



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:23 AM GMT

PDB ID : 2QJR  
Title : dipeptidyl peptidase IV in complex with inhibitor PZF  
Authors : Shenping, L.  
Deposited on : 2007-07-09  
Resolution : 2.20 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

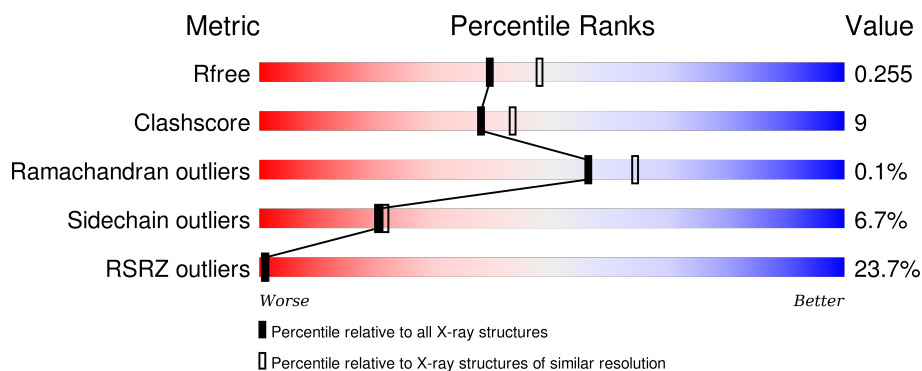
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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. 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  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	748	
1	B	748	

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	A	800	-	-	-	X
3	LGU	A	802	X	-	-	-
3	LGU	A	804	X	-	-	-
4	NAG	B	796	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12532 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Dipeptidyl peptidase 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5957	3825	980	1126	26			
1	B	728	Total	C	N	O	S	0	0	0
			5957	3825	980	1126	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	767	LEU	-	EXPRESSION TAG	UNP P27487
A	768	VAL	-	EXPRESSION TAG	UNP P27487
A	769	PRO	-	EXPRESSION TAG	UNP P27487
A	770	ARG	-	EXPRESSION TAG	UNP P27487
A	771	GLY	-	EXPRESSION TAG	UNP P27487
A	772	SER	-	EXPRESSION TAG	UNP P27487
A	773	HIS	-	EXPRESSION TAG	UNP P27487
A	774	HIS	-	EXPRESSION TAG	UNP P27487
A	775	HIS	-	EXPRESSION TAG	UNP P27487
A	776	HIS	-	EXPRESSION TAG	UNP P27487
A	777	HIS	-	EXPRESSION TAG	UNP P27487
A	778	HIS	-	EXPRESSION TAG	UNP P27487
B	767	LEU	-	EXPRESSION TAG	UNP P27487
B	768	VAL	-	EXPRESSION TAG	UNP P27487
B	769	PRO	-	EXPRESSION TAG	UNP P27487
B	770	ARG	-	EXPRESSION TAG	UNP P27487
B	771	GLY	-	EXPRESSION TAG	UNP P27487
B	772	SER	-	EXPRESSION TAG	UNP P27487
B	773	HIS	-	EXPRESSION TAG	UNP P27487
B	774	HIS	-	EXPRESSION TAG	UNP P27487
B	775	HIS	-	EXPRESSION TAG	UNP P27487
B	776	HIS	-	EXPRESSION TAG	UNP P27487
B	777	HIS	-	EXPRESSION TAG	UNP P27487
B	778	HIS	-	EXPRESSION TAG	UNP P27487

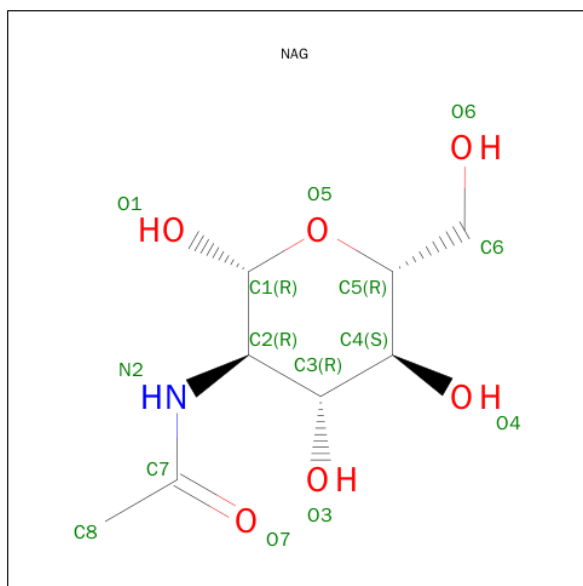
- Molecule 2 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	A	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

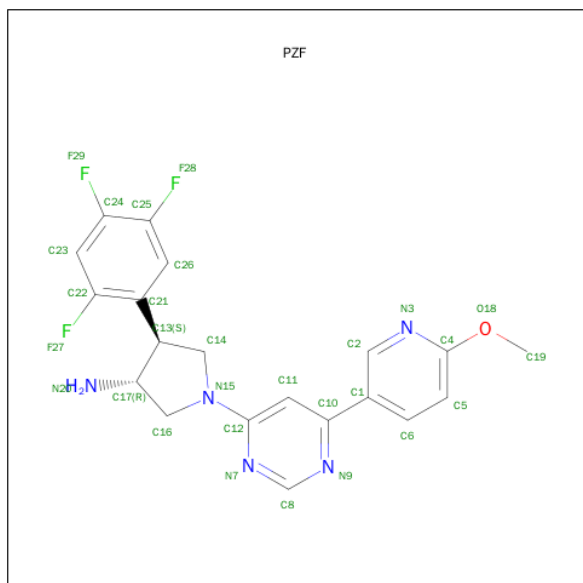


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	2	Total	C	N	O	0	0
			28	16	2	10		
5	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 6 is (3R,4S)-1-[6-(6-METHOXPYRIDIN-3-YL)PYRIMIDIN-4-YL]-4-(2,4,5-TRIFLUOROPHENYL)PYRROLIDIN-3-AMINE (three-letter code: PZF) (formula: C<sub>20</sub>H<sub>18</sub>F<sub>3</sub>N<sub>5</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	F	N	O	0	0
			29	20	3	5	1		
6	B	1	Total	C	F	N	O	0	0
			29	20	3	5	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	105	Total	O	0	0
			105	105		
7	B	226	Total	O	0	0
			226	226		







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.47Å 68.80Å 422.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.90 – 2.20 41.90 – 2.19	Depositor EDS
% Data completeness (in resolution range)	85.7 (41.90-2.20) 85.4 (41.90-2.19)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0003	Depositor
R, $R_{free}$	0.191 , 0.253 0.200 , 0.255	Depositor DCC
$R_{free}$ test set	4236 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	39.1	Xtriage
Anisotropy	0.929	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 67.7	EDS
Estimated twinning fraction	0.055 for k,h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Outliers	2 of 85287 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	12532	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MAN, PZF, NAG, NDG, LGU

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	1.12	6/6129 (0.1%)	1.09	33/8336 (0.4%)
1	B	1.43	42/6129 (0.7%)	1.24	43/8336 (0.5%)
All	All	1.29	48/12258 (0.4%)	1.17	76/16672 (0.5%)

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
3	A	2	0

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	385	CYS	CB-SG	-8.03	1.68	1.82
1	B	250	LYS	CD-CE	6.76	1.68	1.51
1	B	244	GLU	CD-OE1	6.63	1.32	1.25
1	B	83	TYR	CE1-CZ	6.46	1.47	1.38
1	B	82	GLU	CD-OE1	6.43	1.32	1.25
1	A	658	ARG	NE-CZ	6.40	1.41	1.33
1	B	463	LYS	CE-NZ	6.37	1.65	1.49
1	B	669	ARG	CD-NE	-6.30	1.35	1.46
1	B	417	TYR	CD1-CE1	-6.29	1.29	1.39
1	B	480	TYR	CE2-CZ	-6.19	1.30	1.38
1	B	203	TYR	CE1-CZ	6.14	1.46	1.38
1	B	429	ARG	NE-CZ	6.03	1.40	1.33
1	B	347	GLU	CD-OE1	5.92	1.32	1.25
1	B	61	ARG	CG-CD	5.88	1.66	1.51
1	B	271	VAL	CB-CG2	-5.88	1.40	1.52
1	A	379	GLU	CD-OE2	5.84	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	473	SER	CB-OG	-5.82	1.34	1.42
1	B	752	TYR	CD1-CE1	5.79	1.48	1.39
1	B	216	TRP	CG-CD1	5.76	1.44	1.36
1	B	254	VAL	CB-CG1	5.70	1.64	1.52
1	A	39	SER	CA-CB	5.66	1.61	1.52
1	B	423	LYS	CE-NZ	5.63	1.63	1.49
1	B	745	SER	CB-OG	-5.56	1.35	1.42
1	A	256	TYR	CE1-CZ	-5.48	1.31	1.38
1	B	354	VAL	CB-CG2	-5.48	1.41	1.52
1	B	82	GLU	CD-OE2	5.46	1.31	1.25
1	B	106	SER	CB-OG	5.45	1.49	1.42
1	B	403	GLU	CD-OE2	5.39	1.31	1.25
1	B	86	SER	CB-OG	-5.37	1.35	1.42
1	B	225	TYR	CD1-CE1	-5.30	1.31	1.39
1	B	756	SER	CB-OG	5.29	1.49	1.42
1	B	312	SER	CB-OG	-5.27	1.35	1.42
1	B	88	VAL	CB-CG1	-5.26	1.41	1.52
1	A	82	GLU	CD-OE2	5.24	1.31	1.25
1	B	526	TYR	CD1-CE1	-5.23	1.31	1.39
1	B	452	GLU	CD-OE1	5.22	1.31	1.25
1	B	222	PHE	CD1-CE1	5.21	1.49	1.39
1	B	154	TRP	CE3-CZ3	5.17	1.47	1.38
1	B	585	TYR	CE1-CZ	-5.11	1.31	1.38
1	B	391	LYS	CE-NZ	5.11	1.61	1.49
1	B	467	TYR	CE1-CZ	-5.10	1.31	1.38
1	A	589	LYS	CE-NZ	5.08	1.61	1.49
1	B	347	GLU	CD-OE2	5.07	1.31	1.25
1	B	379	GLU	CD-OE1	5.06	1.31	1.25
1	B	453	ARG	CZ-NH1	-5.05	1.26	1.33
1	B	456	TYR	CZ-OH	5.05	1.46	1.37
1	B	474	GLY	C-O	-5.03	1.15	1.23
1	B	457	TYR	CD2-CE2	5.00	1.46	1.39

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	669	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	A	669	ARG	NE-CZ-NH1	12.26	126.43	120.30
1	B	453	ARG	NE-CZ-NH1	-10.82	114.89	120.30
1	B	61	ARG	NE-CZ-NH2	-10.66	114.97	120.30
1	A	658	ARG	NE-CZ-NH1	10.27	125.44	120.30
1	B	453	ARG	NE-CZ-NH2	9.92	125.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	329	ASP	CB-CG-OD2	8.99	126.39	118.30
1	B	429	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	A	501	ASP	CB-CG-OD2	8.88	126.30	118.30
1	B	302	ASP	CB-CG-OD2	8.68	126.11	118.30
1	A	579	ASP	CB-CG-OD2	8.51	125.96	118.30
1	B	515	ASP	CB-CG-OD2	8.18	125.66	118.30
1	A	367	ASP	CB-CG-OD2	8.17	125.65	118.30
1	B	678	ASP	CB-CG-OD2	8.13	125.61	118.30
1	B	230	ASP	CB-CG-OD2	8.10	125.59	118.30
1	A	691	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	B	316	LEU	CB-CG-CD1	7.99	124.58	111.00
1	B	60	LEU	CA-CB-CG	7.98	133.66	115.30
1	B	725	ASP	CB-CG-OD2	7.96	125.46	118.30
1	A	393	ASP	CB-CG-OD2	7.75	125.27	118.30
1	A	133	ASP	CB-CG-OD2	7.46	125.01	118.30
1	A	515	ASP	CB-CG-OD2	7.41	124.97	118.30
1	A	560	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	678	ASP	CB-CG-OD2	7.18	124.76	118.30
1	A	65	ASP	CB-CG-OD2	7.08	124.67	118.30
1	A	401	THR	OG1-CB-CG2	-7.04	93.80	110.00
1	B	271	VAL	CB-CA-C	-7.02	98.06	111.40
1	A	535	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	302	ASP	CB-CG-OD2	6.98	124.58	118.30
1	B	729	ASP	CB-CG-OD2	6.96	124.56	118.30
1	B	556	ASP	CB-CG-OD2	6.94	124.55	118.30
1	A	104	ASP	CB-CG-OD1	6.92	124.53	118.30
1	B	61	ARG	NE-CZ-NH1	6.75	123.67	120.30
1	B	438	ASP	CB-CG-OD2	6.67	124.31	118.30
1	A	243	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	133	ASP	CB-CG-OD2	6.63	124.27	118.30
1	B	47	ASP	CB-CG-OD2	6.63	124.26	118.30
1	B	390	ASP	CB-CG-OD2	6.61	124.25	118.30
1	B	316	LEU	CB-CG-CD2	-6.59	99.79	111.00
1	B	501	ASP	CB-CG-OD2	6.52	124.17	118.30
1	B	321	ASN	CB-CA-C	-6.51	97.37	110.40
1	A	691	ARG	NE-CZ-NH2	-6.39	117.10	120.30
1	B	669	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	669	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	B	413	ASP	CB-CG-OD2	6.16	123.84	118.30
1	B	65	ASP	CB-CG-OD2	6.14	123.82	118.30
1	A	443	THR	OG1-CB-CG2	-6.09	96.00	110.00
1	B	385	CYS	CA-CB-SG	-6.03	103.16	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	329	ASP	CB-CG-OD2	5.78	123.50	118.30
1	A	737	ASP	CB-CG-OD1	5.75	123.48	118.30
1	B	171	ASP	CB-CG-OD2	5.68	123.41	118.30
1	B	243	ASP	CB-CG-OD1	5.66	123.39	118.30
1	B	560	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	A	708	ASP	CB-CG-OD1	5.65	123.39	118.30
1	B	104	ASP	CB-CG-OD2	5.65	123.38	118.30
1	A	560	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	67	GLU	OE1-CD-OE2	-5.61	116.57	123.30
1	A	620	ASP	CB-CG-OD2	5.60	123.34	118.30
1	A	588	ASP	CB-CG-OD2	5.58	123.32	118.30
1	A	605	ASP	CB-CG-OD2	5.54	123.28	118.30
1	A	501	ASP	CB-CG-OD1	-5.46	113.38	118.30
1	B	60	LEU	CB-CG-CD2	5.44	120.25	111.00
1	B	759	ILE	CG1-CB-CG2	-5.44	99.44	111.40
1	B	394	CYS	N-CA-C	-5.33	96.61	111.00
1	B	274	ASP	CB-CG-OD2	5.32	123.09	118.30
1	B	546	VAL	CG1-CB-CG2	-5.28	102.46	110.90
1	A	110	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	115	LEU	CA-CB-CG	5.26	127.39	115.30
1	B	206	GLU	CB-CA-C	-5.25	99.90	110.40
1	B	560	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	A	271	VAL	CB-CA-C	-5.21	101.50	111.40
1	B	110	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	321	ASN	N-CA-CB	-5.14	101.35	110.60
1	B	78	VAL	CB-CA-C	-5.12	101.68	111.40
1	A	488	ASP	CB-CG-OD2	5.11	122.90	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	802	LGU	C5
3	A	804	LGU	C5

There are no planarity outliers.

## 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	5957	0	5672	94	0
1	B	5957	0	5672	125	0
2	A	56	0	50	1	0
2	B	28	0	25	1	0
3	A	61	0	48	0	0
4	A	14	0	13	0	0
4	B	14	0	13	1	0
5	B	56	0	50	2	0
6	A	29	0	18	1	0
6	B	29	0	18	0	0
7	A	105	0	0	10	0
7	B	226	0	0	21	0
All	All	12532	0	11579	218	0

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

All (218) 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:39:SER:O	1:A:40:ARG:CZ	1.79	1.29
1:B:40:ARG:HD3	1:B:40:ARG:N	1.64	1.12
1:B:39:SER:HB2	1:B:40:ARG:HD2	1.31	1.08
1:B:597:ARG:HD3	7:B:1038:HOH:O	1.56	1.02
1:A:621:ASN:C	1:A:621:ASN:HD22	1.64	0.99
1:B:39:SER:HB2	1:B:40:ARG:CD	1.91	0.99
1:B:74:ASN:HB2	7:B:941:HOH:O	1.63	0.94
1:B:401:THR:O	1:B:401:THR:HG22	1.74	0.87
1:B:39:SER:O	7:B:1122:HOH:O	1.93	0.87
1:B:40:ARG:H	1:B:40:ARG:HD3	1.29	0.87
1:B:147:ARG:HD3	7:B:953:HOH:O	1.75	0.87
1:A:434:ILE:HD12	1:A:442:VAL:HG22	1.59	0.85
1:A:630:SER:OG	1:A:740:HIS:NE2	2.09	0.84
1:B:499:ALA:O	1:B:502:LYS:HG2	1.78	0.84
1:B:65:ASP:OD1	1:B:463:LYS:O	1.95	0.83
1:B:236:ILE:HG12	1:B:712:HIS:CE1	2.13	0.82
1:A:39:SER:O	1:A:40:ARG:NH1	2.14	0.80
1:A:39:SER:O	1:A:40:ARG:NH2	2.16	0.79
1:B:598:LEU:O	1:B:682:HIS:HE1	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASN:HB2	1:B:308:GLN:OE1	1.85	0.75
1:B:61:ARG:HD3	7:B:1119:HOH:O	1.85	0.75
1:A:345:HIS:HD2	7:A:1005:HOH:O	1.70	0.74
5:B:800:NDG:H8C1	7:B:1113:HOH:O	1.87	0.74
1:B:66:HIS:HD2	7:B:1008:HOH:O	1.71	0.74
1:B:306:ALA:HB3	1:B:310:ARG:HG2	1.70	0.73
1:B:389:ILE:O	7:B:1045:HOH:O	2.06	0.73
1:A:658:ARG:NE	7:A:1002:HOH:O	1.93	0.72
1:B:66:HIS:CD2	7:B:1008:HOH:O	2.42	0.72
1:B:477:LEU:HD22	1:B:500:LEU:HD13	1.73	0.71
1:A:463:LYS:O	1:A:464:GLU:HB2	1.91	0.70
1:A:177:GLU:HB2	1:A:180:LEU:HD22	1.73	0.70
1:A:499:ALA:O	1:A:502:LYS:HG3	1.91	0.69
1:B:74:ASN:O	1:B:75:ASN:OD1	2.10	0.69
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.11	0.68
1:B:55:LEU:HD23	1:B:500:LEU:CD1	2.23	0.68
1:A:89:PHE:CE2	1:A:107:ILE:HD13	2.29	0.68
1:B:57:LEU:HD23	7:B:1067:HOH:O	1.94	0.68
1:A:71:LYS:NZ	1:A:92:ASN:HD21	1.92	0.68
1:B:89:PHE:CE2	1:B:107:ILE:HD13	2.30	0.67
1:B:71:LYS:NZ	1:B:74:ASN:HA	2.09	0.67
1:A:761:GLN:NE2	7:A:957:HOH:O	2.26	0.66
1:B:39:SER:CB	1:B:40:ARG:HH11	2.09	0.66
1:A:621:ASN:HD22	1:A:622:LYS:N	1.93	0.65
1:B:503:MET:O	1:B:506:ASN:HB2	1.97	0.65
1:B:147:ARG:NH1	7:B:953:HOH:O	2.29	0.64
1:A:345:HIS:CD2	7:A:1005:HOH:O	2.46	0.64
1:A:621:ASN:ND2	1:A:621:ASN:C	2.42	0.63
1:B:680:LEU:HD22	1:B:684:ARG:HD3	1.80	0.63
1:B:89:PHE:HE2	1:B:107:ILE:HD13	1.64	0.63
1:B:429:ARG:NE	7:B:916:HOH:O	2.18	0.63
1:B:414:TYR:CD1	1:B:433:LYS:HD2	2.32	0.63
1:A:298:HIS:HE1	7:A:916:HOH:O	1.81	0.63
1:B:598:LEU:O	1:B:682:HIS:CE1	2.49	0.63
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.65	0.62
1:A:111:GLY:O	1:A:137:LEU:HD12	2.00	0.62
1:B:621:ASN:C	1:B:621:ASN:HD22	2.02	0.62
1:B:358:ARG:HB2	1:B:359:PRO:HD2	1.80	0.62
1:A:500:LEU:HD22	1:A:504:LEU:HG	1.82	0.62
1:B:640:LEU:HD11	1:B:650:GLY:HA3	1.80	0.62
1:A:361:GLU:OE2	1:A:363:HIS:HE1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:LYS:HZ1	1:B:74:ASN:HA	1.65	0.61
1:B:40:ARG:CD	1:B:40:ARG:N	2.48	0.61
1:B:163:LYS:NZ	1:B:274:ASP:OD1	2.31	0.61
1:B:39:SER:HB2	1:B:40:ARG:HD3	1.80	0.60
4:B:796:NAG:C4	7:B:1062:HOH:O	2.49	0.60
1:B:401:THR:O	1:B:401:THR:CG2	2.44	0.60
1:B:40:ARG:CB	1:B:506:ASN:O	2.50	0.59
1:A:39:SER:O	1:A:40:ARG:NE	2.32	0.59
1:A:434:ILE:HD12	1:A:442:VAL:CG2	2.32	0.58
1:B:680:LEU:HD22	1:B:684:ARG:CD	2.32	0.58
1:A:76:ILE:HD12	1:A:90:LEU:HB3	1.85	0.58
1:B:405:ILE:HG13	1:B:429:ARG:CD	2.33	0.58
1:A:71:LYS:HZ1	1:A:92:ASN:HD21	1.52	0.57
1:B:55:LEU:HD23	1:B:500:LEU:HD12	1.85	0.57
1:A:470:LEU:HD12	1:A:483:HIS:CE1	2.40	0.57
1:A:528:MET:HE1	1:A:618:PHE:CZ	2.39	0.57
1:A:481:THR:OG1	1:A:483:HIS:HE1	1.88	0.57
1:B:535:ASP:OD2	1:B:538:LYS:NZ	2.38	0.57
1:B:55:LEU:HD23	1:B:500:LEU:HD11	1.87	0.56
1:B:39:SER:OG	1:B:40:ARG:NH1	2.39	0.56
1:B:562:ASN:HD22	1:B:562:ASN:C	2.08	0.56
1:A:89:PHE:HE2	1:A:107:ILE:HD13	1.71	0.55
1:B:597:ARG:CD	7:B:1038:HOH:O	2.30	0.55
1:A:207:VAL:HG12	1:A:208:PHE:CD1	2.42	0.55
1:A:134:ILE:HD11	1:A:164:LEU:CD1	2.37	0.54
1:B:40:ARG:HB2	1:B:506:ASN:O	2.07	0.54
1:B:296:GLY:O	1:B:298:HIS:HD2	1.90	0.54
1:B:325:MET:HE1	1:B:327:ILE:HD11	1.88	0.53
1:A:65:ASP:OD1	1:A:65:ASP:N	2.27	0.53
1:B:399:LYS:NZ	7:B:1066:HOH:O	2.42	0.53
1:A:314:GLN:HE22	1:A:362:PRO:HD3	1.73	0.53
1:A:726:VAL:CG1	1:A:728:VAL:HG23	2.39	0.53
1:A:219:ASN:HB2	1:A:308:GLN:OE1	2.08	0.53
1:A:320:GLN:OE1	1:A:669:ARG:HD3	2.10	0.52
1:A:624:ILE:HD12	7:A:933:HOH:O	2.07	0.52
1:A:675:THR:HB	1:A:677:GLU:OE1	2.09	0.52
1:A:594:ILE:CD1	1:A:601:PHE:HB2	2.40	0.52
1:A:230:ASP:OD1	1:A:264:PRO:HB3	2.09	0.51
1:A:191:GLU:O	1:A:192:ASP:HB2	2.10	0.51
1:A:378:GLU:CG	7:A:991:HOH:O	2.58	0.51
1:A:546:VAL:HG21	1:A:626:ILE:HD11	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.92	0.51
1:B:693:GLU:CD	1:B:726:VAL:HG21	2.32	0.51
1:A:528:MET:HE1	1:A:618:PHE:HZ	1.74	0.50
1:A:296:GLY:O	1:A:298:HIS:HD2	1.94	0.50
1:A:596:ARG:NH2	1:A:678:ASP:OD1	2.42	0.50
1:B:463:LYS:O	1:B:464:GLU:HB2	2.12	0.50
1:B:87:SER:OG	2:B:794:NAG:O7	2.29	0.50
1:B:621:ASN:HD22	1:B:622:LYS:N	2.09	0.50
1:B:325:MET:CE	1:B:327:ILE:HD11	2.43	0.49
1:B:594:ILE:CD1	1:B:601:PHE:HB2	2.42	0.49
1:B:146:GLU:O	1:B:175:LYS:NZ	2.42	0.49
1:A:40:ARG:HA	1:A:40:ARG:NE	2.24	0.49
1:B:477:LEU:CD2	1:B:500:LEU:HD13	2.42	0.49
1:B:611:ARG:O	1:B:615:LYS:HG2	2.13	0.49
1:B:206:GLU:HG3	1:B:665:VAL:HB	1.95	0.49
1:B:200:ASP:OD2	1:B:264:PRO:HG3	2.12	0.49
1:A:594:ILE:HG23	1:A:594:ILE:O	2.13	0.49
1:B:463:LYS:O	1:B:464:GLU:CB	2.58	0.48
1:B:41:LYS:HE2	1:B:53:TYR:OH	2.13	0.48
1:A:473:SER:OG	7:A:974:HOH:O	2.20	0.48
1:B:224:ALA:HB1	1:B:268:PHE:CZ	2.48	0.48
1:A:757:HIS:HD2	1:B:729:ASP:OD2	1.97	0.48
1:A:726:VAL:HG13	1:A:728:VAL:HG23	1.94	0.48
1:A:477:LEU:HD22	1:A:500:LEU:HD13	1.95	0.48
1:A:522:THR:HG22	1:A:524:PHE:CE2	2.50	0.47
1:B:39:SER:C	1:B:40:ARG:HD3	2.32	0.47
1:A:502:LYS:HE2	1:A:503:MET:HG3	1.95	0.47
1:A:408:GLU:HG3	1:A:418:ILE:HD12	1.97	0.47
1:B:39:SER:CB	1:B:40:ARG:CD	2.81	0.46
1:B:39:SER:N	1:B:40:ARG:HH11	2.14	0.46
1:A:69:LEU:HD13	1:A:107:ILE:HD12	1.98	0.46
1:B:310:ARG:HA	1:B:328:CYS:O	2.15	0.46
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.97	0.46
1:A:413:ASP:OD2	1:A:413:ASP:N	2.49	0.46
1:A:361:GLU:OE2	1:A:363:HIS:CE1	2.68	0.46
1:B:693:GLU:O	1:B:696:LYS:HG3	2.15	0.46
1:A:55:LEU:HD21	1:A:559:PHE:HE2	1.80	0.46
1:A:429:ARG:NE	7:A:945:HOH:O	2.43	0.46
1:A:134:ILE:HD11	1:A:164:LEU:HD11	1.97	0.46
1:B:358:ARG:HB2	1:B:359:PRO:CD	2.46	0.45
1:A:206:GLU:CD	6:A:900:PZF:H202	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:414:TYR:CE1	1:B:433:LYS:HD2	2.50	0.45
1:B:751:ILE:HG23	1:B:752:TYR:N	2.32	0.45
1:B:636:THR:HG21	1:B:651:ILE:O	2.15	0.45
1:B:41:LYS:CE	1:B:53:TYR:OH	2.65	0.45
1:A:375:ILE:HG23	7:A:973:HOH:O	2.17	0.45
1:A:528:MET:HE3	1:A:618:PHE:CE1	2.52	0.45
1:A:415:LEU:HD23	1:A:415:LEU:C	2.37	0.45
1:B:158:SER:HB2	1:B:159:PRO:CD	2.47	0.45
1:B:756:SER:O	1:B:760:LYS:HG3	2.18	0.44
1:B:143:ILE:HD13	1:B:178:PRO:HB2	2.00	0.44
1:B:144:THR:HG22	7:B:1123:HOH:O	2.17	0.44
1:B:306:ALA:CB	1:B:310:ARG:HG2	2.44	0.44
1:A:648:LYS:NZ	1:A:699:GLU:OE1	2.50	0.44
1:B:325:MET:O	1:B:344:GLN:HA	2.18	0.44
1:A:471:ARG:HD2	1:A:480:TYR:CE2	2.53	0.44
1:A:214:LEU:HD23	1:A:225:TYR:HB3	2.00	0.44
1:B:359:PRO:HA	7:B:1102:HOH:O	2.18	0.44
1:B:545:ASP:OD1	1:B:554:LYS:NZ	2.40	0.44
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.98	0.44
1:B:206:GLU:OE2	1:B:663:ASP:OD2	2.36	0.43
1:A:268:PHE:CZ	1:A:313:LEU:HD21	2.54	0.43
1:A:192:ASP:C	1:A:193:ILE:HG13	2.39	0.43
1:B:654:ALA:N	1:B:655:PRO:CD	2.81	0.43
1:A:375:ILE:HG22	1:A:376:SER:N	2.33	0.43
1:B:144:THR:CG2	7:B:1123:HOH:O	2.66	0.43
1:A:598:LEU:O	1:A:682:HIS:NE2	2.39	0.43
1:B:63:ILE:HG21	1:B:69:LEU:CD1	2.48	0.43
1:B:641:GLY:O	1:B:691:ARG:HB3	2.17	0.43
1:A:535:ASP:OD2	1:A:538:LYS:HG2	2.18	0.43
1:B:759:ILE:HD12	1:B:759:ILE:HG23	1.66	0.43
1:A:134:ILE:CD1	1:A:164:LEU:HD11	2.49	0.43
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.54	0.43
1:B:158:SER:HA	1:B:216:TRP:CD1	2.53	0.43
1:B:332:GLU:OE1	5:B:805:NAG:O3	2.36	0.43
1:B:106:SER:HG	1:B:157:TRP:HD1	1.67	0.43
1:A:729:ASP:OD2	1:B:757:HIS:HD2	2.02	0.43
1:A:309:GLU:HB3	1:A:330:TYR:HB3	2.00	0.42
1:A:648:LYS:NZ	1:A:699:GLU:OE2	2.52	0.42
2:A:794:NAG:H61	2:A:797:NAG:C7	2.49	0.42
1:A:418:ILE:HD11	1:A:459:VAL:HG12	2.01	0.42
1:A:172:ILE:HD13	1:A:214:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:627:TRP:HB2	1:B:651:ILE:HB	2.02	0.42
1:A:69:LEU:CD1	1:A:107:ILE:HD12	2.50	0.42
1:A:82:GLU:HB2	1:A:467:TYR:OH	2.19	0.41
1:B:364:PHE:CE2	1:B:389:ILE:HD11	2.51	0.41
1:B:571:GLU:CD	1:B:760:LYS:HD3	2.40	0.41
1:B:71:LYS:HZ3	1:B:74:ASN:HA	1.84	0.41
1:A:711:VAL:CG2	1:A:740:HIS:CE1	3.03	0.41
1:B:448:GLU:OE1	1:B:448:GLU:HA	2.20	0.41
1:B:375:ILE:CD1	1:B:387:PHE:HZ	2.34	0.41
1:B:320:GLN:OE1	1:B:669:ARG:HD3	2.21	0.41
1:B:543:LEU:HD12	1:B:567:LEU:HD13	2.01	0.41
1:A:477:LEU:HD22	1:A:500:LEU:CD1	2.51	0.41
1:A:112:GLN:HB3	1:A:113:PHE:CE2	2.55	0.41
1:B:761:GLN:OE1	1:B:761:GLN:C	2.59	0.41
1:B:208:PHE:O	1:B:209:SER:C	2.58	0.41
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.56	0.41
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.55	0.41
1:B:405:ILE:HG13	1:B:429:ARG:HD3	2.03	0.41
1:B:487:ASN:N	7:B:959:HOH:O	2.34	0.41
1:B:512:LYS:NZ	1:B:556:ASP:O	2.49	0.41
1:A:703:ILE:HD13	1:A:703:ILE:HG21	1.78	0.41
1:B:742:ILE:HG22	1:B:742:ILE:O	2.20	0.41
1:A:196:ASN:OD1	1:A:227:GLN:HG3	2.21	0.41
1:A:177:GLU:HA	1:A:178:PRO:HD3	1.94	0.41
1:B:62:TRP:CG	1:B:462:SER:HA	2.56	0.41
1:A:539:LYS:HE2	1:A:617:GLY:O	2.21	0.41
1:B:39:SER:CB	1:B:40:ARG:HD3	2.49	0.41
1:B:236:ILE:HG12	1:B:712:HIS:ND1	2.34	0.41
1:B:471:ARG:HG3	1:B:480:TYR:CE2	2.56	0.41
1:A:481:THR:OG1	1:A:483:HIS:CE1	2.71	0.40
1:B:435:GLN:NE2	7:B:952:HOH:O	2.51	0.40
1:B:669:ARG:HD2	7:B:1030:HOH:O	2.20	0.40
1:B:285:ILE:HG23	1:B:336:ARG:HH11	1.85	0.40
1:B:562:ASN:ND2	1:B:562:ASN:C	2.73	0.40
1:B:136:ASP:C	1:B:136:ASP:OD1	2.60	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/748 (97%)	694 (96%)	31 (4%)	1 (0%)	56	64
1	B	726/748 (97%)	689 (95%)	36 (5%)	1 (0%)	56	64
All	All	1452/1496 (97%)	1383 (95%)	67 (5%)	2 (0%)	56	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	B	630	SER

### 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	651/669 (97%)	610 (94%)	41 (6%)	22	24
1	B	651/669 (97%)	605 (93%)	46 (7%)	18	19
All	All	1302/1338 (97%)	1215 (93%)	87 (7%)	20	21

All (87) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	50	LYS
1	A	51	ASN
1	A	60	LEU

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Mol	Chain	Res	Type
1	A	65	ASP
1	A	87	SER
1	A	88	VAL
1	A	133	ASP
1	A	145	GLU
1	A	156	THR
1	A	158	SER
1	A	180	LEU
1	A	271	VAL
1	A	278	SER
1	A	300	LEU
1	A	316	LEU
1	A	333	SER
1	A	350	THR
1	A	367	ASP
1	A	385	CYS
1	A	392	LYS
1	A	399	LYS
1	A	412	SER
1	A	413	ASP
1	A	471	ARG
1	A	472	CYS
1	A	479	LEU
1	A	482	LEU
1	A	485	SER
1	A	500	LEU
1	A	502	LYS
1	A	528	MET
1	A	594	ILE
1	A	597	ARG
1	A	615	LYS
1	A	621	ASN
1	A	627	TRP
1	A	677	GLU
1	A	704	HIS
1	A	726	VAL
1	A	762	CYS
1	B	39	SER
1	B	40	ARG
1	B	41	LYS
1	B	51	ASN
1	B	59	SER

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Mol	Chain	Res	Type
1	B	60	LEU
1	B	77	LEU
1	B	88	VAL
1	B	91	GLU
1	B	92	ASN
1	B	140	ARG
1	B	156	THR
1	B	214	LEU
1	B	230	ASP
1	B	236	ILE
1	B	244	GLU
1	B	271	VAL
1	B	279	VAL
1	B	288	THR
1	B	327	ILE
1	B	333	SER
1	B	340	LEU
1	B	350	THR
1	B	358	ARG
1	B	361	GLU
1	B	376	SER
1	B	379	GLU
1	B	389	ILE
1	B	472	CYS
1	B	479	LEU
1	B	500	LEU
1	B	502	LYS
1	B	507	VAL
1	B	536	LYS
1	B	542	LEU
1	B	543	LEU
1	B	562	ASN
1	B	566	TYR
1	B	597	ARG
1	B	621	ASN
1	B	622	LYS
1	B	680	LEU
1	B	684	ARG
1	B	745	SER
1	B	761	GLN
1	B	762	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	92	ASN
1	A	169	ASN
1	A	247	GLN
1	A	263	ASN
1	A	298	HIS
1	A	314	GLN
1	A	338	ASN
1	A	363	HIS
1	A	483	HIS
1	A	533	HIS
1	A	621	ASN
1	A	748	HIS
1	A	757	HIS
1	B	75	ASN
1	B	123	GLN
1	B	169	ASN
1	B	263	ASN
1	B	298	HIS
1	B	383	HIS
1	B	487	ASN
1	B	562	ASN
1	B	586	GLN
1	B	621	ASN
1	B	682	HIS
1	B	697	GLN
1	B	757	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 ⓘ

15 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	A	794	1,2	14,14,15	1.46	3 (21%)	15,19,21	1.61	2 (13%)
3	NAG	A	796	1,3	14,14,15	1.25	2 (14%)	15,19,21	2.04	7 (46%)
2	NAG	A	797	2	14,14,15	0.84	0	15,19,21	2.15	7 (46%)
3	NAG	A	798	3	14,14,15	0.88	0	15,19,21	1.20	1 (6%)
2	NAG	A	800	1,2	14,14,15	0.69	0	15,19,21	2.32	4 (26%)
2	NAG	A	801	2	14,14,15	0.80	1 (7%)	15,19,21	1.30	1 (6%)
3	LGU	A	802	3	11,11,13	0.82	1 (9%)	14,15,19	2.52	5 (35%)
3	MAN	A	803	3	11,11,12	1.04	1 (9%)	14,15,17	1.72	1 (7%)
3	LGU	A	804	3	11,11,13	0.87	0	14,15,19	2.02	4 (28%)
2	NAG	B	794	1,2	14,14,15	1.16	1 (7%)	15,19,21	1.48	3 (20%)
2	NAG	B	797	2	14,14,15	1.16	1 (7%)	15,19,21	1.78	5 (33%)
5	NDG	B	799	1,5	14,14,15	1.11	1 (7%)	15,19,21	1.50	3 (20%)
5	NDG	B	800	1,5	14,14,15	0.85	1 (7%)	15,19,21	1.31	2 (13%)
5	NAG	B	801	5	14,14,15	0.63	0	15,19,21	1.66	3 (20%)
5	NAG	B	805	5	14,14,15	0.52	0	15,19,21	1.60	2 (13%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	794	1,2	-	0/6/23/26	0/1/1/1
3	NAG	A	796	1,3	-	0/6/23/26	0/1/1/1
2	NAG	A	797	2	-	0/6/23/26	0/1/1/1
3	NAG	A	798	3	-	0/6/23/26	0/1/1/1
2	NAG	A	800	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	801	2	-	0/6/23/26	0/1/1/1
3	LGU	A	802	3	1/1/4/6	0/2/19/24	0/1/1/1
3	MAN	A	803	3	-	0/2/19/22	0/1/1/1
3	LGU	A	804	3	1/1/4/6	0/2/19/24	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	794	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	797	2	-	0/6/23/26	0/1/1/1
5	NDG	B	799	1,5	-	0/6/23/26	0/1/1/1
5	NDG	B	800	1,5	-	0/6/23/26	0/1/1/1
5	NAG	B	801	5	-	0/6/23/26	0/1/1/1
5	NAG	B	805	5	-	0/6/23/26	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	797	NAG	O5-C1	-3.44	1.38	1.43
3	A	796	NAG	O5-C1	-3.39	1.38	1.43
2	A	794	NAG	C2-N2	-3.06	1.40	1.46
2	A	794	NAG	O5-C1	-3.05	1.38	1.43
5	B	800	NDG	O-C1	-2.62	1.39	1.43
3	A	803	MAN	O5-C1	-2.61	1.39	1.43
2	B	794	NAG	C2-N2	-2.27	1.42	1.46
3	A	796	NAG	O5-C5	-2.14	1.38	1.43
2	A	794	NAG	C1-C2	2.10	1.55	1.52
3	A	802	LGU	C4-C5	2.12	1.57	1.53
2	A	801	NAG	C1-C2	2.17	1.55	1.52
5	B	799	NDG	C1-C2	2.57	1.56	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	803	MAN	O5-C1-C2	-5.50	101.93	110.86
3	A	802	LGU	C1-C2-C3	-4.85	103.80	109.54
3	A	804	LGU	O5-C1-C2	-4.36	103.78	110.86
3	A	804	LGU	C1-O5-C5	-3.95	107.24	112.25
3	A	796	NAG	O3-C3-C4	-3.16	103.22	110.34
3	A	796	NAG	O6-C6-C5	-3.14	100.97	111.33
3	A	796	NAG	O4-C4-C3	-2.74	104.18	110.34
3	A	798	NAG	O4-C4-C3	-2.69	104.27	110.34
5	B	801	NAG	C3-C4-C5	-2.65	105.58	110.20
2	B	797	NAG	C3-C2-N2	-2.62	104.28	110.56
2	B	794	NAG	O3-C3-C2	-2.49	104.17	109.11
2	B	797	NAG	O4-C4-C3	-2.49	104.73	110.34
2	A	797	NAG	C3-C2-N2	-2.45	104.69	110.56
2	A	797	NAG	O6-C6-C5	-2.42	103.34	111.33
3	A	796	NAG	C2-N2-C7	-2.38	119.98	123.04
3	A	802	LGU	C2-C3-C4	-2.37	107.02	111.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	794	NAG	O7-C7-C8	-2.37	117.72	122.06
2	A	797	NAG	C6-C5-C4	-2.26	107.45	113.02
2	A	800	NAG	O3-C3-C4	-2.17	105.46	110.34
2	A	797	NAG	C3-C4-C5	-2.14	106.47	110.20
3	A	796	NAG	O5-C5-C6	-2.12	102.76	107.35
5	B	799	NDG	O7-C7-C8	-2.09	118.23	122.06
2	A	794	NAG	C3-C2-N2	-2.06	105.62	110.56
5	B	800	NDG	O7-C7-C8	-2.01	118.37	122.06
5	B	799	NDG	C2-N2-C7	2.10	125.73	123.04
3	A	796	NAG	C1-O5-C5	2.17	115.00	112.25
3	A	802	LGU	O5-C1-C2	2.18	114.40	110.86
5	B	805	NAG	O4-C4-C3	2.20	115.30	110.34
2	B	794	NAG	C1-O5-C5	2.24	115.10	112.25
2	A	801	NAG	O5-C5-C6	2.27	112.26	107.35
2	A	800	NAG	O5-C5-C6	2.35	112.43	107.35
2	A	797	NAG	C2-N2-C7	2.36	126.07	123.04
3	A	804	LGU	C2-C3-C4	2.37	115.07	111.04
3	A	804	LGU	C3-C4-C5	2.49	114.54	110.20
2	A	797	NAG	O3-C3-C2	2.53	114.12	109.11
5	B	801	NAG	O4-C4-C5	2.58	116.08	109.24
2	B	797	NAG	C1-O5-C5	2.66	115.62	112.25
2	B	797	NAG	O7-C7-N2	2.70	127.36	121.86
5	B	800	NDG	O7-C7-N2	2.76	127.48	121.86
2	A	800	NAG	C3-C4-C5	3.09	115.58	110.20
3	A	796	NAG	C3-C4-C5	3.09	115.58	110.20
2	B	797	NAG	C3-C4-C5	3.14	115.67	110.20
5	B	799	NDG	O4-C4-C3	3.24	117.62	110.34
3	A	802	LGU	O2-C2-C1	3.41	116.05	109.21
2	A	794	NAG	C2-N2-C7	4.40	128.69	123.04
5	B	801	NAG	C1-O5-C5	4.72	118.24	112.25
5	B	805	NAG	C1-O5-C5	5.22	118.87	112.25
2	A	797	NAG	C1-O5-C5	5.35	119.04	112.25
3	A	802	LGU	C1-O5-C5	5.53	119.27	112.25
2	A	800	NAG	C1-O5-C5	7.37	121.60	112.25

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	802	LGU	C5
3	A	804	LGU	C5

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	794	NAG	1	0
2	A	797	NAG	1	0
2	B	794	NAG	1	0
5	B	800	NDG	1	0
5	B	805	NAG	1	0

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
4	NAG	A	799	1	14,14,15	0.88	0	15,19,21	1.44	2 (13%)
6	PZF	A	900	-	32,32,32	1.03	2 (6%)	41,46,46	2.29	13 (31%)
4	NAG	B	796	1	14,14,15	1.10	1 (7%)	15,19,21	2.37	6 (40%)
6	PZF	B	900	-	32,32,32	1.57	8 (25%)	41,46,46	2.64	15 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	799	1	-	0/6/23/26	0/1/1/1
6	PZF	A	900	-	-	0/14/26/26	0/4/4/4
4	NAG	B	796	1	-	0/6/23/26	0/1/1/1
6	PZF	B	900	-	-	0/14/26/26	0/4/4/4

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	796	NAG	O5-C1	-3.44	1.38	1.43
6	B	900	PZF	C26-C21	-3.18	1.34	1.39
6	B	900	PZF	C21-C13	-3.16	1.47	1.52
6	B	900	PZF	F29-C24	-2.93	1.28	1.35
6	A	900	PZF	C21-C13	-2.78	1.48	1.52
6	A	900	PZF	C2-N3	-2.21	1.29	1.34
6	B	900	PZF	O18-C4	2.03	1.38	1.35
6	B	900	PZF	C11-C10	2.14	1.42	1.39
6	B	900	PZF	C8-N9	2.22	1.38	1.33
6	B	900	PZF	C14-N15	2.41	1.49	1.46
6	B	900	PZF	C4-N3	2.87	1.36	1.32

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	900	PZF	N7-C8-N9	-5.00	120.25	128.67
4	B	796	NAG	O4-C4-C5	-4.77	96.60	109.24
6	B	900	PZF	N7-C8-N9	-4.20	121.59	128.67
6	A	900	PZF	C11-C10-N9	-3.73	117.11	122.02
6	B	900	PZF	C11-C12-N7	-3.30	116.60	122.49
6	B	900	PZF	C11-C10-N9	-3.08	117.96	122.02
6	B	900	PZF	O18-C4-N3	-2.90	114.61	119.92
6	B	900	PZF	C5-C4-N3	-2.85	120.58	124.81
6	A	900	PZF	C26-C25-C24	-2.78	118.61	121.13
6	A	900	PZF	C23-C22-C21	-2.53	121.09	123.78
4	B	796	NAG	C6-C5-C4	-2.48	106.90	113.02
4	A	799	NAG	C2-N2-C7	-2.44	119.91	123.04
6	A	900	PZF	C2-C1-C10	-2.40	116.83	120.89
6	B	900	PZF	C2-C1-C10	-2.29	117.01	120.89
6	B	900	PZF	C26-C25-C24	-2.06	119.26	121.13
4	B	796	NAG	C3-C2-N2	-2.03	105.70	110.56
6	A	900	PZF	N7-C12-N15	2.05	119.92	116.96
6	A	900	PZF	C14-N15-C16	2.09	116.84	112.42
6	A	900	PZF	F28-C25-C24	2.10	124.24	118.51
6	B	900	PZF	C14-C13-C21	2.16	118.17	114.94
4	B	796	NAG	O5-C5-C6	2.19	112.08	107.35
6	B	900	PZF	C11-C10-C1	2.25	124.87	121.89
6	B	900	PZF	C21-C26-C25	2.36	122.37	119.03
6	A	900	PZF	C21-C26-C25	2.44	122.48	119.03
6	A	900	PZF	C2-N3-C4	3.16	119.23	116.72
6	B	900	PZF	C8-N9-C10	3.17	120.19	115.74
4	A	799	NAG	C1-O5-C5	3.18	116.28	112.25
4	B	796	NAG	C3-C4-C5	4.08	117.32	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	796	NAG	C1-O5-C5	4.16	117.53	112.25
6	A	900	PZF	C10-C11-C12	4.21	119.73	116.77
6	B	900	PZF	C2-N3-C4	4.44	120.24	116.72
6	B	900	PZF	O18-C4-C5	4.52	124.78	116.79
6	A	900	PZF	C8-N9-C10	5.62	123.63	115.74
6	B	900	PZF	C10-C11-C12	6.60	121.42	116.77
6	A	900	PZF	C8-N7-C12	6.84	120.09	114.84
6	B	900	PZF	C8-N7-C12	9.40	122.06	114.84

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	900	PZF	1	0
4	B	796	NAG	1	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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	728/748 (97%)	1.58	196 (26%)  	46, 55, 70, 79	0
1	B	728/748 (97%)	1.38	149 (20%)  	44, 55, 71, 79	0
All	All	1456/1496 (97%)	1.48	345 (23%)  	44, 55, 71, 79	0

All (345) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	SER	9.8
1	A	279	VAL	8.9
1	A	74	ASN	8.5
1	A	93	SER	8.0
1	A	94	THR	7.9
1	A	280	THR	7.2
1	A	96	ASP	6.8
1	A	277	SER	6.7
1	B	279	VAL	6.6
1	A	333	SER	6.6
1	A	72	GLN	6.6
1	A	334	SER	6.6
1	A	97	GLU	6.5
1	B	280	THR	6.5
1	A	95	PHE	6.4
1	A	92	ASN	6.4
1	B	333	SER	6.4
1	A	73	GLU	6.0
1	B	74	ASN	5.9
1	A	140	ARG	5.8
1	A	331	ASP	5.8
1	A	537	SER	5.7
1	A	76	ILE	5.7
1	B	73	GLU	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	538	LYS	5.3
1	A	519	LEU	5.2
1	A	135	TYR	5.2
1	B	93	SER	5.2
1	A	91	GLU	5.1
1	B	537	SER	5.1
1	A	136	ASP	5.0
1	A	281	ASN	5.0
1	A	278	SER	4.8
1	B	96	ASP	4.7
1	A	75	ASN	4.7
1	A	99	GLY	4.6
1	A	759	ILE	4.6
1	B	331	ASP	4.6
1	B	681	ASP	4.5
1	A	101	SER	4.5
1	A	521	GLU	4.5
1	B	334	SER	4.5
1	B	94	THR	4.5
1	A	452	GLU	4.4
1	A	138	ASN	4.3
1	B	97	GLU	4.3
1	A	520	ASN	4.3
1	A	522	THR	4.3
1	B	486	VAL	4.3
1	B	505	GLN	4.2
1	A	144	THR	4.1
1	B	92	ASN	4.1
1	A	703	ILE	4.1
1	B	138	ASN	4.1
1	B	335	GLY	4.0
1	A	142	LEU	4.0
1	B	393	ASP	4.0
1	B	617	GLY	3.9
1	A	511	SER	3.9
1	B	538	LYS	3.9
1	A	498	SER	3.8
1	A	276	LEU	3.8
1	A	133	ASP	3.8
1	A	98	PHE	3.7
1	A	616	MET	3.7
1	A	283	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	139	LYS	3.7
1	A	454	CYS	3.6
1	A	535	ASP	3.6
1	A	487	ASN	3.6
1	B	140	ARG	3.6
1	B	616	MET	3.5
1	A	766	PRO	3.5
1	A	100	HIS	3.5
1	B	141	GLN	3.5
1	B	506	ASN	3.5
1	A	651	ILE	3.5
1	B	609	ALA	3.5
1	A	573	ILE	3.4
1	B	533	HIS	3.4
1	B	405	ILE	3.4
1	B	281	ASN	3.4
1	A	407	ILE	3.3
1	A	486	VAL	3.3
1	B	665	VAL	3.3
1	B	701	LEU	3.3
1	B	95	PHE	3.3
1	A	301	CYS	3.3
1	A	500	LEU	3.3
1	B	732	ALA	3.3
1	A	488	ASP	3.3
1	A	533	HIS	3.2
1	B	407	ILE	3.2
1	A	335	GLY	3.2
1	B	651	ILE	3.2
1	A	332	GLU	3.2
1	A	702	LEU	3.2
1	A	39	SER	3.2
1	A	103	ASN	3.2
1	A	544	LEU	3.2
1	B	547	TYR	3.2
1	B	703	ILE	3.2
1	B	719	ILE	3.1
1	A	665	VAL	3.1
1	A	734	TRP	3.1
1	A	179	ASN	3.1
1	B	332	GLU	3.1
1	A	150	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	300	LEU	3.1
1	A	536	LYS	3.1
1	A	374	ILE	3.1
1	A	677	GLU	3.1
1	B	99	GLY	3.1
1	A	275	SER	3.0
1	B	666	TYR	3.0
1	A	422	TYR	3.0
1	B	208	PHE	3.0
1	A	110	ASP	3.0
1	A	313	LEU	3.0
1	B	91	GLU	3.0
1	A	70	TYR	3.0
1	B	357	PHE	3.0
1	A	679	ASN	3.0
1	A	303	VAL	3.0
1	B	374	ILE	2.9
1	A	701	LEU	2.9
1	A	653	VAL	2.9
1	B	356	ARG	2.9
1	B	418	ILE	2.9
1	A	141	GLN	2.9
1	A	89	PHE	2.9
1	B	730	PHE	2.9
1	B	316	LEU	2.9
1	A	177	GLU	2.9
1	A	501	ASP	2.9
1	B	585	TYR	2.9
1	B	389	ILE	2.9
1	A	404	VAL	2.9
1	B	766	PRO	2.9
1	A	51	ASN	2.9
1	B	761	GLN	2.9
1	B	277	SER	2.9
1	A	440	THR	2.8
1	B	384	ILE	2.8
1	A	733	MET	2.8
1	A	676	PRO	2.8
1	A	438	ASP	2.8
1	B	372	TYR	2.8
1	A	539	LYS	2.8
1	B	519	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	700	TYR	2.8
1	B	570	THR	2.8
1	A	325	MET	2.8
1	A	765	LEU	2.8
1	A	547	TYR	2.8
1	A	187	TRP	2.8
1	B	274	ASP	2.8
1	A	640	LEU	2.8
1	B	762	CYS	2.8
1	A	614	SER	2.7
1	A	764	SER	2.7
1	A	656	VAL	2.7
1	A	751	ILE	2.7
1	B	573	ILE	2.7
1	A	546	VAL	2.7
1	B	755	MET	2.7
1	B	223	LEU	2.7
1	A	719	ILE	2.7
1	A	86	SER	2.7
1	B	278	SER	2.7
1	B	350	THR	2.7
1	A	336	ARG	2.7
1	A	652	ALA	2.6
1	A	268	PHE	2.6
1	B	336	ARG	2.6
1	B	551	CYS	2.6
1	B	101	SER	2.6
1	B	635	VAL	2.6
1	A	732	ALA	2.6
1	A	46	THR	2.6
1	A	357	PHE	2.6
1	A	763	PHE	2.6
1	A	394	CYS	2.6
1	B	214	LEU	2.6
1	B	639	VAL	2.6
1	A	52	THR	2.6
1	A	304	THR	2.6
1	B	172	ILE	2.6
1	B	98	PHE	2.6
1	A	678	ASP	2.6
1	B	404	VAL	2.6
1	B	711	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	675	THR	2.6
1	B	52	THR	2.6
1	B	734	TRP	2.6
1	B	110	ASP	2.6
1	B	40	ARG	2.6
1	B	207	VAL	2.6
1	B	656	VAL	2.5
1	A	626	ILE	2.5
1	B	678	ASP	2.5
1	B	54	ARG	2.5
1	A	700	TYR	2.5
1	B	702	LEU	2.5
1	A	108	SER	2.5
1	A	359	PRO	2.5
1	A	85	ASN	2.5
1	B	502	LYS	2.5
1	B	144	THR	2.5
1	B	283	THR	2.5
1	A	476	GLY	2.5
1	A	615	LYS	2.5
1	B	339	CYS	2.5
1	B	546	VAL	2.5
1	A	742	ILE	2.5
1	A	612	GLN	2.5
1	B	338	ASN	2.5
1	A	371	PHE	2.5
1	B	675	THR	2.4
1	B	454	CYS	2.4
1	A	90	LEU	2.4
1	B	677	GLU	2.4
1	B	680	LEU	2.4
1	B	653	VAL	2.4
1	B	724	VAL	2.4
1	A	180	LEU	2.4
1	B	410	LEU	2.4
1	A	713	PHE	2.4
1	B	461	PHE	2.4
1	B	415	LEU	2.4
1	B	544	LEU	2.4
1	A	88	VAL	2.4
1	B	759	ILE	2.4
1	A	413	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	723	LEU	2.4
1	A	666	TYR	2.4
1	A	134	ILE	2.4
1	A	329	ASP	2.4
1	A	418	ILE	2.4
1	A	633	GLY	2.4
1	B	517	ILE	2.4
1	B	364	PHE	2.4
1	B	713	PHE	2.4
1	A	532	PRO	2.4
1	B	543	LEU	2.4
1	A	111	GLY	2.4
1	A	114	ILE	2.4
1	B	303	VAL	2.4
1	B	470	LEU	2.3
1	B	584	GLY	2.3
1	B	631	TYR	2.3
1	B	578	PHE	2.3
1	A	681	ASP	2.3
1	B	650	GLY	2.3
1	A	203	TYR	2.3
1	A	752	TYR	2.3
1	A	451	PRO	2.3
1	A	604	GLU	2.3
1	A	627	TRP	2.3
1	B	482	LEU	2.3
1	A	405	ILE	2.3
1	A	639	VAL	2.3
1	A	735	TYR	2.3
1	A	567	LEU	2.3
1	B	203	TYR	2.3
1	B	459	VAL	2.3
1	B	735	TYR	2.3
1	A	208	PHE	2.3
1	B	243	ASP	2.3
1	A	207	VAL	2.3
1	A	609	ALA	2.3
1	A	758	PHE	2.3
1	B	535	ASP	2.3
1	B	115	LEU	2.3
1	A	315	TRP	2.2
1	A	384	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	548	ALA	2.2
1	B	75	ASN	2.2
1	A	44	THR	2.2
1	A	415	LEU	2.2
1	A	591	MET	2.2
1	A	680	LEU	2.2
1	A	723	LEU	2.2
1	A	356	ARG	2.2
1	A	502	LYS	2.2
1	A	607	ILE	2.2
1	A	146	GLU	2.2
1	B	456	TYR	2.2
1	A	113	PHE	2.2
1	A	364	PHE	2.2
1	A	695	PHE	2.2
1	B	695	PHE	2.2
1	B	359	PRO	2.2
1	A	137	LEU	2.2
1	B	375	ILE	2.2
1	A	635	VAL	2.2
1	B	371	PHE	2.2
1	A	290	PRO	2.2
1	A	116	LEU	2.2
1	B	640	LEU	2.2
1	B	688	VAL	2.1
1	B	417	TYR	2.1
1	B	429	ARG	2.1
1	A	220	GLY	2.1
1	B	457	TYR	2.1
1	A	340	LEU	2.1
1	A	449	LEU	2.1
1	A	274	ASP	2.1
1	A	358	ARG	2.1
1	B	626	ILE	2.1
1	B	108	SER	2.1
1	A	647	PHE	2.1
1	A	563	TRP	2.1
1	A	77	LEU	2.1
1	A	350	THR	2.1
1	B	300	LEU	2.1
1	B	567	LEU	2.1
1	B	362	PRO	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	214	LEU	2.1
1	A	431	LEU	2.1
1	A	84	GLY	2.1
1	B	647	PHE	2.1
1	A	670	TYR	2.1
1	B	530	LEU	2.1
1	B	576	ALA	2.1
1	B	717	ALA	2.1
1	A	106	SER	2.1
1	A	293	MET	2.0
1	A	447	CYS	2.0
1	A	753	THR	2.0
1	B	353	TRP	2.0
1	B	487	ASN	2.0
1	A	316	LEU	2.0
1	A	373	LYS	2.0
1	B	268	PHE	2.0
1	B	306	ALA	2.0
1	B	598	LEU	2.0
1	A	372	TYR	2.0
1	A	360	SER	2.0
1	B	452	GLU	2.0
1	B	525	TRP	2.0
1	A	747	ALA	2.0
1	A	690	SER	2.0
1	A	704	HIS	2.0
1	A	551	CYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	NAG	A	800	14/15	0.73	0.33	4.72	81,87,90,94	0
3	NAG	A	796	14/15	0.85	0.25	1.89	51,59,64,69	0
5	NDG	B	800	14/15	0.86	0.30	1.71	75,84,87,91	0
5	NAG	B	805	14/15	0.80	0.33	1.45	87,91,94,95	0
2	NAG	A	794	14/15	0.92	0.24	0.51	44,48,53,63	0
2	NAG	B	794	14/15	0.92	0.13	-2.22	42,47,56,61	0
2	NAG	A	797	14/15	0.76	0.30	-	75,83,85,86	0
2	NAG	B	797	14/15	0.84	0.28	-	63,68,78,80	0
5	NAG	B	801	14/15	0.69	0.48	-	96,100,102,103	0
3	NAG	A	798	14/15	0.69	0.42	-	65,76,79,83	0
2	NAG	A	801	14/15	0.75	0.52	-	99,102,104,105	0
5	NDG	B	799	14/15	0.84	0.39	-	79,85,92,93	0
3	LGU	A	804	11/13	0.55	0.44	-	87,93,96,98	0
3	MAN	A	803	11/12	0.83	0.40	-	89,91,93,96	0
3	LGU	A	802	11/13	0.83	0.49	-	88,93,97,98	0

## 6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	NAG	B	796	14/15	0.89	0.24	2.16	54,59,68,72	0
6	PZF	A	900	29/29	0.95	0.14	-2.65	44,57,71,80	0
6	PZF	B	900	29/29	0.97	0.12	-3.13	35,44,62,72	0
4	NAG	A	799	14/15	0.78	0.34	-	77,82,87,88	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.