



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 05:56 AM BST

PDB ID : 1NU8  
Title : Crystal structure of human dipeptidyl peptidase IV (DPP-IV) in complex with Diprotin A (IPI)  
Authors : Thoma, R.; Loeffler, B.; Stihle, M.; Huber, W.; Ruf, A.; Hennig, M.  
Deposited on : 2003-01-31  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

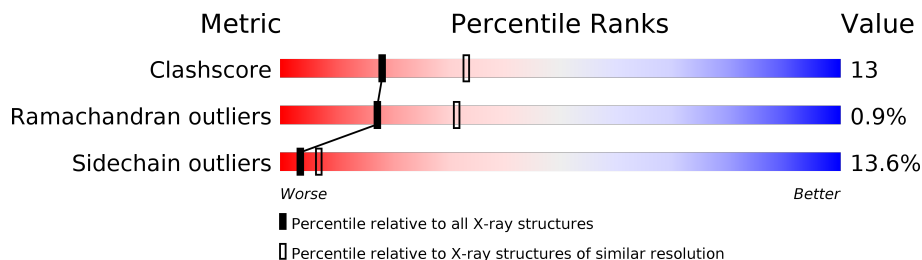
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	728	
1	B	728	
2	D	3	

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
3	NAG	A	794	X	-	-	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 12335 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.

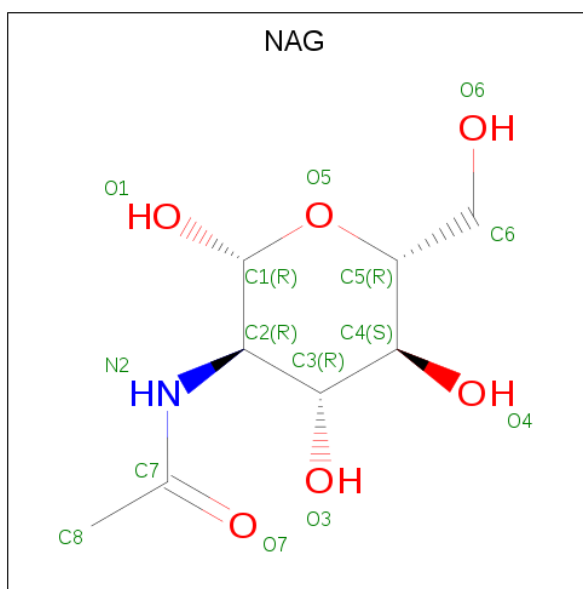
- Molecule 1 is a protein called Dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	728	Total 5963	C 3827	N 982	O 1128	S 26	0	0	0
1	B	728	Total 5963	C 3827	N 982	O 1128	S 26	0	0	0

- Molecule 2 is a protein called 3-mer peptide.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	3	Total 24	C 17	N 3	O 4	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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

- Molecule 4 is water.

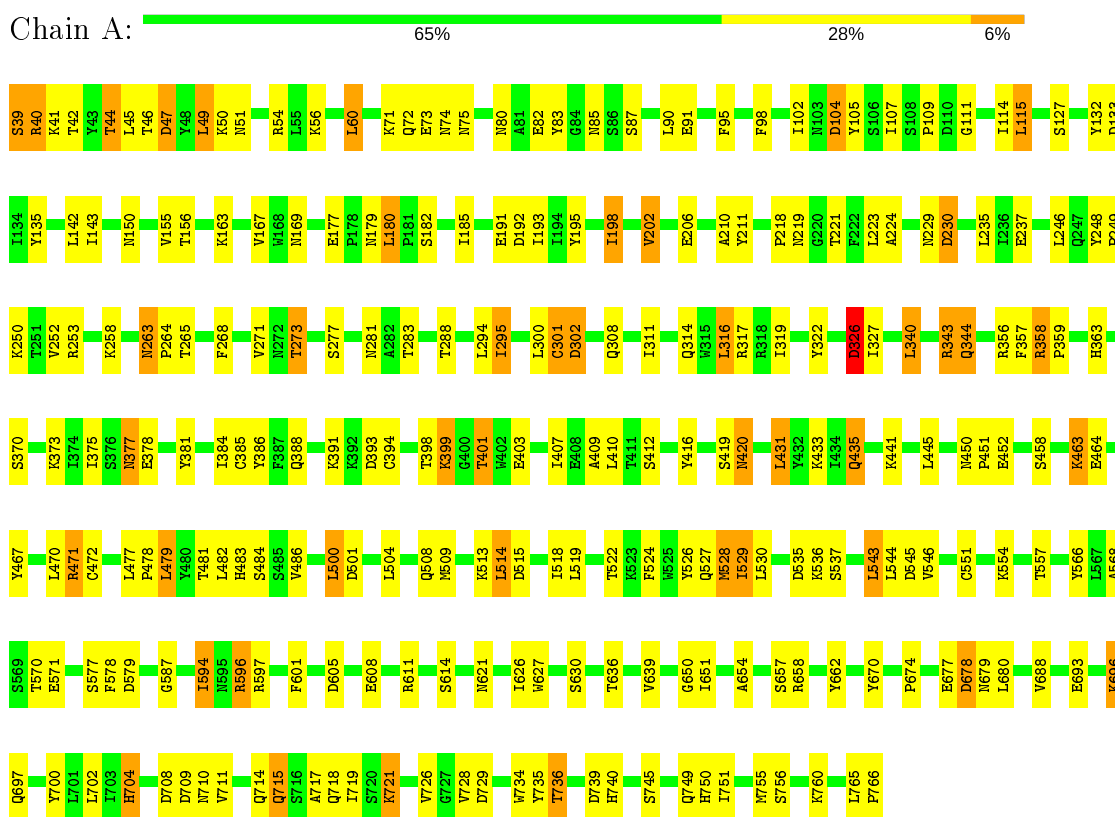
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	122	Total	O	0	0
			122	122		
4	B	150	Total	O	0	0
			150	150		
4	D	1	Total	O	0	0
			1	1		

### 3 Residue-property plots [i](#)

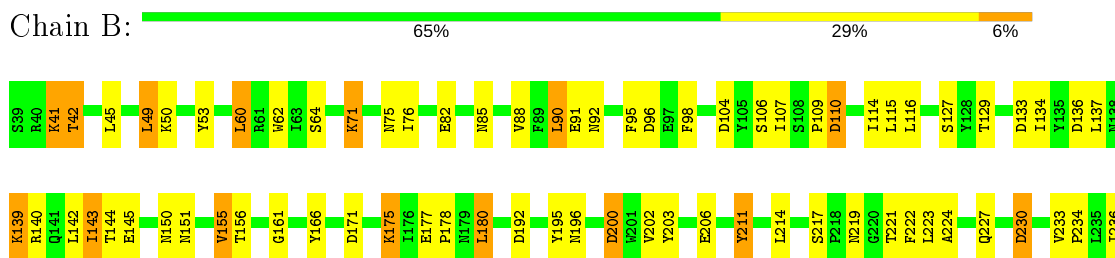
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

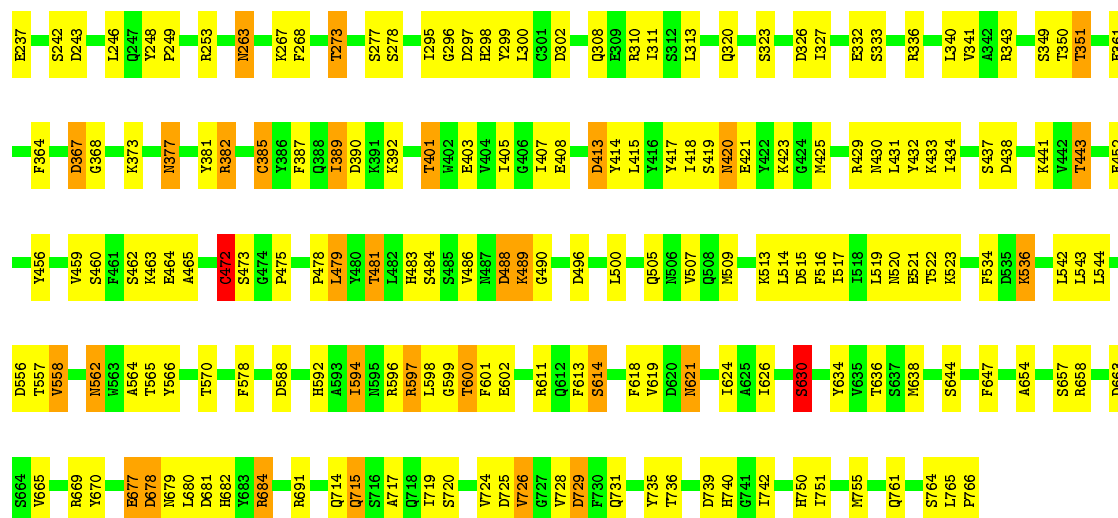
Note EDS was not executed.

- Molecule 1: Dipeptidyl peptidase IV



- Molecule 1: Dipeptidyl peptidase IV





- Molecule 2: 3-mer peptide



## 4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.14Å 67.07Å 419.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (12.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.1	Depositor
R, $R_{free}$	0.225 , 0.282	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	12335	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	32.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:  
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	0.67	0/6135	0.88	16/8344 (0.2%)
1	B	0.71	0/6135	0.90	21/8344 (0.3%)
2	D	1.89	2/24 (8.3%)	1.98	1/31 (3.2%)
All	All	0.69	2/12294 (0.0%)	0.90	38/16719 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
2	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	2	PRO	C-O	6.24	1.35	1.23
2	D	2	PRO	C-N	5.85	1.47	1.34

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	630	SER	CA-CB-OG	8.62	134.49	111.20
2	D	2	PRO	CA-C-N	-8.41	98.70	117.20
1	B	60	LEU	CA-CB-CG	7.66	132.93	115.30
1	B	171	ASP	CB-CG-OD2	7.47	125.03	118.30
1	B	729	ASP	CB-CG-OD2	7.23	124.81	118.30
1	A	678	ASP	CB-CG-OD2	7.08	124.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	ASP	CB-CG-OD2	7.07	124.66	118.30
1	A	47	ASP	CB-CG-OD2	6.37	124.03	118.30
1	B	230	ASP	CB-CG-OD2	6.18	123.87	118.30
1	B	413	ASP	CB-CG-OD2	6.11	123.79	118.30
1	A	709	ASP	CB-CG-OD2	6.09	123.78	118.30
1	B	390	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	488	ASP	CB-CG-OD2	5.98	123.68	118.30
1	A	479	LEU	CA-CB-CG	5.96	129.00	115.30
1	B	678	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	133	ASP	CB-CG-OD2	5.74	123.47	118.30
1	B	472	CYS	CA-CB-SG	5.70	124.27	114.00
1	B	104	ASP	CB-CG-OD2	5.63	123.37	118.30
1	A	545	ASP	CB-CG-OD2	5.60	123.34	118.30
1	B	663	ASP	CB-CG-OD2	5.58	123.32	118.30
1	B	96	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	579	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	297	ASP	CB-CG-OD2	5.36	123.13	118.30
1	B	681	ASP	CB-CG-OD2	5.35	123.12	118.30
1	B	302	ASP	CB-CG-OD2	5.34	123.10	118.30
1	A	326	ASP	CB-CG-OD2	5.28	123.05	118.30
1	A	230	ASP	CB-CG-OD2	5.25	123.02	118.30
1	B	367	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	543	LEU	CA-CB-CG	5.18	127.22	115.30
1	B	588	ASP	CB-CG-OD2	5.14	122.93	118.30
1	B	630	SER	CB-CA-C	5.14	119.87	110.10
1	A	535	ASP	CB-CG-OD2	5.12	122.91	118.30
1	A	302	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	192	ASP	CB-CG-OD2	5.11	122.90	118.30
1	A	104	ASP	CB-CG-OD2	5.11	122.89	118.30
1	A	605	ASP	CB-CG-OD2	5.10	122.89	118.30
1	B	200	ASP	CB-CG-OD2	5.05	122.84	118.30
1	A	501	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	110	ASP	Peptide
2	D	2	PRO	Mainchain

## 5.2 Too-close contacts [i](#)

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	5963	0	5683	157	0
1	B	5963	0	5683	164	2
2	D	24	0	31	3	0
3	A	56	0	52	11	0
3	B	56	0	52	8	0
4	A	122	0	0	15	0
4	B	150	0	0	6	3
4	D	1	0	0	0	0
All	All	12335	0	11501	314	3

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 13.

All (314) 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:370:SER:HA	4:A:892:HOH:O	1.24	1.37
1:A:229:ASN:HD21	3:A:796:NAG:C1	1.43	1.32
1:B:92:ASN:HD21	3:B:797:NAG:C1	1.44	1.26
1:A:82:GLU:HG3	4:A:899:HOH:O	1.35	1.25
1:B:85:ASN:HD21	3:B:794:NAG:C1	1.52	1.22
1:A:150:ASN:HD21	3:A:793:NAG:C1	1.66	1.09
1:B:150:ASN:HD21	3:B:1793:NAG:C1	1.77	0.97
1:A:229:ASN:ND2	3:A:796:NAG:C1	2.28	0.96
1:B:600:THR:CG2	1:B:601:PHE:H	1.79	0.95
1:B:85:ASN:ND2	3:B:794:NAG:C1	2.30	0.94
1:A:221:THR:O	1:A:273:THR:HB	1.68	0.93
1:B:42:THR:CG2	1:B:570:THR:OG1	2.24	0.85
1:B:403:GLU:H	1:B:420:ASN:HD21	1.22	0.85
1:A:44:THR:HG22	1:A:47:ASP:H	1.41	0.85
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.06	0.85
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.11	0.82
1:B:658:ARG:HH22	1:B:684:ARG:HH21	1.27	0.82
1:B:600:THR:CG2	1:B:601:PHE:N	2.42	0.81
1:B:351:THR:HG22	1:B:592:HIS:ND1	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:GLU:C	4:A:899:HOH:O	2.18	0.80
1:A:403:GLU:H	1:A:420:ASN:HD21	1.28	0.80
1:B:373:LYS:NZ	4:B:1863:HOH:O	2.14	0.80
1:A:249:PRO:HD3	1:B:714:GLN:NE2	1.98	0.79
1:B:600:THR:HG22	1:B:601:PHE:H	1.48	0.79
1:B:42:THR:HG21	1:B:570:THR:OG1	1.85	0.77
1:B:600:THR:HG23	1:B:601:PHE:N	2.00	0.76
1:A:163:LYS:HZ3	1:A:273:THR:HG22	1.50	0.75
1:A:401:THR:HG22	1:A:401:THR:O	1.87	0.75
1:B:600:THR:HG23	1:B:601:PHE:H	1.53	0.74
2:D:1:ILE:HG22	2:D:3:ILE:HG22	1.68	0.74
1:A:745:SER:O	1:A:749:GLN:HG3	1.88	0.73
1:B:598:LEU:O	1:B:682:HIS:HE1	1.71	0.72
1:A:281:ASN:HD21	3:A:795:NAG:C1	2.03	0.72
1:A:83:TYR:CG	4:A:899:HOH:O	2.40	0.72
1:A:150:ASN:ND2	3:A:793:NAG:C1	2.49	0.71
1:A:450:ASN:HB2	4:A:819:HOH:O	1.91	0.70
1:B:45:LEU:HG	1:B:49:LEU:HD22	1.72	0.70
1:B:196:ASN:OD1	1:B:227:GLN:HG3	1.92	0.70
1:A:253:ARG:HD2	4:A:876:HOH:O	1.92	0.70
1:B:45:LEU:HG	1:B:49:LEU:CD2	2.23	0.69
1:B:657:SER:H	1:B:715:GLN:NE2	1.91	0.69
1:B:320:GLN:OE1	1:B:669:ARG:HD3	1.92	0.68
1:A:386:TYR:O	1:A:394:CYS:HB2	1.93	0.68
1:B:377:ASN:ND2	1:B:381:TYR:H	1.91	0.68
1:A:594:ILE:HD11	1:A:601:PHE:HB2	1.75	0.67
1:A:693:GLU:O	1:A:696:LYS:CG	2.42	0.67
1:A:177:GLU:HG3	1:A:180:LEU:HD22	1.75	0.67
1:B:237:GLU:OE2	1:B:253:ARG:HD3	1.94	0.67
1:A:431:LEU:HD13	1:A:445:LEU:HD12	1.76	0.67
1:A:107:ILE:HG12	1:A:114:ILE:HD12	1.75	0.67
1:A:80:ASN:HB3	1:A:85:ASN:OD1	1.95	0.66
1:A:594:ILE:HD13	1:A:601:PHE:HB2	1.77	0.66
1:A:83:TYR:CD1	4:A:899:HOH:O	2.48	0.66
1:B:657:SER:H	1:B:715:GLN:HE21	1.43	0.66
1:B:401:THR:O	1:B:401:THR:CG2	2.43	0.65
1:A:674:PRO:O	1:A:680:LEU:HD13	1.96	0.65
1:A:357:PHE:O	1:A:358:ARG:HB3	1.96	0.65
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.80	0.65
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.79	0.64
1:A:693:GLU:O	1:A:696:LYS:HG2	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:377:ASN:ND2	1:A:381:TYR:H	1.97	0.63
1:B:517:ILE:HD12	1:B:519:LEU:HD11	1.81	0.63
1:B:351:THR:CG2	1:B:592:HIS:ND1	2.62	0.62
1:A:167:VAL:HG11	1:A:198:ILE:HG12	1.81	0.62
1:A:163:LYS:NZ	1:A:273:THR:HG22	2.14	0.62
1:A:546:VAL:HG21	1:A:626:ILE:HD11	1.81	0.62
1:B:464:GLU:HA	4:B:1921:HOH:O	1.99	0.62
1:B:405:ILE:HD13	1:B:429:ARG:HD2	1.79	0.62
1:B:726:VAL:HG13	1:B:728:VAL:HG23	1.81	0.62
1:B:109:PRO:HD2	1:B:161:GLY:O	2.00	0.61
1:A:230:ASP:OD1	1:A:264:PRO:HB3	1.99	0.61
1:A:403:GLU:H	1:A:420:ASN:ND2	1.98	0.61
1:B:735:TYR:OH	1:B:750:HIS:HD2	1.83	0.61
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.35	0.61
1:A:258:LYS:HG3	1:B:248:TYR:CZ	2.35	0.61
1:B:401:THR:O	1:B:401:THR:HG22	2.01	0.60
1:A:191:GLU:HG2	1:A:192:ASP:OD2	2.00	0.60
1:A:384:ILE:HD12	1:A:398:THR:HG21	1.83	0.60
1:A:401:THR:CG2	1:A:401:THR:O	2.48	0.60
1:B:405:ILE:HD13	1:B:429:ARG:CD	2.32	0.60
1:A:42:THR:HG23	1:A:570:THR:OG1	2.01	0.60
1:B:134:ILE:HB	1:B:143:ILE:HG12	1.82	0.60
1:B:332:GLU:HG2	1:B:333:SER:N	2.16	0.60
1:A:127:SER:HB3	1:A:211:TYR:CD1	2.37	0.59
1:B:624:ILE:HG22	1:B:647:PHE:CD2	2.38	0.59
1:A:403:GLU:OE2	1:A:587:GLY:HA2	2.01	0.59
1:A:734:TRP:CD1	1:A:736:THR:HG22	2.38	0.59
1:A:281:ASN:ND2	3:A:795:NAG:O5	2.34	0.59
1:B:421:GLU:OE1	4:B:1803:HOH:O	2.16	0.58
1:B:556:ASP:OD1	1:B:558:VAL:HG13	2.03	0.58
1:A:373:LYS:HD3	1:A:375:ILE:HD11	1.84	0.58
1:A:163:LYS:HZ3	1:A:273:THR:CG2	2.17	0.58
1:A:728:VAL:O	1:B:750:HIS:HE1	1.87	0.58
1:A:756:SER:O	1:A:760:LYS:HG3	2.04	0.57
1:B:433:LYS:HB3	1:B:443:THR:HG22	1.85	0.57
1:A:150:ASN:ND2	3:A:793:NAG:HN2	2.02	0.57
1:A:651:ILE:HD13	1:A:755:MET:HG2	1.87	0.57
1:A:734:TRP:NE1	1:A:736:THR:HG22	2.19	0.57
1:B:720:SER:O	1:B:724:VAL:HG23	2.04	0.57
1:A:327:ILE:HB	1:A:343:ARG:HG3	1.86	0.57
1:B:481:THR:HB	1:B:483:HIS:CE1	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:735:TYR:CE1	1:A:750:HIS:HD2	2.23	0.57
1:A:388:GLN:HA	4:A:892:HOH:O	2.03	0.57
1:A:693:GLU:O	1:A:696:LYS:HG3	2.04	0.57
1:A:657:SER:H	1:A:715:GLN:NE2	2.01	0.56
1:A:734:TRP:HE1	1:A:736:THR:HG22	1.70	0.56
1:A:202:VAL:HG22	4:A:863:HOH:O	2.04	0.56
1:A:83:TYR:N	4:A:899:HOH:O	2.37	0.56
1:B:150:ASN:ND2	3:B:1793:NAG:C1	2.59	0.55
1:B:658:ARG:HH22	1:B:684:ARG:NH2	2.00	0.55
1:B:382:ARG:NH2	4:B:1806:HOH:O	2.40	0.55
1:B:751:ILE:O	1:B:755:MET:HG3	2.06	0.54
1:A:377:ASN:C	1:A:377:ASN:HD22	2.11	0.54
1:B:155:VAL:HG13	1:B:166:TYR:HB3	1.90	0.54
1:B:479:LEU:HD23	1:B:496:ASP:HA	1.88	0.54
1:A:688:VAL:HG11	1:A:719:ILE:HD13	1.90	0.54
1:A:237:GLU:HA	1:A:252:VAL:O	2.08	0.53
1:A:458:SER:OG	1:A:471:ARG:HG2	2.08	0.53
1:B:742:ILE:HG22	1:B:742:ILE:O	2.08	0.53
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.89	0.53
1:A:739:ASP:HB2	4:A:895:HOH:O	2.07	0.53
1:A:326:ASP:OD1	1:A:344:GLN:HG3	2.08	0.53
1:B:127:SER:HB3	1:B:211:TYR:CG	2.45	0.52
1:A:163:LYS:NZ	1:A:273:THR:CG2	2.73	0.52
1:A:50:LYS:O	1:A:51:ASN:HB2	2.10	0.52
1:B:341:VAL:C	1:B:343:ARG:H	2.13	0.52
1:B:150:ASN:HD21	3:B:1793:NAG:C2	2.22	0.52
1:A:717:ALA:HB1	1:B:736:THR:HG23	1.92	0.52
1:B:296:GLY:O	1:B:298:HIS:HD2	1.93	0.52
1:B:377:ASN:HD22	1:B:377:ASN:C	2.12	0.52
1:B:417:TYR:CE1	1:B:434:ILE:HD11	2.45	0.52
1:B:611:ARG:O	1:B:614:SER:HB2	2.10	0.52
1:B:739:ASP:HB2	4:B:1939:HOH:O	2.08	0.51
1:B:613:PHE:O	1:B:619:VAL:CG1	2.58	0.51
1:A:356:ARG:HD3	1:A:551:CYS:SG	2.50	0.51
1:A:718:GLN:OE1	1:A:721:LYS:NZ	2.43	0.51
1:B:206:GLU:OE1	1:B:206:GLU:HA	2.10	0.51
1:A:529:ILE:HG22	1:A:568:ALA:HB2	1.91	0.51
1:A:104:ASP:OD1	1:A:105:TYR:N	2.44	0.51
1:A:301:CYS:SG	1:A:316:LEU:HB2	2.50	0.50
1:B:177:GLU:HB2	1:B:180:LEU:CD2	2.41	0.50
1:B:596:ARG:NH2	1:B:678:ASP:OD1	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:ILE:HD12	1:A:179:ASN:HB3	1.93	0.50
1:B:299:TYR:CZ	1:B:665:VAL:HG22	2.46	0.50
1:B:598:LEU:O	1:B:682:HIS:CE1	2.60	0.50
1:A:500:LEU:HD22	1:A:504:LEU:HG	1.94	0.50
1:B:438:ASP:HB3	1:B:441:LYS:HD2	1.93	0.50
1:A:626:ILE:HG23	1:A:636:THR:HG23	1.94	0.50
1:B:418:ILE:HA	1:B:430:ASN:O	2.12	0.49
1:A:44:THR:HG22	1:A:47:ASP:N	2.18	0.49
1:A:708:ASP:CG	1:A:711:VAL:O	2.51	0.49
1:B:219:ASN:HB3	1:B:221:THR:H	1.76	0.49
1:A:39:SER:N	1:A:508:GLN:HG3	2.27	0.49
1:A:409:ALA:HB3	1:A:416:TYR:HB2	1.94	0.49
1:B:517:ILE:CD1	1:B:519:LEU:HD11	2.42	0.49
1:A:82:GLU:HB2	1:A:467:TYR:OH	2.11	0.49
1:B:594:ILE:CD1	1:B:602:GLU:HB3	2.43	0.49
1:A:185:ILE:HG23	1:A:271:VAL:HG21	1.95	0.48
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.78	0.48
1:B:613:PHE:O	1:B:619:VAL:HG13	2.13	0.48
1:A:115:LEU:HD22	1:A:132:TYR:HD1	1.78	0.48
1:A:736:THR:HG21	1:B:717:ALA:O	2.14	0.48
1:B:175:LYS:NZ	1:B:178:PRO:O	2.47	0.48
1:A:219:ASN:HB3	1:A:221:THR:OG1	2.14	0.48
1:A:45:LEU:HG	1:A:49:LEU:HD22	1.96	0.48
1:A:358:ARG:HD3	4:A:816:HOH:O	2.14	0.48
1:B:517:ILE:HD12	1:B:519:LEU:CD1	2.43	0.48
1:B:133:ASP:HB3	1:B:142:LEU:HD22	1.96	0.47
1:B:594:ILE:HD11	1:B:602:GLU:OE1	2.14	0.47
1:A:571:GLU:HA	1:A:571:GLU:OE1	2.15	0.47
1:A:224:ALA:HB1	1:A:268:PHE:CZ	2.49	0.47
1:A:696:LYS:HE3	1:A:697:GLN:HE21	1.79	0.47
1:A:72:GLN:O	1:A:73:GLU:HB2	2.13	0.47
1:A:281:ASN:ND2	3:A:795:NAG:C1	2.76	0.47
1:A:317:ARG:HD2	1:A:322:TYR:HB3	1.96	0.47
1:A:662:TYR:HE1	1:A:710:ASN:OD1	1.97	0.47
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.14	0.47
1:B:562:ASN:HD21	1:B:564:ALA:HB3	1.79	0.47
1:B:657:SER:HB3	1:B:719:ILE:HD11	1.96	0.47
1:B:127:SER:HB3	1:B:211:TYR:CD1	2.50	0.47
1:B:431:LEU:HD13	1:B:459:VAL:HG11	1.97	0.47
1:B:517:ILE:HD11	1:B:578:PHE:CE1	2.49	0.47
1:A:435:GLN:HE21	1:A:441:LYS:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:ASN:HD22	1:B:562:ASN:C	2.18	0.47
1:B:71:LYS:HG3	4:B:1809:HOH:O	2.15	0.47
1:B:62:TRP:CE3	1:B:462:SER:HB3	2.50	0.47
1:B:41:LYS:CE	1:B:53:TYR:OH	2.63	0.47
1:A:518:ILE:HA	1:A:522:THR:O	2.15	0.46
1:A:46:THR:O	1:A:50:LYS:HB2	2.15	0.46
1:A:472:CYS:O	1:A:478:PRO:HA	2.15	0.46
1:B:475:PRO:HA	1:B:557:THR:O	2.16	0.46
1:A:60:LEU:HD13	4:A:880:HOH:O	2.15	0.46
1:B:382:ARG:HG3	1:B:403:GLU:CD	2.36	0.46
1:B:765:LEU:HA	1:B:766:PRO:HD3	1.81	0.46
1:B:630:SER:HA	1:B:654:ALA:O	2.16	0.46
1:A:519:LEU:HB2	1:A:524:PHE:CE2	2.51	0.46
1:A:514:LEU:HD12	1:A:557:THR:HG22	1.98	0.46
1:B:107:ILE:CG1	1:B:114:ILE:HG13	2.46	0.46
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.51	0.46
1:B:221:THR:O	1:B:273:THR:HG22	2.16	0.46
1:B:516:PHE:CE1	1:B:523:LYS:HD3	2.51	0.46
1:B:403:GLU:H	1:B:420:ASN:ND2	2.01	0.45
1:B:42:THR:HG22	1:B:570:THR:OG1	2.12	0.45
1:A:399:LYS:HE2	1:A:399:LYS:HB3	1.80	0.45
1:A:611:ARG:O	1:A:614:SER:HB2	2.16	0.45
1:B:522:THR:HG22	1:B:523:LYS:N	2.31	0.45
1:A:44:THR:O	1:A:47:ASP:HB2	2.16	0.45
1:A:630:SER:HB2	1:A:740:HIS:NE2	2.31	0.45
1:A:73:GLU:HB2	1:A:75:ASN:ND2	2.32	0.45
1:B:630:SER:HB2	1:B:740:HIS:NE2	2.32	0.45
1:A:219:ASN:N	1:A:308:GLN:OE1	2.50	0.45
1:B:90:LEU:HD11	1:B:95:PHE:HE2	1.82	0.45
1:A:529:ILE:HG22	1:A:568:ALA:CB	2.47	0.45
1:A:150:ASN:HD21	3:A:793:NAG:C2	2.25	0.45
1:A:295:ILE:H	1:A:295:ILE:HG13	1.61	0.45
1:B:413:ASP:HB2	1:B:414:TYR:CD2	2.52	0.45
1:B:614:SER:HA	1:B:619:VAL:HG22	1.99	0.45
1:B:206:GLU:OE2	2:D:1:ILE:N	2.50	0.44
1:B:268:PHE:CE2	1:B:313:LEU:HD21	2.52	0.44
1:B:219:ASN:N	1:B:308:GLN:OE1	2.49	0.44
1:B:599:GLY:HA3	1:B:634:TYR:OH	2.18	0.44
1:B:42:THR:HG21	1:B:570:THR:HA	1.99	0.44
1:B:92:ASN:HD22	3:B:797:NAG:C1	2.14	0.44
1:A:477:LEU:HD22	1:A:500:LEU:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:LEU:HD22	1:A:509:MET:SD	2.58	0.44
1:A:95:PHE:HB3	1:A:98:PHE:HB2	1.99	0.44
1:B:726:VAL:CG1	1:B:728:VAL:HG23	2.47	0.44
1:A:750:HIS:HE1	1:B:728:VAL:O	2.01	0.44
1:B:594:ILE:HD11	1:B:602:GLU:H	1.83	0.44
1:A:463:LYS:O	1:A:464:GLU:HB2	2.18	0.44
1:B:95:PHE:CZ	1:B:116:LEU:HD11	2.52	0.44
1:A:363:HIS:CE1	1:A:407:ILE:HB	2.53	0.43
1:A:73:GLU:HB3	1:A:74:ASN:H	1.55	0.43
1:B:327:ILE:HD13	1:B:389:ILE:HG12	1.99	0.43
1:B:64:SER:HA	1:B:463:LYS:HD2	1.99	0.43
1:B:242:SER:OG	1:B:243:ASP:N	2.50	0.43
1:B:536:LYS:HG2	1:B:536:LYS:H	1.62	0.43
1:B:677:GLU:H	1:B:677:GLU:CD	2.21	0.43
2:D:1:ILE:HG22	2:D:3:ILE:CG2	2.43	0.43
1:A:451:PRO:HB2	4:A:910:HOH:O	2.17	0.43
1:A:44:THR:HB	1:A:47:ASP:OD2	2.19	0.43
1:B:481:THR:CB	1:B:483:HIS:CE1	3.01	0.43
1:A:206:GLU:OE1	1:A:206:GLU:HA	2.18	0.43
1:B:520:ASN:O	1:B:521:GLU:HB2	2.18	0.43
1:A:192:ASP:HA	1:A:195:TYR:OH	2.18	0.43
1:A:714:GLN:NE2	1:B:249:PRO:HD3	2.34	0.43
1:A:554:LYS:HB3	1:A:577:SER:HB3	2.01	0.42
1:A:73:GLU:HB2	1:A:75:ASN:HD22	1.84	0.42
1:B:217:SER:HB2	1:B:222:PHE:HB2	2.00	0.42
1:B:341:VAL:C	1:B:343:ARG:N	2.73	0.42
1:B:263:ASN:HA	1:B:263:ASN:HD22	1.60	0.42
1:B:408:GLU:HG3	1:B:418:ILE:HD12	2.01	0.42
1:B:626:ILE:HG23	1:B:636:THR:HG23	2.01	0.42
1:A:358:ARG:HB2	1:A:359:PRO:HD2	2.01	0.42
1:A:750:HIS:HE1	1:B:729:ASP:HA	1.84	0.42
1:B:136:ASP:CG	1:B:139:LYS:HG3	2.39	0.42
1:B:110:ASP:CG	1:B:161:GLY:H	2.23	0.42
1:B:419:SER:OG	1:B:432:TYR:CE1	2.73	0.42
1:B:596:ARG:HA	1:B:670:TYR:O	2.19	0.42
1:B:596:ARG:N	1:B:670:TYR:O	2.47	0.42
1:B:200:ASP:OD1	1:B:203:TYR:HB2	2.19	0.42
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.54	0.42
1:B:71:LYS:HA	1:B:75:ASN:O	2.19	0.42
1:A:319:ILE:HD12	4:A:860:HOH:O	2.19	0.42
1:B:484:SER:O	1:B:488:ASP:HA	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:TYR:O	1:B:638:MET:HG2	2.18	0.42
1:A:700:TYR:OH	1:A:702:LEU:HD13	2.20	0.42
1:A:626:ILE:O	1:A:650:GLY:HA2	2.19	0.42
1:B:98:PHE:CD1	1:B:142:LEU:HD11	2.54	0.42
1:B:76:ILE:HD12	1:B:90:LEU:HB3	2.01	0.42
1:A:150:ASN:ND2	3:A:793:NAG:N2	2.65	0.42
1:A:384:ILE:HD12	1:A:398:THR:CG2	2.48	0.42
1:A:528:MET:HE3	1:A:530:LEU:HD21	2.01	0.42
1:A:185:ILE:CG2	1:A:271:VAL:HG21	2.49	0.42
1:B:385:CYS:HB3	1:B:387:PHE:CE1	2.55	0.42
1:A:594:ILE:HA	1:A:594:ILE:HD12	1.69	0.42
1:A:596:ARG:N	1:A:670:TYR:O	2.43	0.42
1:B:420:ASN:ND2	1:B:420:ASN:H	2.18	0.41
1:A:105:TYR:HB2	1:A:114:ILE:HD11	2.01	0.41
1:A:42:THR:CG2	1:A:570:THR:OG1	2.66	0.41
1:A:526:TYR:HB3	1:A:578:PHE:HD1	1.85	0.41
1:A:150:ASN:ND2	3:A:793:NAG:C2	2.83	0.41
1:B:134:ILE:HD13	1:B:178:PRO:HB3	2.01	0.41
1:B:621:ASN:HA	1:B:624:ILE:HD12	2.02	0.41
1:B:735:TYR:HE1	1:B:750:HIS:CD2	2.38	0.41
1:B:429:ARG:HG2	1:B:456:TYR:CE2	2.55	0.41
1:B:507:VAL:CG2	1:B:509:MET:SD	3.09	0.41
1:B:107:ILE:HG13	1:B:114:ILE:HG13	2.01	0.41
1:B:562:ASN:ND2	1:B:565:THR:H	2.18	0.41
1:B:597:ARG:O	1:B:600:THR:HB	2.20	0.41
1:B:735:TYR:CE1	1:B:750:HIS:CD2	3.07	0.41
1:B:377:ASN:HD21	1:B:381:TYR:H	1.65	0.41
1:A:127:SER:HB3	1:A:211:TYR:CG	2.55	0.41
1:A:85:ASN:N	1:A:85:ASN:OD1	2.52	0.41
1:B:195:TYR:O	1:B:227:GLN:HA	2.20	0.41
1:B:534:PHE:HZ	1:B:618:PHE:CG	2.39	0.41
1:B:85:ASN:CG	3:B:794:NAG:C1	2.87	0.41
1:A:654:ALA:HA	1:A:704:HIS:CE1	2.55	0.41
1:B:233:VAL:HA	1:B:234:PRO:HD3	1.98	0.41
1:B:544:LEU:HD23	1:B:626:ILE:HD12	2.02	0.41
1:A:114:ILE:HG23	1:A:135:TYR:HB3	2.02	0.41
1:B:310:ARG:NH2	1:B:368:GLY:O	2.54	0.41
1:A:340:LEU:HB3	1:A:343:ARG:HD2	2.02	0.41
1:A:218:PRO:HB2	1:A:308:GLN:HE22	1.85	0.40
1:A:735:TYR:OH	1:A:750:HIS:HD2	2.05	0.40
1:A:765:LEU:HA	1:A:766:PRO:HD3	1.80	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:407:ILE:HG23	1:B:415:LEU:HD21	2.02	0.40
1:B:41:LYS:HE3	1:B:53:TYR:OH	2.21	0.40
1:B:489:LYS:HD3	1:B:490:GLY:O	2.21	0.40
1:A:263:ASN:HA	1:A:263:ASN:HD22	1.66	0.40
1:B:418:ILE:HD11	1:B:459:VAL:HG12	2.04	0.40
1:B:472:CYS:O	1:B:478:PRO:HA	2.21	0.40
1:A:433:LYS:HD2	1:A:445:LEU:HD21	2.03	0.40
1:B:459:VAL:HG22	1:B:460:SER:N	2.36	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:GLU:O	4:B:1934:HOH:O[3_745]	1.84	0.36
1:B:437:SER:CB	4:B:1924:HOH:O[3_755]	1.93	0.27
4:B:1837:HOH:O	4:B:1884:HOH:O[1_455]	2.15	0.05

## 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	726/728 (100%)	666 (92%)	52 (7%)	8 (1%)	14	26
1	B	726/728 (100%)	677 (93%)	44 (6%)	5 (1%)	22	39
2	D	1/3 (33%)	1 (100%)	0	0	100	100
All	All	1453/1459 (100%)	1344 (92%)	96 (7%)	13 (1%)	17	31

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	111	GLY
1	B	486	VAL

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Mol	Chain	Res	Type
1	A	40	ARG
1	B	465	ALA
1	A	210	ALA
1	A	358	ARG
1	A	536	LYS
1	B	423	LYS
1	B	630	SER
1	B	725	ASP
1	A	109	PRO
1	A	486	VAL
1	A	639	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	653/653 (100%)	565 (86%)	88 (14%)	4	7
1	B	653/653 (100%)	564 (86%)	89 (14%)	3	7
2	D	3/3 (100%)	2 (67%)	1 (33%)	0	0
All	All	1309/1309 (100%)	1131 (86%)	178 (14%)	3	7

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	SER
1	A	40	ARG
1	A	41	LYS
1	A	44	THR
1	A	49	LEU
1	A	54	ARG
1	A	56	LYS
1	A	60	LEU
1	A	71	LYS
1	A	87	SER
1	A	90	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	91	GLU
1	A	102	ILE
1	A	115	LEU
1	A	142	LEU
1	A	155	VAL
1	A	156	THR
1	A	169	ASN
1	A	180	LEU
1	A	182	SER
1	A	193	ILE
1	A	198	ILE
1	A	202	VAL
1	A	223	LEU
1	A	235	LEU
1	A	246	LEU
1	A	250	LYS
1	A	263	ASN
1	A	273	THR
1	A	277	SER
1	A	283	THR
1	A	288	THR
1	A	294	LEU
1	A	295	ILE
1	A	300	LEU
1	A	301	CYS
1	A	311	ILE
1	A	316	LEU
1	A	326	ASP
1	A	340	LEU
1	A	343	ARG
1	A	344	GLN
1	A	377	ASN
1	A	378	GLU
1	A	385	CYS
1	A	391	LYS
1	A	393	ASP
1	A	399	LYS
1	A	401	THR
1	A	410	LEU
1	A	412	SER
1	A	419	SER
1	A	420	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	431	LEU
1	A	435	GLN
1	A	452	GLU
1	A	463	LYS
1	A	471	ARG
1	A	479	LEU
1	A	482	LEU
1	A	484	SER
1	A	500	LEU
1	A	513	LYS
1	A	514	LEU
1	A	515	ASP
1	A	527	GLN
1	A	528	MET
1	A	529	ILE
1	A	537	SER
1	A	543	LEU
1	A	544	LEU
1	A	566	TYR
1	A	594	ILE
1	A	596	ARG
1	A	597	ARG
1	A	608	GLU
1	A	621	ASN
1	A	627	TRP
1	A	658	ARG
1	A	677	GLU
1	A	679	ASN
1	A	696	LYS
1	A	704	HIS
1	A	715	GLN
1	A	721	LYS
1	A	726	VAL
1	A	736	THR
1	A	751	ILE
1	B	41	LYS
1	B	42	THR
1	B	49	LEU
1	B	50	LYS
1	B	60	LEU
1	B	71	LYS
1	B	88	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	90	LEU
1	B	91	GLU
1	B	106	SER
1	B	115	LEU
1	B	129	THR
1	B	137	LEU
1	B	139	LYS
1	B	140	ARG
1	B	143	ILE
1	B	144	THR
1	B	145	GLU
1	B	151	ASN
1	B	155	VAL
1	B	156	THR
1	B	175	LYS
1	B	180	LEU
1	B	202	VAL
1	B	211	TYR
1	B	214	LEU
1	B	223	LEU
1	B	230	ASP
1	B	236	ILE
1	B	246	LEU
1	B	263	ASN
1	B	267	LYS
1	B	273	THR
1	B	277	SER
1	B	278	SER
1	B	295	ILE
1	B	300	LEU
1	B	311	ILE
1	B	323	SER
1	B	326	ASP
1	B	336	ARG
1	B	340	LEU
1	B	349	SER
1	B	350	THR
1	B	351	THR
1	B	361	GLU
1	B	367	ASP
1	B	377	ASN
1	B	382	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	385	CYS
1	B	389	ILE
1	B	392	LYS
1	B	401	THR
1	B	420	ASN
1	B	425	MET
1	B	443	THR
1	B	452	GLU
1	B	472	CYS
1	B	473	SER
1	B	479	LEU
1	B	481	THR
1	B	489	LYS
1	B	500	LEU
1	B	505	GLN
1	B	513	LYS
1	B	514	LEU
1	B	515	ASP
1	B	536	LYS
1	B	542	LEU
1	B	543	LEU
1	B	558	VAL
1	B	562	ASN
1	B	566	TYR
1	B	594	ILE
1	B	597	ARG
1	B	600	THR
1	B	614	SER
1	B	621	ASN
1	B	644	SER
1	B	677	GLU
1	B	679	ASN
1	B	680	LEU
1	B	684	ARG
1	B	691	ARG
1	B	715	GLN
1	B	726	VAL
1	B	731	GLN
1	B	761	GLN
1	B	764	SER
2	D	3	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such

sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	119	ASN
1	A	123	GLN
1	A	150	ASN
1	A	229	ASN
1	A	247	GLN
1	A	263	ASN
1	A	281	ASN
1	A	377	ASN
1	A	420	ASN
1	A	430	ASN
1	A	435	GLN
1	A	483	HIS
1	A	508	GLN
1	A	533	HIS
1	A	586	GLN
1	A	621	ASN
1	A	679	ASN
1	A	697	GLN
1	A	715	GLN
1	A	731	GLN
1	A	748	HIS
1	A	750	HIS
1	B	85	ASN
1	B	150	ASN
1	B	162	HIS
1	B	169	ASN
1	B	263	ASN
1	B	298	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	483	HIS
1	B	562	ASN
1	B	586	GLN
1	B	621	ASN
1	B	679	ASN
1	B	715	GLN
1	B	748	HIS
1	B	750	HIS



### 5.3.3 RNA [i](#)

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](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

8 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$
3	NAG	A	795	-	14,14,15	0.54	0	17,19,21	1.02	2 (11%)
3	NAG	B	794	1	14,14,15	0.68	0	17,19,21	1.25	2 (11%)
3	NAG	A	796	-	14,14,15	0.50	0	17,19,21	1.31	3 (17%)
3	NAG	B	796	1	14,14,15	0.56	0	17,19,21	1.55	1 (5%)
3	NAG	B	797	1	14,14,15	0.64	0	17,19,21	0.75	0
3	NAG	B	1793	-	14,14,15	0.56	0	17,19,21	3.07	9 (52%)
3	NAG	A	793	-	14,14,15	0.62	0	17,19,21	1.89	4 (23%)
3	NAG	A	794	1	14,14,15	0.73	0	17,19,21	1.48	5 (29%)

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	795	-	-	3/6/23/26	0/1/1/1
3	NAG	B	794	1	-	0/6/23/26	0/1/1/1
3	NAG	A	796	-	-	2/6/23/26	0/1/1/1
3	NAG	B	796	1	-	2/6/23/26	0/1/1/1
3	NAG	B	797	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1793	-	-	5/6/23/26	0/1/1/1
3	NAG	A	793	-	-	5/6/23/26	0/1/1/1
3	NAG	A	794	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1793	NAG	C2-N2-C7	6.07	131.55	122.90
3	B	1793	NAG	C1-O5-C5	5.61	119.80	112.19
3	B	796	NAG	C1-O5-C5	5.44	119.56	112.19
3	B	1793	NAG	C4-C3-C2	-5.08	103.58	111.02
3	B	1793	NAG	C1-C2-N2	5.01	119.05	110.49
3	A	793	NAG	C3-C4-C5	4.34	117.98	110.24
3	A	793	NAG	O5-C1-C2	-3.93	105.08	111.29
3	A	793	NAG	C2-N2-C7	3.73	128.21	122.90
3	B	1793	NAG	O5-C5-C4	3.05	118.24	110.83
3	B	794	NAG	O5-C1-C2	-2.86	106.77	111.29
3	A	794	NAG	C1-O5-C5	2.81	116.00	112.19
3	B	1793	NAG	C3-C4-C5	2.69	115.05	110.24
3	A	794	NAG	C3-C4-C5	-2.67	105.47	110.24
3	A	796	NAG	O7-C7-N2	2.57	126.68	121.95
3	B	1793	NAG	O5-C1-C2	-2.54	107.28	111.29
3	A	796	NAG	C2-N2-C7	2.50	126.46	122.90
3	A	794	NAG	O5-C1-C2	-2.37	107.55	111.29
3	A	795	NAG	C1-O5-C5	2.34	115.36	112.19
3	B	794	NAG	C6-C5-C4	2.22	118.19	113.00
3	A	796	NAG	O7-C7-C8	-2.20	117.97	122.06
3	B	1793	NAG	O5-C5-C6	2.17	110.60	107.20
3	A	793	NAG	O5-C5-C6	2.15	110.58	107.20
3	B	1793	NAG	C6-C5-C4	-2.14	108.00	113.00
3	A	794	NAG	O4-C4-C5	2.13	114.58	109.30
3	A	795	NAG	O5-C5-C6	2.09	110.48	107.20
3	A	794	NAG	O5-C5-C4	-2.00	105.96	110.83

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	794	NAG	C1

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	1793	NAG	C8-C7-N2-C2
3	B	1793	NAG	O7-C7-N2-C2
3	A	793	NAG	C3-C2-N2-C7
3	A	793	NAG	C8-C7-N2-C2
3	A	793	NAG	O7-C7-N2-C2
3	A	795	NAG	O5-C5-C6-O6
3	A	793	NAG	O5-C5-C6-O6
3	B	797	NAG	C4-C5-C6-O6
3	A	793	NAG	C4-C5-C6-O6
3	A	795	NAG	C4-C5-C6-O6
3	B	1793	NAG	O5-C5-C6-O6
3	A	796	NAG	O5-C5-C6-O6
3	B	797	NAG	O5-C5-C6-O6
3	A	796	NAG	C4-C5-C6-O6
3	B	1793	NAG	C1-C2-N2-C7
3	B	1793	NAG	C4-C5-C6-O6
3	B	796	NAG	C8-C7-N2-C2
3	B	796	NAG	O7-C7-N2-C2
3	A	795	NAG	C8-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	795	NAG	3	0
3	B	794	NAG	3	0
3	A	796	NAG	2	0
3	B	797	NAG	2	0
3	B	1793	NAG	3	0
3	A	793	NAG	6	0

## 5.7 Other polymers [i](#)

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.