



Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:10 PM GMT

PDB ID : 2QTB
Title : Human dipeptidyl peptidase iv/cd26 in complex with a 4-aryl cyclohexylalanine inhibitor
Authors : Scapin, G.
Deposited on : 2007-08-01
Resolution : 2.25 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>

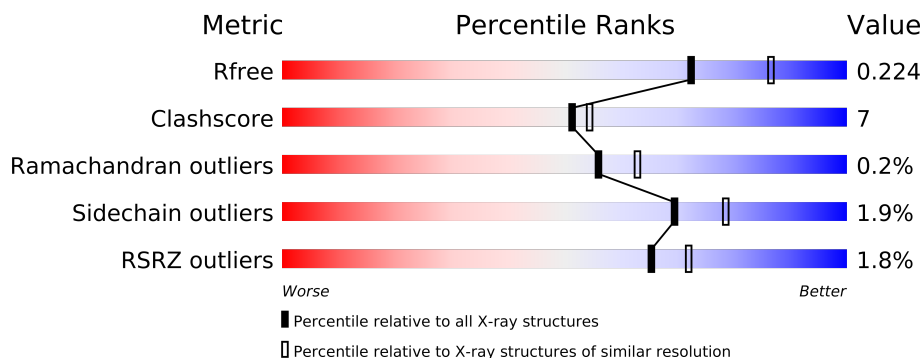
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.25 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	1108 (2.28-2.24)
Clashscore	79885	1326 (2.28-2.24)
Ramachandran outliers	78287	1291 (2.28-2.24)
Sidechain outliers	78261	1291 (2.28-2.24)
RSRZ outliers	66119	1110 (2.28-2.24)

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	766	
1	B	766	

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

Mol	Type	Chain	Res	Geometry	Electron density
3	NAG	A	1520	-	X
3	NAG	B	2150	-	X
3	NAG	B	2321	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13252 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	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			
1	B	728	Total	C	N	O	S	0	0	0
			5965	3828	982	1129	26			

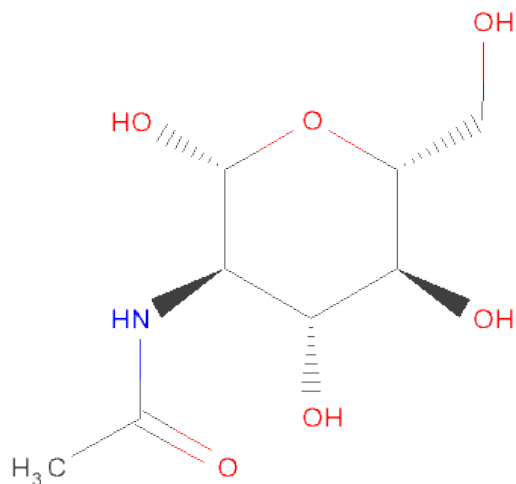
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	39	THR	SER	ENGINEERED	UNP P27487
B	39	THR	SER	ENGINEERED	UNP P27487

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

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

- 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		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	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	M	2	Total	C	N	O	0	0
			28	16	2	10		
4	P	2	Total	C	N	O	0	0
			28	16	2	10		

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

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

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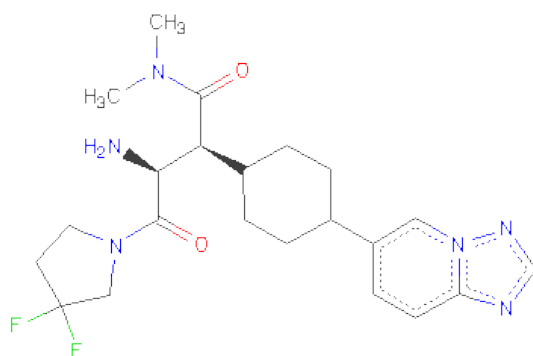
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	Q	2	Total	C	N	O	0	0
			28	16	2	10		
5	R	2	Total	C	N	O	0	0
			28	16	2	10		
5	S	2	Total	C	N	O	0	0
			28	16	2	10		
5	T	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Na	0	0
			1	1		

- Molecule 7 is (2S,3S)-3-AMINO-4-(3,3-DIFLUOROPYRROLIDIN-1-YL)-N,N-DIMETHYL-4-OXO-2-(TRANS-4-[1,2,4]TRIAZOLO[1,5-A]PYRIDIN-6-YLCYCLOHEXYL)BUTANAMIDE (three-letter code: 474) (formula: C₂₂H₃₀F₂N₆O₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	F	N	O	0	0
			32	22	2	6	2		
7	B	1	Total	C	F	N	O	0	0
			32	22	2	6	2		

- Molecule 8 is water.

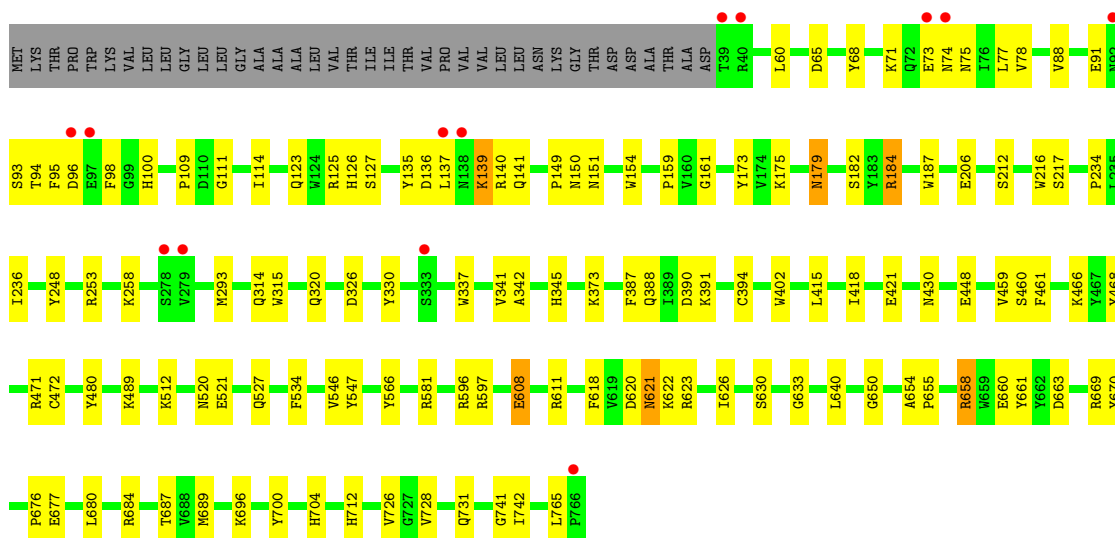
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	453	Total 453	O 453	0	0
8	B	455	Total 455	O 455	0	0
8	M	2	Total 2	O 2	0	0
8	O	1	Total 1	O 1	0	0
8	Q	1	Total 1	O 1	0	0
8	R	2	Total 2	O 2	0	0
8	S	3	Total 3	O 3	0	0
8	T	4	Total 4	O 4	0	0

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.

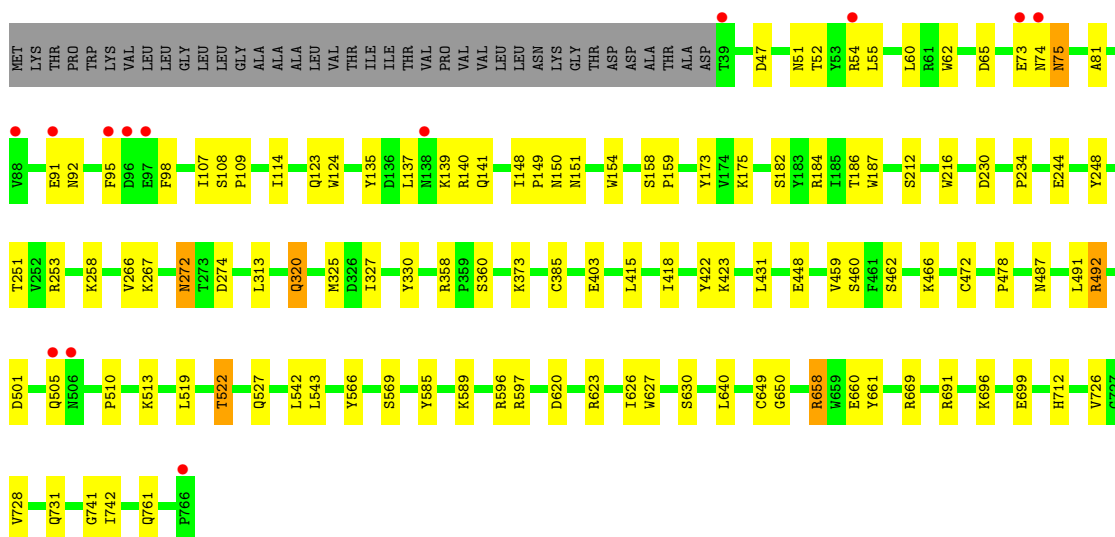
• Molecule 1: Dipeptidyl peptidase 4

Chain A: 



• Molecule 1: Dipeptidyl peptidase 4

Chain B: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	117.86Å 125.63Å 136.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.25 43.07 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.25) 99.6 (43.07-2.25)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.94 (at 2.24Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.187 , 0.228 0.185 , 0.224	Depositor DCC
R_{free} test set	4852 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.475	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 27.9	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	0 of 96565 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13252	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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: NA, NDG, 474, 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	0.48	0/6137	0.68	0/8346
1	B	0.48	0/6137	0.68	0/8346
All	All	0.48	0/12274	0.68	0/16692

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	700	TYR	Sidechain

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	5965	0	5676	93	0
1	B	5965	0	5679	81	0
2	L	28	0	25	2	0
2	O	28	0	25	3	0
3	A	42	0	39	4	0
3	B	42	0	39	1	0
4	M	28	0	25	4	0
4	P	28	0	25	1	0
5	M	28	0	25	1	0
5	Q	28	0	25	0	0
5	R	28	0	25	1	0
5	S	28	0	25	0	0
5	T	28	0	25	1	0
6	A	1	0	0	0	0
7	A	32	0	30	1	0
7	B	32	0	30	5	0
8	A	453	0	0	3	0
8	B	455	0	0	2	0
8	M	2	0	0	0	0
8	O	1	0	0	0	0
8	Q	1	0	0	0	0
8	R	2	0	0	0	0
8	S	3	0	0	0	0
8	T	4	0	0	1	0
All	All	13252	0	11718	175	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 7.

All (175) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:581:ARG:NH1	3:A:1520:NAG:H62	1.91	0.85
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.60	0.81
2:O:1229:NAG:H61	2:O:1230:NDG:O	1.83	0.78
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.65	0.77
1:A:581:ARG:CZ	3:A:1520:NAG:H62	2.15	0.77
1:B:358:ARG:HD3	7:B:2322:474:N56	2.00	0.77
1:A:596:ARG:O	1:A:597:ARG:HD2	1.86	0.76
1:B:184:ARG:HD3	1:B:186:THR:O	1.86	0.75
1:A:139:LYS:HG3	1:A:141:GLN:HB3	1.68	0.73
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.87	0.72
1:A:258:LYS:HZ1	1:A:712:HIS:HD2	1.38	0.72
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.89	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.91	0.70
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.27	0.70
1:B:691:ARG:HD2	8:B:2356:HOH:O	1.90	0.70
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.40	0.69
1:B:630:SER:OG	7:B:2322:474:H212	1.93	0.69
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.30	0.67
1:B:251:THR:HG21	1:B:253:ARG:NH1	2.08	0.67
1:A:65:ASP:OD2	1:A:466:LYS:HB2	1.96	0.65
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.77	0.65
1:B:272:ASN:HD22	1:B:272:ASN:C	1.99	0.65
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.79	0.65
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.27	0.65
1:B:184:ARG:HD2	1:B:187:TRP:CE2	2.33	0.64
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.79	0.64
1:A:630:SER:OG	7:A:1521:474:H212	1.96	0.64
1:A:621:ASN:HD22	1:A:622:LYS:N	1.96	0.64
1:B:360:SER:O	1:B:373:LYS:HE3	1.97	0.63
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.33	0.63
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.81	0.62
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.17	0.62
1:A:179:ASN:H	1:A:179:ASN:HD22	1.47	0.61
1:A:621:ASN:C	1:A:621:ASN:HD22	2.02	0.61
1:B:55:LEU:HD11	1:B:478:PRO:HD2	1.83	0.61
1:A:77:LEU:HD23	1:A:88:VAL:HA	1.84	0.60
1:A:314:GLN:HE22	1:A:373:LYS:NZ	2.00	0.60
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.66	0.60
1:B:107:ILE:HD12	1:B:107:ILE:N	2.17	0.60
1:A:75:ASN:HD21	3:A:1092:NAG:HN2	1.48	0.59
1:B:81:ALA:O	1:B:492:ARG:NH2	2.33	0.59
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.02	0.59
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.37	0.58
1:A:415:LEU:HD23	1:A:415:LEU:C	2.24	0.58
1:B:65:ASP:OD2	1:B:466:LYS:HB2	2.03	0.57
1:B:491:LEU:O	1:B:492:ARG:HB3	2.05	0.57
1:B:91:GLU:OE1	1:B:91:GLU:HA	2.04	0.57
1:B:519:LEU:O	1:B:522:THR:HG23	2.04	0.57
1:B:60:LEU:HD12	1:B:60:LEU:C	2.25	0.56
2:O:1230:NDG:O7	2:O:1230:NDG:H3	2.05	0.56
1:A:676:PRO:HG2	1:A:677:GLU:OE2	2.05	0.56
1:A:60:LEU:HD12	1:A:60:LEU:C	2.26	0.56
1:A:91:GLU:HB2	1:A:94:THR:OG1	2.05	0.56
1:B:501:ASP:O	1:B:505:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.36	0.55
1:B:139:LYS:HB3	1:B:141:GLN:HE21	1.70	0.55
1:B:422:TYR:CE2	1:B:423:LYS:HE2	2.42	0.55
1:A:149:PRO:HA	4:M:1150:NDG:C8	2.37	0.54
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.72	0.54
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.37	0.54
1:B:137:LEU:O	1:B:140:ARG:HD3	2.07	0.54
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.43	0.54
1:B:251:THR:HG21	1:B:253:ARG:HH12	1.72	0.54
1:A:620:ASP:OD2	1:A:623:ARG:HD3	2.08	0.53
1:A:314:GLN:HE22	1:A:373:LYS:HZ3	1.56	0.53
1:A:390:ASP:O	1:A:391:LYS:HD2	2.09	0.52
1:A:71:LYS:HE3	1:A:74:ASN:HA	1.91	0.52
1:B:658:ARG:HD3	1:B:660:GLU:HB2	1.90	0.51
1:B:47:ASP:HA	1:B:52:THR:HG23	1.92	0.51
1:B:173:TYR:CE2	1:B:184:ARG:HG3	2.46	0.51
1:A:621:ASN:ND2	1:A:621:ASN:C	2.65	0.51
1:B:51:ASN:OD1	1:B:54:ARG:HD3	2.11	0.51
1:A:73:GLU:O	1:A:74:ASN:HB2	2.11	0.50
1:A:330:TYR:HB2	1:A:337:TRP:CH2	2.46	0.50
1:A:125:ARG:HG2	1:A:126:HIS:CE1	2.46	0.50
1:B:358:ARG:CD	7:B:2322:474:N56	2.74	0.50
1:A:253:ARG:HH21	1:B:253:ARG:CZ	2.25	0.50
1:A:608:GLU:OE1	1:A:611:ARG:HD2	2.11	0.50
1:A:471:ARG:HG3	1:A:480:TYR:CE2	2.47	0.50
1:B:415:LEU:HD23	1:B:415:LEU:C	2.32	0.49
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.47	0.49
1:B:626:ILE:O	1:B:650:GLY:HA2	2.12	0.49
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.95	0.49
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.95	0.49
1:A:330:TYR:CE2	5:M:1220:NAG:H83	2.47	0.49
1:B:75:ASN:HB3	1:B:92:ASN:H	1.77	0.48
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.95	0.48
1:A:633:GLY:HA3	1:A:655:PRO:HB3	1.95	0.48
1:A:136:ASP:CG	1:A:139:LYS:HG2	2.33	0.48
1:B:107:ILE:HG22	1:B:108:SER:O	2.13	0.48
1:A:293:MET:HG2	1:A:315:TRP:HB3	1.95	0.48
1:B:358:ARG:HD2	7:B:2322:474:H49	1.95	0.48
1:B:513:LYS:O	1:B:527:GLN:HA	2.14	0.48
1:B:741:GLY:O	1:B:742:ILE:C	2.51	0.47
1:B:542:LEU:HD23	1:B:543:LEU:N	2.29	0.47
1:A:75:ASN:ND2	3:A:1092:NAG:HN2	2.12	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:253:ARG:HH21	1:B:253:ARG:NH1	2.13	0.47
1:A:626:ILE:O	1:A:650:GLY:HA2	2.15	0.47
1:B:596:ARG:O	1:B:597:ARG:HD2	2.15	0.46
1:B:175:LYS:HG3	1:B:182:SER:HB3	1.97	0.46
4:M:1150:NDG:H4	4:M:1151:NAG:H2	1.69	0.46
1:B:649:CYS:HB3	1:B:699:GLU:HB2	1.97	0.46
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.34	0.46
1:B:95:PHE:HB3	1:B:98:PHE:HB2	1.98	0.46
1:B:418:ILE:HD13	1:B:431:LEU:HA	1.97	0.46
1:B:272:ASN:ND2	1:B:274:ASP:H	2.15	0.45
1:B:272:ASN:HD22	1:B:274:ASP:H	1.65	0.45
1:A:387:PHE:CD1	1:A:394:CYS:HB3	2.51	0.45
4:P:1321:NDG:O3	4:P:1322:NAG:N2	2.50	0.45
1:A:111:GLY:O	1:A:137:LEU:HD12	2.17	0.45
1:A:512:LYS:HE3	1:A:527:GLN:OE1	2.17	0.45
1:A:150:ASN:O	1:A:151:ASN:HB2	2.16	0.45
1:A:546:VAL:CG2	1:A:547:TYR:N	2.80	0.45
1:A:184:ARG:NH1	1:A:187:TRP:HA	2.32	0.44
1:A:93:SER:HB2	1:A:96:ASP:OD2	2.16	0.44
2:O:1229:NAG:H61	2:O:1230:NDG:C1	2.47	0.44
1:B:459:VAL:HG22	1:B:460:SER:N	2.32	0.44
1:A:731:GLN:NE2	8:A:1972:HOH:O	2.49	0.44
1:B:658:ARG:HG3	1:B:658:ARG:O	2.18	0.44
8:A:1972:HOH:O	1:B:731:GLN:NE2	2.51	0.44
1:A:658:ARG:HB2	1:A:687:THR:HG22	2.00	0.44
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.53	0.44
1:B:358:ARG:HD2	7:B:2322:474:C49	2.48	0.44
1:A:658:ARG:HD3	1:A:660:GLU:HB2	2.00	0.44
1:A:345:HIS:HE1	1:A:391:LYS:O	2.01	0.44
1:A:726:VAL:HG23	1:A:728:VAL:HG23	2.00	0.43
1:A:109:PRO:HD2	1:A:161:GLY:O	2.17	0.43
1:A:139:LYS:HB3	1:A:139:LYS:NZ	2.33	0.43
1:A:489:LYS:HE3	8:A:1822:HOH:O	2.18	0.43
1:A:236:ILE:HG12	1:A:712:HIS:CE1	2.53	0.43
1:A:125:ARG:HG2	1:A:126:HIS:NE2	2.33	0.43
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.52	0.43
1:A:149:PRO:HA	4:M:1150:NDG:H8C1	2.01	0.43
1:A:418:ILE:HA	1:A:430:ASN:O	2.19	0.43
1:A:341:VAL:HG13	1:A:342:ALA:N	2.33	0.43
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.49	0.42
1:B:109:PRO:HG2	1:B:158:SER:O	2.19	0.42
1:A:149:PRO:HA	4:M:1150:NDG:H8C3	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.19	0.42
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.54	0.42
1:A:534:PHE:HZ	1:A:618:PHE:CG	2.37	0.42
1:B:330:TYR:CE2	5:R:2220:NAG:H83	2.54	0.42
1:A:623:ARG:NH2	1:A:765:LEU:HD21	2.33	0.42
5:T:2282:NAG:H2	8:T:483:HOH:O	2.19	0.42
1:A:60:LEU:HB2	1:A:68:TYR:CD1	2.54	0.42
1:A:546:VAL:HG22	1:A:547:TYR:N	2.34	0.42
1:B:123:GLN:HG2	1:B:124:TRP:N	2.34	0.42
1:B:62:TRP:CD2	1:B:462:SER:HA	2.54	0.42
1:A:689:MET:HE3	1:B:244:GLU:HG3	2.02	0.42
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.55	0.42
2:L:1085:NAG:H62	2:L:1086:NDG:HA	1.84	0.42
1:A:78:VAL:HG13	2:L:1085:NAG:H81	2.01	0.42
1:B:542:LEU:HD23	1:B:542:LEU:C	2.41	0.41
1:B:325:MET:HE2	1:B:327:ILE:HG12	2.02	0.41
1:A:139:LYS:O	1:A:140:ARG:C	2.58	0.41
1:A:489:LYS:HB2	1:A:489:LYS:NZ	2.35	0.41
1:B:148:ILE:HA	1:B:149:PRO:HD3	1.90	0.41
1:A:253:ARG:NH2	1:B:253:ARG:NH1	2.68	0.41
1:A:159:PRO:HG3	1:A:217:SER:O	2.20	0.41
1:A:512:LYS:HE3	1:A:527:GLN:CD	2.40	0.41
1:B:251:THR:CG2	1:B:253:ARG:NH1	2.82	0.41
1:B:75:ASN:HB3	1:B:92:ASN:N	2.35	0.41
1:B:266:VAL:HG22	1:B:267:LYS:N	2.34	0.41
1:A:136:ASP:HB3	1:A:139:LYS:HG2	2.03	0.41
1:B:73:GLU:OE1	3:B:2092:NAG:H83	2.21	0.41
1:B:150:ASN:O	1:B:151:ASN:HB2	2.20	0.41
1:B:589:LYS:HB3	8:B:2489:HOH:O	2.21	0.41
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.56	0.41
1:A:520:ASN:O	1:A:521:GLU:HB2	2.21	0.41
1:A:123:GLN:HB3	1:A:127:SER:OG	2.21	0.41
1:A:741:GLY:O	1:A:742:ILE:C	2.59	0.41
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.51	0.40
1:A:459:VAL:HG22	1:A:460:SER:N	2.36	0.40
1:A:654:ALA:HA	1:A:704:HIS:CE1	2.56	0.40
1:B:184:ARG:HD2	1:B:187:TRP:CD2	2.55	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	726/766 (95%)	697 (96%)	28 (4%)	1 (0%)	59	68
1	B	726/766 (95%)	696 (96%)	28 (4%)	2 (0%)	50	54
All	All	1452/1532 (95%)	1393 (96%)	56 (4%)	3 (0%)	56	63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	320	GLN
1	A	320	GLN
1	B	492	ARG

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	653/683 (96%)	642 (98%)	11 (2%)	73	82
1	B	653/683 (96%)	639 (98%)	14 (2%)	66	75
All	All	1306/1366 (96%)	1281 (98%)	25 (2%)	69	78

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	LYS
1	A	179	ASN
1	A	184	ARG
1	A	326	ASP
1	A	388	GLN
1	A	448	GLU

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Mol	Chain	Res	Type
1	A	472	CYS
1	A	566	TYR
1	A	608	GLU
1	A	621	ASN
1	A	658	ARG
1	B	74	ASN
1	B	75	ASN
1	B	230	ASP
1	B	272	ASN
1	B	313	LEU
1	B	385	CYS
1	B	448	GLU
1	B	472	CYS
1	B	487	ASN
1	B	522	THR
1	B	566	TYR
1	B	627	TRP
1	B	658	ARG
1	B	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	123	GLN
1	A	141	GLN
1	A	169	ASN
1	A	179	ASN
1	A	314	GLN
1	A	338	ASN
1	A	505	GLN
1	A	621	ASN
1	A	712	HIS
1	A	731	GLN
1	B	74	ASN
1	B	141	GLN
1	B	169	ASN
1	B	272	ASN
1	B	487	ASN
1	B	533	HIS
1	B	621	ASN
1	B	712	HIS
1	B	731	GLN

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Mol	Chain	Res	Type
1	B	761	GLN

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 ⓘ

18 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	L	1085	1,2	12,14,15	0.59	0	15,19,21	1.17	2 (13%)
2	NDG	L	1086	2	12,14,15	0.71	0	15,19,21	0.87	1 (6%)
4	NDG	M	1150	1,4	12,14,15	0.45	0	15,19,21	0.96	1 (6%)
4	NAG	M	1151	4	12,14,15	0.60	0	15,19,21	0.69	0
5	NAG	M	1219	1,5	12,14,15	0.52	0	15,19,21	0.77	0
5	NAG	M	1220	5	12,14,15	0.51	0	15,19,21	0.64	0
2	NAG	O	1229	1,2	12,14,15	0.48	0	15,19,21	1.09	1 (6%)
2	NDG	O	1230	2	12,14,15	0.54	0	15,19,21	1.00	1 (6%)
4	NDG	P	1321	1,4	12,14,15	0.47	0	15,19,21	0.95	1 (6%)
4	NAG	P	1322	4	12,14,15	0.72	0	15,19,21	0.68	0
5	NAG	Q	2085	1,5	12,14,15	0.53	0	15,19,21	0.61	0
5	NAG	Q	2086	5	12,14,15	0.61	0	15,19,21	0.76	0
5	NAG	R	2219	1,5	12,14,15	0.52	0	15,19,21	0.69	0
5	NAG	R	2220	5	12,14,15	0.48	0	15,19,21	0.84	1 (6%)
5	NAG	S	2229	1,5	12,14,15	0.57	0	15,19,21	0.92	1 (6%)
5	NAG	S	2230	5	12,14,15	0.56	0	15,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	NAG	T	2281	1,5	12,14,15	0.49	0	15,19,21	0.75	0
5	NAG	T	2282	5	12,14,15	0.62	0	15,19,21	0.76	0

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	L	1085	1,2	-	0/6/23/26	0/1/1/1
2	NDG	L	1086	2	-	0/6/23/26	0/1/1/1
4	NDG	M	1150	1,4	-	0/6/23/26	0/1/1/1
4	NAG	M	1151	4	-	0/6/23/26	0/1/1/1
5	NAG	M	1219	1,5	-	0/6/23/26	0/1/1/1
5	NAG	M	1220	5	-	0/6/23/26	0/1/1/1
2	NAG	O	1229	1,2	-	0/6/23/26	0/1/1/1
2	NDG	O	1230	2	-	0/6/23/26	0/1/1/1
4	NDG	P	1321	1,4	-	0/6/23/26	0/1/1/1
4	NAG	P	1322	4	-	0/6/23/26	0/1/1/1
5	NAG	Q	2085	1,5	-	0/6/23/26	0/1/1/1
5	NAG	Q	2086	5	-	0/6/23/26	0/1/1/1
5	NAG	R	2219	1,5	-	0/6/23/26	0/1/1/1
5	NAG	R	2220	5	-	0/6/23/26	0/1/1/1
5	NAG	S	2229	1,5	-	0/6/23/26	0/1/1/1
5	NAG	S	2230	5	-	0/6/23/26	0/1/1/1
5	NAG	T	2281	1,5	-	0/6/23/26	0/1/1/1
5	NAG	T	2282	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	2229	NAG	C3-C2-N2	-2.64	107.74	111.76
4	P	1321	NDG	C3-C2-N2	-2.57	107.84	111.76
2	O	1229	NAG	C3-C2-N2	-2.52	107.93	111.76
4	M	1150	NDG	C3-C2-N2	-2.51	107.94	111.76
2	O	1230	NDG	C3-C2-N2	-2.50	107.96	111.76
2	L	1085	NAG	C4-C3-C2	-2.48	105.25	111.32
5	R	2220	NAG	C3-C2-N2	-2.16	108.48	111.76
2	L	1085	NAG	C2-N2-C7	-2.05	119.64	123.09
2	L	1086	NDG	C3-C4-C5	2.05	113.87	110.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

Of 9 ligands modelled in this entry, 1 is monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	A	1092	1	12,14,15	0.48	0	15,19,21	0.79	0
3	NAG	A	1281	1	12,14,15	0.48	0	15,19,21	0.74	0
3	NAG	A	1520	1	12,14,15	0.60	0	15,19,21	0.74	0
7	474	A	1521	-	35,35,35	2.81	10 (28%)	52,52,52	2.04	12 (23%)
3	NAG	B	2092	1	12,14,15	0.60	0	15,19,21	0.66	0
3	NAG	B	2150	1	12,14,15	0.61	0	15,19,21	0.74	1 (6%)
3	NAG	B	2321	1	12,14,15	0.59	0	15,19,21	0.85	1 (6%)
7	474	B	2322	-	35,35,35	2.75	14 (40%)	52,52,52	2.02	11 (21%)

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	1092	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1281	1	-	0/6/23/26	0/1/1/1
3	NAG	A	1520	1	-	0/6/23/26	0/1/1/1
7	474	A	1521	-	-	0/28/49/49	0/2/4/4
3	NAG	B	2092	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2150	1	-	0/6/23/26	0/1/1/1
3	NAG	B	2321	1	-	0/6/23/26	0/1/1/1
7	474	B	2322	-	-	0/28/49/49	0/2/4/4

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	2322	474	N54-N53	-8.48	1.24	1.36
7	A	1521	474	N54-N53	-7.39	1.25	1.36
7	B	2322	474	C50-C51	7.35	1.51	1.39
7	A	1521	474	C50-C51	7.20	1.51	1.39
7	A	1521	474	C49-C48	6.09	1.49	1.40
7	A	1521	474	C1-C5	-5.85	1.41	1.51
7	B	2322	474	C49-C48	5.08	1.48	1.40
7	B	2322	474	C1-C5	-5.07	1.43	1.51
7	A	1521	474	C52-N53	4.79	1.50	1.38
7	A	1521	474	C5-N9	4.39	1.40	1.34
7	B	2322	474	C5-N9	4.08	1.40	1.34
7	B	2322	474	F62-C19	-3.33	1.33	1.37
7	A	1521	474	F62-C19	-3.20	1.33	1.37
7	B	2322	474	C1-C32	3.19	1.61	1.54
7	B	2322	474	C52-N53	3.06	1.46	1.38
7	A	1521	474	C1-C32	2.93	1.61	1.54
7	A	1521	474	C33-C32	2.90	1.59	1.53
7	B	2322	474	C48-N56	2.50	1.35	1.33
7	B	2322	474	C33-C32	2.47	1.58	1.53
7	B	2322	474	F28-C19	-2.16	1.35	1.37
7	B	2322	474	C34-C33	2.08	1.58	1.52
7	B	2322	474	C55-N54	2.08	1.35	1.32
7	B	2322	474	C1-C2	2.03	1.57	1.55
7	A	1521	474	F28-C19	-2.01	1.35	1.37

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1521	474	C52-C51-C29	-6.19	105.38	120.86
7	B	2322	474	C52-C51-C29	-5.93	106.02	120.86
7	A	1521	474	C50-C51-C29	5.26	133.09	121.19
7	B	2322	474	C50-C51-C29	5.22	132.99	121.19
7	A	1521	474	O8-C5-C1	-4.79	112.86	121.74
7	A	1521	474	C1-C5-N9	4.52	126.59	117.68
7	B	2322	474	O8-C5-C1	-4.38	113.62	121.74
7	A	1521	474	C51-C52-N53	-4.30	117.30	123.63
7	B	2322	474	C1-C5-N9	4.25	126.05	117.68
7	B	2322	474	C52-N53-N54	3.71	128.31	125.21
7	A	1521	474	C49-C48-N53	3.52	120.71	117.93
7	B	2322	474	C20-C21-N4	-3.45	100.62	103.86
7	B	2322	474	C51-C52-N53	-3.42	118.60	123.63
7	B	2322	474	C49-C48-N53	3.36	120.59	117.93
7	A	1521	474	C20-C21-N4	-3.35	100.71	103.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	2322	474	C55-N54-N53	3.25	105.74	102.51
7	A	1521	474	C52-N53-N54	2.98	127.71	125.21
7	B	2322	474	C2-C1-C5	2.97	114.34	109.17
7	B	2322	474	C34-C29-C51	-2.85	106.70	112.89
7	A	1521	474	C55-N54-N53	2.51	105.00	102.51
7	A	1521	474	C34-C29-C51	-2.50	107.45	112.89
7	A	1521	474	C2-C1-C5	2.43	113.39	109.17
7	A	1521	474	C31-C30-C29	2.05	114.44	110.34
3	B	2321	NAG	C2-N2-C7	-2.04	119.66	123.09
3	B	2150	NAG	C2-N2-C7	-2.00	119.72	123.09

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	728/766 (95%)	-0.24	13 (1%) 65 72	13, 24, 45, 59	0
1	B	728/766 (95%)	-0.32	13 (1%) 65 72	13, 24, 43, 58	0
All	All	1456/1532 (95%)	-0.28	26 (1%) 65 72	13, 24, 44, 59	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	39	THR	6.2
1	A	766	PRO	3.9
1	B	39	THR	3.8
1	A	92	ASN	3.7
1	B	766	PRO	3.7
1	A	73	GLU	3.3
1	A	97	GLU	3.3
1	B	73	GLU	3.2
1	B	96	ASP	3.0
1	A	40	ARG	2.9
1	B	138	ASN	2.7
1	A	138	ASN	2.7
1	B	74	ASN	2.7
1	B	91	GLU	2.6
1	A	279	VAL	2.6
1	B	97	GLU	2.5
1	B	95	PHE	2.4
1	A	278	SER	2.3
1	B	506	ASN	2.3
1	A	137	LEU	2.3
1	A	333	SER	2.2
1	A	96	ASP	2.2
1	B	505	GLN	2.2
1	B	88	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	54	ARG	2.1
1	A	74	ASN	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

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	NDG	O	1230	14/15	0.24	9.17	48,52,54,55	0
4	NDG	P	1321	14/15	0.29	7.14	44,48,49,53	0
5	NAG	R	2219	14/15	0.13	6.04	32,37,40,41	0
5	NAG	T	2282	14/15	0.20	5.89	44,46,48,48	0
4	NAG	P	1322	14/15	0.43	5.13	54,56,59,60	0
4	NDG	M	1150	14/15	0.29	4.78	53,54,56,57	0
5	NAG	M	1219	14/15	0.15	2.72	39,42,44,44	0
5	NAG	M	1220	14/15	0.21	2.71	44,47,49,50	0
5	NAG	T	2281	14/15	0.11	1.36	30,31,38,40	0
5	NAG	R	2220	14/15	0.17	1.27	41,42,46,46	0
5	NAG	Q	2085	14/15	0.15	0.74	46,50,54,57	0
5	NAG	S	2230	14/15	0.27	0.59	43,45,47,48	0
5	NAG	S	2229	14/15	0.12	0.54	29,32,39,40	0
2	NAG	O	1229	14/15	0.12	0.48	36,39,43,46	0
2	NAG	L	1085	14/15	0.13	0.15	40,44,49,52	0
4	NAG	M	1151	14/15	0.31	-	55,58,61,62	0
5	NAG	Q	2086	14/15	0.43	-	59,61,63,63	0
2	NDG	L	1086	14/15	0.32	-	55,57,58,59	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(Å ²)	Q<0.9
3	NAG	B	2321	14/15	0.31	6.92	42,45,47,48	0
3	NAG	B	2150	14/15	0.27	6.60	46,49,51,52	0
3	NAG	A	1520	14/15	0.35	5.70	55,56,58,58	0
7	474	B	2322	32/32	0.17	1.48	17,19,22,25	0
3	NAG	A	1092	14/15	0.43	1.46	59,59,61,61	0
7	474	A	1521	32/32	0.18	1.36	19,21,23,25	0
3	NAG	B	2092	14/15	0.32	0.27	55,57,58,59	0
3	NAG	A	1281	14/15	0.16	-0.28	45,46,48,48	0
6	NA	A	1522	1/1	0.08	-0.63	27,27,27,27	0

6.5 Other polymers ⓘ

There are no such residues in this entry.