



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 02:02 AM UTC

PDB ID : 4MC7 / pdb_00004mc7
Title : Crystal structure of a subtype N11 neuraminidase-like protein of A/flat-faced bat/Peru/033/2010 (H18N11)
Authors : Yang, H.; Carney, P.J.; Chang, J.C.; Guo, Z.; Stevens, J.
Deposited on : 2013-08-21
Resolution : 2.99 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

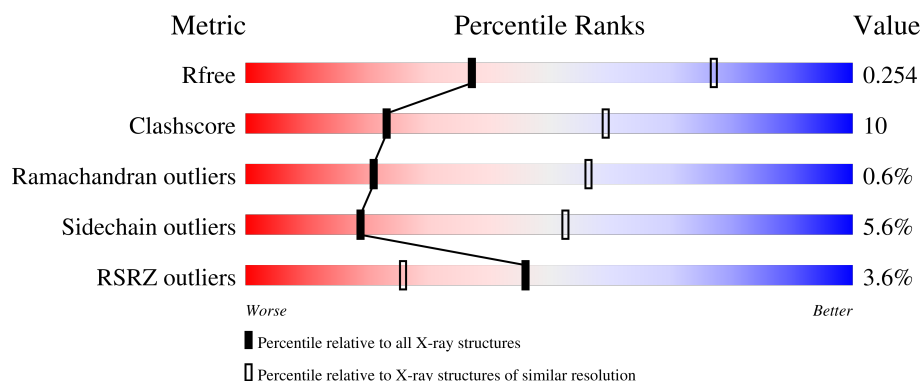
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	374	2% 72% 22% ...
1	B	374	4% 74% 21% ..
1	C	374	4% 71% 24% ...
1	D	374	4% 73% 22% ..

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 11225 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 NEURAMINIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	363	Total	C	N	O	S	0	0	0
			2791	1763	461	548	19			
1	B	363	Total	C	N	O	S	0	0	0
			2791	1763	461	548	19			
1	C	363	Total	C	N	O	S	0	0	0
			2791	1763	461	548	19			
1	D	363	Total	C	N	O	S	0	0	0
			2791	1763	461	548	19			

- 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
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		

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

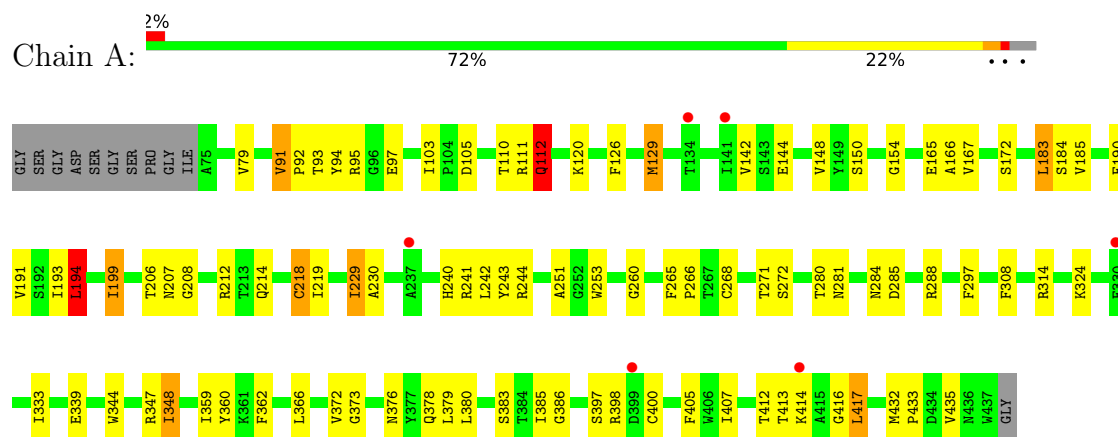
- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		
3	B	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		

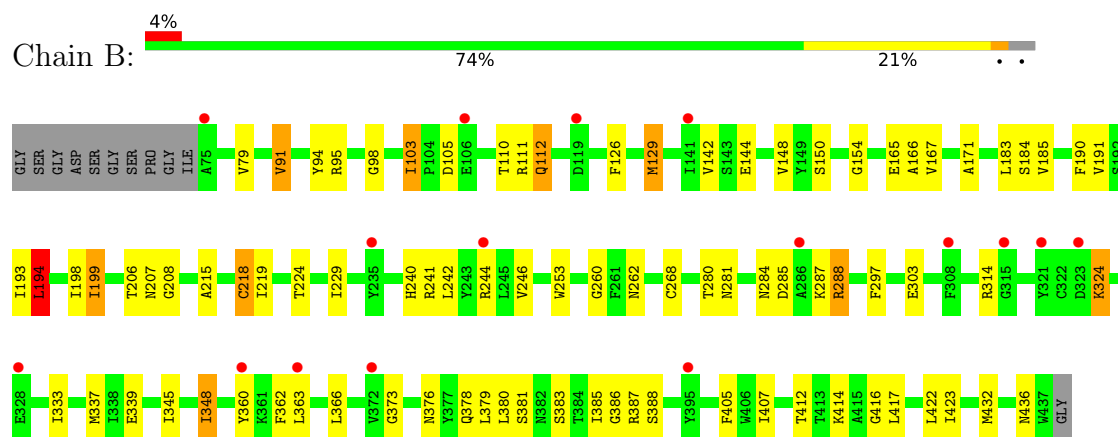
3 Residue-property plots

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.

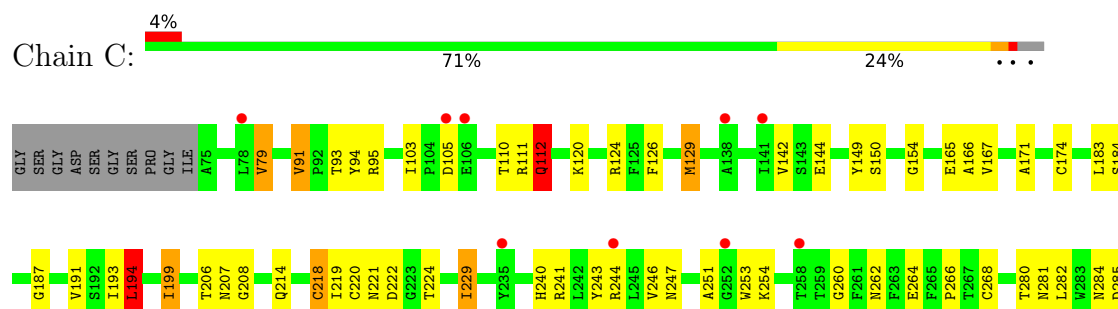
• Molecule 1: NEURAMINIDASE

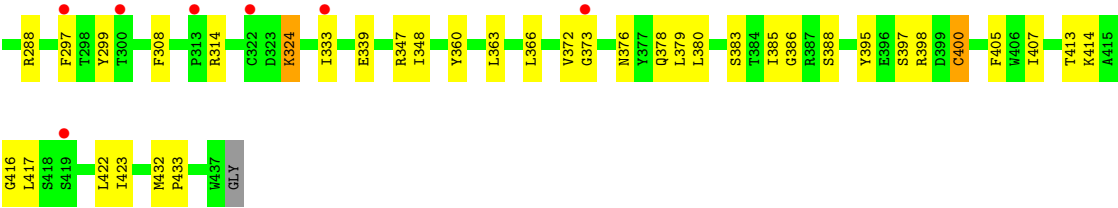


• Molecule 1: NEURAMINIDASE

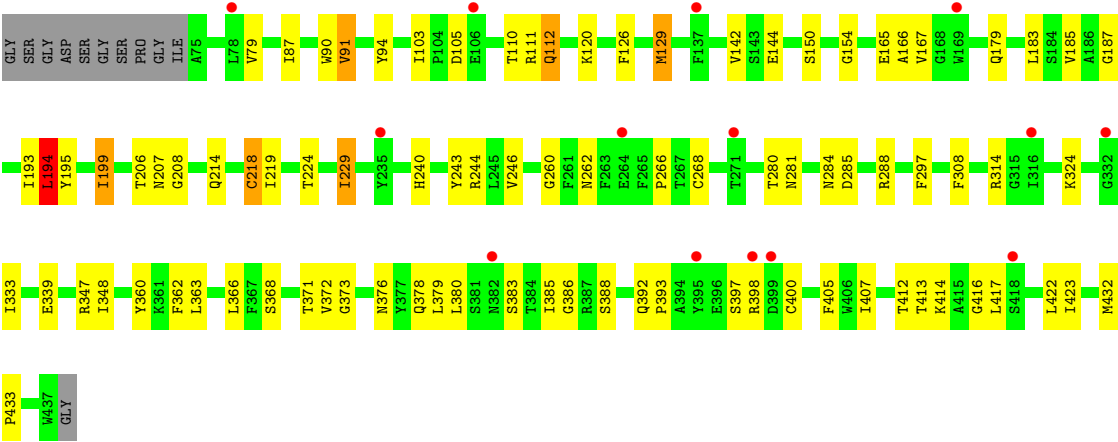


• Molecule 1: NEURAMINIDASE





● Molecule 1: NEURAMINIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.37Å 164.36Å 214.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	44.84 – 2.99 44.84 – 2.99	Depositor EDS
% Data completeness (in resolution range)	93.6 (44.84-2.99) 93.7 (44.84-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0111	Depositor
R, R_{free}	0.214 , 0.260 0.211 , 0.254	Depositor DCC
R_{free} test set	2121 reflections (4.77%)	wwPDB-VP
Wilson B-factor (Å ²)	74.6	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11225	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: CA, 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	0.94	2/2860 (0.1%)	1.03	3/3886 (0.1%)
1	B	0.91	2/2860 (0.1%)	0.99	3/3886 (0.1%)
1	C	0.86	2/2860 (0.1%)	0.98	4/3886 (0.1%)
1	D	0.86	2/2860 (0.1%)	0.98	3/3886 (0.1%)
All	All	0.89	8/11440 (0.1%)	0.99	13/15544 (0.1%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	378	GLN	CD-OE1	5.39	1.33	1.23
1	B	378	GLN	CD-OE1	5.36	1.33	1.23
1	A	378	GLN	CD-OE1	5.32	1.33	1.23
1	C	378	GLN	CD-OE1	5.20	1.33	1.23
1	C	112	GLN	CD-OE1	5.16	1.33	1.23
1	A	112	GLN	CD-NE2	-5.10	1.22	1.33
1	D	185	VAL	CA-CB	-5.08	1.48	1.54
1	B	288	ARG	CA-C	-5.01	1.47	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	240	HIS	CB-CG-CD2	-6.88	122.25	131.20
1	D	240	HIS	CB-CG-CD2	-6.86	122.28	131.20
1	B	240	HIS	CB-CG-CD2	-6.80	122.35	131.20
1	C	240	HIS	CB-CG-CD2	-6.41	122.87	131.20
1	D	194	LEU	N-CA-C	6.22	119.04	108.90
1	C	194	LEU	N-CA-C	6.07	118.80	108.90
1	C	251	ALA	N-CA-C	-5.74	105.59	112.59
1	A	240	HIS	CB-CG-ND1	5.74	131.31	122.70
1	B	194	LEU	N-CA-C	5.69	118.18	108.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	194	LEU	N-CA-C	5.67	118.15	108.90
1	B	240	HIS	CB-CG-ND1	5.65	131.17	122.70
1	D	240	HIS	CB-CG-ND1	5.45	130.87	122.70
1	C	240	HIS	CB-CG-ND1	5.37	130.75	122.70

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	2791	0	2650	64	1
1	B	2791	0	2650	59	1
1	C	2791	0	2650	67	0
1	D	2791	0	2650	51	0
2	A	14	0	13	0	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	11225	0	10652	226	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 10.

All (226) 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:112:GLN:O	1:A:112:GLN:HG3	1.42	1.10
1:B:112:GLN:O	1:B:112:GLN:HG3	1.41	1.09
1:D:112:GLN:O	1:D:112:GLN:HG3	1.35	1.09
1:C:112:GLN:HG3	1:C:112:GLN:O	1.34	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:112:GLN:O	1:D:112:GLN:CG	2.19	0.89
1:A:105:ASP:OD1	1:A:414:LYS:HB3	1.78	0.82
1:C:219:ILE:HD11	1:C:268:CYS:HB2	1.60	0.82
1:A:339:GLU:OE1	1:A:366:LEU:HD12	1.79	0.82
1:B:105:ASP:OD1	1:B:414:LYS:HB3	1.80	0.81
1:B:199:ILE:HD12	1:C:91:VAL:HG21	1.62	0.81
1:A:219:ILE:HD11	1:A:268:CYS:HB2	1.62	0.81
1:C:112:GLN:O	1:C:112:GLN:CG	2.20	0.80
1:D:219:ILE:HD11	1:D:268:CYS:HB2	1.64	0.79
1:B:112:GLN:O	1:B:112:GLN:CG	2.27	0.79
1:C:105:ASP:OD1	1:C:414:LYS:HB3	1.81	0.79
1:C:339:GLU:OE1	1:C:366:LEU:HD12	1.84	0.78
1:B:219:ILE:HD11	1:B:268:CYS:HB2	1.67	0.77
1:B:199:ILE:HD12	1:C:91:VAL:CG2	2.15	0.76
1:D:105:ASP:OD1	1:D:414:LYS:HB3	1.87	0.75
1:B:288:ARG:NH2	1:B:333:ILE:O	2.22	0.73
1:D:339:GLU:OE1	1:D:366:LEU:HD12	1.88	0.72
1:B:339:GLU:OE1	1:B:366:LEU:HD12	1.89	0.72
1:D:219:ILE:CD1	1:D:268:CYS:HB2	2.22	0.69
1:A:112:GLN:O	1:A:112:GLN:CG	2.32	0.69
1:D:288:ARG:NH2	1:D:333:ILE:O	2.26	0.68
1:D:166:ALA:HB2	1:D:194:LEU:HD21	1.76	0.68
1:C:183:LEU:HD23	1:C:193:ILE:HG12	1.76	0.67
1:A:199:ILE:HD12	1:D:91:VAL:HG21	1.76	0.66
1:B:360:TYR:CD1	1:B:376:ASN:HB2	2.31	0.66
1:B:314:ARG:NH2	1:B:348:ILE:O	2.30	0.65
1:C:219:ILE:CD1	1:C:268:CYS:HB2	2.26	0.65
1:B:218:CYS:C	1:B:219:ILE:HD12	2.23	0.64
1:A:288:ARG:NH2	1:A:333:ILE:O	2.31	0.64
1:B:199:ILE:HG13	1:C:93:THR:HG22	1.80	0.63
1:A:94:TYR:CE1	1:A:154:GLY:HA2	2.33	0.63
1:B:219:ILE:CD1	1:B:268:CYS:HB2	2.29	0.63
1:B:183:LEU:HD23	1:B:193:ILE:HG12	1.80	0.63
1:A:219:ILE:CD1	1:A:268:CYS:HB2	2.28	0.63
1:C:94:TYR:CE1	1:C:154:GLY:HA2	2.34	0.62
1:C:385:ILE:HG22	1:C:386:GLY:N	2.15	0.62
1:D:314:ARG:NH2	1:D:348:ILE:O	2.32	0.62
1:B:360:TYR:HD1	1:B:376:ASN:HB2	1.64	0.62
1:A:416:GLY:C	1:A:417:LEU:HG	2.24	0.62
1:C:288:ARG:NH2	1:C:333:ILE:O	2.33	0.62
1:C:416:GLY:C	1:C:417:LEU:HG	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:LEU:HD23	1:A:193:ILE:HG12	1.82	0.61
1:A:110:THR:HG22	1:A:126:PHE:CE1	2.36	0.61
1:D:214:GLN:HG2	1:D:266:PRO:HG2	1.81	0.60
1:D:405:PHE:HE2	1:D:407:ILE:HD11	1.67	0.60
1:B:385:ILE:HG22	1:B:386:GLY:N	2.17	0.60
1:D:183:LEU:HD23	1:D:193:ILE:HG12	1.84	0.59
1:C:241:ARG:NH2	1:C:253:TRP:CZ2	2.70	0.59
1:D:260:GLY:O	1:D:284:ASN:ND2	2.36	0.59
1:B:167:VAL:HG23	1:B:167:VAL:O	2.03	0.59
1:A:218:CYS:C	1:A:219:ILE:HD12	2.28	0.58
1:B:416:GLY:C	1:B:417:LEU:HG	2.28	0.58
1:D:360:TYR:CD1	1:D:376:ASN:HB2	2.39	0.58
1:D:281:ASN:HB3	1:D:285:ASP:HB3	1.86	0.57
1:A:432:MET:HE3	1:A:433:PRO:HD2	1.87	0.57
1:C:432:MET:HE3	1:C:433:PRO:HD2	1.87	0.56
1:B:198:ILE:HG21	1:C:395:TYR:CZ	2.40	0.56
1:D:360:TYR:HD1	1:D:376:ASN:HB2	1.70	0.56
1:A:314:ARG:NH2	1:A:348:ILE:O	2.38	0.56
1:B:94:TYR:CE1	1:B:154:GLY:HA2	2.40	0.56
1:D:218:CYS:C	1:D:219:ILE:HD12	2.30	0.56
1:A:360:TYR:CD1	1:A:376:ASN:HB2	2.40	0.56
1:A:110:THR:HG22	1:A:126:PHE:CD1	2.41	0.56
1:C:229:ILE:HG13	1:C:243:TYR:CD1	2.41	0.56
1:D:385:ILE:HG22	1:D:386:GLY:N	2.21	0.56
1:A:93:THR:HG22	1:C:199:ILE:HG13	1.88	0.56
1:A:97:GLU:OE1	1:C:149:TYR:OH	2.21	0.56
1:D:167:VAL:HG23	1:D:167:VAL:O	2.06	0.55
1:D:94:TYR:CE1	1:D:154:GLY:HA2	2.41	0.55
1:C:214:GLN:HG2	1:C:266:PRO:HG2	1.89	0.55
1:C:142:VAL:HG22	1:C:144:GLU:OE1	2.06	0.55
1:A:91:VAL:HG21	1:C:199:ILE:HD12	1.89	0.55
1:C:111:ARG:HB3	1:C:129:MET:SD	2.48	0.54
1:B:337:MET:HG2	1:B:345:ILE:HG12	1.88	0.53
1:B:244:ARG:HB2	1:B:297:PHE:HZ	1.71	0.53
1:A:360:TYR:HD1	1:A:376:ASN:HB2	1.73	0.53
1:D:416:GLY:C	1:D:417:LEU:HG	2.34	0.53
1:A:142:VAL:HG22	1:A:144:GLU:OE1	2.08	0.53
1:C:360:TYR:CD1	1:C:376:ASN:HB2	2.44	0.52
1:D:142:VAL:HG22	1:D:144:GLU:OE1	2.09	0.52
1:C:110:THR:HG22	1:C:126:PHE:CE1	2.45	0.52
1:B:166:ALA:HB2	1:B:194:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ILE:HD12	1:B:219:ILE:N	2.24	0.52
1:A:219:ILE:HD12	1:A:219:ILE:N	2.24	0.52
1:D:308:PHE:CE2	1:D:347:ARG:HD3	2.45	0.52
1:A:92:PRO:HG2	1:C:167:VAL:HG21	1.91	0.52
1:A:167:VAL:HG23	1:A:167:VAL:O	2.10	0.52
1:A:405:PHE:HE2	1:A:407:ILE:HD11	1.74	0.51
1:C:166:ALA:HB2	1:C:194:LEU:HD21	1.93	0.51
1:C:314:ARG:NH2	1:C:348:ILE:O	2.44	0.51
1:A:111:ARG:HB3	1:A:129:MET:SD	2.50	0.51
1:A:214:GLN:HG2	1:A:266:PRO:HG2	1.94	0.50
1:C:281:ASN:HB3	1:C:285:ASP:HB3	1.94	0.50
1:A:150:SER:HB2	1:A:165:GLU:HG3	1.94	0.50
1:B:150:SER:HB2	1:B:165:GLU:HG3	1.93	0.50
1:C:385:ILE:HG22	1:C:386:GLY:H	1.77	0.50
1:C:405:PHE:HE2	1:C:407:ILE:HD11	1.77	0.50
1:B:142:VAL:HG22	1:B:144:GLU:OE1	2.12	0.50
1:C:110:THR:HG22	1:C:126:PHE:CD1	2.46	0.50
1:B:281:ASN:HB3	1:B:285:ASP:HB3	1.94	0.50
1:A:385:ILE:HG22	1:A:386:GLY:N	2.27	0.49
1:B:405:PHE:HE2	1:B:407:ILE:HD11	1.77	0.49
1:C:360:TYR:HD1	1:C:376:ASN:HB2	1.77	0.49
1:C:379:LEU:O	1:C:380:LEU:HD23	2.11	0.49
1:A:281:ASN:HB3	1:A:285:ASP:HB3	1.93	0.49
1:B:244:ARG:HB2	1:B:297:PHE:CZ	2.47	0.49
1:C:218:CYS:C	1:C:219:ILE:HD12	2.37	0.49
1:D:372:VAL:HG12	1:D:373:GLY:O	2.13	0.49
1:D:379:LEU:O	1:D:380:LEU:HD23	2.11	0.49
1:A:241:ARG:NH2	1:A:253:TRP:CZ2	2.81	0.49
1:C:167:VAL:HG23	1:C:167:VAL:O	2.10	0.49
1:A:344:TRP:HE3	1:A:359:ILE:HG12	1.78	0.49
1:A:360:TYR:HD2	1:A:362:PHE:CE2	2.31	0.48
1:A:244:ARG:HB2	1:A:297:PHE:HZ	1.78	0.48
1:A:379:LEU:O	1:A:380:LEU:HD23	2.14	0.48
1:B:379:LEU:O	1:B:380:LEU:HD23	2.13	0.48
1:B:224:THR:HG22	1:B:246:VAL:HG22	1.94	0.48
1:A:285:ASP:CG	1:A:324:LYS:HG3	2.38	0.48
1:B:148:VAL:HG21	1:B:171:ALA:HB2	1.96	0.48
1:B:199:ILE:HG13	1:C:93:THR:CG2	2.42	0.48
1:B:260:GLY:O	1:B:284:ASN:ND2	2.46	0.48
1:B:184:SER:O	1:B:191:VAL:HA	2.14	0.48
1:D:244:ARG:HB2	1:D:297:PHE:HZ	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:THR:HG22	1:B:126:PHE:CE1	2.49	0.47
1:C:308:PHE:CE2	1:C:347:ARG:HD3	2.50	0.47
1:D:224:THR:HG22	1:D:246:VAL:HG22	1.96	0.47
1:A:244:ARG:HG2	1:A:251:ALA:HB3	1.96	0.47
1:D:281:ASN:CB	1:D:285:ASP:HB3	2.45	0.47
1:B:381:SER:HB2	1:B:436:ASN:HD21	1.79	0.47
1:B:111:ARG:HB3	1:B:129:MET:SD	2.55	0.47
1:B:360:TYR:OH	1:B:373:GLY:HA3	2.15	0.46
1:C:260:GLY:O	1:C:284:ASN:ND2	2.45	0.46
1:C:165:GLU:O	1:C:194:LEU:HD11	2.15	0.46
1:D:110:THR:HG22	1:D:126:PHE:CD1	2.50	0.46
1:D:432:MET:HE3	1:D:432:MET:HB3	1.82	0.46
1:A:184:SER:O	1:A:191:VAL:HA	2.16	0.46
1:B:185:VAL:HA	1:B:190:PHE:O	2.15	0.46
1:B:412:THR:HA	1:B:417:LEU:O	2.16	0.46
1:A:435:VAL:HG11	1:C:187:GLY:HA3	1.97	0.46
1:B:422:LEU:HD23	1:B:422:LEU:HA	1.70	0.46
1:C:184:SER:O	1:C:191:VAL:HA	2.15	0.46
1:B:206:THR:C	1:B:208:GLY:H	2.24	0.46
1:D:206:THR:C	1:D:208:GLY:H	2.24	0.46
1:B:148:VAL:O	1:B:165:GLU:HB2	2.17	0.45
1:D:150:SER:HB2	1:D:165:GLU:HG3	1.98	0.45
1:C:244:ARG:HB2	1:C:297:PHE:HZ	1.81	0.45
1:A:91:VAL:CG2	1:C:199:ILE:HD12	2.45	0.45
1:B:285:ASP:CG	1:B:324:LYS:HG3	2.42	0.45
1:A:260:GLY:O	1:A:284:ASN:ND2	2.44	0.45
1:B:165:GLU:O	1:B:194:LEU:HD11	2.16	0.45
1:B:287:LYS:HD2	1:B:303:GLU:OE2	2.16	0.45
1:A:372:VAL:HG12	1:A:373:GLY:O	2.17	0.45
1:A:412:THR:HA	1:A:417:LEU:O	2.17	0.45
1:A:148:VAL:O	1:A:165:GLU:HB2	2.16	0.45
1:A:360:TYR:CD2	1:A:362:PHE:CZ	3.05	0.45
1:D:244:ARG:HB2	1:D:297:PHE:CZ	2.52	0.45
1:C:432:MET:HE3	1:C:432:MET:HB3	1.82	0.44
1:D:432:MET:HE3	1:D:433:PRO:HD2	1.98	0.44
1:B:432:MET:HE3	1:B:432:MET:HB3	1.82	0.44
1:D:111:ARG:HB3	1:D:129:MET:SD	2.57	0.44
1:C:224:THR:HG22	1:C:246:VAL:HG22	1.98	0.44
1:D:87:ILE:HG21	1:D:90:TRP:CZ2	2.51	0.44
1:A:265:PHE:N	1:A:266:PRO:CD	2.81	0.44
1:B:98:GLY:HA3	1:B:103:ILE:HD11	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:360:TYR:CD2	1:D:362:PHE:CZ	3.06	0.44
1:B:385:ILE:CG2	1:B:386:GLY:N	2.81	0.44
1:C:264:GLU:HG3	1:C:282:LEU:HD13	2.00	0.44
1:A:244:ARG:HB2	1:A:297:PHE:CZ	2.53	0.44
1:C:174:CYS:HB2	1:C:220:CYS:SG	2.57	0.44
1:A:413:THR:HG22	1:A:414:LYS:N	2.33	0.44
1:B:241:ARG:NH2	1:B:253:TRP:CZ2	2.86	0.44
1:C:94:TYR:CG	1:C:95:ARG:N	2.86	0.43
1:C:385:ILE:CG2	1:C:386:GLY:N	2.81	0.43
1:B:199:ILE:CG1	1:C:93:THR:HG22	2.47	0.43
1:A:185:VAL:HA	1:A:190:PHE:O	2.19	0.43
1:B:360:TYR:CD2	1:B:362:PHE:CZ	3.06	0.43
1:C:398:ARG:C	1:C:400:CYS:N	2.76	0.43
1:C:206:THR:C	1:C:208:GLY:H	2.27	0.43
1:B:381:SER:HB2	1:B:436:ASN:ND2	2.34	0.43
1:D:110:THR:HG22	1:D:126:PHE:CE1	2.54	0.43
1:A:229:ILE:HG13	1:A:243:TYR:CD1	2.54	0.42
1:C:219:ILE:HD12	1:C:219:ILE:N	2.34	0.42
1:C:171:ALA:HA	1:C:183:LEU:O	2.19	0.42
1:D:229:ILE:HG13	1:D:243:TYR:CD1	2.54	0.42
1:A:166:ALA:HB2	1:A:194:LEU:HD21	2.02	0.42
1:B:215:ALA:O	1:B:387:ARG:NH2	2.52	0.42
1:C:150:SER:HB2	1:C:165:GLU:HG3	2.01	0.42
1:D:412:THR:HA	1:D:417:LEU:O	2.20	0.42
1:A:212:ARG:HB2	1:A:230:ALA:HB3	2.01	0.42
1:D:422:LEU:HD23	1:D:422:LEU:HA	1.62	0.42
1:A:112:GLN:HE21	1:A:112:GLN:HB2	1.63	0.42
1:A:165:GLU:O	1:A:194:LEU:HD11	2.20	0.42
1:A:206:THR:C	1:A:208:GLY:H	2.28	0.42
1:C:372:VAL:HG12	1:C:373:GLY:O	2.20	0.42
1:C:244:ARG:HB2	1:C:297:PHE:CZ	2.54	0.42
1:A:308:PHE:CE2	1:A:347:ARG:HD3	2.54	0.42
1:C:79:VAL:HG22	1:C:222:ASP:OD1	2.20	0.42
1:C:413:THR:HB	1:C:416:GLY:O	2.20	0.42
1:D:368:SER:HB3	1:D:371:THR:HG23	2.01	0.42
1:A:432:MET:HE3	1:A:432:MET:HB3	1.80	0.41
1:B:91:VAL:HG21	1:D:199:ILE:HD12	2.01	0.41
1:B:112:GLN:HE21	1:B:112:GLN:HB2	1.66	0.41
1:D:398:ARG:C	1:D:400:CYS:N	2.78	0.41
1:A:413:THR:HB	1:A:417:LEU:HD12	2.02	0.41
1:C:285:ASP:CG	1:C:324:LYS:HG3	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:422:LEU:HA	1:C:422:LEU:HD23	1.72	0.41
1:C:124:ARG:HD2	1:C:422:LEU:HD12	2.02	0.41
1:D:392:GLN:HA	1:D:393:PRO:HD2	1.97	0.41
1:A:199:ILE:HD12	1:D:91:VAL:CG2	2.48	0.41
1:D:166:ALA:CB	1:D:194:LEU:HD21	2.47	0.41
1:D:179:GLN:HB2	1:D:195:TYR:CZ	2.56	0.41
1:A:94:TYR:CG	1:A:95:ARG:N	2.88	0.41
1:A:271:THR:O	1:A:272:SER:C	2.64	0.41
1:C:221:ASN:O	1:C:222:ASP:HB2	2.21	0.41
1:D:413:THR:CB	1:D:417:LEU:HD12	2.51	0.41
1:A:398:ARG:C	1:A:400:CYS:N	2.78	0.40
1:B:94:TYR:CG	1:B:95:ARG:N	2.89	0.40
1:B:242:LEU:HG	1:B:297:PHE:CE1	2.56	0.40
1:C:254:LYS:HE2	1:C:299:TYR:HE1	1.85	0.40
1:C:246:VAL:O	1:C:247:ASN:C	2.64	0.40
1:D:360:TYR:HD2	1:D:362:PHE:CZ	2.40	0.40
1:A:242:LEU:HG	1:A:297:PHE:CE1	2.56	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)
1:A:253:TRP:CH2	1:B:360:TYR:OH[8_555]	2.01	0.19

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	361/374 (96%)	337 (93%)	22 (6%)	2 (1%)	21 56
1	B	361/374 (96%)	338 (94%)	22 (6%)	1 (0%)	36 70
1	C	361/374 (96%)	341 (94%)	18 (5%)	2 (1%)	21 56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	361/374 (96%)	339 (94%)	19 (5%)	3 (1%)	16	50
All	All	1444/1496 (96%)	1355 (94%)	81 (6%)	8 (1%)	21	56

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	207	ASN
1	A	207	ASN
1	B	207	ASN
1	C	207	ASN
1	A	397	SER
1	C	397	SER
1	D	397	SER
1	D	187	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	306/312 (98%)	290 (95%)	16 (5%)	21	55
1	B	306/312 (98%)	289 (94%)	17 (6%)	19	52
1	C	306/312 (98%)	288 (94%)	18 (6%)	18	50
1	D	306/312 (98%)	289 (94%)	17 (6%)	19	52
All	All	1224/1248 (98%)	1156 (94%)	68 (6%)	19	52

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	79	VAL
1	A	91	VAL
1	A	103	ILE
1	A	112	GLN
1	A	120	LYS
1	A	129	MET

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Mol	Chain	Res	Type
1	A	172	SER
1	A	183	LEU
1	A	194	LEU
1	A	199	ILE
1	A	218	CYS
1	A	229	ILE
1	A	280	THR
1	A	348	ILE
1	A	383	SER
1	A	417	LEU
1	B	79	VAL
1	B	91	VAL
1	B	103	ILE
1	B	112	GLN
1	B	129	MET
1	B	194	LEU
1	B	199	ILE
1	B	218	CYS
1	B	229	ILE
1	B	262	ASN
1	B	280	THR
1	B	324	LYS
1	B	348	ILE
1	B	363	LEU
1	B	383	SER
1	B	388	SER
1	B	423	ILE
1	C	79	VAL
1	C	91	VAL
1	C	103	ILE
1	C	112	GLN
1	C	120	LYS
1	C	129	MET
1	C	194	LEU
1	C	199	ILE
1	C	218	CYS
1	C	229	ILE
1	C	262	ASN
1	C	280	THR
1	C	324	LYS
1	C	363	LEU
1	C	383	SER

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Mol	Chain	Res	Type
1	C	388	SER
1	C	400	CYS
1	C	423	ILE
1	D	79	VAL
1	D	91	VAL
1	D	103	ILE
1	D	112	GLN
1	D	120	LYS
1	D	129	MET
1	D	194	LEU
1	D	199	ILE
1	D	218	CYS
1	D	229	ILE
1	D	262	ASN
1	D	280	THR
1	D	324	LYS
1	D	363	LEU
1	D	383	SER
1	D	388	SER
1	D	423	ILE

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	240	HIS
1	A	374	ASN
1	A	436	ASN
1	B	204	HIS
1	B	240	HIS
1	B	374	ASN
1	C	374	ASN
1	D	240	HIS
1	D	374	ASN
1	D	436	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 5 are monoatomic - leaving 4 for Mogul analysis.

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	D	501	1	14,14,15	0.77	0	17,19,21	1.61	4 (23%)
2	NAG	A	501	1	14,14,15	0.79	0	17,19,21	2.42	9 (52%)
2	NAG	B	501	1	14,14,15	0.48	0	17,19,21	1.99	5 (29%)
2	NAG	C	501	1	14,14,15	1.09	2 (14%)	17,19,21	2.09	9 (52%)

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	D	501	1	-	2/6/23/26	0/1/1/1
2	NAG	A	501	1	-	0/6/23/26	0/1/1/1
2	NAG	B	501	1	-	0/6/23/26	0/1/1/1
2	NAG	C	501	1	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	NAG	C1-C2	2.58	1.55	1.52
2	C	501	NAG	C3-C2	2.35	1.57	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	NAG	C1-O5-C5	5.82	119.99	112.19
2	B	501	NAG	C1-O5-C5	5.20	119.15	112.19
2	C	501	NAG	O5-C1-C2	-4.37	104.53	111.29
2	D	501	NAG	C1-C2-N2	-3.42	105.04	110.43
2	B	501	NAG	C6-C5-C4	-3.20	105.16	113.02
2	C	501	NAG	C1-O5-C5	2.92	116.10	112.19
2	A	501	NAG	O4-C4-C3	2.85	117.08	110.38
2	A	501	NAG	C6-C5-C4	-2.76	106.23	113.02
2	C	501	NAG	O3-C3-C2	2.76	115.12	109.40
2	D	501	NAG	O5-C5-C6	-2.70	102.41	107.66
2	C	501	NAG	O7-C7-C8	-2.67	117.30	122.05
2	B	501	NAG	O5-C5-C6	2.63	112.78	107.66
2	A	501	NAG	O3-C3-C4	-2.63	104.18	110.38
2	A	501	NAG	C4-C3-C2	2.62	114.86	111.02
2	A	501	NAG	O7-C7-C8	-2.57	117.47	122.05
2	B	501	NAG	C4-C3-C2	-2.54	107.30	111.02
2	A	501	NAG	O4-C4-C5	2.45	115.36	109.32
2	C	501	NAG	O6-C6-C5	-2.32	103.43	111.33
2	C	501	NAG	O4-C4-C3	2.29	115.78	110.38
2	C	501	NAG	C3-C4-C5	-2.29	106.09	110.23
2	A	501	NAG	O5-C1-C2	-2.26	107.79	111.29
2	C	501	NAG	O3-C3-C4	-2.14	105.32	110.38
2	D	501	NAG	O6-C6-C5	-2.12	104.11	111.33
2	D	501	NAG	O5-C1-C2	-2.11	108.03	111.29
2	C	501	NAG	O7-C7-N2	2.05	125.60	121.98
2	A	501	NAG	O6-C6-C5	-2.04	104.38	111.33
2	B	501	NAG	O4-C4-C5	2.01	114.27	109.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	501	NAG	O5-C5-C6-O6
2	D	501	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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	363/374 (97%)	0.13	6 (1%)	69 45	32, 68, 122, 216	0
1	B	363/374 (97%)	0.26	16 (4%)	39 21	35, 72, 126, 222	0
1	C	363/374 (97%)	0.33	16 (4%)	39 21	42, 78, 129, 227	0
1	D	363/374 (97%)	0.34	14 (3%)	43 24	38, 80, 135, 230	0
All	All	1452/1496 (97%)	0.27	52 (3%)	46 26	32, 75, 131, 230	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	308	PHE	4.6
1	D	106	GLU	3.7
1	B	395	TYR	3.5
1	B	360	TYR	3.5
1	C	252	GLY	3.3
1	B	235	TYR	3.2
1	B	286	ALA	3.2
1	B	321	TYR	3.0
1	C	300	THR	3.0
1	B	315	GLY	2.9
1	B	372	VAL	2.9
1	C	235	TYR	2.9
1	A	414	LYS	2.8
1	A	237	ALA	2.7
1	A	134	THR	2.7
1	D	418	SER	2.6
1	C	244	ARG	2.6
1	B	328	GLU	2.6
1	C	138	ALA	2.6
1	D	169	TRP	2.6
1	C	419	SER	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	313	PRO	2.5
1	C	297	PHE	2.5
1	D	332	GLY	2.5
1	B	119	ASP	2.5
1	B	244	ARG	2.5
1	B	363	LEU	2.4
1	B	141	ILE	2.4
1	D	316	ILE	2.4
1	B	106	GLU	2.4
1	B	323	ASP	2.4
1	D	398	ARG	2.4
1	D	235	TYR	2.4
1	C	106	GLU	2.3
1	C	105	ASP	2.3
1	D	264	GLU	2.3
1	D	137	PHE	2.3
1	D	78	LEU	2.3
1	D	399	ASP	2.3
1	C	141	ILE	2.3
1	C	78	LEU	2.2
1	A	141	ILE	2.2
1	C	258	THR	2.2
1	C	322	CYS	2.2
1	D	271	THR	2.2
1	D	382	ASN	2.1
1	A	399	ASP	2.1
1	A	330	GLU	2.1
1	C	373	GLY	2.1
1	C	333	ILE	2.1
1	D	395	TYR	2.0
1	B	75	ALA	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 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(Å ²)	Q<0.9
2	NAG	A	501	14/15	0.78	0.11	56,72,91,113	0
2	NAG	C	501	14/15	0.81	0.12	75,86,103,108	0
2	NAG	D	501	14/15	0.81	0.11	98,113,132,134	0
2	NAG	B	501	14/15	0.84	0.12	88,102,118,125	0
3	CA	D	502	1/1	0.97	0.05	68,68,68,68	0
3	CA	A	503	1/1	0.98	0.08	65,65,65,65	0
3	CA	C	502	1/1	0.98	0.06	63,63,63,63	0
3	CA	A	502	1/1	0.98	0.05	64,64,64,64	0
3	CA	B	502	1/1	0.99	0.04	42,42,42,42	0

6.5 Other polymers [i](#)

There are no such residues in this entry.