



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 01:27 am GMT

PDB ID : 1FZD  
Title : STRUCTURE OF RECOMBINANT ALPHAEC DOMAIN FROM HUMAN FIBRINOGEN-420  
Authors : Spraggon, G.; Applegate, D.; Everse, S.J.; Zhang, J.-Z.; Veerapandian, L.; Redman, C.; Doolittle, R.F.; Grieninger, G.  
Deposited on : 1998-06-22  
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

<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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

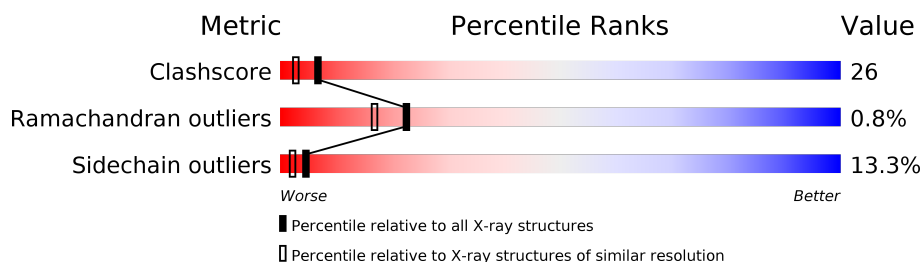
# 1 Overall quality at a glance

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	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (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 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	201	
1	B	201	
1	C	201	
1	D	201	
1	E	201	
1	F	201	
1	G	201	

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Mol	Chain	Length	Quality of chain
1	H	201	

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	MAN	A	13	-	-	X	-
2	MAN	A	14	X	-	X	-
2	MAN	A	15	-	-	X	-
2	NAG	C	12	-	-	X	-
2	MAN	C	13	-	-	X	-
2	MAN	C	14	X	-	X	-
2	MAN	C	15	X	-	-	-
2	NAG	D	10	-	X	-	-
2	NAG	D	12	-	-	X	-
2	MAN	D	13	-	-	X	-
2	MAN	D	15	X	-	-	-
3	NAG	E	10	-	X	X	-
3	NAG	G	10	-	-	X	-
3	NAG	G	11	-	-	X	-
3	NAG	H	10	-	-	X	-
3	NAG	H	11	-	-	X	-
4	NAG	B	12	-	-	X	-
4	MAN	B	13	-	-	X	-
4	MAN	B	14	X	-	X	-

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 13595 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 FIBRINOGEN-420.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	B	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	C	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	D	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	E	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	F	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	G	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			
1	H	197	Total	C	N	O	S	0	0	0
			1585	992	273	315	5			

- Molecule 2 is a polymer of unknown type called SUGAR (6-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	6	Total	C	N	O	0	0
			75	42	3	30		
2	C	6	Total	C	N	O	0	0
			75	42	3	30		
2	D	6	Total	C	N	O	0	0
			75	42	3	30		

- Molecule 3 is SUGAR (6-MER) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is a polymer of unknown type called SUGAR (5-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	5	Total	C	N	O	0	0
			60	34	2	24		

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	F	2	Total	C	N	O	1	0
			28	16	2	10		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	1	Total 1	Ca 1	0	0
6	D	1	Total 1	Ca 1	0	0
6	E	1	Total 1	Ca 1	0	0
6	H	1	Total 1	Ca 1	0	0
6	B	1	Total 1	Ca 1	0	0
6	C	1	Total 1	Ca 1	0	0
6	A	1	Total 1	Ca 1	0	0
6	F	1	Total 1	Ca 1	0	0

- Molecule 7 is water.

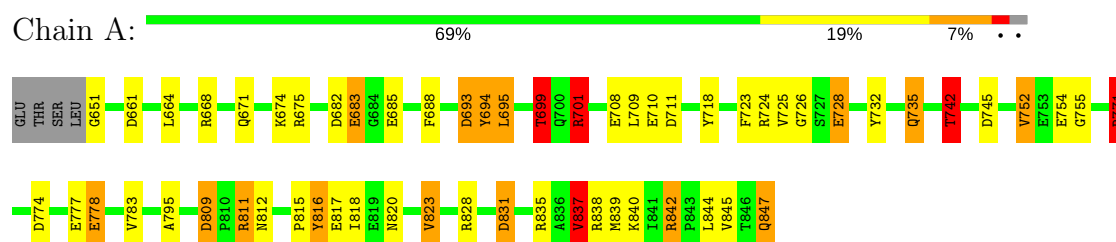
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	70	Total 70	O 70	0	0
7	B	76	Total 76	O 76	0	0
7	C	71	Total 71	O 71	0	0
7	D	74	Total 74	O 74	0	0
7	E	52	Total 52	O 52	0	0
7	F	63	Total 63	O 63	0	0
7	G	56	Total 56	O 56	0	0
7	H	34	Total 34	O 34	0	0

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

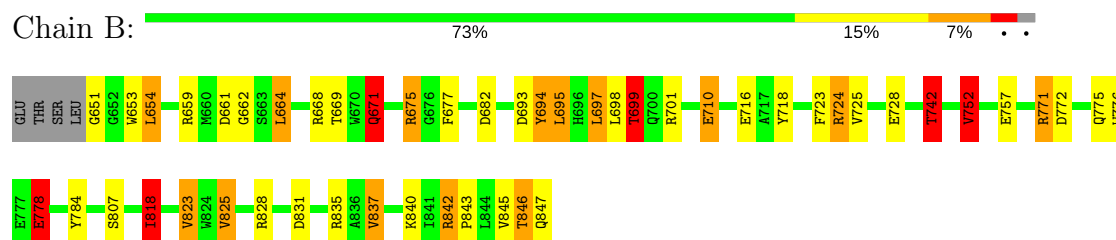
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

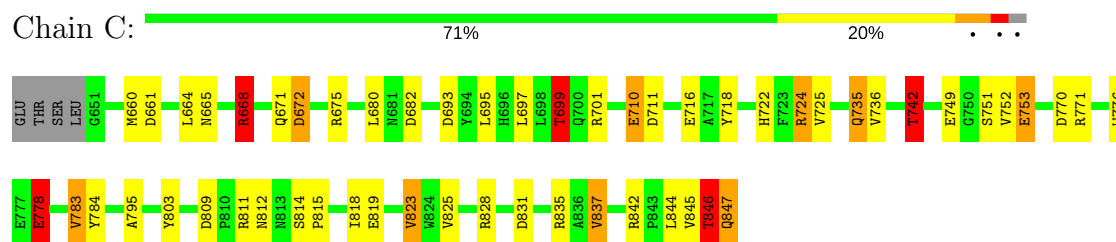
#### • Molecule 1: FIBRINOGEN-420



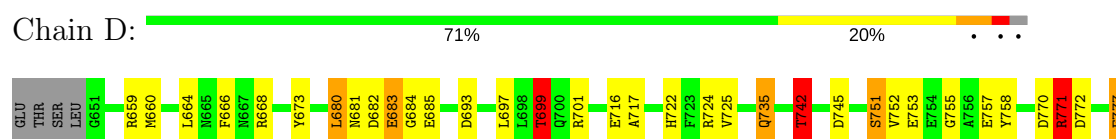
#### • Molecule 1: FIBRINOGEN-420



#### • Molecule 1: FIBRINOGEN-420



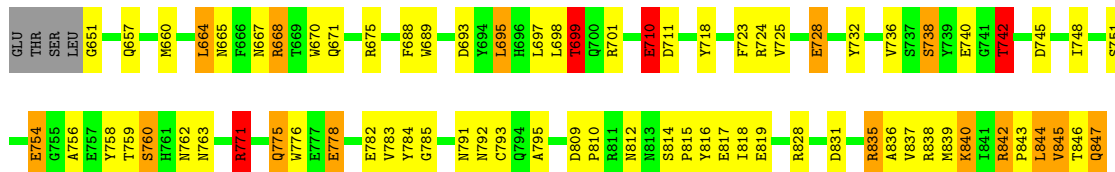
#### • Molecule 1: FIBRINOGEN-420





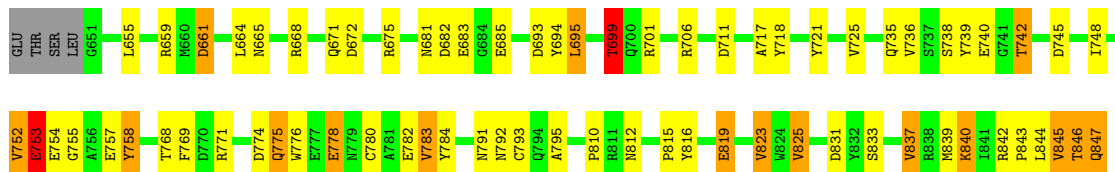
## ● Molecule 1: FIBRINOGEN-420

Chain E:



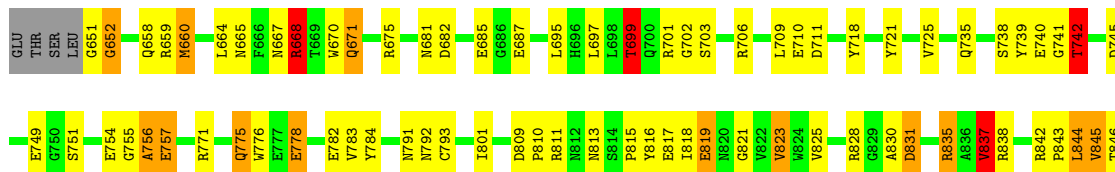
## ● Molecule 1: FIBRINOGEN-420

Chain F:



## ● Molecule 1: FIBRINOGEN-420

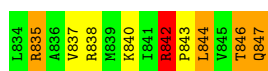
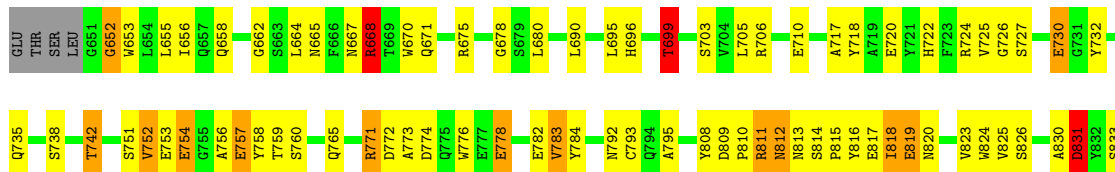
Chain G:



Q847

## ● Molecule 1: FIBRINOGEN-420

Chain H:





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.25Å 105.18Å 71.14Å 104.60° 108.95° 71.47°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	91.2 (20.00-2.10)	Depositor
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	REFMAC, X-PLOR	Depositor
R, $R_{free}$	0.195 , 0.255	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	13595	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	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: CA, NAG, NDG, MAN

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	0.85	0/1628	1.96	46/2208 (2.1%)
1	B	0.82	0/1628	1.81	37/2208 (1.7%)
1	C	0.77	0/1628	1.66	28/2208 (1.3%)
1	D	0.79	0/1628	1.75	29/2208 (1.3%)
1	E	0.60	0/1628	1.41	26/2208 (1.2%)
1	F	0.58	0/1628	1.35	14/2208 (0.6%)
1	G	0.56	0/1628	1.34	12/2208 (0.5%)
1	H	0.52	0/1628	1.41	16/2208 (0.7%)
All	All	0.70	0/13024	1.60	208/17664 (1.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	2
1	G	0	1
2	A	1	0
2	C	2	0
2	D	1	0
4	B	1	0
All	All	5	8

There are no bond length outliers.

All (208) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	771	ARG	CD-NE-CZ	37.32	175.85	123.60
1	B	771	ARG	CD-NE-CZ	28.31	163.23	123.60
1	D	668	ARG	NE-CZ-NH2	-17.90	111.35	120.30
1	D	659	ARG	NE-CZ-NH1	16.59	128.60	120.30
1	B	840	LYS	CA-CB-CG	13.12	142.26	113.40
1	A	842	ARG	NE-CZ-NH1	12.51	126.56	120.30
1	B	828	ARG	NE-CZ-NH2	-12.36	114.12	120.30
1	C	701	ARG	NE-CZ-NH2	-12.29	114.16	120.30
1	C	845	VAL	C-N-CA	12.28	152.40	121.70
1	A	828	ARG	NE-CZ-NH2	-11.79	114.41	120.30
1	A	831	ASP	CB-CG-OD2	-11.76	107.72	118.30
1	H	706	ARG	NE-CZ-NH2	-11.49	114.55	120.30
1	D	842	ARG	NE-CZ-NH1	11.02	125.81	120.30
1	D	771	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	H	706	ARG	NE-CZ-NH1	10.81	125.70	120.30
1	D	840	LYS	CA-CB-CG	10.48	136.46	113.40
1	D	771	ARG	CD-NE-CZ	10.33	138.06	123.60
1	A	728	GLU	OE1-CD-OE2	-9.97	111.33	123.30
1	D	838	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	D	668	ARG	NE-CZ-NH1	9.93	125.26	120.30
1	B	710	GLU	OE1-CD-OE2	9.73	134.97	123.30
1	B	772	ASP	CB-CG-OD1	9.64	126.98	118.30
1	H	724	ARG	CD-NE-CZ	9.62	137.06	123.60
1	C	742	THR	N-CA-CB	-9.57	92.11	110.30
1	B	659	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	B	842	ARG	NE-CZ-NH2	9.55	125.07	120.30
1	A	823	VAL	N-CA-CB	-9.54	90.52	111.50
1	D	772	ASP	CB-CG-OD1	9.48	126.83	118.30
1	A	701	ARG	CD-NE-CZ	9.20	136.48	123.60
1	B	661	ASP	CB-CG-OD1	9.19	126.57	118.30
1	H	724	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	G	711	ASP	CB-CG-OD1	9.11	126.50	118.30
1	G	668	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	A	693	ASP	CB-CG-OD2	-8.87	110.32	118.30
1	B	742	THR	N-CA-CB	-8.57	94.01	110.30
1	A	742	THR	N-CA-CB	-8.44	94.26	110.30
1	C	771	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	B	693	ASP	CB-CG-OD2	-8.37	110.76	118.30
1	D	742	THR	N-CA-CB	-8.36	94.41	110.30
1	A	752	VAL	CB-CA-C	-8.30	95.64	111.40
1	C	828	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	C	831	ASP	CB-CG-OD1	8.20	125.68	118.30
1	E	745	ASP	CB-CG-OD2	-8.15	110.96	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	823	VAL	N-CA-CB	-8.04	93.80	111.50
1	F	659	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	C	778	GLU	OE1-CD-OE2	8.02	132.92	123.30
1	A	835	ARG	NE-CZ-NH2	-7.99	116.31	120.30
1	D	825	VAL	CB-CA-C	-7.94	96.32	111.40
1	C	661	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	B	671	GLN	CB-CG-CD	7.79	131.86	111.60
1	D	716	GLU	OE1-CD-OE2	-7.79	113.95	123.30
1	D	693	ASP	CB-CG-OD1	7.77	125.30	118.30
1	E	840	LYS	CA-CB-CG	7.75	130.46	113.40
1	D	831	ASP	CB-CG-OD1	7.74	125.27	118.30
1	A	771	ARG	NE-CZ-NH1	7.68	124.14	120.30
1	F	701	ARG	CD-NE-CZ	7.64	134.30	123.60
1	C	701	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	B	699	THR	N-CA-CB	-7.50	96.04	110.30
1	C	693	ASP	CB-CG-OD1	7.50	125.05	118.30
1	B	724	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	C	710	GLU	OE1-CD-OE2	7.39	132.17	123.30
1	D	659	ARG	NH1-CZ-NH2	-7.39	111.27	119.40
1	F	711	ASP	CB-CG-OD1	7.39	124.95	118.30
1	C	668	ARG	CD-NE-CZ	7.35	133.90	123.60
1	C	660	MET	CA-CB-CG	7.31	125.72	113.30
1	A	694	TYR	CB-CG-CD1	7.31	125.38	121.00
1	E	771	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	D	699	THR	N-CA-CB	-7.30	96.43	110.30
1	A	809	ASP	CB-CG-OD1	7.29	124.86	118.30
1	H	831	ASP	CB-CG-OD2	-7.26	111.77	118.30
1	B	668	ARG	NE-CZ-NH1	7.26	123.93	120.30
1	F	706	ARG	NE-CZ-NH1	-7.23	116.68	120.30
1	B	728	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	C	835	ARG	CD-NE-CZ	7.16	133.62	123.60
1	A	668	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	D	831	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	G	699	THR	N-CA-CB	-7.05	96.91	110.30
1	D	842	ARG	CD-NE-CZ	7.03	133.44	123.60
1	E	828	ARG	NE-CZ-NH1	-7.03	116.79	120.30
1	C	749	GLU	OE1-CD-OE2	7.02	131.72	123.30
1	C	823	VAL	N-CA-CB	-6.96	96.18	111.50
1	F	721	TYR	CB-CG-CD2	-6.92	116.85	121.00
1	A	745	ASP	CB-CG-OD1	6.91	124.52	118.30
1	F	659	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	A	688	PHE	N-CA-CB	-6.89	98.20	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	837	VAL	N-CA-CB	-6.85	96.44	111.50
1	G	835	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	840	LYS	CA-CB-CG	6.80	128.36	113.40
1	C	711	ASP	CB-CG-OD1	6.80	124.42	118.30
1	E	742	THR	N-CA-CB	-6.75	97.47	110.30
1	H	835	ARG	NE-CZ-NH1	6.75	123.68	120.30
1	C	837	VAL	N-CA-CB	-6.74	96.67	111.50
1	H	842	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	A	778	GLU	OE1-CD-OE2	6.64	131.27	123.30
1	A	839	MET	CG-SD-CE	-6.63	89.60	100.20
1	F	839	MET	CG-SD-CE	6.61	110.78	100.20
1	G	706	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	E	837	VAL	N-CA-CB	-6.56	97.07	111.50
1	C	699	THR	N-CA-CB	-6.52	97.91	110.30
1	G	823	VAL	N-CA-CB	-6.52	97.15	111.50
1	A	831	ASP	OD1-CG-OD2	6.51	135.66	123.30
1	A	661	ASP	CB-CG-OD1	6.48	124.13	118.30
1	B	823	VAL	N-CA-CB	-6.45	97.32	111.50
1	H	658	GLN	CB-CG-CD	6.43	128.31	111.60
1	H	838	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	847	GLN	CB-CG-CD	6.38	128.18	111.60
1	A	694	TYR	CB-CG-CD2	-6.38	117.17	121.00
1	E	771	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	H	811	ARG	CD-NE-CZ	6.36	132.50	123.60
1	D	701	ARG	CD-NE-CZ	6.34	132.48	123.60
1	A	711	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	771	ARG	NH1-CZ-NH2	-6.31	112.46	119.40
1	F	661	ASP	CB-CG-OD1	6.29	123.97	118.30
1	A	711	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	D	837	VAL	N-CA-CB	-6.26	97.72	111.50
1	E	688	PHE	N-CA-CB	-6.26	99.34	110.60
1	H	668	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	828	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	E	835	ARG	CD-NE-CZ	6.21	132.30	123.60
1	C	668	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	A	823	VAL	CG1-CB-CG2	6.19	120.80	110.90
1	E	838	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	668	ARG	NE-CZ-NH2	-6.19	117.21	120.30
1	E	699	THR	N-CA-CB	-6.19	98.54	110.30
1	B	675	ARG	NE-CZ-NH2	6.11	123.36	120.30
1	B	842	ARG	NE-CZ-NH1	-6.11	117.25	120.30
1	B	823	VAL	CA-CB-CG2	6.09	120.04	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	745	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	G	742	THR	N-CA-CB	-6.06	98.78	110.30
1	D	758	TYR	CB-CG-CD1	6.04	124.62	121.00
1	D	745	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	699	THR	N-CA-CB	-6.02	98.87	110.30
1	B	752	VAL	CB-CA-C	-6.00	99.99	111.40
1	H	655	LEU	CA-CB-CG	6.00	129.10	115.30
1	C	672	ASP	CB-CG-OD2	6.00	123.69	118.30
1	B	825	VAL	CG1-CB-CG2	-5.96	101.36	110.90
1	A	668	ARG	CD-NE-CZ	5.94	131.91	123.60
1	A	809	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	B	701	ARG	CD-NE-CZ	5.92	131.89	123.60
1	B	778	GLU	OE1-CD-OE2	5.92	130.40	123.30
1	A	811	ARG	CD-NE-CZ	5.92	131.88	123.60
1	A	842	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	E	740	GLU	CA-CB-CG	5.84	126.26	113.40
1	B	772	ASP	OD1-CG-OD2	-5.84	112.20	123.30
1	E	664	LEU	CA-CB-CG	5.84	128.74	115.30
1	E	724	ARG	CD-NE-CZ	5.83	131.76	123.60
1	E	745	ASP	CB-CG-OD1	5.81	123.53	118.30
1	C	831	ASP	CB-CG-OD2	-5.77	113.11	118.30
1	A	837	VAL	CA-CB-CG1	5.77	119.55	110.90
1	C	828	ARG	CD-NE-CZ	-5.76	115.54	123.60
1	E	785	GLY	N-CA-C	5.75	127.47	113.10
1	A	723	PHE	CB-CG-CD1	5.72	124.81	120.80
1	D	673	TYR	CB-CG-CD2	5.70	124.42	121.00
1	E	723	PHE	N-CA-CB	-5.69	100.36	110.60
1	E	828	ARG	NE-CZ-NH2	5.65	123.12	120.30
1	E	668	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	A	774	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	694	TYR	CB-CG-CD2	-5.54	117.67	121.00
1	E	842	ARG	CD-NE-CZ	5.54	131.36	123.60
1	F	721	TYR	CB-CG-CD1	5.52	124.31	121.00
1	A	778	GLU	CB-CG-CD	-5.51	99.32	114.20
1	B	654	LEU	CA-CB-CG	5.49	127.93	115.30
1	G	721	TYR	CB-CG-CD1	5.47	124.28	121.00
1	A	837	VAL	N-CA-CB	-5.46	99.50	111.50
1	B	659	ARG	CD-NE-CZ	5.46	131.24	123.60
1	A	708	GLU	OE1-CD-OE2	-5.45	116.76	123.30
1	C	803	TYR	CB-CG-CD2	-5.41	117.75	121.00
1	C	770	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	701	ARG	NE-CZ-NH1	5.40	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	724	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	842	ARG	CD-NE-CZ	5.38	131.13	123.60
1	E	847	GLN	CB-CG-CD	5.35	125.50	111.60
1	A	675	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	G	828	ARG	NE-CZ-NH1	-5.33	117.63	120.30
1	B	771	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	F	840	LYS	CA-CB-CG	5.32	125.11	113.40
1	E	710	GLU	CA-CB-CG	5.32	125.10	113.40
1	D	783	VAL	CA-CB-CG1	5.31	118.87	110.90
1	B	677	PHE	CB-CG-CD1	5.31	124.52	120.80
1	C	711	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	H	842	ARG	NE-CZ-NH2	5.29	122.94	120.30
1	B	664	LEU	CA-CB-CG	5.26	127.41	115.30
1	E	775	GLN	CA-CB-CG	5.26	124.98	113.40
1	A	671	GLN	CB-CG-CD	5.26	125.27	111.60
1	B	837	VAL	N-CA-CB	-5.24	99.97	111.50
1	A	755	GLY	CA-C-O	5.24	130.03	120.60
1	E	701	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	H	837	VAL	N-CA-CB	-5.23	99.99	111.50
1	A	838	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	D	745	ASP	OD1-CG-OD2	-5.19	113.44	123.30
1	D	660	MET	CA-CB-CG	5.19	122.12	113.30
1	G	837	VAL	CA-CB-CG1	5.18	118.68	110.90
1	B	699	THR	CA-CB-CG2	5.18	119.66	112.40
1	H	771	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	842	ARG	NE-CZ-NH1	-5.16	117.72	120.30
1	H	699	THR	CA-CB-CG2	5.12	119.56	112.40
1	F	659	ARG	N-CA-CB	5.11	119.80	110.60
1	E	724	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	783	VAL	CA-CB-CG1	5.10	118.55	110.90
1	F	699	THR	N-CA-CB	-5.10	100.61	110.30
1	D	770	ASP	CB-CG-OD2	5.09	122.89	118.30
1	B	837	VAL	CA-CB-CG1	5.09	118.54	110.90
1	G	687	GLU	OE1-CD-OE2	-5.09	117.19	123.30
1	B	818	ILE	N-CA-CB	-5.09	99.09	110.80
1	E	711	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	675	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	D	745	ASP	CB-CG-OD1	5.04	122.83	118.30
1	A	668	ARG	NE-CZ-NH1	5.02	122.81	120.30

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	14	MAN	C1
4	B	14	MAN	C1
2	C	14	MAN	C1
2	C	15	MAN	C1
2	D	15	MAN	C1

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	795	ALA	Mainchain
1	B	723	PHE	Mainchain
1	C	846	THR	Mainchain
1	D	666	PHE	Mainchain
1	D	803	TYR	Mainchain
1	E	738	SER	Mainchain
1	E	840	LYS	Mainchain
1	G	825	VAL	Mainchain

## 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	1585	0	1421	29	0
1	B	1585	0	1418	42	0
1	C	1585	0	1420	31	5
1	D	1585	0	1421	33	1
1	E	1585	0	1422	58	0
1	F	1585	0	1421	108	0
1	G	1585	0	1422	107	0
1	H	1585	0	1422	114	6
2	A	75	0	64	19	0
2	C	75	0	64	27	0
2	D	75	0	64	12	0
3	B	14	0	10	5	0
3	E	28	0	26	17	0
3	G	28	0	26	13	0
3	H	28	0	26	17	0
4	B	60	0	49	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	F	28	0	25	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
7	A	70	0	0	4	0
7	B	76	0	0	8	0
7	C	71	0	0	0	0
7	D	74	0	0	7	0
7	E	52	0	0	5	0
7	F	63	0	0	3	0
7	G	56	0	0	7	0
7	H	34	0	0	6	0
All	All	13595	0	11721	641	6

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 26.

All (641) 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:F:758:TYR:CD1	1:F:792:ASN:HB3	1.25	1.63
3:B:10:NAG:C2	3:B:10:NAG:C3	1.76	1.61
1:F:842:ARG:CZ	1:F:847:GLN:HB2	1.25	1.61
1:E:667:ASN:HD21	3:E:10:NAG:C1	0.99	1.61
1:F:842:ARG:CZ	1:F:847:GLN:CB	1.83	1.56
1:F:843:PRO:HG2	1:F:846:THR:CG2	1.34	1.55
1:G:667:ASN:HD21	3:G:10:NAG:C1	0.97	1.55
1:H:667:ASN:HD21	3:H:10:NAG:C1	1.25	1.50
3:E:10:NAG:C4	3:E:10:NAG:O4	1.64	1.45
1:F:843:PRO:CG	1:F:846:THR:HG21	1.48	1.44
1:F:842:ARG:NE	1:F:847:GLN:HB2	1.15	1.43
3:E:10:NAG:O5	3:E:10:NAG:C1	1.68	1.42
1:F:843:PRO:CD	1:F:846:THR:HG21	1.51	1.39
1:G:671:GLN:NE2	1:G:675:ARG:HE	1.18	1.39
1:F:758:TYR:CD1	1:F:792:ASN:CB	2.07	1.36
2:C:14:MAN:H62	2:C:13:MAN:C5	1.53	1.33

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:846:THR:HB	1:H:847:GLN:OE1	1.21	1.33
1:F:842:ARG:CG	1:F:846:THR:HG23	1.58	1.32
3:E:10:NAG:C5	3:E:10:NAG:O5	1.77	1.31
1:F:843:PRO:CG	1:F:846:THR:CG2	2.07	1.27
1:F:842:ARG:HG2	1:F:846:THR:CG2	1.64	1.27
1:F:819:GLU:OE2	1:F:831:ASP:HB3	1.17	1.26
1:F:758:TYR:CE1	1:F:792:ASN:CB	2.20	1.25
1:H:818:ILE:HD13	1:H:819:GLU:N	1.51	1.24
1:E:846:THR:O	1:E:847:GLN:CG	1.85	1.24
1:F:842:ARG:NH1	1:F:847:GLN:CB	1.99	1.23
1:F:843:PRO:HG2	1:F:846:THR:CB	1.69	1.22
2:C:13:MAN:H4	2:C:12:NAG:C1	1.70	1.20
1:F:842:ARG:CZ	1:F:847:GLN:HB3	1.71	1.20
1:G:784:TYR:OH	1:G:818:ILE:HD11	1.44	1.17
4:B:14:MAN:H61	4:B:13:MAN:C5	1.75	1.17
1:G:702:GLY:C	1:G:844:LEU:CD1	2.13	1.16
1:G:702:GLY:C	1:G:844:LEU:HD12	1.68	1.14
2:C:14:MAN:H61	2:C:13:MAN:H3	1.18	1.13
2:D:14:MAN:H61	2:D:13:MAN:C5	1.78	1.12
1:G:671:GLN:NE2	1:G:675:ARG:NE	1.96	1.12
4:B:14:MAN:H3	4:B:15:MAN:C3	1.72	1.12
1:E:846:THR:O	1:E:847:GLN:HG2	0.94	1.11
4:B:14:MAN:C6	4:B:13:MAN:H5	1.80	1.11
3:E:10:NAG:O4	3:E:11:NAG:H2	1.49	1.10
1:G:652:GLY:HA3	1:G:847:GLN:OE1	1.49	1.10
2:C:14:MAN:C6	2:C:13:MAN:H5	1.80	1.10
1:F:843:PRO:HD2	1:F:846:THR:HG21	1.28	1.09
2:D:14:MAN:H61	2:D:13:MAN:H5	1.21	1.09
1:F:843:PRO:O	1:F:846:THR:HG22	1.52	1.09
4:B:14:MAN:H3	4:B:15:MAN:H3	1.08	1.07
1:F:842:ARG:HG2	1:F:846:THR:HG23	1.10	1.06
1:F:758:TYR:CE1	1:F:792:ASN:HB2	1.84	1.06
1:F:819:GLU:OE2	1:F:831:ASP:CB	2.04	1.06
4:B:13:MAN:H4	4:B:12:NAG:C1	1.87	1.05
1:F:842:ARG:NH1	1:F:847:GLN:HB3	1.68	1.04
1:E:783:VAL:HG12	1:E:818:ILE:HD13	1.39	1.04
1:B:825:VAL:HB	7:B:492:HOH:O	1.54	1.03
1:F:842:ARG:CD	1:F:847:GLN:HB2	1.87	1.03
1:F:842:ARG:NH1	1:F:847:GLN:CG	2.20	1.03
1:G:782:GLU:OE2	1:G:816:TYR:OH	1.78	1.02
1:G:703:SER:N	1:G:844:LEU:HD11	1.74	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:710:GLU:HG3	1:E:836:ALA:HB3	1.41	1.02
1:B:843:PRO:HB2	1:B:846:THR:HG22	1.38	1.01
1:G:842:ARG:HD2	1:G:847:GLN:OXT	1.60	1.01
1:G:843:PRO:HD2	1:G:847:GLN:HB3	1.40	1.01
1:H:754:GLU:HG3	1:H:759:THR:HG21	1.41	1.01
1:F:758:TYR:CZ	1:F:792:ASN:ND2	2.28	1.00
1:F:842:ARG:HH11	1:F:847:GLN:HG3	1.26	1.00
1:D:846:THR:O	1:D:847:GLN:HG3	1.60	1.00
1:G:847:GLN:HA	7:G:438:HOH:O	1.61	1.00
1:H:818:ILE:HD13	1:H:819:GLU:H	0.84	1.00
1:F:842:ARG:NH1	1:F:847:GLN:HG3	1.76	0.99
1:F:843:PRO:CD	1:F:846:THR:CG2	2.38	0.99
1:F:842:ARG:HD2	1:F:846:THR:O	1.61	0.99
1:H:751:SER:CB	1:H:754:GLU:HB2	1.93	0.99
1:F:842:ARG:NH2	1:F:844:LEU:O	1.96	0.99
1:H:818:ILE:CD1	1:H:819:GLU:H	1.76	0.98
2:C:14:MAN:C6	2:C:13:MAN:H3	1.94	0.98
1:H:751:SER:HB3	1:H:754:GLU:HB2	1.42	0.98
1:F:845:VAL:O	1:F:847:GLN:N	1.98	0.97
1:G:703:SER:N	1:G:844:LEU:CD1	2.27	0.97
4:B:14:MAN:H61	4:B:13:MAN:H5	0.97	0.97
2:C:13:MAN:C4	2:C:12:NAG:C1	2.42	0.97
1:D:846:THR:O	1:D:847:GLN:CG	2.13	0.96
1:E:844:LEU:HD12	7:E:478:HOH:O	1.63	0.96
1:E:695:LEU:O	1:E:699:THR:HB	1.65	0.96
2:C:14:MAN:C6	2:C:13:MAN:C5	2.41	0.96
1:F:842:ARG:NE	1:F:847:GLN:CB	2.12	0.95
2:C:11:NAG:O3	2:C:14:MAN:H2	1.66	0.95
1:G:819:GLU:OE2	1:G:831:ASP:HB3	1.67	0.95
1:G:681:ASN:HD21	1:G:685:GLU:CG	1.79	0.94
1:H:782:GLU:HG3	3:H:10:NAG:O4	1.69	0.93
1:H:710:GLU:OE2	1:H:835:ARG:NH2	2.01	0.93
2:A:14:MAN:H62	2:A:14:MAN:O2	1.69	0.93
1:H:757:GLU:OE1	1:H:758:TYR:CE1	2.20	0.93
3:E:10:NAG:O5	3:E:10:NAG:C6	2.15	0.92
1:F:758:TYR:HD1	1:F:792:ASN:HB3	1.27	0.92
1:E:783:VAL:CG1	1:E:818:ILE:HD13	2.00	0.92
1:F:842:ARG:HH11	1:F:847:GLN:CG	1.80	0.92
1:D:783:VAL:HG13	1:D:818:ILE:HD13	1.51	0.92
1:F:843:PRO:HG2	1:F:846:THR:HB	1.47	0.92
1:D:699:THR:HG21	1:D:725:VAL:H	1.35	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:845:VAL:HG23	7:A:905:HOH:O	1.69	0.91
1:G:681:ASN:HD21	1:G:685:GLU:HG2	1.36	0.90
1:H:667:ASN:HD21	3:H:10:NAG:C2	1.82	0.90
1:G:681:ASN:ND2	1:G:685:GLU:HG2	1.86	0.90
1:F:681:ASN:HD21	1:F:685:GLU:CD	1.74	0.90
1:G:784:TYR:OH	1:G:818:ILE:CD1	2.20	0.90
1:C:699:THR:HG21	1:C:725:VAL:H	1.36	0.90
1:E:844:LEU:CD1	7:E:478:HOH:O	2.17	0.90
1:E:846:THR:C	1:E:847:GLN:HG2	1.91	0.90
1:H:846:THR:CB	1:H:847:GLN:OE1	2.16	0.90
1:G:842:ARG:CD	1:G:847:GLN:OXT	2.18	0.90
1:H:653:TRP:CE3	1:H:842:ARG:HG3	2.07	0.89
1:H:776:TRP:CE2	1:H:778:GLU:HB2	2.07	0.89
1:B:843:PRO:HB2	1:B:846:THR:CG2	2.01	0.89
1:G:776:TRP:HA	1:G:792:ASN:HD21	1.35	0.89
2:C:14:MAN:H61	2:C:13:MAN:C3	2.01	0.88
1:C:783:VAL:HG13	1:C:818:ILE:HD13	1.56	0.88
1:H:818:ILE:CD1	1:H:819:GLU:N	2.35	0.88
1:F:842:ARG:HD3	1:F:847:GLN:HG2	1.56	0.88
1:F:842:ARG:CD	1:F:847:GLN:HG2	2.04	0.87
2:D:14:MAN:C6	2:D:13:MAN:H5	2.02	0.87
1:G:702:GLY:O	1:G:844:LEU:HD12	1.74	0.87
1:G:776:TRP:HA	1:G:792:ASN:ND2	1.88	0.87
1:A:818:ILE:HD11	1:A:820:ASN:HB3	1.54	0.86
1:G:671:GLN:HE22	1:G:675:ARG:NE	1.60	0.86
2:C:14:MAN:C6	2:C:13:MAN:C3	2.52	0.86
1:E:758:TYR:HB3	1:E:792:ASN:HB3	1.59	0.85
3:B:10:NAG:C2	3:B:10:NAG:O3	2.22	0.85
3:B:10:NAG:N2	3:B:10:NAG:C3	2.40	0.84
1:G:842:ARG:CB	1:G:847:GLN:OXT	2.24	0.84
1:A:815:PRO:HG2	1:A:816:TYR:CE1	2.11	0.84
2:A:15:MAN:H61	2:A:15:MAN:O2	1.78	0.84
1:H:718:TYR:H	1:H:742:THR:HG22	1.42	0.84
3:B:10:NAG:C1	3:B:10:NAG:C3	2.56	0.84
2:D:13:MAN:O5	2:D:12:NAG:C1	2.26	0.84
1:H:816:TYR:HB2	7:H:389:HOH:O	1.76	0.84
1:F:843:PRO:HG2	1:F:846:THR:HG22	1.58	0.83
1:G:681:ASN:ND2	1:G:685:GLU:CG	2.42	0.83
1:B:842:ARG:HE	1:B:847:GLN:HA	1.44	0.83
1:H:765:GLN:HE22	1:H:771:ARG:HH22	1.26	0.83
1:F:758:TYR:CE1	1:F:792:ASN:ND2	2.46	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:843:PRO:HD2	1:G:847:GLN:CB	2.09	0.83
1:E:842:ARG:NH2	1:E:847:GLN:O	2.12	0.82
1:F:718:TYR:H	1:F:742:THR:HG22	1.44	0.82
4:B:13:MAN:C4	4:B:12:NAG:C1	2.54	0.82
1:C:724:ARG:HB2	1:C:735:GLN:HG3	1.62	0.82
1:E:699:THR:CG2	1:E:725:VAL:H	1.91	0.82
1:H:754:GLU:HG3	1:H:759:THR:CG2	2.09	0.82
3:H:10:NAG:C4	3:H:11:NAG:C1	2.58	0.81
2:C:14:MAN:H62	2:C:13:MAN:H5	0.84	0.81
1:H:795:ALA:O	1:H:825:VAL:HG13	1.81	0.81
1:G:809:ASP:OD1	1:G:811:ARG:HG3	1.80	0.80
1:G:819:GLU:HG2	1:G:830:ALA:O	1.81	0.80
1:H:776:TRP:CD2	1:H:778:GLU:HB2	2.16	0.80
3:E:10:NAG:HO4	3:E:11:NAG:H2	1.44	0.80
1:F:758:TYR:CG	1:F:792:ASN:HB3	2.14	0.80
1:H:752:VAL:HG23	1:H:753:GLU:H	1.46	0.80
1:C:795:ALA:O	1:C:825:VAL:HG23	1.81	0.80
1:H:751:SER:HB3	1:H:754:GLU:CB	2.11	0.80
2:D:14:MAN:C6	2:D:13:MAN:C5	2.57	0.80
2:C:13:MAN:O6	2:C:12:NAG:H61	1.80	0.80
1:G:671:GLN:HE21	1:G:675:ARG:HE	1.30	0.80
1:H:754:GLU:CG	1:H:759:THR:HG21	2.11	0.80
4:B:14:MAN:C3	4:B:15:MAN:H3	2.02	0.79
1:G:671:GLN:HE22	1:G:675:ARG:HE	0.80	0.79
1:E:776:TRP:CZ3	1:E:778:GLU:HB3	2.18	0.79
1:E:810:PRO:O	1:E:817:GLU:HA	1.83	0.79
2:A:14:MAN:H2	2:A:15:MAN:H3	1.66	0.78
1:G:846:THR:OG1	1:G:847:GLN:N	2.12	0.78
1:G:842:ARG:HB2	1:G:847:GLN:OXT	1.83	0.78
1:F:758:TYR:HE1	1:F:792:ASN:HB2	1.47	0.78
1:H:671:GLN:CD	1:H:675:ARG:HH21	1.88	0.77
1:C:671:GLN:HG2	1:C:675:ARG:HE	1.48	0.77
1:E:718:TYR:H	1:E:742:THR:HG22	1.48	0.77
1:F:681:ASN:ND2	1:F:685:GLU:OE2	2.17	0.77
1:D:783:VAL:CG1	1:D:818:ILE:HD13	2.13	0.77
1:G:749:GLU:O	1:G:756:ALA:HB2	1.86	0.76
1:F:842:ARG:CD	1:F:847:GLN:CB	2.61	0.76
1:A:724:ARG:HB3	1:A:735:GLN:HG3	1.66	0.76
1:F:842:ARG:HG3	1:F:846:THR:HG23	1.68	0.76
1:G:665:ASN:O	1:G:668:ARG:HD3	1.84	0.76
1:A:701:ARG:HG2	1:A:701:ARG:HH11	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:815:PRO:HG2	1:H:816:TYR:CE1	2.21	0.75
1:F:842:ARG:CD	1:F:846:THR:HG23	2.16	0.75
2:C:15:MAN:O2	2:C:15:MAN:H62	1.87	0.75
1:G:845:VAL:HG13	1:G:846:THR:H	1.51	0.74
1:D:722:HIS:CD2	7:D:494:HOH:O	2.39	0.74
1:G:718:TYR:H	1:G:742:THR:HG22	1.53	0.74
1:H:699:THR:CG2	1:H:725:VAL:H	2.00	0.74
1:F:758:TYR:CE1	1:F:792:ASN:HB3	1.91	0.74
1:A:699:THR:CG2	1:A:725:VAL:H	2.00	0.74
1:G:671:GLN:HE21	1:G:675:ARG:NE	1.86	0.73
1:H:751:SER:OG	1:H:754:GLU:HB2	1.86	0.73
2:A:14:MAN:H3	2:A:15:MAN:O4	1.89	0.73
1:B:776:TRP:CE3	1:B:778:GLU:HB3	2.23	0.73
1:E:699:THR:HG21	1:E:725:VAL:H	1.52	0.73
1:F:845:VAL:O	1:F:847:GLN:OXT	2.06	0.73
1:B:842:ARG:NE	1:B:847:GLN:HA	2.03	0.72
2:C:13:MAN:C6	2:C:12:NAG:H5	2.19	0.72
3:E:10:NAG:O5	3:E:10:NAG:C2	2.33	0.72
3:G:10:NAG:O4	3:G:11:NAG:C1	2.38	0.72
3:H:10:NAG:H4	3:H:11:NAG:C1	2.20	0.72
2:A:14:MAN:C6	2:A:14:MAN:O2	2.38	0.72
2:A:11:NAG:O3	2:A:15:MAN:H3	1.88	0.72
1:H:667:ASN:ND2	3:H:10:NAG:C2	2.47	0.72
2:A:13:MAN:H4	2:A:12:NAG:C1	2.20	0.72
4:B:14:MAN:C6	4:B:13:MAN:C5	2.51	0.72
2:A:14:MAN:C2	2:A:15:MAN:H3	2.20	0.71
3:E:10:NAG:O5	3:E:10:NAG:H62	1.89	0.71
1:E:776:TRP:CE3	1:E:778:GLU:HB3	2.25	0.71
2:C:13:MAN:H61	2:C:12:NAG:H5	1.73	0.71
1:F:845:VAL:CG1	1:F:846:THR:N	2.53	0.71
4:B:14:MAN:H61	4:B:13:MAN:C3	2.21	0.71
1:F:699:THR:CG2	1:F:725:VAL:H	2.03	0.71
1:A:718:TYR:H	1:A:742:THR:HG22	1.54	0.71
1:D:699:THR:CG2	1:D:725:VAL:H	2.03	0.71
1:F:843:PRO:CG	1:F:846:THR:HG22	2.13	0.71
1:H:815:PRO:HG2	1:H:816:TYR:CD1	2.26	0.71
1:C:846:THR:OG1	1:C:847:GLN:N	2.20	0.71
1:B:653:TRP:CH2	1:B:842:ARG:NH1	2.58	0.70
1:F:699:THR:HG21	1:F:725:VAL:H	1.56	0.70
1:G:695:LEU:O	1:G:699:THR:HB	1.92	0.70
1:F:810:PRO:HG3	1:F:819:GLU:HG3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:842:ARG:CD	1:F:847:GLN:CG	2.69	0.70
1:G:818:ILE:CG1	1:G:819:GLU:H	2.05	0.70
1:G:842:ARG:HD2	1:G:847:GLN:C	2.11	0.70
1:H:776:TRP:CZ3	1:H:778:GLU:HB3	2.27	0.69
4:B:14:MAN:H61	4:B:13:MAN:H3	1.73	0.69
2:C:13:MAN:O6	2:C:12:NAG:C5	2.40	0.69
1:F:783:VAL:HG12	1:F:784:TYR:CD1	2.28	0.69
1:C:718:TYR:H	1:C:742:THR:HG22	1.57	0.69
1:B:784:TYR:OH	1:B:818:ILE:HD11	1.92	0.69
1:F:681:ASN:CG	1:F:685:GLU:HG2	2.13	0.69
1:D:771:ARG:CD	7:D:427:HOH:O	2.40	0.69
1:F:842:ARG:CD	1:F:846:THR:O	2.38	0.69
1:H:823:VAL:HG23	7:H:379:HOH:O	1.92	0.69
1:D:777:GLU:HG2	1:D:778:GLU:OE1	1.93	0.69
1:G:843:PRO:CD	1:G:847:GLN:HB3	2.20	0.69
1:G:699:THR:CG2	1:G:725:VAL:H	2.06	0.68
1:C:809:ASP:OD2	1:C:812:ASN:OD1	2.11	0.68
1:H:765:GLN:NE2	1:H:771:ARG:HH22	1.90	0.68
2:C:13:MAN:O6	2:C:12:NAG:C6	2.41	0.68
1:F:745:ASP:OD2	1:F:748:ILE:HB	1.94	0.67
2:C:15:MAN:O2	2:C:15:MAN:C6	2.43	0.67
1:G:755:GLY:O	1:G:757:GLU:N	2.27	0.67
1:A:771:ARG:NH2	7:A:917:HOH:O	2.20	0.67
1:C:671:GLN:HE21	1:C:675:ARG:NE	1.92	0.67
1:F:843:PRO:HG2	1:F:846:THR:HG21	1.13	0.67
1:F:842:ARG:CG	1:F:846:THR:CG2	2.39	0.67
3:G:10:NAG:C4	3:G:11:NAG:C1	2.73	0.66
1:G:658:GLN:HE21	1:G:838:ARG:HE	1.43	0.66
1:F:774:ASP:OD2	1:F:780:CYS:SG	2.53	0.66
1:G:776:TRP:CA	1:G:792:ASN:ND2	2.58	0.66
2:A:14:MAN:C1	2:A:15:MAN:O4	2.43	0.66
2:C:14:MAN:H62	2:C:13:MAN:C4	2.24	0.66
1:H:665:ASN:O	1:H:668:ARG:HD3	1.94	0.66
1:G:819:GLU:OE2	1:G:831:ASP:CB	2.43	0.66
1:A:817:GLU:C	1:A:818:ILE:HG23	2.17	0.65
1:B:651:GLY:N	1:B:847:GLN:OXT	2.29	0.65
1:E:844:LEU:HD12	1:E:845:VAL:H	1.61	0.65
1:C:710:GLU:HG2	1:C:716:GLU:HG2	1.78	0.65
1:F:775:GLN:HG3	1:F:791:ASN:OD1	1.96	0.65
1:F:843:PRO:HD2	1:F:846:THR:CG2	2.14	0.65
1:A:817:GLU:C	1:A:818:ILE:CG2	2.65	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:724:ARG:HB2	1:D:735:GLN:HG3	1.79	0.65
1:G:681:ASN:CG	1:G:685:GLU:HG2	2.16	0.65
1:G:703:SER:N	1:G:844:LEU:HD12	2.03	0.65
1:G:842:ARG:HB2	1:G:847:GLN:HB3	1.79	0.65
3:E:10:NAG:C5	3:E:10:NAG:O4	2.43	0.64
1:F:681:ASN:ND2	1:F:685:GLU:CG	2.60	0.64
1:H:846:THR:O	1:H:847:GLN:HG2	1.98	0.64
1:F:782:GLU:HG3	5:F:10:NAG:O4	1.97	0.64
1:F:681:ASN:HD21	1:F:685:GLU:CG	2.09	0.64
1:E:775:GLN:CG	1:E:791:ASN:OD1	2.45	0.64
3:G:10:NAG:H4	3:G:11:NAG:O5	1.96	0.64
1:B:776:TRP:CE2	1:B:778:GLU:HB2	2.33	0.64
1:G:818:ILE:HG13	1:G:819:GLU:H	1.62	0.64
1:D:771:ARG:HD3	7:D:427:HOH:O	1.98	0.64
1:A:699:THR:HG21	1:A:725:VAL:H	1.63	0.63
1:G:775:GLN:O	1:G:792:ASN:ND2	2.31	0.63
1:G:702:GLY:CA	1:G:844:LEU:CD1	2.76	0.63
1:E:748:ILE:O	1:E:760:SER:OG	2.15	0.63
1:C:671:GLN:NE2	1:C:675:ARG:CZ	2.61	0.63
1:F:681:ASN:OD1	1:F:685:GLU:HG2	1.99	0.63
1:G:740:GLU:HG2	1:G:741:GLY:N	2.12	0.63
1:C:699:THR:CG2	1:C:725:VAL:H	2.11	0.63
1:H:699:THR:HG23	1:H:725:VAL:H	1.62	0.63
1:B:776:TRP:CZ3	1:B:778:GLU:HB3	2.34	0.63
1:E:756:ALA:O	1:E:760:SER:HB2	1.99	0.63
1:F:842:ARG:HD3	1:F:847:GLN:CG	2.27	0.63
3:E:10:NAG:C4	3:E:10:NAG:HO4	2.07	0.63
1:A:818:ILE:CD1	1:A:820:ASN:HB3	2.28	0.62
3:B:10:NAG:C2	3:B:10:NAG:C4	2.75	0.62
4:B:12:NAG:C3	4:B:12:NAG:O7	2.47	0.62
1:C:671:GLN:NE2	1:C:675:ARG:NH2	2.47	0.62
1:F:681:ASN:ND2	1:F:685:GLU:HG2	2.14	0.62
1:G:652:GLY:CA	1:G:847:GLN:OE1	2.38	0.62
1:H:776:TRP:CZ2	1:H:778:GLU:HB2	2.34	0.62
1:B:699:THR:CG2	1:B:725:VAL:H	2.12	0.62
1:B:784:TYR:CZ	1:B:818:ILE:CD1	2.82	0.62
1:B:662:GLY:HA2	7:B:98:HOH:O	2.00	0.62
1:E:697:LEU:HD23	1:E:698:LEU:HD23	1.81	0.62
1:F:843:PRO:O	1:F:846:THR:CG2	2.40	0.62
1:D:783:VAL:O	1:D:818:ILE:HD11	1.98	0.62
1:F:843:PRO:C	1:F:846:THR:HG22	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:695:LEU:O	1:A:699:THR:HB	2.01	0.61
1:D:783:VAL:CG1	1:D:818:ILE:CD1	2.78	0.61
1:H:809:ASP:OD1	1:H:811:ARG:HB2	2.00	0.61
3:G:10:NAG:H62	3:G:11:NAG:C1	2.31	0.61
1:B:784:TYR:OH	1:B:818:ILE:CD1	2.49	0.61
1:C:783:VAL:HG13	1:C:818:ILE:CD1	2.30	0.61
1:G:810:PRO:O	1:G:817:GLU:HG2	2.01	0.61
1:D:783:VAL:HG13	1:D:818:ILE:CD1	2.29	0.61
1:E:665:ASN:O	1:E:668:ARG:HD3	2.01	0.61
1:D:681:ASN:OD1	1:D:684:GLY:N	2.33	0.60
1:A:817:GLU:O	1:A:818:ILE:HG22	2.01	0.60
1:F:845:VAL:C	1:F:847:GLN:H	1.96	0.60
1:H:782:GLU:CG	3:H:10:NAG:O4	2.47	0.60
1:G:818:ILE:CG1	1:G:819:GLU:N	2.64	0.60
1:H:667:ASN:ND2	3:H:10:NAG:H2	2.16	0.60
1:H:842:ARG:NE	1:H:847:GLN:OE1	2.35	0.60
1:D:771:ARG:NE	7:D:427:HOH:O	2.32	0.60
1:D:795:ALA:O	1:D:825:VAL:HG22	2.01	0.60
1:B:843:PRO:CB	1:B:846:THR:CG2	2.77	0.60
1:G:819:GLU:OE2	1:G:831:ASP:OD2	2.18	0.60
1:G:702:GLY:C	1:G:844:LEU:HD11	2.02	0.60
1:G:671:GLN:NE2	1:G:675:ARG:CZ	2.63	0.60
1:H:842:ARG:CZ	1:H:847:GLN:OE1	2.50	0.60
1:H:754:GLU:CB	1:H:759:THR:HG21	2.32	0.59
1:A:815:PRO:HG2	1:A:816:TYR:CD1	2.37	0.59
1:B:842:ARG:HE	1:B:847:GLN:CA	2.13	0.59
2:D:13:MAN:O5	2:D:12:NAG:O5	2.18	0.59
1:H:782:GLU:CD	3:H:11:NAG:H2	2.23	0.59
1:H:653:TRP:CZ3	1:H:842:ARG:HG3	2.36	0.59
1:G:778:GLU:HG2	7:G:339:HOH:O	2.02	0.59
1:B:695:LEU:O	1:B:699:THR:HB	2.03	0.59
1:E:699:THR:HG23	1:E:725:VAL:H	1.67	0.59
1:F:758:TYR:CE1	1:F:792:ASN:CG	2.76	0.59
1:A:710:GLU:OE1	7:A:916:HOH:O	2.17	0.59
1:A:844:LEU:HB2	7:A:905:HOH:O	2.02	0.59
4:B:14:MAN:H4	4:B:13:MAN:H3	1.83	0.58
1:H:792:ASN:N	1:H:793:CYS:HA	2.17	0.58
2:C:13:MAN:O6	2:C:12:NAG:H5	2.03	0.58
1:E:809:ASP:O	1:E:812:ASN:HB2	2.03	0.58
1:E:844:LEU:HG	7:E:271:HOH:O	2.03	0.58
2:A:11:NAG:O4	2:A:14:MAN:H62	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:783:VAL:HG12	1:G:818:ILE:HG21	1.84	0.58
1:B:718:TYR:H	1:B:742:THR:HG22	1.68	0.58
2:C:13:MAN:O5	2:C:12:NAG:O5	2.21	0.58
2:C:14:MAN:O3	2:C:15:MAN:H62	2.03	0.58
1:E:783:VAL:CG1	1:E:818:ILE:CD1	2.80	0.58
1:F:845:VAL:HG12	1:F:846:THR:H	1.69	0.58
1:G:681:ASN:OD1	1:G:685:GLU:HG2	2.03	0.57
1:H:784:TYR:CE1	1:H:818:ILE:HD12	2.38	0.57
1:C:814:SER:HA	1:C:815:PRO:C	2.24	0.57
1:E:845:VAL:HB	7:E:478:HOH:O	2.03	0.57
1:F:815:PRO:HG2	1:F:816:TYR:CE2	2.39	0.57
1:B:675:ARG:NH1	7:B:437:HOH:O	2.23	0.57
1:G:775:GLN:HB2	1:G:791:ASN:O	2.05	0.57
1:H:653:TRP:CZ2	1:H:842:ARG:HD3	2.39	0.57
1:E:775:GLN:HG3	1:E:791:ASN:OD1	2.04	0.57
1:H:810:PRO:HA	1:H:813:ASN:OD1	2.04	0.57
1:D:699:THR:HG21	1:D:725:VAL:N	2.13	0.57
1:D:846:THR:O	1:D:847:GLN:CB	2.52	0.57
1:C:671:GLN:HE21	1:C:675:ARG:CZ	2.18	0.57
1:E:784:TYR:CZ	1:E:818:ILE:HD11	2.40	0.56
1:G:652:GLY:O	1:G:847:GLN:HG3	2.06	0.56
1:G:784:TYR:CZ	1:G:818:ILE:CD1	2.89	0.56
3:G:10:NAG:C4	3:G:11:NAG:O5	2.54	0.56
1:G:782:GLU:HG3	3:G:10:NAG:O4	2.06	0.56
1:B:710:GLU:OE1	1:B:835:ARG:NH1	2.39	0.56
1:H:756:ALA:O	1:H:760:SER:HB3	2.06	0.56
1:H:846:THR:HG22	1:H:847:GLN:H	1.70	0.56
1:E:759:THR:HB	1:E:795:ALA:HB2	1.88	0.55
1:H:703:SER:HB2	1:H:842:ARG:O	2.06	0.55
1:D:722:HIS:CG	7:D:494:HOH:O	2.58	0.55
1:G:775:GLN:C	1:G:792:ASN:HD22	2.09	0.55
1:B:699:THR:HG23	1:B:724:ARG:HA	1.87	0.55
1:F:665:ASN:O	1:F:668:ARG:HD3	2.06	0.55
1:C:783:VAL:HG12	1:C:784:TYR:CD2	2.42	0.55
1:E:775:GLN:HG2	1:E:791:ASN:OD1	2.06	0.55
1:F:842:ARG:NH2	1:F:847:GLN:HB3	2.20	0.55
4:B:13:MAN:C5	4:B:12:NAG:H5	2.36	0.55
2:D:13:MAN:C1	2:D:12:NAG:O5	2.53	0.55
1:B:697:LEU:HD23	1:B:698:LEU:N	2.22	0.55
1:H:662:GLY:HA2	7:H:391:HOH:O	2.07	0.55
1:H:783:VAL:HG13	1:H:816:TYR:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:811:ARG:HA	1:D:817:GLU:HG2	1.87	0.54
1:H:823:VAL:HG22	1:H:824:TRP:N	2.21	0.54
3:H:10:NAG:C3	3:H:11:NAG:C1	2.85	0.54
1:H:656:ILE:HG22	1:H:690:LEU:HD22	1.89	0.54
2:D:13:MAN:H4	2:D:12:NAG:C1	2.38	0.54
3:H:10:NAG:H4	3:H:11:NAG:N2	2.22	0.54
1:H:810:PRO:HB2	1:H:817:GLU:O	2.07	0.54
1:H:776:TRP:CZ3	1:H:778:GLU:CB	2.90	0.54
4:B:13:MAN:O5	4:B:12:NAG:C5	2.56	0.54
1:A:817:GLU:O	1:A:818:ILE:CG2	2.55	0.54
2:D:13:MAN:C4	2:D:12:NAG:C1	2.86	0.54
3:H:10:NAG:O4	3:H:11:NAG:C1	2.55	0.54
1:G:671:GLN:NE2	1:G:675:ARG:HH21	2.07	0.53
1:D:680:LEU:HD13	1:D:684:GLY:C	2.28	0.53
1:H:717:ALA:HB1	1:H:742:THR:CG2	2.39	0.53
1:F:842:ARG:HD2	1:F:847:GLN:HG2	1.85	0.53
1:F:845:VAL:HG12	1:F:846:THR:N	2.24	0.53
4:B:14:MAN:C4	4:B:13:MAN:H3	2.38	0.53
1:F:845:VAL:N	7:F:314:HOH:O	2.38	0.53
1:H:776:TRP:CH2	1:H:778:GLU:CB	2.91	0.53
1:H:809:ASP:HB3	1:H:812:ASN:ND2	2.22	0.53
2:D:13:MAN:C5	2:D:12:NAG:C1	2.87	0.53
1:H:846:THR:HB	1:H:847:GLN:CD	2.17	0.53
2:A:11:NAG:O3	2:A:14:MAN:H2	2.09	0.52
1:G:670:TRP:CZ3	1:G:771:ARG:HD2	2.44	0.52
1:B:710:GLU:HG2	1:B:716:GLU:HG2	1.90	0.52
1:A:699:THR:HG23	1:A:725:VAL:H	1.74	0.52
1:G:792:ASN:N	1:G:793:CYS:HA	2.22	0.52
1:G:681:ASN:HD21	1:G:685:GLU:CD	2.12	0.52
1:H:670:TRP:CZ3	1:H:771:ARG:HD3	2.44	0.52
1:B:784:TYR:CZ	1:B:818:ILE:HD12	2.44	0.52
1:G:709:LEU:HD23	1:G:837:VAL:HG22	1.92	0.52
1:H:818:ILE:HD13	1:H:819:GLU:CA	2.37	0.52
1:C:671:GLN:CD	1:C:675:ARG:HH21	2.13	0.52
1:C:695:LEU:O	1:C:699:THR:HB	2.10	0.52
1:E:667:ASN:ND2	3:E:10:NAG:O5	2.42	0.52
3:G:10:NAG:H4	3:G:11:NAG:C1	2.39	0.52
1:G:816:TYR:HE1	3:G:10:NAG:HO3	1.57	0.52
1:H:816:TYR:CB	7:H:389:HOH:O	2.48	0.52
1:F:695:LEU:O	1:F:699:THR:HB	2.09	0.52
1:G:755:GLY:C	1:G:757:GLU:H	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:670:TRP:CE3	1:H:771:ARG:HD2	2.45	0.52
2:A:13:MAN:O3	2:A:12:NAG:N2	2.43	0.51
1:G:835:ARG:HD2	7:G:419:HOH:O	2.09	0.51
1:H:696:HIS:HD2	7:H:370:HOH:O	1.93	0.51
1:E:815:PRO:HG2	1:E:816:TYR:CE2	2.45	0.51
1:F:845:VAL:HG13	1:F:846:THR:N	2.25	0.51
1:B:845:VAL:HG13	1:B:846:THR:N	2.25	0.51
1:E:810:PRO:O	1:E:817:GLU:CA	2.57	0.51
1:F:776:TRP:CE3	1:F:778:GLU:HB3	2.46	0.51
1:H:670:TRP:CD2	1:H:771:ARG:HD2	2.45	0.51
2:A:13:MAN:C4	2:A:12:NAG:C1	2.83	0.51
1:B:699:THR:HG21	1:B:725:VAL:H	1.76	0.51
1:B:825:VAL:CB	7:B:492:HOH:O	2.30	0.51
2:C:11:NAG:O3	2:C:14:MAN:C2	2.49	0.51
1:H:772:ASP:OD1	1:H:773:ALA:N	2.44	0.51
1:G:703:SER:CA	1:G:844:LEU:HD12	2.41	0.51
1:G:842:ARG:CG	1:G:847:GLN:OXT	2.58	0.51
1:B:842:ARG:NH1	7:B:113:HOH:O	2.43	0.51
2:C:14:MAN:C6	2:C:13:MAN:C4	2.87	0.50
1:C:671:GLN:CG	1:C:675:ARG:HE	2.21	0.50
3:G:10:NAG:O4	3:G:11:NAG:C2	2.60	0.50
1:G:671:GLN:NE2	1:G:675:ARG:NH2	2.60	0.50
1:A:709:LEU:HD23	1:A:837:VAL:HG22	1.94	0.50
1:E:728:GLU:HB2	1:E:732:TYR:CZ	2.46	0.50
1:G:778:GLU:HB3	7:G:339:HOH:O	2.11	0.50
1:H:695:LEU:O	1:H:699:THR:HB	2.12	0.50
1:H:752:VAL:HG23	1:H:753:GLU:N	2.22	0.50
1:H:842:ARG:HD2	1:H:847:GLN:HE22	1.76	0.50
4:B:13:MAN:O5	4:B:12:NAG:H5	2.12	0.50
1:C:809:ASP:OD2	1:C:811:ARG:HB2	2.12	0.50
1:F:753:GLU:O	1:F:755:GLY:N	2.44	0.50
1:G:703:SER:CA	1:G:844:LEU:CD1	2.88	0.50
1:G:835:ARG:CD	7:G:419:HOH:O	2.59	0.50
1:G:702:GLY:HA3	1:G:844:LEU:HD13	1.94	0.50
1:G:699:THR:HG21	1:G:725:VAL:H	1.77	0.50
1:H:754:GLU:HB3	1:H:759:THR:HG21	1.92	0.50
1:H:652:GLY:O	1:H:842:ARG:HG2	2.12	0.50
1:H:671:GLN:CG	1:H:675:ARG:HH21	2.25	0.50
1:H:846:THR:C	1:H:847:GLN:CG	2.81	0.49
4:B:12:NAG:O7	4:B:12:NAG:O3	2.25	0.49
1:C:844:LEU:O	1:C:846:THR:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:792:ASN:N	1:D:793:CYS:HA	2.27	0.49
1:A:683:GLU:HG3	1:A:685:GLU:CD	2.33	0.49
1:G:751:SER:O	1:G:755:GLY:N	2.36	0.49
1:G:813:ASN:O	1:G:817:GLU:HG3	2.12	0.49
1:G:658:GLN:NE2	1:G:838:ARG:HE	2.08	0.49
1:H:776:TRP:CE3	1:H:778:GLU:HB2	2.46	0.49
1:H:776:TRP:CE3	1:H:778:GLU:CB	2.96	0.49
1:A:651:GLY:HA2	1:A:842:ARG:HH12	1.77	0.49
3:E:10:NAG:O4	3:E:10:NAG:H5	2.12	0.49
1:G:699:THR:HG23	1:G:725:VAL:H	1.77	0.49
1:E:710:GLU:CG	1:E:836:ALA:HB3	2.29	0.49
3:G:10:NAG:O4	3:G:11:NAG:H2	2.13	0.49
1:B:843:PRO:CB	1:B:846:THR:HG22	2.28	0.49
1:H:823:VAL:CG2	1:H:824:TRP:N	2.76	0.49
1:F:843:PRO:CA	1:F:846:THR:HG22	2.43	0.48
1:D:717:ALA:HB1	1:D:742:THR:HG22	1.95	0.48
1:G:651:GLY:O	1:G:847:GLN:O	2.31	0.48
1:H:653:TRP:CH2	1:H:842:ARG:HD3	2.48	0.48
1:H:825:VAL:HG23	1:H:826:SER:N	2.28	0.48
1:D:811:ARG:HB2	1:D:811:ARG:HE	1.44	0.48
1:H:671:GLN:HG2	1:H:675:ARG:NH2	2.28	0.48
1:A:674:LYS:NZ	1:A:728:GLU:OE1	2.42	0.48
4:B:14:MAN:C6	4:B:13:MAN:H3	2.43	0.48
1:F:683:GLU:HB2	1:F:685:GLU:OE2	2.13	0.48
1:H:783:VAL:CG1	1:H:816:TYR:CD2	2.96	0.48
2:C:13:MAN:O5	2:C:12:NAG:C1	2.62	0.48
1:B:843:PRO:HD2	1:B:846:THR:HG23	1.95	0.48
1:E:776:TRP:CE2	1:E:778:GLU:HB2	2.48	0.48
1:H:670:TRP:CZ3	1:H:771:ARG:CD	2.97	0.48
1:C:665:ASN:O	1:C:668:ARG:HD3	2.14	0.48
1:D:783:VAL:HG12	1:D:818:ILE:CD1	2.44	0.48
1:E:651:GLY:N	1:E:847:GLN:O	2.47	0.48
1:H:783:VAL:HG12	1:H:816:TYR:CG	2.48	0.48
1:H:808:TYR:CE1	1:H:831:ASP:HA	2.49	0.48
1:C:752:VAL:HG13	1:C:753:GLU:N	2.28	0.48
1:H:813:ASN:HB3	1:H:816:TYR:O	2.13	0.48
1:B:776:TRP:CD2	1:B:778:GLU:CB	2.98	0.47
1:C:783:VAL:O	1:C:818:ILE:HD11	2.14	0.47
1:F:843:PRO:CG	1:F:846:THR:HB	2.31	0.47
1:H:705:LEU:O	1:H:720:GLU:HA	2.14	0.47
1:H:727:SER:OG	1:H:730:GLU:OE1	2.31	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:13:MAN:C6	2:C:12:NAG:C5	2.90	0.47
1:E:782:GLU:O	3:E:10:NAG:N2	2.31	0.47
1:E:792:ASN:N	1:E:793:CYS:HA	2.29	0.47
1:F:758:TYR:HD1	1:F:792:ASN:CB	1.98	0.47
1:H:846:THR:C	1:H:847:GLN:HG2	2.34	0.47
1:B:697:LEU:C	1:B:697:LEU:HD23	2.35	0.47
1:H:759:THR:HB	1:H:795:ALA:HB2	1.96	0.47
1:D:752:VAL:HA	7:D:214:HOH:O	2.14	0.47
1:G:771:ARG:HD3	1:G:771:ARG:O	2.15	0.47
2:A:14:MAN:O4	2:A:13:MAN:H5	2.14	0.47
2:C:13:MAN:C5	2:C:12:NAG:C1	2.93	0.47
1:E:651:GLY:C	1:E:842:ARG:HH12	2.17	0.47
1:G:702:GLY:HA3	1:G:844:LEU:CD1	2.43	0.47
1:H:699:THR:HG21	1:H:725:VAL:H	1.78	0.47
1:G:815:PRO:HG2	1:G:816:TYR:CE1	2.50	0.47
3:H:10:NAG:H3	3:H:11:NAG:C1	2.45	0.47
1:C:699:THR:HG21	1:C:725:VAL:N	2.18	0.47
1:D:751:SER:C	7:D:214:HOH:O	2.53	0.47
1:E:776:TRP:CH2	1:E:778:GLU:HB3	2.48	0.47
1:H:809:ASP:OD1	1:H:811:ARG:HD3	2.14	0.47
1:F:758:TYR:OH	1:F:775:GLN:O	2.20	0.46
1:F:792:ASN:N	1:F:793:CYS:HA	2.26	0.46
3:H:10:NAG:C4	3:H:11:NAG:N2	2.78	0.46
3:H:10:NAG:H5	3:H:11:NAG:H82	1.95	0.46
2:A:14:MAN:H3	2:A:15:MAN:C4	2.45	0.46
4:B:15:MAN:O2	4:B:15:MAN:C6	2.64	0.46
1:E:699:THR:HG21	1:E:725:VAL:N	2.26	0.46
1:H:842:ARG:HB3	1:H:843:PRO:HD2	1.96	0.46
1:H:667:ASN:ND2	3:H:10:NAG:O5	2.43	0.46
1:B:752:VAL:HA	7:B:102:HOH:O	2.15	0.46
1:D:809:ASP:O	1:D:812:ASN:HB2	2.16	0.46
1:E:651:GLY:N	1:E:842:ARG:HH22	2.14	0.46
1:A:699:THR:HG21	1:A:725:VAL:N	2.31	0.46
2:D:13:MAN:O5	2:D:12:NAG:C5	2.64	0.46
1:G:658:GLN:HE21	1:G:838:ARG:NE	2.11	0.46
1:H:776:TRP:CZ2	1:H:778:GLU:CB	2.98	0.46
1:H:809:ASP:HB3	1:H:812:ASN:HD21	1.81	0.46
1:B:843:PRO:CG	1:B:846:THR:CG2	2.93	0.46
1:F:843:PRO:CB	1:F:846:THR:HG22	2.45	0.46
1:F:842:ARG:NH2	1:F:847:GLN:CB	2.65	0.46
4:B:13:MAN:O5	4:B:12:NAG:O5	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:669:THR:OG1	1:B:671:GLN:HG3	2.15	0.45
1:C:776:TRP:CZ3	1:C:778:GLU:HB3	2.52	0.45
1:F:668:ARG:NE	1:F:672:ASP:OD2	2.46	0.45
1:H:776:TRP:CH2	1:H:778:GLU:HB3	2.51	0.45
2:A:14:MAN:C4	2:A:13:MAN:H5	2.47	0.45
1:F:752:VAL:HG23	7:F:475:HOH:O	2.15	0.45
1:F:846:THR:OG1	7:F:487:HOH:O	2.20	0.45
1:E:657:GLN:HG3	1:E:689:TRP:CZ3	2.51	0.45
1:C:672:ASP:OD1	1:C:675:ARG:NH2	2.50	0.45
1:D:683:GLU:OE1	1:D:685:GLU:OE2	2.34	0.45
1:F:845:VAL:C	1:F:847:GLN:N	2.60	0.45
1:G:811:ARG:HA	1:G:817:GLU:HG2	1.99	0.45
2:D:13:MAN:O6	2:D:12:NAG:H5	2.16	0.45
1:F:842:ARG:NE	1:F:846:THR:C	2.70	0.45
1:G:703:SER:HA	1:G:844:LEU:HD12	1.97	0.45
1:H:717:ALA:HB1	1:H:742:THR:HG23	1.99	0.45
4:B:11:NDG:O3	4:B:14:MAN:C1	2.64	0.45
1:E:783:VAL:HG11	1:E:818:ILE:CD1	2.46	0.45
1:H:816:TYR:CA	7:H:389:HOH:O	2.65	0.45
2:A:11:NAG:O3	2:A:15:MAN:C3	2.63	0.44
1:E:670:TRP:CZ3	1:E:771:ARG:HD3	2.53	0.44
1:E:843:PRO:HA	7:E:271:HOH:O	2.17	0.44
1:C:671:GLN:NE2	1:C:675:ARG:NE	2.63	0.44
1:H:670:TRP:CE3	1:H:771:ARG:CD	3.01	0.44
1:D:846:THR:C	1:D:847:GLN:CG	2.80	0.44
1:F:847:GLN:HA	1:F:847:GLN:OE1	2.18	0.44
1:B:776:TRP:CD2	1:B:778:GLU:HB3	2.52	0.44
1:F:776:TRP:CZ3	1:F:778:GLU:HB3	2.53	0.44
1:H:813:ASN:CB	1:H:816:TYR:O	2.65	0.44
1:G:843:PRO:CD	1:G:847:GLN:CB	2.89	0.44
1:C:722:HIS:O	1:C:736:VAL:HA	2.17	0.43
1:G:739:TYR:CG	1:G:740:GLU:N	2.86	0.43
1:E:844:LEU:HD12	1:E:845:VAL:N	2.30	0.43
1:G:819:GLU:HG2	1:G:830:ALA:C	2.38	0.43
1:F:758:TYR:CE2	1:F:792:ASN:ND2	2.77	0.43
1:G:845:VAL:HG22	1:G:846:THR:N	2.34	0.43
1:B:825:VAL:CG1	7:B:492:HOH:O	2.66	0.43
1:F:843:PRO:N	1:F:846:THR:CG2	2.80	0.43
3:G:10:NAG:C6	3:G:11:NAG:C1	2.97	0.43
1:G:816:TYR:HE1	3:G:10:NAG:O3	2.01	0.43
1:E:754:GLU:HG2	1:E:754:GLU:H	1.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:784:TYR:HE1	1:H:818:ILE:HD12	1.82	0.43
1:A:651:GLY:CA	1:A:842:ARG:HH12	2.32	0.42
4:B:14:MAN:H5	4:B:15:MAN:H3	2.00	0.42
1:H:810:PRO:O	1:H:817:GLU:HA	2.18	0.42
1:H:671:GLN:HG2	1:H:675:ARG:HH21	1.82	0.42
1:B:845:VAL:CG1	1:B:846:THR:N	2.83	0.42
1:H:717:ALA:HA	1:H:742:THR:CG2	2.49	0.42
1:H:718:TYR:N	1:H:742:THR:HG22	2.21	0.42
1:C:671:GLN:CD	1:C:675:ARG:NH2	2.72	0.42
1:A:809:ASP:O	1:A:812:ASN:HB2	2.19	0.42
1:H:809:ASP:OD1	1:H:811:ARG:CB	2.66	0.42
3:E:10:NAG:C5	3:E:10:NAG:C1	2.94	0.42
1:G:660:MET:HB2	7:G:321:HOH:O	2.19	0.42
1:F:795:ALA:O	1:F:825:VAL:HB	2.19	0.42
1:A:701:ARG:NH1	1:A:701:ARG:HG2	2.22	0.42
4:B:13:MAN:C1	4:B:12:NAG:O5	2.67	0.42
2:A:14:MAN:C1	2:A:15:MAN:H3	2.49	0.42
1:F:717:ALA:HB1	1:F:742:THR:HG23	2.01	0.42
1:E:667:ASN:ND2	3:E:10:NAG:C2	2.67	0.42
1:H:813:ASN:O	1:H:816:TYR:C	2.57	0.42
1:E:651:GLY:CA	1:E:842:ARG:HH12	2.33	0.41
1:F:842:ARG:HH21	1:F:844:LEU:C	2.12	0.41
1:F:739:TYR:CG	1:F:740:GLU:N	2.88	0.41
1:G:842:ARG:HB3	1:G:847:GLN:OXT	2.15	0.41
1:H:726:GLY:O	1:H:732:TYR:HA	2.20	0.41
1:B:842:ARG:HE	1:B:847:GLN:CB	2.32	0.41
1:G:784:TYR:HH	1:G:818:ILE:HD11	1.71	0.41
1:E:657:GLN:HB3	1:E:839:MET:HB2	2.02	0.41
1:F:671:GLN:O	1:F:675:ARG:HG3	2.19	0.41
1:D:809:ASP:OD2	1:D:811:ARG:CZ	2.68	0.41
3:E:10:NAG:C4	3:E:10:NAG:O5	2.58	0.41
1:A:724:ARG:O	1:A:735:GLN:HG2	2.21	0.41
3:H:11:NAG:O3	3:H:11:NAG:H61	2.20	0.41
1:G:775:GLN:HB2	1:G:791:ASN:C	2.41	0.41
1:H:819:GLU:HB3	1:H:830:ALA:O	2.20	0.41
1:E:846:THR:O	1:E:847:GLN:CB	2.60	0.41
1:E:842:ARG:CZ	1:E:847:GLN:HA	2.51	0.41
1:G:775:GLN:C	1:G:792:ASN:ND2	2.74	0.41
1:G:778:GLU:CB	7:G:339:HOH:O	2.69	0.41
2:A:14:MAN:O4	2:A:13:MAN:C5	2.68	0.40
1:G:801:ILE:O	1:G:821:GLY:HA2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:762:ASN:O	1:E:763:ASN:HB2	2.22	0.40
4:B:14:MAN:C6	4:B:13:MAN:C3	2.96	0.40
1:B:775:GLN:NE2	7:B:106:HOH:O	2.51	0.40
1:D:751:SER:HB2	1:D:825:VAL:HG21	2.02	0.40
1:G:818:ILE:HG12	1:G:819:GLU:H	1.84	0.40
1:A:726:GLY:O	1:A:732:TYR:HA	2.21	0.40
1:B:776:TRP:CE2	1:B:778:GLU:CB	3.02	0.40
1:H:818:ILE:HG23	1:H:820:ASN:HB3	2.04	0.40
1:F:768:THR:O	1:F:769:PHE:C	2.59	0.40
1:H:842:ARG:HD2	1:H:847:GLN:NE2	2.36	0.40

All (6) 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:C:847:GLN:OXT	1:H:678:GLY:O[1_445]	0.94	1.26
1:D:847:GLN:O	1:H:722:HIS:ND1[1_545]	1.73	0.47
1:C:847:GLN:C	1:H:678:GLY:O[1_445]	1.88	0.32
1:C:847:GLN:NE2	1:H:680:LEU:O[1_445]	2.03	0.17
1:C:847:GLN:OXT	1:H:678:GLY:C[1_445]	2.13	0.07
1:C:680:LEU:O	1:H:847:GLN:O[1_445]	2.18	0.02

## 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	195/201 (97%)	184 (94%)	11 (6%)	0	100	100
1	B	195/201 (97%)	188 (96%)	7 (4%)	0	100	100
1	C	195/201 (97%)	184 (94%)	10 (5%)	1 (0%)	32	28
1	D	195/201 (97%)	183 (94%)	11 (6%)	1 (0%)	32	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	195/201 (97%)	187 (96%)	7 (4%)	1 (0%)	32	28
1	F	195/201 (97%)	181 (93%)	10 (5%)	4 (2%)	8	3
1	G	195/201 (97%)	176 (90%)	16 (8%)	3 (2%)	12	6
1	H	195/201 (97%)	175 (90%)	17 (9%)	3 (2%)	12	6
All	All	1560/1608 (97%)	1458 (94%)	89 (6%)	13 (1%)	22	17

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	846	THR
1	G	756	ALA
1	C	846	THR
1	F	754	GLU
1	H	652	GLY
1	F	753	GLU
1	G	652	GLY
1	H	752	VAL
1	F	661	ASP
1	H	844	LEU
1	E	660	MET
1	G	845	VAL
1	D	755	GLY

### 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	159/163 (98%)	138 (87%)	21 (13%)	5	2
1	B	159/163 (98%)	140 (88%)	19 (12%)	6	3
1	C	159/163 (98%)	143 (90%)	16 (10%)	9	5
1	D	159/163 (98%)	141 (89%)	18 (11%)	7	3
1	E	159/163 (98%)	137 (86%)	22 (14%)	4	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	159/163 (98%)	131 (82%)	28 (18%)	2	1
1	G	159/163 (98%)	137 (86%)	22 (14%)	4	2
1	H	159/163 (98%)	136 (86%)	23 (14%)	4	2
All	All	1272/1304 (98%)	1103 (87%)	169 (13%)	4	2

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	664	LEU
1	A	682	ASP
1	A	683	GLU
1	A	693	ASP
1	A	694	TYR
1	A	695	LEU
1	A	699	THR
1	A	701	ARG
1	A	735	GLN
1	A	742	THR
1	A	752	VAL
1	A	754	GLU
1	A	771	ARG
1	A	777	GLU
1	A	778	GLU
1	A	811	ARG
1	A	816	TYR
1	A	823	VAL
1	A	831	ASP
1	A	837	VAL
1	A	847	GLN
1	B	654	LEU
1	B	664	LEU
1	B	671	GLN
1	B	682	ASP
1	B	694	TYR
1	B	695	LEU
1	B	697	LEU
1	B	699	THR
1	B	742	THR
1	B	752	VAL
1	B	757	GLU
1	B	771	ARG

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Mol	Chain	Res	Type
1	B	778	GLU
1	B	807	SER
1	B	818	ILE
1	B	823	VAL
1	B	831	ASP
1	B	837	VAL
1	B	846	THR
1	C	664	LEU
1	C	668	ARG
1	C	682	ASP
1	C	697	LEU
1	C	699	THR
1	C	735	GLN
1	C	742	THR
1	C	751	SER
1	C	753	GLU
1	C	778	GLU
1	C	783	VAL
1	C	819	GLU
1	C	823	VAL
1	C	837	VAL
1	C	846	THR
1	C	847	GLN
1	D	664	LEU
1	D	680	LEU
1	D	682	ASP
1	D	683	GLU
1	D	697	LEU
1	D	699	THR
1	D	735	GLN
1	D	742	THR
1	D	751	SER
1	D	753	GLU
1	D	757	GLU
1	D	771	ARG
1	D	777	GLU
1	D	778	GLU
1	D	811	ARG
1	D	825	VAL
1	D	837	VAL
1	D	845	VAL
1	E	664	LEU

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Mol	Chain	Res	Type
1	E	671	GLN
1	E	675	ARG
1	E	693	ASP
1	E	695	LEU
1	E	699	THR
1	E	710	GLU
1	E	728	GLU
1	E	736	VAL
1	E	738	SER
1	E	742	THR
1	E	751	SER
1	E	754	GLU
1	E	760	SER
1	E	771	ARG
1	E	778	GLU
1	E	814	SER
1	E	819	GLU
1	E	831	ASP
1	E	835	ARG
1	E	844	LEU
1	E	845	VAL
1	F	655	LEU
1	F	664	LEU
1	F	682	ASP
1	F	693	ASP
1	F	694	TYR
1	F	695	LEU
1	F	699	THR
1	F	735	GLN
1	F	736	VAL
1	F	738	SER
1	F	742	THR
1	F	752	VAL
1	F	753	GLU
1	F	757	GLU
1	F	758	TYR
1	F	771	ARG
1	F	775	GLN
1	F	778	GLU
1	F	783	VAL
1	F	812	ASN
1	F	819	GLU

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Mol	Chain	Res	Type
1	F	823	VAL
1	F	825	VAL
1	F	833	SER
1	F	837	VAL
1	F	840	LYS
1	F	845	VAL
1	F	847	GLN
1	G	659	ARG
1	G	660	MET
1	G	664	LEU
1	G	668	ARG
1	G	671	GLN
1	G	682	ASP
1	G	697	LEU
1	G	699	THR
1	G	701	ARG
1	G	710	GLU
1	G	735	GLN
1	G	738	SER
1	G	742	THR
1	G	754	GLU
1	G	757	GLU
1	G	775	GLN
1	G	778	GLU
1	G	819	GLU
1	G	823	VAL
1	G	831	ASP
1	G	837	VAL
1	G	844	LEU
1	H	664	LEU
1	H	668	ARG
1	H	699	THR
1	H	730	GLU
1	H	735	GLN
1	H	738	SER
1	H	742	THR
1	H	754	GLU
1	H	757	GLU
1	H	774	ASP
1	H	778	GLU
1	H	783	VAL
1	H	812	ASN

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Mol	Chain	Res	Type
1	H	814	SER
1	H	818	ILE
1	H	819	GLU
1	H	831	ASP
1	H	833	SER
1	H	840	LYS
1	H	842	ARG
1	H	844	LEU
1	H	846	THR
1	H	847	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	775	GLN
1	A	813	ASN
1	A	847	GLN
1	B	775	GLN
1	B	813	ASN
1	C	671	GLN
1	E	667	ASN
1	F	763	ASN
1	F	813	ASN
1	G	658	GLN
1	G	667	ASN
1	G	671	GLN
1	G	763	ASN
1	G	775	GLN
1	G	792	ASN
1	H	667	ASN
1	H	765	GLN
1	H	812	ASN

### 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 ⓘ

25 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	10	1,2	14,14,15	0.87	1 (7%)	15,19,21	0.79	0
2	NAG	A	11	2	14,14,15	0.55	0	15,19,21	1.29	2 (13%)
2	NAG	A	12	2	14,14,15	0.60	0	15,19,21	1.43	2 (13%)
2	MAN	A	13	2	11,11,12	0.81	0	13,15,17	0.76	0
2	MAN	A	14	2	11,11,12	0.91	1 (9%)	13,15,17	1.82	3 (23%)
2	MAN	A	15	2	11,11,12	0.98	0	13,15,17	1.82	2 (15%)
4	NDG	B	11	3,4	14,14,15	0.84	0	15,19,21	0.80	0
4	NAG	B	12	4	14,14,15	0.86	0	15,19,21	1.46	2 (13%)
4	MAN	B	13	4	11,11,12	1.48	2 (18%)	13,15,17	1.72	3 (23%)
4	MAN	B	14	4	11,11,12	0.88	0	13,15,17	2.25	3 (23%)
4	MAN	B	15	4	9,10,12	0.69	0	13,14,17	1.09	1 (7%)
2	NAG	C	10	1,2	14,14,15	0.46	0	15,19,21	0.74	0
2	NAG	C	11	2	14,14,15	0.67	0	15,19,21	1.33	1 (6%)
2	NAG	C	12	2	14,14,15	0.90	0	15,19,21	0.80	0
2	MAN	C	13	2	11,11,12	0.67	0	13,15,17	1.08	1 (7%)
2	MAN	C	14	2	11,11,12	0.61	0	13,15,17	1.10	1 (7%)
2	MAN	C	15	2	11,11,12	0.96	1 (9%)	13,15,17	1.12	2 (15%)
2	NAG	D	10	1,2	14,14,15	6.08	11 (78%)	15,19,21	7.20	13 (86%)
2	NAG	D	11	2	14,14,15	0.79	1 (7%)	15,19,21	0.84	1 (6%)
2	NAG	D	12	2	14,14,15	0.89	0	15,19,21	2.08	5 (33%)
2	MAN	D	13	2	11,11,12	0.83	0	13,15,17	1.20	1 (7%)
2	MAN	D	14	2	11,11,12	1.04	1 (9%)	13,15,17	1.76	4 (30%)
2	MAN	D	15	2	11,11,12	0.71	0	13,15,17	1.33	2 (15%)
5	NAG	F	10	1,5	14,14,15	0.64	0	15,19,21	1.09	1 (6%)
5	NAG	F	11	5	14,14,15	0.78	0	15,19,21	1.55	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	10	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	11	2	-	0/6/23/26	0/1/1/1
2	NAG	A	12	2	-	0/6/23/26	0/1/1/1
2	MAN	A	13	2	-	0/2/19/22	0/1/1/1
2	MAN	A	14	2	1/1/4/5	0/2/19/22	1/1/1/1
2	MAN	A	15	2	-	0/2/19/22	0/1/1/1
4	NDG	B	11	3,4	-	0/6/23/26	0/1/1/1
4	NAG	B	12	4	-	0/6/23/26	0/1/1/1
4	MAN	B	13	4	-	0/2/19/22	0/1/1/1
4	MAN	B	14	4	1/1/4/5	0/2/19/22	0/1/1/1
4	MAN	B	15	4	-	0/0/17/22	0/1/1/1
2	NAG	C	10	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	11	2	-	0/6/23/26	0/1/1/1
2	NAG	C	12	2	-	0/6/23/26	0/1/1/1
2	MAN	C	13	2	-	0/2/19/22	0/1/1/1
2	MAN	C	14	2	1/1/4/5	0/2/19/22	0/1/1/1
2	MAN	C	15	2	1/1/4/5	0/2/19/22	1/1/1/1
2	NAG	D	10	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	11	2	-	0/6/23/26	0/1/1/1
2	NAG	D	12	2	-	0/6/23/26	0/1/1/1
2	MAN	D	13	2	-	0/2/19/22	0/1/1/1
2	MAN	D	14	2	-	0/2/19/22	0/1/1/1
2	MAN	D	15	2	1/1/4/5	0/2/19/22	0/1/1/1
5	NAG	F	10	1,5	-	0/6/23/26	0/1/1/1
5	NAG	F	11	5	-	0/6/23/26	0/1/1/1

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	10	NAG	O7-C7	-9.57	1.00	1.23
2	D	10	NAG	C8-C7	-7.32	1.34	1.50
2	D	10	NAG	C4-C5	-2.99	1.46	1.53
2	D	14	MAN	C2-C3	-2.47	1.49	1.52
2	A	14	MAN	O5-C1	2.10	1.47	1.43
2	C	15	MAN	O5-C5	2.11	1.47	1.43
4	B	13	MAN	C1-C2	2.33	1.57	1.52
2	D	11	NAG	C1-C2	2.37	1.55	1.52
2	A	10	NAG	C1-C2	2.49	1.55	1.52
2	D	10	NAG	O4-C4	2.56	1.48	1.43
2	D	10	NAG	C3-C2	3.49	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	13	MAN	C2-C3	3.76	1.57	1.52
2	D	10	NAG	O5-C5	3.82	1.51	1.43
2	D	10	NAG	C6-C5	4.62	1.67	1.51
2	D	10	NAG	C7-N2	5.70	1.55	1.34
2	D	10	NAG	O5-C1	7.54	1.56	1.43
2	D	10	NAG	C1-C2	10.01	1.66	1.52
2	D	10	NAG	C2-N2	10.57	1.65	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	10	NAG	O5-C1-C2	-16.82	88.07	111.47
2	D	10	NAG	O7-C7-N2	-10.01	102.65	121.92
2	D	10	NAG	O4-C4-C3	-8.44	91.99	110.36
2	D	10	NAG	O6-C6-C5	-6.65	88.96	111.34
2	D	10	NAG	C3-C4-C5	-6.36	99.01	110.22
2	D	12	NAG	C2-N2-C7	-5.38	115.09	122.94
4	B	14	MAN	C3-C4-C5	-5.33	100.82	110.22
4	B	13	MAN	C3-C4-C5	-4.37	102.52	110.22
2	D	14	MAN	C3-C4-C5	-4.30	102.64	110.22
4	B	14	MAN	C1-C2-C3	-4.20	104.32	109.65
2	A	14	MAN	C2-C3-C4	-3.97	103.95	110.88
2	C	11	NAG	C4-C3-C2	-3.87	105.34	111.02
2	D	10	NAG	O3-C3-C2	-3.79	101.27	109.39
2	A	14	MAN	C1-C2-C3	-3.74	104.91	109.65
2	D	10	NAG	O4-C4-C5	-3.73	99.90	109.28
4	B	12	NAG	C1-O5-C5	-3.69	107.08	112.17
2	A	12	NAG	C2-N2-C7	-2.98	118.59	122.94
2	D	10	NAG	C2-N2-C7	-2.93	118.67	122.94
2	C	15	MAN	C1-C2-C3	-2.86	106.03	109.65
2	A	12	NAG	O5-C1-C2	-2.85	107.51	111.47
2	D	12	NAG	C4-C3-C2	-2.82	106.88	111.02
2	D	10	NAG	C8-C7-N2	-2.75	111.14	116.11
2	D	12	NAG	O5-C1-C2	-2.72	107.69	111.47
2	D	12	NAG	C1-O5-C5	-2.66	108.50	112.17
2	D	15	MAN	O5-C1-C2	-2.63	106.67	110.79
2	D	13	MAN	C1-C2-C3	-2.56	106.41	109.65
2	D	15	MAN	C1-C2-C3	-2.38	106.63	109.65
2	A	14	MAN	C3-C4-C5	-2.31	106.15	110.22
2	D	14	MAN	C1-C2-C3	-2.29	106.75	109.65
2	D	11	NAG	C2-N2-C7	-2.18	119.77	122.94
2	C	14	MAN	C2-C3-C4	-2.14	107.14	110.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	15	MAN	C2-C3-C4	-2.14	107.15	110.88
4	B	14	MAN	O5-C1-C2	-2.02	107.62	110.79
4	B	12	NAG	C3-C4-C5	2.13	113.97	110.22
2	D	14	MAN	O5-C1-C2	2.13	114.13	110.79
4	B	15	MAN	C1-C2-C3	2.17	112.41	109.65
5	F	11	NAG	C3-C4-C5	2.20	114.10	110.22
2	D	14	MAN	C1-O5-C5	2.20	115.20	112.17
2	D	12	NAG	C6-C5-C4	2.25	118.27	113.00
2	A	11	NAG	C4-C3-C2	2.32	114.42	111.02
4	B	13	MAN	C6-C5-C4	2.37	118.54	113.00
2	A	11	NAG	C3-C4-C5	2.41	114.47	110.22
2	C	13	MAN	C1-O5-C5	2.47	115.57	112.17
5	F	10	NAG	C4-C3-C2	2.55	114.75	111.02
4	B	13	MAN	C1-C2-C3	2.67	113.03	109.65
2	D	10	NAG	C1-O5-C5	3.06	116.38	112.17
2	D	10	NAG	C6-C5-C4	3.70	121.67	113.00
2	D	10	NAG	C4-C3-C2	3.74	116.50	111.02
2	A	15	MAN	C1-C2-C3	4.07	114.81	109.65
2	A	15	MAN	C1-O5-C5	4.23	118.00	112.17
5	F	11	NAG	C4-C3-C2	4.54	117.67	111.02
2	D	10	NAG	O7-C7-C8	12.45	144.71	122.06

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	14	MAN	C1
2	D	15	MAN	C1
2	A	14	MAN	C1
4	B	14	MAN	C1
2	C	15	MAN	C1

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	14	MAN	C1-C2-C3-C4-C5-O5
2	C	15	MAN	C1-C2-C3-C4-C5-O5

19 monomers are involved in 84 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	11	NAG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	12	NAG	3	0
2	A	13	MAN	6	0
2	A	14	MAN	13	0
2	A	15	MAN	9	0
4	B	11	NDG	1	0
4	B	12	NAG	9	0
4	B	13	MAN	17	0
4	B	14	MAN	15	0
4	B	15	MAN	5	0
2	C	11	NAG	2	0
2	C	12	NAG	12	0
2	C	13	MAN	22	0
2	C	14	MAN	13	0
2	C	15	MAN	3	0
2	D	12	NAG	8	0
2	D	13	MAN	12	0
2	D	14	MAN	4	0
5	F	10	NAG	1	0

## 5.6 Ligand geometry

Of 15 ligands modelled in this entry, 8 are monoatomic - leaving 7 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	$\# Z  > 2$
3	NAG	B	10	1,4	14,14,15	6.95	12 (85%)	15,19,21	4.24	10 (66%)
3	NAG	E	10	1,3	14,14,15	8.38	11 (78%)	15,19,21	5.57	12 (80%)
3	NAG	E	11	3	14,14,15	0.59	0	15,19,21	0.74	0
3	NAG	G	10	1	14,14,15	0.55	0	15,19,21	1.45	2 (13%)
3	NAG	G	11	-	14,14,15	0.52	0	15,19,21	1.27	3 (20%)
3	NAG	H	10	1	14,14,15	0.50	0	15,19,21	1.12	1 (6%)
3	NAG	H	11	-	14,14,15	0.71	0	15,19,21	0.82	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	B	10	1,4	-	0/6/23/26	0/1/1/1
3	NAG	E	10	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	11	3	-	0/6/23/26	0/1/1/1
3	NAG	G	10	1	-	0/6/23/26	0/1/1/1
3	NAG	G	11	-	-	0/6/23/26	0/1/1/1
3	NAG	H	10	1	-	0/6/23/26	0/1/1/1
3	NAG	H	11	-	-	0/6/23/26	0/1/1/1

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	10	NAG	C1-C2	-15.91	1.30	1.52
3	B	10	NAG	O3-C3	-14.33	1.10	1.43
3	B	10	NAG	C1-C2	-6.36	1.43	1.52
3	B	10	NAG	O4-C4	-4.90	1.31	1.43
3	B	10	NAG	C6-C5	-4.87	1.35	1.51
3	E	10	NAG	C2-N2	-4.78	1.37	1.46
3	B	10	NAG	C2-N2	-2.72	1.41	1.46
3	E	10	NAG	O7-C7	2.42	1.28	1.23
3	E	10	NAG	C4-C3	2.98	1.59	1.52
3	E	10	NAG	C7-N2	4.03	1.49	1.34
3	B	10	NAG	C4-C3	4.13	1.62	1.52
3	B	10	NAG	O5-C5	4.20	1.52	1.43
3	E	10	NAG	O6-C6	4.34	1.60	1.42
3	B	10	NAG	O6-C6	4.63	1.61	1.42
3	B	10	NAG	C4-C5	6.25	1.66	1.53
3	E	10	NAG	C3-C2	6.42	1.66	1.52
3	E	10	NAG	C8-C7	6.48	1.64	1.50
3	B	10	NAG	C7-N2	6.90	1.59	1.34
3	E	10	NAG	O4-C4	9.16	1.64	1.43
3	B	10	NAG	O5-C1	10.43	1.60	1.43
3	B	10	NAG	C3-C2	10.87	1.76	1.52
3	E	10	NAG	O5-C1	14.89	1.68	1.43
3	E	10	NAG	O5-C5	16.32	1.77	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	10	NAG	C2-N2-C7	-10.42	107.74	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	10	NAG	O7-C7-N2	-9.56	103.52	121.92
3	E	10	NAG	C1-C2-N2	-7.38	97.89	110.49
3	B	10	NAG	C1-C2-N2	-7.25	98.10	110.49
3	E	10	NAG	O6-C6-C5	-7.20	87.10	111.34
3	E	10	NAG	O5-C1-C2	-6.39	102.58	111.47
3	E	10	NAG	O7-C7-C8	-4.63	113.63	122.06
3	B	10	NAG	O3-C3-C2	-4.58	99.58	109.39
3	B	10	NAG	O5-C1-C2	-4.27	105.54	111.47
3	B	10	NAG	C2-N2-C7	-3.82	117.38	122.94
3	E	10	NAG	O4-C4-C5	-3.38	100.77	109.28
3	G	11	NAG	C4-C3-C2	-3.19	106.34	111.02
3	B	10	NAG	O4-C4-C5	-2.92	101.93	109.28
3	H	11	NAG	C2-N2-C7	-2.50	119.30	122.94
3	G	11	NAG	C2-N2-C7	-2.28	119.62	122.94
3	G	10	NAG	C2-N2-C7	-2.13	119.84	122.94
3	G	11	NAG	O5-C1-C2	-2.03	108.65	111.47
3	B	10	NAG	C3-C4-C5	2.10	113.92	110.22
3	E	10	NAG	O3-C3-C4	2.33	115.42	110.36
3	B	10	NAG	C1-O5-C5	2.37	115.44	112.17
3	H	10	NAG	C3-C4-C5	2.82	115.19	110.22
3	E	10	NAG	C1-O5-C5	3.41	116.87	112.17
3	G	10	NAG	C3-C4-C5	3.81	116.93	110.22
3	E	10	NAG	C8-C7-N2	4.31	123.89	116.11
3	E	10	NAG	O4-C4-C3	4.35	119.83	110.36
3	B	10	NAG	C6-C5-C4	4.43	123.37	113.00
3	B	10	NAG	C8-C7-N2	4.71	124.61	116.11
3	E	10	NAG	C3-C4-C5	5.41	119.75	110.22
3	E	10	NAG	C6-C5-C4	9.42	135.04	113.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 52 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	10	NAG	5	0
3	E	10	NAG	17	0
3	E	11	NAG	2	0
3	G	10	NAG	13	0
3	G	11	NAG	9	0
3	H	10	NAG	15	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	11	NAG	10	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.