



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 04:17 PM GMT

PDB ID : 3CCB  
Title : Crystal Structure of Human DPP4 in complex with a benzimidazole derivative  
Authors : Wallace, M.B.; Skene, R.J.  
Deposited on : 2008-02-25  
Resolution : 2.49 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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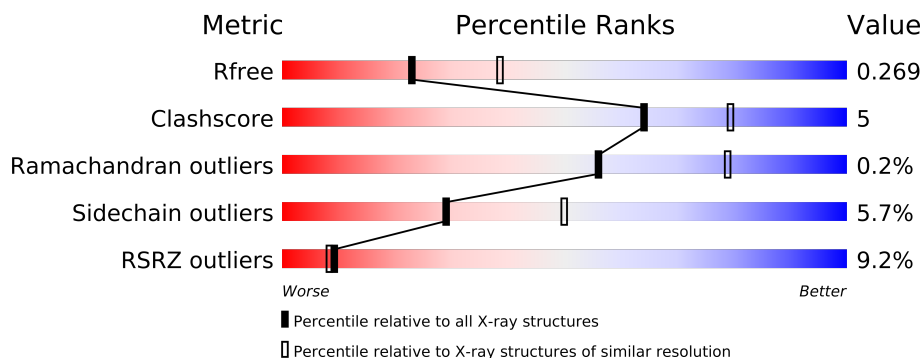
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.49 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	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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
2	NAG	A	808	-	X
2	NAG	B	803	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24805 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	724	Total	C	N	O	S	0	1	0
			5935	3812	977	1120	26			
1	B	729	Total	C	N	O	S	0	0	0
			5965	3830	983	1126	26			
1	C	724	Total	C	N	O	S	0	1	0
			5936	3813	977	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 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
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

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

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

There are 60 discrepancies between the modelled and reference sequences:

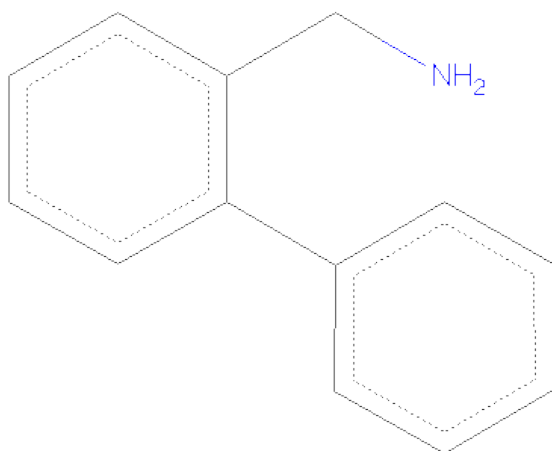
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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 4 is 1-BIPHENYL-2-YLMETHANAMINE (three-letter code: B2Y) (formula: C<sub>13</sub>H<sub>13</sub>N).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			14	13	1		
4	B	1	Total	C	N	0	0
			14	13	1		
4	C	1	Total	C	N	0	0
			14	13	1		
4	D	1	Total	C	N	0	0
			14	13	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	206	Total	O	0	0
			206	206		
5	B	191	Total	O	0	0
			191	191		
5	C	189	Total	O	0	0
			189	189		
5	D	90	Total	O	0	0
			90	90		

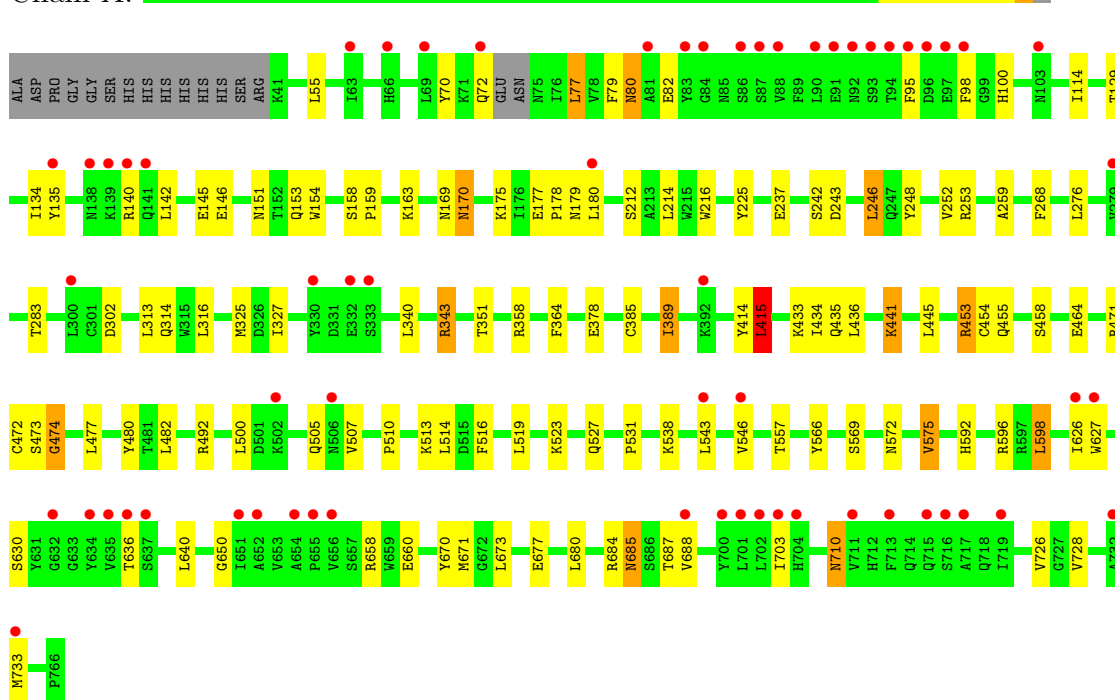


### 3 Residue-property plots

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.

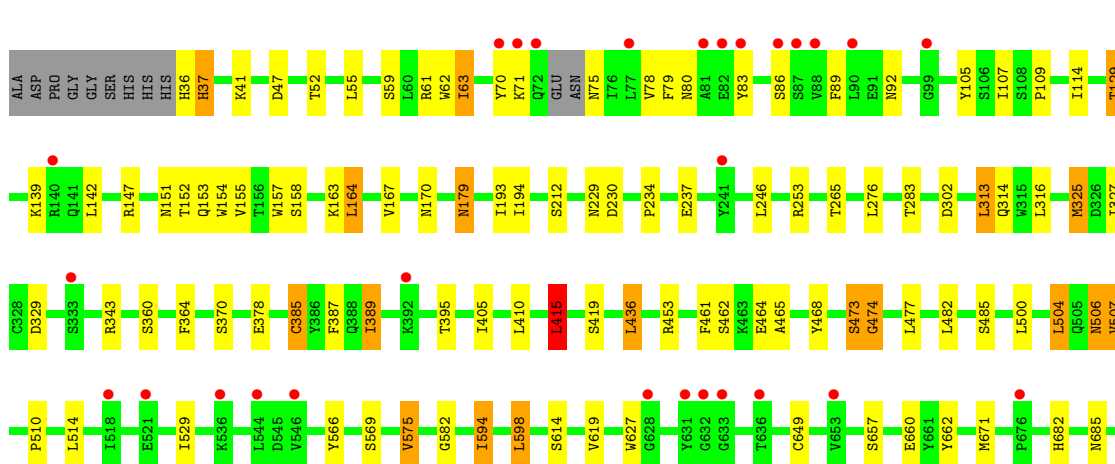
- Molecule 1: Dipeptidyl peptidase 4

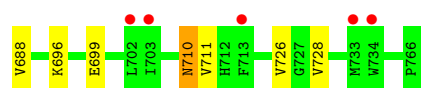
Chain A:



- Molecule 1: Dipeptidyl peptidase 4

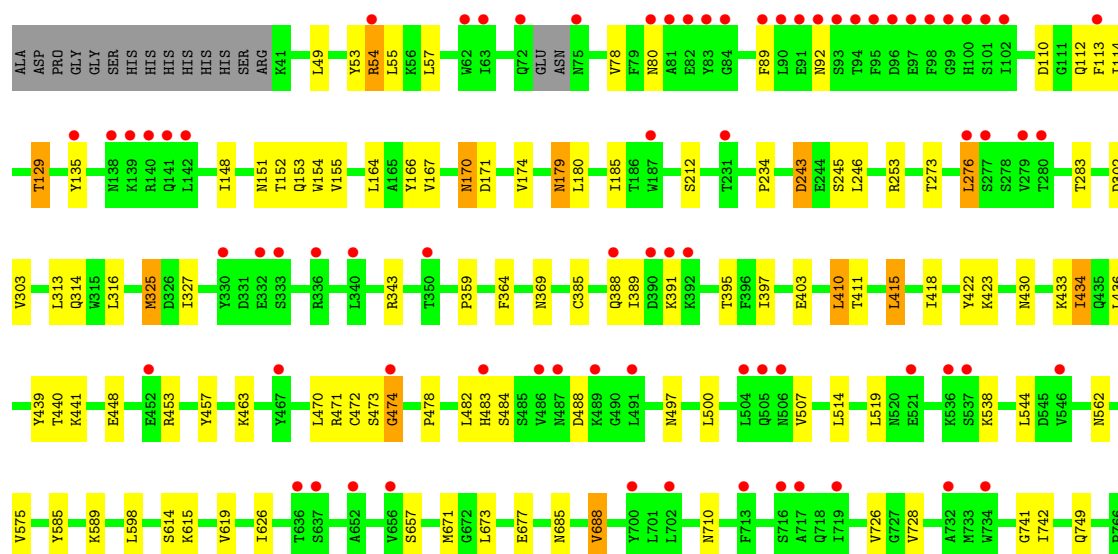
Chain B:





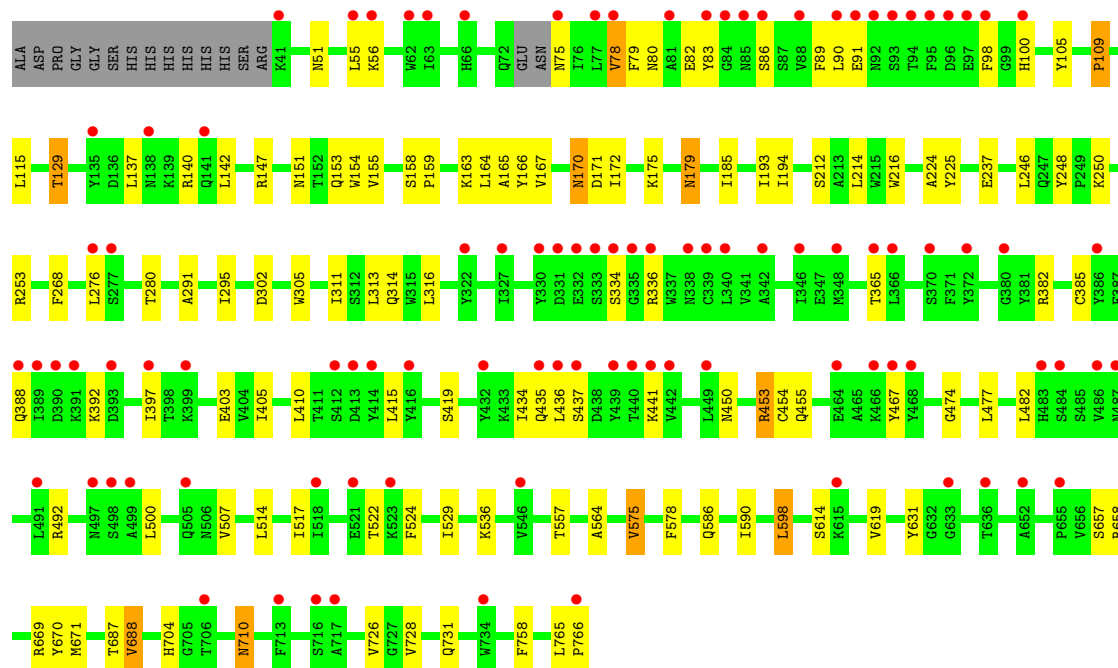
• Molecule 1: Dipeptidyl peptidase 4

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, $\alpha$ , $\beta$ , $\gamma$	122.09Å 123.01Å 144.65Å 90.00° 114.84° 90.00°	Depositor
Resolution (Å)	32.80 – 2.49 32.82 – 2.49	Depositor EDS
% Data completeness (in resolution range)	98.3 (32.80-2.49) 98.3 (32.82-2.49)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.37 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.200 , 0.244 0.234 , 0.269	Depositor DCC
$R_{free}$ test set	6732 reflections (5.03%)	DCC
Wilson B-factor (Å <sup>2</sup> )	44.1	Xtriage
Anisotropy	0.049	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 32.0	EDS
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 133885 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	24805	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 3.41% 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: NAG, B2Y

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	0.45	0/6111	0.62	1/8311 (0.0%)
1	B	0.44	0/6138	0.62	1/8348 (0.0%)
1	C	0.44	0/6111	0.61	1/8311 (0.0%)
1	D	0.42	0/6100	0.58	0/8296
All	All	0.44	0/24460	0.61	3/33266 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	415	LEU	CA-CB-CG	5.83	128.71	115.30
1	A	415	LEU	CA-CB-CG	5.37	127.66	115.30
1	B	415	LEU	CA-CB-CG	5.13	127.11	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	5935	0	5657	72	0
1	B	5965	0	5672	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5936	0	5660	65	0
1	D	5929	0	5651	61	0
2	A	56	0	52	0	0
2	B	56	0	52	1	0
2	C	28	0	26	0	0
2	D	28	0	26	1	0
3	A	56	0	50	0	0
3	B	28	0	25	1	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	A	206	0	0	2	0
5	B	191	0	0	0	0
5	C	189	0	0	1	0
5	D	90	0	0	0	0
All	All	24805	0	22973	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:C:343:ARG:HD2	1:C:389:ILE:HG22	1.42	0.98
1:C:153:GLN:HE22	1:C:170:ASN:H	1.14	0.93
1:A:153:GLN:HE22	1:A:170:ASN:H	1.18	0.90
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.14	0.90
1:C:54:ARG:HH21	1:C:54:ARG:HG2	1.39	0.88
1:A:325:MET:HE3	1:A:327:ILE:HD11	1.56	0.88
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.71	0.88
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.71	0.87
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.58	0.85
1:D:153:GLN:HE22	1:D:170:ASN:H	1.22	0.84
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.88	0.83
1:B:343:ARG:HD3	1:B:389:ILE:HG23	1.59	0.82
1:B:153:GLN:HE22	1:B:170:ASN:H	1.27	0.82
1:A:325:MET:CE	1:A:327:ILE:HD11	2.11	0.81
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.64	0.79
1:C:434:ILE:HD11	1:C:439:TYR:HB2	1.67	0.74
1:A:129:THR:HG23	1:A:151:ASN:HA	1.70	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.73	0.70
1:D:179:ASN:H	1:D:179:ASN:HD22	1.42	0.67
1:A:129:THR:CG2	1:A:151:ASN:HA	2.25	0.67
1:C:726:VAL:HG23	1:C:728:VAL:HG23	1.79	0.64
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.92	0.64
1:B:36:HIS:O	1:B:37:HIS:HB2	1.98	0.63
1:B:614:SER:HA	1:B:619:VAL:HB	1.79	0.63
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.28	0.63
1:C:343:ARG:HD2	1:C:389:ILE:CG2	2.23	0.62
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.80	0.62
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.82	0.62
1:C:153:GLN:NE2	1:C:170:ASN:H	1.94	0.62
1:D:147:ARG:HE	2:D:801:NAG:H83	1.66	0.61
1:A:135:TYR:HD1	1:A:142:LEU:HD13	1.65	0.61
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.83	0.61
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.36	0.60
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.83	0.60
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.92	0.60
1:D:564:ALA:HB1	1:D:575:VAL:HG11	1.84	0.60
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.84	0.60
1:D:155:VAL:HG12	1:D:166:TYR:HB3	1.85	0.59
1:C:314:GLN:HG2	1:C:325:MET:HB2	1.85	0.59
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.85	0.59
1:B:711:VAL:CG2	4:B:800:B2Y:H11	2.32	0.58
1:C:388:GLN:HB2	1:C:391:LYS:HG2	1.84	0.58
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.86	0.58
1:B:529:ILE:HB	1:B:575:VAL:HG13	1.84	0.58
1:C:472:CYS:O	1:C:478:PRO:HA	2.04	0.57
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.67	0.57
1:D:522:THR:HB	1:D:524:PHE:CE2	2.40	0.57
1:D:415:LEU:HB2	1:D:436:LEU:HD11	1.86	0.57
1:D:382:ARG:H	1:D:403:GLU:HG2	1.69	0.57
1:D:529:ILE:HB	1:D:575:VAL:HG13	1.87	0.56
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.86	0.56
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.40	0.56
1:C:152:THR:HG21	1:C:155:VAL:HG13	1.88	0.55
1:B:582:GLY:HA2	1:B:594:ILE:HD12	1.88	0.55
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.71	0.55
1:D:78:VAL:HG22	1:D:89:PHE:HB2	1.88	0.55
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.89	0.55
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.42	0.54
1:C:153:GLN:HE22	1:C:170:ASN:N	1.95	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:343:ARG:HD3	1:B:389:ILE:CG2	2.32	0.54
1:D:172:ILE:HG22	1:D:185:ILE:HD13	1.89	0.54
1:B:89:PHE:HE1	1:B:107:ILE:HD12	1.73	0.54
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.91	0.54
1:D:614:SER:HA	1:D:619:VAL:HB	1.89	0.53
1:A:340:LEU:HD22	1:A:343:ARG:HH11	1.74	0.53
1:C:174:VAL:HG23	1:C:185:ILE:CD1	2.39	0.53
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.89	0.53
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.90	0.52
1:A:135:TYR:HE2	1:A:140:ARG:HG2	1.74	0.52
1:C:170:ASN:N	1:C:170:ASN:HD22	2.08	0.52
1:A:170:ASN:N	1:A:170:ASN:HD22	2.08	0.51
1:C:53:TYR:HB3	1:C:500:LEU:HD11	1.92	0.51
1:C:174:VAL:CG2	1:C:185:ILE:HD11	2.40	0.51
1:D:657:SER:HA	1:D:688:VAL:HG13	1.91	0.51
1:B:179:ASN:H	1:B:179:ASN:HD22	1.57	0.51
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.93	0.51
1:D:453:ARG:NH2	1:D:477:LEU:O	2.43	0.51
1:B:154:TRP:CE2	1:B:212:SER:HB3	2.46	0.51
1:B:147:ARG:HE	2:B:802:NAG:H83	1.75	0.51
1:C:369:ASN:C	1:C:389:ILE:HG12	2.32	0.51
1:C:369:ASN:O	1:C:389:ILE:HG12	2.11	0.50
1:C:273:THR:HA	1:C:276:LEU:HD22	1.93	0.50
1:C:153:GLN:NE2	1:C:167:VAL:HG12	2.27	0.50
1:D:598:LEU:HG	1:D:631:TYR:OH	2.12	0.49
1:D:334:SER:HB2	1:D:336:ARG:H	1.77	0.49
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.93	0.49
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.94	0.49
1:C:54:ARG:NH2	1:C:54:ARG:HG2	2.16	0.49
1:B:158:SER:HB3	1:B:163:LYS:HB2	1.93	0.49
1:B:79:PHE:HA	1:B:86:SER:HB3	1.94	0.49
1:B:504:LEU:HA	1:B:507:VAL:CG1	2.43	0.49
1:A:153:GLN:NE2	1:A:170:ASN:H	1.99	0.49
1:B:47:ASP:HA	1:B:52:THR:OG1	2.12	0.49
1:B:80:ASN:HD22	1:B:83:TYR:H	1.59	0.49
1:B:229:ASN:HB3	1:B:265:THR:OG1	2.13	0.49
1:D:82:GLU:HG2	1:D:467:TYR:OH	2.13	0.49
1:C:327:ILE:HD13	1:C:389:ILE:HG23	1.95	0.48
1:C:110:ASP:OD2	1:C:112:GLN:HG2	2.13	0.48
1:C:129:THR:HG23	1:C:151:ASN:HA	1.93	0.48
1:D:75:ASN:OD1	1:D:91:GLU:HG3	2.12	0.48
1:C:473:SER:O	1:C:474:GLY:O	2.32	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:598:LEU:HB2	1:B:671:MET:SD	2.54	0.48
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.48	0.48
1:B:329:ASP:OD2	1:B:343:ARG:NH1	2.46	0.48
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.95	0.48
1:A:435:GLN:OE1	1:A:441:LYS:HE2	2.14	0.48
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.96	0.47
1:B:473:SER:O	1:B:474:GLY:O	2.32	0.47
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.13	0.47
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.48	0.47
1:C:179:ASN:HD22	1:C:179:ASN:C	2.18	0.47
1:B:71:LYS:HA	1:B:75:ASN:O	2.14	0.47
1:A:153:GLN:HE22	1:A:170:ASN:N	2.00	0.47
1:B:109:PRO:HG2	1:B:158:SER:O	2.14	0.47
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.96	0.47
1:D:305:TRP:CE2	1:D:311:ILE:HD12	2.49	0.47
3:B:804:NAG:H62	3:B:805:NAG:N2	2.30	0.47
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.96	0.47
1:C:364:PHE:HE2	1:C:389:ILE:HD11	1.80	0.47
1:D:80:ASN:HD22	1:D:83:TYR:HB2	1.80	0.47
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.96	0.47
1:D:435:GLN:HE21	1:D:437:SER:HG	1.63	0.47
1:B:465:ALA:O	1:B:485:SER:OG	2.25	0.47
1:C:303:VAL:HG22	1:C:313:LEU:HD12	1.97	0.47
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.49	0.46
1:D:586:GLN:HB3	1:D:590:ILE:HD12	1.97	0.46
1:D:158:SER:OG	1:D:163:LYS:HB2	2.15	0.46
1:D:170:ASN:N	1:D:170:ASN:HD22	2.14	0.46
1:A:685:ASN:ND2	5:A:866:HOH:O	2.48	0.46
1:D:710:ASN:C	1:D:710:ASN:HD22	2.19	0.46
1:B:314:GLN:HG2	1:B:325:MET:HB2	1.97	0.46
1:C:55:LEU:HD23	1:C:500:LEU:HD22	1.98	0.46
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.98	0.46
1:A:710:ASN:C	1:A:710:ASN:HD22	2.20	0.46
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.98	0.46
1:C:657:SER:HA	1:C:688:VAL:HG13	1.98	0.46
1:D:193:ILE:HG22	1:D:194:ILE:HG12	1.98	0.46
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.31	0.45
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.80	0.45
1:D:405:ILE:HG12	1:D:419:SER:HA	1.98	0.45
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.98	0.45
1:C:741:GLY:O	1:C:742:ILE:C	2.55	0.45
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.98	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:669:ARG:HD2	1:D:670:TYR:CZ	2.52	0.45
1:D:214:LEU:HD23	1:D:225:TYR:HB3	1.98	0.45
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.97	0.45
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.47	0.45
1:A:455:GLN:HE21	1:A:557:THR:HG21	1.82	0.45
1:B:129:THR:HG23	1:B:151:ASN:HA	1.97	0.45
1:C:410:LEU:HD22	1:C:411:THR:O	2.16	0.45
1:B:153:GLN:NE2	1:B:170:ASN:H	2.06	0.45
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.52	0.45
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.94	0.45
1:D:129:THR:HG23	1:D:151:ASN:HA	1.98	0.45
1:D:731:GLN:HG3	1:D:758:PHE:HE1	1.82	0.44
1:A:135:TYR:CE2	1:A:140:ARG:HA	2.52	0.44
1:B:62:TRP:CG	1:B:462:SER:HA	2.53	0.44
1:A:242:SER:HB3	1:A:246:LEU:HD12	1.99	0.44
1:B:75:ASN:ND2	1:B:92:ASN:HD22	2.15	0.44
1:C:614:SER:HA	1:C:619:VAL:HB	2.00	0.44
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.33	0.44
1:A:98:PHE:CD1	1:A:100:HIS:HB2	2.52	0.44
1:B:152:THR:HG21	1:B:155:VAL:HG22	1.98	0.44
1:B:193:ILE:HG22	1:B:194:ILE:HG12	2.00	0.44
1:B:378:GLU:H	1:B:378:GLU:CD	2.21	0.44
1:D:455:GLN:HE21	1:D:557:THR:HG21	1.82	0.44
1:B:75:ASN:HD21	1:B:92:ASN:HD22	1.66	0.43
1:D:517:ILE:HD11	1:D:578:PHE:CE1	2.53	0.43
1:C:422:TYR:CE1	1:C:423:LYS:HE3	2.54	0.43
1:C:78:VAL:HG23	1:C:89:PHE:HB2	2.00	0.43
1:B:405:ILE:HG12	1:B:419:SER:HA	2.00	0.43
1:D:397:ILE:HD12	1:D:434:ILE:HD13	2.01	0.43
1:B:302:ASP:HB3	1:B:314:GLN:HB2	2.00	0.43
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.53	0.43
1:C:544:LEU:HD23	1:C:626:ILE:HD12	2.00	0.43
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.54	0.43
1:A:473:SER:O	1:A:474:GLY:O	2.36	0.43
1:D:291:ALA:O	1:D:295:ILE:HG23	2.18	0.43
1:D:165:ALA:HB2	1:D:216:TRP:CZ2	2.54	0.43
1:D:268:PHE:CD2	1:D:313:LEU:HD21	2.54	0.43
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.54	0.43
1:A:596:ARG:HA	1:A:670:TYR:O	2.19	0.43
1:C:112:GLN:HG3	1:C:113:PHE:CD2	2.53	0.43
1:C:148:ILE:HD11	1:C:164:LEU:HD21	2.01	0.43
1:A:453:ARG:HG3	1:A:454:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:268:PHE:CE2	1:D:313:LEU:HD11	2.54	0.42
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.49	0.42
1:A:72:GLN:HB2	1:A:77:LEU:HD21	2.01	0.42
1:B:415:LEU:HB2	1:B:436:LEU:HD11	2.02	0.42
1:A:80:ASN:HD22	1:A:82:GLU:H	1.66	0.42
1:A:268:PHE:CD2	1:A:313:LEU:HD21	2.54	0.42
1:C:54:ARG:HH21	1:C:54:ARG:CG	2.19	0.42
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.50	0.42
1:C:418:ILE:HA	1:C:430:ASN:O	2.19	0.42
1:A:433:LYS:HE2	1:A:445:LEU:HD21	2.01	0.42
1:A:129:THR:HG22	5:A:1002:HOH:O	2.18	0.42
1:C:155:VAL:HG12	1:C:166:TYR:HB3	2.01	0.42
1:D:450:ASN:O	1:D:454:CYS:HB2	2.20	0.42
1:A:596:ARG:N	1:A:670:TYR:O	2.47	0.42
1:C:179:ASN:HD22	1:C:180:LEU:N	2.17	0.42
1:D:435:GLN:OE1	1:D:441:LYS:HD3	2.19	0.42
1:D:765:LEU:HA	1:D:766:PRO:HD3	1.91	0.42
1:C:167:VAL:HA	1:C:171:ASP:O	2.20	0.41
1:B:70:TYR:CG	1:B:71:LYS:N	2.88	0.41
1:B:313:LEU:O	1:B:325:MET:HA	2.19	0.41
1:A:259:ALA:HB3	1:A:660:GLU:HA	2.02	0.41
1:A:658:ARG:HB2	1:A:687:THR:HG22	2.01	0.41
1:C:302:ASP:HB3	1:C:314:GLN:HB2	2.01	0.41
1:C:397:ILE:HD12	1:C:434:ILE:HD13	2.03	0.41
1:B:506:ASN:HB2	1:C:440:THR:CG2	2.49	0.41
1:A:378:GLU:CD	1:A:378:GLU:H	2.23	0.41
1:A:513:LYS:O	1:A:527:GLN:HA	2.20	0.41
1:D:98:PHE:CD1	1:D:100:HIS:HB2	2.55	0.41
1:D:79:PHE:CD2	1:D:86:SER:HB3	2.54	0.41
1:D:237:GLU:HG2	1:D:253:ARG:HG2	2.02	0.41
1:A:458:SER:OG	1:A:471:ARG:HB3	2.21	0.41
1:D:598:LEU:HB2	1:D:671:MET:SD	2.60	0.41
1:C:457:TYR:HA	1:C:471:ARG:O	2.20	0.41
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.55	0.41
1:A:703:ILE:HA	1:A:733:MET:O	2.21	0.41
1:B:662:TYR:HE1	1:B:710:ASN:HD22	1.69	0.41
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.56	0.41
1:D:105:TYR:HA	1:D:115:LEU:O	2.20	0.41
1:A:135:TYR:CE2	1:A:140:ARG:HG2	2.55	0.41
1:C:478:PRO:HB2	1:C:497:ASN:ND2	2.36	0.41
1:D:598:LEU:HD22	1:D:671:MET:HG2	2.02	0.41
1:A:98:PHE:CE1	1:A:100:HIS:HB2	2.56	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:55:LEU:HD23	1:D:500:LEU:HD22	2.02	0.41
1:B:657:SER:HA	1:B:688:VAL:HG13	2.02	0.41
1:C:49:LEU:HD22	1:C:749:GLN:HA	2.03	0.41
1:A:242:SER:OG	1:A:243:ASP:N	2.53	0.41
1:D:167:VAL:HA	1:D:171:ASP:O	2.21	0.41
1:A:598:LEU:HB2	1:A:671:MET:SD	2.60	0.41
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.77	0.41
1:B:598:LEU:O	1:B:682:HIS:NE2	2.52	0.41
1:A:154:TRP:CD2	1:A:212:SER:HB3	2.56	0.41
1:A:177:GLU:HB2	1:A:180:LEU:HG	2.02	0.41
1:B:55:LEU:HD23	1:B:500:LEU:CD2	2.51	0.41
1:A:146:GLU:O	1:A:175:LYS:NZ	2.52	0.41
1:C:562:ASN:HB2	5:C:841:HOH:O	2.20	0.41
1:A:543:LEU:O	1:A:575:VAL:HA	2.22	0.41
1:B:582:GLY:CA	1:B:594:ILE:HD12	2.50	0.40
1:D:55:LEU:HD23	1:D:500:LEU:CD2	2.51	0.40
1:C:484:SER:O	1:C:488:ASP:HA	2.20	0.40
1:A:546:VAL:HG12	1:A:627:TRP:O	2.21	0.40
1:D:164:LEU:HB3	1:D:175:LYS:HB2	2.03	0.40
1:B:649:CYS:HB3	1:B:699:GLU:HB2	2.02	0.40
1:A:158:SER:OG	1:A:163:LYS:HB2	2.22	0.40
1:A:237:GLU:HA	1:A:252:VAL:O	2.21	0.40
1:A:414:TYR:CE2	1:A:433:LYS:HD3	2.57	0.40
1:B:63:ILE:HA	1:B:63:ILE:HD12	1.81	0.40
1:C:243:ASP:C	1:C:245:SER:N	2.75	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	721/740 (97%)	684 (95%)	36 (5%)	1 (0%)	59	81
1	B	725/740 (98%)	698 (96%)	25 (3%)	2 (0%)	50	73
1	C	721/740 (97%)	688 (95%)	31 (4%)	2 (0%)	50	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	720/740 (97%)	684 (95%)	34 (5%)	2 (0%)	50 73
All	All	2887/2960 (98%)	2754 (95%)	126 (4%)	7 (0%)	56 79

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	474	GLY
1	A	474	GLY
1	B	37	HIS
1	B	474	GLY
1	D	474	GLY
1	C	92	ASN
1	D	109	PRO

### 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%)	611 (94%)	39 (6%)	27 47
1	B	652/662 (98%)	611 (94%)	41 (6%)	25 44
1	C	650/662 (98%)	614 (94%)	36 (6%)	30 52
1	D	649/662 (98%)	617 (95%)	32 (5%)	35 59
All	All	2601/2648 (98%)	2453 (94%)	148 (6%)	29 50

All (148) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	77	LEU
1	A	80	ASN
1	A	95	PHE
1	A	145	GLU
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	246	LEU

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Mol	Chain	Res	Type
1	A	276	LEU
1	A	283	THR
1	A	316	LEU
1	A	343	ARG
1	A	358[A]	ARG
1	A	358[B]	ARG
1	A	385	CYS
1	A	389	ILE
1	A	415	LEU
1	A	436	LEU
1	A	441	LYS
1	A	453	ARG
1	A	464	GLU
1	A	472	CYS
1	A	477	LEU
1	A	482	LEU
1	A	492	ARG
1	A	505	GLN
1	A	507	VAL
1	A	514	LEU
1	A	519	LEU
1	A	538	LYS
1	A	566	TYR
1	A	575	VAL
1	A	598	LEU
1	A	630	SER
1	A	673	LEU
1	A	677	GLU
1	A	685	ASN
1	A	688	VAL
1	A	710	ASN
1	B	41	LYS
1	B	59	SER
1	B	61	ARG
1	B	63	ILE
1	B	129	THR
1	B	139	LYS
1	B	142	LEU
1	B	164	LEU
1	B	179	ASN
1	B	230	ASP
1	B	246	LEU

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Mol	Chain	Res	Type
1	B	276	LEU
1	B	283	THR
1	B	313	LEU
1	B	316	LEU
1	B	325	MET
1	B	360	SER
1	B	370	SER
1	B	385	CYS
1	B	389	ILE
1	B	395	THR
1	B	410	LEU
1	B	415	LEU
1	B	436	LEU
1	B	453	ARG
1	B	464	GLU
1	B	473	SER
1	B	477	LEU
1	B	482	LEU
1	B	504	LEU
1	B	506	ASN
1	B	507	VAL
1	B	514	LEU
1	B	566	TYR
1	B	575	VAL
1	B	594	ILE
1	B	598	LEU
1	B	627	TRP
1	B	660	GLU
1	B	685	ASN
1	B	710	ASN
1	C	54	ARG
1	C	57	LEU
1	C	80	ASN
1	C	129	THR
1	C	170	ASN
1	C	179	ASN
1	C	243	ASP
1	C	246	LEU
1	C	276	LEU
1	C	283	THR
1	C	316	LEU
1	C	325	MET

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Mol	Chain	Res	Type
1	C	385	CYS
1	C	395	THR
1	C	410	LEU
1	C	415	LEU
1	C	433	LYS
1	C	434	ILE
1	C	436	LEU
1	C	441	LYS
1	C	448	GLU
1	C	453	ARG
1	C	463	LYS
1	C	482	LEU
1	C	507	VAL
1	C	514	LEU
1	C	519	LEU
1	C	538	LYS
1	C	575	VAL
1	C	589	LYS
1	C	615	LYS
1	C	673	LEU
1	C	677	GLU
1	C	685	ASN
1	C	688	VAL
1	C	710	ASN
1	D	51	ASN
1	D	56	LYS
1	D	78	VAL
1	D	90	LEU
1	D	109	PRO
1	D	129	THR
1	D	137	LEU
1	D	140	ARG
1	D	142	LEU
1	D	170	ASN
1	D	179	ASN
1	D	246	LEU
1	D	250	LYS
1	D	276	LEU
1	D	280	THR
1	D	316	LEU
1	D	365	THR
1	D	385	CYS

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Mol	Chain	Res	Type
1	D	388	GLN
1	D	392	LYS
1	D	410	LEU
1	D	453	ARG
1	D	482	LEU
1	D	492	ARG
1	D	507	VAL
1	D	514	LEU
1	D	536	LYS
1	D	575	VAL
1	D	598	LEU
1	D	688	VAL
1	D	704	HIS
1	D	710	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	80	ASN
1	A	100	HIS
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
1	A	592	HIS
1	A	710	ASN
1	B	80	ASN
1	B	92	ASN
1	B	123	GLN
1	B	138	ASN
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN
1	B	179	ASN
1	B	430	ASN
1	B	455	GLN
1	B	505	GLN

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Mol	Chain	Res	Type
1	B	506	ASN
1	B	508	GLN
1	B	572	ASN
1	B	592	HIS
1	B	710	ASN
1	C	51	ASN
1	C	80	ASN
1	C	100	HIS
1	C	123	GLN
1	C	138	ASN
1	C	141	GLN
1	C	153	GLN
1	C	170	ASN
1	C	179	ASN
1	C	344	GLN
1	C	430	ASN
1	C	455	GLN
1	C	505	GLN
1	C	697	GLN
1	C	710	ASN
1	C	748	HIS
1	D	80	ASN
1	D	138	ASN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	179	ASN
1	D	344	GLN
1	D	430	ASN
1	D	455	GLN
1	D	508	GLN
1	D	572	ASN
1	D	592	HIS
1	D	621	ASN
1	D	710	ASN
1	D	748	HIS

### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates ⓘ

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$
3	NAG	A	804	1,3	12,14,15	0.69	1 (8%)	15,19,21	0.75	0
3	NAG	A	805	3	12,14,15	0.52	0	15,19,21	1.27	1 (6%)
3	NAG	A	806	1,3	12,14,15	0.48	0	15,19,21	1.30	1 (6%)
3	NAG	A	807	3	12,14,15	0.59	0	15,19,21	0.55	0
3	NAG	B	804	1,3	12,14,15	0.71	1 (8%)	15,19,21	1.13	1 (6%)
3	NAG	B	805	3	12,14,15	0.64	0	15,19,21	1.01	1 (6%)
3	NAG	C	803	1,3	12,14,15	0.73	1 (8%)	15,19,21	1.32	3 (20%)
3	NAG	C	804	3	12,14,15	0.74	0	15,19,21	1.10	2 (13%)
3	NAG	D	802	1,3	12,14,15	0.53	0	15,19,21	0.76	0
3	NAG	D	803	3	12,14,15	0.62	0	15,19,21	1.41	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	805	3	-	0/6/23/26	0/1/1/1
3	NAG	A	806	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	807	3	-	0/6/23/26	0/1/1/1
3	NAG	B	804	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	805	3	-	0/6/23/26	0/1/1/1
3	NAG	C	803	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	804	3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	802	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	803	3	-	0/6/23/26	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	803	NAG	O5-C5	-2.19	1.41	1.45
3	A	804	NAG	O5-C5	-2.06	1.41	1.45
3	B	804	NAG	O5-C5	-2.02	1.41	1.45

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	806	NAG	O5-C5-C6	3.80	110.97	106.98
3	D	803	NAG	O5-C5-C6	3.70	110.86	106.98
3	A	805	NAG	O5-C5-C6	3.64	110.80	106.98
3	B	804	NAG	C3-C2-N2	-3.27	106.78	111.76
3	C	803	NAG	O5-C5-C4	-2.52	107.45	110.65
3	C	803	NAG	O5-C5-C6	2.49	109.59	106.98
3	D	803	NAG	O5-C5-C4	-2.44	107.55	110.65
3	B	805	NAG	C3-C2-N2	-2.38	108.14	111.76
3	C	803	NAG	C3-C2-N2	-2.34	108.19	111.76
3	C	804	NAG	C3-C4-C5	2.20	114.13	110.20
3	C	804	NAG	C4-C3-C2	2.19	116.68	111.32
3	D	803	NAG	C3-C2-N2	-2.18	108.44	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
4	B2Y	A	800	-	15,15,15	0.44	0	19,19,19	0.67	0
2	NAG	A	801	1	12,14,15	0.51	0	15,19,21	0.85	0
2	NAG	A	802	1	12,14,15	0.53	0	15,19,21	0.89	1 (6%)
2	NAG	A	803	1	12,14,15	0.67	0	15,19,21	1.02	1 (6%)
2	NAG	A	808	1	12,14,15	0.60	0	15,19,21	0.94	1 (6%)
4	B2Y	B	800	-	15,15,15	0.47	0	19,19,19	0.53	0
2	NAG	B	801	1	12,14,15	0.67	0	15,19,21	1.73	2 (13%)
2	NAG	B	802	1	12,14,15	0.57	0	15,19,21	0.92	1 (6%)
2	NAG	B	803	1	12,14,15	0.57	0	15,19,21	0.76	0
2	NAG	B	806	1	12,14,15	0.47	0	15,19,21	1.30	1 (6%)
4	B2Y	C	800	-	15,15,15	0.46	0	19,19,19	0.66	0
2	NAG	C	801	1	12,14,15	0.46	0	15,19,21	0.92	0
2	NAG	C	802	1	12,14,15	0.70	0	15,19,21	1.16	1 (6%)
4	B2Y	D	800	-	15,15,15	0.45	0	19,19,19	0.59	0
2	NAG	D	801	1	12,14,15	0.52	0	15,19,21	1.23	1 (6%)
2	NAG	D	804	1	12,14,15	0.58	0	15,19,21	1.56	2 (13%)

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	B2Y	A	800	-	-	0/6/6/6	0/2/2/2
2	NAG	A	801	1	-	0/6/23/26	0/1/1/1
2	NAG	A	802	1	-	0/6/23/26	0/1/1/1
2	NAG	A	803	1	-	0/6/23/26	0/1/1/1
2	NAG	A	808	1	-	0/6/23/26	0/1/1/1
4	B2Y	B	800	-	-	0/6/6/6	0/2/2/2
2	NAG	B	801	1	-	0/6/23/26	0/1/1/1
2	NAG	B	802	1	-	0/6/23/26	0/1/1/1
2	NAG	B	803	1	-	0/6/23/26	0/1/1/1
2	NAG	B	806	1	-	0/6/23/26	0/1/1/1
4	B2Y	C	800	-	-	0/6/6/6	0/2/2/2
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	802	1	-	0/6/23/26	0/1/1/1
4	B2Y	D	800	-	-	0/6/6/6	0/2/2/2
2	NAG	D	801	1	-	0/6/23/26	0/1/1/1
2	NAG	D	804	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	NAG	O5-C5-C6	5.09	112.32	106.98
2	D	804	NAG	O5-C5-C6	3.94	111.11	106.98
2	B	806	NAG	O5-C5-C6	3.92	111.09	106.98
2	D	801	NAG	O5-C5-C6	3.40	110.55	106.98
2	B	801	NAG	O5-C5-C4	-2.56	107.41	110.65
2	B	802	NAG	O5-C5-C6	2.37	109.47	106.98
2	D	804	NAG	C3-C4-C5	-2.33	106.03	110.20
2	A	802	NAG	O5-C5-C6	2.30	109.40	106.98
2	C	802	NAG	C4-C3-C2	2.15	116.59	111.32
2	A	803	NAG	O5-C5-C6	2.13	109.22	106.98
2	A	808	NAG	C3-C2-N2	-2.01	108.70	111.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	804	NAG	C1

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	724/740 (97%)	0.55	62 (8%) 11 10	37, 48, 68, 104	0
1	B	729/740 (98%)	0.30	33 (4%) 32 33	36, 47, 67, 83	0
1	C	724/740 (97%)	0.59	74 (10%) 7 7	37, 48, 69, 101	0
1	D	724/740 (97%)	0.69	99 (13%) 4 3	36, 51, 69, 107	0
All	All	2901/2960 (98%)	0.53	268 (9%) 9 8	36, 48, 68, 107	0

All (268) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	95	PHE	8.2
1	D	83	TYR	7.6
1	D	93	SER	7.2
1	C	135	TYR	6.7
1	C	279	VAL	6.4
1	D	94	THR	5.7
1	C	94	THR	5.4
1	D	386	TYR	5.3
1	C	93	SER	5.3
1	A	88	VAL	5.2
1	A	135	TYR	5.0
1	C	96	ASP	4.9
1	D	97	GLU	4.9
1	C	83	TYR	4.9
1	A	92	ASN	4.9
1	C	99	GLY	4.8
1	D	77	LEU	4.6
1	D	414	TYR	4.6
1	D	333	SER	4.5
1	C	92	ASN	4.4
1	C	141	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	95	PHE	4.3
1	A	96	ASP	4.3
1	A	333	SER	4.3
1	D	88	VAL	4.3
1	A	140	ARG	4.2
1	C	187	TRP	4.2
1	D	322	TYR	4.2
1	A	97	GLU	4.2
1	B	518	ILE	4.1
1	C	102	ILE	4.1
1	D	498	SER	4.1
1	A	138	ASN	4.0
1	D	330	TYR	4.0
1	D	487	ASN	4.0
1	B	81	ALA	3.9
1	C	97	GLU	3.9
1	D	518	ILE	3.9
1	C	280	THR	3.9
1	D	334	SER	3.8
1	D	96	ASP	3.7
1	A	332	GLU	3.7
1	A	86	SER	3.7
1	D	412	SER	3.7
1	D	468	TYR	3.7
1	A	93	SER	3.6
1	D	366	LEU	3.6
1	D	734	TRP	3.6
1	D	766	PRO	3.5
1	D	441	LYS	3.5
1	A	635	VAL	3.5
1	B	83	TYR	3.5
1	D	135	TYR	3.5
1	D	491	LEU	3.5
1	D	55	LEU	3.5
1	C	81	ALA	3.5
1	D	505	GLN	3.4
1	D	436	LEU	3.4
1	C	392	LYS	3.4
1	C	489	LYS	3.4
1	C	332	GLU	3.4
1	A	69	LEU	3.4
1	D	467	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	546	VAL	3.3
1	B	72	GLN	3.3
1	C	467	TYR	3.3
1	C	486	VAL	3.3
1	D	439	TYR	3.3
1	B	87	SER	3.3
1	B	88	VAL	3.2
1	D	92	ASN	3.2
1	C	734	TRP	3.2
1	C	487	ASN	3.2
1	D	389	ILE	3.2
1	D	399	LYS	3.2
1	D	81	ALA	3.1
1	D	98	PHE	3.1
1	D	713	PHE	3.1
1	D	85	ASN	3.1
1	C	340	LEU	3.1
1	A	81	ALA	3.1
1	A	180	LEU	3.1
1	C	506	ASN	3.1
1	D	56	LYS	3.1
1	A	713	PHE	3.1
1	A	702	LEU	3.1
1	C	702	LEU	3.1
1	A	636	THR	3.0
1	B	86	SER	3.0
1	A	98	PHE	3.0
1	D	100	HIS	3.0
1	B	392	LYS	3.0
1	D	62	TRP	3.0
1	D	66	HIS	3.0
1	D	413	ASP	3.0
1	D	486	VAL	2.9
1	D	332	GLU	2.9
1	D	437	SER	2.9
1	D	331	ASP	2.9
1	C	142	LEU	2.9
1	C	390	ASP	2.9
1	A	634	TYR	2.9
1	A	700	TYR	2.9
1	D	91	GLU	2.9
1	C	98	PHE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	703	ILE	2.9
1	C	140	ARG	2.8
1	D	277	SER	2.8
1	C	636	THR	2.8
1	D	338	ASN	2.8
1	A	655	PRO	2.8
1	D	370	SER	2.8
1	D	340	LEU	2.8
1	D	706	THR	2.8
1	A	637	SER	2.7
1	D	84	GLY	2.7
1	B	734	TRP	2.7
1	A	716	SER	2.7
1	A	279	VAL	2.7
1	D	435	GLN	2.7
1	C	536	LYS	2.7
1	D	335	GLY	2.7
1	A	719	ILE	2.7
1	D	276	LEU	2.7
1	A	651	ILE	2.7
1	C	138	ASN	2.7
1	B	70	TYR	2.6
1	A	141	GLN	2.6
1	D	327	ILE	2.6
1	D	78	VAL	2.6
1	A	656	VAL	2.6
1	C	713	PHE	2.6
1	C	719	ILE	2.6
1	D	483	HIS	2.6
1	A	506	ASN	2.6
1	A	502	LYS	2.6
1	A	626	ILE	2.5
1	D	41	LYS	2.5
1	D	86	SER	2.5
1	C	474	GLY	2.5
1	D	346	ILE	2.5
1	D	365	THR	2.5
1	C	504	LEU	2.5
1	A	139	LYS	2.5
1	A	392	LYS	2.5
1	D	388	GLN	2.5
1	D	655	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	632	GLY	2.5
1	D	339	CYS	2.5
1	C	91	GLU	2.5
1	D	432	TYR	2.5
1	A	701	LEU	2.5
1	A	94	THR	2.5
1	C	72	GLN	2.5
1	D	397	ILE	2.5
1	C	80	ASN	2.5
1	A	652	ALA	2.5
1	A	654	ALA	2.5
1	C	90	LEU	2.5
1	A	72	GLN	2.4
1	A	711	VAL	2.4
1	D	652	ALA	2.4
1	D	466	LYS	2.4
1	C	84	GLY	2.4
1	A	627	TRP	2.4
1	C	391	LYS	2.4
1	C	101	SER	2.4
1	D	464	GLU	2.4
1	C	62	TRP	2.4
1	D	95	PHE	2.4
1	D	716	SER	2.4
1	A	715	GLN	2.4
1	B	676	PRO	2.4
1	C	100	HIS	2.4
1	C	700	TYR	2.4
1	B	90	LEU	2.4
1	C	716	SER	2.4
1	B	82	GLU	2.3
1	C	54	ARG	2.3
1	D	442	VAL	2.3
1	D	372	TYR	2.3
1	B	77	LEU	2.3
1	D	90	LEU	2.3
1	A	84	GLY	2.3
1	D	380	GLY	2.3
1	B	703	ILE	2.3
1	C	717	ALA	2.3
1	D	348	MET	2.3
1	C	505	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	63	ILE	2.3
1	D	636	THR	2.3
1	A	66	HIS	2.3
1	B	521	GLU	2.3
1	D	390	ASP	2.3
1	C	276	LEU	2.3
1	A	704	HIS	2.3
1	C	732	ALA	2.3
1	D	615	LYS	2.3
1	D	633	GLY	2.3
1	C	63	ILE	2.3
1	D	497	ASN	2.2
1	B	702	LEU	2.2
1	B	628	GLY	2.2
1	B	653	VAL	2.2
1	D	523	LYS	2.2
1	D	546	VAL	2.2
1	B	99	GLY	2.2
1	A	688	VAL	2.2
1	C	330	TYR	2.2
1	A	543	LEU	2.2
1	C	82	GLU	2.2
1	A	732	ALA	2.2
1	D	499	ALA	2.2
1	C	89	PHE	2.2
1	A	546	VAL	2.2
1	B	333	SER	2.2
1	C	350	THR	2.2
1	C	336	ARG	2.2
1	A	87	SER	2.2
1	D	138	ASN	2.2
1	B	71	LYS	2.2
1	B	713	PHE	2.2
1	C	656	VAL	2.2
1	A	90	LEU	2.2
1	D	336	ARG	2.2
1	C	491	LEU	2.1
1	B	632	GLY	2.1
1	D	342	ALA	2.1
1	C	637	SER	2.1
1	C	388	GLN	2.1
1	B	140	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	83	TYR	2.1
1	A	717	ALA	2.1
1	D	393	ASP	2.1
1	D	391	LYS	2.1
1	B	733	MET	2.1
1	A	330	TYR	2.1
1	C	546	VAL	2.1
1	C	139	LYS	2.1
1	C	652	ALA	2.1
1	A	733	MET	2.1
1	D	521	GLU	2.1
1	C	231	THR	2.1
1	A	91	GLU	2.1
1	A	300	LEU	2.1
1	D	63	ILE	2.1
1	B	631	TYR	2.1
1	A	103	ASN	2.1
1	B	544	LEU	2.1
1	C	277	SER	2.1
1	C	452	GLU	2.0
1	D	717	ALA	2.0
1	C	537	SER	2.0
1	D	449	LEU	2.0
1	B	536	LYS	2.0
1	B	636	THR	2.0
1	C	75	ASN	2.0
1	C	113	PHE	2.0
1	D	75	ASN	2.0
1	C	333	SER	2.0
1	D	484	SER	2.0
1	C	521	GLU	2.0
1	B	241	TYR	2.0
1	D	416	TYR	2.0
1	C	483	HIS	2.0
1	D	141	GLN	2.0
1	B	633	GLY	2.0
1	D	440	THR	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
3	NAG	D	803	14/15	0.27	11.94	67,68,72,72	0
3	NAG	B	805	14/15	0.39	4.64	80,82,83,83	0
3	NAG	A	805	14/15	0.28	3.29	68,70,71,71	0
3	NAG	C	804	14/15	0.34	2.52	73,76,78,78	0
3	NAG	B	804	14/15	0.20	1.40	67,69,73,77	0
3	NAG	A	806	14/15	0.22	0.61	73,76,79,80	0
3	NAG	D	802	14/15	0.17	0.35	55,58,61,63	0
3	NAG	A	807	14/15	0.33	0.07	83,84,85,85	0
3	NAG	A	804	14/15	0.18	-0.11	58,60,62,66	0
3	NAG	C	803	14/15	0.16	-0.59	63,65,68,72	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
2	NAG	B	803	14/15	0.33	10.64	63,65,68,68	0
2	NAG	A	808	14/15	0.31	4.23	61,63,64,64	0
2	NAG	C	801	14/15	0.20	1.77	55,55,56,57	0
2	NAG	C	802	14/15	0.27	1.72	68,70,74,74	0
2	NAG	A	802	14/15	0.28	1.71	65,66,68,68	0
2	NAG	A	803	14/15	0.28	1.46	71,73,76,77	0
4	B2Y	B	800	14/14	0.27	1.41	60,62,63,64	0
2	NAG	D	804	14/15	0.21	1.21	78,80,82,82	0
2	NAG	B	802	14/15	0.19	0.88	63,64,66,66	0
4	B2Y	C	800	14/14	0.24	0.65	50,54,55,55	0
2	NAG	D	801	14/15	0.20	0.65	58,60,62,63	0
2	NAG	A	801	14/15	0.30	0.39	72,73,74,74	0
4	B2Y	A	800	14/14	0.23	0.15	53,56,58,58	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	B2Y	D	800	14/14	0.16	-0.12	42,44,46,46	0
2	NAG	B	806	14/15	0.14	-0.50	67,69,73,74	0
2	NAG	B	801	14/15	0.22	-1.19	78,79,80,80	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.