



# Full wwPDB X-ray Structure Validation Report

Feb 26, 2014 – 09:55 PM GMT

PDB ID : 3C43  
Title : Human dipeptidyl peptidase IV/CD26 in complex with a flouroolefin inhibitor  
Authors : Scapin, G.; Edmondson, S.D.; Weber, A.E.  
Deposited on : 2008-01-29  
Resolution : 2.30 Å(reported)

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

---

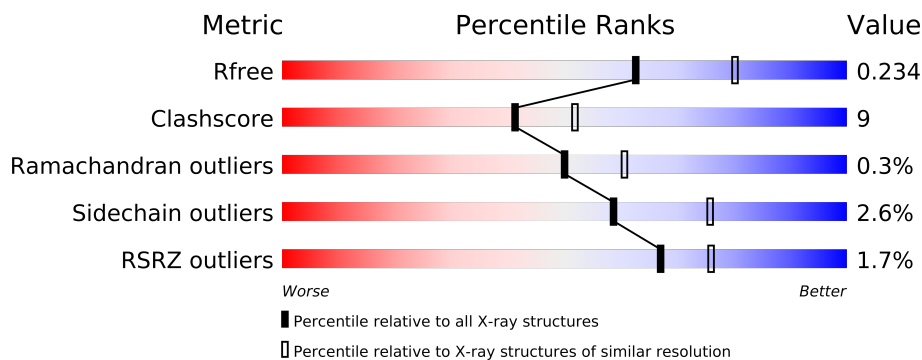
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.30 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	2929 (2.30-2.30)
Clashscore	79885	3679 (2.30-2.30)
Ramachandran outliers	78287	3642 (2.30-2.30)
Sidechain outliers	78261	3641 (2.30-2.30)
RSRZ outliers	66119	2930 (2.30-2.30)

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  $\geq 3$ , 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	728	
1	B	728	

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
6	315	A	1	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13049 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

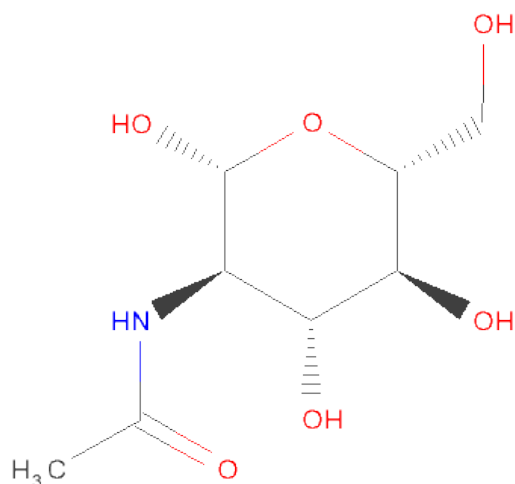
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

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

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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	A	2	Total	C	N	O	0	0
			28	16	2	10		

There is a discrepancy between the modelled and reference sequences:

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

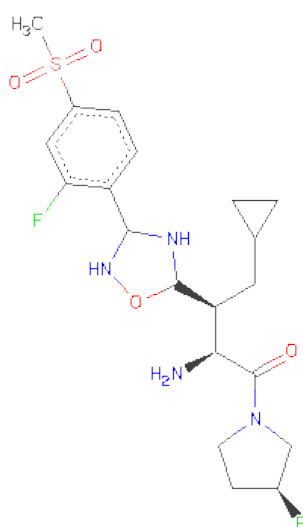
- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

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

There are 6 discrepancies between the modelled and reference sequences:

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

- Molecule 6 is (2S,3S)-4-CYCLOPROPYL-3-[(3R,5R)-3-[2-FLUORO-4-(METHYLSULFONYL)PHENYL]-1,2,4-OXADIAZOLIDIN-5-YL]-1-[(3S)-3-FLUOROPYRROLIDIN-1-YL]-1-OXOBUTAN-2-AMINE (three-letter code: 315) (formula: C<sub>20</sub>H<sub>28</sub>F<sub>2</sub>N<sub>4</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	S	0	0
			31	20	2	4	4	1		
6	B	1	Total	C	F	N	O	S	0	0
			31	20	2	4	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	362	Total	O	0	0
			362	362		
7	B	359	Total	O	0	0
			359	359		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.86Å 125.83Å 136.71Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.30 29.76 – 2.28	Depositor EDS
% Data completeness (in resolution range)	94.5 (30.00-2.30) 95.9 (29.76-2.28)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.68 (at 2.29Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.194 , 0.234 0.193 , 0.234	Depositor DCC
$R_{free}$ test set	4476 reflections (5.31%)	DCC
Wilson B-factor (Å <sup>2</sup> )	28.2	Xtriage
Anisotropy	0.466	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 23.2	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 88749 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13049	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.71% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities 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: 315, 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	0.46	0/6137	0.67	2/8346 (0.0%)
1	B	0.46	0/6137	0.67	1/8346 (0.0%)
All	All	0.46	0/12274	0.67	3/16692 (0.0%)

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
1	B	0	1
2	A	1	0
All	All	1	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	388	GLN	N-CA-C	-5.49	96.17	111.00
1	A	458	SER	N-CA-C	-5.46	96.25	111.00
1	A	300	LEU	N-CA-C	-5.24	96.86	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1230	NDG	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	700	TYR	Sidechain
1	B	735	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	5677	112	0
1	B	5965	0	5679	106	0
2	A	56	0	50	3	0
3	A	42	0	39	4	0
3	B	42	0	39	0	0
4	A	28	0	25	6	0
5	A	56	0	50	1	0
5	B	112	0	100	4	0
6	A	31	0	24	0	0
6	B	31	0	24	0	0
7	A	362	0	0	7	0
7	B	359	0	0	7	0
All	All	13049	0	11707	221	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 9.

All (221) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:651:ILE:HG21	1:B:755:MET:HE2	1.43	1.00
1:A:253:ARG:HH22	1:B:253:ARG:NH1	1.74	0.85
2:A:1230:NDG:O7	2:A:1230:NDG:H3	1.75	0.85
1:A:139:LYS:O	1:A:141:GLN:HG2	1.79	0.83
1:B:760:LYS:HA	1:B:765:LEU:HD23	1.62	0.80
1:A:581:ARG:NH1	3:A:1520:NAG:H62	1.96	0.80
1:A:581:ARG:CZ	3:A:1520:NAG:H62	2.12	0.80
1:A:173:TYR:CE2	1:A:184:ARG:HG2	2.17	0.80
5:B:2086:NAG:O7	5:B:2086:NAG:O3	2.01	0.79
1:A:253:ARG:HH22	1:B:253:ARG:HH12	1.26	0.78

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:596:ARG:O	1:A:597:ARG:HD2	1.86	0.76
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.68	0.75
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.69	0.75
1:B:75:ASN:HB3	1:B:92:ASN:H	1.53	0.74
1:A:149:PRO:HA	4:A:1150:NDG:H8C3	1.71	0.73
1:A:253:ARG:NH2	1:B:253:ARG:HH12	1.87	0.73
1:A:75:ASN:HD21	3:A:1092:NAG:HN2	1.36	0.72
1:B:651:ILE:HG21	1:B:755:MET:CE	2.18	0.72
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.70	0.71
1:A:258:LYS:NZ	1:A:712:HIS:HD2	1.89	0.71
1:A:336:ARG:HG3	1:A:336:ARG:HH11	1.57	0.68
1:A:320:GLN:OE1	1:A:669:ARG:HD3	1.92	0.68
1:A:676:PRO:HG2	1:A:677:GLU:OE2	1.94	0.68
1:A:658:ARG:HG2	1:A:661:TYR:CE2	2.29	0.67
1:B:422:TYR:CE2	1:B:423:LYS:HE2	2.29	0.67
1:A:184:ARG:NH1	1:A:187:TRP:HA	2.10	0.67
1:B:258:LYS:NZ	1:B:712:HIS:HD2	1.92	0.66
1:A:390:ASP:O	1:A:391:LYS:HD2	1.95	0.66
1:A:691:ARG:HD2	7:A:1525:HOH:O	1.95	0.66
1:B:391:LYS:HE3	7:B:2599:HOH:O	1.96	0.66
1:A:293:MET:HE3	1:A:315:TRP:HB2	1.79	0.65
1:A:184:ARG:HH11	1:A:187:TRP:HA	1.63	0.64
1:B:272:ASN:HD21	1:B:274:ASP:HB2	1.63	0.64
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.81	0.63
1:B:272:ASN:C	1:B:272:ASN:HD22	2.02	0.63
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.80	0.63
1:A:620:ASP:OD2	1:A:623:ARG:HD3	1.99	0.62
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.30	0.62
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.99	0.62
1:B:620:ASP:OD2	1:B:623:ARG:HD3	2.00	0.62
1:B:60:LEU:C	1:B:60:LEU:HD12	2.21	0.61
1:B:173:TYR:CE2	1:B:184:ARG:HG2	2.36	0.61
1:B:691:ARG:HD2	7:B:2383:HOH:O	2.01	0.60
1:B:77:LEU:N	1:B:77:LEU:HD12	2.17	0.60
1:A:258:LYS:HZ3	1:A:712:HIS:CD2	2.19	0.59
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.84	0.59
1:B:75:ASN:HD22	1:B:92:ASN:ND2	1.99	0.59
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.37	0.59
5:B:2085:NAG:H4	5:B:2086:NAG:HN2	1.67	0.58
1:A:170:ASN:HD22	1:A:170:ASN:N	2.01	0.58
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.39	0.58
1:B:82:GLU:HG2	1:B:83:TYR:CZ	2.38	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:491:LEU:O	1:B:492:ARG:HB3	2.03	0.58
1:A:149:PRO:CA	4:A:1150:NDG:H8C3	2.34	0.57
1:A:621:ASN:HD22	1:A:622:LYS:N	2.03	0.57
1:A:388:GLN:HB3	1:A:391:LYS:HB2	1.87	0.57
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.86	0.56
1:B:487:ASN:C	1:B:487:ASN:HD22	2.07	0.56
1:A:175:LYS:HG3	1:A:182:SER:HB3	1.86	0.56
1:B:459:VAL:HG22	1:B:460:SER:N	2.20	0.56
1:B:501:ASP:O	1:B:505:GLN:HG2	2.05	0.56
1:B:765:LEU:HB2	1:B:766:PRO:O	2.06	0.56
1:A:149:PRO:HA	4:A:1150:NDG:C8	2.35	0.56
1:B:765:LEU:N	1:B:766:PRO:HA	2.21	0.55
1:A:65:ASP:OD2	1:A:466:LYS:HB2	2.06	0.55
1:A:60:LEU:C	1:A:60:LEU:HD12	2.27	0.55
1:A:91:GLU:HB2	1:A:94:THR:OG1	2.06	0.55
1:B:75:ASN:HB3	1:B:92:ASN:N	2.21	0.55
1:A:153:GLN:HE22	1:A:170:ASN:ND2	2.05	0.55
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.42	0.54
1:A:459:VAL:HG22	1:A:460:SER:N	2.22	0.54
1:B:47:ASP:HA	1:B:52:THR:HG23	1.90	0.53
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.43	0.53
1:A:112:GLN:HG2	1:A:138:ASN:HD21	1.72	0.53
1:B:487:ASN:ND2	1:B:489:LYS:H	2.06	0.53
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.38	0.53
1:B:658:ARG:HD3	1:B:660:GLU:HB2	1.91	0.53
1:A:214:LEU:O	1:A:214:LEU:HD12	2.08	0.53
1:A:726:VAL:HG23	1:A:728:VAL:HG12	1.90	0.53
1:A:392:LYS:HD3	7:A:1777:HOH:O	2.08	0.52
1:B:345:HIS:HD2	7:B:2401:HOH:O	1.92	0.52
1:A:253:ARG:NH2	1:B:253:ARG:NH1	2.49	0.52
1:A:489:LYS:HE3	7:A:1731:HOH:O	2.08	0.52
1:B:109:PRO:HG2	1:B:158:SER:O	2.09	0.52
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.39	0.52
1:B:184:ARG:NH1	1:B:187:TRP:HA	2.24	0.52
1:A:136:ASP:HB3	1:A:139:LYS:HG2	1.91	0.52
1:A:98:PHE:CD2	1:A:100:HIS:HB2	2.45	0.52
1:B:450:ASN:HB2	7:B:2416:HOH:O	2.10	0.51
1:A:319:ILE:HG12	7:A:1706:HOH:O	2.10	0.51
1:B:415:LEU:C	1:B:415:LEU:HD23	2.30	0.51
1:B:487:ASN:HD22	1:B:488:ASP:N	2.09	0.51
1:B:504:LEU:HA	1:B:507:VAL:HG12	1.93	0.51
1:B:272:ASN:HD22	1:B:274:ASP:H	1.59	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:110:ASP:OD2	1:A:112:GLN:HB2	2.12	0.50
1:B:513:LYS:O	1:B:527:GLN:HA	2.12	0.50
2:A:1230:NDG:C3	2:A:1230:NDG:O7	2.49	0.50
1:A:489:LYS:HB2	1:A:489:LYS:HZ2	1.76	0.50
1:A:623:ARG:NH2	1:A:765:LEU:HD21	2.26	0.50
1:A:107:ILE:HG22	1:A:108:SER:O	2.11	0.50
1:A:723:LEU:HB3	1:A:728:VAL:HG13	1.94	0.49
1:A:150:ASN:O	1:A:151:ASN:HB2	2.12	0.49
4:A:1150:NDG:O3	4:A:1151:NAG:N2	2.45	0.49
1:A:489:LYS:HB2	1:A:489:LYS:NZ	2.27	0.49
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.47	0.49
1:B:310:ARG:HH12	1:B:343:ARG:NH1	2.11	0.49
1:A:669:ARG:HD2	7:A:1688:HOH:O	2.12	0.49
1:B:65:ASP:CG	1:B:464:GLU:HB2	2.33	0.49
1:A:159:PRO:HG3	1:A:217:SER:O	2.13	0.49
1:B:258:LYS:HZ1	1:B:712:HIS:HD2	1.58	0.49
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.95	0.49
1:A:293:MET:HG2	1:A:315:TRP:HB3	1.95	0.49
1:A:81:ALA:O	1:A:492:ARG:NH2	2.41	0.49
1:B:125:ARG:HG2	1:B:126:HIS:CD2	2.48	0.49
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.93	0.49
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.43	0.49
1:B:649:CYS:HB3	1:B:699:GLU:HB2	1.95	0.49
1:A:217:SER:HB3	1:A:222:PHE:HB2	1.96	0.48
1:B:167:VAL:HG21	1:B:198:ILE:HG23	1.95	0.48
1:A:312:SER:O	1:A:313:LEU:HD12	2.14	0.48
1:B:756:SER:O	1:B:760:LYS:HG3	2.14	0.47
5:B:2086:NAG:C7	5:B:2086:NAG:HO3	2.13	0.47
1:A:330:TYR:HB2	1:A:337:TRP:CH2	2.49	0.47
1:B:258:LYS:HZ3	1:B:712:HIS:CD2	2.33	0.47
1:B:81:ALA:O	1:B:492:ARG:NH2	2.44	0.47
2:A:1229:NAG:H61	2:A:1230:NDG:O	2.15	0.47
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.97	0.47
1:A:621:ASN:C	1:A:621:ASN:HD22	2.18	0.47
1:B:272:ASN:ND2	1:B:274:ASP:H	2.13	0.47
1:B:123:GLN:HG2	1:B:124:TRP:N	2.30	0.47
1:B:171:ASP:HB2	7:B:2378:HOH:O	2.14	0.46
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.98	0.46
1:B:589:LYS:HB3	7:B:2503:HOH:O	2.16	0.46
1:A:295:ILE:HG13	1:A:296:GLY:N	2.31	0.46
1:A:534:PHE:HZ	1:A:618:PHE:CG	2.33	0.46
1:A:336:ARG:HG3	1:A:336:ARG:NH1	2.28	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:312:SER:HB2	1:A:325:MET:CE	2.46	0.46
1:B:626:ILE:O	1:B:650:GLY:HA2	2.16	0.46
1:A:41:LYS:HG3	7:A:1606:HOH:O	2.15	0.46
1:A:546:VAL:CG2	1:A:547:TYR:N	2.79	0.45
1:B:254:VAL:HA	1:B:255:PRO:HD3	1.85	0.45
1:A:258:LYS:HZ1	1:A:712:HIS:HD2	1.61	0.45
1:B:156:THR:HG21	1:B:214:LEU:HD11	1.97	0.45
1:B:532:PRO:HD3	1:B:569:SER:HA	1.97	0.45
1:A:546:VAL:HG22	1:A:547:TYR:N	2.31	0.45
1:B:40:ARG:HG2	1:B:506:ASN:HD22	1.81	0.45
1:B:98:PHE:CD2	1:B:100:HIS:HB2	2.51	0.45
1:B:82:GLU:HG2	1:B:83:TYR:CE1	2.52	0.45
1:B:196:ASN:OD1	1:B:227:GLN:HG3	2.17	0.45
1:A:160:VAL:HG12	1:A:161:GLY:N	2.32	0.45
1:B:158:SER:HB3	1:B:163:LYS:HB2	1.99	0.45
1:A:312:SER:HB2	1:A:325:MET:HE2	1.99	0.45
1:A:258:LYS:HZ3	1:A:712:HIS:HD2	1.51	0.45
1:A:415:LEU:C	1:A:415:LEU:HD23	2.38	0.44
1:B:111:GLY:O	1:B:137:LEU:HD12	2.17	0.44
4:A:1150:NDG:H4	4:A:1151:NAG:H2	1.67	0.44
1:B:741:GLY:O	1:B:742:ILE:C	2.55	0.44
1:A:73:GLU:HB3	3:A:1092:NAG:H3	1.98	0.44
1:B:658:ARG:HG3	1:B:658:ARG:O	2.17	0.44
1:B:80:ASN:OD1	1:B:82:GLU:HB3	2.17	0.44
1:B:463:LYS:HD3	1:B:463:LYS:HA	1.84	0.44
1:A:240:PHE:HB3	1:A:250:LYS:HG2	2.00	0.44
1:B:760:LYS:HB3	1:B:766:PRO:O	2.18	0.44
1:A:693:GLU:HB2	7:A:1561:HOH:O	2.18	0.43
1:B:651:ILE:CG2	1:B:755:MET:HE2	2.30	0.43
1:A:388:GLN:CB	1:A:391:LYS:HB2	2.47	0.43
1:A:539:LYS:HD3	1:A:617:GLY:O	2.18	0.43
1:B:418:ILE:HA	1:B:430:ASN:O	2.18	0.43
1:A:123:GLN:HB3	1:A:127:SER:OG	2.18	0.43
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.36	0.43
1:B:313:LEU:O	1:B:325:MET:HA	2.18	0.43
1:B:765:LEU:HB2	1:B:766:PRO:C	2.38	0.43
1:A:689:MET:HE3	1:B:244:GLU:HG3	2.01	0.43
1:B:184:ARG:HH11	1:B:187:TRP:HA	1.84	0.43
1:A:387:PHE:CD1	1:A:394:CYS:HB3	2.53	0.43
1:B:310:ARG:NH1	1:B:329:ASP:OD1	2.52	0.43
1:B:614:SER:HA	1:B:619:VAL:HB	2.01	0.43
1:A:193:ILE:HG22	1:A:194:ILE:HG12	2.01	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:143:ILE:CD1	1:A:178:PRO:HB2	2.48	0.42
1:B:125:ARG:HG2	1:B:126:HIS:NE2	2.34	0.42
1:A:139:LYS:O	1:A:140:ARG:C	2.56	0.42
1:A:626:ILE:HG23	1:A:636:THR:HG23	2.01	0.42
1:A:109:PRO:HD2	1:A:161:GLY:O	2.20	0.42
1:B:334:SER:O	1:B:336:ARG:HG2	2.18	0.42
1:B:57:LEU:HA	1:B:480:TYR:CE1	2.54	0.42
1:A:73:GLU:O	1:A:74:ASN:HB2	2.19	0.42
1:B:596:ARG:O	1:B:597:ARG:HD2	2.19	0.42
1:A:289:ALA:HB2	1:A:315:TRP:CH2	2.55	0.42
1:A:175:LYS:NZ	1:A:178:PRO:O	2.42	0.42
1:A:77:LEU:HD23	1:A:88:VAL:HA	2.00	0.42
1:B:66:HIS:HB3	1:B:467:TYR:HE2	1.84	0.42
1:B:150:ASN:O	1:B:151:ASN:HB2	2.20	0.42
1:B:422:TYR:CZ	1:B:423:LYS:HE2	2.55	0.41
1:A:621:ASN:ND2	1:A:621:ASN:C	2.73	0.41
5:B:2085:NAG:H4	5:B:2086:NAG:N2	2.34	0.41
1:A:658:ARG:HD3	1:A:660:GLU:HB2	2.02	0.41
1:B:107:ILE:HD12	1:B:107:ILE:N	2.35	0.41
1:A:197:GLY:C	1:A:213:ALA:HB3	2.40	0.41
1:B:258:LYS:HZ3	1:B:712:HIS:HD2	1.61	0.41
1:A:489:LYS:CB	1:A:489:LYS:NZ	2.83	0.41
1:B:378:GLU:HG2	7:B:2667:HOH:O	2.20	0.41
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.50	0.41
1:B:405:ILE:HG13	1:B:429:ARG:CD	2.50	0.41
1:B:484:SER:OG	1:B:486:VAL:HG12	2.21	0.41
1:A:390:ASP:OD1	1:A:390:ASP:N	2.50	0.41
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.01	0.41
1:A:536:LYS:H	1:A:536:LYS:HG2	1.58	0.41
1:B:544:LEU:HD21	1:B:606:GLN:HG3	2.01	0.41
1:A:626:ILE:O	1:A:650:GLY:HA2	2.21	0.41
1:A:312:SER:C	1:A:313:LEU:HD12	2.40	0.41
1:A:114:ILE:HG23	1:A:135:TYR:HB3	2.03	0.41
5:A:1321:NAG:H61	5:A:1322:NAG:O5	2.21	0.41
1:A:236:ILE:CG2	1:A:254:VAL:HG13	2.50	0.41
1:A:588:ASP:O	1:A:592:HIS:HB2	2.21	0.40
1:B:677:GLU:N	1:B:677:GLU:OE1	2.45	0.40
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.56	0.40
1:B:546:VAL:CG2	1:B:547:TYR:N	2.83	0.40
1:A:149:PRO:HB3	4:A:1150:NDG:H8C3	2.03	0.40
1:B:658:ARG:HG2	1:B:661:TYR:CZ	2.56	0.40
1:A:751:ILE:HG23	1:A:752:TYR:N	2.36	0.40

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:224:ALA:HB1	1:B:268:PHE:CZ	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	726/728 (100%)	696 (96%)	28 (4%)	2 (0%)	50	60
1	B	726/728 (100%)	687 (95%)	37 (5%)	2 (0%)	50	60
All	All	1452/1456 (100%)	1383 (95%)	65 (4%)	4 (0%)	50	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	40	ARG
1	A	40	ARG
1	A	320	GLN
1	B	320	GLN

### 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	653/653 (100%)	633 (97%)	20 (3%)	52	68
1	B	653/653 (100%)	639 (98%)	14 (2%)	66	83
All	All	1306/1306 (100%)	1272 (97%)	34 (3%)	59	76

All (34) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	41	LYS
1	A	96	ASP
1	A	147	ARG
1	A	170	ASN
1	A	184	ARG
1	A	230	ASP
1	A	253	ARG
1	A	254	VAL
1	A	278	SER
1	A	326	ASP
1	A	333	SER
1	A	388	GLN
1	A	391	LYS
1	A	448	GLU
1	A	472	CYS
1	A	507	VAL
1	A	566	TYR
1	A	608	GLU
1	A	621	ASN
1	A	658	ARG
1	B	54	ARG
1	B	66	HIS
1	B	184	ARG
1	B	230	ASP
1	B	254	VAL
1	B	272	ASN
1	B	385	CYS
1	B	472	CYS
1	B	487	ASN
1	B	506	ASN
1	B	597	ARG
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 (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	74	ASN
1	A	75	ASN
1	A	123	GLN
1	A	138	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	151	ASN
1	A	169	ASN
1	A	170	ASN
1	A	572	ASN
1	A	621	ASN
1	A	712	HIS
1	B	51	ASN
1	B	74	ASN
1	B	75	ASN
1	B	119	ASN
1	B	169	ASN
1	B	272	ASN
1	B	338	ASN
1	B	345	HIS
1	B	435	GLN
1	B	487	ASN
1	B	506	ASN
1	B	533	HIS
1	B	712	HIS
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	A	1085	1,2	12,14,15	0.47	0	15,19,21	1.17	1 (6%)
2	NDG	A	1086	2	12,14,15	0.75	0	15,19,21	0.82	0
4	NDG	A	1150	1,4	12,14,15	0.49	0	15,19,21	0.72	0
4	NAG	A	1151	4	12,14,15	0.58	0	15,19,21	0.82	0
5	NAG	A	1219	1,5	12,14,15	0.53	0	15,19,21	0.78	0
5	NAG	A	1220	5	12,14,15	0.56	0	15,19,21	0.69	0
2	NAG	A	1229	1,2	12,14,15	0.44	0	15,19,21	0.95	1 (6%)
2	NDG	A	1230	2	12,14,15	0.41	0	15,19,21	1.42	3 (20%)
5	NAG	A	1321	1,5	12,14,15	0.67	0	15,19,21	0.79	0
5	NAG	A	1322	5	12,14,15	0.49	0	15,19,21	0.59	0
5	NAG	B	2085	1,5	12,14,15	0.65	0	15,19,21	0.73	0
5	NAG	B	2086	5	12,14,15	0.48	0	15,19,21	0.96	0
5	NAG	B	2219	1,5	12,14,15	0.58	0	15,19,21	0.73	0
5	NAG	B	2220	5	12,14,15	0.52	0	15,19,21	1.03	0
5	NAG	B	2229	1,5	12,14,15	0.54	0	15,19,21	1.02	2 (13%)
5	NAG	B	2230	5	12,14,15	0.49	0	15,19,21	0.99	0
5	NAG	B	2281	1,5	12,14,15	0.51	0	15,19,21	0.72	0
5	NAG	B	2282	5	12,14,15	0.50	0	15,19,21	0.97	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	A	1085	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	1086	2	-	0/6/23/26	0/1/1/1
4	NDG	A	1150	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	1151	4	-	0/6/23/26	0/1/1/1
5	NAG	A	1219	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1220	5	-	0/6/23/26	0/1/1/1
2	NAG	A	1229	1,2	-	0/6/23/26	0/1/1/1
2	NDG	A	1230	2	1/1/5/7	0/6/23/26	0/1/1/1
5	NAG	A	1321	1,5	-	0/6/23/26	0/1/1/1
5	NAG	A	1322	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2085	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2086	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2219	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2220	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2229	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	2230	5	-	0/6/23/26	0/1/1/1
5	NAG	B	2281	1,5	-	0/6/23/26	0/1/1/1

*Continued on next page...*

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NAG	B	2282	5	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1230	NDG	O-C5-C6	2.70	109.81	106.98
2	A	1229	NAG	C3-C2-N2	-2.58	107.83	111.76
2	A	1085	NAG	C4-C3-C2	-2.50	105.19	111.32
5	B	2229	NAG	C2-N2-C7	-2.44	118.98	123.09
5	B	2229	NAG	C3-C2-N2	-2.37	108.15	111.76
2	A	1230	NDG	C8-C7-N2	2.34	120.68	116.11
2	A	1230	NDG	C2-N2-C7	-2.33	119.19	123.09

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1230	NDG	C1

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

8 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	$\# Z  > 2$
6	315	A	1	-	34,34,34	3.38	15 (44%)	51,51,51	2.89	11 (21%)
3	NAG	A	1092	1	12,14,15	0.69	0	15,19,21	0.66	0
3	NAG	A	1281	1	12,14,15	0.59	0	15,19,21	0.75	0
3	NAG	A	1520	1	12,14,15	0.57	0	15,19,21	0.75	0
6	315	B	2	-	34,34,34	3.44	14 (41%)	51,51,51	2.94	10 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NAG	B	2092	1	12,14,15	0.57	0	15,19,21	0.63	0
3	NAG	B	2150	1	12,14,15	0.57	0	15,19,21	0.91	1 (6%)
3	NAG	B	2321	1	12,14,15	0.63	0	15,19,21	0.71	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
6	315	A	1	-	2/2/9/11	0/29/50/50	0/2/4/4
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
6	315	B	2	-	2/2/9/11	0/29/50/50	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

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2	315	O38-N37	-9.20	1.33	1.45
6	A	1	315	C2-N6	-8.94	1.15	1.47
6	A	1	315	O38-N37	-8.75	1.34	1.45
6	B	2	315	C2-N6	-8.47	1.17	1.47
6	B	2	315	C1-C33	6.81	1.62	1.52
6	A	1	315	C36-N37	-6.38	1.35	1.47
6	B	2	315	C36-N35	-6.29	1.35	1.47
6	A	1	315	C1-C33	6.19	1.62	1.52
6	B	2	315	C39-C44	6.15	1.46	1.38
6	A	1	315	C36-N35	-5.97	1.36	1.47
6	B	2	315	C36-N37	-5.95	1.36	1.47
6	A	1	315	C39-C44	5.45	1.45	1.38
6	A	1	315	C2-C3	3.99	1.58	1.52
6	B	2	315	C2-C3	3.76	1.58	1.52
6	A	1	315	C33-N35	-3.49	1.31	1.44
6	B	2	315	C39-C36	-3.38	1.49	1.52
6	A	1	315	O38-C33	-3.34	1.34	1.44
6	B	2	315	O38-C33	-3.23	1.34	1.44
6	B	2	315	C33-N35	-3.19	1.32	1.44
6	A	1	315	C1-C2	2.83	1.59	1.54

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1	315	C8-C23	2.60	1.58	1.53
6	A	1	315	C40-C39	2.39	1.43	1.39
6	B	2	315	C1-C2	2.34	1.58	1.54
6	B	2	315	C41-C42	2.28	1.42	1.38
6	A	1	315	C39-C36	-2.23	1.50	1.52
6	A	1	315	C8-C1	2.15	1.56	1.54
6	A	1	315	C43-C44	2.12	1.41	1.37
6	B	2	315	C8-C1	2.07	1.56	1.54
6	B	2	315	C40-C39	2.06	1.42	1.39

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2	315	C8-C23-C26	-9.97	106.29	120.51
6	A	1	315	C39-C36-N35	9.78	127.00	111.58
6	B	2	315	C39-C36-N35	9.36	126.33	111.58
6	A	1	315	C8-C23-C26	-9.29	107.26	120.51
6	B	2	315	O38-N37-C36	6.80	108.66	103.90
6	B	2	315	C39-C36-N37	6.79	122.17	111.51
6	A	1	315	C39-C36-N37	6.58	121.85	111.51
6	A	1	315	O38-N37-C36	6.41	108.39	103.90
6	B	2	315	O38-C33-N35	6.25	117.95	104.45
6	A	1	315	O38-C33-N35	6.07	117.58	104.45
6	A	1	315	C1-C33-N35	5.89	127.24	113.49
6	B	2	315	C1-C33-N35	5.68	126.76	113.49
6	B	2	315	F48-C44-C39	4.84	123.89	118.28
6	A	1	315	F48-C44-C39	4.25	123.21	118.28
6	B	2	315	C40-C39-C36	-2.77	116.60	121.64
6	A	1	315	C8-C23-C27	2.61	124.25	120.51
6	A	1	315	C40-C39-C36	-2.45	117.18	121.64
6	A	1	315	C12-C11-N4	2.30	105.83	103.05
6	B	2	315	O51-S49-C42	-2.12	106.58	108.23
6	B	2	315	C36-N35-C33	-2.11	99.98	106.67
3	B	2150	NAG	C2-N2-C7	-2.09	119.59	123.09
6	A	1	315	C8-C1-C33	-2.03	106.87	111.56

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	2	315	C33
6	B	2	315	C36
6	A	1	315	C33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atom
6	A	1	315	C36

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	728/728 (100%)	-0.30	13 (1%) 65 74	15, 25, 47, 61	0
1	B	728/728 (100%)	-0.26	10 (1%) 72 80	15, 26, 45, 62	0
All	All	1456/1456 (100%)	-0.28	23 (1%) 67 77	15, 26, 46, 62	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	766	PRO	7.0
1	B	39	THR	6.2
1	A	39	THR	5.8
1	B	765	LEU	5.6
1	A	766	PRO	4.3
1	A	73	GLU	3.6
1	B	74	ASN	3.6
1	A	279	VAL	3.2
1	A	97	GLU	3.1
1	B	138	ASN	3.1
1	A	92	ASN	3.1
1	B	73	GLU	3.0
1	A	96	ASP	2.9
1	B	506	ASN	2.7
1	A	138	ASN	2.6
1	B	71	LYS	2.6
1	A	521	GLU	2.5
1	A	74	ASN	2.3
1	A	278	SER	2.3
1	A	336	ARG	2.2
1	A	333	SER	2.2
1	B	97	GLU	2.1
1	B	334	SER	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	NAG	A	1322	14/15	0.45	13.26	59,60,63,64	0
5	NAG	A	1321	14/15	0.29	12.14	45,48,51,56	0
5	NAG	A	1219	14/15	0.22	5.31	40,44,47,48	0
4	NDG	A	1150	14/15	0.36	4.88	55,58,62,62	0
5	NAG	B	2219	14/15	0.19	4.30	34,40,42,44	0
5	NAG	B	2281	14/15	0.14	2.89	30,34,42,45	0
2	NAG	A	1085	14/15	0.15	2.40	43,47,52,56	0
2	NAG	A	1229	14/15	0.16	2.31	35,38,42,45	0
5	NAG	B	2220	14/15	0.25	2.17	45,47,50,50	0
5	NAG	B	2085	14/15	0.14	2.01	45,52,54,58	0
5	NAG	A	1220	14/15	0.26	1.84	47,48,50,51	0
5	NAG	B	2229	14/15	0.16	1.37	28,31,36,40	0
5	NAG	B	2230	14/15	0.39	0.81	43,46,50,53	0
5	NAG	B	2282	14/15	0.32	-	49,52,54,54	0
2	NDG	A	1230	14/15	0.37	-	45,52,59,61	0
4	NAG	A	1151	14/15	0.37	-	58,62,64,64	0
2	NDG	A	1086	14/15	0.35	-	60,62,63,63	0
5	NAG	B	2086	14/15	0.33	-	60,62,63,64	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, 95<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	2150	14/15	0.34	8.32	53,55,57,58	0
3	NAG	A	1520	14/15	0.40	5.61	56,59,61,62	0
3	NAG	B	2321	14/15	0.24	4.73	40,43,44,46	0
6	315	A	1	31/31	0.14	2.35	20,36,38,43	0
3	NAG	A	1092	14/15	0.45	1.76	60,62,63,63	0
3	NAG	B	2092	14/15	0.39	1.56	59,60,62,62	0
6	315	B	2	31/31	0.13	1.02	21,32,37,41	0
3	NAG	A	1281	14/15	0.20	-0.16	48,50,51,51	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.