



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:33 AM GMT

PDB ID : 3I2T
Title : Crystal structure of the unliganded Drosophila Epidermal Growth Factor Receptor ectodomain
Authors : Alvarado, D.; Klein, D.E.; Lemmon, M.A.
Deposited on : 2009-06-29
Resolution : 2.70 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>

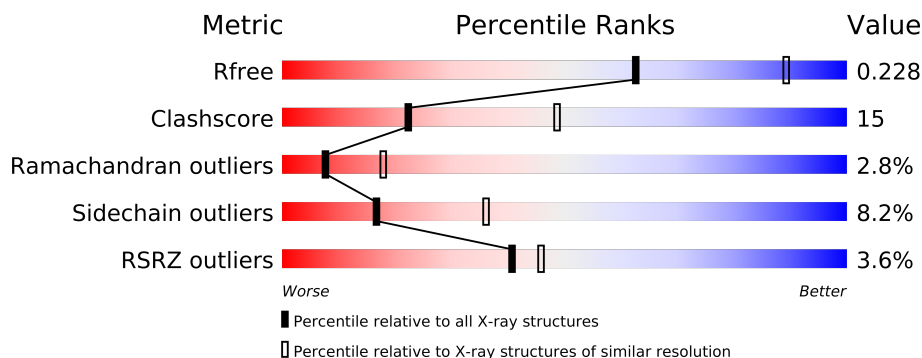
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
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 2.70 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}	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (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 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.

Mol	Chain	Length	Quality of chain
1	A	551	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4381 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, isoform A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	542	Total	C	N	O	S	0	0	0
			4203	2617	737	798	51			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-4	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-3	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-2	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-1	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	0	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	2	ILE	VAL	SEE REMARK 999	UNP Q8MLW0
A	493	ASN	THR	SEE REMARK 999	UNP Q8MLW0

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

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-4	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-3	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-2	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-1	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	0	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	2	ILE	VAL	SEE REMARK 999	UNP Q8MLW0
A	493	ASN	THR	SEE REMARK 999	UNP Q8MLW0

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-4	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-3	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-2	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-1	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	0	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	2	ILE	VAL	SEE REMARK 999	UNP Q8MLW0
A	493	ASN	THR	SEE REMARK 999	UNP Q8MLW0

- Molecule 4 is a polymer of unknown type called SUGAR (3-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		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-4	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-3	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-2	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-1	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	0	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	2	ILE	VAL	SEE REMARK 999	UNP Q8MLW0
A	493	ASN	THR	SEE REMARK 999	UNP Q8MLW0
A	-5	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-4	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-3	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-2	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-1	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	0	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	2	ILE	VAL	SEE REMARK 999	UNP Q8MLW0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ASN	THR	SEE REMARK 999	UNP Q8MLW0

- Molecule 5 is a polymer of unknown type called SUGAR (3-MER).

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

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-4	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-3	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-2	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	-1	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	0	HIS	-	EXPRESSION TAG	UNP Q8MLW0
A	2	ILE	VAL	SEE REMARK 999	UNP Q8MLW0
A	493	ASN	THR	SEE REMARK 999	UNP Q8MLW0

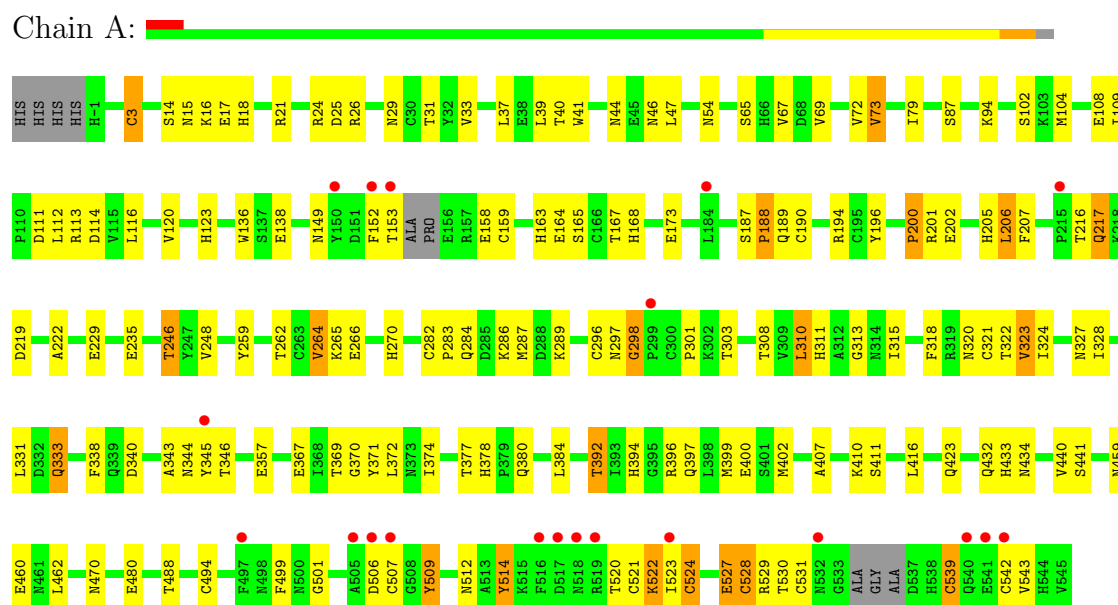
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	5	Total	O	0	0
			5	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 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 ($\text{RSRZ} > 2$). 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: Epidermal growth factor receptor, isoform A



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	74.38Å 174.80Å 161.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.68 – 2.70 36.68 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (36.68-2.70) 99.2 (36.68-2.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.68Å)	Xtriage
Refinement program	REFMAC 5.5.0044	Depositor
R, R_{free}	0.224 , 0.264 0.227 , 0.228	Depositor DCC
R_{free} test set	1481 reflections (5.10%)	DCC
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.030	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 35.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 29077 reflections (0.007%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4381	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 5.19% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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, NDG

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	0.65	2/4298 (0.0%)	0.73	3/5826 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	3	CYS	CB-SG	-9.53	1.66	1.82
1	A	159	CYS	CB-SG	-6.49	1.71	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	3	CYS	CB-CA-C	-7.32	95.76	110.40
1	A	494	CYS	CA-CB-SG	-6.96	101.47	114.00
1	A	26	ARG	NE-CZ-NH2	-5.82	117.39	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4203	0	3924	126	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	28	0	25	5	0
3	A	28	0	25	2	0
4	A	78	0	68	0	0
5	A	39	0	34	4	0
6	A	5	0	0	0	0
All	All	4381	0	4076	126	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 15.

All (126) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:320:ASN:ND2	3:A:3200:NAG:C1	1.71	1.47
1:A:470:ASN:HD21	5:A:4700:NDG:C1	1.28	1.44
1:A:29:ASN:ND2	2:A:546:NDG:C1	1.88	1.36
1:A:470:ASN:ND2	5:A:4700:NDG:C1	1.90	1.32
1:A:470:ASN:HD21	5:A:4700:NDG:C2	1.65	1.09
1:A:114:ASP:OD2	1:A:116:LEU:HD23	1.59	1.02
1:A:205:HIS:ND1	1:A:216:THR:HG23	1.76	0.99
1:A:311:HIS:HD2	1:A:313:GLY:H	1.10	0.96
1:A:29:ASN:HD21	2:A:546:NDG:C1	1.60	0.92
1:A:378:HIS:HD2	1:A:380:GLN:H	1.21	0.87
1:A:15:ASN:HD22	1:A:18:HIS:H	1.22	0.86
1:A:531:CYS:CB	1:A:539:CYS:HB3	2.06	0.85
1:A:530:THR:O	1:A:539:CYS:HB2	1.75	0.85
1:A:205:HIS:CD2	1:A:206:LEU:H	1.97	0.83
1:A:303:THR:HG22	1:A:323:VAL:HG13	1.60	0.81
1:A:399:MET:HE1	1:A:407:ALA:HB3	1.62	0.80
1:A:327:ASN:HD22	1:A:371:TYR:H	1.27	0.78
1:A:188:PRO:C	1:A:190:CYS:H	1.86	0.78
1:A:200:PRO:O	1:A:202:GLU:N	2.18	0.76
1:A:399:MET:CE	1:A:407:ALA:HB3	2.16	0.76
1:A:246:THR:HG22	1:A:248:VAL:HG23	1.67	0.75
1:A:378:HIS:CD2	1:A:380:GLN:H	2.04	0.75
1:A:114:ASP:OD2	1:A:116:LEU:CD2	2.33	0.74
1:A:459:ASN:HD22	1:A:460:GLU:HG3	1.52	0.73
1:A:531:CYS:HB2	1:A:539:CYS:HB3	1.69	0.73
1:A:111:ASP:OD1	1:A:113:ARG:NH1	2.21	0.72
1:A:163:HIS:HD2	1:A:165:SER:OG	1.73	0.72
1:A:512:ASN:HD22	1:A:524:CYS:HB2	1.55	0.71
1:A:320:ASN:ND2	3:A:3200:NAG:O5	2.25	0.69
1:A:378:HIS:HD2	1:A:380:GLN:N	1.92	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:311:HIS:HD2	1:A:313:GLY:N	1.88	0.66
1:A:400:GLU:H	1:A:400:GLU:CD	2.00	0.64
1:A:301:PRO:O	1:A:303:THR:HG23	1.97	0.64
1:A:531:CYS:HB3	1:A:539:CYS:HB3	1.79	0.64
1:A:399:MET:CE	1:A:407:ALA:CB	2.75	0.64
1:A:324:ILE:HD13	1:A:328:ILE:HD11	1.80	0.63
1:A:311:HIS:CD2	1:A:313:GLY:H	2.02	0.63
1:A:399:MET:HE3	1:A:407:ALA:CB	2.29	0.63
1:A:29:ASN:CG	2:A:546:NDG:C1	2.66	0.62
1:A:470:ASN:ND2	5:A:4700:NDG:C2	2.48	0.62
1:A:512:ASN:HB3	1:A:524:CYS:H	1.65	0.61
1:A:246:THR:HG22	1:A:248:VAL:CG2	2.29	0.61
1:A:512:ASN:ND2	1:A:524:CYS:HB2	2.15	0.61
1:A:246:THR:CG2	1:A:248:VAL:HG23	2.30	0.60
1:A:196:TYR:CZ	1:A:202:GLU:HB2	2.36	0.60
1:A:297:ASN:O	1:A:298:GLY:O	2.20	0.60
1:A:399:MET:HE3	1:A:407:ALA:HB2	1.84	0.60
1:A:367:GLU:OE1	1:A:394:HIS:HE1	1.85	0.60
1:A:44:ASN:HB3	1:A:47:LEU:HG	1.85	0.59
1:A:259:TYR:O	1:A:262:THR:HB	2.02	0.58
1:A:411:SER:H	1:A:434:ASN:HD22	1.52	0.58
1:A:205:HIS:HD2	1:A:207:PHE:H	1.50	0.58
1:A:411:SER:H	1:A:434:ASN:ND2	2.00	0.58
1:A:24:ARG:NH1	1:A:25:ASP:OD2	2.37	0.57
1:A:528:CYS:C	1:A:530:THR:H	2.08	0.57
1:A:338:PHE:HE2	1:A:340:ASP:OD1	1.88	0.56
1:A:521:CYS:O	1:A:522:LYS:CB	2.53	0.56
1:A:109:ILE:HG22	1:A:112:LEU:HB2	1.86	0.56
1:A:512:ASN:HB3	1:A:524:CYS:HB2	1.86	0.55
1:A:205:HIS:HD2	1:A:206:LEU:H	1.53	0.54
1:A:246:THR:CG2	1:A:248:VAL:CG2	2.86	0.54
1:A:327:ASN:HD22	1:A:371:TYR:N	2.02	0.54
1:A:188:PRO:C	1:A:190:CYS:N	2.57	0.53
1:A:318:PHE:HA	1:A:321:CYS:SG	2.49	0.52
1:A:187:SER:O	1:A:190:CYS:HB2	2.10	0.52
1:A:310:LEU:HD11	1:A:315:ILE:HD12	1.92	0.52
1:A:138:GLU:O	1:A:194:ARG:NH2	2.42	0.52
1:A:531:CYS:HB3	1:A:539:CYS:CB	2.40	0.51
1:A:343:ALA:C	1:A:345:TYR:H	2.12	0.51
1:A:73:VAL:HB	1:A:108:GLU:HB2	1.92	0.51
1:A:21:ARG:HG3	1:A:24:ARG:HH22	1.75	0.51
1:A:123:HIS:HD2	1:A:149:ASN:HB3	1.76	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:327:ASN:ND2	1:A:370:GLY:HA3	2.26	0.50
1:A:205:HIS:HB2	1:A:217:GLN:H	1.76	0.50
1:A:527:GLU:O	1:A:528:CYS:SG	2.70	0.50
1:A:29:ASN:HD21	2:A:546:NDG:C2	2.21	0.49
1:A:205:HIS:ND1	1:A:216:THR:CG2	2.64	0.49
1:A:109:ILE:CG2	1:A:112:LEU:HB2	2.43	0.49
1:A:205:HIS:CG	1:A:206:LEU:H	2.29	0.49
1:A:528:CYS:O	1:A:530:THR:N	2.44	0.48
1:A:287:MET:HE2	1:A:296:CYS:SG	2.53	0.48
1:A:188:PRO:O	1:A:189:GLN:HB2	2.13	0.48
1:A:512:ASN:HB3	1:A:524:CYS:N	2.29	0.48
1:A:163:HIS:CD2	1:A:165:SER:OG	2.61	0.47
1:A:15:ASN:ND2	1:A:18:HIS:H	2.01	0.47
1:A:289:LYS:HA	1:A:289:LYS:HD2	1.58	0.47
1:A:303:THR:HA	1:A:323:VAL:O	2.16	0.46
1:A:67:VAL:O	1:A:102:SER:HB3	2.15	0.46
1:A:297:ASN:C	1:A:298:GLY:O	2.53	0.45
1:A:514:TYR:CD1	1:A:514:TYR:C	2.89	0.45
1:A:369:THR:HA	1:A:394:HIS:HB2	1.98	0.45
1:A:270:HIS:HA	1:A:396:ARG:HG2	1.98	0.45
1:A:392:THR:HB	1:A:423:GLN:HB3	1.99	0.45
1:A:531:CYS:CB	1:A:539:CYS:CB	2.86	0.45
1:A:283:PRO:HG2	1:A:286:LYS:HG3	1.99	0.44
1:A:205:HIS:CD2	1:A:207:PHE:H	2.34	0.44
1:A:416:LEU:HD11	1:A:440:VAL:HG12	1.99	0.44
1:A:287:MET:HE3	1:A:296:CYS:HA	1.99	0.44
1:A:499:PHE:C	1:A:501:GLY:H	2.20	0.44
1:A:87:SER:OG	1:A:94:LYS:HD3	2.18	0.44
1:A:120:VAL:HG11	1:A:136:TRP:CZ3	2.53	0.44
1:A:512:ASN:HD22	1:A:524:CYS:CB	2.27	0.43
1:A:433:HIS:HA	1:A:460:GLU:O	2.18	0.43
1:A:15:ASN:HD22	1:A:18:HIS:N	2.04	0.43
1:A:512:ASN:CB	1:A:524:CYS:HB2	2.48	0.43
1:A:506:ASP:O	1:A:507:CYS:CB	2.67	0.43
1:A:372:LEU:HD11	1:A:374:ILE:HD11	1.99	0.43
1:A:29:ASN:ND2	2:A:546:NDG:N2	2.67	0.43
1:A:152:PHE:O	1:A:153:THR:CB	2.67	0.42
1:A:402:MET:HA	1:A:402:MET:CE	2.50	0.42
1:A:167:THR:OG1	1:A:168:HIS:CD2	2.73	0.42
1:A:322:THR:HG22	1:A:323:VAL:HG12	2.01	0.42
1:A:79:ILE:HD13	1:A:222:ALA:HB3	2.02	0.42
1:A:327:ASN:HD22	1:A:370:GLY:HA3	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:410:LYS:HA	1:A:433:HIS:O	2.19	0.41
1:A:15:ASN:HD21	1:A:17:GLU:HB2	1.85	0.41
1:A:287:MET:HG2	1:A:296:CYS:SG	2.61	0.41
1:A:432:GLN:HA	1:A:459:ASN:O	2.20	0.41
1:A:114:ASP:OD1	1:A:194:ARG:NH1	2.54	0.41
1:A:264:VAL:HG13	1:A:266:GLU:O	2.21	0.41
1:A:3:CYS:HB2	1:A:33:VAL:HA	2.03	0.41
1:A:31:THR:HA	1:A:54:ASN:O	2.20	0.41
1:A:40:THR:HA	1:A:65:SER:O	2.21	0.40
1:A:333:GLN:H	1:A:333:GLN:CD	2.24	0.40
1:A:282:CYS:HB3	1:A:286:LYS:HB2	2.03	0.40
1:A:16:LYS:HE3	1:A:41:TRP:CE3	2.57	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	536/551 (97%)	463 (86%)	58 (11%)	15 (3%)	8	18

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ARG
1	A	217	GLN
1	A	229	GLU
1	A	522	LYS
1	A	529	ARG
1	A	200	PRO
1	A	298	GLY
1	A	344	ASN
1	A	528	CYS
1	A	539	CYS
1	A	520	THR

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Mol	Chain	Res	Type
1	A	543	VAL
1	A	14	SER
1	A	509	TYR
1	A	188	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	463/489 (95%)	425 (92%)	38 (8%)	17	36

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	39	LEU
1	A	46	ASN
1	A	69	VAL
1	A	72	VAL
1	A	73	VAL
1	A	104	MET
1	A	158	GLU
1	A	164	GLU
1	A	173	GLU
1	A	206	LEU
1	A	219	ASP
1	A	235	GLU
1	A	246	THR
1	A	264	VAL
1	A	265	LYS
1	A	284	GLN
1	A	308	THR
1	A	310	LEU
1	A	323	VAL
1	A	331	LEU
1	A	333	GLN
1	A	346	THR
1	A	357	GLU

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Mol	Chain	Res	Type
1	A	377	THR
1	A	384	LEU
1	A	392	THR
1	A	397	GLN
1	A	441	SER
1	A	462	LEU
1	A	480	GLU
1	A	488	THR
1	A	509	TYR
1	A	514	TYR
1	A	523	ILE
1	A	524	CYS
1	A	527	GLU
1	A	542	CYS

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	15	ASN
1	A	29	ASN
1	A	46	ASN
1	A	54	ASN
1	A	123	HIS
1	A	135	GLN
1	A	163	HIS
1	A	168	HIS
1	A	205	HIS
1	A	284	GLN
1	A	311	HIS
1	A	327	ASN
1	A	333	GLN
1	A	378	HIS
1	A	394	HIS
1	A	423	GLN
1	A	434	ASN
1	A	459	ASN
1	A	470	ASN
1	A	512	ASN
1	A	518	ASN

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 ⓘ

13 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$
3	NAG	A	3200	3	12,14,15	0.71	0	15,19,21	1.25	1 (6%)
3	NAG	A	3201	3	12,14,15	0.66	0	15,19,21	1.67	1 (6%)
4	NAG	A	3440	1,4	12,14,15	0.54	0	15,19,21	1.69	5 (33%)
4	NAG	A	3441	4	12,14,15	0.69	0	15,19,21	1.51	2 (13%)
4	BMA	A	3442	4	10,11,12	0.85	0	11,15,17	1.00	0
4	NAG	A	3830	1,4	12,14,15	0.67	0	15,19,21	1.61	2 (13%)
4	NAG	A	3831	4	12,14,15	0.68	0	15,19,21	1.32	2 (13%)
4	BMA	A	3832	4	10,11,12	0.79	0	11,15,17	2.48	4 (36%)
5	NDG	A	4700	5	12,14,15	0.66	0	15,19,21	1.52	3 (20%)
5	NDG	A	4701	5	12,14,15	0.70	0	15,19,21	1.43	3 (20%)
5	BMA	A	4702	5	10,11,12	0.92	0	11,15,17	1.04	1 (9%)
2	NDG	A	546	2	12,14,15	0.69	1 (8%)	15,19,21	1.14	1 (6%)
2	NAG	A	547	2	12,14,15	0.67	0	15,19,21	1.08	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	3200	3	-	0/6/23/26	0/1/1/1
3	NAG	A	3201	3	-	0/6/23/26	0/1/1/1
4	NAG	A	3440	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3441	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3442	4	-	0/2/19/22	0/1/1/1
4	NAG	A	3830	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	3831	4	-	0/6/23/26	0/1/1/1
4	BMA	A	3832	4	-	0/2/19/22	0/1/1/1
5	NDG	A	4700	5	-	0/6/23/26	0/1/1/1
5	NDG	A	4701	5	-	0/6/23/26	0/1/1/1
5	BMA	A	4702	5	-	0/2/19/22	0/1/1/1
2	NDG	A	546	2	-	0/6/23/26	0/1/1/1
2	NAG	A	547	2	-	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)
2	A	546	NDG	O-C5	-2.09	1.41	1.45

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	3832	BMA	O5-C5-C6	6.38	113.68	106.98
3	A	3201	NAG	O5-C5-C6	5.63	112.89	106.98
4	A	3830	NAG	C2-N2-C7	-4.22	116.00	123.09
5	A	4701	NDG	C2-N2-C7	-3.58	117.08	123.09
4	A	3441	NAG	C3-C2-N2	-3.55	106.35	111.76
4	A	3831	NAG	O5-C5-C6	3.54	110.70	106.98
5	A	4700	NDG	O-C5-C4	3.48	115.08	110.65
4	A	3440	NAG	O5-C5-C6	3.46	110.61	106.98
4	A	3441	NAG	O5-C5-C6	3.42	110.57	106.98
4	A	3832	BMA	O5-C5-C4	-2.83	107.06	110.65
4	A	3440	NAG	O5-C5-C4	2.82	114.23	110.65
3	A	3200	NAG	O5-C5-C6	2.81	109.93	106.98
4	A	3440	NAG	C2-N2-C7	2.73	127.67	123.09
2	A	547	NAG	O5-C5-C6	2.42	109.52	106.98
5	A	4701	NDG	O-C5-C6	2.41	109.51	106.98
2	A	546	NDG	O-C5-C4	-2.38	107.63	110.65
5	A	4700	NDG	O-C5-C6	2.34	109.44	106.98
4	A	3440	NAG	O7-C7-C8	-2.30	117.56	122.04
4	A	3830	NAG	O3-C3-C4	-2.27	105.26	110.35
4	A	3832	BMA	O3-C3-C4	2.26	115.42	110.35
4	A	3832	BMA	C3-C4-C5	-2.17	106.33	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	4700	NDG	O4-C4-C5	-2.09	103.79	109.28
5	A	4702	BMA	O3-C3-C4	2.08	115.01	110.35
5	A	4701	NDG	O-C5-C4	2.05	113.26	110.65
4	A	3440	NAG	C3-C2-N2	2.04	114.86	111.76
4	A	3831	NAG	C3-C2-N2	-2.03	108.68	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 ⓘ

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	542/551 (98%)	0.12	20 (3%)	39 44	31, 45, 69, 78	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	152	PHE	4.5
1	A	153	THR	4.5
1	A	541	GLU	4.2
1	A	215	PRO	3.9
1	A	184	LEU	3.9
1	A	506	ASP	3.7
1	A	505	ALA	3.4
1	A	507	CYS	3.2
1	A	523	ILE	3.0
1	A	516	PHE	3.0
1	A	497	PHE	2.9
1	A	150	TYR	2.8
1	A	542	CYS	2.8
1	A	518	ASN	2.8
1	A	540	GLN	2.6
1	A	345	TYR	2.4
1	A	532	ASN	2.4
1	A	519	ARG	2.2
1	A	299	PRO	2.2
1	A	517	ASP	2.1

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 ⓘ

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	NAG	A	3200	14/15	0.33	15.41	89,94,97,100	0
2	NDG	A	546	14/15	0.25	4.59	85,88,90,95	0
4	NAG	A	3441	14/15	0.23	1.78	80,85,87,91	0
5	NDG	A	4700	14/15	0.19	0.98	69,72,77,79	0
5	NDG	A	4701	14/15	0.22	0.80	66,69,71,72	0
4	NAG	A	3830	14/15	0.14	-1.53	76,82,86,86	0
4	NAG	A	3440	14/15	0.10	-2.54	56,64,68,73	0
4	BMA	A	3832	11/12	0.31	-	96,98,100,101	0
4	BMA	A	3442	11/12	0.29	-	94,98,99,100	0
4	NAG	A	3831	14/15	0.23	-	89,91,96,96	0
2	NAG	A	547	14/15	0.34	-	98,100,102,102	0
5	BMA	A	4702	11/12	0.26	-	73,75,77,78	0
3	NAG	A	3201	14/15	0.43	-	99,102,103,103	0

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.