



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 12:31 PM GMT

PDB ID : 1NQL
Title : Structure of the extracellular domain of human epidermal growth factor (EGF) receptor in an inactive (low pH) complex with EGF.
Authors : Ferguson, K.M.; Lemmon, M.A.
Deposited on : 2003-01-21
Resolution : 2.80 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

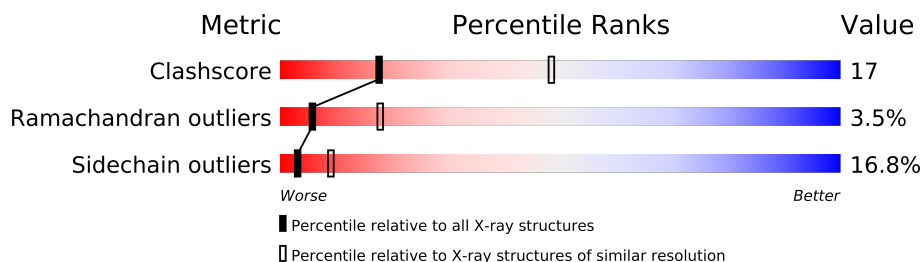
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.80 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))
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	624	
2	B	53	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 5150 atoms, of which 0 are hydrogen and 0 are deuterium.

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 epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	612	Total	C	N	O	S	10	0	0
			4597	2836	817	885	59			

- Molecule 2 is a protein called epidermal growth factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	48	Total	C	N	O	S	0	0	0
			377	235	62	73	7			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	3	Total	C	N	O	0	0
			39	22	2	15		
4	A	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

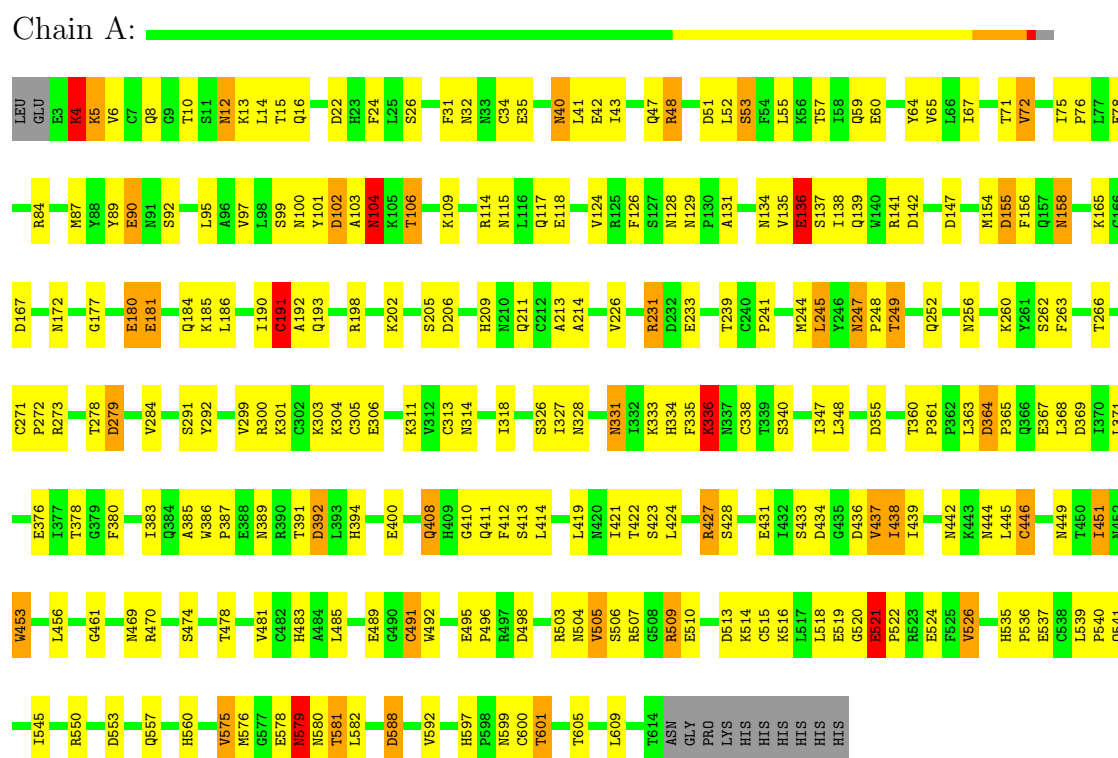
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	2	Total	C	N	O	0	0
			28	16	2	10		

3 Residue-property plots

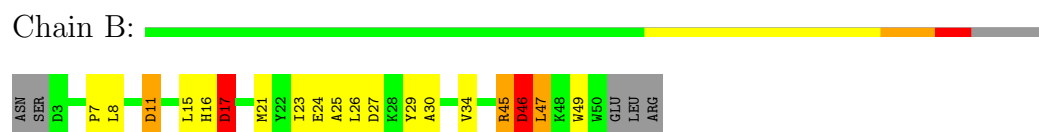
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

- Molecule 1: epidermal growth factor receptor



- Molecule 2: epidermal growth factor



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	119.17Å 103.66Å 101.49Å 90.00° 119.27° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.241 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5150	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, 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	0.85	4/4688 (0.1%)	0.98	22/6365 (0.3%)
2	B	0.57	0/386	0.92	3/523 (0.6%)
All	All	0.83	4/5074 (0.1%)	0.97	25/6888 (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	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	LYS	C-N	-35.46	0.52	1.34
1	A	4	LYS	CB-CG	-9.44	1.27	1.52
1	A	244	MET	CG-SD	7.65	2.01	1.81
1	A	90	GLU	CD-OE2	6.72	1.33	1.25

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	LYS	O-C-N	17.58	150.83	122.70
1	A	4	LYS	CA-C-N	-15.53	83.04	117.20
1	A	4	LYS	CB-CG-CD	-10.81	83.50	111.60
1	A	4	LYS	CA-CB-CG	10.07	135.56	113.40
1	A	142	ASP	CB-CG-OD2	8.02	125.52	118.30
1	A	4	LYS	C-N-CA	-7.68	102.50	121.70
1	A	434	ASP	CB-CG-OD2	6.80	124.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	102	ASP	CB-CG-OD2	6.61	124.25	118.30
1	A	22	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	355	ASP	CB-CG-OD2	6.26	123.93	118.30
2	B	11	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	206	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	231	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	A	579	ASN	N-CA-C	5.94	127.05	111.00
1	A	155	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	364	ASP	CB-CG-OD2	5.68	123.41	118.30
1	A	491	CYS	CB-CA-C	-5.57	99.26	110.40
1	A	244	MET	CA-CB-CG	5.50	122.66	113.30
1	A	167	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	588	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	369	ASP	CB-CG-OD2	5.19	122.97	118.30
2	B	46	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	392	ASP	CB-CG-OD2	5.12	122.91	118.30
2	B	17	ASP	CB-CG-OD2	5.12	122.90	118.30
1	A	279	ASP	CB-CG-OD2	5.03	122.83	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	521	GLU	Peptide
1	A	578	GLU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4597	0	4316	166	0
2	B	377	0	328	10	0
3	A	70	0	65	13	0
4	A	78	0	68	0	0
5	A	28	0	25	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5150	0	4802	172	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 17.

All (172) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:516:LYS:HB3	1:A:520:GLY:HA3	1.33	1.05
1:A:576:MET:SD	3:A:5791:NAG:O3	2.15	1.05
1:A:576:MET:CG	3:A:5791:NAG:H4	2.05	0.86
1:A:256:ASN:HD21	3:A:5791:NAG:C6	1.89	0.85
1:A:541:GLN:HE22	1:A:557:GLN:HE21	1.24	0.84
1:A:209:HIS:HD2	1:A:211:GLN:H	1.26	0.83
1:A:576:MET:SD	3:A:5791:NAG:H4	2.19	0.82
1:A:245:LEU:HB3	1:A:256:ASN:HB2	1.61	0.82
1:A:516:LYS:CB	1:A:520:GLY:HA3	2.10	0.82
1:A:100:ASN:HD22	1:A:129:ASN:ND2	1.76	0.82
2:B:17:ASP:HB3	2:B:34:VAL:HG21	1.63	0.80
1:A:256:ASN:HD21	3:A:5791:NAG:H62	1.47	0.79
1:A:51:ASP:OD1	1:A:53:SER:HB2	1.82	0.79
1:A:483:HIS:HD2	1:A:485:LEU:H	1.37	0.72
1:A:213:ALA:HB3	1:A:226:VAL:HG12	1.71	0.71
1:A:99:SER:HA	1:A:128:ASN:O	1.91	0.70
1:A:514:LYS:NZ	1:A:518:LEU:H	1.90	0.70
1:A:521:GLU:HB2	1:A:522:PRO:CD	2.23	0.68
1:A:326:SER:HB3	1:A:348:LEU:HG	1.74	0.68
1:A:48:ARG:HG2	1:A:48:ARG:HH11	1.58	0.68
1:A:439:ILE:HG22	1:A:469:ASN:HD21	1.57	0.68
1:A:34:CYS:O	1:A:57:THR:HG22	1.94	0.67
1:A:101:TYR:HA	1:A:106:THR:O	1.95	0.67
1:A:136:GLU:HG2	1:A:137:SER:N	2.09	0.66
1:A:521:GLU:CB	1:A:522:PRO:CD	2.74	0.66
1:A:247:ASN:C	1:A:247:ASN:HD22	1.99	0.65
1:A:541:GLN:HE22	1:A:557:GLN:NE2	1.94	0.65
1:A:421:ILE:HD12	1:A:445:LEU:HD13	1.78	0.65
1:A:134:ASN:HD22	1:A:177:GLY:HA2	1.60	0.65
1:A:256:ASN:ND2	3:A:5791:NAG:H62	2.13	0.64
1:A:600:CYS:O	1:A:601:THR:HB	1.98	0.63
1:A:537:GLU:OE1	1:A:560:HIS:HD2	1.80	0.63
1:A:180:GLU:HG2	1:A:181:GLU:N	2.14	0.63
1:A:100:ASN:HD22	1:A:129:ASN:HD21	1.46	0.63
1:A:576:MET:SD	3:A:5791:NAG:C3	2.88	0.62

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:333:LYS:O	1:A:336:LYS:HG2	1.99	0.62
1:A:24:PHE:HE1	1:A:52:LEU:HD23	1.65	0.61
1:A:193:GLN:HA	1:A:193:GLN:OE1	2.00	0.61
1:A:535:HIS:HD2	1:A:537:GLU:H	1.48	0.61
1:A:241:PRO:HG2	1:A:260:LYS:HB2	1.81	0.61
1:A:576:MET:SD	3:A:5791:NAG:C4	2.88	0.60
1:A:134:ASN:ND2	1:A:177:GLY:HA2	2.17	0.59
1:A:48:ARG:HG2	1:A:48:ARG:NH1	2.17	0.59
1:A:328:ASN:HB2	1:A:331:ASN:HB2	1.85	0.59
1:A:516:LYS:HB3	1:A:520:GLY:CA	2.20	0.59
1:A:95:LEU:HD23	1:A:124:VAL:HG13	1.83	0.59
1:A:247:ASN:HD21	1:A:249:THR:HB	1.67	0.58
1:A:576:MET:HG2	3:A:5791:NAG:H4	1.82	0.58
1:A:328:ASN:H	1:A:331:ASN:CB	2.16	0.58
1:A:12:ASN:N	1:A:42:GLU:OE1	2.37	0.58
1:A:541:GLN:NE2	1:A:557:GLN:HE21	2.00	0.57
1:A:109:LYS:HA	1:A:131:ALA:O	2.05	0.57
1:A:453:TRP:HA	1:A:456:LEU:HD12	1.86	0.57
1:A:581:THR:HG22	1:A:582:LEU:H	1.70	0.57
1:A:521:GLU:HB2	1:A:522:PRO:HD2	1.85	0.56
1:A:247:ASN:HD22	1:A:249:THR:H	1.53	0.56
1:A:256:ASN:ND2	3:A:5791:NAG:C6	2.64	0.56
1:A:32:ASN:HD21	3:A:625:NAG:H2	1.71	0.56
1:A:347:ILE:HD12	1:A:383:ILE:HG12	1.87	0.55
1:A:451:ILE:HD12	1:A:491:CYS:O	2.05	0.55
1:A:233:GLU:OE1	1:A:233:GLU:HA	2.05	0.55
1:A:509:ARG:HG3	1:A:509:ARG:NH1	2.22	0.54
1:A:483:HIS:CD2	1:A:485:LEU:H	2.21	0.54
1:A:521:GLU:CB	1:A:522:PRO:HD3	2.38	0.54
1:A:588:ASP:OD1	1:A:592:VAL:N	2.41	0.53
1:A:516:LYS:CG	1:A:520:GLY:HA3	2.38	0.53
1:A:414:LEU:HB3	1:A:437:VAL:HG22	1.90	0.53
1:A:158:ASN:H	1:A:158:ASN:HD22	1.56	0.53
1:A:496:PRO:HB2	1:A:510:GLU:HG2	1.92	0.52
1:A:516:LYS:HD3	1:A:521:GLU:H	1.73	0.52
2:B:46:ASP:O	2:B:47:LEU:HB2	2.09	0.52
1:A:504:ASN:OD1	3:A:5041:NAG:O5	2.25	0.52
1:A:41:LEU:HD21	1:A:43:ILE:HD11	1.90	0.52
1:A:135:VAL:HA	1:A:138:ILE:CD1	2.39	0.51
1:A:539:LEU:HD12	1:A:540:PRO:HD2	1.92	0.51
1:A:247:ASN:ND2	1:A:249:THR:H	2.08	0.51
1:A:576:MET:CE	3:A:5791:NAG:O3	2.59	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:495:GLU:HB2	1:A:498:ASP:OD2	2.11	0.51
1:A:385:ALA:O	1:A:386:TRP:HB2	2.11	0.50
1:A:35:GLU:HG2	1:A:59:GLN:HE21	1.77	0.50
1:A:209:HIS:CD2	1:A:211:GLN:H	2.18	0.50
1:A:535:HIS:HD2	1:A:537:GLU:N	2.09	0.50
1:A:311:LYS:HB3	1:A:338:CYS:HA	1.93	0.49
1:A:365:PRO:HB3	1:A:387:PRO:CG	2.43	0.49
1:A:514:LYS:HZ1	1:A:518:LEU:H	1.56	0.49
1:A:48:ARG:CG	1:A:48:ARG:HH11	2.25	0.49
1:A:507:ARG:NH2	1:A:516:LYS:HG3	2.28	0.49
1:A:24:PHE:HE1	1:A:52:LEU:CD2	2.25	0.48
2:B:24:GLU:O	2:B:26:LEU:O	2.30	0.48
1:A:41:LEU:HD23	1:A:65:VAL:HG13	1.94	0.48
1:A:263:PHE:O	1:A:266:THR:HB	2.12	0.48
1:A:421:ILE:CD1	1:A:445:LEU:HD13	2.43	0.48
1:A:78:GLU:OE1	1:A:114:ARG:NH2	2.46	0.48
1:A:364:ASP:HB3	1:A:367:GLU:HG3	1.95	0.48
1:A:291:SER:HB3	1:A:303:LYS:O	2.14	0.48
1:A:192:ALA:O	1:A:193:GLN:C	2.52	0.47
1:A:514:LYS:HD3	1:A:515:CYS:O	2.14	0.47
1:A:328:ASN:H	1:A:331:ASN:HB2	1.78	0.47
1:A:516:LYS:HD3	1:A:521:GLU:N	2.28	0.47
1:A:509:ARG:HG3	1:A:509:ARG:HH11	1.80	0.47
1:A:78:GLU:OE1	1:A:114:ARG:NH1	2.48	0.47
1:A:47:GLN:O	1:A:72:VAL:HG13	2.15	0.47
1:A:380:PHE:HB2	1:A:413:SER:O	2.15	0.47
1:A:360:THR:HA	1:A:361:PRO:HD2	1.81	0.47
1:A:446:CYS:SG	1:A:470:ARG:HD3	2.54	0.47
1:A:514:LYS:HZ3	1:A:518:LEU:H	1.63	0.47
1:A:509:ARG:HH11	1:A:509:ARG:CG	2.28	0.47
1:A:14:LEU:CD1	2:B:23:ILE:HD13	2.45	0.47
1:A:515:CYS:SG	1:A:526:VAL:HG13	2.55	0.46
1:A:575:VAL:O	1:A:582:LEU:HA	2.15	0.46
1:A:16:GLN:HB3	2:B:21:MET:CE	2.45	0.46
1:A:521:GLU:HB3	1:A:522:PRO:HD3	1.97	0.46
1:A:184:GLN:HG2	1:A:186:LEU:HD23	1.97	0.46
1:A:247:ASN:HA	1:A:248:PRO:HD3	1.78	0.46
1:A:600:CYS:O	1:A:601:THR:CB	2.64	0.46
1:A:67:ILE:HB	1:A:97:VAL:HG22	1.98	0.46
1:A:60:GLU:OE2	1:A:84:ARG:NH2	2.49	0.46
1:A:52:LEU:O	1:A:76:PRO:HG2	2.16	0.46
1:A:438:ILE:O	1:A:438:ILE:HG22	2.14	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:57:THR:O	1:A:57:THR:HG22	2.16	0.46
1:A:411:GLN:HG3	1:A:436:ASP:OD2	2.16	0.46
1:A:190:ILE:O	1:A:190:ILE:HD12	2.17	0.45
1:A:10:THR:OG1	1:A:12:ASN:ND2	2.50	0.45
1:A:100:ASN:HD22	1:A:129:ASN:HD22	1.60	0.45
1:A:597:HIS:CD2	1:A:599:ASN:H	2.34	0.45
1:A:516:LYS:N	1:A:524:GLU:OE1	2.40	0.45
1:A:57:THR:O	1:A:57:THR:CG2	2.64	0.45
1:A:505:VAL:HG11	1:A:515:CYS:SG	2.56	0.45
1:A:328:ASN:H	1:A:331:ASN:HB3	1.79	0.45
1:A:16:GLN:HB3	2:B:21:MET:HE1	1.99	0.45
1:A:135:VAL:HA	1:A:138:ILE:HD13	1.99	0.45
1:A:597:HIS:CD2	1:A:599:ASN:HB2	2.52	0.44
1:A:444:ASN:HA	1:A:470:ARG:HD2	1.99	0.44
1:A:117:GLN:HB2	1:A:214:ALA:HB1	1.98	0.44
1:A:412:PHE:CE2	1:A:438:ILE:HG13	2.53	0.44
1:A:408:GLN:C	1:A:410:GLY:H	2.20	0.44
1:A:135:VAL:O	1:A:136:GLU:C	2.56	0.44
1:A:419:LEU:HB2	1:A:442:ASN:OD1	2.18	0.44
1:A:515:CYS:SG	1:A:526:VAL:CG1	3.07	0.43
1:A:333:LYS:C	1:A:335:PHE:H	2.21	0.43
1:A:126:PHE:HD1	1:A:154:MET:CE	2.31	0.43
1:A:118:GLU:HG3	1:A:198:ARG:NH2	2.33	0.43
1:A:424:LEU:O	1:A:492:TRP:O	2.36	0.43
1:A:400:GLU:HA	1:A:428:SER:O	2.18	0.43
1:A:365:PRO:HB3	1:A:387:PRO:HG3	2.00	0.43
1:A:31:PHE:CZ	1:A:41:LEU:HD12	2.54	0.43
1:A:12:ASN:O	1:A:15:THR:HB	2.19	0.43
2:B:16:HIS:CE1	2:B:45:ARG:HH21	2.36	0.43
1:A:75:ILE:HA	1:A:76:PRO:HD3	1.79	0.42
2:B:7:PRO:HG2	2:B:29:TYR:CG	2.53	0.42
1:A:427:ARG:H	1:A:427:ARG:HG2	1.69	0.42
1:A:271:CYS:HA	1:A:272:PRO:HD3	1.84	0.42
1:A:581:THR:HG22	1:A:582:LEU:N	2.34	0.42
1:A:78:GLU:O	1:A:115:ASN:ND2	2.49	0.42
1:A:5:LYS:HD2	1:A:6:VAL:N	2.34	0.42
1:A:516:LYS:HD3	1:A:520:GLY:HA3	2.02	0.42
1:A:333:LYS:O	1:A:335:PHE:N	2.53	0.42
1:A:89:TYR:CE2	1:A:90:GLU:HG3	2.56	0.41
1:A:40:ASN:HB3	1:A:64:TYR:O	2.20	0.41
1:A:138:ILE:CG2	1:A:139:GLN:N	2.83	0.41
1:A:408:GLN:C	1:A:410:GLY:N	2.74	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:102:ASP:O	1:A:104:ASN:N	2.53	0.41
1:A:71:THR:HG22	1:A:71:THR:O	2.21	0.41
2:B:25:ALA:C	2:B:26:LEU:O	2.57	0.41
1:A:78:GLU:OE1	1:A:114:ARG:CZ	2.69	0.41
1:A:483:HIS:HD2	1:A:485:LEU:N	2.09	0.41
1:A:191:CYS:HB3	1:A:192:ALA:H	1.65	0.41
1:A:35:GLU:CG	1:A:59:GLN:HE21	2.34	0.41
1:A:41:LEU:HD21	1:A:43:ILE:CD1	2.51	0.40
1:A:15:THR:HA	2:B:30:ALA:HB1	2.03	0.40
1:A:503:ARG:HG3	1:A:504:ASN:N	2.35	0.40
1:A:516:LYS:NZ	1:A:521:GLU:HG3	2.37	0.40

There are no symmetry-related clashes.

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	610/624 (98%)	514 (84%)	73 (12%)	23 (4%)	5	15
2	B	46/53 (87%)	37 (80%)	9 (20%)	0	100	100
All	All	656/677 (97%)	551 (84%)	82 (12%)	23 (4%)	6	18

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	5	LYS
1	A	104	ASN
1	A	191	CYS
1	A	521	GLU
1	A	579	ASN
1	A	172	ASN
1	A	273	ARG
1	A	314	ASN

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Mol	Chain	Res	Type
1	A	453	TRP
1	A	580	ASN
1	A	13	LYS
1	A	55	LEU
1	A	136	GLU
1	A	334	HIS
1	A	92	SER
1	A	103	ALA
1	A	389	ASN
1	A	601	THR
1	A	336	LYS
1	A	292	TYR
1	A	461	GLY
1	A	536	PRO

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	507/545 (93%)	424 (84%)	83 (16%)	3	10
2	B	40/47 (85%)	31 (78%)	9 (22%)	1	3
All	All	547/592 (92%)	455 (83%)	92 (17%)	3	9

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	8	GLN
1	A	12	ASN
1	A	26	SER
1	A	40	ASN
1	A	48	ARG
1	A	53	SER
1	A	72	VAL
1	A	87	MET
1	A	104	ASN
1	A	106	THR

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Mol	Chain	Res	Type
1	A	136	GLU
1	A	141	ARG
1	A	147	ASP
1	A	155	ASP
1	A	156	PHE
1	A	158	ASN
1	A	165	LYS
1	A	180	GLU
1	A	181	GLU
1	A	185	LYS
1	A	191	CYS
1	A	202	LYS
1	A	205	SER
1	A	231	ARG
1	A	239	THR
1	A	245	LEU
1	A	247	ASN
1	A	249	THR
1	A	252	GLN
1	A	262	SER
1	A	278	THR
1	A	279	ASP
1	A	284	VAL
1	A	299	VAL
1	A	300	ARG
1	A	301	LYS
1	A	304	LYS
1	A	305	CYS
1	A	306	GLU
1	A	313	CYS
1	A	318	ILE
1	A	327	ILE
1	A	331	ASN
1	A	336	LYS
1	A	340	SER
1	A	363	LEU
1	A	368	LEU
1	A	371	LEU
1	A	376	GLU
1	A	378	THR
1	A	391	THR
1	A	392	ASP

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Mol	Chain	Res	Type
1	A	394	HIS
1	A	408	GLN
1	A	422	THR
1	A	423	SER
1	A	427	ARG
1	A	431	GLU
1	A	433	SER
1	A	437	VAL
1	A	438	ILE
1	A	446	CYS
1	A	449	ASN
1	A	451	ILE
1	A	474	SER
1	A	478	THR
1	A	481	VAL
1	A	489	GLU
1	A	505	VAL
1	A	506	SER
1	A	509	ARG
1	A	513	ASP
1	A	519	GLU
1	A	526	VAL
1	A	545	ILE
1	A	550	ARG
1	A	553	ASP
1	A	575	VAL
1	A	579	ASN
1	A	581	THR
1	A	605	THR
1	A	609	LEU
2	B	8	LEU
2	B	11	ASP
2	B	15	LEU
2	B	17	ASP
2	B	27	ASP
2	B	45	ARG
2	B	46	ASP
2	B	47	LEU
2	B	49	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	12	ASN
1	A	59	GLN
1	A	79	ASN
1	A	81	GLN
1	A	104	ASN
1	A	128	ASN
1	A	129	ASN
1	A	134	ASN
1	A	158	ASN
1	A	209	HIS
1	A	210	ASN
1	A	247	ASN
1	A	480	GLN
1	A	483	HIS
1	A	535	HIS
1	A	557	GLN
1	A	560	HIS
1	A	597	HIS
1	A	599	ASN
2	B	16	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 carbohydrates 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
4	NAG	A	3281	1,4	12,14,15	0.59	0	15,19,21	1.37	3 (20%)
4	NAG	A	3282	4	12,14,15	0.71	0	15,19,21	1.45	3 (20%)
4	BMA	A	3283	4	10,11,12	0.71	0	11,15,17	1.28	1 (9%)
4	NAG	A	3371	1,4	12,14,15	0.64	0	15,19,21	1.36	3 (20%)
4	NAG	A	3372	4	12,14,15	0.62	0	15,19,21	0.96	0
4	BMA	A	3373	4	10,11,12	0.74	0	11,15,17	1.11	1 (9%)
5	NAG	A	5441	1,5	12,14,15	0.79	0	15,19,21	1.90	6 (40%)
5	NAG	A	5442	5	12,14,15	0.60	0	15,19,21	1.13	1 (6%)

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
4	NAG	A	3281	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3282	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3283	4	-	0/2/19/22	0/1/1/1
4	NAG	A	3371	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3372	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3373	4	-	0/2/19/22	0/1/1/1
5	NAG	A	5441	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	5442	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3373	BMA	O5-C5-C6	3.20	110.34	106.98
4	A	3282	NAG	C2-N2-C7	-3.05	117.98	123.09
5	A	5441	NAG	C3-C2-N2	-3.04	107.12	111.76
5	A	5441	NAG	O3-C3-C2	-2.94	102.92	109.09
5	A	5442	NAG	C3-C2-N2	-2.70	107.66	111.76
4	A	3281	NAG	O6-C6-C5	-2.55	102.59	111.36
5	A	5441	NAG	C6-C5-C4	-2.55	106.84	113.00
4	A	3283	BMA	O5-C5-C6	2.46	109.56	106.98
5	A	5441	NAG	O3-C3-C4	-2.42	104.92	110.35
5	A	5441	NAG	C2-N2-C7	-2.41	119.05	123.09
4	A	3371	NAG	C3-C2-N2	-2.39	108.12	111.76
4	A	3281	NAG	C3-C2-N2	-2.37	108.15	111.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3282	NAG	O4-C4-C3	-2.33	105.14	110.35
5	A	5441	NAG	C3-C4-C5	2.32	114.35	110.20
4	A	3371	NAG	C4-C3-C2	2.25	116.83	111.32
4	A	3282	NAG	O5-C5-C4	2.19	113.44	110.65
4	A	3371	NAG	C3-C4-C5	2.17	114.07	110.20
4	A	3281	NAG	O7-C7-C8	-2.14	117.86	122.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

5 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$
3	NAG	A	4201	1	12,14,15	0.75	0	15,19,21	1.66	2 (13%)
3	NAG	A	4202	-	12,14,15	0.64	0	15,19,21	1.66	2 (13%)
3	NAG	A	5041	1	12,14,15	0.47	0	15,19,21	1.39	3 (20%)
3	NAG	A	5791	1	12,14,15	1.12	1 (8%)	15,19,21	1.35	3 (20%)
3	NAG	A	625	-	12,14,15	0.66	0	15,19,21	1.28	1 (6%)

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
3	NAG	A	4201	1	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	A	4202	-	-	0/6/23/26	0/1/1/1
3	NAG	A	5041	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	5791	1	-	0/6/23/26	0/1/1/1
3	NAG	A	625	-	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	5791	NAG	O5-C5	-3.28	1.39	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4201	NAG	O5-C5-C6	4.31	111.50	106.98
3	A	4202	NAG	C3-C4-C5	4.10	117.53	110.20
3	A	625	NAG	O5-C5-C6	4.05	111.24	106.98
3	A	4202	NAG	O5-C5-C4	3.56	115.17	110.65
3	A	4201	NAG	O5-C5-C4	-3.19	106.61	110.65
3	A	5791	NAG	O5-C5-C4	-3.12	106.69	110.65
3	A	5041	NAG	O5-C5-C6	3.10	110.23	106.98
3	A	5791	NAG	C3-C2-N2	-2.82	107.47	111.76
3	A	5041	NAG	C6-C5-C4	-2.38	107.25	113.00
3	A	5041	NAG	O5-C5-C4	2.10	113.31	110.65
3	A	5791	NAG	O6-C6-C5	-2.03	104.37	111.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	4201	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.