Full wwPDB X-ray Structure Validation Report (i)

Sep 19, 2023 – 03:25 AM EDT

PDB ID	:	4YC2
Title	:	Crystal structure of the stabilized inner domain of clade A/E HIV-1 gp120 from E. coli in complex with the antibody A32.
Authors	:	Tolbert, W.D.; Gohain, N.; Pazgier, M.
Deposited on	:	2015-02-19
Resolution	:	3.02 Å(reported)

The following versions of software and data (see references (i)) 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 ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	Percentile Ranks	Value
Rfree		0.284
Clashscore		12
Ramachandran outliers		3.6%
Sidechain outliers		4.6%
RSRZ outliers		2.0%

Worse ← → *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
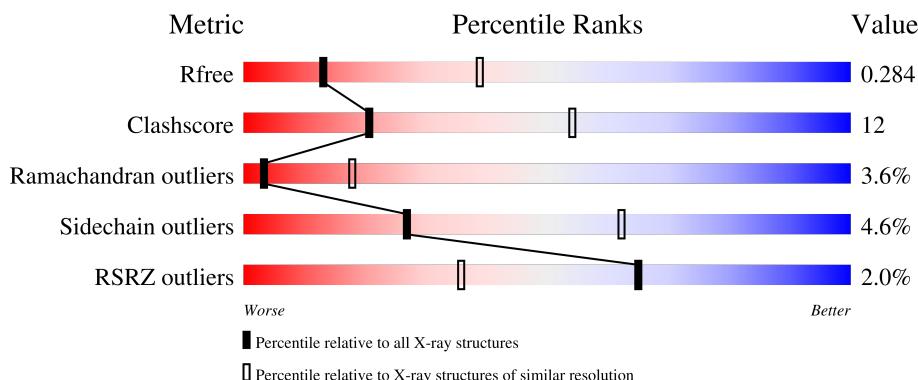
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	2399 (3.04-3.00)
Clashscore	141614	2734 (3.04-3.00)
Ramachandran outliers	138981	2640 (3.04-3.00)
Sidechain outliers	138945	2643 (3.04-3.00)
RSRZ outliers	127900	2287 (3.04-3.00)

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 <=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	156	9%　49% 24% 10% · 16%
1	G	156	.%　58% 22% · · 15%
2	B	224	2%　79% 16% · ·
2	H	224	.%　79% 15% · ·
3	C	210	90% 9% ·
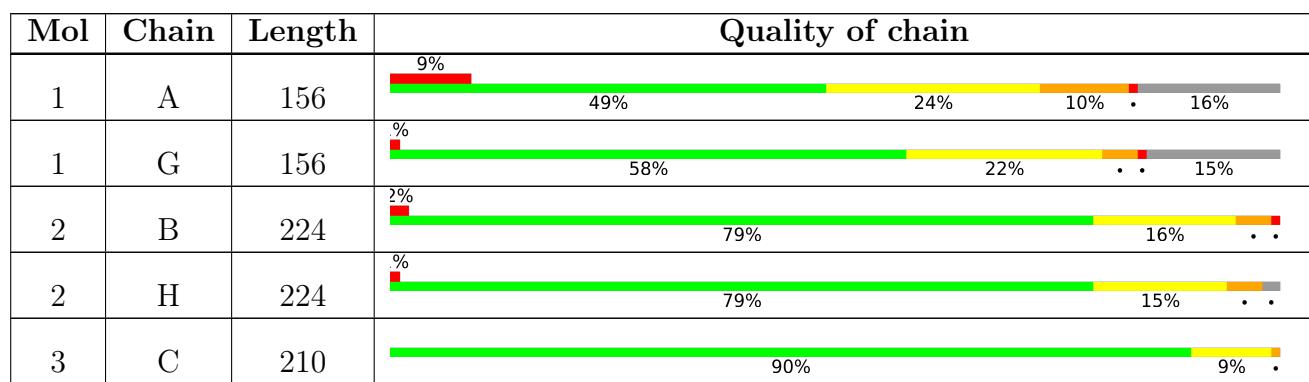
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	L	210	88% · · · · 12%

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 8604 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 The stabilized inner domain of clade A/E HIV-1 gp120 from E. coli.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	133	Total	C	N	O	S	0	0	0
			1071	676	181	203	11			
1	A	131	Total	C	N	O	S	0	0	0
			1054	666	177	200	11			

- Molecule 2 is a protein called The antibody A32 Fab heavy chain..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	220	Total	C	N	O	S	0	0	0
			1666	1052	286	323	5			
2	B	223	Total	C	N	O	S	0	0	0
			1685	1062	289	329	5			

- Molecule 3 is a protein called The antibody A32 Fab light chain..

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	210	Total	C	N	O	S	0	0	0
			1562	977	261	320	4			
3	C	210	Total	C	N	O	S	0	0	0
			1562	977	261	320	4			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total	O	0	0
			1	1		
4	B	2	Total	O	0	0
			2	2		
4	C	1	Total	O	0	0
			1	1		

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: The stabilized inner domain of clade A/E HIV-1 gp120 from E. coli
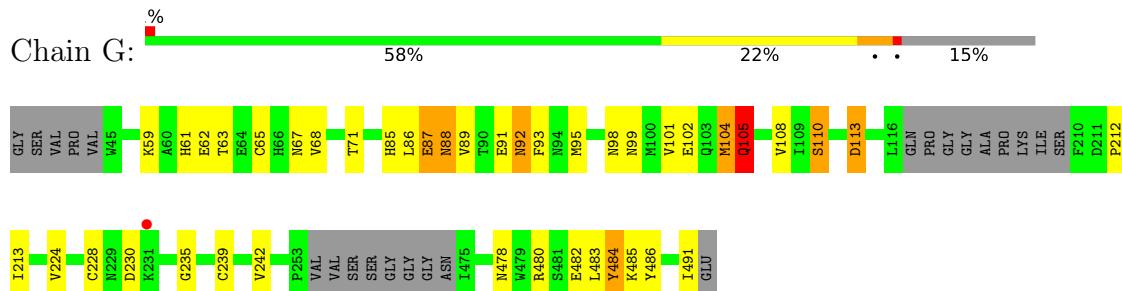
Chain G:

• Molecule 1: The stabilized inner domain of clade A/E HIV-1 gp120 from E. coli

Chain A:

• Molecule 2: The antibody A32 Fab heavy chain.

Chain H:

• Molecule 2: The antibody A32 Fab heavy chain.

Chain B:

Full wwPDB X-ray Structure Validation Report

Q1 V2 E6 S7 G8 Q16 S19 L20 T23 G26 GLY S28 S29 S30 S31 G32 A33 W35A Y40 P41 G42 K43 G44 Y50 Y53 L63 K64 S65 R66 I67 S74 L80 K81 L82 N82A T87 C92 A93 R94 T110 S113 A114 S115

P126 S127 S128 K129 G133 A137 C140 L178 V181 V182 T183 K214

• Molecule 3: The antibody A32 Fab light chain.

Chain L:

88%   12%

V4 S34 W35 Y36 H39 P40 G41 L46 S49 N53 D60 R61 L73 Q79 A84 T92 D93 I94 H95 N95A V115 L132 V133 C134 L135 E160 T161 T162 T163 L178 V195 K204 P208

• Molecule 3: The antibody A32 Fab light chain.

Chain C:

90%   9%

V4 S34 D60 E81 S89 T92 D93 I94 V115 S121 E124 T131 L135 D151 N170 S179 H197 E198 G199 S200 T201 K204 P208
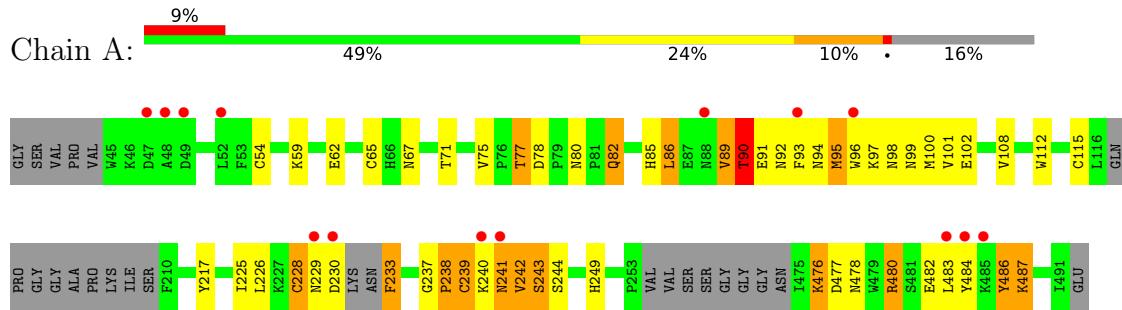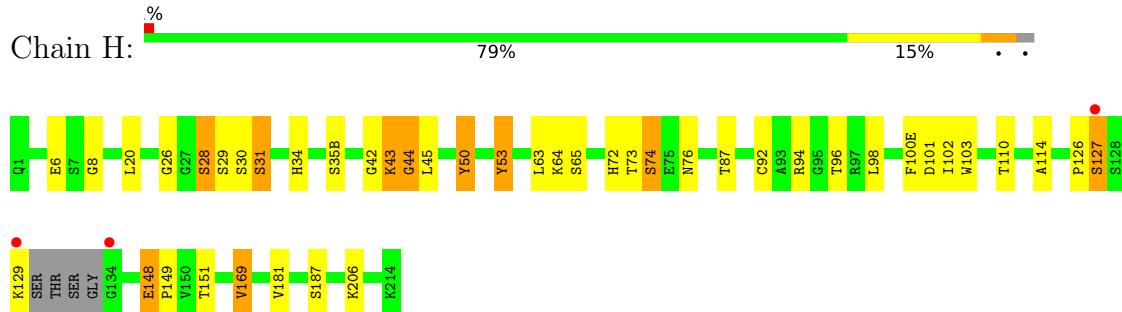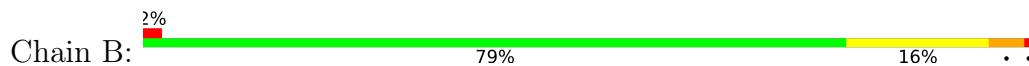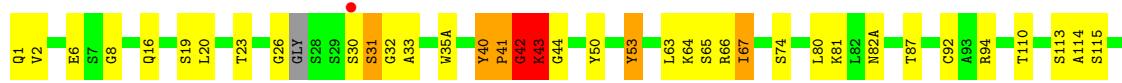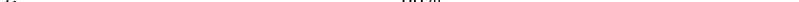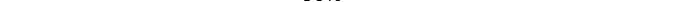
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	75.80Å 211.80Å 72.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.02 47.07 – 3.02	Depositor EDS
% Data completeness (in resolution range)	86.2 (50.00-3.02) 86.3 (47.07-3.02)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0103, PHENIX, CNS	Depositor
R, R_{free}	0.227 , 0.288 0.229 , 0.284	Depositor DCC
R_{free} test set	1087 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å^2)	85.4	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 42.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8604	wwPDB-VP
Average B, all atoms (Å^2)	90.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.58% of the height of the origin peak. No significant pseudotranslation is detected.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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	0.52	0/1082	0.89	4/1473 (0.3%)
1	G	0.40	0/1100	0.71	1/1498 (0.1%)
2	B	0.41	0/1727	0.74	3/2355 (0.1%)
2	H	0.38	0/1708	0.70	0/2329
3	C	0.37	0/1603	0.58	0/2191
3	L	0.35	0/1603	0.57	0/2191
All	All	0.40	0/8823	0.69	8/12037 (0.1%)

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	4
2	B	0	2
All	All	0	6

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	228	CYS	CA-CB-SG	-7.95	99.69	114.00
2	B	40	TYR	C-N-CD	-7.36	104.41	120.60
2	B	40	TYR	N-CA-C	7.24	130.54	111.00
1	A	90	THR	CA-CB-CG2	-6.10	103.86	112.40
1	A	86	LEU	CB-CG-CD1	5.55	120.44	111.00
1	A	90	THR	N-CA-C	5.49	125.81	111.00
2	B	43	LYS	N-CA-C	5.48	125.79	111.00
1	G	105	GLN	N-CA-C	5.47	125.77	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	241	ASN	Peptide
1	A	77	THR	Peptide
1	A	89	VAL	Peptide
1	A	90	THR	Peptide
2	B	35(A)	TRP	Peptide
2	B	42	GLY	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	1054	0	982	96	0
1	G	1071	0	1002	41	0
2	B	1685	0	1659	28	0
2	H	1666	0	1642	33	0
3	C	1562	0	1499	8	1
3	L	1562	0	1499	9	0
4	B	2	0	0	0	0
4	C	1	0	0	0	0
4	H	1	0	0	0	0
All	All	8604	0	8283	208	1

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 12.

All (208) 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:249:HIS:ND1	1:A:486:TYR:OH	1.69	1.25
1:A:230:ASP:CG	1:A:233:PHE:HB2	1.58	1.21
1:A:230:ASP:OD2	1:A:233:PHE:HB2	1.45	1.14
1:A:233:PHE:HE1	1:A:239:CYS:HB2	1.08	1.10
1:A:233:PHE:CE1	1:A:239:CYS:HB2	1.89	1.07
1:A:480:ARG:HA	1:A:484:TYR:CE2	1.93	1.04
2:H:30:SER:O	2:H:53:TYR:CD1	2.11	1.03

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:HG21	1:A:240:LYS:HA	1.42	0.98
1:A:249:HIS:HD1	1:A:486:TYR:HH	1.03	0.96
1:A:93:PHE:HZ	1:A:486:TYR:O	1.48	0.95
1:G:86:LEU:HD22	1:G:242:VAL:HB	1.46	0.94
1:A:77:THR:HG22	1:A:78:ASP:O	1.70	0.90
2:B:63:LEU:HB2	2:B:67:ILE:HD11	1.54	0.90
2:B:41:PRO:O	2:B:42:GLY:C	2.11	0.89
1:A:486:TYR:O	1:A:487:LYS:HG3	1.74	0.88
3:C:92:THR:O	3:C:93:ASP:O	1.91	0.88
1:A:230:ASP:CG	1:A:233:PHE:CB	2.43	0.85
1:A:249:HIS:CE1	1:A:486:TYR:OH	2.30	0.84
1:G:104:MET:HB3	1:G:105:GLN:NE2	1.94	0.82
1:A:90:THR:CG2	1:A:240:LYS:HA	2.09	0.82
1:A:86:LEU:HD12	1:A:86:LEU:O	1.79	0.81
1:A:93:PHE:CZ	1:A:486:TYR:O	2.32	0.81
1:G:101:VAL:CG2	1:G:483:LEU:HD22	2.12	0.80
1:A:90:THR:HG21	1:A:239:CYS:O	1.82	0.79
1:A:93:PHE:HZ	1:A:486:TYR:C	1.86	0.78
1:G:86:LEU:CD2	1:G:242:VAL:HB	2.14	0.76
2:H:30:SER:HG	2:H:53:TYR:HE1	1.33	0.76
1:G:91:GLU:OE2	1:G:92:ASN:ND2	2.18	0.76
1:G:86:LEU:HD11	1:G:89:VAL:HB	1.67	0.76
1:A:82:GLN:H	1:A:82:GLN:HE21	1.34	0.76
1:G:101:VAL:HG23	1:G:483:LEU:HD22	1.66	0.75
2:B:66:ARG:NH1	2:B:82(A):ASN:O	2.20	0.74
1:A:90:THR:HG21	1:A:240:LYS:CA	2.19	0.73
1:G:101:VAL:HG11	1:G:480:ARG:HE	1.53	0.73
1:A:101:VAL:HG21	1:A:484:TYR:OH	1.89	0.73
2:H:34:HIS:CE1	2:H:94:ARG:CZ	2.72	0.72
1:A:233:PHE:CE1	1:A:239:CYS:CB	2.72	0.72
1:A:92:ASN:HA	1:A:238:PRO:HA	1.71	0.72
1:A:230:ASP:OD2	1:A:233:PHE:CB	2.32	0.71
1:G:85:HIS:ND1	1:G:86:LEU:O	2.23	0.71
1:A:249:HIS:CE1	1:A:486:TYR:HH	2.07	0.70
1:A:67:ASN:O	1:A:71:THR:HG23	1.91	0.70
2:H:101:ASP:OD1	2:H:102:ILE:N	2.24	0.70
1:A:477:ASP:OD1	1:A:478:ASN:N	2.24	0.70
2:B:41:PRO:O	2:B:43:LYS:HB2	1.92	0.69
1:A:93:PHE:CE1	1:A:487:LYS:HD2	2.28	0.68
1:A:92:ASN:HA	1:A:238:PRO:CA	2.24	0.67
1:A:91:GLU:O	1:A:238:PRO:CB	2.43	0.66

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:101:VAL:HG11	1:G:480:ARG:NE	2.09	0.66
2:H:96:THR:HG22	2:H:98:LEU:H	1.60	0.65
1:A:82:GLN:HE21	1:A:82:GLN:N	1.94	0.65
1:A:94:ASN:CB	1:A:97:LYS:HB3	2.27	0.64
1:A:86:LEU:HD23	1:A:242:VAL:C	2.18	0.64
1:A:94:ASN:HB2	1:A:97:LYS:HB3	1.80	0.64
1:A:228:CYS:HA	1:A:242:VAL:HA	1.78	0.64
1:G:478:ASN:O	1:G:482:GLU:OE1	2.16	0.64
1:A:230:ASP:CB	1:A:233:PHE:HB2	2.26	0.63
1:A:86:LEU:HB2	1:A:89:VAL:HG22	1.80	0.63
2:H:74:SER:HB3	2:B:53:TYR:CE1	2.34	0.63
2:H:28:SER:O	2:H:76:ASN:ND2	2.31	0.62
1:A:228:CYS:O	1:A:230:ASP:OD1	2.17	0.62
1:G:105:GLN:CD	1:G:105:GLN:N	2.50	0.62
1:A:480:ARG:CD	1:A:484:TYR:HE2	2.12	0.62
2:H:30:SER:OG	2:H:53:TYR:HE1	1.81	0.62
1:A:75:VAL:HG11	2:B:33:ALA:HB1	1.81	0.62
1:A:239:CYS:SG	1:A:240:LYS:N	2.72	0.61
2:H:30:SER:C	2:H:53:TYR:CD1	2.75	0.61
2:B:1:GLN:O	2:B:26:GLY:HA2	2.01	0.60
1:A:86:LEU:O	1:A:86:LEU:CD1	2.49	0.60
1:A:477:ASP:O	1:A:480:ARG:HB3	2.01	0.60
1:A:90:THR:CG2	1:A:239:CYS:O	2.50	0.60
1:A:480:ARG:HD3	1:A:484:TYR:HE2	1.67	0.60
1:G:99:ASN:HA	1:G:102:GLU:HG2	1.83	0.59
2:H:87:THR:HG23	2:H:110:THR:HA	1.85	0.59
1:A:77:THR:HG22	1:A:78:ASP:C	2.22	0.59
2:B:53:TYR:O	2:B:53:TYR:CD1	2.56	0.58
1:A:101:VAL:HG22	1:A:483:LEU:HD12	1.85	0.58
1:A:93:PHE:CZ	1:A:486:TYR:C	2.73	0.57
2:H:6:GLU:HG3	2:H:92:CYS:SG	2.44	0.57
2:B:87:THR:HG23	2:B:110:THR:HA	1.87	0.57
2:B:2:VAL:HG13	2:B:2:VAL:O	2.05	0.56
1:A:95:MET:O	1:A:487:LYS:NZ	2.38	0.56
1:A:225:ILE:HA	1:A:487:LYS:O	2.06	0.56
1:A:78:ASP:O	1:A:78:ASP:OD1	2.24	0.56
1:A:92:ASN:ND2	1:A:238:PRO:HD3	2.21	0.55
2:H:30:SER:O	2:H:53:TYR:CE1	2.57	0.55
1:G:92:ASN:ND2	1:G:92:ASN:O	2.39	0.55
1:A:86:LEU:O	1:A:86:LEU:CG	2.55	0.55
1:A:59:LYS:HD2	1:A:62:GLU:HB2	1.89	0.55

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:41:PRO:O	2:B:43:LYS:CB	2.53	0.54
2:B:6:GLU:OE2	2:B:92:CYS:SG	2.64	0.54
1:A:86:LEU:HD23	1:A:243:SER:N	2.23	0.54
2:B:63:LEU:O	2:B:65:SER:N	2.41	0.54
2:B:41:PRO:O	2:B:42:GLY:O	2.26	0.53
1:A:101:VAL:HG11	1:A:476:LYS:HD2	1.90	0.53
1:A:92:ASN:CA	1:A:238:PRO:HB3	2.38	0.53
1:A:100:MET:SD	1:A:487:LYS:HA	2.49	0.53
1:A:101:VAL:HG21	1:A:484:TYR:CZ	2.44	0.53
1:A:90:THR:HG21	1:A:239:CYS:C	2.28	0.53
2:H:30:SER:O	2:H:53:TYR:CG	2.61	0.52
2:H:28:SER:HB2	2:H:31:SER:HB3	1.91	0.52
2:H:35(B):SER:HB3	2:H:50:TYR:HB3	1.92	0.52
1:A:86:LEU:HD21	1:A:241:ASN:HA	1.92	0.52
2:H:42:GLY:O	2:H:44:GLY:HA3	2.09	0.52
1:A:77:THR:HG22	1:A:78:ASP:N	2.25	0.52
1:G:99:ASN:HA	1:G:102:GLU:CG	2.40	0.52
1:A:108:VAL:O	1:A:112:TRP:HD1	1.94	0.51
1:A:229:ASN:O	1:A:230:ASP:O	2.28	0.51
2:B:8:GLY:HA3	2:B:20:LEU:HD23	1.93	0.51
1:A:95:MET:HB3	1:A:96:TRP:CE3	2.47	0.50
1:A:480:ARG:CD	1:A:484:TYR:CE2	2.94	0.49
1:G:67:ASN:O	1:G:71:THR:HG23	2.12	0.49
1:A:93:PHE:CZ	1:A:487:LYS:HB2	2.46	0.49
1:A:92:ASN:HA	1:A:238:PRO:HB3	1.93	0.49
2:H:28:SER:O	2:H:76:ASN:CG	2.51	0.49
2:H:28:SER:CB	2:H:31:SER:HB3	2.42	0.49
1:A:242:VAL:HG12	1:A:243:SER:H	1.78	0.49
2:B:127:SER:HB3	2:B:129:LYS:HG2	1.95	0.48
2:H:28:SER:O	2:H:76:ASN:OD1	2.30	0.48
1:G:230:ASP:OD2	1:G:239:CYS:HA	2.14	0.48
1:G:87:GLU:O	1:G:88:ASN:OD1	2.31	0.48
1:A:228:CYS:HB3	1:A:233:PHE:CZ	2.48	0.48
1:A:237:GLY:O	1:A:238:PRO:O	2.31	0.48
2:H:43:LYS:CB	2:H:44:GLY:CA	2.92	0.48
3:L:132:LEU:HD12	3:L:178:LEU:HD23	1.95	0.48
1:G:480:ARG:HA	1:G:483:LEU:HB3	1.94	0.48
1:G:59:LYS:HD3	1:G:61:HIS:CE1	2.49	0.48
1:G:62:GLU:CD	1:G:63:THR:H	2.17	0.48
2:H:74:SER:HB3	2:B:53:TYR:CD1	2.48	0.48
1:A:249:HIS:CE1	1:A:482:GLU:HB3	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:137:ALA:HB2	2:B:183:THR:HG22	1.96	0.48
1:A:230:ASP:CG	1:A:233:PHE:CG	2.87	0.47
3:C:93:ASP:O	3:C:94:ILE:C	2.53	0.47
1:G:484:TYR:CE1	1:G:485:LYS:CG	2.98	0.47
3:C:34:SER:OG	3:C:89:SER:OG	2.32	0.47
1:G:98:ASN:ND2	1:G:486:TYR:O	2.47	0.47
1:A:92:ASN:HA	1:A:238:PRO:CB	2.43	0.47
1:A:94:ASN:HB3	1:A:97:LYS:HB3	1.95	0.47
1:G:104:MET:N	1:G:105:GLN:HE22	2.12	0.47
1:G:99:ASN:ND2	1:G:99:ASN:O	2.47	0.47
1:A:226:LEU:HD23	1:A:244:SER:OG	2.15	0.46
1:A:480:ARG:HD2	1:A:484:TYR:CE2	2.50	0.46
3:C:197:HIS:CE1	3:C:198:GLU:HG2	2.50	0.46
2:H:100(E):PHE:O	2:H:103:TRP:NE1	2.48	0.46
2:H:63:LEU:O	2:H:65:SER:N	2.48	0.46
2:B:53:TYR:CD1	2:B:53:TYR:C	2.87	0.46
3:C:121:SER:HB2	3:C:124:GLU:H	1.81	0.46
1:G:93:PHE:CE2	1:G:228:CYS:HB2	2.51	0.46
1:A:486:TYR:O	1:A:487:LYS:CG	2.54	0.46
2:B:127:SER:HB3	2:B:129:LYS:H	1.80	0.46
1:A:95:MET:HG3	1:A:484:TYR:CD2	2.51	0.45
1:A:99:ASN:HA	1:A:102:GLU:HB2	1.99	0.45
2:B:30:SER:HB2	2:B:94:ARG:HH11	1.81	0.45
3:L:49:SER:O	3:L:53:ASN:HB3	2.16	0.45
1:A:82:GLN:N	1:A:82:GLN:NE2	2.62	0.45
2:H:29:SER:HB3	2:H:76:ASN:OD1	2.17	0.45
1:A:91:GLU:O	1:A:238:PRO:HB2	2.14	0.45
2:B:129:LYS:HD3	2:B:129:LYS:N	2.32	0.45
2:B:126:PRO:O	2:B:127:SER:CB	2.65	0.44
3:C:131:THR:HG22	3:C:179:SER:HA	1.99	0.44
1:G:101:VAL:C	1:G:105:GLN:NE2	2.71	0.44
2:B:30:SER:O	2:B:31:SER:OG	2.26	0.44
1:G:87:GLU:C	1:G:88:ASN:OD1	2.56	0.44
2:B:181:VAL:HG11	3:C:135:LEU:HD11	1.99	0.44
1:G:65:CYS:O	1:G:68:VAL:HB	2.17	0.44
1:A:92:ASN:OD1	1:A:93:PHE:N	2.51	0.44
1:G:483:LEU:O	1:G:485:LYS:N	2.51	0.43
3:L:39:HIS:CD2	3:L:84:ALA:HB2	2.53	0.43
1:A:476:LYS:HZ3	1:A:480:ARG:HD3	1.82	0.43
1:G:85:HIS:CE1	1:G:86:LEU:O	2.71	0.43
1:G:105:GLN:HA	1:G:108:VAL:HG13	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:181:VAL:HG11	3:L:135:LEU:HD11	2.00	0.43
2:H:30:SER:C	2:H:53:TYR:CE1	2.92	0.43
3:L:92:THR:O	3:L:95(A):ASN:HB3	2.18	0.43
1:A:86:LEU:O	1:A:86:LEU:HG	2.19	0.43
1:G:101:VAL:HG21	1:G:480:ARG:HG2	2.01	0.43
1:A:99:ASN:O	1:A:99:ASN:OD1	2.37	0.43
1:G:101:VAL:HG12	1:G:101:VAL:O	2.19	0.43
3:L:115:VAL:O	3:L:204:LYS:NZ	2.40	0.43
1:A:54:CYS:HB3	1:A:217:TYR:CE1	2.54	0.43
3:L:61:ARG:NH2	3:L:79:GLN:OE1	2.51	0.43
1:G:110:SER:HA	1:G:113:ASP:HB3	2.00	0.43
2:H:72:HIS:NE2	1:A:80:ASN:O	2.52	0.42
1:A:229:ASN:O	1:A:230:ASP:CG	2.58	0.42
2:B:19:SER:HA	2:B:80:LEU:O	2.19	0.42
3:C:115:VAL:O	3:C:204:LYS:HD2	2.19	0.42
1:A:59:LYS:CD	1:A:62:GLU:HB2	2.49	0.42
1:A:233:PHE:CE1	1:A:238:PRO:O	2.73	0.42
1:G:484:TYR:OH	1:G:485:LYS:NZ	2.33	0.42
1:G:95:MET:SD	1:G:235:GLY:HA3	2.60	0.41
2:H:148:GLU:CG	2:H:149:PRO:HA	2.51	0.41
1:A:80:ASN:O	1:A:80:ASN:CG	2.59	0.41
1:G:224:VAL:HG12	1:G:491:ILE:HD11	2.03	0.41
3:L:36:TYR:CE1	3:L:46:LEU:HD13	2.56	0.41
2:B:43:LYS:HB2	2:B:44:GLY:HA2	2.02	0.41
2:H:8:GLY:HA3	2:H:20:LEU:HD23	2.03	0.40
2:H:30:SER:HB2	2:H:73:THR:HA	2.03	0.40
1:A:480:ARG:HA	1:A:484:TYR:HE2	1.67	0.40
1:G:483:LEU:O	1:G:483:LEU:HG	2.18	0.40
2:H:34:HIS:ND1	2:H:94:ARG:CD	2.84	0.40
1:A:480:ARG:HA	1:A:484:TYR:CD2	2.50	0.40
2:H:169:VAL:HG13	3:L:160:GLU:HB3	2.04	0.40
1:A:86:LEU:HD22	1:A:242:VAL:HB	2.04	0.40
2:H:30:SER:OG	2:H:53:TYR:CE1	2.62	0.40
2:B:40:TYR:HD2	2:B:44:GLY:O	2.04	0.40
1:G:86:LEU:HB3	1:G:242:VAL:O	2.21	0.40
1:G:483:LEU:O	1:G:484:TYR:C	2.59	0.40
1:A:480:ARG:O	1:A:484:TYR:CD2	2.75	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:93:ASP:OD2	3:C:151:ASP:OD2[2_455]	2.17	0.03

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	123/156 (79%)	103 (84%)	13 (11%)	7 (6%)	1	9
1	G	127/156 (81%)	118 (93%)	5 (4%)	4 (3%)	4	21
2	B	219/224 (98%)	186 (85%)	22 (10%)	11 (5%)	2	12
2	H	216/224 (96%)	184 (85%)	21 (10%)	11 (5%)	2	11
3	C	208/210 (99%)	187 (90%)	17 (8%)	4 (2%)	8	34
3	L	208/210 (99%)	180 (86%)	25 (12%)	3 (1%)	11	41
All	All	1101/1180 (93%)	958 (87%)	103 (9%)	40 (4%)	3	18

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	88	ASN
1	G	104	MET
1	G	105	GLN
2	H	64	LYS
2	H	126	PRO
2	H	127	SER
3	L	60	ASP
1	A	238	PRO
1	A	239	CYS
1	A	242	VAL
1	A	243	SER
2	B	41	PRO
2	B	64	LYS
2	B	127	SER
3	C	93	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	94	ILE
1	G	484	TYR
2	H	26	GLY
2	H	31	SER
2	H	43	LYS
2	H	53	TYR
2	B	31	SER
2	B	42	GLY
2	B	114	ALA
2	B	126	PRO
2	H	114	ALA
2	H	187	SER
1	A	95	MET
2	B	16	GLN
1	A	487	LYS
3	L	94	ILE
1	A	85	HIS
3	C	170	ASN
2	H	74	SER
3	L	41	GLY
2	B	32	GLY
2	B	43	LYS
3	C	60	ASP
2	H	44	GLY
2	B	133	GLY

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	120/138 (87%)	111 (92%)	9 (8%)	13	42
1	G	122/138 (88%)	115 (94%)	7 (6%)	20	54
2	B	193/193 (100%)	182 (94%)	11 (6%)	20	54
2	H	190/193 (98%)	181 (95%)	9 (5%)	26	61
3	C	177/177 (100%)	174 (98%)	3 (2%)	60	85

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	L	177/177 (100%)	171 (97%)	6 (3%)	37	72
All	All	979/1016 (96%)	934 (95%)	45 (5%)	27	62

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	87	GLU
1	G	92	ASN
1	G	105	GLN
1	G	110	SER
1	G	113	ASP
1	G	212	PRO
1	G	213	ILE
2	H	28	SER
2	H	45	LEU
2	H	50	TYR
2	H	127	SER
2	H	129	LYS
2	H	148	GLU
2	H	151	THR
2	H	169	VAL
2	H	206	LYS
3	L	34	SER
3	L	73	LEU
3	L	134	CYS
3	L	162	THR
3	L	163	THR
3	L	195	VAL
1	A	65	CYS
1	A	82	GLN
1	A	90	THR
1	A	98	ASN
1	A	115	CYS
1	A	233	PHE
1	A	476	LYS
1	A	480	ARG
1	A	486	TYR
2	B	23	THR
2	B	50	TYR
2	B	53	TYR
2	B	67	ILE
2	B	74	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	81	LYS
2	B	113	SER
2	B	115	SER
2	B	129	LYS
2	B	140	CYS
2	B	178	LEU
3	C	81	GLU
3	C	200	SER
3	C	201	THR

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

Mol	Chain	Res	Type
1	G	92	ASN
1	G	232	ASN
1	A	82	GLN
1	A	241	ASN
2	B	39	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers ⓘ

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	131/156 (83%)	0.56	14 (10%)	6	2	85, 130, 178, 187	0
1	G	133/156 (85%)	0.03	1 (0%)	86	65	86, 120, 150, 156	0
2	B	223/224 (99%)	-0.19	4 (1%)	68	39	54, 75, 113, 129	0
2	H	220/224 (98%)	-0.24	3 (1%)	75	48	59, 76, 102, 127	0
3	C	210/210 (100%)	-0.34	0	100	100	55, 72, 94, 104	0
3	L	210/210 (100%)	-0.32	0	100	100	63, 78, 101, 110	0
All	All	1127/1180 (95%)	-0.14	22 (1%)	65	36	54, 82, 146, 187	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	229	ASN	3.7
1	A	93	PHE	3.6
1	A	240	LYS	3.6
1	G	231	LYS	3.3
1	A	230	ASP	3.2
2	H	129	LYS	3.0
1	A	96	TRP	2.9
1	A	88	ASN	2.8
1	A	241	ASN	2.8
2	B	128	SER	2.8
2	H	134	GLY	2.7
1	A	48	ALA	2.5
1	A	52	LEU	2.5
2	H	127	SER	2.3
1	A	485	LYS	2.2
1	A	47	ASP	2.2
2	B	30	SER	2.1
1	A	483	LEU	2.1
1	A	484	TYR	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	127	SER	2.1
2	B	133	GLY	2.0
1	A	49	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.