



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 13, 2024 – 12:28 PM EDT

PDB ID : 1NU6  
Title : Crystal structure of human Dipeptidyl Peptidase IV (DPP-IV)  
Authors : Hennig, M.; Stihle, M.; Thoma, R.; Ruf, A.  
Deposited on : 2003-01-31  
Resolution : 2.10 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)
Xtriage (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)	:	2.36.2

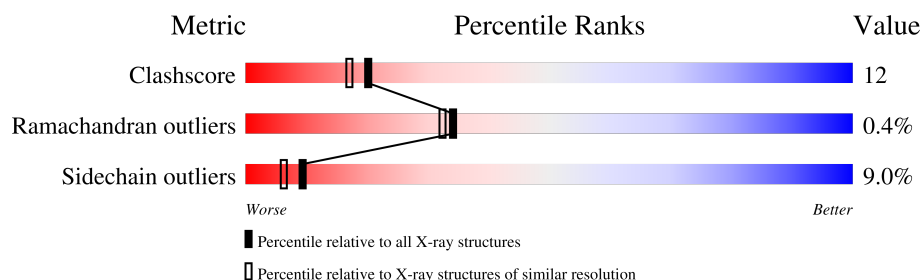
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 of 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	

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	B	797	X	-	-	-

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12366 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
1	A	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			
1	B	728	Total	C	N	O	S	0	0	0
			5963	3827	982	1128	26			

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (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		

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

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	Hg	0	0
			3	3		
3	B	3	Total	Hg	0	0
			3	3		

- Molecule 4 is water.

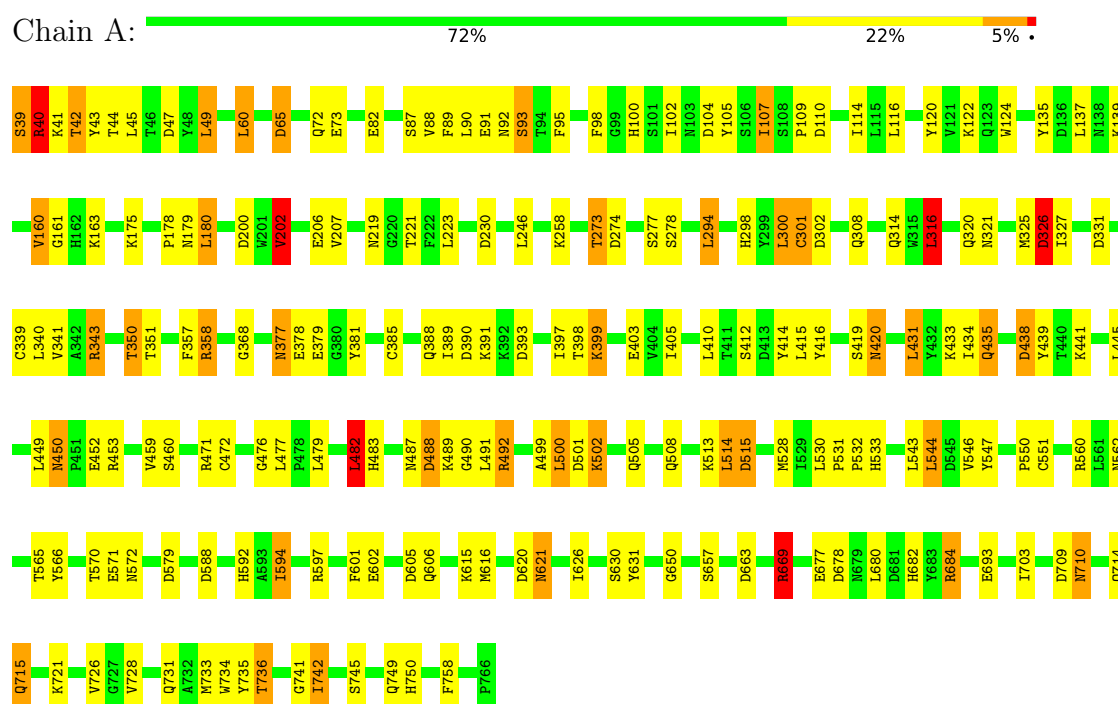
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total	O	0	0
			152	152		
4	B	170	Total	O	0	0
			170	170		

### 3 Residue-property plots

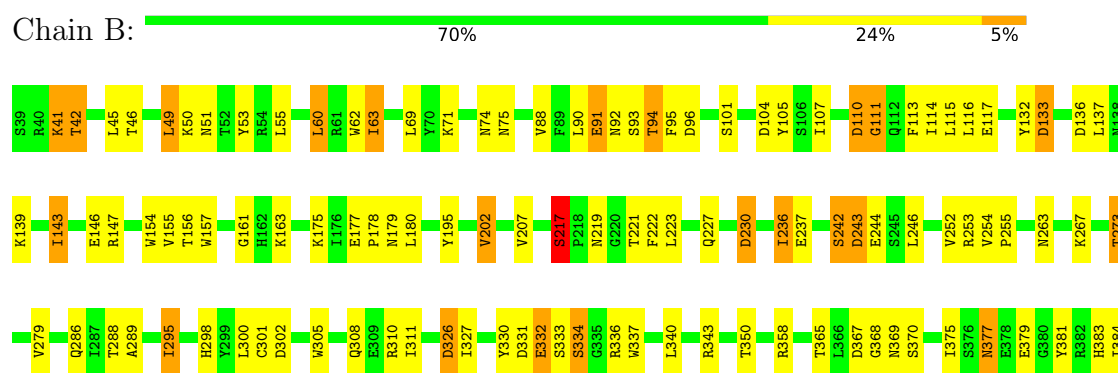
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



C385	Y386	F387	Q388	I389	D390	K391	K392	D393	C394	I397	T398	K399	G400	E403	V404	I405	D413	N420	E421	Y422	R429	Y439	E448	P451	E452	V459	S460	F461	S462	Y468	Q469	L470	R471	C472	P478	L479	H483	S484	S485	V486	N487	D488	L500	L504
V507	K513	L514	I517	N520	E521	T522	K523	Q527	M528	I529	D535	L543	L544	D556	T557	V558	N562	W563	Y566	T570	F578	Y585	I594	L598	G599	T600	F601	E602	S614	K615	M616	G617	F618	V619	D620	N621	K622	R623	W627	K648	S657			
E677	D678	N679	L680	D681	H682	Y683	R684	H704	D709	M710	V711	H712	Q715	S716	A717	K721	V726	G727	V728	D729	M733	D739	H740	G741	I742	H750	F758	I759	K760	Q761	C762	F763	F766											

## 4 Data and refinement statistics

Xtriage (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, $\alpha$ , $\beta$ , $\gamma$	65.50Å 68.24Å 419.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.10	Depositor
% Data completeness (in resolution range)	83.0 (12.00-2.10)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC 5.0	Depositor
R, $R_{free}$	0.215 , 0.266	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12366	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	34.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, HG

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	0.84	2/6135 (0.0%)	1.00	29/8344 (0.3%)
1	B	0.86	4/6135 (0.1%)	1.01	26/8344 (0.3%)
All	All	0.85	6/12270 (0.0%)	1.00	55/16688 (0.3%)

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	A	1	0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	301	CYS	CB-SG	9.21	1.98	1.82
1	B	301	CYS	CB-SG	8.79	1.97	1.82
1	B	558	VAL	CB-CG1	-5.87	1.40	1.52
1	A	301	CYS	CA-CB	5.63	1.66	1.53
1	B	721	LYS	CD-CE	5.18	1.64	1.51
1	B	507	VAL	CB-CG1	-5.08	1.42	1.52

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	110	ASP	CB-CG-OD2	9.34	126.70	118.30
1	B	620	ASP	CB-CG-OD2	7.71	125.23	118.30
1	A	620	ASP	CB-CG-OD2	7.26	124.84	118.30
1	B	111	GLY	N-CA-C	7.26	131.24	113.10
1	A	202	VAL	CB-CA-C	-6.78	98.53	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	243	ASP	CB-CG-OD2	6.75	124.37	118.30
1	B	133	ASP	CB-CG-OD2	6.74	124.37	118.30
1	B	390	ASP	CB-CG-OD2	6.70	124.33	118.30
1	B	678	ASP	CB-CG-OD2	6.53	124.18	118.30
1	A	390	ASP	CB-CG-OD2	6.47	124.12	118.30
1	A	60	LEU	CA-CB-CG	6.43	130.10	115.30
1	A	501	ASP	CB-CG-OD2	6.29	123.96	118.30
1	B	230	ASP	CB-CG-OD2	6.20	123.88	118.30
1	A	579	ASP	CB-CG-OD2	6.14	123.82	118.30
1	B	202	VAL	CB-CA-C	-6.02	99.96	111.40
1	A	316	LEU	CA-CB-CG	5.97	129.04	115.30
1	B	739	ASP	CB-CG-OD1	5.95	123.66	118.30
1	B	709	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	110	ASP	CB-CG-OD2	5.87	123.58	118.30
1	A	492	ARG	CB-CA-C	-5.86	98.68	110.40
1	A	492	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	A	40	ARG	N-CA-C	5.80	126.65	111.00
1	A	482	LEU	CA-CB-CG	5.79	128.62	115.30
1	B	721	LYS	CD-CE-NZ	5.78	125.00	111.70
1	A	302	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	438	ASP	CB-CG-OD2	5.69	123.42	118.30
1	B	681	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	678	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	60	LEU	CB-CG-CD2	5.56	120.45	111.00
1	A	588	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	326	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	544	LEU	CA-CB-CG	5.53	128.02	115.30
1	B	217	SER	CB-CA-C	-5.51	99.63	110.10
1	A	709	ASP	CB-CG-OD2	5.51	123.25	118.30
1	B	60	LEU	CA-CB-CG	5.50	127.94	115.30
1	A	104	ASP	CB-CG-OD2	5.46	123.21	118.30
1	A	274	ASP	CB-CG-OD2	5.45	123.20	118.30
1	A	515	ASP	CB-CG-OD1	5.44	123.20	118.30
1	A	560	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	605	ASP	CB-CG-OD2	5.42	123.17	118.30
1	B	96	ASP	CB-CG-OD2	5.40	123.16	118.30
1	A	47	ASP	CB-CG-OD2	5.37	123.14	118.30
1	B	729	ASP	CB-CG-OD2	5.35	123.11	118.30
1	B	155	VAL	CB-CA-C	-5.34	101.25	111.40
1	A	669	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	104	ASP	CB-CG-OD2	5.23	123.01	118.30
1	B	244	GLU	CB-CA-C	-5.22	99.96	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	115	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	200	ASP	CB-CG-OD2	5.14	122.92	118.30
1	B	331	ASP	CB-CG-OD2	5.13	122.91	118.30
1	B	413	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	326	ASP	CB-CG-OD2	5.08	122.87	118.30
1	B	535	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	60	LEU	CB-CG-CD2	5.04	119.58	111.00
1	A	65	ASP	CB-CG-OD2	5.04	122.83	118.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	40	ARG	CA

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	5963	0	5678	133	1
1	B	5963	0	5679	158	0
2	A	56	0	52	2	0
2	B	56	0	52	3	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
4	A	152	0	0	7	0
4	B	170	0	0	4	0
All	All	12366	0	11461	290	1

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 12.

All (290) 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:160:VAL:HG12	1:A:160:VAL:O	1.59	1.01
1:B:620:ASP:OD1	1:B:620:ASP:O	1.91	0.88
1:B:543:LEU:HD23	1:B:544:LEU:N	1.91	0.86
1:B:267:LYS:HD2	1:B:286:GLN:NE2	1.90	0.85
1:B:403:GLU:H	1:B:420:ASN:HD21	1.24	0.84
1:B:600:THR:CG2	1:B:601:PHE:H	1.90	0.84
1:B:175:LYS:NZ	1:B:178:PRO:O	2.11	0.83
1:B:600:THR:HG22	1:B:601:PHE:H	1.43	0.83
1:B:267:LYS:CE	1:B:286:GLN:HE22	1.91	0.83
1:B:680:LEU:HD22	1:B:684:ARG:HD3	1.59	0.82
1:B:163:LYS:NZ	1:B:273:THR:HG22	1.94	0.81
1:B:163:LYS:HZ3	1:B:273:THR:HG22	1.45	0.81
1:B:46:THR:HG22	1:B:50:LYS:HD3	1.63	0.80
1:A:412:SER:HB2	4:A:1421:HOH:O	1.82	0.79
1:B:620:ASP:OD1	1:B:620:ASP:C	2.21	0.79
1:A:657:SER:H	1:A:715:GLN:NE2	1.80	0.78
1:A:175:LYS:NZ	1:A:178:PRO:O	2.16	0.78
1:B:594:ILE:HD11	1:B:602:GLU:H	1.49	0.77
1:B:543:LEU:HD21	1:B:627:TRP:HD1	1.49	0.77
1:A:487:ASN:O	1:A:489:LYS:N	2.17	0.77
1:B:163:LYS:HZ3	1:B:273:THR:CG2	1.98	0.76
1:B:163:LYS:NZ	1:B:273:THR:CG2	2.49	0.76
1:B:42:THR:HG23	1:B:570:THR:OG1	1.86	0.76
1:A:657:SER:H	1:A:715:GLN:HE21	1.34	0.75
1:B:543:LEU:CD2	1:B:543:LEU:C	2.54	0.75
1:A:160:VAL:O	1:A:160:VAL:CG1	2.31	0.74
1:B:42:THR:CG2	1:B:570:THR:OG1	2.35	0.74
1:B:543:LEU:HD23	1:B:543:LEU:C	2.05	0.74
1:A:377:ASN:C	1:A:377:ASN:HD22	1.91	0.74
1:B:236:ILE:HD12	1:B:712:HIS:CD2	2.24	0.72
1:B:657:SER:H	1:B:715:GLN:NE2	1.87	0.72
1:B:600:THR:CG2	1:B:601:PHE:N	2.50	0.72
1:A:528:MET:CE	1:A:530:LEU:HD21	2.19	0.71
1:B:405:ILE:CD1	1:B:429:ARG:HD3	2.20	0.71
1:A:403:GLU:H	1:A:420:ASN:HD21	1.37	0.71
1:B:267:LYS:NZ	1:B:286:GLN:HE22	1.89	0.71
1:B:520:ASN:O	1:B:521:GLU:HB2	1.92	0.70
1:B:221:THR:O	1:B:273:THR:HB	1.92	0.70
1:B:46:THR:CG2	1:B:50:LYS:HD3	2.22	0.70
1:B:267:LYS:HD2	1:B:286:GLN:HE21	1.57	0.69
1:B:648:LYS:HE3	1:B:762:CYS:O	1.92	0.69
1:A:477:LEU:HD22	1:A:500:LEU:HD12	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:320:GLN:OE1	1:A:669:ARG:HG3	1.94	0.68
1:B:63:ILE:CD1	1:B:69:LEU:CD1	2.72	0.67
1:B:133:ASP:OD1	1:B:147:ARG:NH1	2.28	0.67
1:A:680:LEU:HD11	1:A:684:ARG:NE	2.10	0.67
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.26	0.66
1:B:377:ASN:C	1:B:377:ASN:HD22	2.00	0.66
1:A:44:THR:HG22	1:A:45:LEU:N	2.11	0.65
1:B:598:LEU:O	1:B:682:HIS:HE1	1.79	0.65
1:A:482:LEU:HD13	1:A:491:LEU:HD12	1.79	0.65
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.79	0.63
1:B:267:LYS:CD	1:B:286:GLN:NE2	2.62	0.63
1:B:621:ASN:C	1:B:621:ASN:HD22	2.03	0.62
1:B:726:VAL:HG12	1:B:728:VAL:HG23	1.80	0.62
1:A:602:GLU:OE2	1:A:631:TYR:OH	2.16	0.62
1:A:405:ILE:HD12	1:A:419:SER:HA	1.82	0.61
1:B:63:ILE:CD1	1:B:69:LEU:HD11	2.30	0.61
1:B:95:PHE:CZ	1:B:116:LEU:HD11	2.34	0.61
1:B:177:GLU:HB2	1:B:180:LEU:HD23	1.83	0.60
1:B:657:SER:H	1:B:715:GLN:HE21	1.48	0.60
1:B:680:LEU:HD22	1:B:684:ARG:CD	2.30	0.60
1:A:301:CYS:SG	1:A:316:LEU:HD12	2.42	0.60
1:B:594:ILE:HD11	1:B:602:GLU:N	2.16	0.60
1:B:107:ILE:HG12	1:B:114:ILE:HG13	1.85	0.59
1:B:143:ILE:HG13	1:B:143:ILE:O	2.02	0.59
1:A:221:THR:O	1:A:273:THR:HB	2.03	0.59
1:A:403:GLU:H	1:A:420:ASN:ND2	2.01	0.59
1:A:431:LEU:HD13	1:A:445:LEU:HD12	1.85	0.59
1:B:563:TRP:HH2	1:B:759:ILE:HD12	1.68	0.58
1:B:621:ASN:HD22	1:B:622:LYS:N	2.01	0.58
1:B:405:ILE:HD13	1:B:429:ARG:HD3	1.84	0.58
1:A:514:LEU:C	1:A:514:LEU:HD23	2.24	0.58
1:A:514:LEU:HD23	1:A:515:ASP:N	2.18	0.58
1:A:179:ASN:OD1	1:A:180:LEU:HD22	2.04	0.57
1:B:422:TYR:OH	1:B:448:GLU:OE2	2.16	0.57
1:A:528:MET:HE2	1:A:530:LEU:HD21	1.87	0.57
1:B:117:GLU:HG3	1:B:132:TYR:CE1	2.39	0.57
1:B:600:THR:HG23	1:B:601:PHE:N	2.19	0.57
1:A:300:LEU:C	1:A:300:LEU:CD2	2.73	0.57
1:A:414:TYR:CE1	1:A:435:GLN:HG3	2.39	0.57
1:A:736:THR:HG21	1:B:717:ALA:O	2.04	0.57
1:B:403:GLU:H	1:B:420:ASN:ND2	2.00	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:PRO:HD2	1:A:161:GLY:O	2.05	0.56
1:A:483:HIS:CD2	1:A:490:GLY:HA2	2.40	0.56
1:A:42:THR:CG2	1:A:570:THR:OG1	2.52	0.56
1:A:219:ASN:ND2	4:A:1398:HOH:O	2.37	0.56
1:B:387:PHE:CE2	1:B:394:CYS:HB3	2.40	0.56
1:B:236:ILE:HD12	1:B:712:HIS:NE2	2.20	0.56
1:B:563:TRP:CH2	1:B:759:ILE:HD12	2.41	0.56
1:A:388:GLN:OE1	1:A:391:LYS:HD2	2.07	0.55
1:A:721:LYS:NZ	1:B:242:SER:O	2.31	0.55
1:B:556:ASP:OD1	1:B:558:VAL:HG13	2.07	0.55
1:B:405:ILE:HD13	1:B:429:ARG:CD	2.35	0.55
1:B:484:SER:O	1:B:488:ASP:HA	2.07	0.54
1:B:267:LYS:NZ	1:B:286:GLN:NE2	2.54	0.54
1:A:39:SER:HB3	1:A:505:GLN:O	2.08	0.54
1:B:136:ASP:O	1:B:139:LYS:O	2.25	0.54
1:A:499:ALA:O	1:A:502:LYS:HG3	2.06	0.54
1:A:735:TYR:OH	1:A:750:HIS:HD2	1.90	0.54
1:A:44:THR:HG23	4:A:1346:HOH:O	2.08	0.53
1:A:397:ILE:HG22	1:A:439:TYR:CE2	2.42	0.53
1:B:332:GLU:HG2	1:B:333:SER:N	2.23	0.53
1:B:598:LEU:O	1:B:682:HIS:CE1	2.60	0.53
1:A:42:THR:HG23	1:A:570:THR:OG1	2.08	0.53
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.90	0.53
1:B:514:LEU:HD12	1:B:557:THR:HG22	1.91	0.53
1:A:734:TRP:HE1	1:A:736:THR:HG22	1.73	0.53
1:B:343:ARG:NH2	4:B:2469:HOH:O	2.42	0.53
1:B:63:ILE:HD11	1:B:69:LEU:HD11	1.90	0.53
1:B:334:SER:OG	1:B:336:ARG:HB2	2.09	0.53
1:A:562:ASN:O	1:A:565:THR:HB	2.09	0.53
1:B:758:PHE:O	1:B:761:GLN:HG3	2.09	0.52
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.90	0.52
1:A:320:GLN:OE1	1:A:669:ARG:CG	2.58	0.52
1:A:90:LEU:HD23	1:A:90:LEU:C	2.31	0.52
1:A:550:PRO:O	1:A:551:CYS:HB2	2.10	0.52
1:A:415:LEU:HD23	1:A:415:LEU:C	2.31	0.51
2:B:793:NAG:H3	2:B:793:NAG:H83	1.91	0.51
1:A:98:PHE:CE2	1:A:100:HIS:HB2	2.46	0.51
1:B:156:THR:HG22	1:B:157:TRP:O	2.11	0.51
1:B:377:ASN:ND2	1:B:379:GLU:H	2.09	0.51
1:A:514:LEU:C	1:A:514:LEU:CD2	2.79	0.51
1:A:122:LYS:HE3	1:A:124:TRP:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:326:ASP:OD2	1:A:339:CYS:HB3	2.10	0.50
1:A:43:TYR:CD2	1:A:565:THR:HG22	2.46	0.50
1:B:386:TYR:HB2	1:B:397:ILE:CD1	2.42	0.50
1:A:594:ILE:HD11	1:A:601:PHE:HB2	1.92	0.50
1:A:40:ARG:O	1:A:508:GLN:OE1	2.30	0.50
1:A:546:VAL:HG22	1:A:606:GLN:OE1	2.10	0.50
1:B:616:MET:O	1:B:618:PHE:N	2.45	0.50
1:A:626:ILE:O	1:A:650:GLY:HA2	2.11	0.50
1:A:377:ASN:ND2	1:A:379:GLU:H	2.10	0.50
1:B:563:TRP:HH2	1:B:759:ILE:CD1	2.25	0.50
1:A:741:GLY:O	1:A:742:ILE:C	2.50	0.49
1:B:46:THR:CG2	1:B:50:LYS:CD	2.88	0.49
1:B:110:ASP:CG	1:B:161:GLY:H	2.15	0.49
1:B:163:LYS:HZ2	1:B:273:THR:CG2	2.23	0.49
1:A:680:LEU:HD11	1:A:684:ARG:CZ	2.43	0.48
4:A:1312:HOH:O	1:B:750:HIS:CD2	2.66	0.48
1:B:680:LEU:CD2	1:B:684:ARG:HD3	2.38	0.48
1:B:310:ARG:NH2	1:B:389:ILE:HD13	2.28	0.48
1:A:397:ILE:HD12	1:A:434:ILE:HD13	1.95	0.48
1:A:433:LYS:HD2	1:A:445:LEU:HD21	1.95	0.48
1:B:91:GLU:CD	1:B:94:THR:OG1	2.51	0.48
1:A:459:VAL:HG22	1:A:460:SER:N	2.29	0.48
1:B:383:HIS:HD2	1:B:398:THR:CB	2.26	0.48
1:B:500:LEU:HD22	1:B:504:LEU:HG	1.95	0.48
1:B:726:VAL:HG13	1:B:726:VAL:O	2.14	0.48
1:A:734:TRP:NE1	1:A:736:THR:HG22	2.29	0.48
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.49	0.48
1:A:728:VAL:O	1:B:750:HIS:CE1	2.68	0.47
1:B:55:LEU:HD22	1:B:478:PRO:HG2	1.96	0.47
1:B:367:ASP:OD1	1:B:369:ASN:HB2	2.14	0.47
1:A:202:VAL:HG22	4:A:1396:HOH:O	2.14	0.47
1:A:477:LEU:CD2	1:A:500:LEU:HD12	2.42	0.47
1:B:387:PHE:CD2	1:B:394:CYS:HB3	2.49	0.47
1:B:179:ASN:OD1	1:B:180:LEU:HD22	2.15	0.47
1:A:90:LEU:HD23	1:A:91:GLU:N	2.29	0.47
1:A:340:LEU:HD12	1:A:340:LEU:HA	1.71	0.47
1:B:137:LEU:C	1:B:139:LYS:H	2.16	0.47
1:B:217:SER:OG	1:B:222:PHE:HB2	2.15	0.47
1:A:316:LEU:HD22	1:A:320:GLN:HA	1.97	0.47
1:A:693:GLU:HA	1:A:726:VAL:HG11	1.97	0.47
1:B:62:TRP:CG	1:B:462:SER:HA	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASN:N	1:B:308:GLN:OE1	2.48	0.47
1:A:102:ILE:HD13	1:A:116:LEU:HD22	1.97	0.46
1:A:314:GLN:CG	1:A:325:MET:HG3	2.45	0.46
1:A:397:ILE:HG22	1:A:439:TYR:CD2	2.50	0.46
1:B:377:ASN:C	1:B:377:ASN:ND2	2.66	0.46
1:A:350:THR:HG22	1:A:351:THR:HG23	1.98	0.46
1:B:377:ASN:ND2	1:B:381:TYR:H	2.13	0.46
1:A:44:THR:HG22	1:A:45:LEU:H	1.77	0.46
1:A:615:LYS:O	1:A:616:MET:C	2.54	0.46
1:B:405:ILE:HD12	1:B:429:ARG:HD3	1.96	0.46
2:B:793:NAG:H3	2:B:793:NAG:C8	2.45	0.46
1:B:343:ARG:HG3	1:B:389:ILE:HG23	1.98	0.46
1:B:383:HIS:HE1	1:B:400:GLY:O	1.98	0.46
1:A:621:ASN:C	1:A:621:ASN:HD22	2.19	0.46
1:B:105:TYR:CD1	1:B:105:TYR:C	2.89	0.46
1:A:89:PHE:HE2	1:A:107:ILE:HD13	1.80	0.46
1:B:343:ARG:O	1:B:343:ARG:HG2	2.15	0.46
1:A:92:ASN:OD1	1:A:93:SER:N	2.49	0.46
1:A:368:GLY:O	1:A:389:ILE:HD12	2.16	0.46
1:B:63:ILE:CD1	1:B:69:LEU:HG	2.46	0.46
1:B:113:PHE:CZ	1:B:178:PRO:HG2	2.51	0.46
1:B:267:LYS:CD	1:B:286:GLN:HE22	2.22	0.45
2:B:793:NAG:H82	2:B:793:NAG:C1	2.45	0.45
1:A:137:LEU:O	1:A:139:LYS:O	2.34	0.45
1:A:377:ASN:C	1:A:377:ASN:ND2	2.63	0.45
1:A:44:THR:CG2	1:A:45:LEU:N	2.80	0.45
1:A:98:PHE:CD2	1:A:100:HIS:HB2	2.51	0.45
1:B:529:ILE:HD13	4:B:2356:HOH:O	2.15	0.45
1:A:163:LYS:HZ3	1:A:273:THR:HG22	1.82	0.45
2:A:793:NAG:H83	2:A:793:NAG:H3	1.99	0.45
1:A:300:LEU:HD23	1:A:301:CYS:N	2.31	0.45
1:B:146:GLU:O	1:B:175:LYS:HE3	2.16	0.45
1:B:207:VAL:O	1:B:358:ARG:NH1	2.49	0.45
1:B:517:ILE:HD11	1:B:578:PHE:CE1	2.52	0.45
1:A:65:ASP:N	1:A:65:ASP:OD1	2.49	0.45
1:A:482:LEU:HD12	1:A:492:ARG:NH1	2.32	0.44
1:A:415:LEU:HD23	1:A:416:TYR:N	2.33	0.44
1:A:449:LEU:C	1:A:450:ASN:ND2	2.71	0.44
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.52	0.44
1:B:461:PHE:CD1	1:B:468:TYR:HB3	2.52	0.44
1:A:321:ASN:ND2	4:A:1448:HOH:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:405:ILE:HD13	1:B:429:ARG:NE	2.32	0.44
1:B:41:LYS:HE3	1:B:53:TYR:OH	2.17	0.44
1:B:267:LYS:CE	1:B:286:GLN:NE2	2.69	0.44
1:B:392:LYS:H	1:B:392:LYS:HG3	1.62	0.44
1:B:520:ASN:O	1:B:521:GLU:CB	2.63	0.44
1:A:731:GLN:HE22	1:A:758:PHE:HD2	1.65	0.44
1:B:403:GLU:OE1	1:B:585:TYR:HA	2.17	0.44
1:A:487:ASN:O	1:A:488:ASP:C	2.56	0.44
1:A:90:LEU:C	1:A:90:LEU:CD2	2.86	0.44
1:A:745:SER:O	1:A:749:GLN:HG3	2.18	0.44
1:A:414:TYR:CE1	1:A:433:LYS:HE2	2.53	0.43
1:B:295:ILE:HG21	1:B:295:ILE:HD13	1.73	0.43
1:B:379:GLU:CD	1:B:379:GLU:N	2.71	0.43
1:A:163:LYS:HZ3	1:A:273:THR:CG2	2.32	0.43
1:A:300:LEU:C	1:A:300:LEU:HD23	2.39	0.43
1:A:710:ASN:HD22	1:A:710:ASN:C	2.22	0.43
1:B:63:ILE:HD11	1:B:69:LEU:CD1	2.46	0.43
1:A:90:LEU:HD11	1:A:95:PHE:HE2	1.84	0.43
1:A:163:LYS:NZ	1:A:273:THR:HG22	2.32	0.43
1:A:546:VAL:HG12	1:A:547:TYR:N	2.34	0.43
1:B:365:THR:HG21	1:B:370:SER:OG	2.19	0.42
1:A:416:TYR:CE2	1:A:433:LYS:HG3	2.55	0.42
1:B:298:HIS:HE1	4:B:2463:HOH:O	2.03	0.42
1:A:750:HIS:HE1	1:B:728:VAL:O	2.02	0.42
2:A:793:NAG:C1	2:A:793:NAG:H82	2.48	0.42
1:A:258:LYS:NZ	1:A:714:GLN:OE1	2.51	0.42
1:B:105:TYR:HB2	1:B:114:ILE:HD11	2.02	0.42
1:B:522:THR:HG22	1:B:523:LYS:N	2.34	0.42
1:B:49:LEU:HD12	1:B:49:LEU:HA	1.79	0.42
1:A:294:LEU:HD12	1:A:294:LEU:HA	1.77	0.42
1:B:254:VAL:HA	1:B:255:PRO:HD3	1.93	0.42
1:A:327:ILE:HB	1:A:343:ARG:HG3	2.02	0.42
1:A:502:LYS:HG3	1:A:502:LYS:HZ2	1.51	0.42
1:A:45:LEU:HG	1:A:49:LEU:HD22	2.01	0.42
1:B:334:SER:OG	1:B:336:ARG:N	2.53	0.42
1:B:562:ASN:C	1:B:562:ASN:HD22	2.24	0.42
1:A:728:VAL:O	1:B:750:HIS:HE1	2.03	0.41
1:B:513:LYS:O	1:B:527:GLN:HA	2.21	0.41
1:A:435:GLN:NE2	1:A:441:LYS:HD3	2.36	0.41
1:A:597:ARG:HA	1:A:682:HIS:CD2	2.55	0.41
1:A:398:THR:C	1:A:399:LYS:HG2	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:LEU:HG	1:B:49:LEU:HD22	2.02	0.41
1:B:383:HIS:CD2	1:B:399:LYS:N	2.88	0.41
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.38	0.41
1:A:438:ASP:C	1:A:438:ASP:OD1	2.58	0.41
1:B:459:VAL:HG22	1:B:460:SER:N	2.35	0.41
1:B:594:ILE:HD13	1:B:602:GLU:HB3	2.02	0.41
1:A:114:ILE:HG23	1:A:135:TYR:HB3	2.02	0.41
1:A:207:VAL:O	1:A:358:ARG:NH1	2.54	0.41
1:B:113:PHE:CE1	1:B:178:PRO:HG2	2.55	0.41
1:B:154:TRP:NE1	1:B:156:THR:OG1	2.54	0.41
1:B:237:GLU:HA	1:B:252:VAL:O	2.21	0.41
1:A:314:GLN:HG2	1:A:325:MET:HG3	2.02	0.41
1:A:571:GLU:O	1:A:572:ASN:HB2	2.21	0.41
1:B:485:SER:O	1:B:486:VAL:C	2.59	0.41
1:A:357:PHE:CZ	1:A:551:CYS:HB2	2.55	0.41
1:A:377:ASN:ND2	1:A:381:TYR:H	2.19	0.41
1:A:703:ILE:HA	1:A:733:MET:O	2.21	0.41
1:B:327:ILE:HD13	1:B:389:ILE:HG12	2.03	0.41
1:B:383:HIS:CD2	1:B:399:LYS:HA	2.55	0.41
1:B:623:ARG:HB3	1:B:763:PHE:CD1	2.55	0.41
1:B:648:LYS:CE	1:B:762:CYS:O	2.65	0.41
1:B:741:GLY:O	1:B:742:ILE:C	2.59	0.41
1:A:532:PRO:O	1:A:533:HIS:HB2	2.21	0.41
1:A:750:HIS:CE1	1:B:728:VAL:O	2.74	0.41
1:B:75:ASN:OD1	1:B:92:ASN:HB3	2.21	0.41
1:A:298:HIS:HE1	4:A:1326:HOH:O	2.03	0.40
1:B:237:GLU:HG2	1:B:253:ARG:HG2	2.03	0.40
1:B:242:SER:HB2	1:B:243:ASP:H	1.60	0.40
1:A:219:ASN:HB2	1:A:308:GLN:OE1	2.21	0.40
1:A:331:ASP:C	1:A:331:ASP:OD1	2.60	0.40
1:B:305:TRP:CZ3	1:B:311:ILE:HG12	2.55	0.40
1:B:383:HIS:HD2	1:B:398:THR:OG1	2.04	0.40
1:B:397:ILE:HG13	1:B:439:TYR:CD2	2.56	0.40
1:A:72:GLN:O	1:A:73:GLU:HB2	2.21	0.40
1:B:288:THR:HG22	1:B:289:ALA:O	2.21	0.40
1:B:368:GLY:O	1:B:389:ILE:CD1	2.70	0.40
1:B:384:ILE:HG13	1:B:404:VAL:HG21	2.03	0.40
1:A:453:ARG:HG3	1:A:476:GLY:HA3	2.02	0.40
1:A:530:LEU:HA	1:A:531:PRO:HD3	1.89	0.40
1:B:195:TYR:O	1:B:227:GLN:HA	2.21	0.40
1:B:529:ILE:HD11	4:B:2440:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:614:SER:HA	1:B:619:VAL:CG2	2.50	0.40
1:B:375:ILE:HD13	1:B:387:PHE:HZ	1.87	0.40

All (1) 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:A:41:LYS:NZ	1:A:341:VAL:O[1_655]	2.12	0.08

## 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%)	683 (94%)	39 (5%)	4 (1%)	25	21
1	B	726/728 (100%)	683 (94%)	41 (6%)	2 (0%)	41	41
All	All	1452/1456 (100%)	1366 (94%)	80 (6%)	6 (0%)	34	32

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	488	ASP
1	B	74	ASN
1	B	111	GLY
1	A	393	ASP
1	A	160	VAL
1	A	742	ILE

### 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%)	597 (91%)	56 (9%)	10	7
1	B	653/653 (100%)	591 (90%)	62 (10%)	8	5
All	All	1306/1306 (100%)	1188 (91%)	118 (9%)	9	6

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

Mol	Chain	Res	Type
1	A	39	SER
1	A	40	ARG
1	A	42	THR
1	A	49	LEU
1	A	60	LEU
1	A	82	GLU
1	A	87	SER
1	A	88	VAL
1	A	93	SER
1	A	107	ILE
1	A	120	TYR
1	A	180	LEU
1	A	202	VAL
1	A	223	LEU
1	A	230	ASP
1	A	246	LEU
1	A	273	THR
1	A	277	SER
1	A	278	SER
1	A	294	LEU
1	A	300	LEU
1	A	316	LEU
1	A	326	ASP
1	A	343	ARG
1	A	350	THR
1	A	358	ARG
1	A	377	ASN
1	A	378	GLU
1	A	385	CYS
1	A	399	LYS
1	A	410	LEU

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Mol	Chain	Res	Type
1	A	420	ASN
1	A	431	LEU
1	A	435	GLN
1	A	450	ASN
1	A	452	GLU
1	A	471	ARG
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	500	LEU
1	A	502	LYS
1	A	513	LYS
1	A	514	LEU
1	A	543	LEU
1	A	544	LEU
1	A	566	TYR
1	A	594	ILE
1	A	621	ASN
1	A	630	SER
1	A	669	ARG
1	A	677	GLU
1	A	684	ARG
1	A	710	ASN
1	A	715	GLN
1	A	736	THR
1	B	41	LYS
1	B	42	THR
1	B	49	LEU
1	B	51	ASN
1	B	60	LEU
1	B	63	ILE
1	B	71	LYS
1	B	88	VAL
1	B	90	LEU
1	B	91	GLU
1	B	93	SER
1	B	94	THR
1	B	101	SER
1	B	143	ILE
1	B	202	VAL
1	B	217	SER
1	B	223	LEU

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Mol	Chain	Res	Type
1	B	230	ASP
1	B	236	ILE
1	B	242	SER
1	B	246	LEU
1	B	263	ASN
1	B	273	THR
1	B	279	VAL
1	B	295	ILE
1	B	300	LEU
1	B	302	ASP
1	B	326	ASP
1	B	332	GLU
1	B	334	SER
1	B	340	LEU
1	B	350	THR
1	B	377	ASN
1	B	385	CYS
1	B	389	ILE
1	B	392	LYS
1	B	397	ILE
1	B	420	ASN
1	B	451	PRO
1	B	452	GLU
1	B	472	CYS
1	B	479	LEU
1	B	486	VAL
1	B	500	LEU
1	B	507	VAL
1	B	514	LEU
1	B	543	LEU
1	B	558	VAL
1	B	562	ASN
1	B	566	TYR
1	B	594	ILE
1	B	600	THR
1	B	619	VAL
1	B	620	ASP
1	B	621	ASN
1	B	677	GLU
1	B	680	LEU
1	B	684	ARG
1	B	704	HIS

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Mol	Chain	Res	Type
1	B	710	ASN
1	B	715	GLN
1	B	733	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	GLN
1	A	169	ASN
1	A	247	GLN
1	A	263	ASN
1	A	298	HIS
1	A	377	ASN
1	A	420	ASN
1	A	435	GLN
1	A	450	ASN
1	A	483	HIS
1	A	508	GLN
1	A	533	HIS
1	A	586	GLN
1	A	592	HIS
1	A	621	ASN
1	A	679	ASN
1	A	710	ASN
1	A	715	GLN
1	A	731	GLN
1	A	748	HIS
1	A	750	HIS
1	B	66	HIS
1	B	169	ASN
1	B	263	ASN
1	B	286	GLN
1	B	298	HIS
1	B	377	ASN
1	B	383	HIS
1	B	420	ASN
1	B	435	GLN
1	B	483	HIS
1	B	562	ASN
1	B	586	GLN
1	B	621	ASN
1	B	679	ASN

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Mol	Chain	Res	Type
1	B	682	HIS
1	B	710	ASN
1	B	715	GLN
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](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	B	793	1	14,14,15	0.43	0	17,19,21	2.40	6 (35%)
2	NAG	B	796	1	14,14,15	0.98	1 (7%)	17,19,21	1.92	5 (29%)
2	NAG	B	797	1	14,14,15	0.66	0	17,19,21	1.79	5 (29%)
2	NAG	A	795	1	14,14,15	0.57	0	17,19,21	1.15	1 (5%)
2	NAG	A	796	1	14,14,15	0.72	0	17,19,21	1.61	4 (23%)
2	NAG	B	794	1	14,14,15	0.59	0	17,19,21	1.57	4 (23%)
2	NAG	A	794	1	14,14,15	0.71	0	17,19,21	1.51	2 (11%)
2	NAG	A	793	1	14,14,15	0.62	0	17,19,21	1.70	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
2	NAG	B	797	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	B	793	1	-	5/6/23/26	0/1/1/1
2	NAG	B	796	1	-	2/6/23/26	0/1/1/1
2	NAG	A	795	1	-	3/6/23/26	0/1/1/1
2	NAG	A	796	1	-	0/6/23/26	0/1/1/1
2	NAG	B	794	1	-	0/6/23/26	0/1/1/1
2	NAG	A	794	1	-	0/6/23/26	0/1/1/1
2	NAG	A	793	1	-	5/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	796	NAG	O5-C1	-3.05	1.38	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	793	NAG	C1-O5-C5	5.61	119.79	112.19
2	B	796	NAG	O5-C1-C2	-5.21	103.06	111.29
2	B	793	NAG	O5-C1-C2	4.28	118.04	111.29
2	B	797	NAG	C1-O5-C5	4.19	117.87	112.19
2	B	793	NAG	C4-C3-C2	-4.18	104.89	111.02
2	B	797	NAG	C3-C4-C5	-3.65	103.73	110.24
2	A	795	NAG	C4-C3-C2	-3.40	106.04	111.02
2	A	793	NAG	O5-C1-C2	-3.36	105.98	111.29
2	B	794	NAG	C1-O5-C5	3.32	116.70	112.19
2	A	796	NAG	O5-C1-C2	-3.19	106.25	111.29
2	B	793	NAG	O3-C3-C2	3.18	116.05	109.47
2	B	796	NAG	O6-C6-C5	-2.90	101.33	111.29
2	A	793	NAG	C1-O5-C5	2.84	116.04	112.19
2	B	794	NAG	O5-C1-C2	-2.78	106.91	111.29
2	B	794	NAG	O7-C7-N2	2.76	127.03	121.95
2	B	796	NAG	C1-C2-N2	2.61	114.95	110.49
2	B	797	NAG	C2-N2-C7	-2.60	119.20	122.90
2	A	794	NAG	C4-C3-C2	-2.58	107.24	111.02
2	A	796	NAG	C3-C4-C5	-2.57	105.65	110.24
2	B	796	NAG	C6-C5-C4	-2.55	107.02	113.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	796	NAG	O6-C6-C5	-2.44	102.92	111.29
2	A	793	NAG	O3-C3-C2	2.40	114.43	109.47
2	A	796	NAG	C1-C2-N2	2.36	114.52	110.49
2	B	794	NAG	C1-C2-N2	-2.35	106.47	110.49
2	B	793	NAG	C8-C7-N2	2.27	119.94	116.10
2	A	794	NAG	O5-C1-C2	-2.12	107.94	111.29
2	B	797	NAG	C4-C3-C2	-2.11	107.93	111.02
2	B	797	NAG	O4-C4-C5	2.09	114.49	109.30
2	B	793	NAG	O7-C7-C8	-2.04	118.26	122.06
2	B	796	NAG	O5-C5-C4	2.03	115.76	110.83
2	A	793	NAG	C8-C7-N2	2.02	119.52	116.10
2	A	793	NAG	O7-C7-C8	-2.01	118.32	122.06

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	797	NAG	C1

All (17) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	793	NAG	3	0
2	A	793	NAG	2	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

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.