



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:13 PM UTC

PDB ID : 1NU6 / pdb_00001nu6
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

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>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

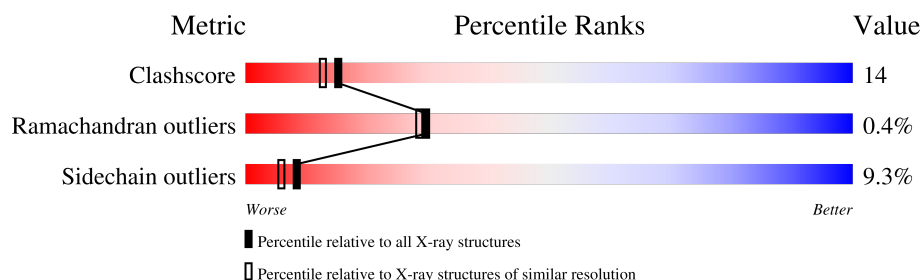
1 Overall quality at a glance

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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 ≥ 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	 71% 22% 6%
1	B	728	 70% 24% 5%

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](#)

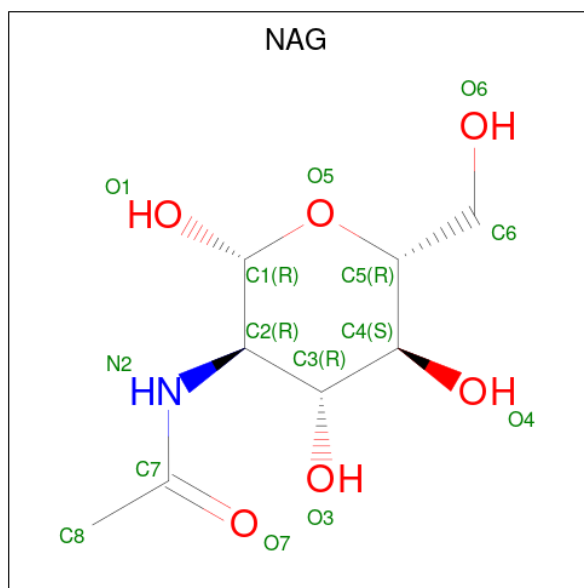
There are 4 unique types of molecules in this entry. The entry contains 12366 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: 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 (CCD ID: 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.

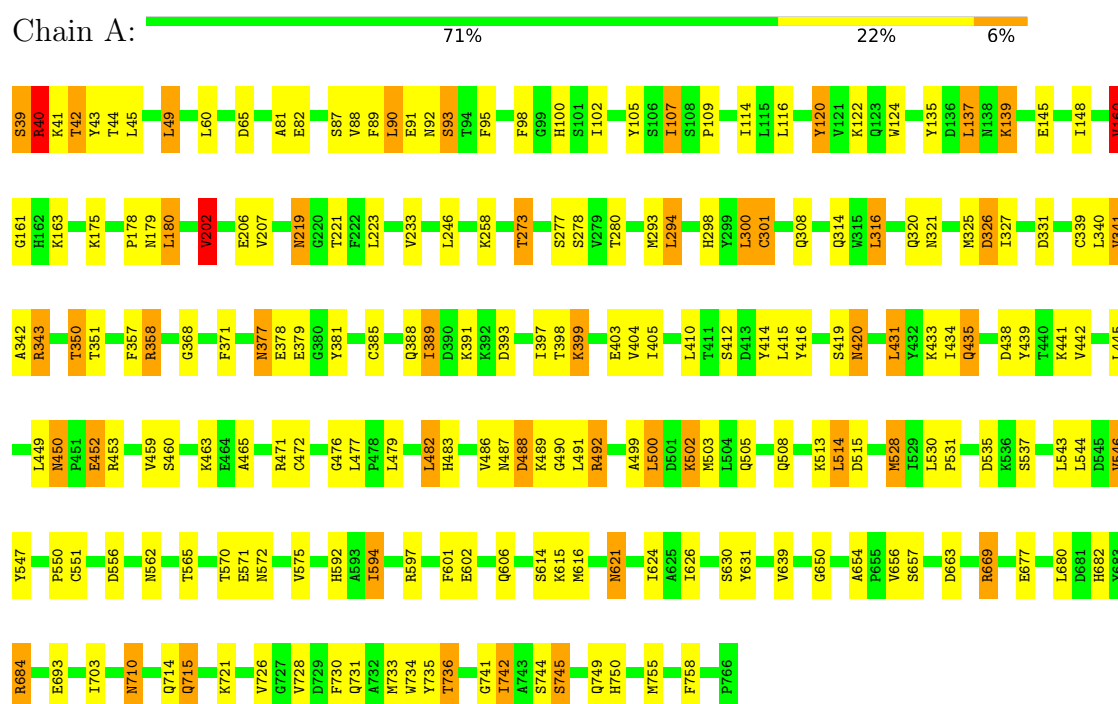
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	152	Total	O	0	0
			152	152		
4	B	170	Total	O	0	0
			170	170		

3 Residue-property plots

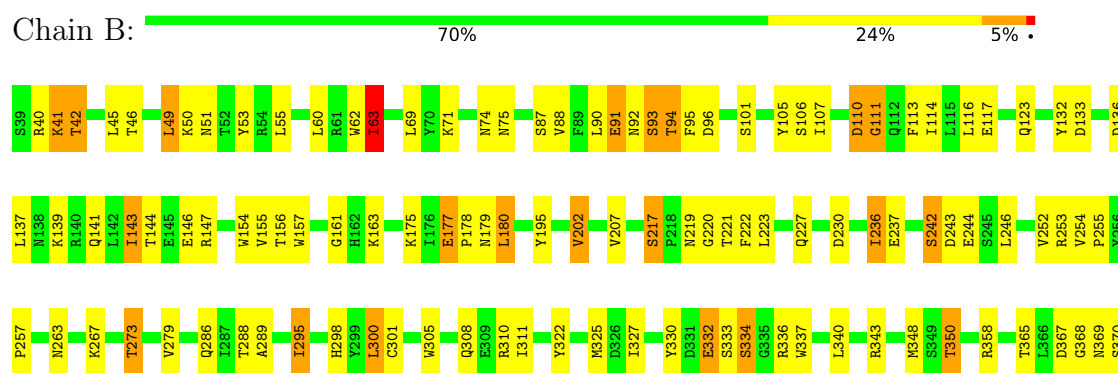
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

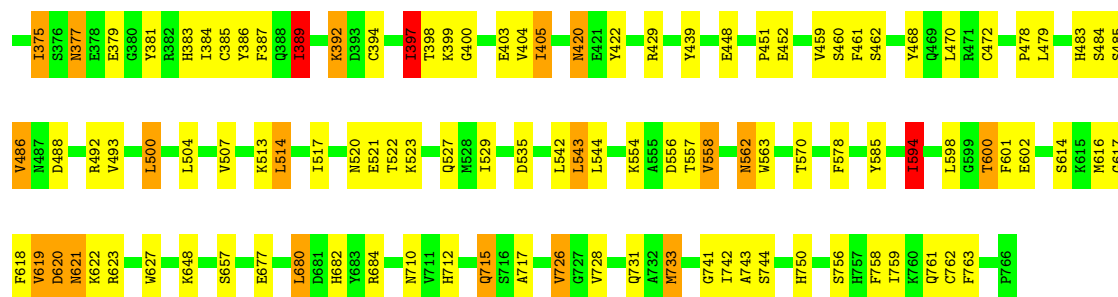
Note EDS was not executed.

• Molecule 1: Dipeptidyl peptidase IV



• Molecule 1: Dipeptidyl peptidase IV





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, α , β , γ	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 ²)	34.0	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: HG, 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	1.04	9/6135 (0.1%)	1.16	21/8344 (0.3%)
1	B	1.04	7/6135 (0.1%)	1.17	21/8344 (0.3%)
All	All	1.04	16/12270 (0.1%)	1.17	42/16688 (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 (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	528	MET	SD-CE	-9.43	1.55	1.79
1	A	301	CYS	CA-CB	8.67	1.66	1.54
1	B	733	MET	SD-CE	-7.55	1.60	1.79
1	B	301	CYS	CA-C	6.55	1.60	1.52
1	A	654	ALA	C-O	-6.39	1.20	1.23
1	B	301	CYS	CA-CB	6.17	1.62	1.54
1	A	404	VAL	CA-CB	-5.95	1.46	1.54
1	A	575	VAL	CA-CB	-5.91	1.46	1.53
1	B	405	ILE	CA-CB	-5.70	1.46	1.54
1	A	755	MET	SD-CE	-5.62	1.65	1.79
1	A	301	CYS	CA-C	5.45	1.59	1.52
1	B	325	MET	SD-CE	-5.39	1.66	1.79
1	B	123	GLN	CA-C	5.20	1.55	1.52
1	A	624	ILE	CA-CB	-5.17	1.48	1.54
1	B	177	GLU	CA-C	-5.09	1.48	1.52
1	A	301	CYS	CB-SG	5.05	1.98	1.81

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	202	VAL	CB-CA-C	-10.30	98.53	112.02
1	B	389	ILE	N-CA-C	9.81	121.80	110.62
1	A	389	ILE	N-CA-C	8.89	123.43	111.17
1	B	202	VAL	CB-CA-C	-8.89	99.96	112.22
1	B	96	ASP	N-CA-C	-8.57	101.53	112.93
1	A	202	VAL	N-CA-CB	7.88	120.65	110.57
1	B	111	GLY	N-CA-C	7.62	131.24	113.18
1	B	397	ILE	N-CA-CB	-7.48	103.43	112.33
1	A	40	ARG	N-CA-C	7.44	126.65	110.80
1	A	656	VAL	N-CA-C	-6.87	99.86	109.21
1	B	257	PRO	CB-CA-C	-6.62	106.31	111.87
1	A	139	LYS	N-CA-C	-6.56	99.69	109.86
1	A	492	ARG	CB-CA-C	-6.42	98.68	110.62
1	A	301	CYS	CB-CA-C	6.30	119.65	109.07
1	B	301	CYS	CB-CA-C	6.28	119.61	109.07
1	B	594	ILE	N-CA-CB	-6.23	104.00	112.28
1	A	137	LEU	N-CA-C	6.20	118.12	111.36
1	A	486	VAL	CB-CA-C	-6.08	103.91	111.70
1	B	451	PRO	N-CA-C	6.03	121.68	113.84
1	B	141	GLN	N-CA-C	5.72	118.79	109.24
1	B	756	SER	N-CA-C	-5.62	105.07	111.14
1	B	217	SER	CB-CA-C	-5.61	99.63	109.61
1	A	148	ILE	N-CA-C	-5.57	102.83	108.96
1	A	293	MET	N-CA-C	-5.57	106.62	113.41
1	B	63	ILE	N-CA-CB	-5.56	105.13	112.36
1	A	486	VAL	N-CA-C	5.55	116.00	110.23
1	B	155	VAL	CB-CA-C	-5.47	101.25	110.71
1	B	244	GLU	CB-CA-C	-5.41	99.96	110.46
1	B	300	LEU	N-CA-C	-5.33	100.48	108.96
1	A	452	GLU	N-CA-C	-5.33	105.92	112.90
1	B	220	GLY	N-CA-C	-5.31	107.78	115.27
1	B	493	VAL	N-CA-C	-5.27	100.48	108.17
1	A	744	SER	N-CA-C	-5.21	103.26	110.35
1	A	639	VAL	CB-CA-C	-5.21	105.20	112.02
1	A	81	ALA	N-CA-C	5.18	117.00	111.36
1	B	350	THR	N-CA-C	-5.11	107.17	113.41
1	A	219	ASN	CB-CA-C	-5.10	101.19	110.63
1	B	110	ASP	N-CA-C	-5.10	97.68	107.57
1	A	233	VAL	N-CA-C	-5.08	104.27	108.63
1	A	546	VAL	N-CA-C	5.06	116.64	108.85
1	B	202	VAL	N-CA-CB	5.03	118.13	110.58
1	A	442	VAL	CB-CA-C	-5.01	103.65	110.77

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	140	1
1	B	5963	0	5679	179	0
2	A	56	0	52	2	0
2	B	56	0	52	4	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	316	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 14.

All (316) 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:620:ASP:OD1	1:B:620:ASP:C	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:LEU:HD23	1:B:543:LEU:C	2.05	0.81
1:B:163:LYS:NZ	1:B:273:THR:HG22	1.94	0.81
1:B:543:LEU:C	1:B:543:LEU:CD2	2.54	0.80
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:A:377:ASN:C	1:A:377:ASN:HD22	1.91	0.78
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: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: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: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:163:LYS:HZ3	1:B:273:THR:HG22	1.53	0.71
1:B:267:LYS:NZ	1:B:286:GLN:HE22	1.89	0.71
1:B:377:ASN:C	1:B:377:ASN:HD22	2.00	0.70
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
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:621:ASN:C	1:B:621:ASN:HD22	2.03	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: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:44:THR:HG22	1:A:45:LEU:N	2.11	0.64
1:B:163:LYS:HZ2	1:B:273:THR:CG2	2.10	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.79	0.63
1:A:514:LEU:C	1:A:514:LEU:HD23	2.24	0.63
1:B:267:LYS:CD	1:B:286:GLN:NE2	2.62	0.63
1:B:726:VAL:HG12	1:B:728:VAL:HG23	1.80	0.62
1:A:528:MET:HE3	1:A:530:LEU:HD21	1.82	0.62
1:A:602:GLU:OE2	1:A:631:TYR:OH	2.16	0.62
1:A:300:LEU:C	1:A:300:LEU:CD2	2.73	0.61
1:A:405:ILE:HD12	1:A:419:SER:HA	1.82	0.61
1:A:730:PHE:CZ	1:B:733:MET:HE1	2.35	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:A:730:PHE:CE2	1:B:733:MET:HE1	2.37	0.59
1:B:107:ILE:HG12	1:B:114:ILE:HG13	1.85	0.59
1:B:143:ILE:O	1:B:143:ILE:HG13	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:HD23	1:A:515:ASP:N	2.18	0.58
1:B:163:LYS:HZ3	1:B:273:THR:CG2	2.11	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: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: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
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:A:90:LEU:HD23	1:A:90:LEU:C	2.31	0.56
1:A:415:LEU:HD23	1:A:415:LEU:C	2.31	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ILE:HD12	1:B:712:HIS:NE2	2.20	0.56
1:A:514:LEU:C	1:A:514:LEU:CD2	2.79	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:A:741:GLY:O	1:A:742:ILE:C	2.50	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:B:110:ASP:CG	1:B:161:GLY:H	2.15	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:137:LEU:C	1:B:139:LYS:H	2.16	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: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:91:GLU:CD	1:B:94:THR:OG1	2.51	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:B:163:LYS:HZ2	1:B:273:THR:HG22	1.72	0.52
1:B:87:SER:OG	2:B:794:NAG:O7	2.26	0.52
1:A:550:PRO:O	1:A:551:CYS:HB2	2.10	0.52
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:615:LYS:O	1:A:616:MET:C	2.54	0.51
1:A:122:LYS:HE3	1:A:124:TRP:O	2.11	0.51
1:B:105:TYR:CD1	1:B:105:TYR:C	2.89	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:621:ASN:C	1:A:621:ASN:HD22	2.19	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:322:TYR:HE1	1:B:348:MET:HE2	1.77	0.50
1:B:563:TRP:HH2	1:B:759:ILE:CD1	2.25	0.50
1:A:377:ASN:C	1:A:377:ASN:ND2	2.63	0.49
1:B:46:THR:CG2	1:B:50:LYS:CD	2.88	0.49
1:A:449:LEU:C	1:A:450:ASN:ND2	2.71	0.49
1:A:500:LEU:HA	1:A:503:MET:HE3	1.94	0.49
1:A:487:ASN:O	1:A:488:ASP:C	2.56	0.48
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:91:GLU:CD	1:B:94:THR:HG1	2.21	0.48
1:B:310:ARG:NH2	1:B:389:ILE:HD13	2.28	0.48
1:A:90:LEU:C	1:A:90:LEU:CD2	2.86	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:379:GLU:CD	1:B:379:GLU:N	2.71	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:A:300:LEU:C	1:A:300:LEU:HD23	2.39	0.48
1:A:710:ASN:HD22	1:A:710:ASN:C	2.22	0.48
1:B:470:LEU:HD12	1:B:483:HIS:CE1	2.49	0.48
1:A:528:MET:HE2	1:A:530:LEU:HD21	1.95	0.48
1:A:325:MET:HE1	1:A:371:PHE:CZ	2.49	0.48
1:A:535:ASP:CG	1:A:537:SER:HG	2.22	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:562:ASN:C	1:B:562:ASN:HD22	2.24	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:459:VAL:HG22	1:A:460:SER:N	2.29	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: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:485:SER:O	1:B:486:VAL:C	2.59	0.46
1:B:267:LYS:CD	1:B:286:GLN:HE22	2.22	0.45
1:B:741:GLY:O	1:B:742:ILE:C	2.59	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:398:THR:C	1:A:399:LYS:HG2	2.40	0.45
1:A:438:ASP:OD1	1:A:438:ASP:C	2.58	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
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:A:614:SER:O	1:A:615:LYS:C	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:B:743:ALA:O	1:B:744:SER:C	2.59	0.44
1:A:331:ASP:OD1	1:A:331:ASP:C	2.60	0.44
1:A:535:ASP:C	1:A:537:SER:H	2.24	0.44
1:A:745:SER:O	1:A:749:GLN:HG3	2.18	0.44
1:B:616:MET:C	1:B:618:PHE:N	2.76	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:A:340:LEU:C	1:A:342:ALA:N	2.73	0.43
1:B:543:LEU:C	1:B:543:LEU:HD22	2.41	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:120:TYR:CD1	1:A:120:TYR:C	2.97	0.43
1:A:463:LYS:C	1:A:465:ALA:H	2.26	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:535:ASP:C	1:B:535:ASP:OD1	2.61	0.43
1:B:365:THR:HG21	1:B:370:SER:OG	2.19	0.42
1:A:300:LEU:C	1:A:300:LEU:HD22	2.43	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:B:616:MET:C	1:B:618:PHE:H	2.27	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:728:VAL:O	1:B:750:HIS:HE1	2.03	0.41
1:B:137:LEU:C	1:B:139:LYS:N	2.77	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:B:45:LEU:HG	1:B:49:LEU:HD22	2.02	0.41
1:B:267:LYS:HZ1	1:B:286:GLN:HE22	1.67	0.41
1:B:383:HIS:CD2	1:B:399:LYS:N	2.88	0.41
1:B:522:THR:HG22	1:B:523:LYS:N	2.34	0.41
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.38	0.41
1:B:163:LYS:HZ2	1:B:273:THR:HG21	1.84	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:B:322:TYR:CE1	1:B:348:MET:HE2	2.56	0.41
1:B:542:LEU:C	1:B:542:LEU:HD23	2.45	0.41
1:B:710:ASN:HD22	1:B:710:ASN:C	2.29	0.41
1:B:616:MET:O	1:B:617:GLY:C	2.64	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:106:SER:HG	1:B:157:TRP:CD1	2.39	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:93:SER:O	1:B:94:THR:C	2.63	0.41
1:B:327:ILE:HD13	1:B:389:ILE:HG12	2.03	0.41
1:B:383:HIS:CD2	1:B:398:THR:C	2.99	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:A:750:HIS:CE1	1:B:728:VAL:O	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:556:ASP:OD1	1:A:556:ASP:C	2.64	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
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%)	21	18
1	B	726/728 (100%)	683 (94%)	41 (6%)	2 (0%)	36	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1452/1456 (100%)	1366 (94%)	80 (6%)	6 (0%)	30	28

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 ⓘ

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%)	593 (91%)	60 (9%)	8	6
1	B	653/653 (100%)	592 (91%)	61 (9%)	8	6
All	All	1306/1306 (100%)	1185 (91%)	121 (9%)	8	6

All (121) 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	90	LEU
1	A	93	SER
1	A	107	ILE
1	A	120	TYR

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Mol	Chain	Res	Type
1	A	145	GLU
1	A	160	VAL
1	A	180	LEU
1	A	202	VAL
1	A	223	LEU
1	A	246	LEU
1	A	273	THR
1	A	277	SER
1	A	278	SER
1	A	280	THR
1	A	294	LEU
1	A	300	LEU
1	A	316	LEU
1	A	326	ASP
1	A	341	VAL
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
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	594	ILE
1	A	621	ASN
1	A	630	SER
1	A	669	ARG

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Mol	Chain	Res	Type
1	A	677	GLU
1	A	684	ARG
1	A	710	ASN
1	A	715	GLN
1	A	736	THR
1	A	745	SER
1	B	40	ARG
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	144	THR
1	B	180	LEU
1	B	202	VAL
1	B	223	LEU
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	332	GLU
1	B	334	SER
1	B	340	LEU
1	B	350	THR
1	B	375	ILE
1	B	377	ASN
1	B	385	CYS
1	B	389	ILE

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Mol	Chain	Res	Type
1	B	392	LYS
1	B	397	ILE
1	B	420	ASN
1	B	452	GLU
1	B	472	CYS
1	B	479	LEU
1	B	486	VAL
1	B	492	ARG
1	B	500	LEU
1	B	507	VAL
1	B	514	LEU
1	B	543	LEU
1	B	554	LYS
1	B	558	VAL
1	B	562	ASN
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	715	GLN
1	B	726	VAL
1	B	731	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (43) 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	314	GLN
1	A	377	ASN
1	A	420	ASN
1	A	430	ASN
1	A	435	GLN
1	A	450	ASN
1	A	483	HIS
1	A	508	GLN

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Mol	Chain	Res	Type
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	750	HIS
1	B	103	ASN
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	430	ASN
1	B	435	GLN
1	B	483	HIS
1	B	562	ASN
1	B	595	ASN
1	B	606	GLN
1	B	621	ASN
1	B	679	ASN
1	B	682	HIS
1	B	710	ASN
1	B	715	GLN
1	B	731	GLN
1	B	750	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	794	1	14,14,15	0.57	0	17,19,21	1.61	5 (29%)
2	NAG	A	793	1	14,14,15	0.62	0	17,19,21	1.71	5 (29%)
2	NAG	B	793	1	14,14,15	0.42	0	17,19,21	2.42	6 (35%)
2	NAG	A	796	1	14,14,15	0.71	0	17,19,21	1.60	4 (23%)
2	NAG	A	794	1	14,14,15	0.70	0	17,19,21	1.49	3 (17%)
2	NAG	B	796	1	14,14,15	0.95	1 (7%)	17,19,21	1.94	5 (29%)
2	NAG	A	795	1	14,14,15	0.58	0	17,19,21	1.16	1 (5%)
2	NAG	B	797	1	14,14,15	0.68	0	17,19,21	1.77	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	794	1	-	0/6/23/26	0/1/1/1
2	NAG	A	793	1	-	5/6/23/26	0/1/1/1
2	NAG	A	796	1	-	0/6/23/26	0/1/1/1
2	NAG	B	797	1	1/1/5/7	2/6/23/26	0/1/1/1
2	NAG	A	794	1	-	0/6/23/26	0/1/1/1
2	NAG	B	793	1	-	5/6/23/26	0/1/1/1
2	NAG	A	795	1	-	3/6/23/26	0/1/1/1
2	NAG	B	796	1	-	2/6/23/26	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	-2.88	1.38	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	793	NAG	C1-O5-C5	5.68	119.79	112.19
2	B	796	NAG	O5-C1-C2	-5.32	103.06	111.29
2	B	793	NAG	O5-C1-C2	4.36	118.04	111.29
2	B	797	NAG	C1-O5-C5	4.24	117.87	112.19
2	B	793	NAG	C4-C3-C2	-4.18	104.89	111.02
2	B	797	NAG	C3-C4-C5	-3.59	103.73	110.23
2	A	793	NAG	O5-C1-C2	-3.43	105.98	111.29
2	A	795	NAG	C4-C3-C2	-3.40	106.04	111.02
2	B	794	NAG	C1-O5-C5	3.37	116.70	112.19
2	A	796	NAG	O5-C1-C2	-3.26	106.25	111.29
2	B	793	NAG	O3-C3-C2	3.20	116.05	109.40
2	B	796	NAG	O6-C6-C5	-2.94	101.33	111.33
2	A	793	NAG	C1-O5-C5	2.87	116.04	112.19
2	B	796	NAG	C1-C2-N2	2.87	114.95	110.43
2	B	794	NAG	O7-C7-N2	2.86	127.03	121.98
2	B	794	NAG	O5-C1-C2	-2.83	106.91	111.29
2	B	797	NAG	C2-N2-C7	-2.76	119.20	122.90
2	A	796	NAG	C1-C2-N2	2.59	114.52	110.43
2	A	794	NAG	C4-C3-C2	-2.58	107.24	111.02
2	A	796	NAG	C3-C4-C5	-2.53	105.65	110.23
2	B	794	NAG	C1-C2-N2	-2.51	106.47	110.43
2	A	796	NAG	O6-C6-C5	-2.47	102.92	111.33
2	B	796	NAG	C6-C5-C4	-2.44	107.02	113.02
2	A	793	NAG	O3-C3-C2	2.42	114.43	109.40
2	B	793	NAG	C8-C7-N2	2.30	119.94	116.12
2	A	794	NAG	O5-C1-C2	-2.17	107.94	111.29
2	B	793	NAG	O7-C7-C8	-2.13	118.26	122.05
2	B	797	NAG	C4-C3-C2	-2.11	107.93	111.02
2	B	797	NAG	O4-C4-C5	2.10	114.49	109.32
2	A	793	NAG	O7-C7-C8	-2.10	118.32	122.05
2	A	793	NAG	C8-C7-N2	2.05	119.52	116.12
2	B	796	NAG	O5-C5-C4	2.03	115.76	110.83
2	B	794	NAG	C8-C7-N2	-2.02	112.76	116.12
2	A	794	NAG	O7-C7-N2	2.02	125.55	121.98

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

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	794	NAG	1	0
2	A	793	NAG	2	0
2	B	793	NAG	3	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.