



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:22 PM GMT

PDB ID : 3CCC
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 : 2.71 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>

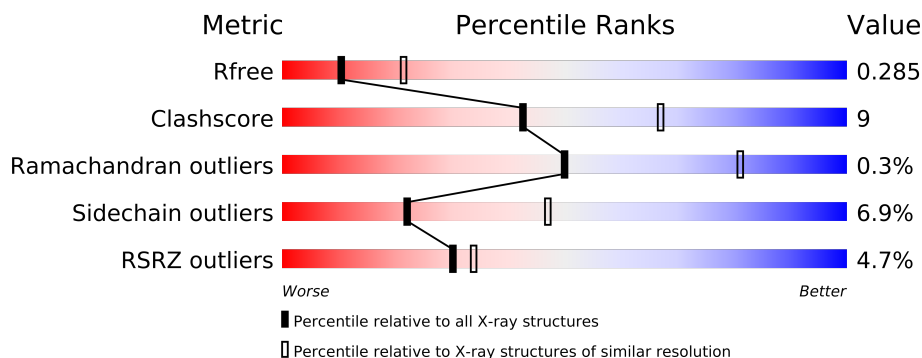
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.71 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	1770 (2.74-2.70)
Clashscore	79885	2183 (2.74-2.70)
Ramachandran outliers	78287	2147 (2.74-2.70)
Sidechain outliers	78261	2148 (2.74-2.70)
RSRZ outliers	66119	1772 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	C	805	-	X
4	7AC	B	800	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24357 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	0	0
			5929	3809	974	1120	26			
1	B	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			
1	C	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			
1	D	724	Total	C	N	O	S	0	0	0
			5929	3809	974	1120	26			

There are 48 discrepancies between the modelled and reference sequences:

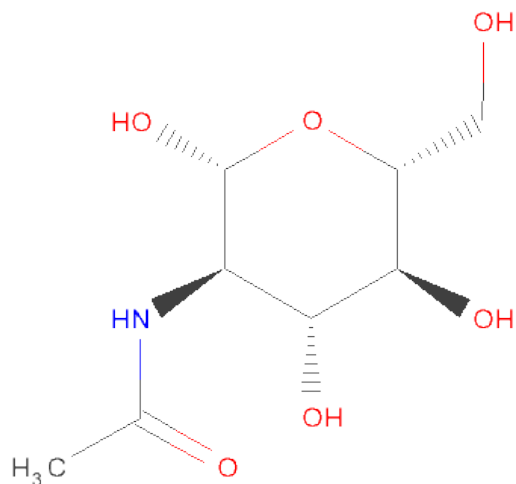
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487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

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

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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	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	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	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 48 discrepancies between the modelled and reference sequences:

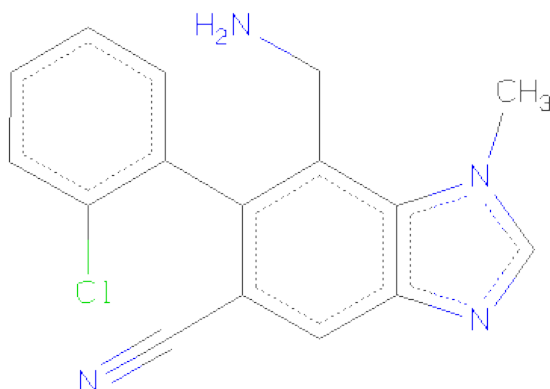
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	ALA	-	EXPRESSION TAG	UNP P27487
A	28	ASP	-	EXPRESSION TAG	UNP P27487
A	29	PRO	-	EXPRESSION TAG	UNP P27487
A	30	GLY	-	EXPRESSION TAG	UNP P27487
A	31	GLY	-	EXPRESSION TAG	UNP P27487
A	32	SER	-	EXPRESSION TAG	UNP P27487
A	33	HIS	-	EXPRESSION TAG	UNP P27487
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
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 4 is 7-(AMINOMETHYL)-6-(2-CHLOROPHENYL)-1-METHYL-1H-BENZIMIDAZOLE-5-CARBONITRILE (three-letter code: 7AC) (formula: C₁₆H₁₃ClN₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	Cl	N	0	0
			21	16	1	4		
4	B	1	Total	C	Cl	N	0	0
			21	16	1	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	Cl	N	0	0
			21	16	1	4		
4	D	1	Total	C	Cl	N	0	0
			21	16	1	4		

- Molecule 5 is water.

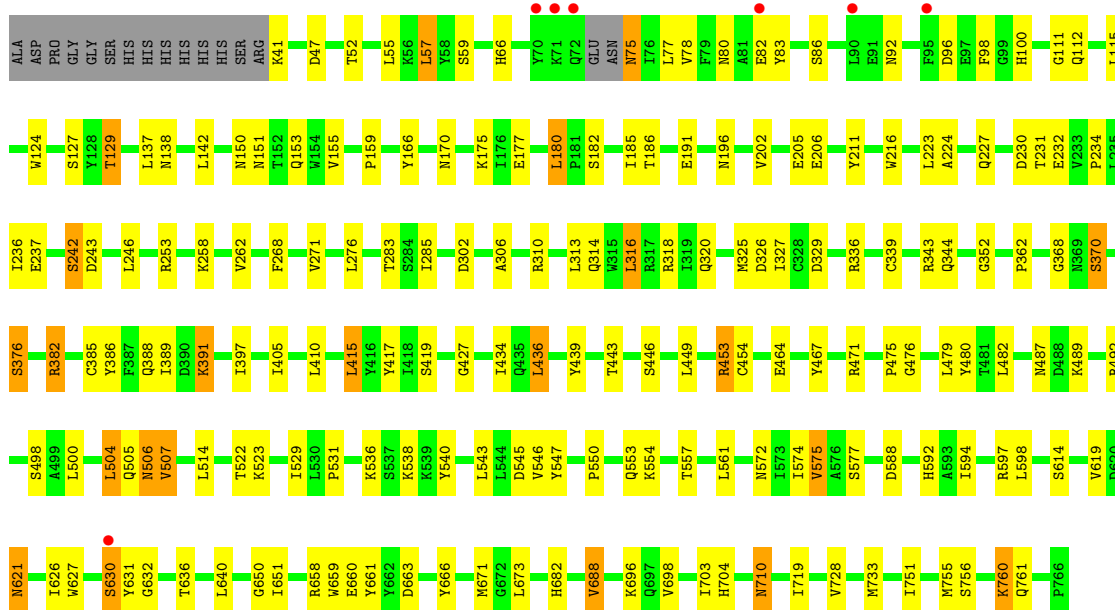
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	85	Total	O	0	0
			85	85		
5	B	106	Total	O	0	0
			106	106		
5	C	56	Total	O	0	0
			56	56		
5	D	30	Total	O	0	0
			30	30		

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.

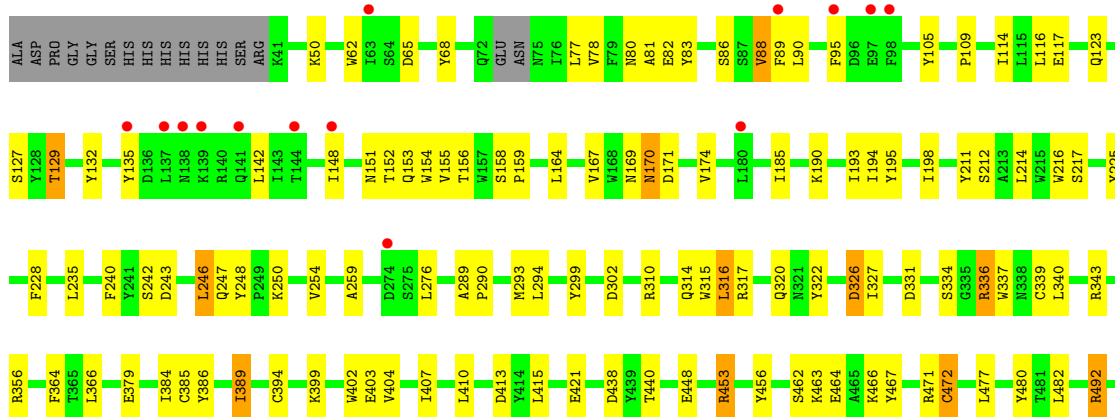
• Molecule 1: Dipeptidyl peptidase 4

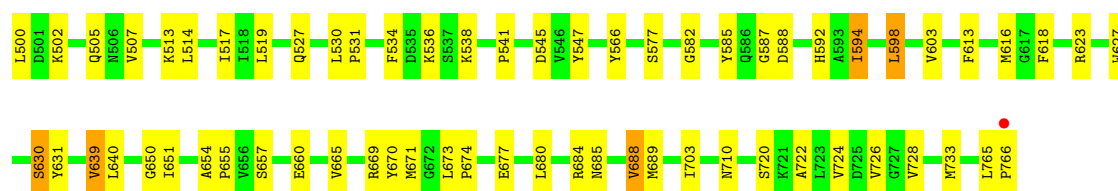
Chain A: 



• Molecule 1: Dipeptidyl peptidase 4

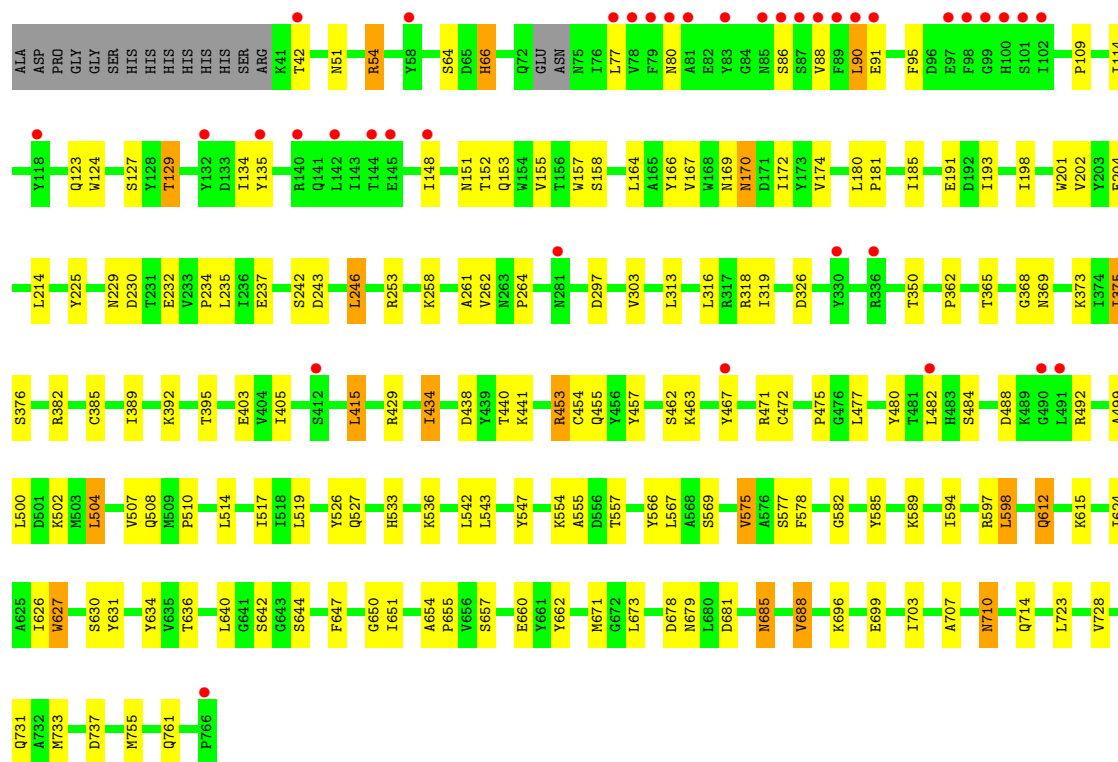
Chain B: 





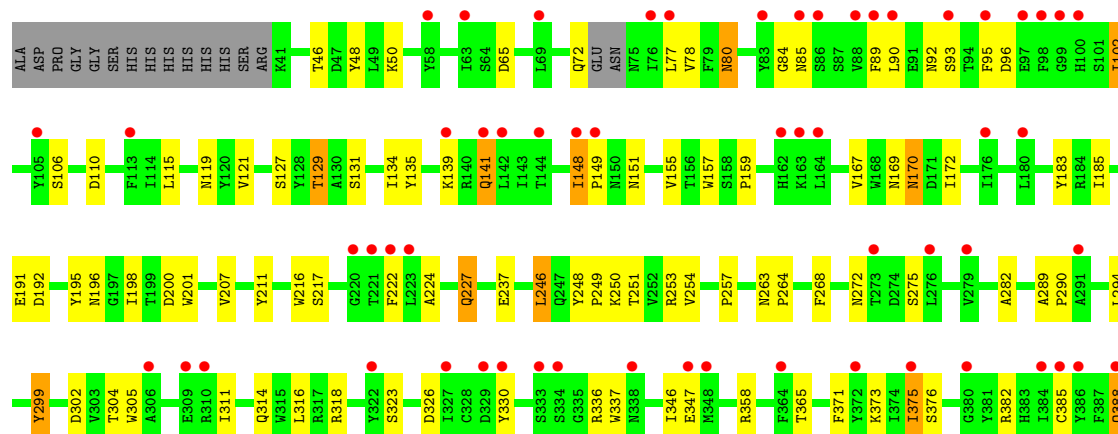
• Molecule 1: Dipeptidyl peptidase 4

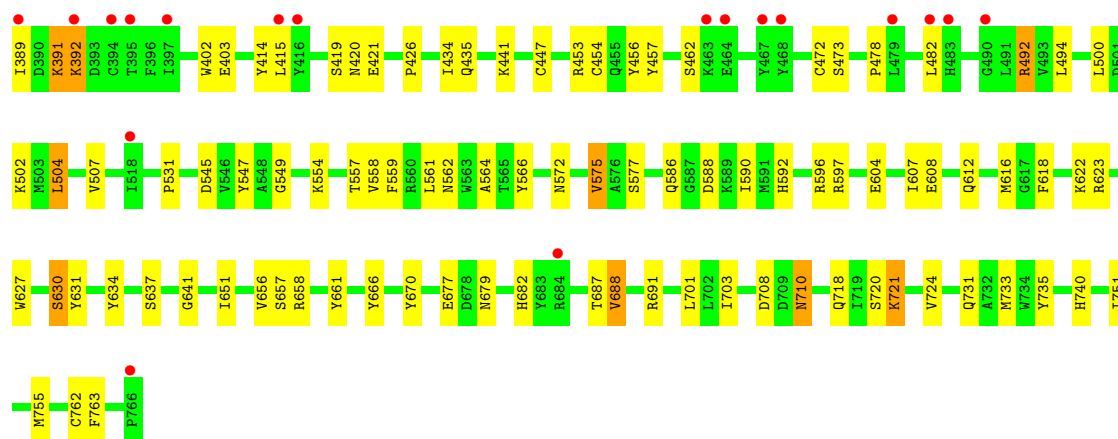
Chain C:



• 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	121.90Å 121.96Å 144.28Å 90.00° 114.94° 90.00°	Depositor
Resolution (Å)	46.13 – 2.71 44.75 – 2.71	Depositor EDS
% Data completeness (in resolution range)	90.9 (46.13-2.71) 91.0 (44.75-2.71)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.267 0.225 , 0.285	Depositor DCC
R_{free} test set	4718 reflections (4.99%)	DCC
Wilson B-factor (Å ²)	57.3	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 22.8	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 94570 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24357	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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: 7AC, 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	0.47	0/6100	0.62	1/8296 (0.0%)
1	B	0.49	0/6100	0.64	0/8296
1	C	0.46	0/6100	0.61	0/8296
1	D	0.42	0/6100	0.59	0/8296
All	All	0.46	0/24400	0.62	1/33184 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	LEU	CA-CB-CG	5.06	126.94	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	5929	0	5649	109	0
1	B	5929	0	5649	109	0
1	C	5929	0	5649	97	0
1	D	5929	0	5651	114	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	56	0	52	0	0
2	B	42	0	39	0	0
2	C	42	0	39	0	0
2	D	28	0	26	0	0
3	A	28	0	25	0	0
3	B	28	0	25	0	0
3	C	28	0	25	0	0
3	D	28	0	25	0	0
4	A	21	0	13	3	0
4	B	21	0	13	3	0
4	C	21	0	13	1	0
4	D	21	0	13	2	0
5	A	85	0	0	1	0
5	B	106	0	0	0	0
5	C	56	0	0	0	0
5	D	30	0	0	0	0
All	All	24357	0	22906	420	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (420) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:651:ILE:HD13	1:A:755:MET:HG2	1.40	1.01
1:C:253:ARG:HH21	1:D:253:ARG:HH21	1.05	0.99
1:D:658:ARG:HB2	1:D:687:THR:HG22	1.50	0.93
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.54	0.90
1:C:235:LEU:HD23	1:C:253:ARG:HB3	1.54	0.86
1:D:720:SER:O	1:D:724:VAL:HG23	1.77	0.82
1:B:78:VAL:HG23	1:B:89:PHE:HB2	1.59	0.82
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.78	0.81
1:A:153:GLN:HE22	1:A:170:ASN:H	1.27	0.80
1:D:414:TYR:HE2	1:D:435:GLN:HG2	1.45	0.79
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.83	0.77
1:A:388:GLN:HB2	1:A:391:LYS:HG2	1.68	0.76
1:A:550:PRO:HG3	1:A:594:ILE:HD11	1.69	0.74
1:D:623:ARG:HH11	1:D:763:PHE:HB3	1.55	0.71
1:D:139:LYS:HG3	1:D:141:GLN:HE22	1.56	0.71
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.71	0.71
1:A:82:GLU:HG2	1:A:467:TYR:OH	1.91	0.71
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.71	0.70
1:C:237:GLU:HG2	1:C:253:ARG:HG2	1.73	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:388:GLN:H	1:D:391:LYS:HE2	1.57	0.69
1:B:336:ARG:HB2	1:B:336:ARG:HH11	1.57	0.69
1:B:630:SER:HB2	4:B:800:7AC:N9	2.08	0.68
1:A:471:ARG:HG3	1:A:480:TYR:CE1	2.28	0.68
1:A:77:LEU:HD23	1:A:86:SER:OG	1.94	0.67
1:A:504:LEU:HA	1:A:507:VAL:CG1	2.25	0.66
1:D:80:ASN:O	1:D:84:GLY:HA2	1.96	0.66
1:B:386:TYR:O	1:B:394:CYS:HB2	1.96	0.65
1:A:554:LYS:HB3	1:A:577:SER:HB3	1.78	0.65
1:B:720:SER:O	1:B:724:VAL:HG23	1.97	0.65
1:B:78:VAL:CG2	1:B:89:PHE:HB2	2.27	0.65
1:A:329:ASP:OD2	1:A:343:ARG:NH1	2.30	0.65
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.77	0.64
1:D:588:ASP:HB3	1:D:592:HIS:CD2	2.33	0.64
1:D:102:ILE:HD13	1:D:102:ILE:H	1.63	0.64
1:C:66:HIS:HB3	1:C:467:TYR:HE1	1.63	0.63
1:B:153:GLN:HE22	1:B:170:ASN:H	1.44	0.63
1:D:72:GLN:HG3	1:D:77:LEU:HD22	1.80	0.63
1:B:588:ASP:HB3	1:B:592:HIS:HD2	1.64	0.63
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.79	0.62
1:B:148:ILE:HD11	1:B:164:LEU:HD21	1.80	0.62
1:D:402:TRP:CD2	1:D:421:GLU:HB2	2.33	0.62
1:A:316:LEU:HD13	1:A:320:GLN:HG2	1.82	0.62
1:D:473:SER:HB3	1:D:558:VAL:HG13	1.82	0.62
1:C:543:LEU:HD23	1:C:567:LEU:HD13	1.82	0.62
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.82	0.62
1:C:153:GLN:HE22	1:C:170:ASN:H	1.48	0.61
1:A:614:SER:HA	1:A:619:VAL:HB	1.82	0.61
1:D:290:PRO:HG3	1:D:326:ASP:OD1	2.00	0.61
1:C:152:THR:HG21	1:C:155:VAL:HG22	1.82	0.61
1:D:121:VAL:HB	1:D:129:THR:HG22	1.83	0.61
1:A:185:ILE:HG22	1:A:186:THR:HG23	1.81	0.61
1:C:51:ASN:HD21	1:C:54:ARG:HD2	1.64	0.61
1:C:170:ASN:N	1:C:170:ASN:HD22	1.97	0.61
1:A:175:LYS:HG2	1:A:182:SER:HB3	1.83	0.61
1:C:510:PRO:HD3	1:C:569:SER:HB2	1.83	0.61
1:A:703:ILE:HG21	1:A:751:ILE:HD12	1.82	0.60
1:A:756:SER:O	1:A:760:LYS:HB2	2.00	0.60
1:A:98:PHE:CE1	1:A:100:HIS:HB2	2.36	0.60
1:C:155:VAL:HG13	1:C:166:TYR:HB3	1.84	0.60
1:D:346:ILE:H	1:D:392:LYS:NZ	2.00	0.60
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.83	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:82:GLU:HG2	1:B:467:TYR:OH	2.02	0.60
1:A:115:LEU:HD21	1:A:155:VAL:HG21	1.82	0.60
1:C:630:SER:HB2	4:C:800:7AC:N9	2.17	0.59
1:A:543:LEU:HD21	1:A:627:TRP:CD1	2.37	0.59
1:B:114:ILE:CG2	1:B:135:TYR:HB3	2.32	0.58
1:D:272:ASN:ND2	1:D:275:SER:HB3	2.17	0.58
1:B:598:LEU:HD22	1:B:671:MET:HG2	1.85	0.58
1:A:388:GLN:HG3	1:A:391:LYS:HE2	1.85	0.58
1:A:155:VAL:HG12	1:A:166:TYR:CB	2.34	0.57
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.05	0.57
1:D:78:VAL:HG23	1:D:89:PHE:HB2	1.87	0.57
1:B:159:PRO:HG3	1:B:217:SER:O	2.05	0.57
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.87	0.56
1:A:242:SER:OG	1:A:243:ASP:N	2.38	0.56
1:C:124:TRP:HB2	1:C:204:GLU:OE1	2.05	0.56
1:D:630:SER:HB2	4:D:800:7AC:N9	2.21	0.56
1:A:531:PRO:HB3	1:A:572:ASN:HD22	1.71	0.56
1:B:135:TYR:HD1	1:B:142:LEU:HD13	1.70	0.56
1:D:346:ILE:H	1:D:392:LYS:HZ1	1.50	0.56
1:B:657:SER:HA	1:B:688:VAL:CG1	2.35	0.56
1:D:148:ILE:HG22	1:D:149:PRO:HD2	1.88	0.56
1:B:170:ASN:N	1:B:170:ASN:HD22	2.03	0.56
1:D:347:GLU:OE2	1:D:375:ILE:HG23	2.05	0.56
1:A:545:ASP:OD2	1:A:554:LYS:NZ	2.38	0.56
1:C:731:GLN:HE22	1:D:731:GLN:NE2	2.04	0.55
1:D:172:ILE:HG22	1:D:185:ILE:HD13	1.89	0.55
1:A:397:ILE:HD12	1:A:434:ILE:HD13	1.88	0.55
1:A:155:VAL:HG12	1:A:166:TYR:HB3	1.89	0.55
1:C:77:LEU:HD23	1:C:86:SER:HB2	1.88	0.55
1:A:237:GLU:HG2	1:A:253:ARG:HB3	1.89	0.55
1:A:540:TYR:HB2	1:A:574:ILE:HD12	1.88	0.55
1:C:180:LEU:HB3	1:C:181:PRO:HD2	1.89	0.55
1:D:207:VAL:O	1:D:358:ARG:HD3	2.07	0.54
1:C:438:ASP:OD2	1:C:440:THR:HB	2.07	0.54
1:C:454:CYS:HB3	1:C:457:TYR:CZ	2.42	0.54
1:C:114:ILE:HG23	1:C:135:TYR:HB3	1.88	0.54
1:B:477:LEU:HD22	1:B:500:LEU:HD23	1.90	0.54
1:D:224:ALA:HB1	1:D:268:PHE:CZ	2.43	0.54
1:D:608:GLU:O	1:D:612:GLN:HG2	2.08	0.54
1:D:554:LYS:HB3	1:D:577:SER:HB3	1.90	0.53
1:D:651:ILE:HD13	1:D:755:MET:HG2	1.90	0.53
1:D:389:ILE:HG22	1:D:389:ILE:O	2.09	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:48:TYR:CE1	1:D:562:ASN:HA	2.43	0.53
1:A:150:ASN:O	1:A:151:ASN:HB2	2.09	0.53
1:C:731:GLN:NE2	1:D:731:GLN:HE22	2.06	0.53
1:C:90:LEU:HD21	1:C:95:PHE:HE2	1.73	0.53
1:A:159:PRO:HD3	1:A:216:TRP:HB3	1.90	0.53
1:B:174:VAL:HG23	1:B:185:ILE:HD11	1.90	0.53
1:D:72:GLN:HB2	1:D:77:LEU:HD13	1.90	0.53
1:D:263:ASN:ND2	1:D:299:TYR:HE1	2.07	0.53
1:D:708:ASP:OD2	1:D:740:HIS:HB2	2.08	0.53
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.09	0.53
1:B:240:PHE:HB3	1:B:250:LYS:HG3	1.90	0.53
1:D:414:TYR:CE2	1:D:435:GLN:HG2	2.36	0.52
1:A:310:ARG:NH1	1:A:368:GLY:O	2.41	0.52
1:D:323:SER:HB3	1:D:347:GLU:HB3	1.91	0.52
1:D:106:SER:HB3	1:D:115:LEU:HB3	1.91	0.52
1:C:526:TYR:HB3	1:C:578:PHE:HD1	1.74	0.52
1:B:154:TRP:HD1	1:B:214:LEU:HD12	1.74	0.52
1:C:598:LEU:HG	1:C:631:TYR:OH	2.09	0.52
1:A:314:GLN:NE2	1:A:362:PRO:HD3	2.25	0.52
1:C:153:GLN:OE1	1:C:170:ASN:ND2	2.43	0.52
4:B:800:7AC:H19A	4:B:800:7AC:C1	2.40	0.52
1:C:554:LYS:HB3	1:C:577:SER:HB3	1.91	0.52
1:B:582:GLY:HA2	1:B:594:ILE:HD12	1.92	0.52
1:C:731:GLN:HE22	1:D:731:GLN:HE22	1.57	0.51
1:A:597:ARG:HA	1:A:682:HIS:CD2	2.45	0.51
1:C:484:SER:O	1:C:488:ASP:HA	2.09	0.51
1:C:234:PRO:HB2	1:D:248:TYR:CZ	2.45	0.51
1:C:64:SER:HA	1:C:463:LYS:HE2	1.91	0.51
1:C:453:ARG:NH2	1:C:477:LEU:O	2.43	0.51
1:D:679:ASN:OD1	1:D:682:HIS:HB3	2.11	0.51
1:D:93:SER:HA	1:D:96:ASP:HB2	1.92	0.51
1:C:258:LYS:HB3	1:C:660:GLU:O	2.11	0.51
1:D:115:LEU:HD21	1:D:155:VAL:HG21	1.92	0.51
1:B:703:ILE:HG12	1:B:733:MET:HB3	1.93	0.51
1:A:75:ASN:HB3	1:A:92:ASN:HD22	1.76	0.51
1:C:471:ARG:HG3	1:C:480:TYR:CE1	2.46	0.51
1:C:651:ILE:HG21	1:C:755:MET:HG2	1.93	0.51
1:A:453:ARG:HB2	1:A:476:GLY:HA3	1.93	0.51
1:B:627:TRP:HB2	1:B:651:ILE:HB	1.91	0.51
1:C:543:LEU:HD11	1:C:627:TRP:HD1	1.76	0.50
1:A:80:ASN:HD22	1:A:83:TYR:H	1.59	0.50
1:A:327:ILE:HD13	1:A:389:ILE:CD1	2.41	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:318:ARG:HG2	5:A:873:HOH:O	2.11	0.50
1:B:331:ASP:HB3	1:B:334:SER:HB3	1.94	0.50
1:A:159:PRO:HD3	1:A:216:TRP:CB	2.42	0.50
1:B:195:TYR:HB2	1:B:228:PHE:HB2	1.94	0.50
1:D:634:TYR:HD2	1:D:656:VAL:O	1.94	0.50
1:D:46:THR:O	1:D:50:LYS:HB2	2.11	0.50
1:B:242:SER:HB3	1:B:246:LEU:HD12	1.92	0.50
1:C:500:LEU:HG	1:C:504:LEU:HD22	1.93	0.50
1:C:375:ILE:HD12	1:C:376:SER:O	2.11	0.50
1:A:327:ILE:HG21	1:A:389:ILE:HD11	1.93	0.50
1:D:472:CYS:O	1:D:478:PRO:HA	2.11	0.50
1:B:65:ASP:CG	1:B:464:GLU:HB3	2.32	0.50
1:B:123:GLN:HB3	1:B:127:SER:OG	2.11	0.50
1:D:106:SER:HG	1:D:157:TRP:HD1	1.57	0.50
1:D:382:ARG:H	1:D:403:GLU:HG2	1.77	0.49
1:B:403:GLU:OE1	1:B:587:GLY:HA2	2.12	0.49
1:B:153:GLN:NE2	1:B:167:VAL:HG12	2.26	0.49
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.93	0.49
1:C:369:ASN:O	1:C:389:ILE:HB	2.11	0.49
1:B:159:PRO:HD3	1:B:216:TRP:CB	2.41	0.49
1:A:626:ILE:O	1:A:650:GLY:HA2	2.11	0.49
1:C:714:GLN:NE2	1:D:249:PRO:HD3	2.28	0.49
1:C:696:LYS:HG3	1:C:728:VAL:HG22	1.95	0.49
1:A:206:GLU:CD	1:A:666:TYR:HB2	2.33	0.49
1:D:545:ASP:OD2	1:D:554:LYS:HE3	2.13	0.49
1:C:681:ASP:O	1:C:685:ASN:HB2	2.13	0.49
1:C:167:VAL:HG11	1:C:198:ILE:HG12	1.93	0.49
1:C:543:LEU:HD11	1:C:627:TRP:CD1	2.47	0.49
1:D:718:GLN:OE1	1:D:721:LYS:NZ	2.45	0.49
1:B:517:ILE:HD12	1:B:519:LEU:HD13	1.95	0.49
1:D:492:ARG:HH21	1:D:492:ARG:HB3	1.78	0.49
1:D:371:PHE:HE1	1:D:373:LYS:HG2	1.77	0.49
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.40	0.49
1:B:613:PHE:O	1:B:616:MET:HB2	2.13	0.49
1:A:41:LYS:HD3	1:A:506:ASN:HB3	1.95	0.49
1:C:362:PRO:HA	1:C:373:LYS:HB3	1.95	0.49
1:B:193:ILE:HG22	1:B:194:ILE:HG12	1.95	0.48
1:D:588:ASP:HB3	1:D:592:HIS:HD2	1.77	0.48
1:A:206:GLU:HG3	1:A:663:ASP:OD1	2.12	0.48
1:C:129:THR:HG23	1:C:151:ASN:HA	1.95	0.48
1:B:156:THR:HG23	1:B:216:TRP:HE1	1.77	0.48
1:D:631:TYR:HD1	4:D:800:7AC:H13	1.77	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:123:GLN:HB3	1:C:127:SER:OG	2.12	0.48
1:D:500:LEU:HG	1:D:504:LEU:HD22	1.94	0.48
1:D:616:MET:HB3	1:D:618:PHE:CE1	2.49	0.48
1:D:415:LEU:O	1:D:434:ILE:HG22	2.13	0.48
1:A:232:GLU:HB3	1:A:262:VAL:HG11	1.93	0.48
1:A:453:ARG:NH2	1:A:479:LEU:HB2	2.28	0.48
1:A:313:LEU:O	1:A:325:MET:HA	2.14	0.48
1:B:95:PHE:HE1	1:B:135:TYR:CD1	2.30	0.48
1:D:549:GLY:HA2	1:D:631:TYR:CE2	2.49	0.48
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.79	0.48
1:B:471:ARG:HG3	1:B:480:TYR:CE1	2.49	0.48
1:A:415:LEU:HB2	1:A:436:LEU:HD11	1.96	0.48
1:A:703:ILE:HG21	1:A:751:ILE:CD1	2.44	0.48
1:A:326:ASP:OD2	1:A:344:GLN:HG2	2.14	0.48
1:D:637:SER:HB3	1:D:688:VAL:HG21	1.96	0.48
1:D:375:ILE:HG22	1:D:376:SER:N	2.29	0.47
1:A:75:ASN:HB3	1:A:92:ASN:H	1.79	0.47
1:B:534:PHE:HZ	1:B:618:PHE:CG	2.32	0.47
1:B:660:GLU:OE2	1:B:684:ARG:NH2	2.47	0.47
1:B:456:TYR:O	1:B:472:CYS:HA	2.14	0.47
1:A:529:ILE:HB	1:A:575:VAL:HG13	1.96	0.47
1:A:155:VAL:HG12	1:A:166:TYR:HB2	1.97	0.47
1:B:185:ILE:N	1:B:185:ILE:HD12	2.29	0.47
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.97	0.47
1:C:626:ILE:O	1:C:650:GLY:HA2	2.13	0.47
1:D:482:LEU:HB2	1:D:494:LEU:HD21	1.97	0.47
1:A:710:ASN:C	1:A:710:ASN:HD22	2.18	0.47
1:B:116:LEU:O	1:B:132:TYR:HA	2.14	0.47
1:C:543:LEU:O	1:C:575:VAL:HA	2.15	0.47
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.97	0.47
1:D:586:GLN:HB3	1:D:590:ILE:HD12	1.96	0.47
1:B:410:LEU:HD13	1:B:415:LEU:HD23	1.96	0.47
1:B:669:ARG:HD2	1:B:670:TYR:CZ	2.50	0.47
1:D:420:ASN:HB2	1:D:426:PRO:HA	1.97	0.47
1:B:129:THR:HG23	1:B:151:ASN:HA	1.97	0.47
1:A:352:GLY:HA3	1:A:592:HIS:ND1	2.30	0.47
1:C:626:ILE:HG23	1:C:636:THR:HG23	1.97	0.46
1:C:365:THR:O	1:C:368:GLY:N	2.45	0.46
1:D:196:ASN:OD1	1:D:227:GLN:HG3	2.15	0.46
1:C:157:TRP:CE3	1:C:164:LEU:HD13	2.50	0.46
1:A:112:GLN:HG2	1:A:138:ASN:HD21	1.80	0.46
1:A:127:SER:HB3	1:A:211:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:95:PHE:HE1	1:D:135:TYR:CD1	2.33	0.46
1:B:317:ARG:HD2	1:B:322:TYR:HB3	1.96	0.46
1:B:334:SER:OG	1:B:336:ARG:HG3	2.15	0.46
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.49	0.46
1:B:154:TRP:CE2	1:B:212:SER:HB2	2.50	0.46
1:D:492:ARG:HB3	1:D:492:ARG:NH2	2.30	0.46
1:D:289:ALA:HB3	1:D:294:LEU:HD21	1.96	0.46
1:D:224:ALA:HB1	1:D:268:PHE:HZ	1.79	0.46
1:A:453:ARG:HG3	1:A:454:CYS:SG	2.55	0.46
1:C:174:VAL:HG23	1:C:185:ILE:HD11	1.98	0.46
1:A:129:THR:HG22	1:A:151:ASN:HA	1.97	0.46
1:C:499:ALA:O	1:C:502:LYS:HB3	2.16	0.46
1:D:305:TRP:CE2	1:D:311:ILE:HD12	2.51	0.46
1:D:564:ALA:HB1	1:D:575:VAL:HG21	1.97	0.46
1:B:438:ASP:OD2	1:B:440:THR:HB	2.15	0.46
1:C:657:SER:HA	1:C:688:VAL:HG13	1.97	0.46
1:A:598:LEU:HB2	1:A:671:MET:SD	2.56	0.46
1:A:376:SER:HA	1:A:382:ARG:HA	1.96	0.46
1:C:201:TRP:CZ2	1:C:710:ASN:HA	2.51	0.46
1:C:455:GLN:HB2	1:C:475:PRO:HD3	1.98	0.46
1:D:657:SER:HA	1:D:688:VAL:CG1	2.46	0.45
1:B:289:ALA:HB3	1:B:294:LEU:CD2	2.46	0.45
1:D:148:ILE:H	1:D:148:ILE:HD12	1.81	0.45
1:D:376:SER:HA	1:D:382:ARG:HA	1.98	0.45
1:D:119:ASN:HB2	1:D:131:SER:HB2	1.98	0.45
1:B:530:LEU:HA	1:B:531:PRO:HD2	1.83	0.45
1:A:446:SER:HA	1:A:449:LEU:HG	1.98	0.45
1:D:302:ASP:HB3	1:D:314:GLN:HB2	1.98	0.45
1:A:543:LEU:O	1:A:575:VAL:HA	2.16	0.45
1:C:662:TYR:OH	1:C:710:ASN:ND2	2.49	0.45
1:A:688:VAL:HG22	1:A:719:ILE:HG12	1.99	0.45
1:C:527:GLN:HG2	1:C:555:ALA:HA	1.97	0.45
1:A:370:SER:OG	1:A:386:TYR:CE2	2.68	0.45
1:B:689:MET:HG3	1:B:722:ALA:HB2	1.98	0.45
1:A:640:LEU:HB3	1:A:698:VAL:HG21	1.98	0.45
1:C:232:GLU:HB2	1:C:262:VAL:HG11	1.98	0.45
1:A:397:ILE:CD1	1:A:434:ILE:HD13	2.46	0.45
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.99	0.45
1:A:546:VAL:HG23	1:A:632:GLY:HA2	1.99	0.45
1:C:517:ILE:CD1	1:C:612:GLN:HG3	2.47	0.45
1:B:466:LYS:HD2	1:B:467:TYR:CE1	2.51	0.45
1:B:235:LEU:HA	1:B:254:VAL:O	2.17	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:258:LYS:HD2	1:B:247:GLN:HG2	1.98	0.45
1:C:415:LEU:HB3	1:C:434:ILE:HG13	1.97	0.45
1:D:65:ASP:HA	1:D:462:SER:HB2	1.98	0.45
1:B:195:TYR:HB3	1:B:198:ILE:O	2.17	0.45
1:D:169:ASN:O	1:D:170:ASN:HB2	2.17	0.45
1:C:90:LEU:HD21	1:C:95:PHE:CE2	2.52	0.44
1:B:471:ARG:CG	1:B:480:TYR:CE1	3.00	0.44
1:D:191:GLU:O	1:D:192:ASP:HB2	2.17	0.44
1:C:237:GLU:OE2	1:D:251:THR:OG1	2.27	0.44
1:A:153:GLN:HB3	1:A:211:TYR:CE1	2.52	0.44
1:D:454:CYS:HB3	1:D:457:TYR:CE2	2.52	0.44
1:D:733:MET:HG3	1:D:735:TYR:CE2	2.53	0.44
1:B:81:ALA:O	1:B:492:ARG:NH1	2.51	0.44
1:B:336:ARG:HB2	1:B:336:ARG:NH1	2.29	0.44
1:B:598:LEU:HB2	1:B:671:MET:SD	2.57	0.44
1:D:666:TYR:CE1	1:D:670:TYR:HE2	2.36	0.44
1:B:152:THR:HG21	1:B:155:VAL:HG22	1.98	0.44
1:D:217:SER:HB3	1:D:222:PHE:HB2	2.00	0.44
1:D:559:PHE:CZ	1:D:561:LEU:HD21	2.53	0.44
1:C:582:GLY:HA2	1:C:594:ILE:HG12	1.99	0.44
1:C:109:PRO:HG2	1:C:158:SER:O	2.18	0.44
1:D:148:ILE:CG2	1:D:149:PRO:HD2	2.47	0.44
1:C:723:LEU:HD22	1:C:728:VAL:HG11	2.00	0.44
1:C:191:GLU:O	1:C:193:ILE:HD12	2.17	0.44
1:A:621:ASN:H	1:A:621:ASN:ND2	2.14	0.44
1:A:453:ARG:HH21	1:A:479:LEU:HB2	1.83	0.43
1:A:285:ILE:HG21	1:A:336:ARG:HA	2.00	0.43
1:D:263:ASN:ND2	1:D:299:TYR:CE1	2.86	0.43
1:D:564:ALA:CB	1:D:575:VAL:HG21	2.49	0.43
1:C:214:LEU:HD23	1:C:225:TYR:HB3	2.00	0.43
1:A:554:LYS:HB3	1:A:577:SER:CB	2.47	0.43
1:D:703:ILE:HG12	1:D:733:MET:HB3	2.00	0.43
1:B:603:VAL:HG13	1:B:639:VAL:HG23	1.99	0.43
1:C:261:ALA:O	1:C:318:ARG:NH1	2.42	0.43
1:B:62:TRP:CG	1:B:462:SER:HA	2.53	0.43
1:C:597:ARG:NH1	1:C:679:ASN:OD1	2.52	0.43
1:C:415:LEU:HB3	1:C:434:ILE:CG1	2.48	0.43
1:D:246:LEU:HD23	1:D:246:LEU:HA	1.92	0.43
1:A:405:ILE:HG12	1:A:419:SER:HA	2.00	0.43
1:C:242:SER:HB3	1:C:246:LEU:HD12	2.01	0.43
1:D:604:GLU:HA	1:D:607:ILE:HD12	1.99	0.43
1:C:134:ILE:HG22	1:C:135:TYR:N	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:657:SER:HA	1:D:688:VAL:HG12	2.00	0.43
1:D:531:PRO:HB3	1:D:572:ASN:HD22	1.84	0.43
1:D:710:ASN:C	1:D:710:ASN:HD22	2.21	0.43
1:C:642:SER:OG	1:C:644:SER:HB3	2.18	0.43
1:B:327:ILE:HG12	1:B:389:ILE:HD12	2.00	0.43
1:A:588:ASP:O	1:A:592:HIS:HB2	2.18	0.43
1:C:475:PRO:HA	1:C:557:THR:O	2.19	0.43
1:B:316:LEU:HD22	1:B:320:GLN:HA	2.01	0.43
1:A:427:GLY:HA2	1:A:553:GLN:OE1	2.19	0.43
1:B:77:LEU:HD13	1:B:88:VAL:HA	2.00	0.43
1:D:651:ILE:HG12	1:D:701:LEU:HB3	2.01	0.43
1:B:242:SER:OG	1:B:243:ASP:N	2.47	0.43
1:B:356:ARG:NH2	1:B:403:GLU:OE2	2.47	0.43
1:B:77:LEU:HD12	1:B:86:SER:HB2	1.99	0.43
1:C:42:THR:HG22	1:C:508:GLN:HG3	2.00	0.43
1:A:561:LEU:HA	1:A:561:LEU:HD23	1.90	0.43
1:B:407:ILE:HG23	1:B:415:LEU:HD21	2.00	0.42
1:D:195:TYR:O	1:D:227:GLN:HA	2.18	0.42
1:D:735:TYR:OH	1:D:751:ILE:HA	2.18	0.42
1:A:417:TYR:HE1	1:A:419:SER:HB3	1.84	0.42
1:B:109:PRO:HG2	1:B:158:SER:O	2.19	0.42
1:B:674:PRO:O	1:B:680:LEU:HD13	2.19	0.42
1:D:167:VAL:HG21	1:D:198:ILE:HG23	1.99	0.42
1:A:598:LEU:O	1:A:682:HIS:NE2	2.50	0.42
1:D:201:TRP:CZ2	1:D:710:ASN:HA	2.54	0.42
1:A:696:LYS:HG3	1:A:728:VAL:CG2	2.43	0.42
1:D:596:ARG:C	1:D:597:ARG:HD2	2.40	0.42
1:D:159:PRO:HD3	1:D:216:TRP:CB	2.49	0.42
1:C:376:SER:HA	1:C:382:ARG:HA	2.01	0.42
1:B:290:PRO:HD3	1:B:315:TRP:CD1	2.55	0.42
1:B:159:PRO:HD3	1:B:216:TRP:HB3	2.01	0.42
1:B:389:ILE:HD13	1:B:389:ILE:HA	1.86	0.42
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.54	0.42
1:D:661:TYR:OH	1:D:718:GLN:HG3	2.20	0.42
1:B:259:ALA:HB3	1:B:660:GLU:HA	2.01	0.42
1:A:417:TYR:CE1	1:A:419:SER:HB3	2.55	0.42
1:B:513:LYS:O	1:B:527:GLN:HA	2.20	0.42
1:B:598:LEU:HG	1:B:631:TYR:OH	2.20	0.42
1:B:117:GLU:HB2	1:B:132:TYR:CE2	2.55	0.42
1:D:183:TYR:O	1:D:185:ILE:HD12	2.20	0.42
1:B:340:LEU:HB2	1:B:343:ARG:CG	2.49	0.42
1:A:230:ASP:O	1:A:231:THR:C	2.58	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:167:VAL:HA	1:B:171:ASP:O	2.20	0.42
1:C:303:VAL:HG22	1:C:313:LEU:HD12	2.01	0.42
1:A:487:ASN:OD1	1:A:489:LYS:HG2	2.20	0.42
1:B:384:ILE:HG13	1:B:404:VAL:HG21	2.01	0.42
1:A:153:GLN:NE2	1:A:170:ASN:H	2.07	0.41
1:D:90:LEU:HD21	1:D:95:PHE:HE2	1.84	0.41
1:A:631:TYR:HD1	4:A:800:7AC:H13	1.84	0.41
1:B:379:GLU:HA	1:B:379:GLU:OE2	2.20	0.41
1:D:299:TYR:OH	1:D:318:ARG:HG3	2.20	0.41
1:C:654:ALA:N	1:C:655:PRO:HD3	2.35	0.41
1:B:336:ARG:NH1	1:B:337:TRP:O	2.54	0.41
1:C:627:TRP:HB2	1:C:651:ILE:HB	2.02	0.41
1:C:51:ASN:ND2	1:C:54:ARG:HD2	2.32	0.41
1:B:340:LEU:HB2	1:B:343:ARG:HG3	2.02	0.41
1:A:177:GLU:HB2	1:A:180:LEU:HD13	2.02	0.41
1:A:475:PRO:HA	1:A:557:THR:O	2.19	0.41
1:A:47:ASP:HA	1:A:52:THR:OG1	2.20	0.41
1:B:654:ALA:N	1:B:655:PRO:CD	2.83	0.41
1:C:134:ILE:HD11	1:C:148:ILE:HD11	2.03	0.41
1:C:462:SER:O	1:C:463:LYS:C	2.59	0.41
1:C:172:ILE:HG22	1:C:185:ILE:HD13	2.01	0.41
1:B:299:TYR:CE1	1:B:665:VAL:HG22	2.56	0.41
1:B:310:ARG:HH21	1:B:343:ARG:NH1	2.18	0.41
1:D:127:SER:HB3	1:D:211:TYR:CD2	2.56	0.41
1:B:95:PHE:CE1	1:B:116:LEU:HD11	2.56	0.41
1:B:62:TRP:CE3	1:B:68:TYR:HB3	2.56	0.41
1:A:205:GLU:OE1	4:A:800:7AC:N20	2.53	0.41
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.55	0.41
1:B:214:LEU:HD23	1:B:225:TYR:HB3	2.03	0.41
1:B:293:MET:HG3	1:B:315:TRP:HB3	2.02	0.41
1:D:330:TYR:HB2	1:D:337:TRP:CH2	2.56	0.41
1:D:237:GLU:HG2	1:D:253:ARG:HG2	2.02	0.41
1:A:236:ILE:O	1:A:253:ARG:HA	2.20	0.41
1:B:290:PRO:HG3	1:B:326:ASP:OD1	2.21	0.41
1:A:630:SER:HB2	4:A:800:7AC:N9	2.36	0.41
1:A:223:LEU:HB3	1:A:271:VAL:HG13	2.02	0.41
1:B:630:SER:HB2	1:B:631:TYR:H	1.55	0.41
1:A:598:LEU:HD23	1:A:659:TRP:CE2	2.56	0.41
1:C:703:ILE:HA	1:C:733:MET:O	2.21	0.41
1:B:453:ARG:NH2	1:B:477:LEU:O	2.48	0.40
1:C:229:ASN:O	1:C:264:PRO:HA	2.20	0.40
1:B:545:ASP:HB3	1:B:577:SER:OG	2.21	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:624:ILE:HG22	1:C:647:PHE:CD2	2.57	0.40
1:B:169:ASN:O	1:B:170:ASN:HB2	2.21	0.40
1:B:403:GLU:OE2	1:B:585:TYR:HA	2.21	0.40
1:D:641:GLY:O	1:D:691:ARG:HB3	2.21	0.40
1:B:541:PRO:HG3	1:B:623:ARG:CZ	2.52	0.40
1:A:658:ARG:HD3	1:A:661:TYR:CZ	2.56	0.40
1:D:257:PRO:HG3	1:D:264:PRO:HD3	2.03	0.40
1:C:542:LEU:HD23	1:C:542:LEU:C	2.41	0.40
1:B:765:LEU:HA	1:B:766:PRO:HD3	1.88	0.40
1:A:703:ILE:HA	1:A:733:MET:O	2.22	0.40
1:C:405:ILE:HG13	1:C:429:ARG:CD	2.50	0.40
1:D:456:TYR:HB2	1:D:557:THR:OG1	2.21	0.40
1:A:96:ASP:OD1	1:A:96:ASP:N	2.52	0.40
1:C:319:ILE:HD12	1:C:319:ILE:H	1.86	0.40
1:C:631:TYR:O	1:C:634:TYR:HB3	2.22	0.40
1:D:90:LEU:HD21	1:D:95:PHE:CE2	2.56	0.40
1:C:612:GLN:HA	1:C:612:GLN:HE21	1.86	0.40
1:A:111:GLY:O	1:A:137:LEU:HD12	2.22	0.40
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.57	0.40
4:B:800:7AC:H19A	4:B:800:7AC:H1B	2.02	0.40
1:B:153:GLN:HB3	1:B:211:TYR:CE1	2.56	0.40
1:A:306:ALA:HB3	1:A:310:ARG:HG2	2.03	0.40
1:C:707:ALA:HB2	1:C:737:ASP:HA	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	720/740 (97%)	675 (94%)	44 (6%)	1 (0%)	59	88
1	B	720/740 (97%)	667 (93%)	50 (7%)	3 (0%)	43	76
1	C	720/740 (97%)	668 (93%)	50 (7%)	2 (0%)	50	81
1	D	720/740 (97%)	642 (89%)	76 (11%)	2 (0%)	50	81

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2880/2960 (97%)	2652 (92%)	220 (8%)	8 (0%)	50 81

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	678	ASP
1	B	366	LEU
1	A	124	TRP
1	D	282	ALA
1	D	447	CYS
1	B	389	ILE
1	C	88	VAL
1	B	88	VAL

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	649/662 (98%)	599 (92%)	50 (8%)	18 40
1	B	649/662 (98%)	610 (94%)	39 (6%)	27 55
1	C	649/662 (98%)	602 (93%)	47 (7%)	21 45
1	D	649/662 (98%)	605 (93%)	44 (7%)	22 48
All	All	2596/2648 (98%)	2416 (93%)	180 (7%)	22 47

All (180) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LEU
1	A	59	SER
1	A	66	HIS
1	A	75	ASN
1	A	78	VAL
1	A	129	THR
1	A	142	LEU
1	A	180	LEU

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Mol	Chain	Res	Type
1	A	191	GLU
1	A	202	VAL
1	A	242	SER
1	A	246	LEU
1	A	276	LEU
1	A	283	THR
1	A	316	LEU
1	A	339	CYS
1	A	370	SER
1	A	376	SER
1	A	382	ARG
1	A	385	CYS
1	A	391	LYS
1	A	410	LEU
1	A	415	LEU
1	A	436	LEU
1	A	443	THR
1	A	453	ARG
1	A	464	GLU
1	A	482	LEU
1	A	492	ARG
1	A	498	SER
1	A	504	LEU
1	A	505	GLN
1	A	506	ASN
1	A	507	VAL
1	A	514	LEU
1	A	522	THR
1	A	523	LYS
1	A	536	LYS
1	A	538	LYS
1	A	547	TYR
1	A	575	VAL
1	A	621	ASN
1	A	630	SER
1	A	660	GLU
1	A	673	LEU
1	A	688	VAL
1	A	704	HIS
1	A	710	ASN
1	A	760	LYS
1	A	761	GLN

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Mol	Chain	Res	Type
1	B	50	LYS
1	B	80	ASN
1	B	83	TYR
1	B	90	LEU
1	B	129	THR
1	B	170	ASN
1	B	190	LYS
1	B	246	LEU
1	B	276	LEU
1	B	316	LEU
1	B	326	ASP
1	B	336	ARG
1	B	339	CYS
1	B	385	CYS
1	B	399	LYS
1	B	413	ASP
1	B	448	GLU
1	B	453	ARG
1	B	463	LYS
1	B	472	CYS
1	B	482	LEU
1	B	492	ARG
1	B	502	LYS
1	B	505	GLN
1	B	507	VAL
1	B	514	LEU
1	B	536	LYS
1	B	538	LYS
1	B	547	TYR
1	B	566	TYR
1	B	594	ILE
1	B	598	LEU
1	B	630	SER
1	B	639	VAL
1	B	673	LEU
1	B	677	GLU
1	B	685	ASN
1	B	688	VAL
1	B	710	ASN
1	C	54	ARG
1	C	66	HIS
1	C	80	ASN

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Mol	Chain	Res	Type
1	C	90	LEU
1	C	91	GLU
1	C	129	THR
1	C	169	ASN
1	C	170	ASN
1	C	202	VAL
1	C	230	ASP
1	C	243	ASP
1	C	246	LEU
1	C	297	ASP
1	C	316	LEU
1	C	326	ASP
1	C	350	THR
1	C	375	ILE
1	C	385	CYS
1	C	392	LYS
1	C	395	THR
1	C	415	LEU
1	C	434	ILE
1	C	441	LYS
1	C	453	ARG
1	C	472	CYS
1	C	482	LEU
1	C	492	ARG
1	C	504	LEU
1	C	507	VAL
1	C	514	LEU
1	C	519	LEU
1	C	533	HIS
1	C	536	LYS
1	C	547	TYR
1	C	566	TYR
1	C	575	VAL
1	C	589	LYS
1	C	598	LEU
1	C	612	GLN
1	C	615	LYS
1	C	627	TRP
1	C	673	LEU
1	C	685	ASN
1	C	688	VAL
1	C	699	GLU

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Mol	Chain	Res	Type
1	C	710	ASN
1	C	761	GLN
1	D	80	ASN
1	D	85	ASN
1	D	92	ASN
1	D	102	ILE
1	D	110	ASP
1	D	129	THR
1	D	134	ILE
1	D	141	GLN
1	D	148	ILE
1	D	151	ASN
1	D	170	ASN
1	D	200	ASP
1	D	227	GLN
1	D	246	LEU
1	D	250	LYS
1	D	254	VAL
1	D	299	TYR
1	D	304	THR
1	D	316	LEU
1	D	336	ARG
1	D	365	THR
1	D	375	ILE
1	D	385	CYS
1	D	388	GLN
1	D	391	LYS
1	D	392	LYS
1	D	419	SER
1	D	441	LYS
1	D	453	ARG
1	D	492	ARG
1	D	502	LYS
1	D	504	LEU
1	D	507	VAL
1	D	547	TYR
1	D	566	TYR
1	D	575	VAL
1	D	622	LYS
1	D	627	TRP
1	D	630	SER
1	D	677	GLU

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Mol	Chain	Res	Type
1	D	688	VAL
1	D	710	ASN
1	D	721	LYS
1	D	762	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	80	ASN
1	A	92	ASN
1	A	123	GLN
1	A	138	ASN
1	A	141	GLN
1	A	153	GLN
1	A	170	ASN
1	A	344	GLN
1	A	455	GLN
1	A	505	GLN
1	A	506	ASN
1	A	572	ASN
1	A	621	ASN
1	A	710	ASN
1	A	761	GLN
1	B	80	ASN
1	B	100	HIS
1	B	112	GLN
1	B	123	GLN
1	B	141	GLN
1	B	151	ASN
1	B	153	GLN
1	B	169	ASN
1	B	170	ASN
1	B	338	ASN
1	B	344	GLN
1	B	435	GLN
1	B	455	GLN
1	B	505	GLN
1	B	572	ASN
1	B	592	HIS
1	B	595	ASN
1	B	697	GLN

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Mol	Chain	Res	Type
1	B	710	ASN
1	B	731	GLN
1	C	51	ASN
1	C	80	ASN
1	C	123	GLN
1	C	138	ASN
1	C	151	ASN
1	C	153	GLN
1	C	169	ASN
1	C	170	ASN
1	C	227	GLN
1	C	344	GLN
1	C	430	ASN
1	C	455	GLN
1	C	572	ASN
1	C	592	HIS
1	C	710	ASN
1	D	80	ASN
1	D	85	ASN
1	D	92	ASN
1	D	123	GLN
1	D	138	ASN
1	D	141	GLN
1	D	169	ASN
1	D	170	ASN
1	D	388	GLN
1	D	430	ASN
1	D	505	GLN
1	D	572	ASN
1	D	710	ASN
1	D	731	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

8 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	0.85	0	15,19,21	1.07	1 (6%)
3	NAG	A	805	3	12,14,15	0.62	0	15,19,21	0.66	0
3	NAG	B	803	1,3	12,14,15	0.67	0	15,19,21	1.02	1 (6%)
3	NAG	B	804	3	12,14,15	0.60	0	15,19,21	0.93	0
3	NAG	C	802	1,3	12,14,15	0.73	1 (8%)	15,19,21	1.13	1 (6%)
3	NAG	C	803	3	12,14,15	0.53	0	15,19,21	0.78	0
3	NAG	D	802	1,3	12,14,15	0.53	0	15,19,21	0.99	0
3	NAG	D	803	3	12,14,15	0.59	0	15,19,21	1.53	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
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	B	803	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	804	3	-	0/6/23/26	0/1/1/1
3	NAG	C	802	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	803	3	-	0/6/23/26	0/1/1/1
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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	NAG	O5-C5	-2.10	1.41	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	803	NAG	O5-C5-C6	3.75	110.92	106.98
3	A	804	NAG	C3-C2-N2	-3.34	106.68	111.76
3	C	802	NAG	O5-C5-C6	2.45	109.56	106.98
3	D	803	NAG	O5-C5-C4	-2.21	107.85	110.65
3	B	803	NAG	C2-N2-C7	-2.20	119.40	123.09

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	7AC	A	800	-	23,23,23	0.85	1 (4%)	33,33,33	2.09	4 (12%)
2	NAG	A	801	1	12,14,15	0.53	0	15,19,21	1.53	1 (6%)
2	NAG	A	802	1	12,14,15	0.55	0	15,19,21	1.49	1 (6%)
2	NAG	A	803	1	12,14,15	0.59	0	15,19,21	1.22	1 (6%)
2	NAG	A	806	1	12,14,15	0.41	0	15,19,21	1.52	1 (6%)
4	7AC	B	800	-	23,23,23	0.96	2 (8%)	33,33,33	1.70	3 (9%)
2	NAG	B	801	1	12,14,15	0.58	0	15,19,21	1.35	1 (6%)
2	NAG	B	802	1	12,14,15	0.76	0	15,19,21	1.62	2 (13%)
2	NAG	B	805	1	12,14,15	0.54	0	15,19,21	1.02	1 (6%)
4	7AC	C	800	-	23,23,23	0.96	2 (8%)	33,33,33	1.76	3 (9%)
2	NAG	C	801	1	12,14,15	0.71	0	15,19,21	1.03	1 (6%)
2	NAG	C	804	1	12,14,15	0.67	0	15,19,21	1.77	3 (20%)
2	NAG	C	805	1	12,14,15	0.48	0	15,19,21	1.24	1 (6%)
4	7AC	D	800	-	23,23,23	0.88	1 (4%)	33,33,33	2.14	6 (18%)
2	NAG	D	801	1	12,14,15	0.56	0	15,19,21	1.08	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	D	804	1	12,14,15	0.54	0	15,19,21	0.90	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	7AC	A	800	-	-	0/8/8/8	0/1/3/3
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	806	1	-	0/6/23/26	0/1/1/1
4	7AC	B	800	-	-	0/8/8/8	0/1/3/3
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	805	1	-	0/6/23/26	0/1/1/1
4	7AC	C	800	-	-	0/8/8/8	0/1/3/3
2	NAG	C	801	1	-	0/6/23/26	0/1/1/1
2	NAG	C	804	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	805	1	-	0/6/23/26	0/1/1/1
4	7AC	D	800	-	-	0/8/8/8	0/1/3/3
2	NAG	D	801	1	-	0/6/23/26	0/1/1/1
2	NAG	D	804	1	-	0/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	800	7AC	C3-N4	-2.39	1.29	1.34
4	B	800	7AC	C18-C21	-2.36	1.39	1.43
4	C	800	7AC	C10-C7	2.30	1.43	1.40
4	D	800	7AC	C3-N4	-2.21	1.30	1.34
4	B	800	7AC	C3-N4	-2.15	1.30	1.34
4	A	800	7AC	C3-N4	-2.02	1.30	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	7AC	C18-C21-N2	7.47	135.50	129.15
4	D	800	7AC	C18-C21-N2	7.41	135.45	129.15
4	C	800	7AC	C18-C21-N2	7.19	135.26	129.15
4	D	800	7AC	C10-C11-C16	-6.42	115.40	122.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	800	7AC	C10-C11-C16	-6.07	115.76	122.10
4	B	800	7AC	C18-C21-N2	5.95	134.20	129.15
4	B	800	7AC	C10-C11-C16	-5.35	116.51	122.10
2	A	801	NAG	O5-C5-C6	5.31	112.55	106.98
2	A	806	NAG	O5-C5-C6	4.98	112.20	106.98
2	C	804	NAG	O5-C5-C6	4.96	112.19	106.98
2	A	802	NAG	O5-C5-C6	4.82	112.04	106.98
4	A	800	7AC	C11-C10-C7	-4.39	116.05	120.82
4	C	800	7AC	C10-C11-C16	-4.31	117.60	122.10
2	B	801	NAG	O5-C5-C6	4.11	111.30	106.98
4	D	800	7AC	C11-C10-C7	-3.83	116.66	120.82
2	B	802	NAG	O5-C5-C6	3.32	110.47	106.98
2	A	803	NAG	O5-C5-C6	3.21	110.35	106.98
2	C	804	NAG	O5-C5-C4	-3.20	106.59	110.65
2	C	805	NAG	O5-C5-C6	3.18	110.32	106.98
2	B	805	NAG	O5-C5-C6	2.77	109.89	106.98
4	D	800	7AC	C12-C11-C10	2.75	125.45	118.68
2	B	802	NAG	C4-C3-C2	2.71	117.94	111.32
2	D	801	NAG	O5-C5-C6	2.68	109.79	106.98
4	C	800	7AC	C11-C10-C7	-2.51	118.10	120.82
4	A	800	7AC	C12-C11-C10	2.38	124.53	118.68
4	D	800	7AC	C11-C16-CL17	-2.37	117.93	120.62
2	D	801	NAG	C3-C2-N2	-2.33	108.22	111.76
4	B	800	7AC	C11-C10-C7	-2.32	118.30	120.82
4	D	800	7AC	C1-N2-C21	2.24	128.41	125.61
2	C	804	NAG	C3-C2-N2	-2.21	108.40	111.76
2	C	801	NAG	C4-C3-C2	2.15	116.58	111.32
2	D	804	NAG	O5-C5-C6	2.01	109.08	106.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	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	724/740 (97%)	0.05	7 (0%) 79 84	32, 52, 73, 108	0
1	B	724/740 (97%)	0.11	15 (2%) 60 67	28, 49, 75, 102	0
1	C	724/740 (97%)	0.30	38 (5%) 26 29	30, 57, 84, 99	0
1	D	724/740 (97%)	0.63	76 (10%) 7 7	40, 69, 95, 124	0
All	All	2896/2960 (97%)	0.27	136 (4%) 30 34	28, 55, 86, 124	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	VAL	7.5
1	C	89	PHE	5.8
1	D	99	GLY	5.2
1	D	148	ILE	5.2
1	D	89	PHE	5.1
1	D	97	GLU	4.9
1	D	88	VAL	4.7
1	C	102	ILE	4.6
1	B	148	ILE	4.5
1	D	83	TYR	4.4
1	C	490	GLY	4.3
1	D	90	LEU	4.1
1	D	142	LEU	4.1
1	C	491	LEU	4.0
1	C	100	HIS	3.8
1	D	322	TYR	3.8
1	D	141	GLN	3.7
1	D	176	ILE	3.7
1	D	220	GLY	3.7
1	D	149	PRO	3.6
1	D	276	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	C	99	GLY	3.4
1	D	518	ILE	3.3
1	C	78	VAL	3.3
1	B	137	LEU	3.2
1	D	483	HIS	3.2
1	D	98	PHE	3.2
1	C	79	PHE	3.2
1	D	86	SER	3.2
1	D	388	GLN	3.2
1	D	279	VAL	3.1
1	D	77	LEU	3.1
1	D	334	SER	3.1
1	C	81	ALA	3.1
1	D	63	ILE	3.1
1	C	142	LEU	3.0
1	C	330	TYR	3.0
1	D	330	TYR	3.0
1	D	380	GLY	2.9
1	D	139	LYS	2.9
1	D	479	LEU	2.9
1	D	415	LEU	2.9
1	D	397	ILE	2.9
1	D	273	THR	2.9
1	D	395	THR	2.9
1	D	69	LEU	2.8
1	C	148	ILE	2.8
1	D	221	THR	2.8
1	D	348	MET	2.8
1	D	384	ILE	2.8
1	B	138	ASN	2.8
1	D	95	PHE	2.8
1	D	306	ALA	2.8
1	D	372	TYR	2.7
1	C	766	PRO	2.7
1	C	87	SER	2.7
1	B	180	LEU	2.7
1	D	223	LEU	2.7
1	D	468	TYR	2.7
1	B	139	LYS	2.7
1	D	375	ILE	2.7
1	D	93	SER	2.6
1	D	163	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	482	LEU	2.6
1	D	222	PHE	2.6
1	D	416	TYR	2.6
1	C	132	TYR	2.6
1	C	58	TYR	2.5
1	C	42	THR	2.5
1	C	140	ARG	2.5
1	B	274	ASP	2.5
1	D	164	LEU	2.5
1	C	83	TYR	2.5
1	D	58	TYR	2.5
1	C	482	LEU	2.5
1	D	113	PHE	2.5
1	C	144	THR	2.5
1	D	100	HIS	2.4
1	B	144	THR	2.4
1	C	91	GLU	2.4
1	D	162	HIS	2.4
1	C	98	PHE	2.4
1	D	180	LEU	2.4
1	A	71	LYS	2.4
1	D	386	TYR	2.4
1	C	80	ASN	2.4
1	B	98	PHE	2.4
1	D	392	LYS	2.4
1	C	77	LEU	2.4
1	D	389	ILE	2.4
1	B	135	TYR	2.4
1	D	309	GLU	2.3
1	D	364	PHE	2.3
1	D	385	CYS	2.3
1	D	333	SER	2.3
1	C	90	LEU	2.3
1	C	467	TYR	2.3
1	B	95	PHE	2.3
1	B	97	GLU	2.3
1	C	145	GLU	2.3
1	A	82	GLU	2.3
1	D	327	ILE	2.3
1	D	766	PRO	2.2
1	D	684	ARG	2.2
1	D	464	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	463	LYS	2.2
1	D	144	THR	2.2
1	C	97	GLU	2.2
1	D	467	TYR	2.2
1	C	85	ASN	2.2
1	D	310	ARG	2.2
1	D	338	ASN	2.2
1	A	95	PHE	2.2
1	B	766	PRO	2.2
1	D	394	CYS	2.2
1	A	72	GLN	2.2
1	D	490	GLY	2.2
1	D	76	ILE	2.1
1	C	101	SER	2.1
1	A	70	TYR	2.1
1	C	86	SER	2.1
1	D	329	ASP	2.1
1	B	141	GLN	2.1
1	A	90	LEU	2.1
1	D	85	ASN	2.1
1	B	89	PHE	2.1
1	B	63	ILE	2.1
1	C	118	TYR	2.1
1	D	105	TYR	2.1
1	D	347	GLU	2.1
1	C	336	ARG	2.0
1	C	135	TYR	2.0
1	A	630	SER	2.0
1	D	291	ALA	2.0
1	C	281	ASN	2.0
1	C	412	SER	2.0

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

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

6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 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
3	NAG	C	803	14/15	0.26	6.38	86,89,90,90	0
3	NAG	A	805	14/15	0.24	3.34	82,83,85,86	0
3	NAG	D	803	14/15	0.19	3.00	82,83,84,84	0
3	NAG	B	804	14/15	0.18	0.68	74,75,77,77	0
3	NAG	A	804	14/15	0.18	0.67	67,71,75,79	0
3	NAG	B	803	14/15	0.15	-0.30	63,66,69,71	0
3	NAG	C	802	14/15	0.15	-0.56	71,74,78,82	0
3	NAG	D	802	14/15	0.14	-1.72	76,77,78,80	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(Å ²)	Q<0.9
4	7AC	B	800	21/21	0.27	2.18	55,58,59,59	0
2	NAG	C	805	14/15	0.29	2.15	73,76,77,77	0
4	7AC	A	800	21/21	0.30	1.63	57,58,59,60	0
4	7AC	C	800	21/21	0.25	1.44	55,59,59,59	0
2	NAG	A	803	14/15	0.18	0.97	73,76,78,79	0
2	NAG	B	802	14/15	0.29	0.91	80,83,85,85	0
4	7AC	D	800	21/21	0.26	0.60	67,68,68,68	0
2	NAG	A	802	14/15	0.23	0.53	62,67,69,69	0
2	NAG	C	801	14/15	0.23	0.19	73,75,75,76	0
2	NAG	A	801	14/15	0.18	-0.14	78,80,81,82	0
2	NAG	B	805	14/15	0.15	-0.54	75,78,79,79	0
2	NAG	B	801	14/15	0.18	-0.77	76,77,78,78	0
2	NAG	D	801	14/15	0.18	-0.97	71,72,72,72	0
2	NAG	D	804	14/15	0.12	-1.91	91,92,93,93	0
2	NAG	C	804	14/15	0.17	-2.58	93,95,96,96	0
2	NAG	A	806	14/15	0.11	-2.71	65,68,70,70	0

6.5 Other polymers ⓘ

There are no such residues in this entry.