	L	1630	1555	1555	10	0
5	X	281	262	262	8	0
5	Y	259	208	239	10	0
All	All	18663	18365	18394	136	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 (136) 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
4:L:63:THR:HG1	4:L:74:THR:HG1	1.15	0.88
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
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: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
1:C:612:CYS:O	1:C:613:ILE:C	2.42	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:67:LYS:NZ	3:E:90:ASP:OD2	2.35	0.56
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
4:L:63:THR:OG1	4:L:74:THR:OG1	1.99	0.54
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:519:LEU:C	1:C:521:ARG:H	2.11	0.53
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
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: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
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
5:Y:64:ASN:OD1	5:Y:64:ASN:C	2.52	0.47
1:C:384:PRO:O	1:C:430:ARG:NH1	2.48	0.47
4:F:76:SER:O	4:F:77:ASN:C	2.52	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
1:C:139:PRO:HG3	5:Y:81:TRP:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:518:SER:C	1:C:519:LEU:O	2.54	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
5:Y:64:ASN:O	5:Y:65:LYS:C	2.57	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
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:38:ILE:O	1:A:38:ILE:CG1	2.67	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
3:E:100:LEU:O	3:E:102:PRO:O	2.37	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
2:B:124:PHE:C	2:B:126:ALA:H	2.24	0.41
5:X:66:THR:O	5:X:67:ALA:C	2.59	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
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 [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	653/660 (99%)	617 (94%)	32 (5%)	4 (1%)	25 59

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	653/660 (99%)	610 (93%)	41 (6%)	2 (0%)	41	73
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	8
5	Y	29/35 (83%)	22 (76%)	7 (24%)	0	100	100
All	All	2378/2478 (96%)	2228 (94%)	142 (6%)	8 (0%)	41	73

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 [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	A	561/565 (99%)	549 (98%)	12 (2%)	53	79
1	C	561/565 (99%)	540 (96%)	21 (4%)	34	66
2	B	82/98 (84%)	79 (96%)	3 (4%)	34	66
2	D	81/98 (83%)	80 (99%)	1 (1%)	71	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	E	185/187 (99%)	176 (95%)	9 (5%)	25	57
3	H	185/187 (99%)	178 (96%)	7 (4%)	33	66
4	F	188/189 (100%)	184 (98%)	4 (2%)	53	79
4	L	186/189 (98%)	184 (99%)	2 (1%)	73	89
5	X	32/33 (97%)	30 (94%)	2 (6%)	18	48
5	Y	29/33 (88%)	27 (93%)	2 (7%)	15	45
All	All	2090/2144 (98%)	2027 (97%)	63 (3%)	41	71

All (63) 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	122	LEU
1	A	190	ASP
1	A	275	LYS
1	A	308	THR
1	A	312	CYS
1	A	519	LEU
1	A	584	MET
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	90	GLN
4	L	181	LEU
5	X	65	LYS
5	X	81	TRP
1	C	46	LYS
1	C	95	VAL
1	C	108	HIS

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Mol	Chain	Res	Type
1	C	111	VAL
1	C	190	ASP
1	C	310	ASN
1	C	312	CYS
1	C	335	CYS
1	C	388	VAL
1	C	415	THR
1	C	516	ARG
1	C	519	LEU
1	C	521	ARG
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
2	D	104	LEU
3	E	1	GLU
3	E	30	THR
3	E	58	THR
3	E	60	TYR
3	E	61	ASN
3	E	62	GLN
3	E	63	LYS
3	E	108	GLN
3	E	198	CYS
4	F	77	ASN
4	F	83	LEU
4	F	175	MET
4	F	183	LYS
5	Y	77	LYS
5	Y	81	TRP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA

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 [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%) 10 4	21, 56, 117, 144	0
1	C	655/660 (99%)	0.98	111 (16%) 1 0	19, 60, 149, 178	0
2	B	94/114 (82%)	0.50	7 (7%) 14 5	35, 62, 100, 117	0
2	D	92/114 (80%)	0.45	7 (7%) 13 5	32, 60, 104, 115	0
3	E	214/217 (98%)	0.15	6 (2%) 53 30	20, 40, 70, 119	0
3	H	213/217 (98%)	0.11	2 (0%) 84 69	23, 41, 72, 100	0
4	F	212/213 (99%)	0.44	15 (7%) 16 6	21, 56, 101, 128	0
4	L	210/213 (98%)	0.42	15 (7%) 16 6	26, 59, 88, 95	0
5	X	34/35 (97%)	0.17	1 (2%) 51 28	39, 61, 84, 99	0
5	Y	31/35 (88%)	0.39	2 (6%) 18 8	38, 64, 83, 93	0
All	All	2410/2478 (97%)	0.54	222 (9%) 9 3	19, 54, 125, 178	0

All (222) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	574	SER	13.8
1	C	671	ALA	12.7
1	C	569	SER	10.4
1	C	625	LYS	9.8
1	C	604	ASN	9.1
1	C	663	THR	9.0
1	C	567	GLU	9.0
1	C	589	GLN	9.0
1	C	587	CYS	9.0
1	C	570	THR	8.9
1	A	625	LYS	8.8
2	D	25	ALA	8.5
1	C	624	GLU	8.4

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Mol	Chain	Res	Type	RSRZ
1	C	561	ARG	8.3
1	C	582	VAL	8.1
1	C	674	TYR	8.0
1	C	655	HIS	7.8
1	C	588	SER	7.7
1	C	605	PHE	7.5
1	A	567	GLU	7.3
1	A	569	SER	7.2
1	C	596	PRO	7.0
3	E	61	ASN	6.8
1	C	548	ILE	6.7
1	C	672	GLY	6.7
1	A	674	TYR	6.2
1	C	497	GLN	6.2
1	A	585	ASN	6.2
1	C	654	LEU	6.0
1	C	581	PRO	6.0
1	C	575	SER	6.0
1	C	620	LEU	6.0
1	C	665	GLY	5.9
1	C	551	THR	5.9
1	C	573	LEU	5.9
1	C	669	GLU	5.9
1	C	599	ILE	5.7
1	C	635	THR	5.5
1	C	644	LEU	5.5
1	C	555	SER	5.4
1	C	533	LYS	5.3
1	A	48	PRO	5.3
1	C	565	LEU	5.3
1	C	673	LEU	5.3
1	C	594	GLY	5.3
1	C	603	GLN	5.3
1	A	500	THR	5.2
1	A	521	ARG	5.1
1	A	550	VAL	5.1
1	A	588	SER	5.0
1	C	536	ASP	5.0
1	A	582	VAL	5.0
1	C	500	THR	5.0
1	C	571	THR	4.9
2	D	26	TYR	4.9

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Mol	Chain	Res	Type	RSRZ
1	C	640	GLN	4.8
1	C	639	VAL	4.8
1	A	570	THR	4.8
1	A	437	THR	4.8
1	C	456	ALA	4.8
1	C	534	CYS	4.7
1	A	596	PRO	4.7
1	C	611	SER	4.5
1	C	558	ARG	4.4
1	C	622	TYR	4.3
4	F	151	ASP	4.3
1	C	585	ASN	4.3
1	C	607	ARG	4.3
1	C	656	VAL	4.3
2	D	57	ASP	4.3
1	C	562	GLY	4.2
1	C	576	SER	4.2
1	C	580	SER	4.2
1	C	651	PHE	4.2
2	B	129	ASN	4.2
1	C	499	ALA	4.1
1	C	559	GLU	4.1
1	A	568	ALA	4.1
1	A	594	GLY	3.9
1	C	652	ASP	3.9
1	A	55	LEU	3.9
1	C	600	PRO	3.9
1	C	553	ILE	3.9
4	L	152	GLY	3.9
1	C	572	TYR	3.8
2	B	132	ALA	3.8
1	A	626	GLU	3.8
1	C	616	GLY	3.7
1	C	276	GLY	3.7
1	C	520	GLU	3.7
1	C	657	HIS	3.7
3	H	61	ASN	3.7
1	C	537	ARG	3.7
1	A	435	ASN	3.7
1	C	557	ASP	3.6
4	F	154	GLU	3.5
4	L	12	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	589	GLN	3.5
2	B	84	ASN	3.4
1	A	527	TRP	3.3
3	H	55	ASP	3.3
1	A	657	HIS	3.3
1	A	542	LEU	3.3
4	F	184	ASP	3.3
1	A	533	LYS	3.2
1	C	530	PRO	3.2
4	F	203	SER	3.2
1	A	60	ASN	3.2
1	A	587	CYS	3.2
2	D	83	LEU	3.2
1	A	624	GLU	3.2
1	C	437	THR	3.1
1	C	619	LEU	3.1
4	L	184	ASP	3.1
1	C	108	HIS	3.1
1	C	618	ALA	3.1
1	A	499	ALA	3.0
1	C	550	VAL	3.0
4	L	151	ASP	3.0
1	A	51	SER	3.0
1	A	21	SER	3.0
1	A	59	ALA	3.0
1	A	595	GLU	3.0
5	X	66	THR	2.9
1	A	547	LEU	2.9
1	C	637	GLN	2.9
2	B	128	LEU	2.9
1	A	586	LYS	2.9
1	A	655	HIS	2.9
1	C	610	LYS	2.8
1	A	63	GLU	2.8
1	C	563	SER	2.8
1	A	615	CYS	2.8
2	D	127	ASN	2.8
1	C	606	THR	2.8
1	C	583	ILE	2.8
4	F	190	ASN	2.7
5	Y	69	GLN	2.7
4	F	143	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
3	E	136	ASN	2.6
1	A	22	GLU	2.6
1	A	583	ILE	2.6
1	C	664	ASN	2.6
1	C	560	VAL	2.6
1	C	597	ARG	2.6
2	B	57	ASP	2.5
1	C	547	LEU	2.5
4	L	144	ILE	2.5
1	A	549	ASN	2.5
4	F	139	PHE	2.5
2	B	130	ARG	2.5
1	C	518	SER	2.5
2	D	108	LEU	2.5
3	E	41	PRO	2.5
4	L	149	LYS	2.5
4	F	149	LYS	2.5
1	C	602	ILE	2.5
1	C	650	ASP	2.5
1	A	79	SER	2.5
4	F	204	PRO	2.4
1	A	125	PRO	2.4
4	L	154	GLU	2.4
4	L	197	THR	2.4
1	A	673	LEU	2.4
1	C	612	CYS	2.4
1	A	563	SER	2.4
1	C	653	ASN	2.4
1	A	536	ASP	2.4
1	C	554	ILE	2.4
1	C	643	ILE	2.4
1	C	566	TYR	2.4
1	C	502	ASP	2.4
4	F	148	TRP	2.4
4	F	209	PHE	2.4
4	F	133	VAL	2.3
1	C	595	GLU	2.3
4	F	189	HIS	2.3
4	L	127	SER	2.3
1	C	668	MET	2.3
3	E	130	GLY	2.3
4	L	199	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	591	ALA	2.3
1	C	634	ILE	2.3
1	C	541	VAL	2.3
1	A	558	ARG	2.3
3	E	55	ASP	2.3
1	C	628	LEU	2.2
4	L	109	ALA	2.2
1	A	636	SER	2.2
1	A	669	GLU	2.2
1	C	504	ALA	2.2
1	C	532	TYR	2.2
1	C	568	ALA	2.2
1	A	497	GLN	2.2
1	A	637	GLN	2.2
4	L	145	ASN	2.2
1	A	575	SER	2.2
3	E	171	ALA	2.2
1	A	640	GLN	2.2
1	C	436	VAL	2.2
4	L	157	ASN	2.2
1	C	617	PHE	2.1
1	C	586	LYS	2.1
1	C	556	SER	2.1
1	C	593	ALA	2.1
5	Y	67	ALA	2.1
4	L	105	GLU	2.1
2	D	129	ASN	2.1
4	F	188	ARG	2.1
2	B	58	GLY	2.1
1	C	132	TYR	2.1
4	L	139	PHE	2.1
1	A	559	GLU	2.1
1	C	47	VAL	2.1
1	C	79	SER	2.1
1	C	647	ASN	2.0
1	A	103	ASP	2.0
1	A	534	CYS	2.0
1	C	503	GLN	2.0
1	C	523	ASP	2.0
4	F	191	SER	2.0
1	C	549	ASN	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.