



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:08 PM GMT

PDB ID : 3G0D
Title : Crystal structure of dipeptidyl peptidase IV in complex with a pyrimidinedione inhibitor 2
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 : 2.39 Å(reported)

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

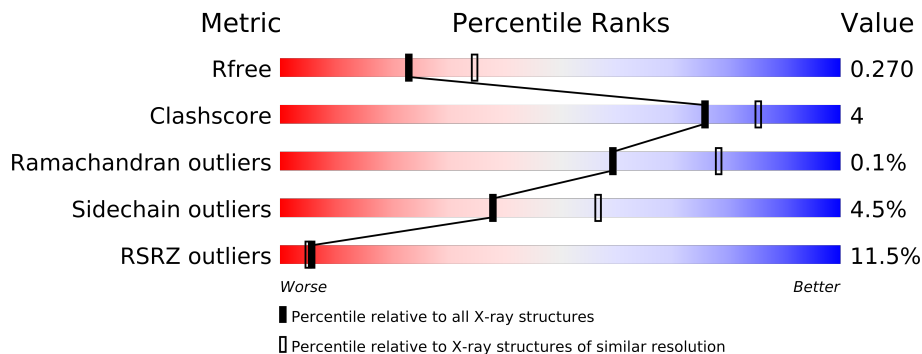
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.39 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	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	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 25530 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	3	0
			5936	3813	977	1120	26			
1	B	728	Total	C	N	O	S	0	3	0
			5970	3833	985	1126	26			
1	C	723	Total	C	N	O	S	0	1	0
			5927	3808	975	1118	26			
1	D	723	Total	C	N	O	S	0	0	0
			5918	3800	973	1119	26			

There are 48 discrepancies between the modelled and reference sequences:

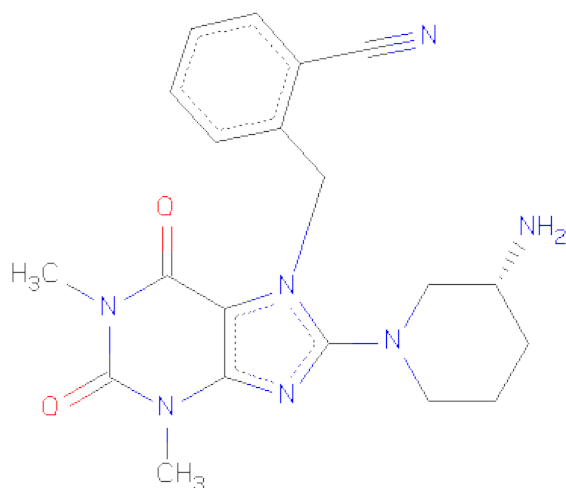
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
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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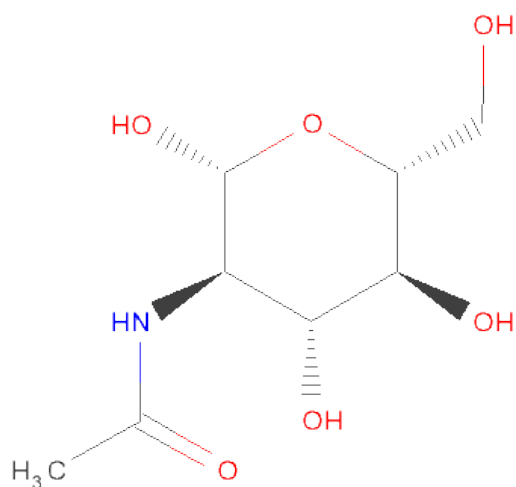
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
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-({8-[(3R)-3-AMINOPIPERIDIN-1-YL]-1,3-DIMETHYL-2,6-DIOXO-1,2,3,6-TETRAHYDRO-7H-PURIN-7-YL}METHYL)BENZONITRILE (three-letter code: XIH) (formula: C₂₀H₂₃N₇O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			29	20	7	2		
2	B	1	Total	C	N	O	0	0
			29	20	7	2		
2	C	1	Total	C	N	O	0	0
			29	20	7	2		
2	D	1	Total	C	N	O	0	0
			29	20	7	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	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		

- 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	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		

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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 5 is water.

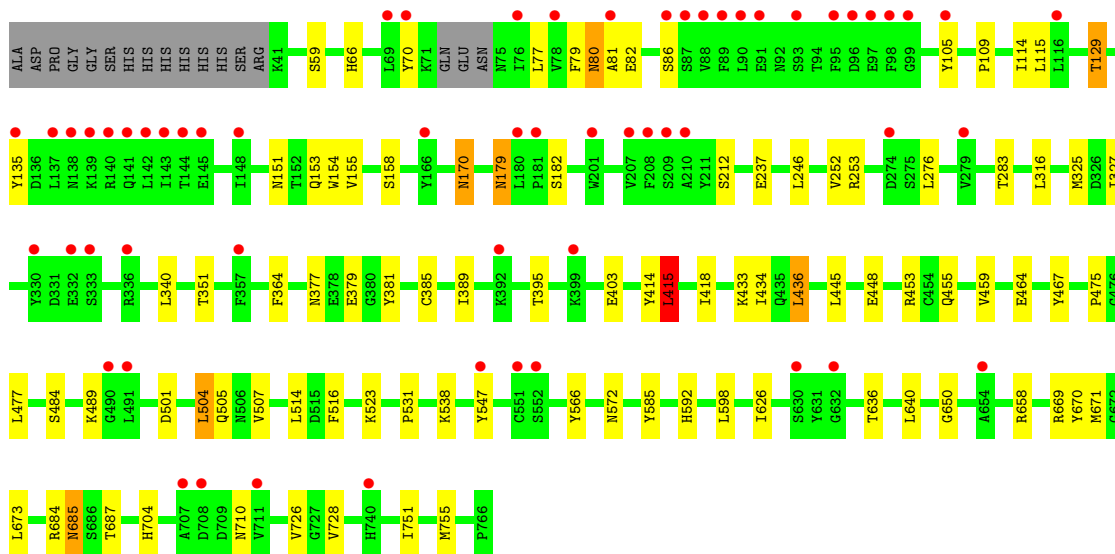
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	394	Total O 394 394	0	0
5	B	370	Total O 370 370	0	0
5	C	348	Total O 348 348	0	0
5	D	215	Total O 215 215	0	0

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.

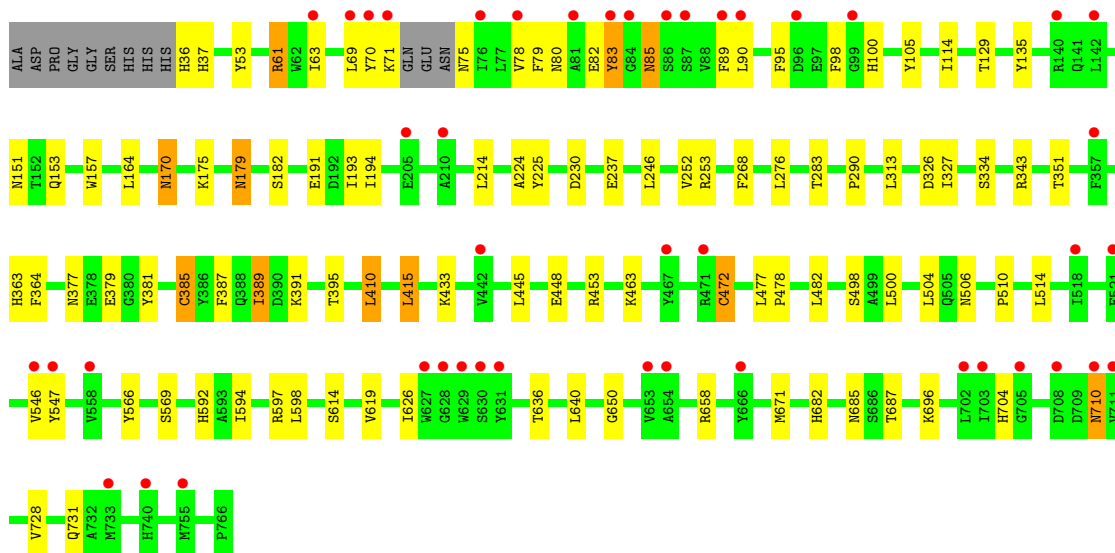
- Molecule 1: Dipeptidyl peptidase 4

Chain A: 



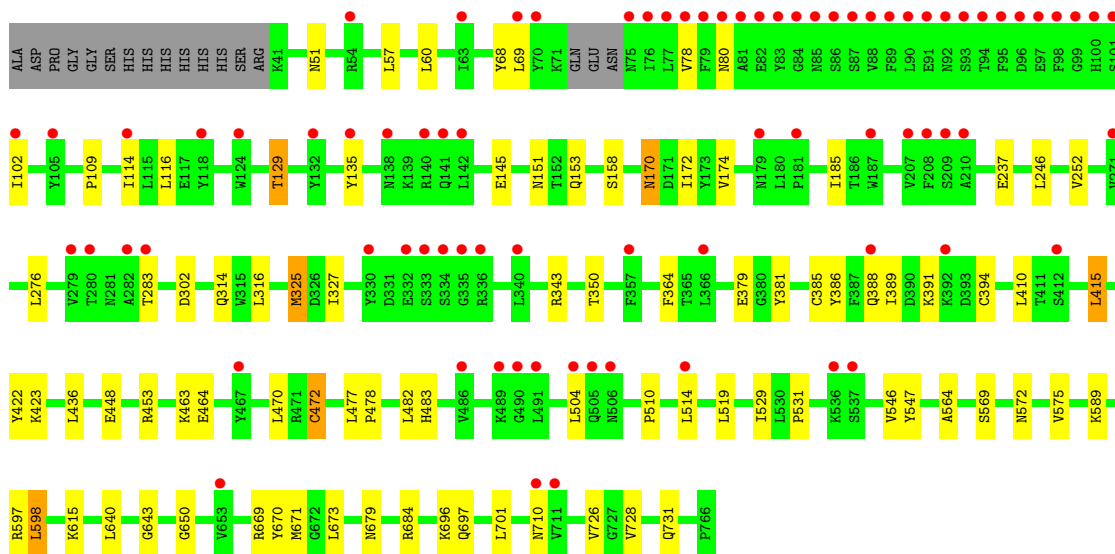
- Molecule 1: Dipeptidyl peptidase 4

Chain B: 



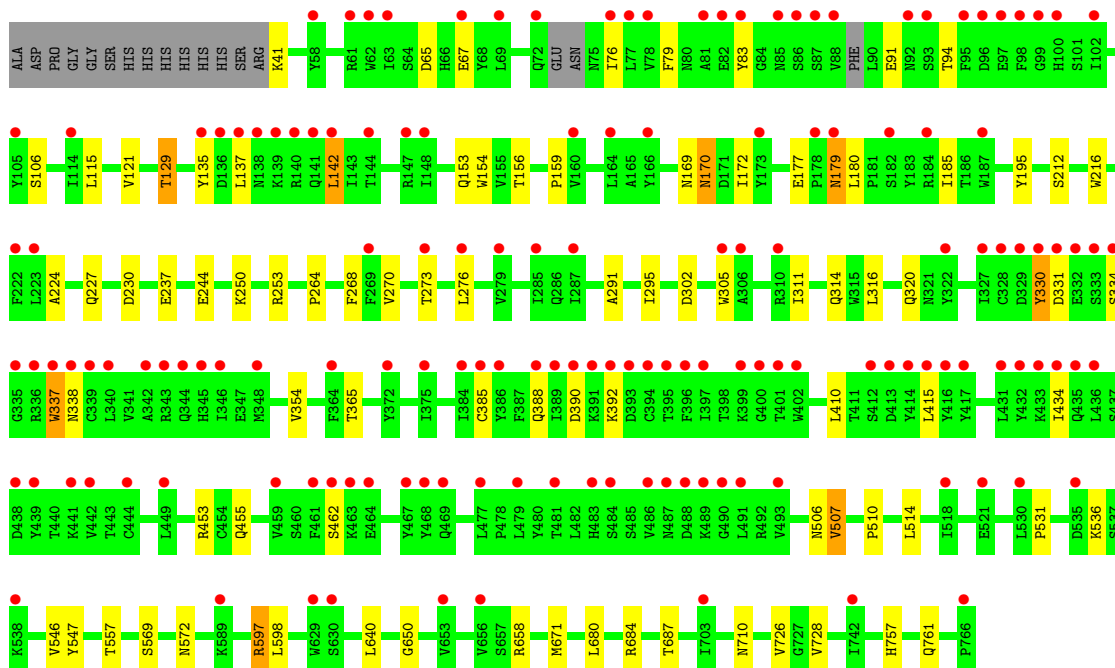
- Molecule 1: Dipeptidyl peptidase 4

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, α , β , γ	122.91Å 123.44Å 145.68Å 90.00° 114.69° 90.00°	Depositor
Resolution (Å)	50.00 – 2.39 48.71 – 2.40	Depositor EDS
% Data completeness (in resolution range)	95.2 (50.00-2.39) 95.2 (48.71-2.40)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.28 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.187 , 0.239 0.231 , 0.270	Depositor DCC
R_{free} test set	7417 reflections (5.02%)	DCC
Wilson B-factor (Å ²)	46.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 38.1	EDS
Estimated twinning fraction	0.004 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 147788 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	25530	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.29% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: XIH, 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	0.45	0/6119	0.60	1/8321 (0.0%)
1	B	0.45	0/6155	0.59	1/8370 (0.0%)
1	C	0.45	0/6102	0.60	1/8298 (0.0%)
1	D	0.48	4/6087 (0.1%)	0.58	4/8277 (0.0%)
All	All	0.45	4/24463 (0.0%)	0.59	7/33266 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	338	ASN	CG-OD1	11.25	1.48	1.24
1	D	337	TRP	CD2-CE2	6.56	1.49	1.41
1	D	338	ASN	C-O	6.05	1.34	1.23
1	D	270	VAL	CB-CG1	5.74	1.65	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	330	TYR	CB-CG-CD1	-9.73	115.16	121.00
1	D	330	TYR	CB-CG-CD2	8.35	126.01	121.00
1	B	415	LEU	CA-CB-CG	6.19	129.53	115.30
1	C	415	LEU	CA-CB-CG	5.86	128.77	115.30
1	A	415	LEU	CA-CB-CG	5.46	127.86	115.30
1	D	142	LEU	CA-CB-CG	5.22	127.31	115.30
1	D	330	TYR	O-C-N	5.12	130.89	122.70

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	5936	0	5655	55	0
1	B	5970	0	5678	53	0
1	C	5927	0	5650	40	0
1	D	5918	0	5641	38	0
2	A	29	0	23	0	0
2	B	29	0	23	1	0
2	C	29	0	23	0	0
2	D	29	0	23	0	0
3	A	56	0	52	0	0
3	B	56	0	52	0	0
3	C	56	0	52	0	0
3	D	28	0	26	0	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	394	0	0	2	0
5	B	370	0	0	1	0
5	C	348	0	0	1	0
5	D	215	0	0	1	0
All	All	25530	0	23023	186	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 4.

All (186) 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	1.11	0.91
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.20	0.90
1:C:153:GLN:HE22	1:C:170:ASN:H	1.19	0.89
1:B:379:GLU:HG3	1:B:381:TYR:HD1	1.39	0.87
1:B:36:HIS:CD2	1:B:37:HIS:H	1.95	0.85
1:B:153:GLN:HE22	1:B:170:ASN:H	1.26	0.84
1:D:153:GLN:HE22	1:D:170:ASN:H	1.29	0.81

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:70:TYR:HB3	1:B:79:PHE:CE1	2.23	0.73
1:B:731[B]:GLN:HG3	5:B:1227:HOH:O	1.90	0.71
1:A:129:THR:HG23	1:A:151:ASN:HA	1.73	0.69
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.75	0.69
1:B:696:LYS:HG3	1:B:728:VAL:HG22	1.75	0.68
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.77	0.67
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.75	0.66
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.76	0.66
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.79	0.65
1:C:564:ALA:HB1	1:C:575:VAL:HG11	1.79	0.64
1:B:129:THR:HG23	1:B:151:ASN:HA	1.80	0.63
1:A:115:LEU:HD21	1:A:155:VAL:HG21	1.82	0.61
1:B:379:GLU:HG3	1:B:381:TYR:CD1	2.29	0.60
1:B:70:TYR:HB3	1:B:79:PHE:HE1	1.65	0.60
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.85	0.59
1:D:237:GLU:HG2	1:D:253:ARG:HG2	1.85	0.59
1:B:237:GLU:HG2	1:B:253:ARG:HG2	1.86	0.58
1:D:331:ASP:HB3	1:D:334:SER:HB2	1.85	0.58
1:C:388:GLN:HG3	1:C:391:LYS:HE3	1.86	0.58
1:D:726:VAL:HG23	1:D:728:VAL:HG23	1.87	0.57
1:A:70:TYR:HB3	1:A:79:PHE:CE1	2.40	0.56
1:A:179:ASN:H	1:A:179:ASN:HD22	1.52	0.56
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.87	0.55
1:C:529:ILE:HB	1:C:575:VAL:HG13	1.89	0.55
1:B:510:PRO:HD3	1:B:569:SER:HB2	1.87	0.55
1:A:379:GLU:HG3	1:A:381:TYR:HD1	1.70	0.55
1:C:174:VAL:CG2	1:C:185:ILE:HD11	2.37	0.55
1:D:598:LEU:HD22	1:D:671:MET:HG2	1.88	0.55
1:C:726:VAL:HG23	1:C:728:VAL:HG23	1.88	0.54
1:C:388:GLN:HB2	1:C:391:LYS:HG2	1.89	0.54
1:B:597:ARG:HH11	1:B:682:HIS:HB2	1.72	0.54
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.89	0.54
1:C:379:GLU:HG3	1:C:381:TYR:HD1	1.71	0.54
1:B:71:LYS:HG3	1:B:75:ASN:HB3	1.90	0.54
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.91	0.53
1:D:195:TYR:O	1:D:227:GLN:HA	2.08	0.53
1:C:364:PHE:HE2	1:C:389:ILE:HD11	1.74	0.53
1:D:273:THR:HA	1:D:276:LEU:HD13	1.91	0.53
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.91	0.53
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.91	0.53
1:A:598:LEU:HB2	1:A:671:MET:SD	2.50	0.52
1:C:343:ARG:HD2	1:C:389:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:510:PRO:HD3	1:D:569:SER:HB2	1.92	0.52
1:A:80:ASN:HD22	1:A:82:GLU:H	1.58	0.52
1:D:291:ALA:O	1:D:295:ILE:HG23	2.09	0.52
1:A:154:TRP:CE2	1:A:212:SER:HB3	2.44	0.52
1:A:455:GLN:HB2	1:A:475:PRO:HD3	1.92	0.52
1:B:614:SER:HA	1:B:619:VAL:HB	1.92	0.51
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.76	0.51
1:D:415:LEU:HB3	1:D:434:ILE:HG23	1.93	0.51
1:B:377:ASN:OD1	1:B:379:GLU:HG2	2.11	0.51
1:A:179:ASN:N	1:A:179:ASN:HD22	2.07	0.51
1:D:177:GLU:HB2	1:D:180:LEU:HG	1.92	0.51
1:C:153:GLN:NE2	1:C:170:ASN:H	1.99	0.51
1:C:531:PRO:HB3	1:C:572:ASN:HD22	1.75	0.51
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.46	0.50
1:A:59:SER:O	1:A:70:TYR:HD1	1.93	0.50
1:D:121:VAL:HB	1:D:129:THR:HG22	1.92	0.50
1:D:305:TRP:CE2	1:D:311:ILE:HD12	2.46	0.50
1:B:179:ASN:H	1:B:179:ASN:HD22	1.60	0.50
1:C:314:GLN:HG2	1:C:325:MET:HB2	1.95	0.49
1:C:597:ARG:NH1	1:C:679:ASN:OD1	2.46	0.49
1:A:153:GLN:NE2	1:A:170:ASN:H	1.92	0.49
1:A:114:ILE:CG2	1:A:135:TYR:HB3	2.43	0.49
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.95	0.49
1:C:172:ILE:HG22	1:C:185:ILE:HD12	1.94	0.49
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.96	0.49
1:A:684[B]:ARG:HD2	5:A:982:HOH:O	2.12	0.49
1:A:325:MET:CE	1:A:327:ILE:HD11	2.42	0.48
1:C:69:LEU:HD23	1:C:78:VAL:HG22	1.95	0.48
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.48	0.48
1:B:90:LEU:HD21	1:B:95:PHE:HE2	1.79	0.48
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.94	0.48
1:B:343:ARG:HD3	1:B:389:ILE:HG23	1.96	0.48
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.95	0.48
1:A:364:PHE:HE2	1:A:389:ILE:HD11	1.79	0.48
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.78	0.48
1:A:77:LEU:HB3	1:A:86:SER:HB2	1.96	0.47
2:B:800:XIH:H101	2:B:800:XIH:H172	1.96	0.47
1:B:80:ASN:HB3	1:B:85:ASN:O	2.15	0.47
1:D:757:HIS:HD2	5:D:1339:HOH:O	1.97	0.47
1:D:91:GLU:HB3	1:D:94:THR:OG1	2.15	0.47
1:A:170:ASN:N	1:A:170:ASN:HD22	2.12	0.47
1:C:170:ASN:N	1:C:170:ASN:HD22	2.13	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.79	0.47
1:A:237:GLU:HG2	1:A:253:ARG:HG2	1.97	0.47
1:A:129:THR:HG21	1:A:151:ASN:HD22	1.79	0.47
1:C:129:THR:HG23	1:C:151:ASN:HA	1.96	0.47
1:B:472:CYS:O	1:B:478:PRO:HA	2.14	0.46
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.50	0.46
1:D:106:SER:HB3	1:D:115:LEU:HB3	1.97	0.46
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.97	0.46
1:C:684[A]:ARG:HD2	5:C:1004:HOH:O	2.15	0.46
1:A:325:MET:HE2	1:A:327:ILE:HD11	1.98	0.46
1:D:179:ASN:ND2	1:D:179:ASN:H	2.11	0.46
1:D:172:ILE:HG22	1:D:185:ILE:HD13	1.98	0.46
1:A:467:TYR:HD2	1:A:484:SER:HA	1.81	0.46
1:C:643:GLY:HA2	1:C:697:GLN:HE22	1.80	0.46
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.98	0.46
1:C:174:VAL:HG23	1:C:185:ILE:CD1	2.44	0.46
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.97	0.46
1:B:433:LYS:HD2	1:B:445:LEU:HD21	1.98	0.46
1:A:237:GLU:HA	1:A:252:VAL:O	2.16	0.45
1:A:377:ASN:OD1	1:A:379:GLU:HG2	2.15	0.45
1:A:414:TYR:CD2	1:A:433:LYS:HD3	2.51	0.45
1:B:351:THR:OG1	1:B:592:HIS:HD2	1.99	0.45
1:B:290:PRO:HD3	1:B:326:ASP:OD1	2.16	0.45
1:C:422:TYR:CE1	1:C:423:LYS:HE3	2.50	0.45
1:A:501:ASP:O	1:A:505[B]:GLN:HG2	2.17	0.45
1:A:415:LEU:HB3	1:A:434:ILE:CG2	2.47	0.45
1:D:67:GLU:HA	1:D:79:PHE:O	2.17	0.45
1:B:36:HIS:CG	1:B:37:HIS:H	2.32	0.45
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.99	0.45
1:D:320:GLN:O	1:D:354:VAL:HG12	2.17	0.45
1:C:302:ASP:HB3	1:C:314:GLN:HB2	1.99	0.44
1:B:626:ILE:HG23	1:B:636:THR:HG23	1.99	0.44
1:B:710:ASN:C	1:B:710:ASN:HD22	2.20	0.44
1:A:179:ASN:H	1:A:179:ASN:ND2	2.15	0.44
1:A:114:ILE:HG23	1:A:135:TYR:HB3	1.98	0.44
1:A:80:ASN:HD22	1:A:81:ALA:N	2.15	0.44
1:D:230:ASP:OD1	1:D:264:PRO:HB3	2.18	0.44
1:A:467:TYR:CD2	1:A:484:SER:HA	2.53	0.44
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.53	0.44
1:D:76:ILE:H	1:D:91:GLU:HA	1.83	0.43
1:B:214:LEU:HD23	1:B:225:TYR:HB3	1.99	0.43
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:135:TYR:CZ	1:D:142:LEU:HB2	2.53	0.43
1:A:66:HIS:HB3	1:A:467:TYR:HE1	1.82	0.43
1:D:154:TRP:CE2	1:D:212:SER:HB3	2.53	0.43
1:D:330:TYR:HB2	1:D:337:TRP:CH2	2.53	0.43
1:A:685:ASN:ND2	5:A:981:HOH:O	2.51	0.43
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.99	0.43
1:A:415:LEU:HB2	1:A:436:LEU:HD11	2.00	0.43
1:D:597:ARG:HA	1:D:597:ARG:HD3	1.84	0.43
1:C:701:LEU:HD13	1:C:731:GLN:HB2	1.99	0.43
1:B:598:LEU:O	1:B:682:HIS:NE2	2.48	0.43
1:B:598:LEU:HB2	1:B:671:MET:SD	2.59	0.43
1:B:105:TYR:HB2	1:B:114:ILE:HD11	2.00	0.43
1:B:626:ILE:O	1:B:650:GLY:HA2	2.18	0.43
1:D:156:THR:HG23	1:D:216:TRP:HE1	1.83	0.43
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.49	0.42
1:A:109:PRO:HG2	1:A:158:SER:O	2.18	0.42
1:B:61:ARG:HG3	1:B:69:LEU:HB2	2.02	0.42
1:C:470:LEU:HD12	1:C:483:HIS:NE2	2.34	0.42
1:A:751:ILE:O	1:A:755:MET:HG3	2.19	0.42
1:B:327:ILE:HD13	1:B:389:ILE:HG13	2.00	0.42
1:C:643:GLY:HA2	1:C:697:GLN:NE2	2.35	0.42
1:A:403:GLU:OE2	1:A:585:TYR:HA	2.19	0.42
1:A:418:ILE:HD11	1:A:459:VAL:HG12	2.02	0.42
1:C:237:GLU:HA	1:C:252:VAL:O	2.20	0.42
1:C:669:ARG:HD2	1:C:670:TYR:CZ	2.54	0.41
1:A:153:GLN:HE22	1:A:170:ASN:N	1.95	0.41
1:B:191:GLU:O	1:B:193:ILE:HD12	2.20	0.41
1:B:175:LYS:HG3	1:B:182:SER:HB3	2.03	0.41
1:A:658:ARG:HB2	1:A:687:THR:HG22	2.01	0.41
1:A:504:LEU:HA	1:A:507:VAL:HG12	2.02	0.41
1:B:363:HIS:HB3	1:B:410:LEU:HD22	2.02	0.41
1:D:65:ASP:HA	1:D:462:SER:HB2	2.02	0.41
1:D:169:ASN:O	1:D:170:ASN:HB2	2.21	0.41
1:B:98:PHE:CE1	1:B:100:HIS:HB2	2.55	0.41
1:B:53:TYR:HB3	1:B:500:LEU:HD11	2.03	0.41
1:C:472:CYS:O	1:C:478:PRO:HA	2.20	0.41
1:C:102:ILE:HD12	1:C:116:LEU:HB3	2.03	0.41
1:D:455:GLN:HE21	1:D:557:THR:HG21	1.86	0.41
1:C:696:LYS:HG3	1:C:728:VAL:HG22	2.02	0.40
1:C:386:TYR:O	1:C:394:CYS:HB2	2.21	0.40
1:C:109:PRO:HG2	1:C:158:SER:O	2.21	0.40
1:B:82:GLU:HB2	1:B:83:TYR:CD1	2.56	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:237:GLU:HA	1:B:252:VAL:O	2.22	0.40
1:D:41:LYS:HG3	1:D:507:VAL:HG12	2.03	0.40
1:A:669:ARG:HD2	1:A:670:TYR:CZ	2.56	0.40
1:D:680:LEU:O	1:D:684:ARG:HG3	2.21	0.40
1:A:433:LYS:HE2	1:A:445:LEU:HD21	2.03	0.40
1:B:658:ARG:HB2	1:B:687:THR:HG22	2.03	0.40
1:C:60:LEU:HB2	1:C:68:TYR:CD1	2.56	0.40
1:C:510:PRO:HD3	1:C:569:SER:HB2	2.04	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	722/740 (98%)	690 (96%)	32 (4%)	0	100	100
1	B	727/740 (98%)	702 (97%)	24 (3%)	1 (0%)	59	78
1	C	720/740 (97%)	692 (96%)	28 (4%)	0	100	100
1	D	717/740 (97%)	687 (96%)	29 (4%)	1 (0%)	59	78
All	All	2886/2960 (98%)	2771 (96%)	113 (4%)	2 (0%)	59	78

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	463	LYS
1	D	390	ASP

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	651/662 (98%)	623 (96%)	28 (4%)	40	59
1	B	654/662 (99%)	620 (95%)	34 (5%)	32	49
1	C	649/662 (98%)	616 (95%)	33 (5%)	33	50
1	D	648/662 (98%)	625 (96%)	23 (4%)	48	69
All	All	2602/2648 (98%)	2484 (96%)	118 (4%)	38	57

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	129	THR
1	A	170	ASN
1	A	179	ASN
1	A	182	SER
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	316	LEU
1	A	340	LEU
1	A	385	CYS
1	A	395	THR
1	A	415	LEU
1	A	436	LEU
1	A	448	GLU
1	A	453	ARG
1	A	464	GLU
1	A	477	LEU
1	A	489	LYS
1	A	504	LEU
1	A	514	LEU
1	A	538	LYS
1	A	547	TYR
1	A	566	TYR
1	A	673	LEU
1	A	685	ASN
1	A	704	HIS
1	A	710	ASN
1	B	61	ARG
1	B	63	ILE
1	B	83	TYR
1	B	85	ASN
1	B	170	ASN

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Mol	Chain	Res	Type
1	B	179	ASN
1	B	230	ASP
1	B	246	LEU
1	B	276	LEU
1	B	283	THR
1	B	313	LEU
1	B	334	SER
1	B	385	CYS
1	B	389	ILE
1	B	391	LYS
1	B	395	THR
1	B	410	LEU
1	B	415	LEU
1	B	448	GLU
1	B	453	ARG
1	B	472	CYS
1	B	477	LEU
1	B	482	LEU
1	B	498	SER
1	B	504	LEU
1	B	506	ASN
1	B	514	LEU
1	B	546	VAL
1	B	547	TYR
1	B	566	TYR
1	B	594	ILE
1	B	685	ASN
1	B	704	HIS
1	B	710	ASN
1	C	51	ASN
1	C	57	LEU
1	C	80	ASN
1	C	129	THR
1	C	145	GLU
1	C	170	ASN
1	C	246	LEU
1	C	276	LEU
1	C	283	THR
1	C	316	LEU
1	C	325	MET
1	C	350	THR
1	C	385	CYS

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Mol	Chain	Res	Type
1	C	410	LEU
1	C	415	LEU
1	C	436	LEU
1	C	448	GLU
1	C	453	ARG
1	C	463	LYS
1	C	464	GLU
1	C	472	CYS
1	C	477	LEU
1	C	482	LEU
1	C	504	LEU
1	C	514	LEU
1	C	519	LEU
1	C	546	VAL
1	C	547	TYR
1	C	589	LYS
1	C	598	LEU
1	C	615	LYS
1	C	673	LEU
1	C	710	ASN
1	D	83	TYR
1	D	129	THR
1	D	137	LEU
1	D	170	ASN
1	D	179	ASN
1	D	244	GLU
1	D	250	LYS
1	D	316	LEU
1	D	365	THR
1	D	385	CYS
1	D	388	GLN
1	D	392	LYS
1	D	410	LEU
1	D	453	ARG
1	D	506	ASN
1	D	507	VAL
1	D	514	LEU
1	D	536	LYS
1	D	546	VAL
1	D	547	TYR
1	D	597	ARG
1	D	710	ASN

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Mol	Chain	Res	Type
1	D	761	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	141	GLN
1	A	151	ASN
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	455	GLN
1	A	572	ASN
1	A	592	HIS
1	A	697	GLN
1	A	710	ASN
1	B	36	HIS
1	B	80	ASN
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN
1	B	179	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	C	80	ASN
1	C	123	GLN
1	C	153	GLN
1	C	170	ASN
1	C	344	GLN
1	C	455	GLN
1	C	572	ASN
1	C	685	ASN
1	C	694	ASN
1	C	697	GLN
1	C	710	ASN
1	D	75	ASN

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Mol	Chain	Res	Type
1	D	112	GLN
1	D	153	GLN
1	D	169	ASN
1	D	170	ASN
1	D	179	ASN
1	D	455	GLN
1	D	572	ASN
1	D	592	HIS
1	D	685	ASN
1	D	710	ASN

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	0.73	1 (8%)	15,19,21	0.96	1 (6%)
4	NAG	A	805	4	12,14,15	0.51	0	15,19,21	0.79	0
4	NAG	A	806	1,4	12,14,15	0.51	0	15,19,21	1.04	1 (6%)
4	NAG	A	807	4	12,14,15	0.63	0	15,19,21	0.64	0
4	NAG	B	804	1,4	12,14,15	0.59	0	15,19,21	0.80	0
4	NAG	B	805	4	12,14,15	0.54	0	15,19,21	0.99	1 (6%)
4	NAG	C	803	1,4	12,14,15	0.67	0	15,19,21	1.25	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	C	804	4	12,14,15	0.57	0	15,19,21	0.87	1 (6%)
4	NAG	D	802	1,4	12,14,15	0.56	0	15,19,21	0.89	0
4	NAG	D	803	4	12,14,15	0.57	0	15,19,21	1.06	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
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	804	NAG	O5-C5	-2.00	1.41	1.45

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	806	NAG	O5-C5-C6	3.00	110.12	106.98
4	C	803	NAG	O5-C5-C6	2.92	110.05	106.98
4	D	803	NAG	O5-C5-C6	2.76	109.88	106.98
4	C	804	NAG	O5-C5-C6	2.61	109.72	106.98
4	B	805	NAG	C3-C2-N2	-2.27	108.30	111.76
4	A	804	NAG	O5-C5-C6	2.09	109.18	106.98

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.6 Ligand geometry ⓘ

18 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	XIH	A	800	-	32,32,32	2.35	8 (25%)	40,47,47	2.42	14 (35%)
3	NAG	A	801	1	12,14,15	0.60	0	15,19,21	0.74	0
3	NAG	A	802	1	12,14,15	0.50	0	15,19,21	0.94	1 (6%)
3	NAG	A	803	1	12,14,15	0.59	0	15,19,21	0.79	0
3	NAG	A	808	1	12,14,15	0.60	0	15,19,21	0.72	0
2	XIH	B	800	-	32,32,32	2.28	9 (28%)	40,47,47	2.37	12 (30%)
3	NAG	B	801	1	12,14,15	0.73	0	15,19,21	1.98	2 (13%)
3	NAG	B	802	1	12,14,15	0.51	0	15,19,21	1.16	1 (6%)
3	NAG	B	803	1	12,14,15	0.60	0	15,19,21	0.91	0
3	NAG	B	806	1	12,14,15	0.49	0	15,19,21	1.36	1 (6%)
2	XIH	C	800	-	32,32,32	2.50	9 (28%)	40,47,47	2.33	16 (40%)
3	NAG	C	801	1	12,14,15	0.64	0	15,19,21	0.93	1 (6%)
3	NAG	C	802	1	12,14,15	0.68	0	15,19,21	1.02	0
3	NAG	C	805	1	12,14,15	0.61	0	15,19,21	1.17	2 (13%)
3	NAG	C	806	1	12,14,15	0.63	0	15,19,21	1.06	2 (13%)
2	XIH	D	800	-	32,32,32	2.55	9 (28%)	40,47,47	2.25	11 (27%)
3	NAG	D	801	1	12,14,15	0.61	0	15,19,21	1.13	2 (13%)
3	NAG	D	804	1	12,14,15	0.66	0	15,19,21	1.44	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
2	XIH	A	800	-	-	0/8/20/20	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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	XIH	B	800	-	-	0/8/20/20	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	XIH	C	800	-	-	0/8/20/20	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
3	NAG	C	805	1	-	0/6/23/26	0/1/1/1
3	NAG	C	806	1	-	0/6/23/26	0/1/1/1
2	XIH	D	800	-	-	0/8/20/20	0/2/4/4
3	NAG	D	801	1	-	0/6/23/26	0/1/1/1
3	NAG	D	804	1	1/1/5/7	0/6/23/26	0/1/1/1

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	800	XIH	C23-C24	-9.55	1.29	1.44
2	D	800	XIH	C23-C24	-9.52	1.29	1.44
2	B	800	XIH	C23-C24	-8.93	1.30	1.44
2	A	800	XIH	C23-C24	-8.64	1.30	1.44
2	D	800	XIH	C3-C5	5.28	1.49	1.41
2	A	800	XIH	C3-C5	5.02	1.49	1.41
2	D	800	XIH	C28-N	4.94	1.43	1.38
2	D	800	XIH	C5-C6	4.87	1.47	1.40
2	C	800	XIH	C3-C5	4.72	1.48	1.41
2	C	800	XIH	C28-N	4.51	1.43	1.38
2	A	800	XIH	C5-C6	4.47	1.47	1.40
2	C	800	XIH	C5-C6	4.07	1.46	1.40
2	B	800	XIH	C3-C5	4.05	1.47	1.41
2	B	800	XIH	C5-C6	3.99	1.46	1.40
2	A	800	XIH	C28-N	3.80	1.42	1.38
2	B	800	XIH	C28-N26	3.52	1.42	1.38
2	A	800	XIH	C28-N26	3.19	1.41	1.38
2	C	800	XIH	C8-N9	3.07	1.39	1.35
2	A	800	XIH	C8-N9	3.04	1.39	1.35
2	D	800	XIH	C28-N26	3.01	1.41	1.38
2	C	800	XIH	C28-N26	2.93	1.41	1.38
2	B	800	XIH	C5-N16	-2.81	1.35	1.39
2	D	800	XIH	C3-N	2.80	1.43	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	XIH	C28-N	2.78	1.41	1.38
2	A	800	XIH	C5-N16	-2.67	1.35	1.39
2	D	800	XIH	C5-N16	-2.56	1.36	1.39
2	D	800	XIH	C8-N9	2.46	1.38	1.35
2	A	800	XIH	C3-N	2.46	1.42	1.35
2	C	800	XIH	C3-N	2.43	1.42	1.35
2	C	800	XIH	C5-N16	-2.42	1.36	1.39
2	C	800	XIH	C6-N7	2.32	1.35	1.33
2	B	800	XIH	C8-N9	2.29	1.38	1.35
2	D	800	XIH	C6-N26	-2.23	1.34	1.38
2	B	800	XIH	C3-N	2.16	1.41	1.35
2	B	800	XIH	C6-N26	-2.11	1.34	1.38

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	800	XIH	N26-C28-N	7.70	122.56	115.69
2	B	800	XIH	N26-C28-N	7.66	122.52	115.69
2	A	800	XIH	N26-C28-N	7.57	122.44	115.69
2	C	800	XIH	N26-C28-N	6.86	121.81	115.69
2	B	800	XIH	C10-N9-C15	6.39	124.64	112.80
2	A	800	XIH	C10-N9-C15	6.30	124.45	112.80
2	D	800	XIH	C10-N9-C15	6.23	124.33	112.80
3	B	801	NAG	O5-C5-C6	6.02	113.30	106.98
2	C	800	XIH	C10-N9-C15	5.76	123.47	112.80
2	C	800	XIH	C18-C17-N16	4.38	120.68	113.26
2	B	800	XIH	C18-C23-C24	4.22	123.52	119.99
2	B	800	XIH	C5-C6-N7	-4.16	107.80	112.46
2	A	800	XIH	C18-C23-C24	4.09	123.41	119.99
2	C	800	XIH	C5-C6-N7	-4.06	107.92	112.46
2	A	800	XIH	C5-C6-N7	-4.05	107.92	112.46
2	D	800	XIH	C18-C17-N16	3.98	120.00	113.26
2	B	800	XIH	C18-C17-N16	3.90	119.87	113.26
2	A	800	XIH	C18-C17-N16	3.85	119.78	113.26
3	B	806	NAG	O5-C5-C6	3.79	110.96	106.98
2	A	800	XIH	C3-C5-C6	-3.66	117.30	119.92
2	D	800	XIH	C5-C6-N7	-3.62	108.41	112.46
3	B	801	NAG	O5-C5-C4	-3.60	106.09	110.65
2	C	800	XIH	C11-C12-C13	-3.43	107.73	112.32
3	D	804	NAG	C3-C2-N2	-3.39	106.60	111.76
2	D	800	XIH	C8-N16-C5	-3.27	102.76	110.19
2	C	800	XIH	C3-N-C28	-3.19	120.57	121.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	XIH	C8-N16-C5	-3.08	103.19	110.19
2	C	800	XIH	C18-C23-C24	3.07	122.56	119.99
2	D	800	XIH	C3-N-C28	-3.07	120.61	121.69
2	A	800	XIH	C8-N16-C5	-3.00	103.39	110.19
2	A	800	XIH	C3-N-C28	-2.99	120.64	121.69
3	A	802	NAG	O5-C5-C6	2.88	110.00	106.98
2	C	800	XIH	C8-N16-C5	-2.82	103.78	110.19
2	D	800	XIH	C10-N9-C8	-2.81	115.95	122.01
2	D	800	XIH	C3-C5-C6	-2.74	117.96	119.92
2	C	800	XIH	C17-C18-C19	-2.70	114.99	121.30
3	C	805	NAG	C3-C2-N2	-2.66	107.70	111.76
2	D	800	XIH	C17-N16-C5	2.65	130.71	125.23
3	D	804	NAG	O5-C5-C4	-2.64	107.30	110.65
2	C	800	XIH	C3-C5-C6	-2.61	118.05	119.92
2	B	800	XIH	C10-N9-C8	-2.57	116.48	122.01
2	A	800	XIH	C17-C18-C19	-2.55	115.36	121.30
3	D	801	NAG	O5-C5-C6	2.54	109.65	106.98
2	A	800	XIH	N7-C8-N9	-2.47	116.03	120.64
2	A	800	XIH	C17-N16-C5	2.47	130.32	125.23
3	D	801	NAG	C3-C2-N2	-2.44	108.04	111.76
2	C	800	XIH	C10-N9-C8	-2.41	116.81	122.01
2	A	800	XIH	C13-C15-N9	2.40	113.27	110.46
2	D	800	XIH	N7-C8-N9	-2.39	116.18	120.64
2	C	800	XIH	C12-C11-C10	2.37	113.84	110.92
2	B	800	XIH	C3-N-C28	-2.26	120.90	121.69
3	C	806	NAG	C3-C2-N2	-2.25	108.33	111.76
2	C	800	XIH	C19-C18-C23	2.24	120.36	117.46
3	B	802	NAG	O5-C5-C6	2.23	109.32	106.98
2	B	800	XIH	C17-C18-C19	-2.22	116.12	121.30
2	B	800	XIH	C3-C5-C6	-2.18	118.36	119.92
2	A	800	XIH	C10-N9-C8	-2.15	117.38	122.01
2	B	800	XIH	C17-C18-C23	2.12	124.72	121.88
2	C	800	XIH	C13-C15-N9	2.12	112.94	110.46
3	C	805	NAG	O5-C5-C6	2.11	109.19	106.98
2	C	800	XIH	N7-C8-N9	-2.10	116.71	120.64
2	D	800	XIH	C18-C23-C24	2.06	121.72	119.99
3	C	806	NAG	O5-C5-C6	2.04	109.12	106.98
2	B	800	XIH	N7-C8-N9	-2.04	116.83	120.64
2	A	800	XIH	C17-C18-C23	2.03	124.61	121.88
2	C	800	XIH	C17-C18-C23	2.02	124.59	121.88
3	C	801	NAG	O5-C5-C6	2.00	109.08	106.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	723/740 (97%)	0.69	59 (8%) 12 10	39, 48, 74, 104	0
1	B	728/740 (98%)	0.53	45 (6%) 20 18	36, 49, 72, 93	0
1	C	723/740 (97%)	0.78	80 (11%) 6 5	39, 49, 73, 93	0
1	D	723/740 (97%)	1.12	151 (20%) 1 1	38, 54, 82, 118	0
All	All	2897/2960 (97%)	0.78	335 (11%) 5 5	36, 50, 76, 118	0

All (335) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	99	GLY	7.8
1	D	77	LEU	7.2
1	A	81	ALA	7.0
1	C	89	PHE	6.4
1	C	279	VAL	6.3
1	B	81	ALA	6.3
1	A	86	SER	6.1
1	D	415	LEU	6.0
1	D	92	ASN	5.9
1	D	372	TYR	5.8
1	D	148	ILE	5.8
1	D	322	TYR	5.7
1	C	83	TYR	5.7
1	C	93	SER	5.5
1	C	87	SER	5.5
1	A	135	TYR	5.5
1	D	98	PHE	5.4
1	D	416	TYR	5.4
1	D	467	TYR	5.4
1	C	76	ILE	5.3
1	D	397	ILE	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	90	LEU	5.2
1	D	491	LEU	5.2
1	D	141	GLN	5.2
1	D	140	ARG	5.2
1	C	90	LEU	5.1
1	D	78	VAL	5.1
1	A	88	VAL	5.1
1	D	135	TYR	5.1
1	D	97	GLU	5.1
1	A	95	PHE	5.0
1	C	88	VAL	5.0
1	D	138	ASN	5.0
1	D	386	TYR	4.9
1	D	333	SER	4.9
1	C	97	GLU	4.9
1	B	78	VAL	4.9
1	A	332	GLU	4.8
1	C	98	PHE	4.6
1	D	81	ALA	4.6
1	B	70	TYR	4.6
1	C	95	PHE	4.5
1	D	468	TYR	4.5
1	C	86	SER	4.5
1	D	392	LYS	4.5
1	D	396	PHE	4.5
1	D	464	GLU	4.5
1	C	96	ASP	4.4
1	C	78	VAL	4.4
1	C	467	TYR	4.3
1	D	389	ILE	4.3
1	D	105	TYR	4.3
1	A	89	PHE	4.2
1	D	391	LYS	4.2
1	D	93	SER	4.2
1	D	137	LEU	4.2
1	D	442	VAL	4.1
1	C	330	TYR	4.1
1	D	414	TYR	4.1
1	D	276	LEU	4.0
1	D	62	TRP	4.0
1	D	463	LYS	4.0
1	D	339	CYS	4.0

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Mol	Chain	Res	Type	RSRZ
1	D	88	VAL	3.9
1	C	85	ASN	3.9
1	D	439	TYR	3.9
1	D	83	TYR	3.8
1	A	140	ARG	3.8
1	D	483	HIS	3.8
1	D	417	TYR	3.7
1	A	93	SER	3.7
1	A	141	GLN	3.7
1	C	138	ASN	3.7
1	D	335	GLY	3.7
1	D	375	ILE	3.7
1	A	91	GLU	3.6
1	C	82	GLU	3.6
1	D	338	ASN	3.6
1	D	395	THR	3.6
1	A	137	LEU	3.6
1	C	101	SER	3.6
1	D	449	LEU	3.6
1	D	436	LEU	3.5
1	C	92	ASN	3.5
1	A	98	PHE	3.5
1	D	222	PHE	3.5
1	C	207	VAL	3.5
1	A	99	GLY	3.5
1	B	89	PHE	3.4
1	D	330	TYR	3.4
1	D	102	ILE	3.4
1	D	348	MET	3.4
1	A	333	SER	3.4
1	D	178	PRO	3.4
1	D	82	GLU	3.4
1	D	173	TYR	3.4
1	D	346	ILE	3.4
1	A	96	ASP	3.3
1	D	385	CYS	3.3
1	C	69	LEU	3.3
1	D	69	LEU	3.3
1	A	138	ASN	3.3
1	D	100	HIS	3.3
1	C	283	THR	3.3
1	D	332	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	76	ILE	3.3
1	B	654	ALA	3.3
1	B	83	TYR	3.3
1	A	69	LEU	3.3
1	A	139	LYS	3.3
1	C	100	HIS	3.2
1	D	96	ASP	3.2
1	C	506	ASN	3.2
1	D	489	LYS	3.2
1	D	345	HIS	3.2
1	A	207	VAL	3.2
1	C	79	PHE	3.2
1	B	740	HIS	3.1
1	D	95	PHE	3.1
1	A	76	ILE	3.1
1	C	504	LEU	3.1
1	C	102	ILE	3.1
1	D	87	SER	3.1
1	D	327	ILE	3.1
1	D	432	TYR	3.1
1	B	471[A]	ARG	3.1
1	D	310	ARG	3.1
1	A	97	GLU	3.1
1	D	342	ALA	3.1
1	D	273	THR	3.1
1	D	413	ASP	3.1
1	A	551	CYS	3.1
1	C	141	GLN	3.1
1	C	94	THR	3.1
1	D	438	ASP	3.1
1	C	54	ARG	3.0
1	C	114	ILE	3.0
1	B	90	LEU	3.0
1	A	70	TYR	3.0
1	B	630	SER	3.0
1	A	105	TYR	3.0
1	B	653	VAL	3.0
1	D	493	VAL	3.0
1	D	393	ASP	3.0
1	D	67	GLU	3.0
1	C	486	VAL	3.0
1	C	210	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	81	ALA	2.9
1	C	142	LEU	2.9
1	B	629	TRP	2.9
1	A	711	VAL	2.9
1	C	282	ALA	2.9
1	D	412	SER	2.9
1	D	462	SER	2.9
1	A	181	PRO	2.9
1	C	80	ASN	2.9
1	C	490	GLY	2.9
1	A	330	TYR	2.9
1	D	58	TYR	2.9
1	B	628	GLY	2.9
1	B	711	VAL	2.9
1	C	209	SER	2.8
1	D	400	GLY	2.8
1	A	392	LYS	2.8
1	C	179	ASN	2.8
1	D	285	ILE	2.8
1	C	91	GLU	2.8
1	C	105	TYR	2.8
1	D	433	LYS	2.8
1	D	435	GLN	2.8
1	D	114	ILE	2.8
1	B	546	VAL	2.8
1	D	384	ILE	2.8
1	D	518	ILE	2.8
1	C	489	LYS	2.7
1	D	469	GLN	2.7
1	B	521	GLU	2.7
1	A	148	ILE	2.7
1	A	547	TYR	2.7
1	D	337	TRP	2.7
1	C	75	ASN	2.7
1	C	340	LEU	2.7
1	D	343	ARG	2.7
1	C	99	GLY	2.7
1	B	733	MET	2.7
1	A	279	VAL	2.7
1	B	142	LEU	2.7
1	C	84	GLY	2.7
1	D	394	CYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	179	ASN	2.7
1	D	629	TRP	2.6
1	D	486	VAL	2.6
1	B	63	ILE	2.6
1	B	442	VAL	2.6
1	D	63	ILE	2.6
1	D	441	LYS	2.6
1	A	209	SER	2.6
1	B	631	TYR	2.6
1	D	331	ASP	2.6
1	D	630	SER	2.6
1	A	166	TYR	2.6
1	D	344	GLN	2.6
1	D	521	GLU	2.6
1	D	431	LEU	2.6
1	B	547	TYR	2.5
1	D	166	TYR	2.5
1	C	392	LYS	2.5
1	D	742	ILE	2.5
1	D	61	ARG	2.5
1	B	666	TYR	2.5
1	C	70	TYR	2.5
1	C	491	LEU	2.5
1	D	334	SER	2.5
1	B	357	PHE	2.5
1	D	402	TRP	2.5
1	D	487	ASN	2.5
1	D	279	VAL	2.5
1	D	490	GLY	2.5
1	D	399	LYS	2.5
1	C	140	ARG	2.5
1	D	653	VAL	2.5
1	C	388	GLN	2.5
1	B	703	ILE	2.5
1	A	145	GLU	2.5
1	A	552	SER	2.5
1	B	87	SER	2.5
1	A	399	LYS	2.5
1	A	210	ALA	2.5
1	D	147	ARG	2.5
1	C	208	PHE	2.4
1	D	340	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	490	GLY	2.4
1	D	477	LEU	2.4
1	C	336	ARG	2.4
1	A	491	LEU	2.4
1	B	71	LYS	2.4
1	C	332	GLU	2.4
1	D	287	ILE	2.3
1	A	201	TRP	2.3
1	C	711	VAL	2.3
1	D	656	VAL	2.3
1	D	703	ILE	2.3
1	D	329	ASP	2.3
1	B	705	GLY	2.3
1	C	505	GLN	2.3
1	A	78	VAL	2.3
1	D	328	CYS	2.3
1	D	481	THR	2.3
1	D	766	PRO	2.3
1	C	366	LEU	2.3
1	B	708	ASP	2.3
1	B	518	ILE	2.3
1	A	208	PHE	2.3
1	C	77	LEU	2.3
1	D	187	TRP	2.3
1	D	72	GLN	2.3
1	D	336	ARG	2.3
1	D	434	ILE	2.3
1	D	269	PHE	2.3
1	B	205	GLU	2.3
1	B	69	LEU	2.3
1	D	164	LEU	2.3
1	D	388	GLN	2.3
1	C	536	LYS	2.2
1	C	271	VAL	2.2
1	D	85	ASN	2.2
1	C	335	GLY	2.2
1	A	116	LEU	2.2
1	A	142	LEU	2.2
1	A	144	THR	2.2
1	D	538	LYS	2.2
1	C	653	VAL	2.2
1	D	459	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	632	GLY	2.2
1	B	210	ALA	2.2
1	C	132	TYR	2.2
1	C	333	SER	2.2
1	D	390	ASP	2.2
1	D	160	VAL	2.2
1	B	86	SER	2.2
1	B	84	GLY	2.2
1	D	306	ALA	2.2
1	A	740	HIS	2.2
1	B	755	MET	2.2
1	C	537	SER	2.2
1	C	63	ILE	2.1
1	B	710	ASN	2.1
1	B	140	ARG	2.1
1	C	118	TYR	2.1
1	A	274	ASP	2.1
1	D	444	CYS	2.1
1	D	488	ASP	2.1
1	B	99	GLY	2.1
1	D	136	ASP	2.1
1	C	181	PRO	2.1
1	C	280	THR	2.1
1	C	514	LEU	2.1
1	D	142	LEU	2.1
1	D	223	LEU	2.1
1	D	535	ASP	2.1
1	B	558	VAL	2.1
1	D	139	LYS	2.1
1	A	357	PHE	2.1
1	D	461	PHE	2.1
1	C	124	TRP	2.1
1	C	187	TRP	2.1
1	B	467	TYR	2.1
1	D	364	PHE	2.1
1	B	702	LEU	2.1
1	D	305	TRP	2.1
1	A	630	SER	2.1
1	B	76	ILE	2.1
1	C	135	TYR	2.1
1	B	96	ASP	2.1
1	D	86	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	144	THR	2.1
1	D	484	SER	2.1
1	A	654	ALA	2.1
1	A	707	ALA	2.1
1	C	357	PHE	2.1
1	C	412	SER	2.0
1	D	401	THR	2.0
1	C	710	ASN	2.0
1	A	708	ASP	2.0
1	A	336	ARG	2.0
1	D	182	SER	2.0
1	D	184	ARG	2.0
1	A	143	ILE	2.0
1	D	589	LYS	2.0
1	A	180	LEU	2.0
1	D	479	LEU	2.0
1	D	530	LEU	2.0
1	A	87	SER	2.0
1	C	334	SER	2.0
1	B	627	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NAG	B	805	14/15	0.27	3.39	77,79,80,80	0
4	NAG	C	804	14/15	0.19	2.00	73,75,77,77	0
4	NAG	B	804	14/15	0.19	1.14	62,65,69,73	0
4	NAG	A	804	14/15	0.16	0.84	56,59,62,65	0
4	NAG	C	803	14/15	0.14	-0.12	60,63,66,70	0
4	NAG	A	807	14/15	0.18	-0.25	90,91,92,92	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
4	NAG	A	806	14/15	0.17	-0.28	80,84,85,87	0
4	NAG	D	803	14/15	0.12	-0.83	73,75,76,77	0
4	NAG	D	802	14/15	0.12	-1.21	60,63,65,69	0
4	NAG	A	805	14/15	0.13	-1.91	67,68,69,69	0

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	NAG	B	803	14/15	0.22	3.34	64,67,70,71	0
3	NAG	C	806	14/15	0.20	1.84	68,73,74,74	0
3	NAG	A	803	14/15	0.22	1.65	69,72,76,77	0
3	NAG	A	808	14/15	0.23	1.39	62,66,68,68	0
3	NAG	A	802	14/15	0.28	1.12	75,78,79,79	0
2	XIH	A	800	29/29	0.26	0.57	38,43,44,44	0
2	XIH	D	800	29/29	0.23	0.48	40,42,43,45	0
3	NAG	B	802	14/15	0.15	0.46	67,68,69,70	0
3	NAG	A	801	14/15	0.28	0.12	95,95,96,96	0
2	XIH	B	800	29/29	0.26	-0.11	35,39,40,41	0
2	XIH	C	800	29/29	0.23	-0.26	35,37,38,39	0
3	NAG	C	801	14/15	0.19	-0.28	60,60,61,62	0
3	NAG	C	802	14/15	0.15	-0.39	70,72,75,75	0
3	NAG	B	806	14/15	0.12	-0.59	69,71,74,74	0
3	NAG	D	801	14/15	0.17	-1.01	65,67,68,69	0
3	NAG	C	805	14/15	0.17	-1.14	78,81,82,82	0
3	NAG	B	801	14/15	0.15	-1.22	79,80,81,81	0
3	NAG	D	804	14/15	0.14	-1.34	81,83,85,85	0

6.5 Other polymers

There are no such residues in this entry.