



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 20, 2018 – 12:31 am 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 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

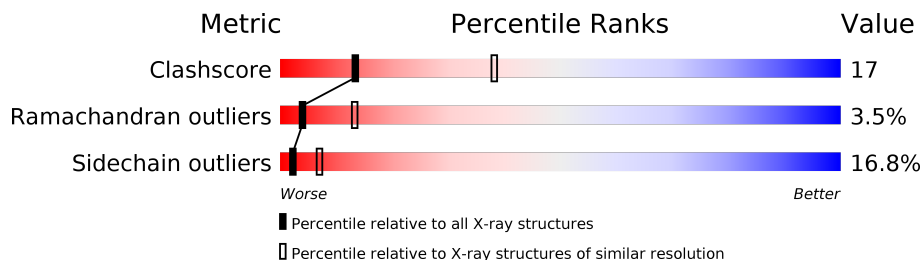
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	122078	3207 (2.80-2.80)
Ramachandran outliers	120005	3156 (2.80-2.80)
Sidechain outliers	119972	3158 (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. 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.

Note EDS was not executed.

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

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	4201	X	-	-	-
3	NAG	A	5791	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5150 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.

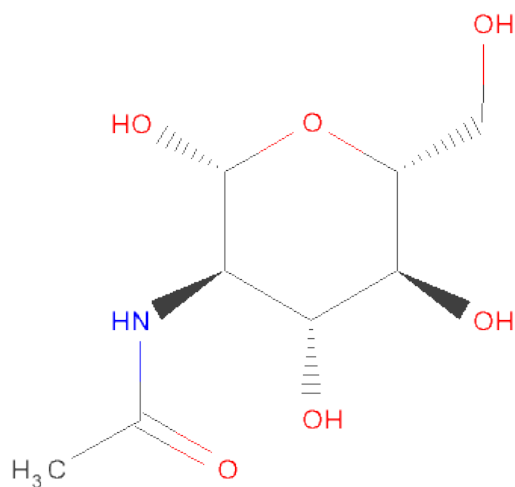
- Molecule 1 is a protein called epidermal growth factor receptor.

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



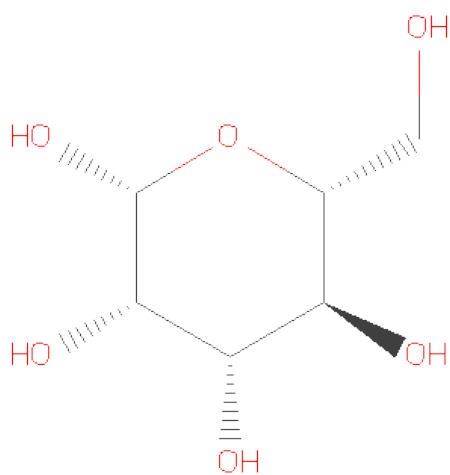
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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		
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		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



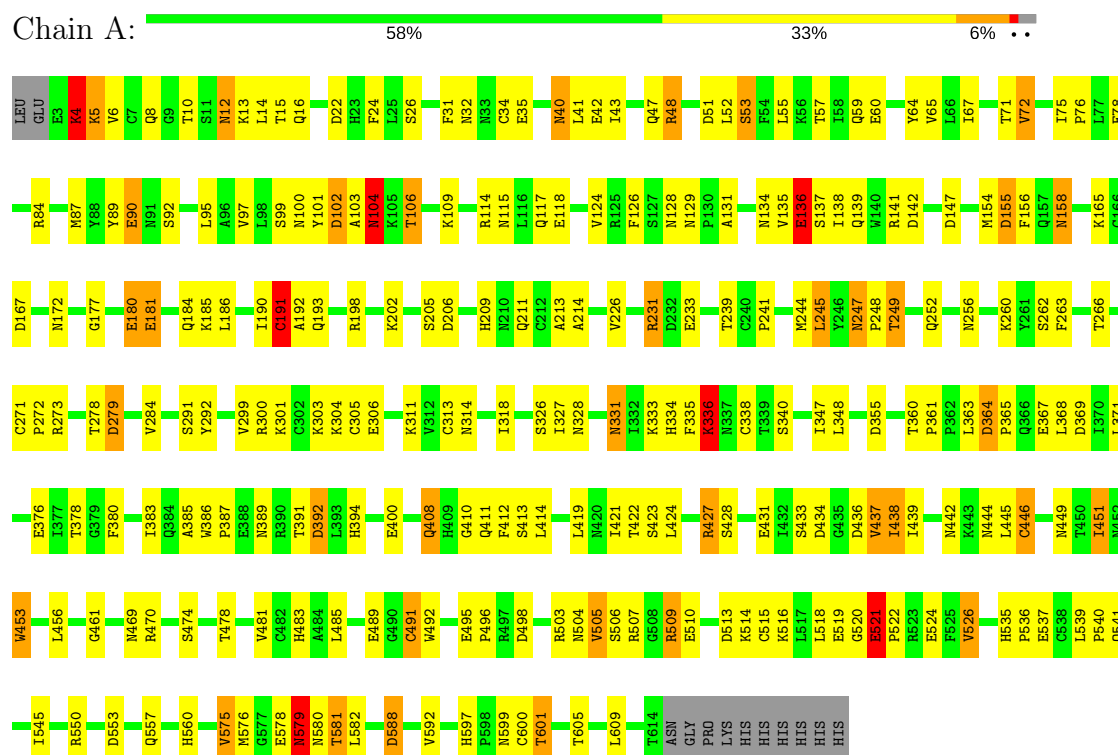
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		

3 Residue-property plots

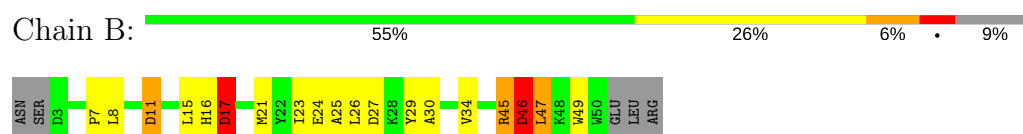
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

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 is therefore 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 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	4597	0	4316	166	0
2	B	377	0	328	10	0
3	A	154	0	138	13	0
4	A	22	0	20	0	0
All	All	5150	0	4802	172	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 17.

All (172) 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: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:100:ASN:HD22	1:A:129:ASN:ND2	1.76	0.82
1:A:516:LYS:CB	1:A:520:GLY:HA3	2.10	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:421:ILE:HD12	1:A:445:LEU:HD13	1.78	0.65
1:A:541:GLN:HE22	1:A:557:GLN:NE2	1.94	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:333:LYS:O	1:A:336:LYS:HG2	1.99	0.62
1:A:576:MET:SD	3:A:5791:NAG:C3	2.88	0.62
1:A:193:GLN:HA	1:A:193:GLN:OE1	2.00	0.61
1:A:24:PHE:HE1	1:A:52:LEU:HD23	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:PRO:HG2	1:A:260:LYS:HB2	1.81	0.61
1:A:535:HIS:HD2	1:A:537:GLU:H	1.48	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:328:ASN:HB2	1:A:331:ASN:HB2	1.85	0.59
1:A:48:ARG:HG2	1:A:48:ARG:NH1	2.17	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:247:ASN:HD22	1:A:249:THR:H	1.53	0.56
1:A:521:GLU:HB2	1:A:522:PRO:HD2	1.85	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:233:GLU:OE1	1:A:233:GLU:HA	2.05	0.55
1:A:451:ILE:HD12	1:A:491:CYS:O	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
1:A:504:ASN:OD1	3:A:5041:NAG:O5	2.25	0.52
2:B:46:ASP:O	2:B:47:LEU:HB2	2.09	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:263:PHE:O	1:A:266:THR:HB	2.12	0.48
1:A:41:LEU:HD23	1:A:65:VAL:HG13	1.94	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:328:ASN:H	1:A:331:ASN:HB2	1.78	0.47
1:A:514:LYS:HD3	1:A:515:CYS:O	2.14	0.47
1:A:516:LYS:HD3	1:A:521:GLU:N	2.28	0.47
1:A:78:GLU:OE1	1:A:114:ARG:NH1	2.48	0.47
1:A:509:ARG:HG3	1:A:509:ARG:HH11	1.80	0.47
1:A:47:GLN:O	1:A:72:VAL:HG13	2.15	0.47
1:A:360:THR:HA	1:A:361:PRO:HD2	1.81	0.47
1:A:380:PHE:HB2	1:A:413:SER:O	2.15	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:14:LEU:CD1	2:B:23:ILE:HD13	2.45	0.47
1:A:509:ARG:HH11	1:A:509:ARG:CG	2.28	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:184:GLN:HG2	1:A:186:LEU:HD23	1.97	0.46
1:A:521:GLU:HB3	1:A:522:PRO:HD3	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
1:A:411:GLN:HG3	1:A:436:ASP:OD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:O	1:A:57:THR:HG22	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:117:GLN:HB2	1:A:214:ALA:HB1	1.98	0.44
1:A:444:ASN:HA	1:A:470:ARG:HD2	1.99	0.44
1:A:408:GLN:C	1:A:410:GLY:H	2.20	0.44
1:A:412:PHE:CE2	1:A:438:ILE:HG13	2.53	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:126:PHE:HD1	1:A:154:MET:CE	2.31	0.43
1:A:333:LYS:C	1:A:335:PHE:H	2.21	0.43
1:A:515:CYS:SG	1:A:526:VAL:CG1	3.07	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:5:LYS:HD2	1:A:6:VAL:N	2.34	0.42
1:A:78:GLU:O	1:A:115:ASN:ND2	2.49	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:102:ASP:O	1:A:104:ASN:N	2.53	0.41
1:A:138:ILE:CG2	1:A:139:GLN:N	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:408:GLN:C	1:A:410:GLY:N	2.74	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: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:483:HIS:HD2	1:A:485:LEU:N	2.09	0.41
1:A:41:LEU:HD21	1:A:43:ILE:CD1	2.51	0.40
1:A:503:ARG:HG3	1:A:504:ASN:N	2.35	0.40
1:A:15:THR:HA	2:B:30:ALA:HB1	2.03	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 [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	610/624 (98%)	514 (84%)	73 (12%)	23 (4%)	3	11
2	B	46/53 (87%)	37 (80%)	9 (20%)	0	100	100
All	All	656/677 (97%)	551 (84%)	82 (12%)	23 (4%)	4	13

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

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Mol	Chain	Res	Type
1	A	273	ARG
1	A	314	ASN
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%)	2	8
2	B	40/47 (85%)	31 (78%)	9 (22%)	1	3
All	All	547/592 (92%)	455 (83%)	92 (17%)	2	7

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

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Mol	Chain	Res	Type
1	A	72	VAL
1	A	87	MET
1	A	104	ASN
1	A	106	THR
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

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Mol	Chain	Res	Type
1	A	376	GLU
1	A	378	THR
1	A	391	THR
1	A	392	ASP
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

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Mol	Chain	Res	Type
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 [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 carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 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	3281	1,3	14,14,15	0.71	1 (7%)	17,19,21	1.56	4 (23%)
3	NAG	A	3282	3,4	14,14,15	0.64	0	17,19,21	1.60	4 (23%)
4	BMA	A	3283	3	11,11,12	0.67	0	15,15,17	1.26	1 (6%)
3	NAG	A	3371	1,3	14,14,15	0.67	0	17,19,21	1.36	3 (17%)
3	NAG	A	3372	3,4	14,14,15	0.55	0	17,19,21	1.24	3 (17%)
4	BMA	A	3373	3	11,11,12	0.70	0	15,15,17	0.78	1 (6%)
3	NAG	A	4201	1	14,14,15	0.66	0	17,19,21	1.29	1 (5%)
3	NAG	A	4202	-	14,14,15	0.57	0	17,19,21	1.82	4 (23%)
3	NAG	A	5041	1	14,14,15	0.57	0	17,19,21	2.32	2 (11%)
3	NAG	A	5441	1,3	14,14,15	0.68	0	17,19,21	2.61	8 (47%)
3	NAG	A	5442	3	14,14,15	0.57	0	17,19,21	1.35	1 (5%)
3	NAG	A	5791	1	14,14,15	0.88	0	17,19,21	1.73	1 (5%)
3	NAG	A	625	-	14,14,15	0.64	0	17,19,21	1.09	2 (11%)

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	3281	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3282	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	3283	3	-	0/2/19/22	0/1/1/1
3	NAG	A	3371	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	3372	3,4	-	0/6/23/26	0/1/1/1
4	BMA	A	3373	3	-	0/2/19/22	0/1/1/1
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	5041	1	-	0/6/23/26	0/1/1/1
3	NAG	A	5441	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	5442	3	-	0/6/23/26	0/1/1/1
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	3281	NAG	C1-C2	2.01	1.55	1.52

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	5791	NAG	C1-O5-C5	-5.96	103.99	112.19
3	A	4202	NAG	O5-C1-C2	-3.76	106.33	111.52
3	A	3282	NAG	C2-N2-C7	-3.40	117.98	122.94
3	A	3282	NAG	O5-C1-C2	-3.15	107.17	111.52
3	A	5441	NAG	O3-C3-C2	-3.02	102.92	109.39
3	A	625	NAG	O5-C1-C2	-2.82	107.62	111.52
3	A	5441	NAG	C2-N2-C7	-2.67	119.05	122.94
3	A	5441	NAG	C6-C5-C4	-2.60	106.84	112.99
3	A	3281	NAG	O6-C6-C5	-2.49	102.59	111.29
3	A	5041	NAG	C6-C5-C4	-2.43	107.25	112.99
3	A	3281	NAG	O7-C7-C8	-2.33	117.86	122.07
3	A	5441	NAG	O3-C3-C4	-2.32	104.92	110.34
3	A	3281	NAG	O5-C1-C2	-2.31	108.33	111.52
3	A	3372	NAG	C4-C3-C2	-2.27	107.70	111.02
3	A	3282	NAG	O4-C4-C3	-2.23	105.14	110.34
3	A	3372	NAG	O5-C1-C2	-2.12	108.59	111.52
3	A	3371	NAG	O3-C3-C2	-2.09	104.90	109.39
4	A	3373	BMA	O5-C5-C6	2.01	110.34	107.15
3	A	5441	NAG	O4-C4-C5	2.02	114.37	109.31
3	A	3371	NAG	C3-C4-C5	2.14	114.07	110.24
3	A	5441	NAG	C3-C4-C5	2.29	114.35	110.24
3	A	5441	NAG	C1-C2-N2	2.38	114.55	110.49
3	A	3372	NAG	C1-C2-N2	2.46	114.68	110.49
3	A	4202	NAG	C1-O5-C5	2.48	115.60	112.19
3	A	625	NAG	O5-C5-C6	2.58	111.24	107.15
3	A	4202	NAG	C4-C3-C2	2.60	114.83	111.02
3	A	3282	NAG	C4-C3-C2	2.67	114.93	111.02
3	A	4201	NAG	O5-C5-C6	2.75	111.50	107.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3283	BMA	C1-C2-C3	3.26	113.79	109.66
3	A	3281	NAG	C1-O5-C5	3.30	116.72	112.19
3	A	3371	NAG	C4-C3-C2	3.96	116.83	111.02
3	A	4202	NAG	C3-C4-C5	4.08	117.53	110.24
3	A	5442	NAG	C1-O5-C5	4.43	118.28	112.19
3	A	5441	NAG	C1-O5-C5	8.09	123.32	112.19
3	A	5041	NAG	C1-O5-C5	8.17	123.43	112.19

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.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5041	NAG	1	0
3	A	5791	NAG	11	0
3	A	625	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	4:LYS	C	5:LYS	N	0.52

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.