



# Full wwPDB X-ray Structure Validation Report i

Feb 28, 2014 – 03:37 PM GMT

PDB ID : 3G0C  
Title : Crystal structure of dipeptidyl peptidase IV in complex with a pyrimidinedione inhibitor 1  
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 : 2.69 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>

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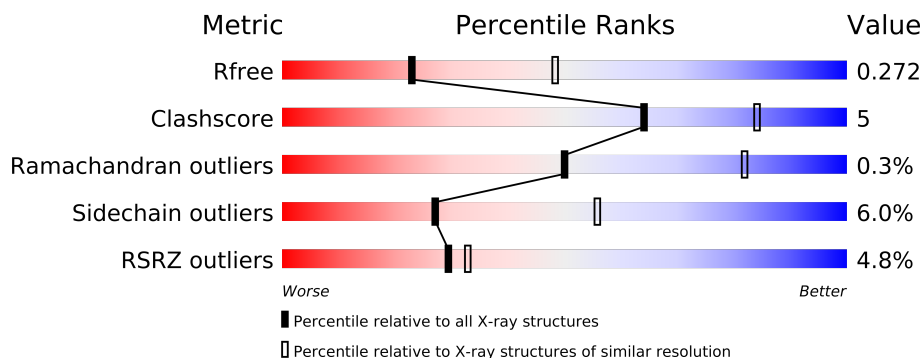
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 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 2.69 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	66092	1557 (2.70-2.70)
Clashscore	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (2.70-2.70)
RSRZ outliers	66119	1559 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	740	
1	B	740	
1	C	740	
1	D	740	

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	B	803	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24940 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	723	Total	C	N	O	S	0	1	0
			5920	3804	972	1118	26			
1	B	729	Total	C	N	O	S	0	1	0
			5972	3834	986	1126	26			
1	C	724	Total	C	N	O	S	0	1	0
			5929	3809	974	1120	26			
1	D	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			

There are 48 discrepancies between the modelled and reference sequences:

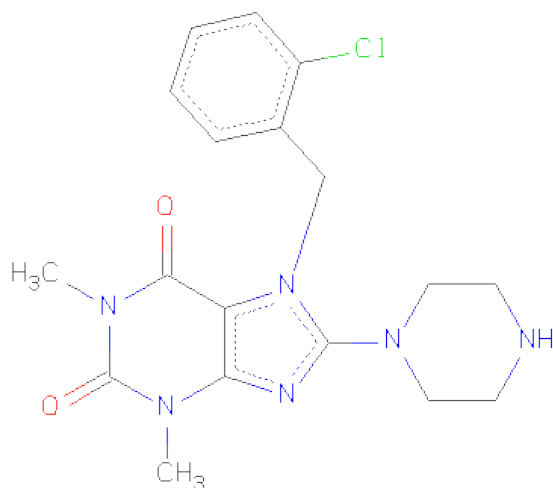
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
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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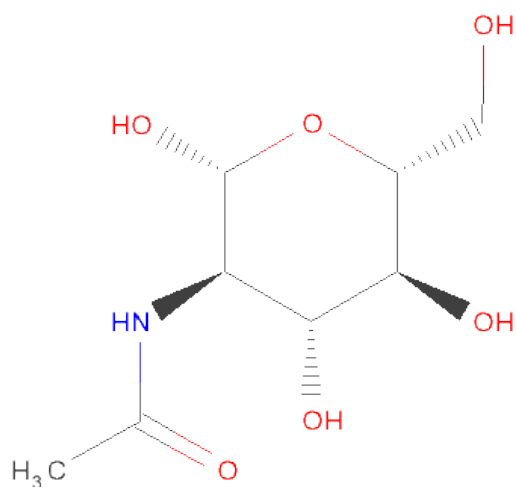
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
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 7-(2-CHLOROBENZYL)-1,3-DIMETHYL-8-PIPERAZIN-1-YL-3,7-DIHYDR O-1H-PURINE-2,6-DIONE (three-letter code: RUF) (formula: C<sub>18</sub>H<sub>21</sub>ClN<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			27	18	1	6	2		
2	B	1	Total	C	Cl	N	O	0	0
			27	18	1	6	2		
2	C	1	Total	C	Cl	N	O	0	0
			27	18	1	6	2		
2	D	1	Total	C	Cl	N	O	0	0
			27	18	1	6	2		

- 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 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	A	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	B	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	C	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0
3	D	1	Total C N O 14 8 1 5	0	0

- 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 28 16 2 10	0	0
4	A	2	Total C N O 28 16 2 10	0	0
4	B	2	Total C N O 28 16 2 10	0	0
4	C	2	Total C N O 28 16 2 10	0	0
4	D	2	Total C N O 28 16 2 10	0	0

There are 60 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	231	Total O 231 231	0	0
5	B	237	Total O 237 237	0	0
5	C	196	Total O 196 196	0	0
5	D	110	Total O 110 110	0	0

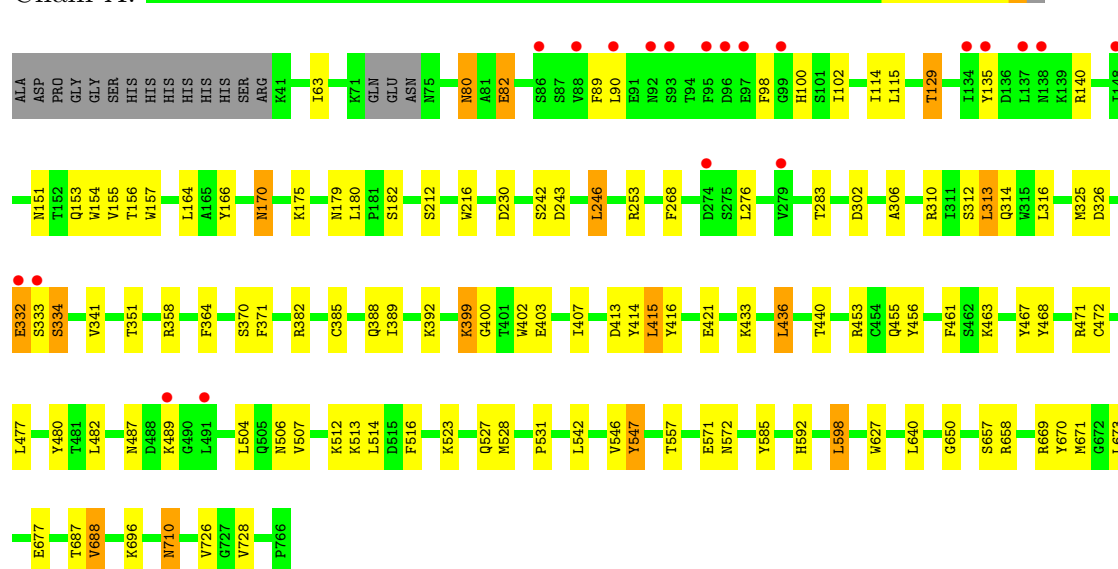


### 3 Residue-property plots

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.

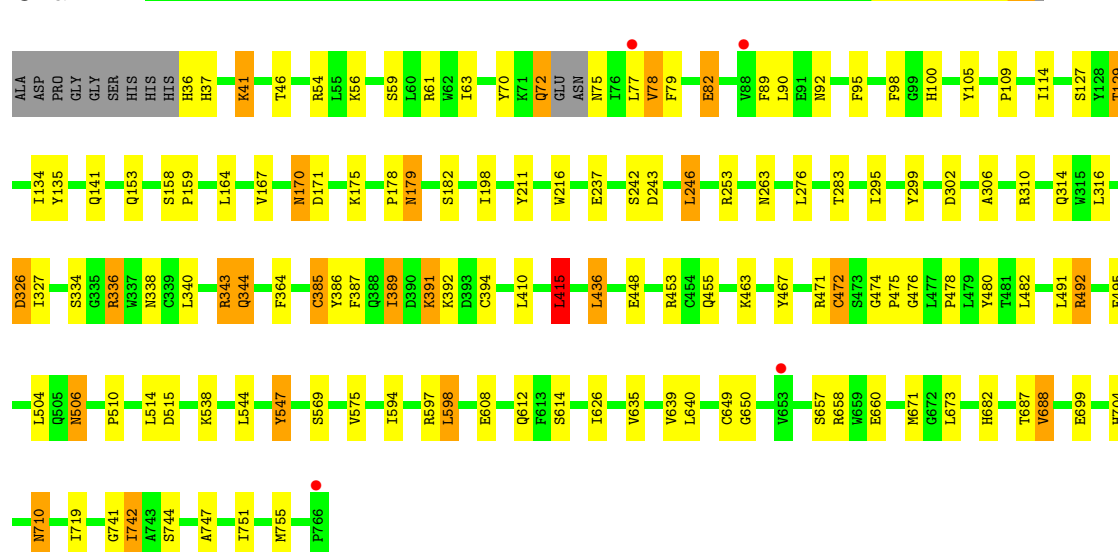
#### • Molecule 1: Dipeptidyl peptidase 4

Chain A:



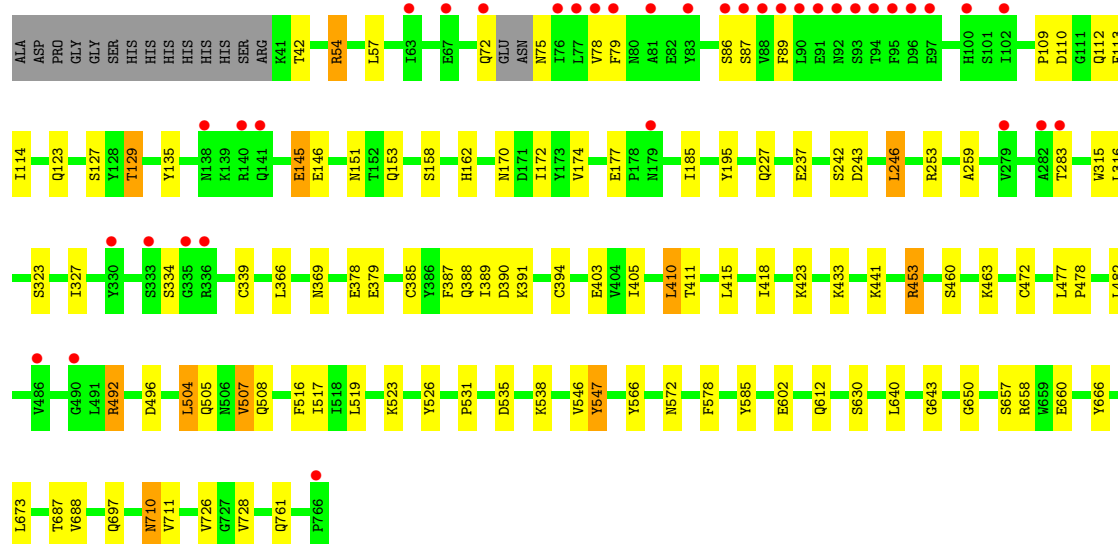
#### • Molecule 1: Dipeptidyl peptidase 4

Chain B:



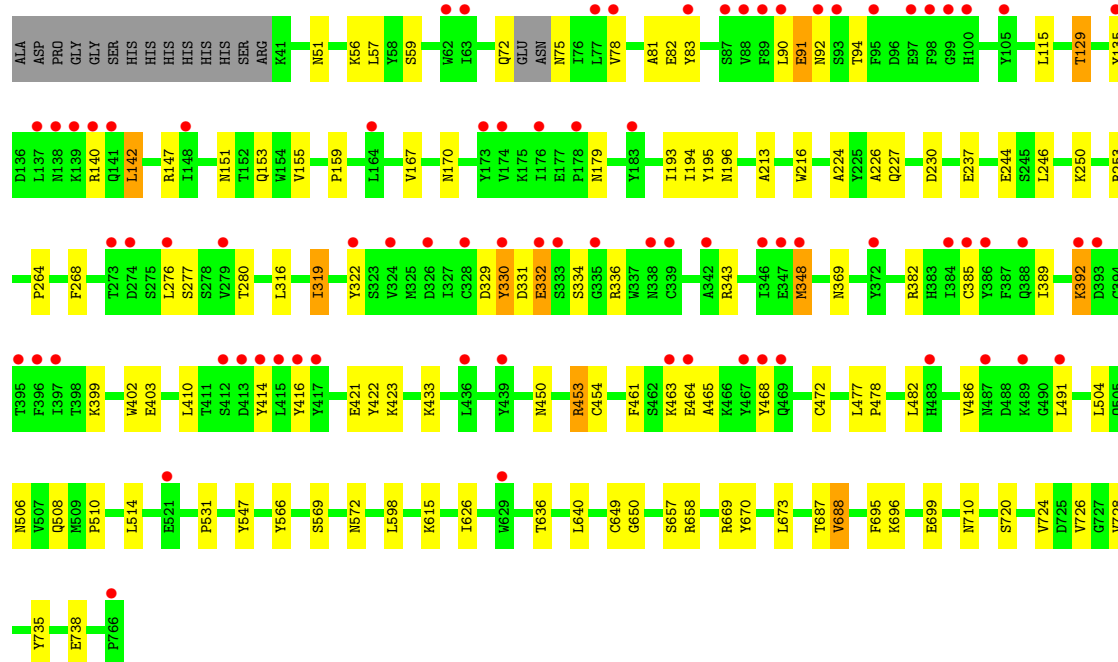
- Molecule 1: Dipeptidyl peptidase 4

Chain C:



- Molecule 1: Dipeptidyl peptidase 4

Chain D:



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	122.84Å 122.77Å 145.11Å 90.00° 114.68° 90.00°	Depositor
Resolution (Å)	50.00 – 2.69 48.57 – 2.69	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.69) 99.2 (48.57-2.69)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.27 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.195 , 0.248 0.234 , 0.272	Depositor DCC
$R_{free}$ test set	5406 reflections (4.99%)	DCC
Wilson B-factor (Å <sup>2</sup> )	48.6	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 19.8	EDS
Estimated twinning fraction	0.007 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 108370 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	24940	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% 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: RUF, 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	0.46	0/6091	0.61	0/8284
1	B	0.47	0/6149	0.61	1/8362 (0.0%)
1	C	0.46	0/6100	0.61	0/8296
1	D	0.50	4/6100 (0.1%)	0.59	1/8296 (0.0%)
All	All	0.47	4/24440 (0.0%)	0.61	2/33238 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	332	GLU	CD-OE1	9.06	1.35	1.25
1	D	332	GLU	CD-OE2	8.97	1.35	1.25
1	D	330	TYR	CE1-CZ	5.96	1.46	1.38
1	D	330	TYR	CG-CD2	5.90	1.46	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	142	LEU	CA-CB-CG	5.87	128.81	115.30
1	B	415	LEU	CA-CB-CG	5.28	127.45	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5920	0	5638	65	0
1	B	5972	0	5681	75	0
1	C	5929	0	5649	52	0
1	D	5929	0	5650	55	0
2	A	27	0	21	2	0
2	B	27	0	21	2	0
2	C	27	0	21	4	0
2	D	27	0	21	2	0
3	A	56	0	52	0	0
3	B	56	0	52	0	0
3	C	28	0	26	0	0
3	D	28	0	26	1	0
4	A	56	0	50	0	0
4	B	28	0	25	0	0
4	C	28	0	25	0	0
4	D	28	0	25	0	0
5	A	231	0	0	3	0
5	B	237	0	0	4	0
5	C	196	0	0	2	0
5	D	110	0	0	1	0
All	All	24940	0	22983	253	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 5.

All (253) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:153:GLN:HE22	1:A:170:ASN:H	1.15	0.91
1:C:153:GLN:HE22	1:C:170:ASN:H	1.10	0.90
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.15	0.90
1:D:90:LEU:HD12	1:D:140:ARG:HH21	1.39	0.87
1:C:54:ARG:HH21	1:C:54:ARG:HG2	1.41	0.86
1:B:153:GLN:HE22	1:B:170:ASN:H	1.27	0.79
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.66	0.77
1:D:277:SER:HB3	1:D:280:THR:HG22	1.70	0.73
1:B:78:VAL:HG22	1:B:89:PHE:HB2	1.70	0.73
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.72	0.72
1:B:391:LYS:HE3	1:B:391:LYS:HA	1.73	0.69
1:D:153:GLN:HE22	1:D:170:ASN:H	1.38	0.69
1:B:82:GLU:HG2	1:B:467:TYR:OH	1.91	0.69

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.75	0.68
1:B:98:PHE:CE1	1:B:100:HIS:HB2	2.30	0.67
1:A:658:ARG:HB2	1:A:687:THR:HG22	1.76	0.65
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.78	0.65
1:B:36:HIS:CD2	1:B:37:HIS:H	2.14	0.64
1:B:338:ASN:OD1	1:B:340:LEU:HD12	1.97	0.64
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.80	0.63
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.79	0.63
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.81	0.62
1:B:98:PHE:HE1	1:B:100:HIS:HB2	1.64	0.62
1:B:179:ASN:H	1:B:179:ASN:HD22	1.45	0.61
1:B:597:ARG:HH11	1:B:682:HIS:HB2	1.65	0.61
1:A:399:LYS:HD2	1:A:400:GLY:N	2.16	0.61
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.82	0.60
1:A:358[A]:ARG:HD2	5:A:903:HOH:O	2.01	0.60
1:D:237:GLU:HG2	1:D:253:ARG:HG2	1.84	0.60
1:B:658:ARG:HB2	1:B:687:THR:HG22	1.83	0.60
1:D:450:ASN:O	1:D:454:CYS:HB2	2.03	0.59
1:B:391:LYS:HD3	1:B:392:LYS:H	1.68	0.58
1:A:546:VAL:HG12	1:A:627:TRP:O	2.03	0.57
1:A:170:ASN:N	1:A:170:ASN:HD22	2.02	0.57
1:D:129:THR:HG23	1:D:151:ASN:HA	1.85	0.57
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.85	0.57
1:D:461:PHE:CD2	1:D:468:TYR:HB3	2.39	0.57
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.86	0.57
1:C:129:THR:HG23	1:C:151:ASN:HA	1.85	0.57
1:D:461:PHE:CD2	1:D:465:ALA:HB1	2.40	0.57
1:D:422:TYR:CE1	1:D:423:LYS:HE2	2.40	0.57
1:A:129:THR:HG23	1:A:151:ASN:HA	1.86	0.57
1:C:531:PRO:HB3	1:C:572:ASN:ND2	2.20	0.56
1:B:334:SER:HB3	1:B:336:ARG:HG3	1.87	0.56
1:D:72:GLN:HB2	1:D:75:ASN:HB2	1.87	0.56
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.87	0.56
2:A:800:RUF:C13	2:A:800:RUF:H11	2.36	0.56
1:B:710:ASN:C	1:B:710:ASN:HD22	2.09	0.55
1:C:54:ARG:HH21	1:C:54:ARG:CG	2.18	0.55
1:B:455:GLN:HB2	1:B:475:PRO:HD3	1.89	0.54
1:B:415:LEU:HB2	1:B:436:LEU:HD11	1.89	0.54
1:B:283:THR:HG22	5:B:849:HOH:O	2.07	0.54
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.42	0.54
2:C:800:RUF:H11	2:C:800:RUF:H13A	1.90	0.54
1:C:112:GLN:HG3	1:C:113:PHE:CD2	2.42	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:41:LYS:HE2	1:B:506:ASN:HB3	1.90	0.54
2:A:800:RUF:H13A	2:A:800:RUF:H11	1.88	0.54
1:A:487:ASN:OD1	1:A:489:LYS:HG2	2.08	0.54
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.74	0.53
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.90	0.53
2:C:800:RUF:H11	2:C:800:RUF:C13	2.37	0.53
1:A:399:LYS:HD2	1:A:400:GLY:H	1.73	0.53
1:C:54:ARG:NH2	1:C:54:ARG:HG2	2.17	0.53
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.92	0.53
1:A:477:LEU:HD12	1:A:477:LEU:H	1.73	0.53
1:D:147:ARG:HE	3:D:801:NAG:H83	1.73	0.53
1:C:535:ASP:HB3	1:C:538:LYS:HG3	1.90	0.52
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.91	0.52
1:D:330:TYR:CE2	1:D:332:GLU:HA	2.44	0.52
1:A:407:ILE:HG23	1:A:415:LEU:CD1	2.38	0.52
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.90	0.52
1:B:657:SER:HA	1:B:688:VAL:HG13	1.90	0.52
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.45	0.51
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.75	0.51
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.93	0.51
2:B:800:RUF:H15	2:B:800:RUF:C21	2.40	0.51
1:C:643:GLY:HA2	1:C:697:GLN:HE22	1.75	0.51
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.91	0.51
1:B:72:GLN:HB2	1:B:75:ASN:HB2	1.93	0.51
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.75	0.51
1:C:505:GLN:HG2	5:C:849:HOH:O	2.10	0.51
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.92	0.51
1:B:608:GLU:O	1:B:612:GLN:HG2	2.11	0.51
1:C:410:LEU:HD22	1:C:411:THR:O	2.11	0.50
1:D:331:ASP:HB3	1:D:334:SER:HB2	1.93	0.50
1:D:657:SER:HA	1:D:688:VAL:HG13	1.93	0.50
1:B:159:PRO:HD3	1:B:216:TRP:HB3	1.93	0.50
2:D:800:RUF:C13	2:D:800:RUF:H11	2.42	0.50
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.12	0.50
1:C:172:ILE:HG22	1:C:185:ILE:HD12	1.94	0.50
1:C:129:THR:HG22	5:C:777:HOH:O	2.11	0.50
1:B:649:CYS:HB3	1:B:699:GLU:HB2	1.94	0.50
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.93	0.50
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.93	0.49
1:B:386:TYR:O	1:B:394:CYS:HB2	2.12	0.49
1:D:196:ASN:OD1	1:D:227:GLN:HG3	2.13	0.49
1:D:508:GLN:HG2	5:D:823:HOH:O	2.12	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:695:PHE:HB3	1:D:728:VAL:HG11	1.95	0.49
1:D:382:ARG:H	1:D:403:GLU:HG2	1.76	0.49
1:D:91:GLU:HB3	1:D:94:THR:H	1.77	0.49
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.95	0.49
1:C:145:GLU:HG2	1:C:146:GLU:HG2	1.95	0.49
1:C:453:ARG:NH2	1:C:477:LEU:O	2.41	0.49
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.77	0.48
1:A:407:ILE:HG23	1:A:415:LEU:HD11	1.94	0.48
1:D:322:TYR:HA	1:D:348:MET:HB3	1.95	0.48
1:B:544:LEU:HD23	1:B:626:ILE:HD12	1.94	0.48
1:C:526:TYR:HB3	1:C:578:PHE:HD1	1.78	0.48
1:A:333:SER:O	1:A:334:SER:HB3	2.13	0.48
1:B:135:TYR:CE1	1:B:141:GLN:HA	2.49	0.48
1:A:80:ASN:HD22	1:A:82:GLU:H	1.61	0.48
1:A:129:THR:HG21	1:A:151:ASN:HD22	1.78	0.48
1:A:415:LEU:HD12	1:A:416:TYR:N	2.27	0.48
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.49	0.48
1:C:315:TRP:O	1:C:323:SER:HB2	2.14	0.48
1:D:482:LEU:HD22	1:D:491:LEU:HD12	1.96	0.48
1:D:75:ASN:HA	1:D:91:GLU:HG3	1.96	0.48
1:A:332:GLU:HA	1:A:332:GLU:OE2	2.14	0.48
2:D:800:RUF:H11	2:D:800:RUF:C14	2.44	0.47
1:A:82:GLU:OE1	1:A:82:GLU:HA	2.14	0.47
1:B:471[A]:ARG:HG3	1:B:480:TYR:CE1	2.50	0.47
1:B:635:VAL:O	1:B:639:VAL:HG23	2.14	0.47
1:D:392:LYS:HD2	1:D:392:LYS:H	1.79	0.47
1:C:504:LEU:HA	1:C:507:VAL:HG13	1.96	0.47
1:D:461:PHE:CE2	1:D:468:TYR:HB3	2.49	0.47
1:C:517:ILE:HD13	1:C:612:GLN:HG3	1.97	0.47
1:A:455:GLN:HE21	1:A:557:THR:HG21	1.79	0.47
1:C:174:VAL:CG2	1:C:185:ILE:HD11	2.45	0.47
1:A:82:GLU:HG2	1:A:467:TYR:OH	2.15	0.47
1:D:91:GLU:HB3	1:D:94:THR:N	2.30	0.46
1:D:135:TYR:CZ	1:D:142:LEU:HB2	2.50	0.46
1:B:472:CYS:O	1:B:478:PRO:HA	2.14	0.46
1:D:369:ASN:O	1:D:389:ILE:HG12	2.16	0.46
1:A:598:LEU:HB2	1:A:671:MET:SD	2.55	0.46
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.50	0.46
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.80	0.46
1:A:414:TYR:CE2	1:A:433:LYS:HD3	2.50	0.46
1:D:657:SER:HA	1:D:688:VAL:CG1	2.46	0.46
1:A:657:SER:HA	1:A:688:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.51	0.46
1:D:193:ILE:HG22	1:D:194:ILE:HG12	1.97	0.46
1:D:115:LEU:HD21	1:D:155:VAL:HG21	1.98	0.46
1:B:109:PRO:HG2	1:B:158:SER:O	2.15	0.46
1:C:643:GLY:HA2	1:C:697:GLN:NE2	2.31	0.46
1:A:102:ILE:H	1:A:102:ILE:HD12	1.80	0.46
1:A:306:ALA:HB3	1:A:310:ARG:HG2	1.98	0.46
1:B:129:THR:HG22	5:B:890:HOH:O	2.16	0.46
1:B:242:SER:OG	1:B:243:ASP:N	2.47	0.45
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.98	0.45
2:B:800:RUF:C14	2:B:800:RUF:H11	2.46	0.45
1:D:696:LYS:HG3	1:D:728:VAL:HG22	1.97	0.45
1:A:312:SER:HA	1:A:326:ASP:O	2.17	0.45
1:D:81:ALA:C	1:D:83:TYR:H	2.19	0.45
1:D:319:ILE:HG13	1:D:319:ILE:H	1.55	0.45
1:B:491:LEU:O	1:B:492:ARG:HB3	2.17	0.45
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.46	0.45
1:A:156:THR:HG23	1:A:216:TRP:HE1	1.82	0.45
1:B:170:ASN:N	1:B:170:ASN:HD22	2.14	0.45
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.52	0.45
1:D:343:ARG:HG2	1:D:389:ILE:HG22	1.99	0.45
1:A:571:GLU:OE2	1:A:571:GLU:HA	2.16	0.45
1:B:56:LYS:HE3	1:B:495:GLU:OE2	2.17	0.45
1:B:340:LEU:HB2	1:B:343:ARG:HG3	2.00	0.44
1:B:134:ILE:HD13	1:B:178:PRO:HB3	1.98	0.44
1:A:710:ASN:C	1:A:710:ASN:HD22	2.21	0.44
1:D:213:ALA:HB1	1:D:226:ALA:HB3	1.99	0.44
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.44
1:A:388:GLN:NE2	5:A:974:HOH:O	2.50	0.44
1:C:109:PRO:HG2	1:C:158:SER:O	2.18	0.44
1:D:640:LEU:HD11	1:D:650:GLY:HA3	2.00	0.44
1:C:242:SER:HB3	1:C:246:LEU:HD12	1.99	0.44
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.98	0.43
1:A:414:TYR:CD2	1:A:433:LYS:HD3	2.53	0.43
1:A:115:LEU:HD21	1:A:155:VAL:HG21	2.00	0.43
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.33	0.43
1:C:110:ASP:OD2	1:C:112:GLN:HG2	2.19	0.43
1:A:513:LYS:O	1:A:527:GLN:HA	2.18	0.43
1:D:230:ASP:OD1	1:D:264:PRO:HB3	2.18	0.43
1:B:92:ASN:ND2	5:B:980:HOH:O	2.51	0.43
1:A:89:PHE:O	1:A:90:LEU:HG	2.19	0.43
1:B:167:VAL:HG11	1:B:198:ILE:HG12	2.01	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.54	0.43
1:B:263:ASN:ND2	1:B:299:TYR:OH	2.51	0.43
1:D:720:SER:O	1:D:724:VAL:HG23	2.19	0.43
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.53	0.43
1:B:127:SER:HB3	1:B:211:TYR:CG	2.54	0.43
1:C:657:SER:HA	1:C:688:VAL:HG13	2.00	0.43
1:A:382:ARG:NH2	5:A:1:HOH:O	2.52	0.42
1:C:259:ALA:HB3	1:C:660:GLU:HA	2.01	0.42
1:B:127:SER:HB3	1:B:211:TYR:CD2	2.53	0.42
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.49	0.42
1:B:72:GLN:HG3	1:B:77:LEU:CD2	2.50	0.42
1:A:98:PHE:CE1	1:A:100:HIS:HB2	2.54	0.42
1:D:416:TYR:CE1	1:D:433:LYS:HE2	2.55	0.42
1:B:167:VAL:HA	1:B:171:ASP:O	2.20	0.42
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.54	0.42
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.50	0.42
1:C:710:ASN:C	1:C:710:ASN:HD22	2.23	0.42
1:B:306:ALA:HB3	1:B:310:ARG:HG2	2.01	0.42
1:A:175:LYS:NZ	1:A:180:LEU:O	2.43	0.42
1:A:403:GLU:OE2	1:A:585:TYR:HA	2.19	0.42
1:B:175:LYS:HG3	1:B:182:SER:HB3	2.02	0.42
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.55	0.42
1:B:741:GLY:O	1:B:742:ILE:C	2.57	0.42
1:D:453:ARG:NH2	1:D:477:LEU:O	2.49	0.42
1:D:195:TYR:O	1:D:227:GLN:HA	2.20	0.42
1:C:516:PHE:CG	1:C:523:LYS:HE3	2.54	0.42
1:C:42:THR:HG22	1:C:508:GLN:HG3	2.02	0.42
1:D:669:ARG:HD2	1:D:670:TYR:CZ	2.55	0.42
1:B:95:PHE:HE1	1:B:135:TYR:CD1	2.37	0.42
1:D:626:ILE:HG23	1:D:636:THR:HG23	2.01	0.42
1:B:54:ARG:HG3	5:B:884:HOH:O	2.20	0.42
1:C:388:GLN:HB2	1:C:391:LYS:HG2	2.02	0.42
1:A:456:TYR:HB2	1:A:557:THR:OG1	2.20	0.41
1:D:472:CYS:O	1:D:478:PRO:HA	2.20	0.41
1:D:649:CYS:HB3	1:D:699:GLU:HB2	2.02	0.41
1:A:325:MET:CE	1:A:371:PHE:CZ	3.03	0.41
1:C:472:CYS:O	1:C:478:PRO:HA	2.19	0.41
1:A:436:LEU:HD12	1:A:436:LEU:HA	1.90	0.41
1:D:735:TYR:HB3	1:D:738:GLU:HG3	2.02	0.41
1:C:726:VAL:HG23	1:C:728:VAL:HG23	2.01	0.41
1:C:387:PHE:CD1	1:C:394:CYS:HB3	2.55	0.41
1:C:369:ASN:C	1:C:389:ILE:HG12	2.41	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:36:HIS:CG	1:B:37:HIS:H	2.38	0.41
1:C:405:ILE:HB	1:C:418:ILE:HG22	2.01	0.41
1:B:688:VAL:HG22	1:B:719:ILE:HG12	2.01	0.41
1:B:744:SER:HB2	1:B:747:ALA:HB3	2.03	0.41
1:A:157:TRP:CE3	1:A:164:LEU:HD13	2.55	0.41
1:C:711:VAL:HG23	2:C:800:RUF:H17	2.02	0.41
1:C:666:TYR:CD1	2:C:800:RUF:H11A	2.56	0.41
1:A:547:TYR:CD1	1:A:547:TYR:C	2.94	0.41
1:C:123:GLN:HB3	1:C:127:SER:OG	2.20	0.41
1:A:402:TRP:CD2	1:A:421:GLU:HB2	2.56	0.41
1:C:79:PHE:CE2	1:C:86:SER:HB3	2.56	0.41
1:D:153:GLN:NE2	1:D:167:VAL:HG12	2.36	0.41
1:B:506:ASN:HA	1:B:506:ASN:HD22	1.60	0.41
1:B:547:TYR:CD1	1:B:547:TYR:C	2.94	0.41
1:C:547:TYR:C	1:C:547:TYR:CD1	2.94	0.41
1:D:726:VAL:HG23	1:D:728:VAL:HG23	2.03	0.40
1:C:162:HIS:NE2	1:C:177:GLU:OE1	2.54	0.40
1:C:602:GLU:OE1	1:C:602:GLU:N	2.51	0.40
1:B:164:LEU:HB3	1:B:175:LYS:HB2	2.04	0.40
1:B:326:ASP:OD2	1:B:344:GLN:HG3	2.21	0.40
1:D:510:PRO:HD3	1:D:569:SER:HB2	2.03	0.40
1:B:474:GLY:HA2	1:B:476:GLY:O	2.21	0.40
1:C:492:ARG:NH2	1:C:492:ARG:HB3	2.37	0.40
1:A:512:LYS:HA	1:A:528:MET:O	2.21	0.40
1:C:78:VAL:HG23	1:C:89:PHE:HB2	2.03	0.40
1:A:155:VAL:HG12	1:A:166:TYR:HB3	2.02	0.40
1:D:414:TYR:CD2	1:D:433:LYS:HG2	2.56	0.40
1:C:658:ARG:HG3	1:C:687:THR:HG22	2.03	0.40
1:B:751:ILE:O	1:B:755:MET:HG3	2.21	0.40
1:C:195:TYR:O	1:C:227:GLN:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	719/740 (97%)	684 (95%)	31 (4%)	4 (1%)	33	66
1	B	726/740 (98%)	698 (96%)	27 (4%)	1 (0%)	59	89
1	C	720/740 (97%)	679 (94%)	39 (5%)	2 (0%)	50	82
1	D	720/740 (97%)	664 (92%)	55 (8%)	1 (0%)	59	89
All	All	2885/2960 (98%)	2725 (94%)	152 (5%)	8 (0%)	50	82

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	332	GLU
1	A	140	ARG
1	A	334	SER
1	A	463	LYS
1	C	423	LYS
1	C	334	SER
1	D	244	GLU
1	B	742	ILE

### 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	648/662 (98%)	611 (94%)	37 (6%)	29	58
1	B	653/662 (99%)	607 (93%)	46 (7%)	21	47
1	C	649/662 (98%)	612 (94%)	37 (6%)	29	58
1	D	649/662 (98%)	613 (94%)	36 (6%)	30	60
All	All	2599/2648 (98%)	2443 (94%)	156 (6%)	27	56

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	63	ILE
1	A	80	ASN
1	A	82	GLU
1	A	129	THR

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Mol	Chain	Res	Type
1	A	170	ASN
1	A	179	ASN
1	A	182	SER
1	A	230	ASP
1	A	243	ASP
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	313	LEU
1	A	316	LEU
1	A	341	VAL
1	A	370	SER
1	A	385	CYS
1	A	392	LYS
1	A	399	LYS
1	A	413	ASP
1	A	415	LEU
1	A	436	LEU
1	A	440	THR
1	A	453	ARG
1	A	472	CYS
1	A	482	LEU
1	A	504	LEU
1	A	506	ASN
1	A	507	VAL
1	A	514	LEU
1	A	542	LEU
1	A	547	TYR
1	A	598	LEU
1	A	673	LEU
1	A	677	GLU
1	A	688	VAL
1	A	710	ASN
1	B	41	LYS
1	B	46	THR
1	B	59	SER
1	B	61	ARG
1	B	63	ILE
1	B	72	GLN
1	B	78	VAL
1	B	82	GLU
1	B	129	THR

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Mol	Chain	Res	Type
1	B	170	ASN
1	B	179	ASN
1	B	246	LEU
1	B	276	LEU
1	B	295	ILE
1	B	316	LEU
1	B	326	ASP
1	B	336	ARG
1	B	343	ARG
1	B	344	GLN
1	B	385	CYS
1	B	389	ILE
1	B	391	LYS
1	B	410	LEU
1	B	415	LEU
1	B	436	LEU
1	B	448	GLU
1	B	453	ARG
1	B	463	LYS
1	B	472	CYS
1	B	482	LEU
1	B	492	ARG
1	B	504	LEU
1	B	506	ASN
1	B	514	LEU
1	B	515	ASP
1	B	538	LYS
1	B	547	TYR
1	B	575	VAL
1	B	594	ILE
1	B	598	LEU
1	B	614	SER
1	B	660	GLU
1	B	673	LEU
1	B	688	VAL
1	B	704	HIS
1	B	710	ASN
1	C	54	ARG
1	C	57	LEU
1	C	72	GLN
1	C	75	ASN
1	C	87	SER

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Mol	Chain	Res	Type
1	C	129	THR
1	C	145	GLU
1	C	243	ASP
1	C	246	LEU
1	C	283	THR
1	C	316	LEU
1	C	339	CYS
1	C	366	LEU
1	C	378	GLU
1	C	379	GLU
1	C	385	CYS
1	C	390	ASP
1	C	410	LEU
1	C	415	LEU
1	C	433	LYS
1	C	441	LYS
1	C	453	ARG
1	C	460	SER
1	C	463	LYS
1	C	482	LEU
1	C	492	ARG
1	C	496	ASP
1	C	504	LEU
1	C	507	VAL
1	C	519	LEU
1	C	546	VAL
1	C	547	TYR
1	C	566	TYR
1	C	630	SER
1	C	673	LEU
1	C	710	ASN
1	C	761	GLN
1	D	51	ASN
1	D	56	LYS
1	D	57	LEU
1	D	59	SER
1	D	78	VAL
1	D	82	GLU
1	D	91	GLU
1	D	92	ASN
1	D	129	THR
1	D	179	ASN

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Mol	Chain	Res	Type
1	D	246	LEU
1	D	250	LYS
1	D	276	LEU
1	D	316	LEU
1	D	319	ILE
1	D	329	ASP
1	D	336	ARG
1	D	348	MET
1	D	385	CYS
1	D	392	LYS
1	D	399	LYS
1	D	410	LEU
1	D	453	ARG
1	D	463	LYS
1	D	464	GLU
1	D	486	VAL
1	D	504	LEU
1	D	506	ASN
1	D	514	LEU
1	D	547	TYR
1	D	566	TYR
1	D	598	LEU
1	D	615	LYS
1	D	673	LEU
1	D	688	VAL
1	D	710	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	80	ASN
1	A	138	ASN
1	A	151	ASN
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	338	ASN
1	A	344	GLN
1	A	455	GLN
1	A	572	ASN

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Mol	Chain	Res	Type
1	A	592	HIS
1	A	710	ASN
1	B	36	HIS
1	B	80	ASN
1	B	141	GLN
1	B	153	GLN
1	B	170	ASN
1	B	179	ASN
1	B	263	ASN
1	B	455	GLN
1	B	505	GLN
1	B	506	ASN
1	B	508	GLN
1	B	572	ASN
1	B	592	HIS
1	B	710	ASN
1	B	731	GLN
1	C	66	HIS
1	C	112	GLN
1	C	141	GLN
1	C	153	GLN
1	C	170	ASN
1	C	344	GLN
1	C	369	ASN
1	C	455	GLN
1	C	572	ASN
1	C	586	GLN
1	C	685	ASN
1	C	697	GLN
1	C	710	ASN
1	D	75	ASN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	272	ASN
1	D	344	GLN
1	D	455	GLN
1	D	572	ASN
1	D	592	HIS
1	D	685	ASN
1	D	710	ASN
1	D	731	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 ⓘ

10 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	12,14,15	0.63	0	15,19,21	1.10	1 (6%)
4	NAG	A	805	4	12,14,15	0.63	0	15,19,21	1.00	1 (6%)
4	NAG	A	806	1,4	12,14,15	0.56	0	15,19,21	1.23	1 (6%)
4	NAG	A	807	4	12,14,15	0.70	1 (8%)	15,19,21	0.91	0
4	NAG	B	804	1,4	12,14,15	0.66	0	15,19,21	1.48	3 (20%)
4	NAG	B	805	4	12,14,15	0.54	0	15,19,21	0.97	1 (6%)
4	NAG	C	803	1,4	12,14,15	0.70	0	15,19,21	1.19	1 (6%)
4	NAG	C	804	4	12,14,15	0.52	0	15,19,21	0.83	1 (6%)
4	NAG	D	802	1,4	12,14,15	0.62	0	15,19,21	0.96	1 (6%)
4	NAG	D	803	4	12,14,15	0.69	0	15,19,21	1.28	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
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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	C	803	1,4	-	0/6/23/26	0/1/1/1
4	NAG	C	804	4	-	0/6/23/26	0/1/1/1
4	NAG	D	802	1,4	-	0/6/23/26	0/1/1/1
4	NAG	D	803	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	807	NAG	O5-C5	-2.05	1.41	1.45

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	804	NAG	O5-C5-C6	3.29	110.44	106.98
4	B	804	NAG	C3-C2-N2	-3.28	106.77	111.76
4	A	804	NAG	O5-C5-C6	3.25	110.39	106.98
4	D	803	NAG	C3-C2-N2	-2.91	107.33	111.76
4	C	803	NAG	C3-C2-N2	-2.54	107.90	111.76
4	C	804	NAG	O5-C5-C6	2.48	109.58	106.98
4	A	806	NAG	C2-N2-C7	-2.31	119.20	123.09
4	B	805	NAG	O5-C5-C6	2.31	109.41	106.98
4	A	805	NAG	O5-C5-C6	2.24	109.34	106.98
4	B	804	NAG	C2-N2-C7	-2.24	119.32	123.09
4	D	802	NAG	C3-C2-N2	-2.22	108.38	111.76

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.6 Ligand geometry ⓘ

16 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	RUF	A	800	-	30,30,30	1.17	3 (10%)	37,44,44	2.54	10 (27%)
3	NAG	A	801	1	12,14,15	0.57	0	15,19,21	1.01	1 (6%)
3	NAG	A	802	1	12,14,15	0.52	0	15,19,21	1.33	1 (6%)
3	NAG	A	803	1	12,14,15	0.76	0	15,19,21	1.21	2 (13%)
3	NAG	A	808	1	12,14,15	0.69	0	15,19,21	0.76	0
2	RUF	B	800	-	30,30,30	1.11	2 (6%)	37,44,44	2.51	9 (24%)
3	NAG	B	801	1	12,14,15	0.70	0	15,19,21	1.58	3 (20%)
3	NAG	B	802	1	12,14,15	0.59	0	15,19,21	1.14	1 (6%)
3	NAG	B	803	1	12,14,15	0.56	0	15,19,21	1.04	0
3	NAG	B	806	1	12,14,15	0.48	0	15,19,21	1.15	1 (6%)
2	RUF	C	800	-	30,30,30	1.13	3 (10%)	37,44,44	2.32	9 (24%)
3	NAG	C	801	1	12,14,15	0.47	0	15,19,21	1.15	1 (6%)
3	NAG	C	802	1	12,14,15	0.71	0	15,19,21	1.71	3 (20%)
2	RUF	D	800	-	30,30,30	1.05	3 (10%)	37,44,44	2.44	10 (27%)
3	NAG	D	801	1	12,14,15	0.60	0	15,19,21	1.00	1 (6%)
3	NAG	D	804	1	12,14,15	0.72	0	15,19,21	1.09	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	RUF	A	800	-	-	0/6/16/16	0/2/4/4
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	RUF	B	800	-	-	0/6/16/16	0/2/4/4
3	NAG	B	801	1	-	0/6/23/26	0/1/1/1
3	NAG	B	802	1	-	0/6/23/26	0/1/1/1
3	NAG	B	803	1	-	0/6/23/26	0/1/1/1
3	NAG	B	806	1	-	0/6/23/26	0/1/1/1
2	RUF	C	800	-	-	0/6/16/16	0/2/4/4
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
2	RUF	D	800	-	-	0/6/16/16	0/2/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	801	1	-	0/6/23/26	0/1/1/1
3	NAG	D	804	1	-	0/6/23/26	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	RUF	C5-N6	4.00	1.40	1.35
2	A	800	RUF	C5-N6	3.97	1.40	1.35
2	C	800	RUF	C5-N6	3.52	1.39	1.35
2	D	800	RUF	C5-N6	3.50	1.39	1.35
2	C	800	RUF	C26-N24	-2.61	1.35	1.38
2	D	800	RUF	C5-N12	2.47	1.38	1.35
2	A	800	RUF	C5-N12	2.34	1.38	1.35
2	A	800	RUF	C26-N24	-2.24	1.36	1.38
2	D	800	RUF	C26-N24	-2.22	1.36	1.38
2	B	800	RUF	C5-N12	2.02	1.37	1.35
2	C	800	RUF	C5-N12	2.01	1.37	1.35

All (53) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	RUF	N4-C3-N2	9.43	134.44	128.19
2	B	800	RUF	N4-C3-N2	9.03	134.18	128.19
2	D	800	RUF	N4-C3-N2	8.49	133.82	128.19
2	C	800	RUF	N4-C3-N2	8.33	133.72	128.19
2	D	800	RUF	N2-C26-N24	7.28	122.18	115.69
2	A	800	RUF	N2-C26-N24	7.23	122.13	115.69
2	B	800	RUF	N2-C26-N24	6.57	121.55	115.69
2	C	800	RUF	N2-C26-N24	6.48	121.46	115.69
2	B	800	RUF	C21-C3-N4	-5.09	106.76	112.46
2	A	800	RUF	C21-C3-N4	-5.07	106.78	112.46
2	B	800	RUF	C14-C13-N12	-5.03	104.74	113.26
2	C	800	RUF	C21-C3-N4	-4.75	107.14	112.46
2	D	800	RUF	C21-C3-N4	-4.34	107.60	112.46
3	B	801	NAG	O5-C5-C6	4.31	111.50	106.98
2	C	800	RUF	C7-N6-C5	-4.24	112.88	122.01
2	D	800	RUF	C22-N24-C26	-4.21	120.21	121.69
3	C	802	NAG	O5-C5-C6	4.01	111.19	106.98
3	A	802	NAG	O5-C5-C6	3.91	111.08	106.98
2	A	800	RUF	C14-C13-N12	-3.88	106.69	113.26
2	A	800	RUF	C22-N24-C26	-3.84	120.34	121.69
2	B	800	RUF	C7-N6-C5	-3.74	113.96	122.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	RUF	C22-N24-C26	-3.60	120.43	121.69
2	D	800	RUF	C7-N6-C5	-3.51	114.45	122.01
3	B	806	NAG	O5-C5-C6	3.43	110.58	106.98
2	A	800	RUF	C7-N6-C5	-3.43	114.62	122.01
3	B	802	NAG	O5-C5-C6	3.16	110.30	106.98
2	D	800	RUF	C14-C13-N12	-3.04	108.11	113.26
3	C	801	NAG	O5-C5-C6	3.02	110.15	106.98
3	D	804	NAG	C2-N2-C7	2.95	128.04	123.09
3	A	803	NAG	O5-C5-C4	-2.90	106.97	110.65
2	C	800	RUF	C14-C13-N12	-2.85	108.42	113.26
3	D	801	NAG	O5-C5-C6	2.84	109.97	106.98
2	D	800	RUF	C11-N6-C5	-2.79	116.00	122.01
3	C	802	NAG	O5-C5-C4	-2.76	107.14	110.65
2	B	800	RUF	C11-N6-C5	-2.67	116.25	122.01
3	A	801	NAG	O5-C5-C6	2.64	109.75	106.98
2	C	800	RUF	C11-N6-C5	-2.61	116.38	122.01
2	D	800	RUF	C21-C3-N2	-2.46	118.59	124.85
2	C	800	RUF	C13-N12-C5	2.41	129.09	125.63
2	A	800	RUF	C13-N12-C5	2.40	129.07	125.63
2	A	800	RUF	C21-C3-N2	-2.39	118.77	124.85
2	B	800	RUF	C21-C3-N2	-2.28	119.06	124.85
2	C	800	RUF	C21-C3-N2	-2.25	119.14	124.85
2	B	800	RUF	N4-C5-N6	2.24	124.83	120.64
2	C	800	RUF	C22-N24-C26	-2.19	120.92	121.69
2	D	800	RUF	N4-C5-N6	2.18	124.72	120.64
3	B	801	NAG	C2-N2-C7	2.16	126.72	123.09
2	D	800	RUF	C13-N12-C5	2.16	128.72	125.63
2	A	800	RUF	C11-N6-C5	-2.15	117.38	122.01
3	A	803	NAG	C4-C3-C2	2.07	116.38	111.32
3	C	802	NAG	C3-C2-N2	-2.03	108.67	111.76
3	B	801	NAG	O7-C7-C8	-2.02	118.11	122.04
2	A	800	RUF	N4-C5-N6	2.00	124.39	120.64

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, 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	723/740 (97%)	0.20	20 (2%) 50 56	35, 46, 62, 81	1 (0%)
1	B	729/740 (98%)	0.05	4 (0%) 88 92	37, 46, 63, 85	0
1	C	724/740 (97%)	0.30	37 (5%) 27 30	37, 46, 64, 82	0
1	D	724/740 (97%)	0.58	78 (10%) 6 6	35, 47, 63, 92	0
All	All	2900/2960 (97%)	0.28	139 (4%) 29 33	35, 46, 63, 92	1 (0%)

All (139) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	97	GLU	7.9
1	D	88	VAL	5.8
1	D	467	TYR	5.4
1	D	137	LEU	5.1
1	C	89	PHE	5.0
1	D	415	LEU	5.0
1	C	81	ALA	4.8
1	D	397	ILE	4.5
1	D	416	TYR	4.5
1	C	88	VAL	4.2
1	C	486	VAL	4.2
1	D	99	GLY	4.2
1	D	148	ILE	4.2
1	D	140	ARG	4.0
1	C	90	LEU	3.9
1	C	78	VAL	3.8
1	A	138	ASN	3.8
1	D	483	HIS	3.8
1	D	392	LYS	3.8
1	C	79	PHE	3.6
1	D	333	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	766	PRO	3.5
1	D	372	TYR	3.5
1	D	89	PHE	3.4
1	D	468	TYR	3.3
1	D	464	GLU	3.3
1	D	174	VAL	3.3
1	D	338	ASN	3.3
1	D	83	TYR	3.3
1	C	330	TYR	3.2
1	D	322	TYR	3.2
1	D	178	PRO	3.2
1	C	83	TYR	3.1
1	D	63	ILE	3.1
1	C	91	GLU	3.1
1	C	102	ILE	3.1
1	C	93	SER	3.0
1	A	99	GLY	3.0
1	C	63	ILE	3.0
1	C	95	PHE	3.0
1	A	97	GLU	3.0
1	D	273	THR	3.0
1	A	86	SER	2.9
1	D	78	VAL	2.9
1	A	332	GLU	2.9
1	A	90	LEU	2.9
1	A	489	LYS	2.9
1	C	97	GLU	2.8
1	D	279	VAL	2.8
1	D	436	LEU	2.8
1	C	335	GLY	2.8
1	A	274	ASP	2.8
1	D	330	TYR	2.7
1	D	439	TYR	2.7
1	D	92	ASN	2.7
1	C	96	ASP	2.7
1	D	62	TRP	2.7
1	D	90	LEU	2.7
1	D	77	LEU	2.7
1	D	93	SER	2.7
1	D	346	ILE	2.7
1	D	395	THR	2.7
1	D	141	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	76	ILE	2.6
1	D	135	TYR	2.6
1	D	332	GLU	2.6
1	D	139	LYS	2.6
1	D	276	LEU	2.6
1	C	100	HIS	2.6
1	D	348	MET	2.6
1	C	72	GLN	2.6
1	D	396	PHE	2.5
1	A	333	SER	2.5
1	D	384	ILE	2.5
1	C	94	THR	2.5
1	D	173	TYR	2.5
1	D	87	SER	2.4
1	D	463	LYS	2.4
1	D	491	LEU	2.4
1	D	489	LYS	2.4
1	D	105	TYR	2.4
1	C	77	LEU	2.4
1	C	87	SER	2.4
1	C	67	GLU	2.4
1	C	490	GLY	2.4
1	D	413	ASP	2.4
1	D	386	TYR	2.4
1	C	279	VAL	2.4
1	D	100	HIS	2.4
1	A	92	ASN	2.4
1	D	347	GLU	2.4
1	C	283	THR	2.4
1	D	412	SER	2.4
1	D	274	ASP	2.3
1	D	326	ASP	2.3
1	D	385	CYS	2.3
1	C	179	ASN	2.3
1	D	138	ASN	2.3
1	D	335	GLY	2.3
1	D	324	VAL	2.3
1	C	766	PRO	2.3
1	A	148	ILE	2.3
1	A	96	ASP	2.2
1	D	393	ASP	2.2
1	C	138	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	328	CYS	2.2
1	D	417	TYR	2.2
1	C	336	ARG	2.2
1	A	134	ILE	2.2
1	B	77	LEU	2.2
1	A	88	VAL	2.2
1	D	342	ALA	2.2
1	D	414	TYR	2.2
1	D	339	CYS	2.2
1	D	469	GLN	2.2
1	A	93	SER	2.2
1	A	135	TYR	2.1
1	D	521	GLU	2.1
1	D	164	LEU	2.1
1	D	98	PHE	2.1
1	D	487	ASN	2.1
1	D	183	TYR	2.1
1	B	88	VAL	2.1
1	B	653	VAL	2.1
1	A	95	PHE	2.1
1	C	140	ARG	2.1
1	C	86	SER	2.1
1	C	141	GLN	2.1
1	D	629	TRP	2.1
1	D	95	PHE	2.1
1	D	176	ILE	2.1
1	C	282	ALA	2.0
1	C	92	ASN	2.0
1	D	388	GLN	2.0
1	A	279	VAL	2.0
1	D	766	PRO	2.0
1	A	137	LEU	2.0
1	A	491	LEU	2.0
1	C	333	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
4	NAG	D	803	14/15	0.21	3.45	61,64,66,67	0
4	NAG	B	805	14/15	0.25	1.32	74,76,78,79	0
4	NAG	C	804	14/15	0.22	1.04	74,76,78,79	0
4	NAG	A	807	14/15	0.15	-0.52	74,75,76,77	0
4	NAG	A	806	14/15	0.16	-0.57	63,67,69,71	0
4	NAG	B	804	14/15	0.15	-0.63	55,61,65,70	0
4	NAG	C	803	14/15	0.13	-0.94	60,63,67,71	0
4	NAG	D	802	14/15	0.12	-1.07	51,53,55,58	0
4	NAG	A	804	14/15	0.14	-1.37	52,54,57,59	0
4	NAG	A	805	14/15	0.14	-3.48	61,62,64,65	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(Å <sup>2</sup> )	Q<0.9
3	NAG	B	803	14/15	0.20	2.13	58,61,64,64	0
3	NAG	A	808	14/15	0.24	0.94	54,58,60,60	0
2	RUF	B	800	27/27	0.28	0.79	54,55,59,59	0
2	RUF	D	800	27/27	0.25	0.53	51,53,54,55	0
3	NAG	B	802	14/15	0.20	0.51	56,60,62,64	0
2	RUF	A	800	27/27	0.24	0.40	52,55,58,59	0
2	RUF	C	800	27/27	0.23	0.38	53,55,55,56	0
3	NAG	A	803	14/15	0.25	0.38	61,64,69,69	0
3	NAG	B	801	14/15	0.17	0.14	68,70,71,71	0
3	NAG	A	802	14/15	0.23	0.04	65,68,68,69	0
3	NAG	C	802	14/15	0.21	-0.09	58,61,64,64	0
3	NAG	C	801	14/15	0.23	-0.36	52,53,55,56	0
3	NAG	A	801	14/15	0.18	-0.77	58,60,61,61	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	806	14/15	0.11	-0.91	61,63,66,66	0
3	NAG	D	801	14/15	0.19	-1.13	55,57,57,58	0
3	NAG	D	804	14/15	0.15	-1.51	73,76,78,78	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.