



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:07 PM UTC

PDB ID : 2RKC / pdb_00002rkc
Title : Crystal structure of the measles virus hemagglutinin
Authors : Colf, L.A.; Juo, Z.S.; Garcia, K.C.
Deposited on : 2007-10-16
Resolution : 2.70 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
Mogul : 2022.3.0, CSD as543be (2022)
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

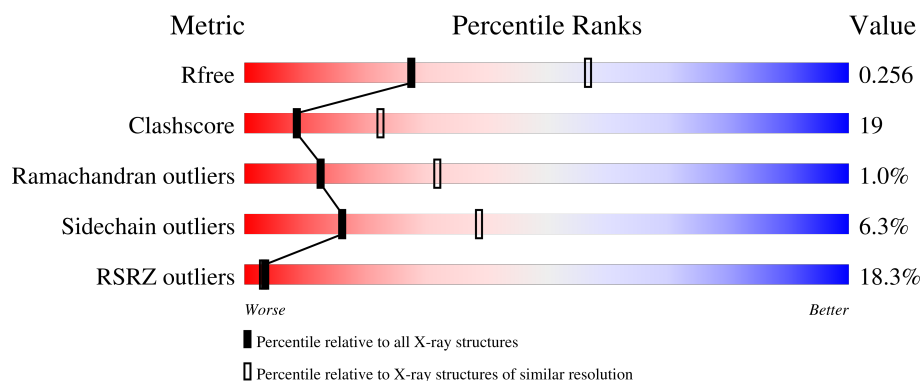
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	462	16% 56% 25% 5% 14%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3203 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hemagglutinin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	399	3109	1995	515	577	22	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	238	ILE	ASN	engineered mutation	UNP Q83531

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	14	8	1	5	0	0
2	A	1	14	8	1	5	0	0

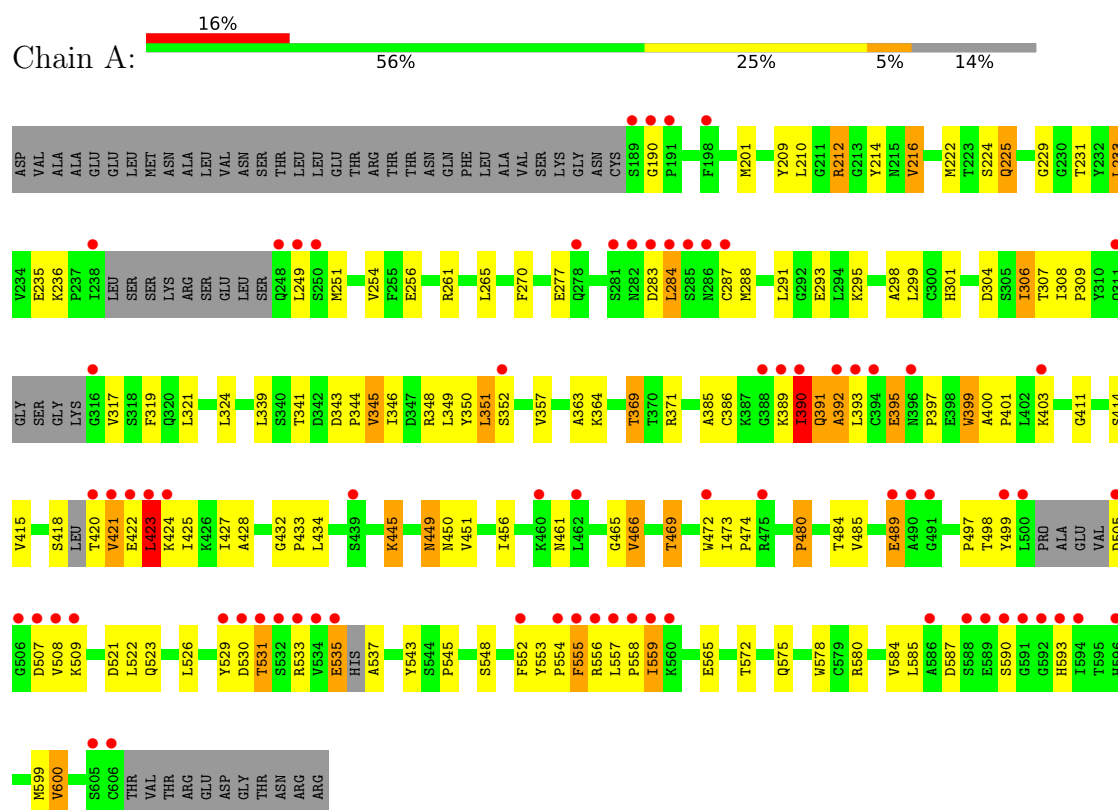
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	66	Total	O	0	0
			66	66		

3 Residue-property plots [i](#)

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

• Molecule 1: Hemagglutinin



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.20Å 134.20Å 100.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.70 40.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.4 (40.00-2.70) 99.4 (40.00-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.69Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.222 , 0.251 0.224 , 0.256	Depositor DCC
R_{free} test set	1279 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3203	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.38% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.46	0/3186	1.03	18/4332 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	LEU	N-CA-C	-11.38	98.89	113.12
1	A	351	LEU	N-CA-C	7.69	122.23	109.46
1	A	489	GLU	N-CA-C	7.36	121.67	111.74
1	A	392	ALA	CB-CA-C	-7.34	99.49	110.06
1	A	480	PRO	CB-CA-C	-7.28	98.67	110.25
1	A	555	PHE	N-CA-C	-6.89	96.11	110.80
1	A	465	GLY	N-CA-C	-6.79	103.03	112.13
1	A	351	LEU	CB-CA-C	-6.40	99.30	109.80
1	A	352	SER	N-CA-C	6.25	124.12	110.80
1	A	390	ILE	CB-CA-C	-5.98	101.49	111.29
1	A	306	ILE	N-CA-C	5.66	116.09	108.17
1	A	261	ARG	N-CA-C	5.36	118.46	110.52
1	A	559	ILE	N-CA-C	-5.36	98.19	109.34
1	A	428	ALA	N-CA-C	-5.25	101.20	109.50
1	A	225	GLN	CB-CA-C	-5.09	110.73	116.63
1	A	391	GLN	CB-CA-C	-5.06	100.97	109.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	423	LEU	N-CA-C	5.04	116.79	110.24
1	A	575	GLN	N-CA-C	5.00	118.96	112.86

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	399	TRP	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	3109	0	3057	116	0
2	A	28	0	26	1	0
3	A	66	0	0	1	0
All	All	3203	0	3083	117	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 19.

All (117) 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:489:GLU:O	1:A:489:GLU:HG2	1.53	1.07
1:A:553:TYR:CE2	1:A:555:PHE:O	2.18	0.97
1:A:537:ALA:HA	1:A:556:ARG:HD3	1.55	0.87
1:A:508:VAL:H	1:A:531:THR:CG2	1.90	0.83
1:A:389:LYS:O	1:A:390:ILE:HG12	1.79	0.82
1:A:559:ILE:HG13	1:A:559:ILE:O	1.81	0.81
1:A:400:ALA:N	1:A:401:PRO:HD2	1.96	0.81
1:A:508:VAL:H	1:A:531:THR:HG22	1.44	0.80
1:A:391:GLN:O	1:A:392:ALA:HB3	1.83	0.78
1:A:339:LEU:HD11	1:A:427:ILE:HD11	1.67	0.77
1:A:535:GLU:HB3	1:A:537:ALA:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:TYR:CD2	1:A:555:PHE:O	2.39	0.75
1:A:456:ILE:HB	1:A:466:VAL:HG13	1.69	0.74
1:A:385:ALA:HB1	1:A:390:ILE:HD11	1.68	0.73
1:A:535:GLU:HG2	1:A:537:ALA:N	2.03	0.73
1:A:357:VAL:HG11	1:A:445:LYS:HD2	1.71	0.73
1:A:556:ARG:HA	1:A:556:ARG:HH11	1.53	0.73
1:A:556:ARG:NH1	1:A:557:LEU:H	1.90	0.69
1:A:235:GLU:CD	1:A:249:LEU:HD13	2.19	0.67
1:A:400:ALA:N	1:A:401:PRO:CD	2.58	0.67
1:A:423:LEU:H	1:A:423:LEU:HD23	1.57	0.67
1:A:254:VAL:HG22	1:A:277:GLU:HG3	1.78	0.66
1:A:553:TYR:HE2	1:A:555:PHE:O	1.79	0.66
1:A:391:GLN:O	1:A:392:ALA:CB	2.45	0.65
1:A:489:GLU:O	1:A:489:GLU:CG	2.35	0.64
1:A:557:LEU:CB	1:A:558:PRO:HD2	2.27	0.64
1:A:469:THR:HG22	3:A:27:HOH:O	1.99	0.62
1:A:509:LYS:HD3	1:A:530:ASP:OD2	1.99	0.62
1:A:535:GLU:HA	1:A:552:PHE:HZ	1.64	0.62
1:A:505:ASP:HB2	1:A:507:ASP:OD1	2.01	0.61
1:A:565:GLU:HB3	1:A:584:VAL:HB	1.83	0.61
1:A:399:TRP:CD1	1:A:400:ALA:H	2.19	0.60
1:A:390:ILE:HG22	1:A:499:TYR:HB2	1.84	0.60
1:A:308:ILE:HD11	1:A:349:LEU:HG	1.84	0.59
1:A:535:GLU:CB	1:A:537:ALA:HB2	2.30	0.59
1:A:552:PHE:O	1:A:554:PRO:HD3	2.02	0.58
1:A:304:ASP:HB2	1:A:351:LEU:O	2.04	0.58
1:A:553:TYR:HE1	1:A:600:VAL:HG22	1.69	0.57
1:A:210:LEU:HD21	1:A:216:VAL:HG22	1.87	0.57
1:A:307:THR:OG1	1:A:348:ARG:NH1	2.37	0.56
1:A:480:PRO:O	1:A:480:PRO:HG2	2.05	0.56
1:A:485:VAL:HG13	1:A:498:THR:HG22	1.88	0.56
1:A:306:ILE:N	1:A:306:ILE:HD12	2.20	0.56
1:A:306:ILE:HG21	1:A:317:VAL:HG11	1.86	0.56
1:A:222:MET:HE2	1:A:291:LEU:HB2	1.89	0.55
1:A:580:ARG:NE	1:A:599:MET:HE3	2.22	0.54
1:A:473:ILE:HG23	1:A:474:PRO:HA	1.90	0.54
1:A:343:ASP:HB3	1:A:346:ILE:HG12	1.89	0.54
1:A:251:MET:HE3	1:A:283:ASP:HB3	1.88	0.54
1:A:309:PRO:HG2	1:A:341:THR:HG22	1.90	0.54
1:A:521:ASP:O	1:A:523:GLN:HG3	2.08	0.54
1:A:531:THR:O	1:A:531:THR:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:ASP:HB3	1:A:590:SER:O	2.07	0.53
1:A:389:LYS:O	1:A:390:ILE:CG1	2.55	0.53
1:A:421:VAL:HG12	1:A:421:VAL:O	2.09	0.53
1:A:390:ILE:HG13	1:A:390:ILE:O	2.09	0.52
1:A:397:PRO:HG2	1:A:403:LYS:HG2	1.90	0.52
1:A:390:ILE:CG1	1:A:390:ILE:O	2.55	0.52
1:A:537:ALA:CA	1:A:556:ARG:HD3	2.34	0.52
1:A:553:TYR:CE1	1:A:600:VAL:HG22	2.46	0.51
1:A:559:ILE:O	1:A:559:ILE:CG1	2.53	0.51
1:A:418:SER:O	1:A:421:VAL:HA	2.10	0.51
1:A:522:LEU:O	1:A:545:PRO:HD3	2.10	0.50
1:A:321:LEU:HD22	1:A:415:VAL:HG21	1.94	0.50
1:A:422:GLU:HA	1:A:422:GLU:OE1	2.12	0.50
1:A:461:ASN:HA	1:A:509:LYS:HB3	1.94	0.49
1:A:400:ALA:H	1:A:401:PRO:HD2	1.77	0.49
1:A:293:GLU:O	1:A:295:LYS:HG3	2.12	0.48
2:A:619:NAG:H83	2:A:619:NAG:H3	1.95	0.48
1:A:201:MET:SD	1:A:265:LEU:HD13	2.53	0.48
1:A:449:ASN:O	1:A:450:ASN:HB2	2.13	0.48
1:A:392:ALA:HA	1:A:395:GLU:HB2	1.95	0.48
1:A:288:MET:CE	1:A:299:LEU:HD23	2.43	0.48
1:A:364:LYS:HE2	1:A:472:TRP:CH2	2.49	0.48
1:A:585:LEU:O	1:A:593:HIS:HA	2.14	0.47
1:A:212:ARG:HE	1:A:212:ARG:CA	2.27	0.47
1:A:209:TYR:O	1:A:214:TYR:HB2	2.15	0.47
1:A:284:LEU:HD12	1:A:284:LEU:O	2.15	0.46
1:A:522:LEU:C	1:A:522:LEU:HD13	2.39	0.46
1:A:557:LEU:CB	1:A:558:PRO:CD	2.92	0.46
1:A:432:GLY:O	1:A:433:PRO:C	2.59	0.46
1:A:369:THR:CG2	1:A:411:GLY:HA3	2.45	0.46
1:A:578:TRP:HA	1:A:600:VAL:O	2.15	0.46
1:A:363:ALA:O	1:A:414:SER:HA	2.16	0.46
1:A:210:LEU:HD21	1:A:216:VAL:CG2	2.47	0.45
1:A:288:MET:O	1:A:298:ALA:HA	2.15	0.45
1:A:350:TYR:CE2	1:A:401:PRO:HB3	2.51	0.45
1:A:309:PRO:HG2	1:A:341:THR:CG2	2.47	0.45
1:A:235:GLU:OE2	1:A:249:LEU:HD13	2.17	0.45
1:A:201:MET:HE1	1:A:265:LEU:HB3	1.99	0.44
1:A:386:CYS:O	1:A:391:GLN:HB2	2.18	0.44
1:A:480:PRO:O	1:A:480:PRO:CG	2.66	0.44
1:A:554:PRO:O	1:A:556:ARG:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:ALA:HA	1:A:395:GLU:CB	2.47	0.44
1:A:543:TYR:HA	1:A:548:SER:HB3	2.00	0.44
1:A:251:MET:HE3	1:A:283:ASP:CB	2.47	0.43
1:A:391:GLN:HG2	1:A:392:ALA:N	2.32	0.43
1:A:345:VAL:O	1:A:371:ARG:HA	2.19	0.43
1:A:216:VAL:HA	1:A:233:LEU:O	2.19	0.43
1:A:251:MET:CE	1:A:283:ASP:HB3	2.49	0.43
1:A:345:VAL:HG23	1:A:371:ARG:HB3	2.01	0.43
1:A:236:LYS:NZ	1:A:277:GLU:OE1	2.49	0.42
1:A:301:HIS:HB2	1:A:319:PHE:CD1	2.54	0.42
1:A:229:GLY:HA2	1:A:256:GLU:O	2.19	0.42
1:A:484:THR:HG22	1:A:497:PRO:HA	2.01	0.42
1:A:270:PHE:CE1	1:A:599:MET:HE1	2.54	0.42
1:A:319:PHE:HB2	1:A:425:ILE:HD11	2.02	0.42
1:A:343:ASP:HA	1:A:344:PRO:HD3	1.79	0.41
1:A:364:LYS:HE2	1:A:472:TRP:CZ2	2.55	0.41
1:A:231:THR:HA	1:A:254:VAL:O	2.21	0.41
1:A:231:THR:HG21	1:A:287:CYS:HB3	2.02	0.41
1:A:299:LEU:HD21	1:A:425:ILE:HD13	2.03	0.41
1:A:224:SER:C	1:A:225:GLN:HG2	2.45	0.41
1:A:343:ASP:HB3	1:A:346:ILE:CG1	2.50	0.40
1:A:420:THR:C	1:A:422:GLU:H	2.29	0.40
1:A:369:THR:HG21	1:A:411:GLY:HA3	2.03	0.40
1:A:529:TYR:HE1	1:A:556:ARG:HH21	1.69	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	387/462 (84%)	358 (92%)	25 (6%)	4 (1%)	12 32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	190	GLY
1	A	390	ILE
1	A	531	THR
1	A	421	VAL

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	348/405 (86%)	326 (94%)	22 (6%)	16	39

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	212	ARG
1	A	216	VAL
1	A	233	LEU
1	A	284	LEU
1	A	324	LEU
1	A	345	VAL
1	A	369	THR
1	A	390	ILE
1	A	395	GLU
1	A	423	LEU
1	A	424	LYS
1	A	434	LEU
1	A	445	LYS
1	A	449	ASN
1	A	451	VAL
1	A	466	VAL
1	A	469	THR
1	A	526	LEU
1	A	533	ARG
1	A	535	GLU
1	A	572	THR

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Mol	Chain	Res	Type
1	A	600	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	278	GLN
1	A	286	ASN
1	A	320	GLN
1	A	334	GLN
1	A	362	GLN
1	A	383	GLN
1	A	391	GLN
1	A	461	ASN
1	A	523	GLN
1	A	581	HIS

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](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	A	618	1	14,14,15	0.64	0	17,19,21	0.66	1 (5%)
2	NAG	A	619	1	14,14,15	0.68	0	17,19,21	0.68	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	618	1	-	4/6/23/26	0/1/1/1
2	NAG	A	619	1	-	6/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	618	NAG	C2-N2-C7	-2.12	120.06	122.90

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	618	NAG	C8-C7-N2-C2
2	A	618	NAG	O7-C7-N2-C2
2	A	619	NAG	C8-C7-N2-C2
2	A	619	NAG	O7-C7-N2-C2
2	A	618	NAG	C4-C5-C6-O6
2	A	619	NAG	C4-C5-C6-O6
2	A	619	NAG	O5-C5-C6-O6
2	A	618	NAG	O5-C5-C6-O6
2	A	619	NAG	C3-C2-N2-C7
2	A	619	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	619	NAG	1	0

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	399/462 (86%)	0.71	73 (18%) 3 3	24, 42, 91, 108	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	555	PHE	7.2
1	A	238	ILE	7.1
1	A	421	VAL	7.1
1	A	534	VAL	7.1
1	A	557	LEU	6.1
1	A	559	ILE	6.0
1	A	591	GLY	5.8
1	A	558	PRO	5.8
1	A	489	GLU	5.7
1	A	248	GLN	5.4
1	A	420	THR	5.1
1	A	500	LEU	4.9
1	A	190	GLY	4.8
1	A	535	GLU	4.7
1	A	533	ARG	4.7
1	A	390	ILE	4.6
1	A	423	LEU	4.6
1	A	281	SER	4.5
1	A	606	CYS	4.5
1	A	596	HIS	4.2
1	A	392	ALA	4.2
1	A	189	SER	4.2
1	A	393	LEU	4.2
1	A	394	CYS	4.1
1	A	283	ASP	4.0
1	A	389	LYS	3.9
1	A	593	HIS	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	592	GLY	3.9
1	A	472	TRP	3.9
1	A	560	LYS	3.8
1	A	588	SER	3.8
1	A	590	SER	3.7
1	A	556	ARG	3.7
1	A	507	ASP	3.6
1	A	508	VAL	3.6
1	A	554	PRO	3.4
1	A	422	GLU	3.4
1	A	594	ILE	3.3
1	A	491	GLY	3.3
1	A	532	SER	3.3
1	A	284	LEU	3.3
1	A	311	GLN	3.2
1	A	506	GLY	3.1
1	A	499	TYR	3.0
1	A	352	SER	2.9
1	A	531	THR	2.9
1	A	460	LYS	2.9
1	A	552	PHE	2.9
1	A	530	ASP	2.8
1	A	191	PRO	2.7
1	A	462	LEU	2.7
1	A	529	TYR	2.7
1	A	589	GLU	2.6
1	A	286	ASN	2.6
1	A	396	ASN	2.6
1	A	278	GLN	2.5
1	A	490	ALA	2.5
1	A	316	GLY	2.5
1	A	285	SER	2.4
1	A	586	ALA	2.4
1	A	475	ARG	2.4
1	A	605	SER	2.4
1	A	509	LYS	2.3
1	A	439	SER	2.3
1	A	424	LYS	2.2
1	A	388	GLY	2.2
1	A	250	SER	2.2
1	A	198	PHE	2.2
1	A	249	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	287	CYS	2.1
1	A	505	ASP	2.1
1	A	282	ASN	2.1
1	A	403	LYS	2.1

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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	A	618	14/15	0.40	0.26	73,78,81,81	0
2	NAG	A	619	14/15	0.51	0.26	78,83,84,84	0

6.5 Other polymers [i](#)

There are no such residues in this entry.