Full wwPDB X-ray Structure Validation Report ⓘ

Apr 8, 2025 – 12:08 PM JST

PDB ID	:	8WJB / pdb_00008wjb
Title	:	Structural insights into the Langya virus attachment glycoprotein
Authors	:	Jun, L.; Chenghai, W.
Deposited on	:	2023-09-25
Resolution	:	2.75 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:

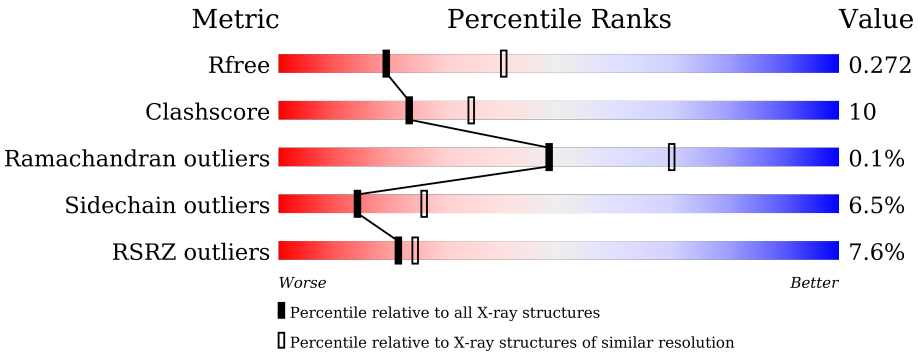
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

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 2.75 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)

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	424	6% 78% 20%
1	B	424	9% 67% 29%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 6529 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 Attachment glycoprotein.

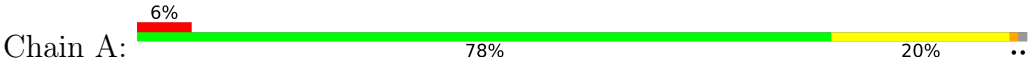
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3259	2069	539	628	23			
1	B	421	Total	C	N	O	S	0	0	0
			3270	2076	541	630	23			

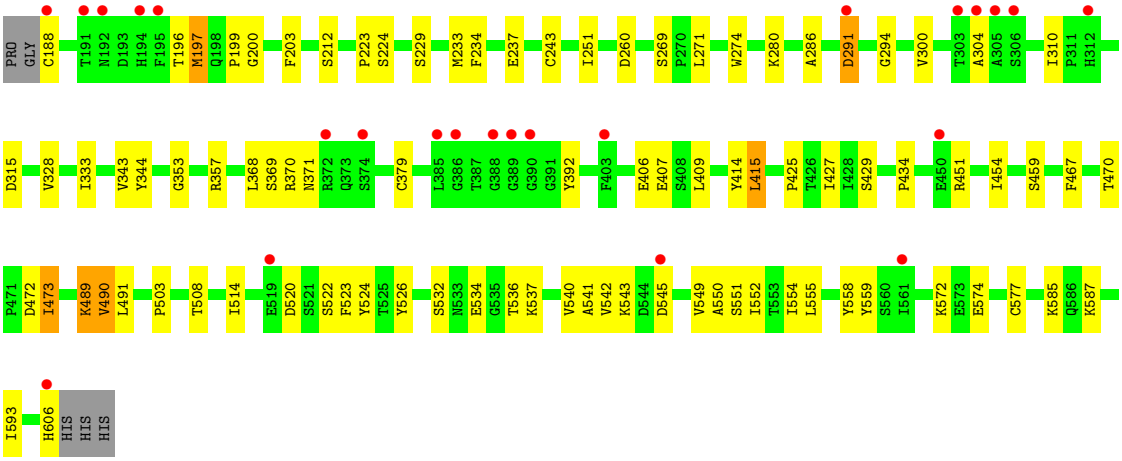
3 Residue-property plots (i)

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: Attachment glycoprotein

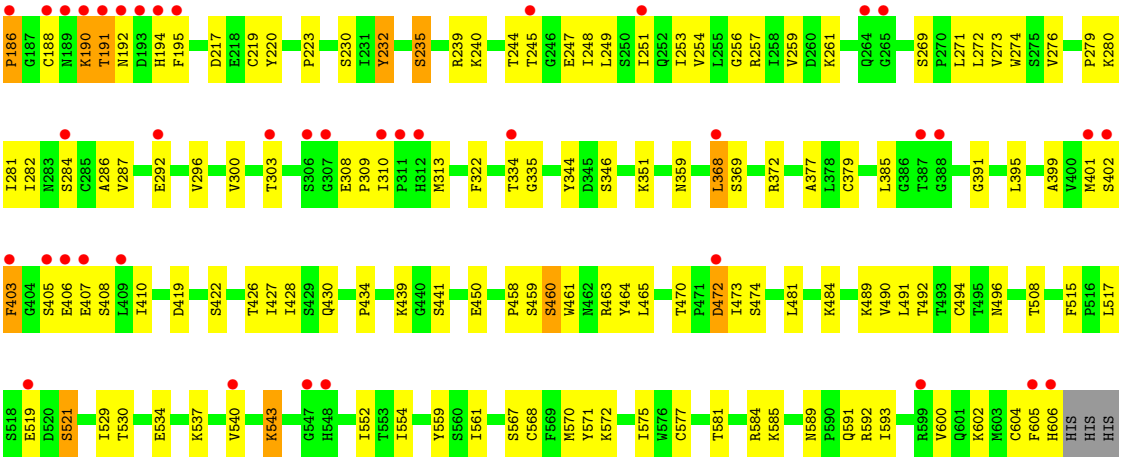
Chain A:





• Molecule 1: Attachment glycoprotein

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	196.77Å 48.56Å 116.92Å 90.00° 122.67° 90.00°	Depositor
Resolution (Å)	46.31 – 2.75 46.31 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.31-2.75) 98.3 (46.31-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.47 (at 2.77Å)	Xtriage
Refinement program	PHENIX (1.18.2_3874: ???)	Depositor
R, R_{free}	0.216 , 0.275 0.216 , 0.272	Depositor DCC
R_{free} test set	1268 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 43.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	6529	wwPDB-VP
Average B, all atoms (Å^2)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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	0.51	2/3340 (0.1%)	0.72	3/4534 (0.1%)
1	B	0.50	0/3352	0.69	1/4550 (0.0%)
All	All	0.50	2/6692 (0.0%)	0.70	4/9084 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	577	CYS	CB-SG	-5.52	1.72	1.81
1	A	243	CYS	CB-SG	-5.33	1.73	1.81

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	291	ASP	CB-CG-OD1	9.06	126.45	118.30
1	A	291	ASP	CB-CG-OD2	-7.55	111.51	118.30
1	B	368	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	415	LEU	CB-CG-CD1	-5.08	102.36	111.00

There are no chirality outliers.

There are no planarity outliers.

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	3259	0	3155	51	0
1	B	3270	0	3166	79	0
All	All	6529	0	6321	130	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 10.

All (130) 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:280:LYS:HD2	1:A:280:LYS:H	1.50	0.77
1:B:279:PRO:HA	1:B:282:ILE:HD12	1.68	0.74
1:B:368:LEU:HD23	1:B:402:SER:OG	1.88	0.74
1:A:451:ARG:HB2	1:A:451:ARG:NH1	2.05	0.71
1:B:223:PRO:HB3	1:B:593:ILE:HD13	1.76	0.68
1:B:441:SER:HB3	1:B:459:SER:HB3	1.77	0.66
1:B:492:THR:HB	1:B:508:THR:HG23	1.79	0.65
1:B:334:THR:HG22	1:B:335:GLY:H	1.61	0.65
1:A:304:ALA:HB2	1:A:310:ILE:HD11	1.79	0.64
1:A:286:ALA:HB1	1:A:353:GLY:HA2	1.79	0.64
1:B:403:PHE:CD2	1:B:407:GLU:HB3	2.33	0.63
1:A:197:MET:HB3	1:A:542:VAL:HG11	1.80	0.63
1:A:451:ARG:HB2	1:A:451:ARG:HH11	1.64	0.61
1:B:391:GLY:O	1:B:395:LEU:HD12	2.02	0.60
1:B:280:LYS:NZ	1:B:308:GLU:OE1	2.21	0.58
1:B:240:LYS:HB2	1:B:249:LEU:HD21	1.84	0.58
1:A:197:MET:HB2	1:A:523:PHE:CD2	2.40	0.57
1:A:490:VAL:HG13	1:A:491:LEU:HG	1.85	0.57
1:A:534:GLU:HG3	1:A:559:TYR:CE1	2.40	0.57
1:B:220:TYR:HB3	1:B:593:ILE:HG13	1.87	0.56
1:B:248:ILE:HG22	1:B:279:PRO:HB2	1.88	0.55
1:B:515:PHE:CD2	1:B:567:SER:HA	2.41	0.55
1:B:540:VAL:HG23	1:B:554:ILE:HD13	1.88	0.55
1:B:254:VAL:HG22	1:B:273:VAL:HG22	1.88	0.55
1:B:561:ILE:HD12	1:B:581:THR:HB	1.89	0.55
1:A:415:LEU:HD11	1:A:427:ILE:HG23	1.89	0.54
1:A:555:LEU:HD22	1:A:558:TYR:CE1	2.43	0.54
1:A:260:ASP:OD2	1:A:572:LYS:NZ	2.31	0.53
1:A:470:THR:OG1	1:A:472:ASP:O	2.18	0.53
1:B:235:SER:HB3	1:B:287:VAL:HG13	1.90	0.53
1:A:514:ILE:HG22	1:A:526:TYR:HB3	1.90	0.53
1:B:458:PRO:HB3	1:B:463:ARG:HA	1.89	0.53
1:B:287:VAL:HG12	1:B:296:VAL:HG22	1.89	0.52
1:B:490:VAL:HG12	1:B:491:LEU:HG	1.92	0.52
1:A:223:PRO:HB3	1:A:593:ILE:HD13	1.93	0.51
1:B:540:VAL:HG23	1:B:554:ILE:HG21	1.93	0.50
1:B:427:ILE:O	1:B:428:ILE:HD13	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:403:PHE:CB	1:B:407:GLU:HB3	2.42	0.50
1:B:584:ARG:NH1	1:B:589:ASN:O	2.45	0.50
1:B:575:ILE:HD11	1:B:602:LYS:NZ	2.26	0.50
1:A:451:ARG:HH11	1:A:451:ARG:CB	2.24	0.50
1:B:346:SER:OG	1:B:368:LEU:HD12	2.12	0.50
1:B:369:SER:O	1:B:408:SER:HA	2.11	0.49
1:A:543:LYS:HG3	1:A:549:VAL:HG22	1.94	0.49
1:B:195:PHE:CZ	1:B:602:LYS:HD3	2.47	0.49
1:A:409:LEU:HD13	1:A:434:PRO:HG3	1.95	0.49
1:B:419:ASP:CG	1:B:422:SER:HB3	2.34	0.49
1:B:459:SER:HA	1:B:508:THR:O	2.12	0.47
1:A:300:VAL:HG23	1:A:315:ASP:HB3	1.95	0.47
1:B:481:LEU:HD11	1:B:521:SER:HB3	1.97	0.47
1:B:186:PRO:HB2	1:B:190:LYS:NZ	2.30	0.47
1:B:410:ILE:H	1:B:410:ILE:HD12	1.79	0.47
1:A:197:MET:HB2	1:A:523:PHE:HD2	1.81	0.46
1:A:199:PRO:HG2	1:A:552:ILE:HD12	1.97	0.46
1:B:217:ASP:OD1	1:B:217:ASP:N	2.48	0.46
1:A:280:LYS:HD2	1:A:280:LYS:N	2.27	0.46
1:B:559:TYR:HB3	1:B:584:ARG:O	2.16	0.46
1:B:568:CYS:HA	1:B:577:CYS:HA	1.98	0.46
1:A:540:VAL:O	1:A:551:SER:HA	2.16	0.46
1:B:571:TYR:CE2	1:B:572:LYS:HG3	2.50	0.45
1:A:280:LYS:H	1:A:280:LYS:CD	2.26	0.45
1:A:371:ASN:HB3	1:A:406:GLU:O	2.15	0.45
1:A:536:THR:O	1:A:537:LYS:HD3	2.16	0.45
1:B:191:THR:O	1:B:192:ASN:C	2.55	0.45
1:A:454:ILE:O	1:A:467:PHE:HA	2.15	0.45
1:B:402:SER:N	1:B:408:SER:O	2.44	0.45
1:B:195:PHE:CE2	1:B:602:LYS:HD3	2.52	0.45
1:A:203:PHE:CZ	1:A:554:ILE:HD12	2.52	0.45
1:A:333:ILE:HD11	1:A:425:PRO:HG2	1.98	0.45
1:B:470:THR:HG23	1:B:472:ASP:O	2.16	0.45
1:B:494:CYS:HB3	1:B:496:ASN:OD1	2.17	0.45
1:A:415:LEU:HD11	1:A:427:ILE:CG2	2.46	0.45
1:B:272:LEU:HD11	1:B:274:TRP:HB2	1.98	0.45
1:B:257:ARG:NH2	1:B:292:GLU:OE2	2.51	0.44
1:B:529:ILE:HG21	1:B:561:ILE:O	2.18	0.44
1:B:244:THR:HG22	1:B:245:THR:HG23	1.99	0.44
1:A:520:ASP:HB3	1:A:522:SER:OG	2.17	0.44
1:B:552:ILE:HD13	1:B:552:ILE:HG21	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:ARG:HG3	1:B:271:LEU:HD11	1.99	0.44
1:A:392:TYR:HB3	1:A:503:PRO:HG2	2.00	0.43
1:B:219:CYS:SG	1:B:591:GLN:HB3	2.58	0.43
1:B:377:ALA:HA	1:B:434:PRO:O	2.17	0.43
1:A:459:SER:HA	1:A:508:THR:O	2.18	0.43
1:B:403:PHE:CG	1:B:407:GLU:HB3	2.54	0.43
1:A:489:LYS:HE2	1:A:489:LYS:HB2	1.52	0.43
1:B:359:ASN:ND2	1:B:419:ASP:HA	2.33	0.43
1:B:310:ILE:HG22	1:B:313:MET:HG3	2.00	0.43
1:A:237:GLU:HG2	1:A:251:ILE:HG12	2.01	0.43
1:A:414:TYR:CD1	1:A:473:ILE:HG23	2.54	0.43
1:B:460:SER:HB3	1:B:461:TRP:H	1.60	0.43
1:B:543:LYS:HB3	1:B:543:LYS:HE3	1.17	0.43
1:B:259:VAL:HG23	1:B:261:LYS:HG3	2.01	0.42
1:B:344:TYR:CE1	1:B:369:SER:HB3	2.53	0.42
1:B:419:ASP:OD1	1:B:422:SER:HB3	2.19	0.42
1:A:371:ASN:O	1:A:407:GLU:HA	2.19	0.42
1:A:558:TYR:CE1	1:A:585:LYS:HE2	2.55	0.42
1:B:251:ILE:HD12	1:B:282:ILE:HD13	2.00	0.42
1:B:239:ARG:HG2	1:B:247:GLU:O	2.20	0.42
1:A:224:SER:O	1:A:234:PHE:HA	2.20	0.42
1:B:274:TRP:HZ3	1:B:276:VAL:HG22	1.85	0.42
1:B:281:ILE:HG22	1:B:309:PRO:HB3	2.01	0.42
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.80	0.41
1:B:575:ILE:H	1:B:575:ILE:HG13	1.73	0.41
1:A:343:VAL:CG1	1:A:370:ARG:HD2	2.50	0.41
1:A:524:TYR:OH	1:A:543:LYS:HD3	2.21	0.41
1:B:220:TYR:HB2	1:B:592:ARG:HA	2.02	0.41
1:A:233:MET:SD	1:A:294:GLY:HA3	2.60	0.41
1:B:489:LYS:NZ	1:B:530:THR:HG22	2.35	0.41
1:B:261:LYS:NZ	1:B:269:SER:HB3	2.35	0.41
1:A:534:GLU:HG3	1:A:559:TYR:HE1	1.83	0.41
1:A:541:ALA:HA	1:A:550:ALA:O	2.21	0.41
1:B:186:PRO:HB2	1:B:190:LYS:HZ2	1.83	0.41
1:B:190:LYS:HE3	1:B:190:LYS:HB2	1.72	0.41
1:B:464:TYR:CD1	1:B:484:LYS:HB3	2.55	0.41
1:A:559:TYR:CD1	1:A:587:LYS:HB2	2.55	0.41
1:B:399:ALA:O	1:B:439:LYS:HD3	2.21	0.41
1:B:517:LEU:HD13	1:B:600:VAL:HG11	2.02	0.41
1:A:200:GLY:O	1:A:552:ILE:HD13	2.21	0.41
1:A:344:TYR:HA	1:A:368:LEU:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:534:GLU:CD	1:B:534:GLU:N	2.75	0.41
1:A:291:ASP:O	1:A:291:ASP:OD1	2.39	0.40
1:A:274:TRP:CD1	1:A:328:VAL:HG21	2.57	0.40
1:B:232:TYR:CE2	1:B:256:GLY:HA3	2.56	0.40
1:B:286:ALA:HB2	1:B:351:LYS:HA	2.03	0.40
1:B:464:TYR:HB3	1:B:465:LEU:H	1.66	0.40
1:A:522:SER:HB3	1:A:545:ASP:OD2	2.21	0.40
1:B:385:LEU:HD23	1:B:385:LEU:C	2.42	0.40
1:B:585:LYS:HE2	1:B:585:LYS:HB2	1.76	0.40
1:B:239:ARG:HA	1:B:247:GLU:O	2.21	0.40
1:B:253:ILE:HG21	1:B:322:PHE:CZ	2.57	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	417/424 (98%)	396 (95%)	21 (5%)	0	100 100
1	B	419/424 (99%)	384 (92%)	34 (8%)	1 (0%)	44 63
All	All	836/848 (99%)	780 (93%)	55 (7%)	1 (0%)	48 70

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	405	SER

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	363/367 (99%)	347 (96%)	16 (4%)	24 43
1	B	364/367 (99%)	333 (92%)	31 (8%)	8 16
All	All	727/734 (99%)	680 (94%)	47 (6%)	14 26

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	188	CYS
1	A	196	THR
1	A	197	MET
1	A	212	SER
1	A	229	SER
1	A	269	SER
1	A	357	ARG
1	A	369	SER
1	A	379	CYS
1	A	429	SER
1	A	473	ILE
1	A	489	LYS
1	A	490	VAL
1	A	532	SER
1	A	574	GLU
1	A	606	HIS
1	B	186	PRO
1	B	188	CYS
1	B	190	LYS
1	B	191	THR
1	B	194	HIS
1	B	230	SER
1	B	232	TYR
1	B	235	SER
1	B	284	SER
1	B	300	VAL
1	B	303	THR
1	B	372	ARG
1	B	379	CYS
1	B	401	MET
1	B	403	PHE
1	B	406	GLU
1	B	426	THR

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Mol	Chain	Res	Type
1	B	430	GLN
1	B	450	GLU
1	B	460	SER
1	B	472	ASP
1	B	473	ILE
1	B	474	SER
1	B	519	GLU
1	B	521	SER
1	B	537	LYS
1	B	543	LYS
1	B	570	MET
1	B	604	CYS
1	B	605	PHE
1	B	606	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	601	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 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, 95^{th} 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	419/424 (98%)	0.17	24 (5%)	30	33	19, 34, 77, 137	0
1	B	421/424 (99%)	0.65	40 (9%)	15	18	25, 47, 93, 153	0
All	All	840/848 (99%)	0.41	64 (7%)	21	24	19, 42, 86, 153	0

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	192	ASN	7.1
1	B	194	HIS	7.0
1	B	403	PHE	5.7
1	B	605	PHE	5.4
1	A	194	HIS	5.0
1	A	312	HIS	4.6
1	A	191	THR	4.6
1	A	390	GLY	4.5
1	B	406	GLU	4.5
1	B	186	PRO	4.4
1	A	188	CYS	4.4
1	B	191	THR	3.8
1	B	548	HIS	3.6
1	A	388	GLY	3.5
1	B	402	SER	3.5
1	B	190	LYS	3.4
1	B	606	HIS	3.4
1	B	306	SER	3.4
1	A	291	ASP	3.3
1	B	387	THR	3.2
1	A	403	PHE	3.2
1	A	195	PHE	3.1
1	A	386	GLY	3.1
1	B	193	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	306	SER	3.0
1	B	401	MET	3.0
1	B	311	PRO	3.0
1	A	192	ASN	3.0
1	A	305	ALA	2.9
1	B	388	GLY	2.9
1	B	312	HIS	2.8
1	A	545	ASP	2.7
1	A	606	HIS	2.7
1	A	372	ARG	2.6
1	B	292	GLU	2.5
1	B	405	SER	2.5
1	A	385	LEU	2.5
1	B	195	PHE	2.4
1	B	472	ASP	2.4
1	A	303	THR	2.4
1	A	374	SER	2.4
1	A	389	GLY	2.4
1	A	519	GLU	2.4
1	B	407	GLU	2.3
1	B	519	GLU	2.3
1	B	307	GLY	2.3
1	A	304	ALA	2.3
1	B	310	ILE	2.2
1	B	188	CYS	2.2
1	B	547	GLY	2.2
1	B	284	SER	2.2
1	A	561	ILE	2.2
1	B	265	GLY	2.2
1	B	599	ARG	2.2
1	B	245	THR	2.1
1	B	540	VAL	2.1
1	B	189	ASN	2.1
1	B	368	LEU	2.1
1	A	450	GLU	2.1
1	B	251	ILE	2.1
1	B	264	GLN	2.1
1	B	303	THR	2.0
1	B	334	THR	2.0
1	B	409	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 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.