Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:50 AM 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

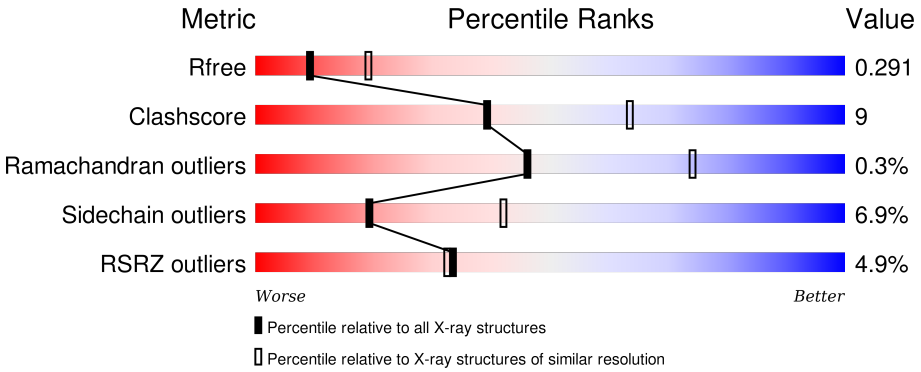
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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}	91344	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	740	% 73% 22%
1	B	740	3% 73% 23%
1	C	740	5% 74% 21%
1	D	740	10% 72% 23%

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	C	804	X	-	-	-
2	NAG	C	805	-	-	-	X
4	7AC	B	800	-	-	-	X

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 24357 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	724	Total	C	N	O	S	0	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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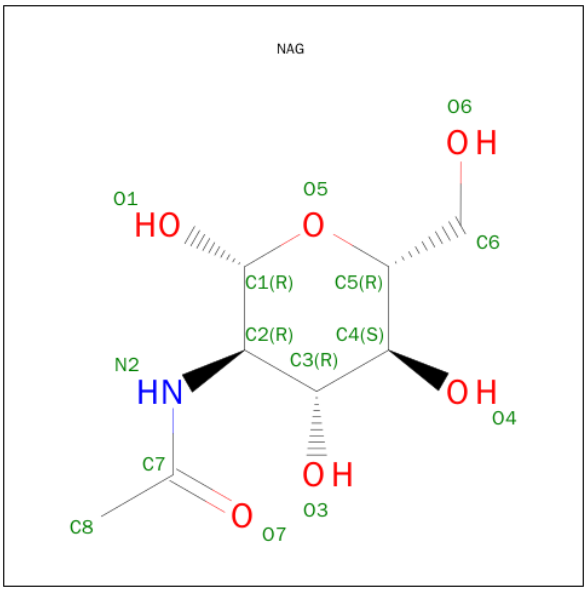
Chain	Residue	Modelled	Actual	Comment	Reference
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	27	ALA	-	EXPRESSION TAG	UNP P27487
C	28	ASP	-	EXPRESSION TAG	UNP P27487
C	29	PRO	-	EXPRESSION TAG	UNP P27487
C	30	GLY	-	EXPRESSION TAG	UNP P27487
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: $C_8H_{15}NO_6$).

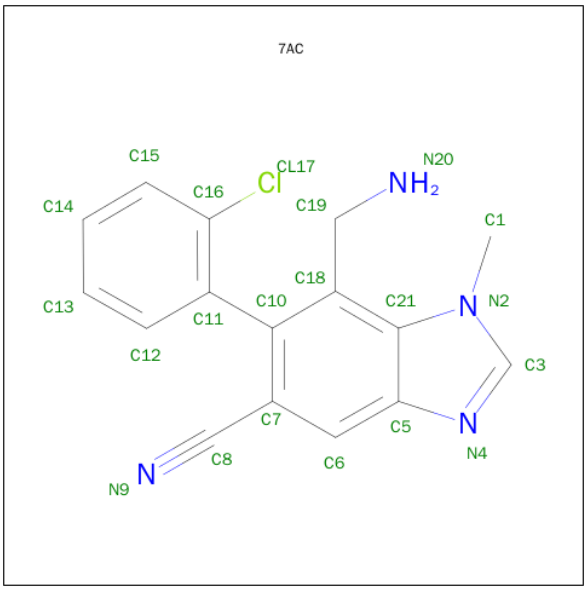


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	A	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	B	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	C	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0
2	D	1	Total C N O 14 8 1 5	0	0

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

- Molecule 4 is 7-(AMINOMETHYL)-6-(2-CHLOROPHENYL)-1-METHYL-1H-BENZIMIDAZOLE-5-CARBONITRILE (three-letter code: 7AC) (formula: $C_{16}H_{13}ClN_4$).



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

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	85	Total O 85 85	0	0

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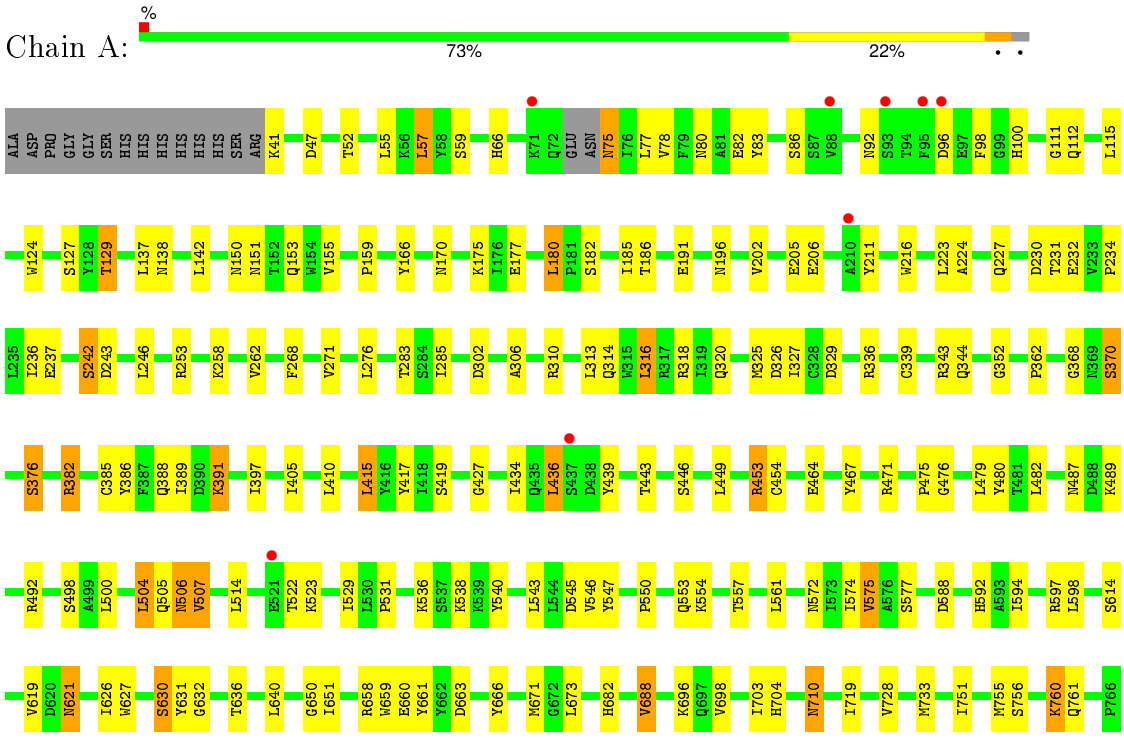
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	106	Total O 106 106	0	0
5	C	56	Total O 56 56	0	0
5	D	30	Total O 30 30	0	0

3 Residue-property plots (i)

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.

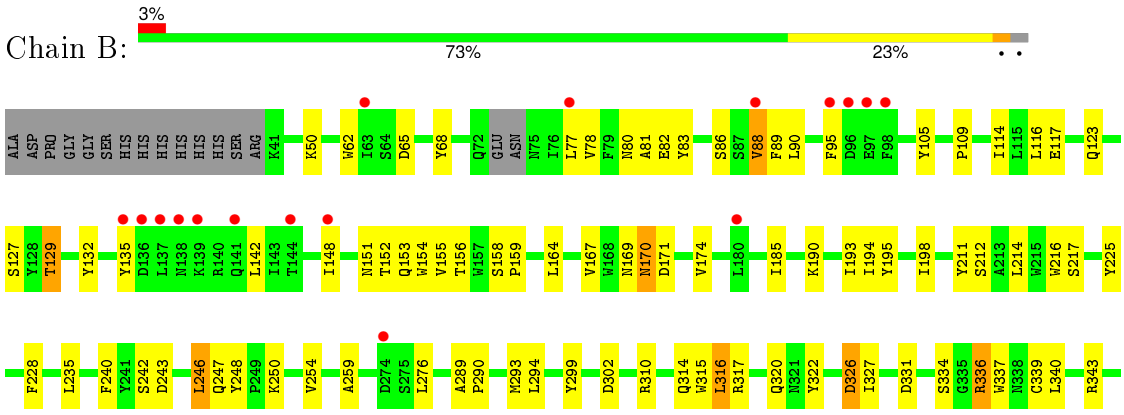
- Molecule 1: Dipeptidyl peptidase 4

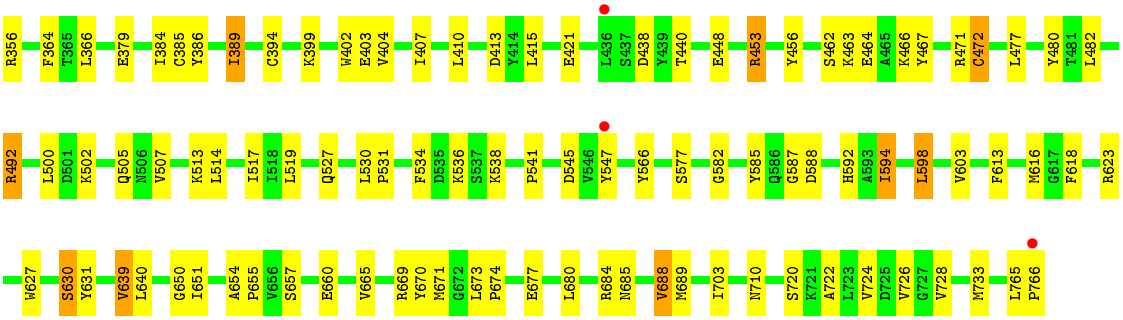
Chain A:



- Molecule 1: Dipeptidyl peptidase 4

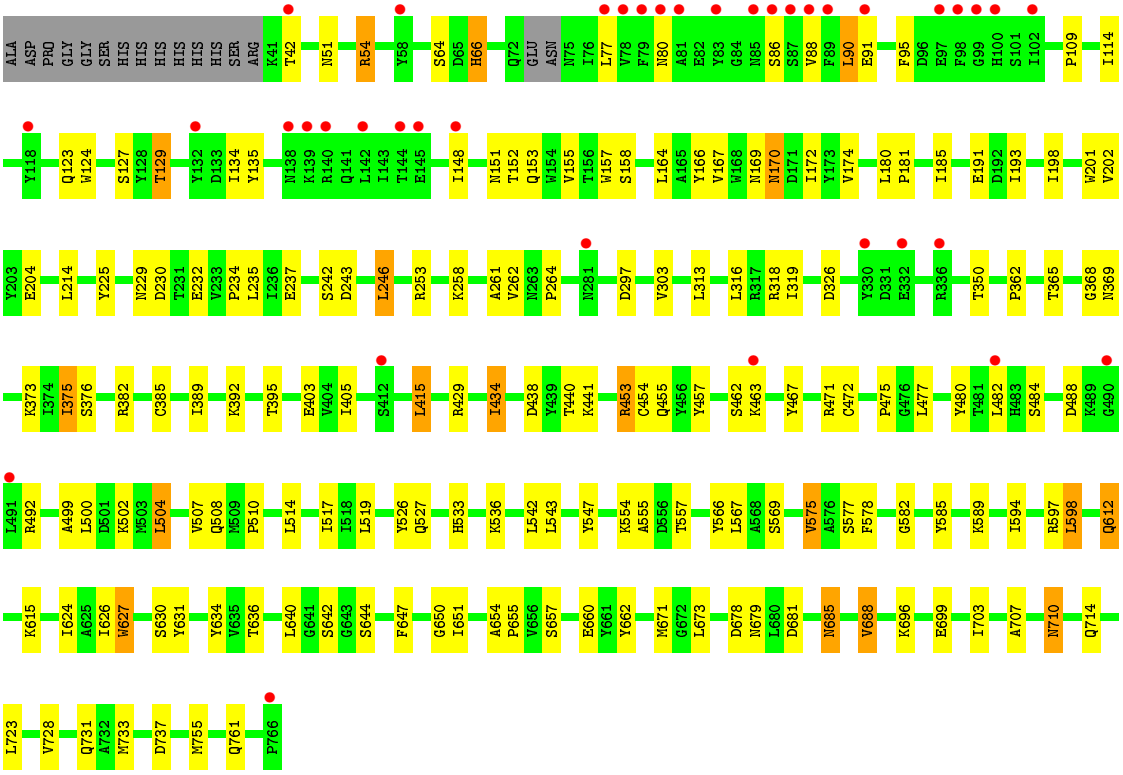
Chain B:





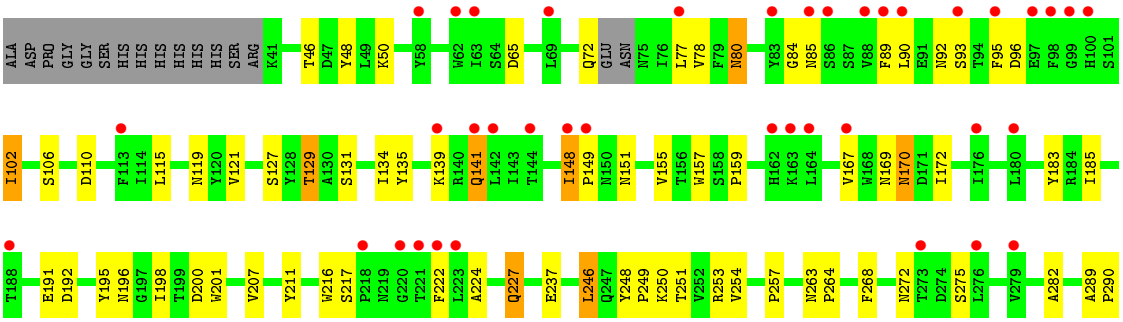
- Molecule 1: Dipeptidyl peptidase 4

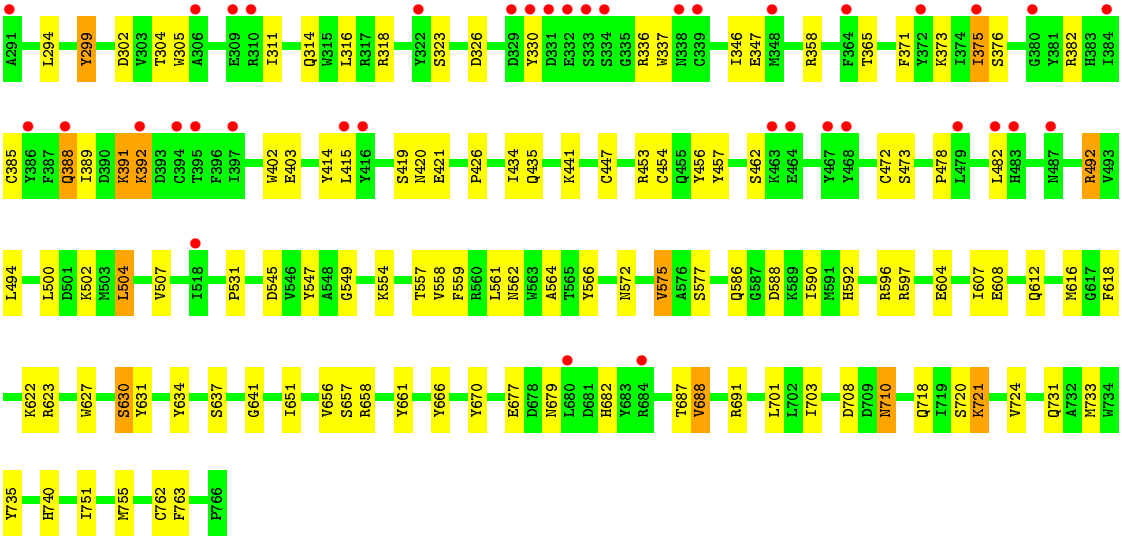
Chain C:



- Molecule 1: Dipeptidyl peptidase 4

Chain D:




A291 L294 Y299 D302 V303 T304 W305 A306 E309 R310 I311 Q314 W315 L316 R317 R318 Y322 S323 D326 D329 Y330 D331 E332 S333 S334 G335 R336 W337 N338 C339 I346 E347 W348 R358 F364 T365 F371 Y372 K373 I374 I375 S376 G380 Y381 R382 H383 I384
C385 Y386 F387 Q388 I389 D390 K391 K392 D393 C394 T395 F396 I397 W402 E403 Y414 L415 Y416 S419 N420 E421 P426 I434 Q435 K441 C447 R453 C454 Q455 Y456 Y457 S462 K463 E464 Y467 Y468 C472 S473 P478 L479 L482 H483 N487 R492 V493
L494 L500 D501 K502 M503 L504 V507 I518 P531 D545 V546 Y547 A548 G549 K554 T557 V558 F559 R560 L561 N562 W563 A564 T565 Y566 N572 V575 A576 S577 Q586 G587 D588 K589 I590 M591 H592 R596 R597 E604 I607 E608 Q612 M616 G617 F618
K622 R623 W627 S630 Y631 Y634 S637 G641 I651 V656 S657 R658 Y661 Y666 Y670 E677 D678 H679 L680 D681 H682 Y683 R684 T687 V688 R691 L701 L702 I703 D708 D709 N710 Q718 I719 S720 K721 V724 Q731 A732 M733 W734
Y735 H740 I751 M755 C762 F763 P766

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.58 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.200 , 0.267 0.225 , 0.291	Depositor DCC
R_{free} test set	4722 reflections (5.26%)	DCC
Wilson B-factor (Å^2)	57.3	Xtriage
Anisotropy	0.180	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 34.7	EDS
Estimated twinning fraction	0.023 for h,-k,-h-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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(^{o})	Ideal(^{o})
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 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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
2	A	56	0	52	0	0
2	B	42	0	39	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 9.

All (420) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:VAL:HG23	1:B:728:VAL:HG23	1.83	0.60
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 (i)

5.3.1 Protein backbone (i)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	720/740 (97%)	675 (94%)	44 (6%)	1 (0%)	56 83
1	B	720/740 (97%)	667 (93%)	50 (7%)	3 (0%)	39 68
1	C	720/740 (97%)	668 (93%)	50 (7%)	2 (0%)	46 74
1	D	720/740 (97%)	642 (89%)	76 (11%)	2 (0%)	46 74
All	All	2880/2960 (97%)	2652 (92%)	220 (8%)	8 (0%)	46 74

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 (i)

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%)	16 35
1	B	649/662 (98%)	610 (94%)	39 (6%)	24 49
1	C	649/662 (98%)	602 (93%)	47 (7%)	18 40
1	D	649/662 (98%)	605 (93%)	44 (7%)	20 43
All	All	2596/2648 (98%)	2416 (93%)	180 (7%)	19 42

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 molecules in this entry.

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

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

5.5 Carbohydrates (i)

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	14,14,15	0.55	0	15,19,21	0.73	0
3	NAG	A	805	3	14,14,15	0.47	0	15,19,21	0.86	0
3	NAG	B	803	1,3	14,14,15	0.50	0	15,19,21	1.12	1 (6%)
3	NAG	B	804	3	14,14,15	0.54	0	15,19,21	1.01	1 (6%)
3	NAG	C	802	1,3	14,14,15	0.63	0	15,19,21	0.85	0
3	NAG	C	803	3	14,14,15	0.48	0	15,19,21	1.20	1 (6%)
3	NAG	D	802	1,3	14,14,15	0.46	0	15,19,21	1.09	1 (6%)
3	NAG	D	803	3	14,14,15	0.61	0	15,19,21	1.26	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	803	NAG	C2-N2-C7	-2.83	119.40	123.04
3	D	802	NAG	C1-O5-C5	2.36	115.25	112.25
3	B	804	NAG	C4-C3-C2	2.38	114.93	111.23
3	C	803	NAG	C1-O5-C5	3.77	117.03	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry (i)

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	-	21,23,23	0.91	2 (9%)	19,33,33	1.30	3 (15%)
2	NAG	A	801	1	14,14,15	0.56	0	15,19,21	1.40	2 (13%)
2	NAG	A	802	1	14,14,15	0.49	0	15,19,21	1.62	2 (13%)
2	NAG	A	803	1	14,14,15	0.63	0	15,19,21	1.03	1 (6%)
2	NAG	A	806	1	14,14,15	0.53	0	15,19,21	1.74	2 (13%)
4	7AC	B	800	-	21,23,23	1.08	2 (9%)	19,33,33	1.00	1 (5%)
2	NAG	B	801	1	14,14,15	0.57	0	15,19,21	1.12	1 (6%)
2	NAG	B	802	1	14,14,15	0.79	1 (7%)	15,19,21	1.66	3 (20%)
2	NAG	B	805	1	14,14,15	0.59	0	15,19,21	1.55	1 (6%)
4	7AC	C	800	-	21,23,23	1.06	3 (14%)	19,33,33	0.94	0
2	NAG	C	801	1	14,14,15	0.69	0	15,19,21	1.24	2 (13%)
2	NAG	C	804	1	14,14,15	0.78	1 (7%)	15,19,21	1.17	2 (13%)
2	NAG	C	805	1	14,14,15	0.61	0	15,19,21	1.58	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	7AC	D	800	-	21,23,23	0.96	2 (9%)	19,33,33	1.29	2 (10%)
2	NAG	D	801	1	14,14,15	0.62	0	15,19,21	1.55	1 (6%)
2	NAG	D	804	1	14,14,15	0.70	1 (7%)	15,19,21	1.42	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	-	-	0/7/8/8	0/3/3/3
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	-	-	0/7/8/8	0/3/3/3
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	-	-	0/7/8/8	0/3/3/3
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	-	-	0/7/8/8	0/3/3/3
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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	800	7AC	C18-C21	-3.18	1.39	1.43
4	C	800	7AC	C18-C21	-2.50	1.40	1.43
4	C	800	7AC	C3-N4	-2.46	1.29	1.34
4	D	800	7AC	C18-C21	-2.41	1.40	1.43
4	D	800	7AC	C3-N4	-2.27	1.30	1.34
4	B	800	7AC	C3-N4	-2.21	1.30	1.34
4	A	800	7AC	C18-C21	-2.19	1.40	1.43
4	A	800	7AC	C3-N4	-2.08	1.30	1.34
2	B	802	NAG	C1-C2	2.10	1.55	1.52
2	D	804	NAG	C1-C2	2.19	1.55	1.52
4	C	800	7AC	C10-C7	2.36	1.43	1.40
2	C	804	NAG	C1-C2	2.37	1.55	1.52

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	800	7AC	C11-C10-C7	-3.40	116.05	120.57
4	D	800	7AC	C11-C10-C7	-2.94	116.66	120.57
2	B	802	NAG	C3-C4-C5	2.01	113.70	110.20
4	B	800	7AC	C12-C11-C16	2.01	120.17	117.50
2	C	801	NAG	C1-O5-C5	2.01	114.80	112.25
2	C	805	NAG	O3-C3-C2	2.05	113.17	109.11
4	A	800	7AC	C7-C10-C18	2.11	120.94	118.99
2	A	802	NAG	O5-C5-C6	2.17	112.04	107.35
2	C	804	NAG	O5-C5-C6	2.24	112.19	107.35
2	A	806	NAG	O5-C5-C6	2.24	112.20	107.35
2	A	801	NAG	O5-C5-C6	2.40	112.55	107.35
4	A	800	7AC	C12-C11-C10	2.46	124.53	118.56
2	C	804	NAG	C4-C3-C2	2.48	115.08	111.23
2	B	802	NAG	C2-N2-C7	2.48	126.23	123.04
2	A	803	NAG	C1-O5-C5	2.56	115.50	112.25
4	D	800	7AC	C12-C11-C10	2.84	125.45	118.56
2	B	801	NAG	C1-O5-C5	3.17	116.27	112.25
2	C	801	NAG	C4-C3-C2	3.44	116.58	111.23
2	A	801	NAG	C1-O5-C5	4.16	117.52	112.25
2	B	802	NAG	C4-C3-C2	4.32	117.94	111.23
2	C	805	NAG	C1-O5-C5	4.42	117.86	112.25
2	A	802	NAG	C1-O5-C5	4.71	118.23	112.25
2	D	804	NAG	C1-O5-C5	4.82	118.36	112.25
2	B	805	NAG	C1-O5-C5	5.22	118.88	112.25
2	D	801	NAG	C1-O5-C5	5.29	118.97	112.25
2	A	806	NAG	C1-O5-C5	5.40	119.10	112.25

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.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	800	7AC	3	0
4	B	800	7AC	3	0
4	C	800	7AC	1	0
4	D	800	7AC	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.07	8 (1%) 82 83	32, 52, 73, 108	0
1	B	724/740 (97%)	0.16	20 (2%) 56 57	28, 49, 75, 102	0
1	C	724/740 (97%)	0.32	38 (5%) 31 30	30, 57, 84, 99	0
1	D	724/740 (97%)	0.66	77 (10%) 8 6	40, 69, 95, 124	0
All	All	2896/2960 (97%)	0.30	143 (4%) 33 32	28, 55, 86, 124	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	88	VAL	7.3
1	D	97	GLU	4.9
1	D	99	GLY	4.9
1	D	83	TYR	4.8
1	C	490	GLY	4.7
1	D	89	PHE	4.4
1	D	148	ILE	4.3
1	C	89	PHE	4.3
1	C	99	GLY	4.2
1	C	102	ILE	4.1
1	D	220	GLY	3.9
1	C	100	HIS	3.8
1	B	148	ILE	3.8
1	D	176	ILE	3.8
1	D	330	TYR	3.6
1	D	149	PRO	3.6
1	C	491	LEU	3.5
1	D	141	GLN	3.5
1	D	276	LEU	3.5
1	D	139	LYS	3.4
1	D	222	PHE	3.4

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Mol	Chain	Res	Type	RSRZ
1	D	395	THR	3.3
1	D	142	LEU	3.3
1	D	322	TYR	3.2
1	C	144	THR	3.2
1	D	380	GLY	3.1
1	C	79	PHE	3.1
1	D	88	VAL	3.1
1	D	415	LEU	3.1
1	B	137	LEU	3.1
1	D	397	ILE	3.1
1	C	330	TYR	3.1
1	D	221	THR	3.1
1	D	306	ALA	3.1
1	D	86	SER	3.0
1	D	483	HIS	3.0
1	B	138	ASN	3.0
1	C	142	LEU	3.0
1	D	90	LEU	3.0
1	D	223	LEU	3.0
1	D	98	PHE	3.0
1	D	63	ILE	3.0
1	D	375	ILE	3.0
1	D	279	VAL	3.0
1	D	334	SER	2.9
1	D	273	THR	2.9
1	B	139	LYS	2.9
1	B	95	PHE	2.8
1	D	69	LEU	2.8
1	C	91	GLU	2.7
1	B	144	THR	2.7
1	B	96	ASP	2.7
1	C	97	GLU	2.7
1	D	77	LEU	2.7
1	B	98	PHE	2.7
1	D	416	TYR	2.7
1	B	97	GLU	2.7
1	D	180	LEU	2.6
1	C	145	GLU	2.6
1	D	164	LEU	2.6
1	C	281	ASN	2.6
1	D	464	GLU	2.6
1	D	163	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	96	ASP	2.6
1	C	132	TYR	2.6
1	D	479	LEU	2.6
1	C	78	VAL	2.6
1	D	348	MET	2.6
1	D	309	GLU	2.6
1	D	482	LEU	2.6
1	B	63	ILE	2.6
1	D	388	GLN	2.6
1	D	518	ILE	2.6
1	D	162	HIS	2.5
1	D	468	TYR	2.5
1	D	218	PRO	2.5
1	D	93	SER	2.5
1	C	81	ALA	2.5
1	D	113	PHE	2.5
1	B	135	TYR	2.5
1	C	140	ARG	2.5
1	B	274	ASP	2.5
1	D	100	HIS	2.5
1	D	463	LYS	2.5
1	D	58	TYR	2.5
1	D	372	TYR	2.5
1	B	88	VAL	2.4
1	A	95	PHE	2.4
1	C	336	ARG	2.4
1	D	333	SER	2.4
1	D	394	CYS	2.4
1	B	141	GLN	2.4
1	C	87	SER	2.4
1	C	148	ILE	2.4
1	A	93	SER	2.3
1	D	384	ILE	2.3
1	C	80	ASN	2.3
1	D	392	LYS	2.3
1	D	467	TYR	2.3
1	C	766	PRO	2.3
1	C	42	THR	2.3
1	D	331	ASP	2.3
1	D	338	ASN	2.3
1	D	188	THR	2.3
1	A	71	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	437	SER	2.2
1	D	329	ASP	2.2
1	C	86	SER	2.2
1	C	139	LYS	2.2
1	C	58	TYR	2.2
1	C	118	TYR	2.2
1	D	95	PHE	2.2
1	D	85	ASN	2.2
1	D	310	ARG	2.2
1	D	144	THR	2.2
1	D	487	ASN	2.2
1	C	332	GLU	2.1
1	D	167	VAL	2.1
1	C	77	LEU	2.1
1	D	62	TRP	2.1
1	A	521	GLU	2.1
1	C	98	PHE	2.1
1	A	210	ALA	2.1
1	D	291	ALA	2.1
1	C	463	LYS	2.1
1	D	386	TYR	2.1
1	B	436	LEU	2.1
1	D	680	LEU	2.1
1	C	83	TYR	2.1
1	D	684	ARG	2.1
1	B	180	LEU	2.1
1	C	482	LEU	2.1
1	D	364	PHE	2.1
1	D	339	CYS	2.1
1	C	412	SER	2.1
1	C	85	ASN	2.0
1	C	138	ASN	2.0
1	B	136	ASP	2.0
1	B	547	TYR	2.0
1	A	88	VAL	2.0
1	B	766	PRO	2.0
1	B	77	LEU	2.0
1	D	332	GLU	2.0

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

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

6.3 Carbohydrates (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	NAG	A	804	14/15	0.94	0.19	0.46	67,71,75,79	0
3	NAG	B	803	14/15	0.93	0.14	-0.68	63,66,69,71	0
3	NAG	C	802	14/15	0.93	0.14	-0.97	71,74,78,82	0
3	NAG	D	802	14/15	0.91	0.15	-1.41	76,77,78,80	0
3	NAG	A	805	14/15	0.88	0.24	-	82,83,85,86	0
3	NAG	B	804	14/15	0.86	0.18	-	74,75,77,77	0
3	NAG	D	803	14/15	0.91	0.19	-	82,83,84,84	0
3	NAG	C	803	14/15	0.84	0.24	-	86,89,90,90	0

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	C	805	14/15	0.85	0.30	2.68	73,76,77,77	0
4	7AC	B	800	21/21	0.95	0.29	2.45	55,58,59,59	0
4	7AC	A	800	21/21	0.94	0.30	1.80	57,58,59,60	0
4	7AC	C	800	21/21	0.94	0.25	1.31	55,59,59,59	0
4	7AC	D	800	21/21	0.94	0.26	0.57	67,68,68,68	0
2	NAG	A	801	14/15	0.74	0.18	-0.09	78,80,81,82	0
2	NAG	D	801	14/15	0.78	0.18	-1.04	71,72,72,72	0
2	NAG	B	801	14/15	0.76	0.19	-1.05	76,77,78,78	0
2	NAG	C	804	14/15	0.78	0.19	-	93,95,96,96	0
2	NAG	D	804	14/15	0.84	0.13	-	91,92,93,93	0
2	NAG	A	802	14/15	0.77	0.25	-	62,67,69,69	0
2	NAG	B	805	14/15	0.87	0.16	-	75,78,79,79	0
2	NAG	A	803	14/15	0.86	0.19	-	73,76,78,79	0
2	NAG	C	801	14/15	0.87	0.24	-	73,75,75,76	0
2	NAG	A	806	14/15	0.90	0.11	-	65,68,70,70	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	B	802	14/15	0.83	0.28	-	80,83,85,85	0

6.5 Other polymers (i)

There are no such residues in this entry.