



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 08:47 AM GMT

PDB ID : 3G0G  
Title : Crystal structure of dipeptidyl peptidase IV in complex with a pyrimidinone inhibitor 3  
Authors : Zhang, Z.; Wallace, M.B.; Feng, J.; Stafford, J.A.; Kaldor, S.W.; Shi, L.; Skene, R.J.; Aertgeerts, K.; Lee, B.; Jennings, A.; Xu, R.; Kassel, D.; Webb, D.R.; Gwaltney, S.L.  
Deposited on : 2009-01-27  
Resolution : 2.45 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

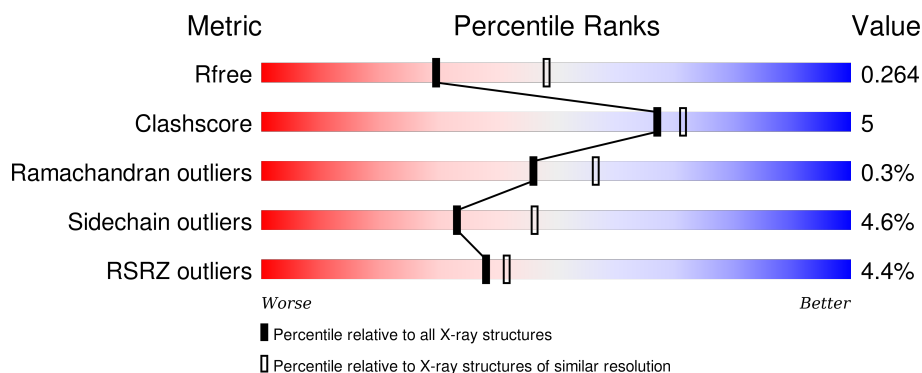
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	740	<div> <div>3%</div> <div>81% 16% ..</div> </div>
1	B	740	<div> <div>%</div> <div>85% 13% ..</div> </div>
1	C	740	<div> <div>5%</div> <div>84% 13% ..</div> </div>
1	D	740	<div> <div>8%</div> <div>80% 12% • 7%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	A	808	-	-	-	X
3	NAG	B	808	-	-	-	X
3	NAG	C	808	-	-	-	X
3	NAG	D	803	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24783 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	2	0
			5933	3811	975	1121	26			
1	B	730	Total	C	N	O	S	0	2	0
			5990	3844	991	1129	26			
1	C	724	Total	C	N	O	S	0	1	0
			5929	3809	974	1120	26			
1	D	690	Total	C	N	O	S	0	1	0
			5649	3631	926	1066	26			

There are 48 discrepancies between the modelled and reference sequences:

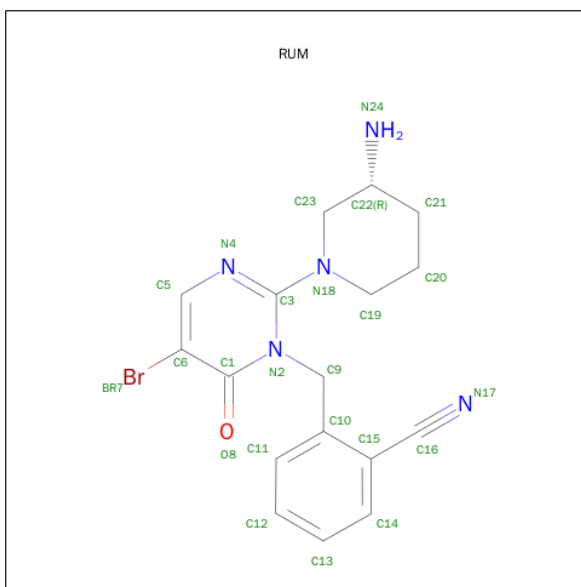
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
A	34	HIS	-	EXPRESSION TAG	UNP P27487
A	35	HIS	-	EXPRESSION TAG	UNP P27487
A	36	HIS	-	EXPRESSION TAG	UNP P27487
A	37	HIS	-	EXPRESSION TAG	UNP P27487
A	38	HIS	-	EXPRESSION TAG	UNP P27487
B	27	ALA	-	EXPRESSION TAG	UNP P27487
B	28	ASP	-	EXPRESSION TAG	UNP P27487
B	29	PRO	-	EXPRESSION TAG	UNP P27487
B	30	GLY	-	EXPRESSION TAG	UNP P27487
B	31	GLY	-	EXPRESSION TAG	UNP P27487
B	32	SER	-	EXPRESSION TAG	UNP P27487
B	33	HIS	-	EXPRESSION TAG	UNP P27487
B	34	HIS	-	EXPRESSION TAG	UNP P27487
B	35	HIS	-	EXPRESSION TAG	UNP P27487

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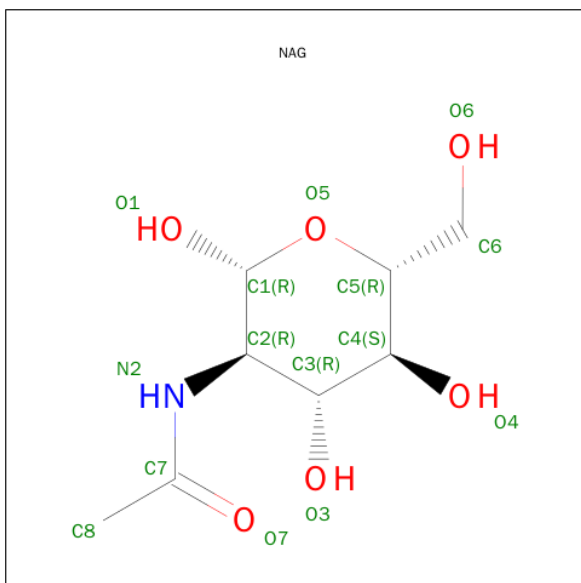
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
C	31	GLY	-	EXPRESSION TAG	UNP P27487
C	32	SER	-	EXPRESSION TAG	UNP P27487
C	33	HIS	-	EXPRESSION TAG	UNP P27487
C	34	HIS	-	EXPRESSION TAG	UNP P27487
C	35	HIS	-	EXPRESSION TAG	UNP P27487
C	36	HIS	-	EXPRESSION TAG	UNP P27487
C	37	HIS	-	EXPRESSION TAG	UNP P27487
C	38	HIS	-	EXPRESSION TAG	UNP P27487
D	27	ALA	-	EXPRESSION TAG	UNP P27487
D	28	ASP	-	EXPRESSION TAG	UNP P27487
D	29	PRO	-	EXPRESSION TAG	UNP P27487
D	30	GLY	-	EXPRESSION TAG	UNP P27487
D	31	GLY	-	EXPRESSION TAG	UNP P27487
D	32	SER	-	EXPRESSION TAG	UNP P27487
D	33	HIS	-	EXPRESSION TAG	UNP P27487
D	34	HIS	-	EXPRESSION TAG	UNP P27487
D	35	HIS	-	EXPRESSION TAG	UNP P27487
D	36	HIS	-	EXPRESSION TAG	UNP P27487
D	37	HIS	-	EXPRESSION TAG	UNP P27487
D	38	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is 2-({2-[(3R)-3-AMINOPIPERIDIN-1-YL]-5-BROMO-6-OXOPYRIMIDIN-1(6H)-YL} METHYL) BENZONITRILE (three-letter code: RUM) (formula: C<sub>17</sub>H<sub>18</sub>BrN<sub>5</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			24	1	17	5	1		
2	B	1	Total	Br	C	N	O	0	0
			24	1	17	5	1		
2	C	1	Total	Br	C	N	O	0	0
			24	1	17	5	1		
2	D	1	Total	Br	C	N	O	0	0
			24	1	17	5	1		

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

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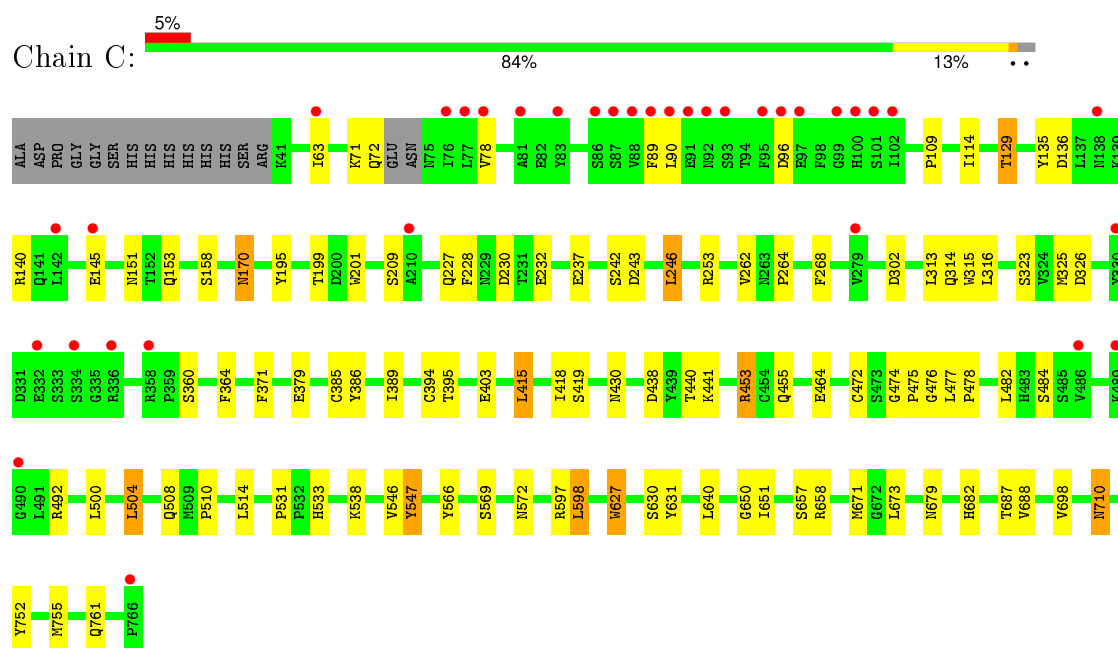
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	C	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		
4	D	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 5 is water.

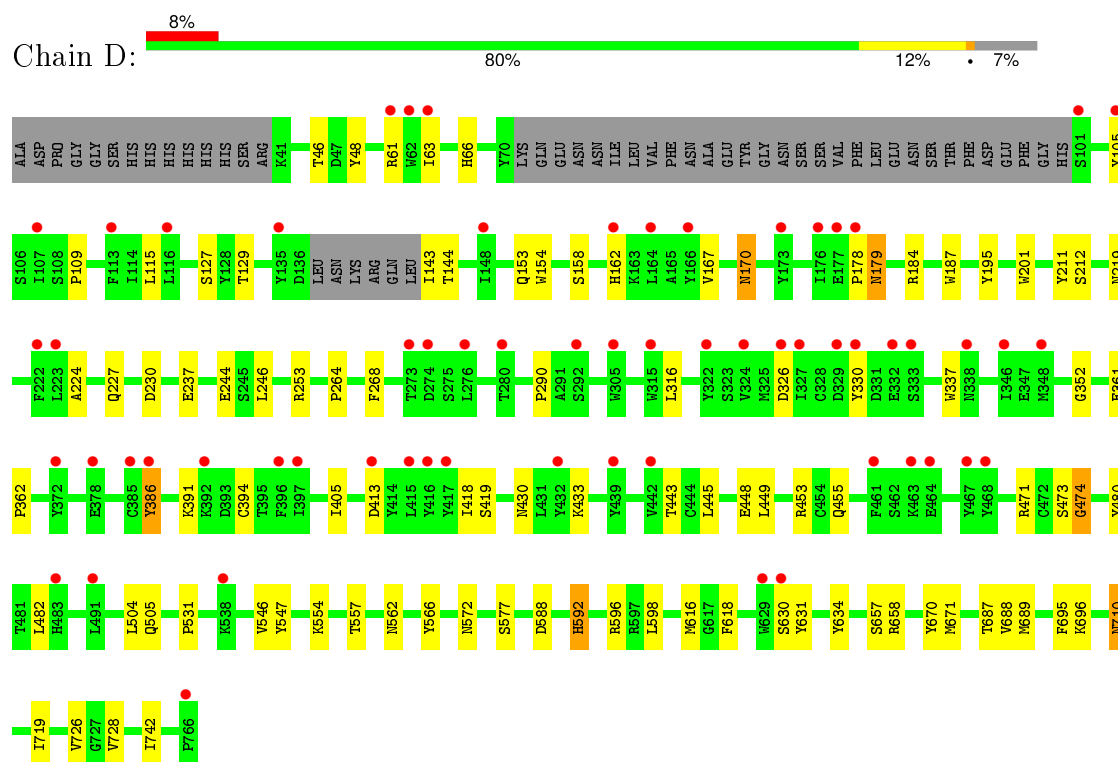
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	699	Total	O	0	0
			699	699		







• Molecule 1: Dipeptidyl peptidase 4



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.91Å 122.92Å 145.09Å 90.00° 114.77° 90.00°	Depositor
Resolution (Å)	50.00 – 2.45 48.52 – 2.45	Depositor EDS
% Data completeness (in resolution range)	95.4 (50.00-2.45) 95.4 (48.52-2.45)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.46 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.210 , 0.265 0.209 , 0.264	Depositor DCC
$R_{free}$ test set	6854 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	47.2	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 46.4	EDS
Estimated twinning fraction	0.012 for h,-k,-h-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 136813 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24783	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, RUM

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	0.49	0/6108	0.61	0/8307
1	B	0.47	0/6169	0.61	0/8389
1	C	0.46	0/6100	0.61	1/8296 (0.0%)
1	D	0.43	0/5813	0.57	0/7908
All	All	0.46	0/24190	0.60	1/32900 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	415	LEU	CA-CB-CG	5.32	127.54	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5933	0	5648	71	0
1	B	5990	0	5692	56	0
1	C	5929	0	5646	48	0
1	D	5649	0	5381	47	0
2	A	24	0	18	3	0
2	B	24	0	18	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	18	3	0
2	D	24	0	18	1	0
3	A	56	0	52	0	0
3	B	56	0	52	0	0
3	C	56	0	52	0	0
3	D	56	0	52	0	0
4	A	56	0	50	0	0
4	B	56	0	50	0	0
4	C	56	0	50	0	0
4	D	56	0	50	0	0
5	A	39	0	0	0	0
5	B	699	0	0	5	0
All	All	24783	0	22847	224	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 224 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:ARG:HH21	1:B:253:ARG:HH21	0.99	0.98
1:C:153:GLN:HE22	1:C:170:ASN:H	1.20	0.87
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.78	0.81
1:A:153:GLN:HE22	1:A:170:ASN:H	1.30	0.79
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.65	0.79

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	721/740 (97%)	680 (94%)	40 (6%)	1 (0%)	56	71
1	B	727/740 (98%)	689 (95%)	37 (5%)	1 (0%)	56	71
1	C	720/740 (97%)	679 (94%)	41 (6%)	0	100	100
1	D	684/740 (92%)	641 (94%)	37 (5%)	6 (1%)	21	25
All	All	2852/2960 (96%)	2689 (94%)	155 (5%)	8 (0%)	46	57

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	474	GLY
1	D	244	GLU
1	D	449	LEU
1	B	244	GLU
1	A	334	SER

### 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	650/662 (98%)	618 (95%)	32 (5%)	31	43
1	B	656/662 (99%)	626 (95%)	30 (5%)	33	46
1	C	649/662 (98%)	617 (95%)	32 (5%)	31	43
1	D	618/662 (93%)	594 (96%)	24 (4%)	39	54
All	All	2573/2648 (97%)	2455 (95%)	118 (5%)	33	46

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	505	GLN
1	C	145	GLU
1	D	453	ARG
1	B	506	ASN
1	B	658	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 55 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	455	GLN
1	C	123	GLN
1	D	455	GLN
1	B	505	GLN
1	B	710	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules 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 ⓘ

16 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	$\# Z  > 2$
4	NAG	A	804	1,4	14,14,15	0.61	0	15,19,21	1.09	1 (6%)
4	NAG	A	805	4	14,14,15	0.51	0	15,19,21	1.13	2 (13%)
4	NAG	A	806	1,4	14,14,15	0.57	0	15,19,21	1.17	1 (6%)
4	NAG	A	807	4	14,14,15	0.56	0	15,19,21	0.75	0
4	NAG	B	804	1,4	14,14,15	0.60	0	15,19,21	0.84	0
4	NAG	B	805	4	14,14,15	0.60	0	15,19,21	1.33	2 (13%)
4	NAG	B	806	1,4	14,14,15	0.49	0	15,19,21	1.02	0
4	NAG	B	807	4	14,14,15	0.55	0	15,19,21	1.17	2 (13%)
4	NAG	C	804	1,4	14,14,15	0.60	0	15,19,21	1.30	1 (6%)
4	NAG	C	805	4	14,14,15	0.53	0	15,19,21	1.01	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	C	806	1,4	14,14,15	0.66	0	15,19,21	1.32	1 (6%)
4	NAG	C	807	4	14,14,15	0.52	0	15,19,21	1.49	3 (20%)
4	NAG	D	804	1,4	14,14,15	0.51	0	15,19,21	0.85	1 (6%)
4	NAG	D	805	4	14,14,15	0.41	0	15,19,21	1.41	4 (26%)
4	NAG	D	806	1,4	14,14,15	0.52	0	15,19,21	1.28	1 (6%)
4	NAG	D	807	4	14,14,15	0.50	0	15,19,21	0.63	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
4	NAG	A	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	805	4	-	0/6/23/26	0/1/1/1
4	NAG	A	806	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	807	4	-	0/6/23/26	0/1/1/1
4	NAG	B	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	805	4	-	0/6/23/26	0/1/1/1
4	NAG	B	806	1,4	-	0/6/23/26	0/1/1/1
4	NAG	B	807	4	-	0/6/23/26	0/1/1/1
4	NAG	C	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	805	4	-	0/6/23/26	0/1/1/1
4	NAG	C	806	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	807	4	-	0/6/23/26	0/1/1/1
4	NAG	D	804	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	805	4	-	0/6/23/26	0/1/1/1
4	NAG	D	806	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	807	4	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	805	NAG	C4-C3-C2	-2.75	106.96	111.23
4	A	805	NAG	C2-N2-C7	-2.45	119.89	123.04
4	D	805	NAG	C2-N2-C7	-2.38	119.99	123.04
4	B	805	NAG	C1-O5-C5	-2.15	109.52	112.25
4	D	805	NAG	C3-C4-C5	-2.04	106.64	110.20

There are no chirality outliers.



There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.6 Ligand geometry ⓘ

20 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$
2	RUM	A	800	-	24,26,26	3.06	4 (16%)	23,36,36	1.88	7 (30%)
3	NAG	A	801	1	14,14,15	0.54	0	15,19,21	1.03	1 (6%)
3	NAG	A	802	1	14,14,15	0.57	0	15,19,21	1.39	2 (13%)
3	NAG	A	803	1	14,14,15	0.60	0	15,19,21	1.02	1 (6%)
3	NAG	A	808	1	14,14,15	0.49	0	15,19,21	1.88	2 (13%)
2	RUM	B	800	-	24,26,26	3.00	4 (16%)	23,36,36	2.01	5 (21%)
3	NAG	B	801	1	14,14,15	0.60	0	15,19,21	1.07	1 (6%)
3	NAG	B	802	1	14,14,15	0.52	0	15,19,21	1.34	1 (6%)
3	NAG	B	803	1	14,14,15	0.60	0	15,19,21	0.88	0
3	NAG	B	808	1	14,14,15	0.51	0	15,19,21	1.44	1 (6%)
2	RUM	C	800	-	24,26,26	3.02	5 (20%)	23,36,36	1.77	6 (26%)
3	NAG	C	801	1	14,14,15	0.61	0	15,19,21	1.08	2 (13%)
3	NAG	C	802	1	14,14,15	0.54	0	15,19,21	1.06	1 (6%)
3	NAG	C	803	1	14,14,15	0.54	0	15,19,21	1.00	1 (6%)
3	NAG	C	808	1	14,14,15	0.70	0	15,19,21	1.33	1 (6%)
2	RUM	D	800	-	24,26,26	3.03	4 (16%)	23,36,36	1.60	2 (8%)
3	NAG	D	801	-	14,14,15	0.51	0	15,19,21	0.96	0
3	NAG	D	802	1	14,14,15	0.55	0	15,19,21	1.49	1 (6%)
3	NAG	D	803	1	14,14,15	0.45	0	15,19,21	0.72	0
3	NAG	D	808	1	14,14,15	0.62	0	15,19,21	0.93	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
2	RUM	A	800	-	-	0/10/20/20	0/3/3/3
3	NAG	A	801	1	-	0/6/23/26	0/1/1/1
3	NAG	A	802	1	-	0/6/23/26	0/1/1/1
3	NAG	A	803	1	-	0/6/23/26	0/1/1/1
3	NAG	A	808	1	-	0/6/23/26	0/1/1/1
2	RUM	B	800	-	-	0/10/20/20	0/3/3/3
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	1/6/23/26	0/1/1/1
3	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NAG	B	808	1	-	0/6/23/26	0/1/1/1
2	RUM	C	800	-	-	0/10/20/20	0/3/3/3
3	NAG	C	801	1	-	0/6/23/26	0/1/1/1
3	NAG	C	802	1	-	0/6/23/26	0/1/1/1
3	NAG	C	803	1	-	0/6/23/26	0/1/1/1
3	NAG	C	808	1	-	0/6/23/26	0/1/1/1
2	RUM	D	800	-	-	0/10/20/20	0/3/3/3
3	NAG	D	801	-	-	0/6/23/26	0/1/1/1
3	NAG	D	802	1	-	0/6/23/26	0/1/1/1
3	NAG	D	803	1	-	0/6/23/26	0/1/1/1
3	NAG	D	808	1	-	0/6/23/26	0/1/1/1

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	RUM	C15-C16	-10.63	1.28	1.44
2	D	800	RUM	C15-C16	-10.46	1.28	1.44
2	A	800	RUM	C15-C16	-9.86	1.29	1.44
2	B	800	RUM	C15-C16	-9.58	1.30	1.44
2	C	800	RUM	C3-N4	2.03	1.37	1.33

The worst 5 of 36 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	RUM	C15-C16-N17	-3.84	171.16	177.82
2	A	800	RUM	C20-C21-C22	-3.31	107.41	111.97
3	A	808	NAG	C2-N2-C7	-2.83	119.40	123.04
2	C	800	RUM	C6-C5-N4	-2.58	119.66	123.23
2	A	800	RUM	BR7-C6-C1	-2.48	117.31	121.48

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	802	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	800	RUM	3	0
2	B	800	RUM	1	0
2	C	800	RUM	3	0
2	D	800	RUM	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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	724/740 (97%)	0.07	20 (2%) 56 60	20, 44, 71, 104	1 (0%)
1	B	730/740 (98%)	0.02	8 (1%) 82 84	21, 45, 68, 103	1 (0%)
1	C	724/740 (97%)	0.23	35 (4%) 34 37	18, 49, 75, 99	1 (0%)
1	D	690/740 (93%)	0.52	62 (8%) 12 12	26, 55, 79, 87	0
All	All	2868/2960 (96%)	0.20	125 (4%) 38 41	18, 47, 76, 104	3 (0%)

The worst 5 of 125 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	464	GLU	6.4
1	D	222	PHE	6.0
1	D	392	LYS	5.7
1	C	89	PHE	5.0
1	C	90	LEU	4.9

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

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

### 6.3 Carbohydrates [i](#)

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	804	14/15	0.92	0.20	1.48	54,57,61,64	0
4	NAG	A	804	14/15	0.93	0.14	1.24	52,55,58,59	0
4	NAG	C	804	14/15	0.91	0.15	0.15	59,63,66,67	0
4	NAG	D	804	14/15	0.93	0.14	-1.00	56,57,58,59	0
4	NAG	D	805	14/15	0.73	0.21	-	60,61,63,63	0
4	NAG	C	807	14/15	0.69	0.31	-	73,75,76,76	0
4	NAG	B	805	14/15	0.75	0.33	-	66,68,68,69	0
4	NAG	B	807	14/15	0.73	0.35	-	71,72,74,74	0
4	NAG	B	806	14/15	0.88	0.12	-	61,64,65,68	0
4	NAG	A	806	14/15	0.84	0.15	-	66,67,69,71	0
4	NAG	D	806	14/15	0.76	0.18	-	91,92,92,93	0
4	NAG	C	805	14/15	0.82	0.31	-	70,71,73,73	0
4	NAG	A	805	14/15	0.88	0.17	-	60,61,62,62	0
4	NAG	C	806	14/15	0.63	0.23	-	68,70,71,73	0
4	NAG	D	807	14/15	0.77	0.36	-	94,94,95,95	0
4	NAG	A	807	14/15	0.82	0.22	-	73,74,75,75	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	808	14/15	0.82	0.30	6.85	57,60,61,62	0
3	NAG	D	803	14/15	0.35	0.59	6.77	89,90,92,92	0
3	NAG	C	808	14/15	0.88	0.28	3.25	64,68,69,69	0
3	NAG	A	808	14/15	0.89	0.24	3.12	58,62,66,66	0
3	NAG	D	808	14/15	0.80	0.26	2.00	66,68,69,69	0
2	RUM	A	800	24/24	0.92	0.20	1.10	38,39,41,42	1
3	NAG	A	801	14/15	0.79	0.25	0.03	71,73,74,74	0
2	RUM	C	800	24/24	0.93	0.17	-0.09	36,40,42,46	1
3	NAG	C	801	14/15	0.69	0.29	-0.16	98,98,99,99	0
2	RUM	B	800	24/24	0.94	0.21	-0.27	41,45,46,49	1
3	NAG	B	801	14/15	0.71	0.14	-0.73	81,82,83,83	0
2	RUM	D	800	24/24	0.92	0.18	-0.96	42,46,47,50	1
3	NAG	C	803	14/15	0.88	0.15	-	66,68,68,68	0
3	NAG	A	802	14/15	0.81	0.31	-	65,65,66,67	0
3	NAG	D	801	14/15	0.64	0.42	-	92,93,93,93	0
3	NAG	B	802	14/15	0.85	0.18	-	59,62,63,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	D	802	14/15	0.68	0.21	-	72,73,73,73	0
3	NAG	C	802	14/15	0.87	0.27	-	62,63,65,65	0
3	NAG	A	803	14/15	0.78	0.29	-	63,65,67,67	0
3	NAG	B	803	14/15	0.83	0.21	-	54,57,59,60	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.