



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 07:02 AM GMT

PDB ID : 2RIP
Title : Structure of DPPIV in complex with an inhibitor
Authors : Qiu, X.
Deposited on : 2007-10-12
Resolution : 2.90 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>

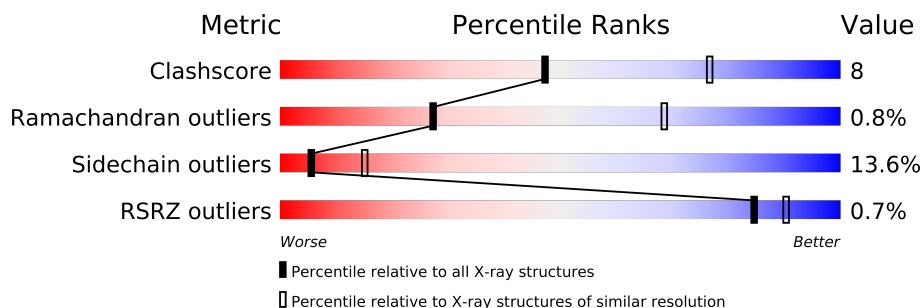
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.90 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	1326 (2.90-2.90)
Ramachandran outliers	78287	1290 (2.90-2.90)
Sidechain outliers	78261	1292 (2.90-2.90)
RSRZ outliers	66119	1054 (2.90-2.90)

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	729	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
4	NAG	A	1219	-	X
4	NAG	A	1321	-	X
5	34Q	A	800	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6158 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 Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	729	Total	C	N	O	S	0	0	0
			5972	3831	983	1132	26			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	4	Total	C	N	O	0	0
			50	28	2	20		

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

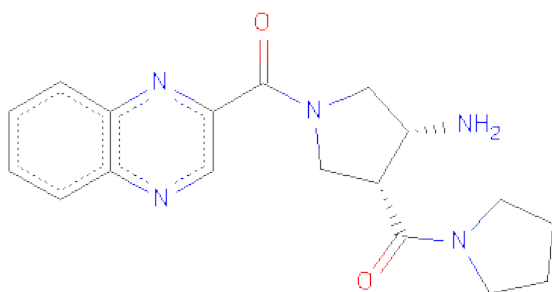
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is (3R,4R)-4-(PYRROLIDIN-1-YLCARBONYL)-1-(QUINOXALIN-2-YLCARBONYL)PYRROLIDIN-3-AMINE (three-letter code: 34Q) (formula: $C_{18}H_{21}N_5O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			25	18	5	2		

- Molecule 6 is water.

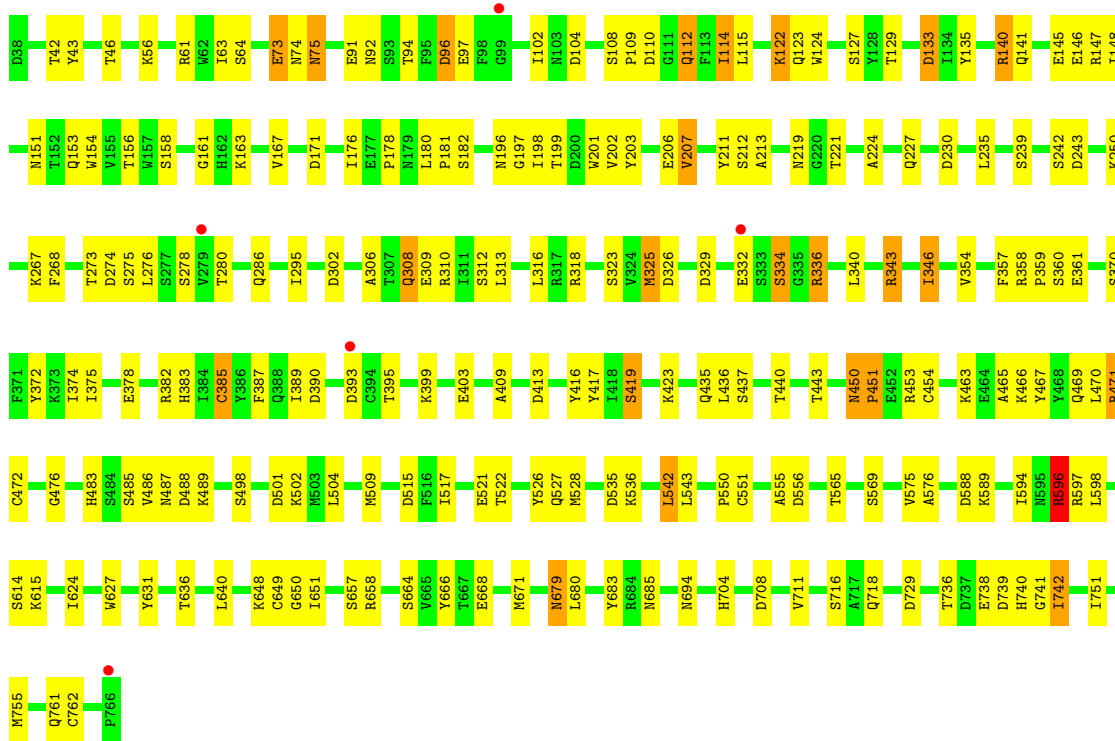
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total	O	0	0
			27	27		

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.

- Molecule 1: Dipeptidyl peptidase 4

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	69.22Å 69.22Å 409.22Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.90 48.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	90.6 (50.00-2.90) 90.5 (48.95-2.90)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.93 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.214 , 0.293 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	49.4	Xtriage
Anisotropy	0.298	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , -2.9	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	1 of 22692 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6158	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.67% 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: NAG, 34Q, MAN

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	0.56	0/6144	0.81	19/8355 (0.2%)

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
2	A	2	0

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	243	ASP	CB-CG-OD2	7.16	124.74	118.30
1	A	171	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	302	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	96	ASP	CB-CG-OD2	6.05	123.74	118.30
1	A	390	ASP	CB-CG-OD2	5.94	123.64	118.30
1	A	588	ASP	CB-CG-OD2	5.91	123.62	118.30
1	A	729	ASP	CB-CG-OD2	5.88	123.59	118.30
1	A	535	ASP	CB-CG-OD2	5.74	123.47	118.30
1	A	393	ASP	CB-CG-OD2	5.68	123.42	118.30
1	A	133	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	488	ASP	CB-CG-OD2	5.59	123.33	118.30
1	A	515	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	501	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	556	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	739	ASP	CB-CG-OD2	5.36	123.12	118.30
1	A	274	ASP	CB-CG-OD2	5.31	123.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	104	ASP	CB-CG-OD2	5.29	123.06	118.30
1	A	230	ASP	CB-CG-OD2	5.19	122.97	118.30
1	A	329	ASP	CB-CG-OD2	5.12	122.91	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2085	NAG	C1
2	A	3085	MAN	C1

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	5972	0	5687	93	0
2	A	50	0	43	1	0
3	A	28	0	25	2	0
4	A	56	0	52	1	0
5	A	25	0	21	1	0
6	A	27	0	0	0	0
All	All	6158	0	5828	96	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 8.

All (96) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:308:GLN:HE21	1:A:308:GLN:HA	1.11	1.11
1:A:704:HIS:HD2	1:A:716:SER:OG	1.38	1.06
1:A:308:GLN:NE2	1:A:308:GLN:HA	1.68	1.02
1:A:648:LYS:HE2	1:A:762:CYS:O	1.74	0.88
1:A:308:GLN:CA	1:A:308:GLN:HE21	1.88	0.86
1:A:704:HIS:CD2	1:A:716:SER:OG	2.28	0.85

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:542:LEU:HD23	1:A:624:ILE:HG23	1.63	0.79
1:A:334:SER:HB2	1:A:336:ARG:HG2	1.67	0.75
1:A:219:ASN:HB2	1:A:308:GLN:CD	2.09	0.73
1:A:146:GLU:HG2	1:A:181:PRO:HA	1.71	0.72
1:A:469:GLN:OE1	1:A:471:ARG:HD3	1.94	0.67
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.77	0.67
1:A:203:TYR:HA	1:A:207:VAL:HG23	1.78	0.65
1:A:153:GLN:HG2	1:A:211:TYR:OH	1.97	0.65
1:A:708:ASP:OD2	1:A:740:HIS:HA	1.98	0.64
1:A:334:SER:HB2	1:A:336:ARG:CG	2.28	0.63
1:A:74:ASN:C	1:A:92:ASN:HB3	2.19	0.62
1:A:122:LYS:HE2	1:A:124:TRP:O	2.01	0.61
1:A:308:GLN:CA	1:A:308:GLN:NE2	2.47	0.59
1:A:664:SER:HB2	1:A:668:GLU:OE2	2.03	0.58
3:A:4086:NAG:H61	3:A:4087:NAG:H83	1.85	0.57
1:A:636:THR:HG21	1:A:651:ILE:O	2.05	0.57
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.86	0.57
1:A:219:ASN:HB2	1:A:308:GLN:NE2	2.19	0.57
1:A:318:ARG:O	1:A:318:ARG:HG3	2.05	0.57
1:A:219:ASN:H	1:A:308:GLN:HE22	1.52	0.55
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.36	0.55
1:A:465:ALA:O	1:A:485:SER:OG	2.20	0.55
3:A:4086:NAG:C6	3:A:4087:NAG:H83	2.37	0.54
1:A:206:GLU:OE2	1:A:666:TYR:HB2	2.06	0.54
1:A:454:CYS:SG	1:A:472:CYS:SG	3.06	0.54
1:A:679:ASN:O	1:A:683:TYR:HD2	1.91	0.53
1:A:527:GLN:HG2	1:A:555:ALA:HA	1.91	0.53
1:A:221:THR:O	1:A:273:THR:OG1	2.27	0.53
1:A:680:LEU:O	1:A:680:LEU:HG	2.09	0.53
1:A:382:ARG:H	1:A:403:GLU:HG2	1.74	0.52
1:A:308:GLN:HB3	4:A:1219:NAG:H61	1.92	0.52
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.45	0.51
1:A:741:GLY:O	1:A:742:ILE:C	2.48	0.51
1:A:306:ALA:HB3	1:A:310:ARG:HB3	1.92	0.51
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.11	0.50
1:A:340:LEU:HB3	1:A:343:ARG:HG3	1.93	0.50
1:A:385:CYS:HB3	1:A:387:PHE:HE1	1.76	0.50
1:A:453:ARG:HG3	1:A:476:GLY:HA3	1.93	0.50
1:A:109:PRO:HG2	1:A:158:SER:O	2.12	0.49
1:A:140:ARG:O	1:A:140:ARG:CG	2.59	0.49
1:A:551:CYS:SG	1:A:551:CYS:O	2.71	0.49
1:A:454:CYS:HG	1:A:472:CYS:HG	1.58	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:385:CYS:HB3	1:A:387:PHE:CE1	2.49	0.48
1:A:199:THR:HB	1:A:203:TYR:HB3	1.94	0.48
1:A:550:PRO:HB3	1:A:594:ILE:HD11	1.96	0.47
1:A:598:LEU:HB2	1:A:671:MET:SD	2.55	0.47
1:A:74:ASN:HB3	1:A:92:ASN:HB2	1.96	0.47
1:A:167:VAL:HG21	1:A:198:ILE:HG23	1.95	0.47
1:A:372:TYR:HA	1:A:385:CYS:O	2.15	0.47
1:A:450:ASN:N	1:A:451:PRO:CD	2.78	0.46
1:A:409:ALA:HB3	1:A:416:TYR:HB2	1.98	0.46
1:A:374:ILE:O	1:A:375:ILE:HD12	2.16	0.46
1:A:738:GLU:HG3	1:A:742:ILE:HG23	1.97	0.46
1:A:374:ILE:HA	1:A:383:HIS:O	2.16	0.45
2:A:1085:NAG:H61	2:A:2085:NAG:HN2	1.81	0.45
1:A:64:SER:O	1:A:463:LYS:HB2	2.15	0.45
1:A:140:ARG:HG2	1:A:140:ARG:O	2.15	0.45
1:A:417:TYR:CE1	1:A:419:SER:HB3	2.52	0.45
1:A:123:GLN:HB3	1:A:127:SER:OG	2.16	0.45
1:A:110:ASP:OD1	1:A:112:GLN:HB2	2.17	0.45
1:A:109:PRO:HD2	1:A:161:GLY:O	2.16	0.45
1:A:649:CYS:HG	1:A:762:CYS:CB	2.30	0.44
1:A:528:MET:HG2	1:A:576:ALA:HB2	1.99	0.44
1:A:346:ILE:HG22	1:A:346:ILE:O	2.18	0.44
1:A:417:TYR:HE1	1:A:419:SER:HB3	1.83	0.44
1:A:704:HIS:HE1	1:A:711:VAL:O	2.00	0.43
1:A:354:VAL:HG12	1:A:359:PRO:HG3	1.99	0.43
1:A:751:ILE:O	1:A:755:MET:HG3	2.18	0.43
1:A:75:ASN:HB3	1:A:91:GLU:HA	2.00	0.43
1:A:504:LEU:HD22	1:A:509:MET:SD	2.58	0.43
1:A:123:GLN:HB3	1:A:124:TRP:H	1.70	0.43
1:A:316:LEU:HD13	1:A:323:SER:HB2	2.00	0.43
1:A:154:TRP:CE2	1:A:212:SER:HB2	2.54	0.43
1:A:201:TRP:CE3	1:A:202:VAL:HA	2.54	0.43
1:A:74:ASN:HB3	1:A:92:ASN:CB	2.50	0.42
1:A:313:LEU:O	1:A:325:MET:HA	2.19	0.42
1:A:467:TYR:HB3	1:A:483:HIS:O	2.19	0.42
1:A:357:PHE:HB2	5:A:800:34Q:C12	2.50	0.42
1:A:596:ARG:O	1:A:597:ARG:NH1	2.53	0.41
1:A:197:GLY:C	1:A:213:ALA:HB3	2.41	0.41
1:A:42:THR:HB	1:A:569:SER:OG	2.19	0.41
1:A:550:PRO:O	1:A:551:CYS:HB3	2.21	0.41
1:A:167:VAL:HG11	1:A:198:ILE:HG12	2.01	0.41
1:A:163:LYS:HG2	1:A:176:ILE:HA	2.03	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:378:GLU:H	1:A:378:GLU:CD	2.24	0.41
1:A:543:LEU:O	1:A:575:VAL:HA	2.21	0.41
1:A:517:ILE:HG23	1:A:526:TYR:CE2	2.56	0.41
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.57	0.40
1:A:43:TYR:N	1:A:569:SER:OG	2.42	0.40
1:A:598:LEU:HD22	1:A:631:TYR:OH	2.21	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	727/729 (100%)	662 (91%)	59 (8%)	6 (1%)	27 68

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	596	ARG
1	A	332	GLU
1	A	73	GLU
1	A	178	PRO
1	A	451	PRO
1	A	450	ASN

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	654/654 (100%)	565 (86%)	89 (14%)	5 15

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	THR
1	A	56	LYS
1	A	61	ARG
1	A	63	ILE
1	A	73	GLU
1	A	75	ASN
1	A	94	THR
1	A	96	ASP
1	A	97	GLU
1	A	102	ILE
1	A	108	SER
1	A	112	GLN
1	A	114	ILE
1	A	115	LEU
1	A	122	LYS
1	A	129	THR
1	A	133	ASP
1	A	140	ARG
1	A	141	GLN
1	A	145	GLU
1	A	147	ARG
1	A	148	ILE
1	A	151	ASN
1	A	156	THR
1	A	180	LEU
1	A	182	SER
1	A	207	VAL
1	A	235	LEU
1	A	239	SER
1	A	242	SER
1	A	250	LYS
1	A	267	LYS
1	A	275	SER
1	A	276	LEU
1	A	278	SER
1	A	280	THR
1	A	286	GLN
1	A	295	ILE
1	A	308	GLN
1	A	309	GLU
1	A	312	SER
1	A	325	MET

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Mol	Chain	Res	Type
1	A	326	ASP
1	A	334	SER
1	A	336	ARG
1	A	343	ARG
1	A	346	ILE
1	A	358	ARG
1	A	360	SER
1	A	361	GLU
1	A	370	SER
1	A	385	CYS
1	A	389	ILE
1	A	395	THR
1	A	399	LYS
1	A	413	ASP
1	A	419	SER
1	A	423	LYS
1	A	435	GLN
1	A	436	LEU
1	A	437	SER
1	A	440	THR
1	A	443	THR
1	A	466	LYS
1	A	471	ARG
1	A	486	VAL
1	A	487	ASN
1	A	489	LYS
1	A	498	SER
1	A	502	LYS
1	A	521	GLU
1	A	522	THR
1	A	536	LYS
1	A	542	LEU
1	A	565	THR
1	A	589	LYS
1	A	596	ARG
1	A	614	SER
1	A	615	LYS
1	A	627	TRP
1	A	657	SER
1	A	658	ARG
1	A	679	ASN
1	A	685	ASN

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Mol	Chain	Res	Type
1	A	694	ASN
1	A	718	GLN
1	A	736	THR
1	A	742	ILE
1	A	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	ASN
1	A	75	ASN
1	A	103	ASN
1	A	162	HIS
1	A	169	ASN
1	A	170	ASN
1	A	308	GLN
1	A	344	GLN
1	A	430	ASN
1	A	483	HIS
1	A	572	ASN
1	A	586	GLN
1	A	595	ASN
1	A	606	GLN
1	A	679	ASN
1	A	685	ASN
1	A	694	ASN
1	A	704	HIS
1	A	718	GLN
1	A	748	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

6 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$
2	NAG	A	1085	1,2	12,14,15	0.87	1 (8%)	15,19,21	1.31	2 (13%)
2	NAG	A	2085	2	12,14,15	0.59	0	15,19,21	1.73	2 (13%)
2	MAN	A	3085	2	10,11,12	0.71	0	11,15,17	0.83	0
2	MAN	A	4085	2	10,11,12	0.78	0	11,15,17	1.71	3 (27%)
3	NAG	A	4086	1,3	12,14,15	0.69	0	15,19,21	1.69	2 (13%)
3	NAG	A	4087	3	12,14,15	0.78	1 (8%)	15,19,21	1.28	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1085	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	2085	2	1/1/5/7	0/6/23/26	0/1/1/1
2	MAN	A	3085	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	A	4085	2	-	0/2/19/22	0/1/1/1
3	NAG	A	4086	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	4087	3	-	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)
3	A	4087	NAG	O5-C5	-2.13	1.41	1.45
2	A	1085	NAG	O5-C5	-2.10	1.41	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2085	NAG	O5-C5-C6	5.82	113.09	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	4086	NAG	O5-C5-C4	5.01	117.01	110.65
2	A	4085	MAN	O5-C5-C6	3.68	110.84	106.98
2	A	1085	NAG	C3-C2-N2	-3.38	106.61	111.76
2	A	4085	MAN	C4-C3-C2	2.72	114.16	110.50
3	A	4087	NAG	O5-C5-C4	-2.66	107.28	110.65
2	A	4085	MAN	O2-C2-C3	2.31	115.16	110.18
3	A	4086	NAG	C3-C4-C5	2.31	114.33	110.20
2	A	2085	NAG	C3-C2-N2	-2.20	108.41	111.76
2	A	1085	NAG	C3-C4-C5	2.11	113.97	110.20
3	A	4087	NAG	O3-C3-C4	-2.08	105.68	110.35
3	A	4087	NAG	O5-C5-C6	2.09	109.17	106.98

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2085	NAG	C1
2	A	3085	MAN	C1

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	$\# Z > 2$
4	NAG	A	1219	1	12,14,15	0.56	0	15,19,21	0.90	1 (6%)
4	NAG	A	1229	1	12,14,15	0.57	0	15,19,21	1.17	1 (6%)
4	NAG	A	1281	1	12,14,15	0.67	0	15,19,21	0.92	0
4	NAG	A	1321	1	12,14,15	0.68	0	15,19,21	1.18	2 (13%)
5	34Q	A	800	-	28,28,28	2.41	8 (28%)	40,40,40	1.49	6 (15%)

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	1219	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1229	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1281	1	-	0/6/23/26	0/1/1/1
4	NAG	A	1321	1	-	0/6/23/26	0/1/1/1
5	34Q	A	800	-	-	0/16/35/35	0/2/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	34Q	C18-C17	7.20	1.52	1.39
5	A	800	34Q	C17-C10	5.50	1.62	1.50
5	A	800	34Q	C15-C14	3.78	1.48	1.41
5	A	800	34Q	C12-C13	3.60	1.48	1.41
5	A	800	34Q	C11-C16	3.43	1.47	1.37
5	A	800	34Q	C13-N5	3.38	1.43	1.37
5	A	800	34Q	C14-C13	-3.19	1.35	1.42
5	A	800	34Q	C11-C12	2.02	1.41	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	34Q	C18-C17-C10	4.16	124.74	119.52
5	A	800	34Q	C9-C3-C2	-3.20	98.72	104.65
4	A	1321	NAG	O5-C5-C6	2.91	110.03	106.98
5	A	800	34Q	C3-C2-C4	2.39	116.00	111.64
5	A	800	34Q	C6-C5-N2	2.35	108.43	103.40
5	A	800	34Q	O1-C4-C2	-2.33	117.50	121.84
5	A	800	34Q	C15-C14-C13	2.26	122.27	119.30
4	A	1229	NAG	C2-N2-C7	-2.26	119.30	123.09
4	A	1219	NAG	O5-C5-C6	2.10	109.19	106.98
4	A	1321	NAG	C4-C3-C2	2.07	116.37	111.32

There are no chirality outliers.

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 ⓘ

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	729/729 (100%)	-0.17	5 (0%) 84 90	13, 37, 59, 80	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	279	VAL	2.6
1	A	99	GLY	2.5
1	A	766	PRO	2.5
1	A	332	GLU	2.4
1	A	393	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
2	MAN	A	4085	11/12	0.45	3.12	87,89,89,89	0
3	NAG	A	4086	14/15	0.28	1.43	61,65,67,71	0
2	NAG	A	1085	14/15	0.23	0.68	45,49,53,59	0
2	NAG	A	2085	14/15	0.29	0.44	64,68,70,73	0
2	MAN	A	3085	11/12	0.29	-	77,79,83,86	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	A	4087	14/15	0.26	-	74,77,78,80	0

6.4 Ligands

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(\AA^2)	Q<0.9
4	NAG	A	1321	14/15	0.25	2.87	58,63,64,66	0
4	NAG	A	1219	14/15	0.25	2.23	64,66,67,67	0
5	34Q	A	800	25/25	0.23	2.20	27,33,39,39	0
4	NAG	A	1281	14/15	0.25	0.36	62,64,66,66	0
4	NAG	A	1229	14/15	0.18	-0.39	39,48,52,54	0

6.5 Other polymers

There are no such residues in this entry.