Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:57 PM GMT

PDB ID	:	1R9M
Title	:	Crystal Structure of Human Dipeptidyl Peptidase IV at 2.1 Ang. Resolution.
Authors	:	Aertgeerts, K.; Ye, S.; Tennant, M.G.; Collins, B.; Rogers, J.; Sang, B.C.; Skene, R.J.; Webb, D.R.; Prasad, G.S.
Deposited on	:	2003-10-30
Resolution	:	2.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

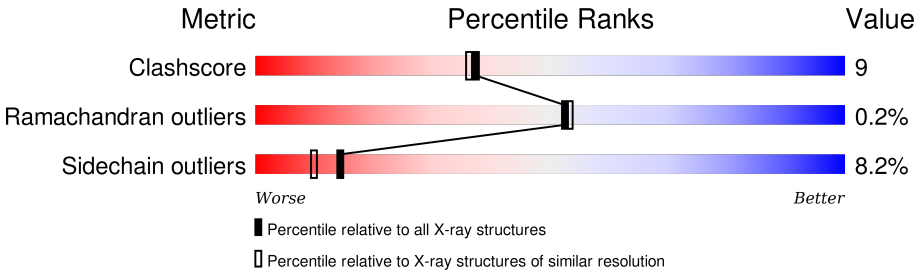
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (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 >=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 <=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	733	71% 23%
1	B	733	73% 23%
1	C	733	74% 22%
1	D	733	75% 20%

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	6851	X	-	-	-
2	NAG	C	1501	X	-	-	-
2	NAG	D	2191	X	-	-	-
2	NAG	D	5201	X	-	-	-
2	NAG	D	6851	X	-	-	-
3	NAG	B	2192	X	-	-	-
6	MAN	C	2294	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 26111 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

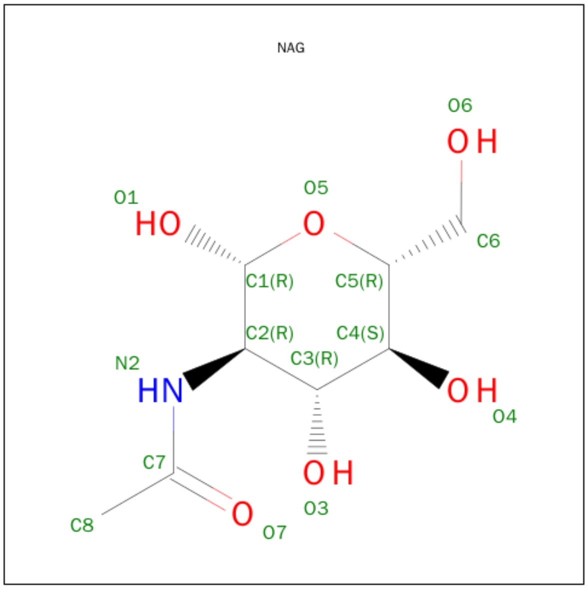
- Molecule 1 is a protein called Dipeptidyl peptidase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	727	Total	C	N	O	S	0	0	0
			5951	3821	978	1126	26			
1	B	733	Total	C	N	O	S	0	0	0
			6013	3857	997	1133	26			
1	C	727	Total	C	N	O	S	0	0	0
			5951	3821	978	1126	26			
1	D	727	Total	C	N	O	S	0	0	0
			5957	3824	981	1126	26			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	HIS	-	EXPRESSION TAG	UNP P27487
A	35	HIS	-	EXPRESSION TAG	UNP P27487
A	36	HIS	-	EXPRESSION TAG	UNP P27487
A	37	HIS	-	EXPRESSION TAG	UNP P27487
A	38	HIS	-	EXPRESSION TAG	UNP P27487
B	34	HIS	-	EXPRESSION TAG	UNP P27487
B	35	HIS	-	EXPRESSION TAG	UNP P27487
B	36	HIS	-	EXPRESSION TAG	UNP P27487
B	37	HIS	-	EXPRESSION TAG	UNP P27487
B	38	HIS	-	EXPRESSION TAG	UNP P27487
C	34	HIS	-	EXPRESSION TAG	UNP P27487
C	35	HIS	-	EXPRESSION TAG	UNP P27487
C	36	HIS	-	EXPRESSION TAG	UNP P27487
C	37	HIS	-	EXPRESSION TAG	UNP P27487
C	38	HIS	-	EXPRESSION TAG	UNP P27487
D	34	HIS	-	EXPRESSION TAG	UNP P27487
D	35	HIS	-	EXPRESSION TAG	UNP P27487
D	36	HIS	-	EXPRESSION TAG	UNP P27487
D	37	HIS	-	EXPRESSION TAG	UNP P27487
D	38	HIS	-	EXPRESSION TAG	UNP P27487

- Molecule 2 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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

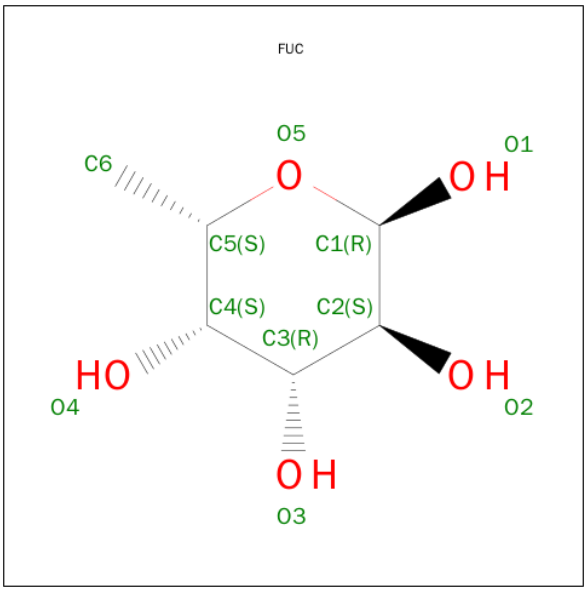
- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 4 is a polymer of unknown type called SUGAR (3-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	3	Total C N O 39 22 2 15	0	0

- Molecule 5 is SUGAR (FUCOSE) (three-letter code: FUC) (formula: $C_6H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total C O 10 6 4	0	0

- Molecule 6 is a polymer of unknown type called SUGAR (4-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	4	Total C N O 50 28 2 20	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	466	Total O 466 466	0	0
7	B	467	Total O 467 467	0	0
7	C	334	Total O 334 334	0	0
7	D	411	Total O 411 411	0	0

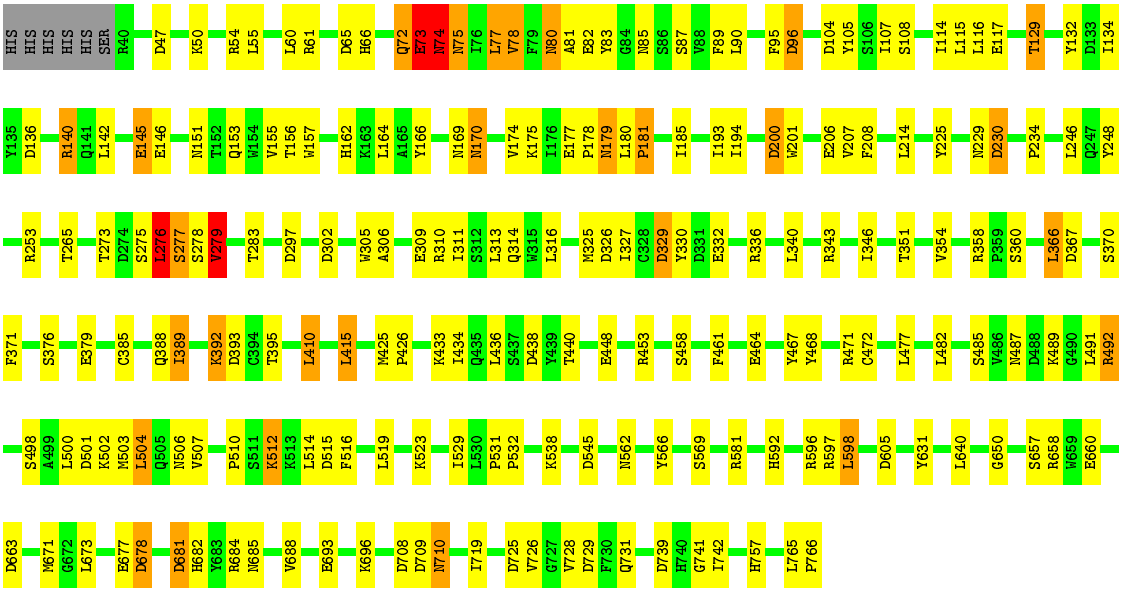
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

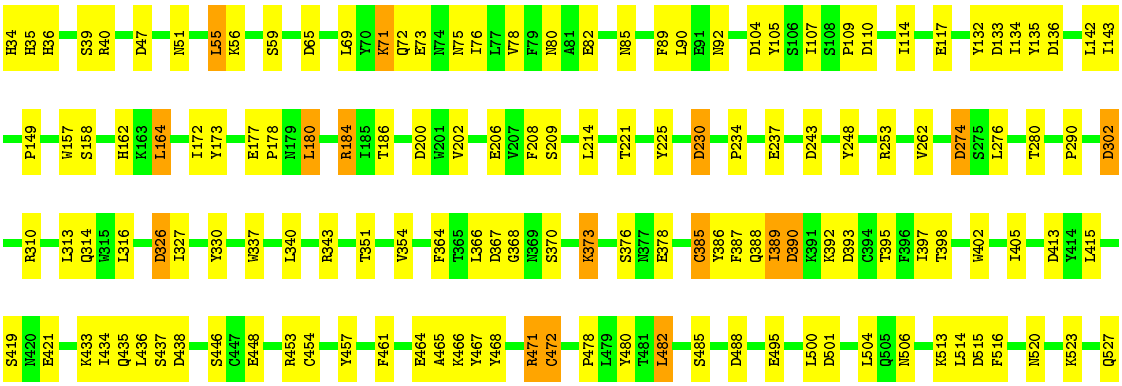
- Molecule 1: Dipeptidyl peptidase IV

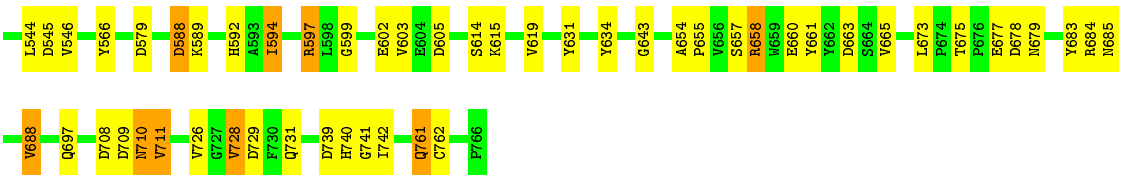
Chain A:



- Molecule 1: Dipeptidyl peptidase IV

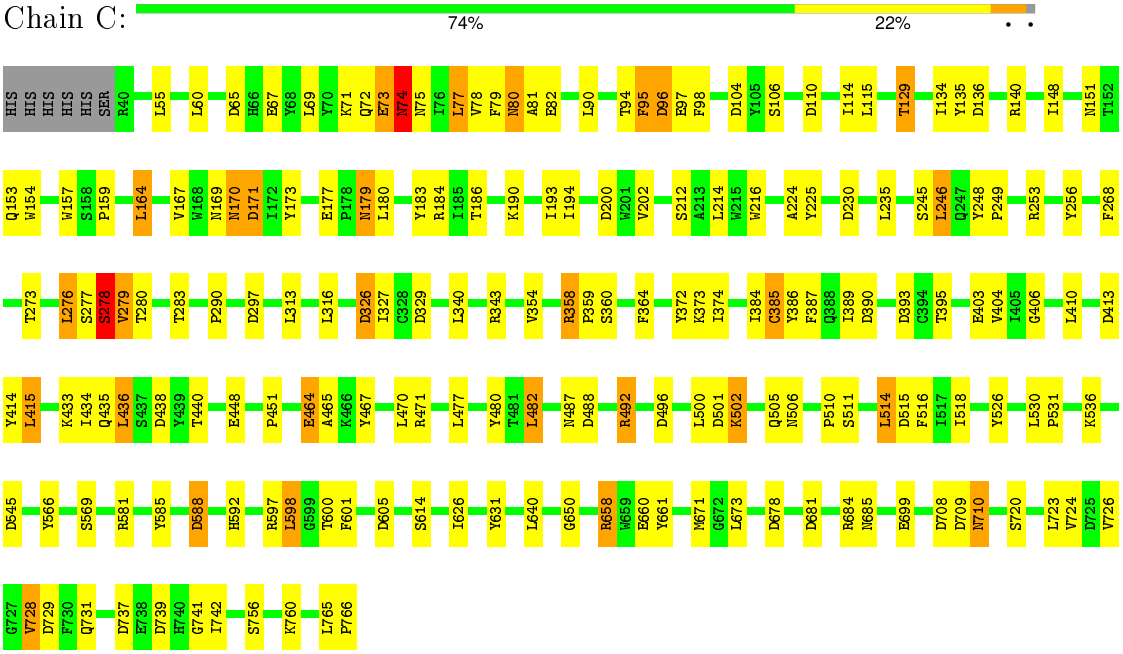
Chain B:





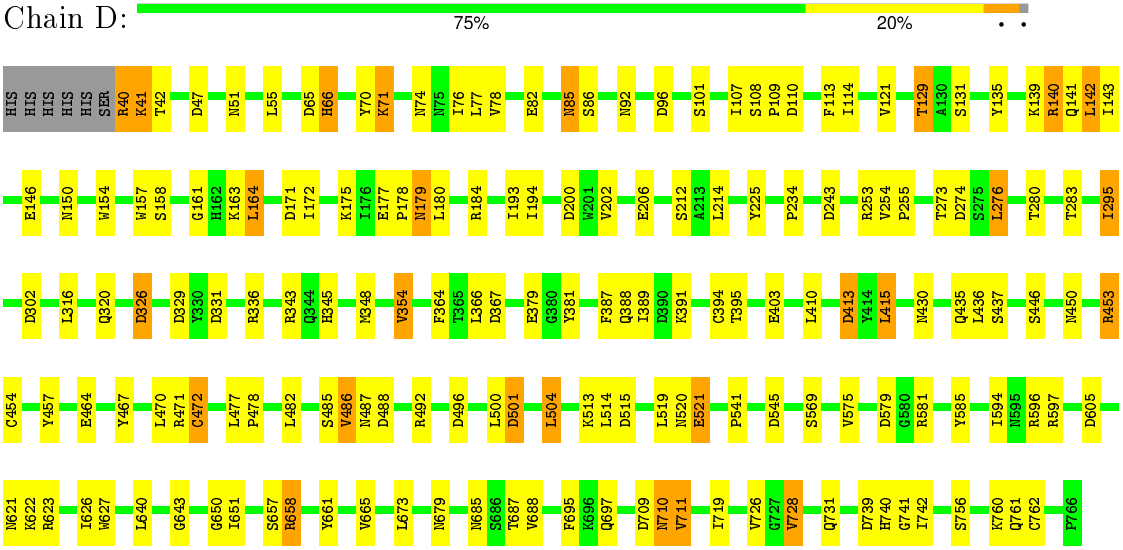
• Molecule 1: Dipeptidyl peptidase IV

Chain C:



• Molecule 1: Dipeptidyl peptidase IV

Chain D:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	121.82Å 124.06Å 144.49Å 90.00° 114.71° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	100.0 (20.00-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
Refinement program	REFMAC 5	Depositor
R, R_{free}	0.218 , 0.249	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	26111	wwPDB-VP
Average B, all atoms (Å^2)	21.0	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: FUC, NAG, 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	0.48	0/6123	0.85	32/8329 (0.4%)
1	B	0.43	0/6190	0.79	25/8419 (0.3%)
1	C	0.41	0/6123	0.85	34/8329 (0.4%)
1	D	0.42	0/6129	0.80	27/8336 (0.3%)
All	All	0.44	0/24565	0.82	118/33413 (0.4%)

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	6
1	C	2	3
3	B	1	0
6	C	1	0
All	All	4	9

There are no bond length outliers.

All (118) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	74	ASN	O-C-N	-15.46	97.96	122.70
1	C	279	VAL	O-C-N	-10.01	106.68	122.70
1	C	74	ASN	CA-C-O	9.21	139.45	120.10
1	A	279	VAL	O-C-N	-9.17	108.03	122.70
1	A	545	ASP	CB-CG-OD2	8.55	126.00	118.30
1	D	739	ASP	CB-CG-OD2	7.87	125.39	118.30
1	A	73	GLU	CA-C-N	-7.85	99.93	117.20
1	C	279	VAL	CA-C-O	7.22	135.27	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	739	ASP	CB-CG-OD2	7.08	124.67	118.30
1	C	739	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	709	ASP	CB-CG-OD2	6.86	124.47	118.30
1	B	390	ASP	CB-CG-OD2	6.84	124.45	118.30
1	A	73	GLU	O-C-N	6.62	133.30	122.70
1	D	326	ASP	CB-CG-OD2	6.57	124.22	118.30
1	D	709	ASP	CB-CG-OD2	6.55	124.19	118.30
1	A	708	ASP	CB-CG-OD2	6.53	124.17	118.30
1	D	545	ASP	CB-CG-OD2	6.51	124.16	118.30
1	C	74	ASN	CB-CA-C	6.42	123.25	110.40
1	C	65	ASP	CB-CG-OD2	6.41	124.07	118.30
1	C	73	GLU	O-C-N	-6.39	112.47	122.70
1	A	276	LEU	O-C-N	-6.38	112.50	122.70
1	C	326	ASP	CB-CG-OD2	6.36	124.03	118.30
1	C	709	ASP	CB-CG-OD2	6.33	123.99	118.30
1	C	496	ASP	CB-CG-OD2	6.32	123.99	118.30
1	C	729	ASP	CB-CG-OD2	6.26	123.94	118.30
1	D	139	LYS	CB-CA-C	-6.26	97.89	110.40
1	B	243	ASP	CB-CG-OD2	6.24	123.91	118.30
1	C	501	ASP	CB-CG-OD2	6.19	123.87	118.30
1	D	501	ASP	CB-CG-OD2	6.18	123.86	118.30
1	C	515	ASP	CB-CG-OD2	6.09	123.78	118.30
1	A	279	VAL	CA-CB-CG1	6.08	120.02	110.90
1	B	326	ASP	CB-CG-OD2	6.04	123.73	118.30
1	B	545	ASP	CB-CG-OD2	6.03	123.72	118.30
1	D	413	ASP	CB-CG-OD2	6.01	123.70	118.30
1	B	709	ASP	CB-CG-OD2	5.99	123.69	118.30
1	C	110	ASP	CB-CG-OD2	5.98	123.68	118.30
1	B	579	ASP	CB-CG-OD2	5.97	123.67	118.30
1	C	393	ASP	CB-CG-OD2	5.94	123.65	118.30
1	B	605	ASP	CB-CG-OD2	5.93	123.64	118.30
1	C	329	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	133	ASP	CB-CG-OD2	5.93	123.64	118.30
1	D	41	LYS	O-C-N	-5.93	113.21	122.70
1	B	515	ASP	CB-CG-OD2	5.91	123.62	118.30
1	C	171	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	96	ASP	CB-CG-OD2	5.86	123.58	118.30
1	A	393	ASP	CB-CG-OD2	5.86	123.57	118.30
1	D	40	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	681	ASP	CB-CG-OD2	5.79	123.51	118.30
1	B	393	ASP	CB-CG-OD2	5.79	123.51	118.30
1	D	40	ARG	NE-CZ-NH2	5.76	123.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	367	ASP	CB-CG-OD2	5.73	123.45	118.30
1	A	605	ASP	CB-CG-OD2	5.72	123.45	118.30
1	C	390	ASP	CB-CG-OD2	5.71	123.44	118.30
1	A	297	ASP	CB-CG-OD2	5.70	123.43	118.30
1	C	708	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	678	ASP	CB-CG-OD2	5.66	123.40	118.30
1	A	729	ASP	CB-CG-OD2	5.65	123.39	118.30
1	A	739	ASP	CB-CG-OD2	5.62	123.36	118.30
1	D	200	ASP	CB-CG-OD2	5.62	123.36	118.30
1	A	277	SER	O-C-N	-5.60	113.74	122.70
1	A	329	ASP	CB-CG-OD2	5.59	123.33	118.30
1	B	200	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	438	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	501	ASP	CB-CG-OD2	5.56	123.31	118.30
1	A	96	ASP	CB-CG-OD2	5.56	123.30	118.30
1	D	302	ASP	CB-CG-OD2	5.54	123.29	118.30
1	C	413	ASP	CB-CG-OD2	5.53	123.28	118.30
1	D	329	ASP	CB-CG-OD2	5.53	123.27	118.30
1	B	438	ASP	CB-CG-OD2	5.52	123.27	118.30
1	D	110	ASP	CB-CG-OD2	5.51	123.26	118.30
1	C	200	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	104	ASP	CB-CG-OD2	5.50	123.25	118.30
1	B	678	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	302	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	274	ASP	CB-CG-OD2	5.45	123.20	118.30
1	D	605	ASP	CB-CG-OD2	5.43	123.19	118.30
1	D	140	ARG	CB-CA-C	5.43	121.26	110.40
1	A	140	ARG	CA-C-O	5.42	131.49	120.10
1	A	725	ASP	CB-CG-OD2	5.39	123.15	118.30
1	D	331	ASP	CB-CG-OD2	5.38	123.14	118.30
1	B	708	ASP	CB-CG-OD2	5.37	123.14	118.30
1	C	737	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	275	SER	C-N-CA	-5.35	108.32	121.70
1	A	367	ASP	CB-CG-OD2	5.35	123.11	118.30
1	C	678	ASP	CB-CG-OD2	5.34	123.11	118.30
1	A	75	ASN	N-CA-CB	-5.34	100.99	110.60
1	C	681	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	515	ASP	CB-CG-OD2	5.32	123.09	118.30
1	D	274	ASP	CB-CG-OD2	5.32	123.08	118.30
1	B	413	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	729	ASP	CB-CG-OD2	5.30	123.07	118.30
1	A	136	ASP	CB-CG-OD2	5.29	123.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	588	ASP	CB-CG-OD2	5.27	123.04	118.30
1	C	438	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	515	ASP	CB-CG-OD2	5.22	123.00	118.30
1	D	171	ASP	CB-CG-OD2	5.21	122.99	118.30
1	B	47	ASP	CB-CG-OD2	5.21	122.98	118.30
1	C	279	VAL	CA-CB-CG1	5.18	118.67	110.90
1	B	230	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	230	ASP	CB-CG-OD2	5.17	122.95	118.30
1	A	200	ASP	CB-CG-OD2	5.17	122.95	118.30
1	C	545	ASP	CB-CG-OD2	5.16	122.95	118.30
1	B	367	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	605	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	96	ASP	CB-CG-OD2	5.12	122.91	118.30
1	D	47	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	588	ASP	CB-CG-OD2	5.09	122.88	118.30
1	B	501	ASP	CB-CG-OD2	5.08	122.87	118.30
1	C	297	ASP	CB-CG-OD2	5.07	122.87	118.30
1	A	65	ASP	CB-CG-OD2	5.07	122.86	118.30
1	D	488	ASP	CB-CG-OD2	5.06	122.85	118.30
1	C	73	GLU	N-CA-CB	-5.05	101.52	110.60
1	B	104	ASP	CB-CG-OD2	5.04	122.83	118.30
1	D	496	ASP	CB-CG-OD2	5.01	122.81	118.30
1	D	243	ASP	CB-CG-OD2	5.01	122.81	118.30
1	D	579	ASP	CB-CG-OD2	5.01	122.81	118.30
1	C	104	ASP	CB-CG-OD2	5.01	122.81	118.30

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	B	2192	NAG	C1
1	C	73	GLU	CA
1	C	74	ASN	CA
6	C	2294	MAN	C1

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	276	LEU	Mainchain
1	A	277	SER	Mainchain
1	A	279	VAL	Mainchain
1	A	72	GLN	Peptide

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Mol	Chain	Res	Type	Group
1	A	74	ASN	Mainchain,Peptide
1	C	277	SER	Mainchain
1	C	278	SER	Mainchain,Peptide

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	5951	0	5660	114	0
1	B	6013	0	5710	110	1
1	C	5951	0	5660	119	0
1	D	5957	0	5673	101	1
2	A	56	0	52	10	0
2	B	84	0	77	9	0
2	C	70	0	65	3	0
2	D	84	0	78	4	0
3	A	84	0	74	1	0
3	B	56	0	50	3	0
3	D	28	0	25	0	0
4	A	39	0	34	2	0
5	B	10	0	10	3	0
6	C	50	0	41	1	0
7	A	466	0	0	3	0
7	B	467	0	0	3	0
7	C	334	0	0	0	0
7	D	411	0	0	0	0
All	All	26111	0	23209	442	1

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

All (442) 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:C:731:GLN:NE2	1:D:731:GLN:HE22	1.46	1.13
1:A:327:ILE:HD13	1:A:389:ILE:CD1	1.80	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1501:NAG:O6	5:B:1502:FUC:C1	2.00	1.10
1:C:731:GLN:HE22	1:D:731:GLN:NE2	1.50	1.08
1:C:731:GLN:NE2	1:D:731:GLN:NE2	2.03	1.06
1:A:327:ILE:HD13	1:A:389:ILE:HD12	1.36	1.04
1:B:82:GLU:HG2	1:B:467:TYR:OH	1.60	1.01
1:C:153:GLN:HE22	1:C:170:ASN:H	1.08	0.99
1:A:72:GLN:HG3	1:A:77:LEU:CD2	1.94	0.97
1:A:72:GLN:HG3	1:A:77:LEU:HD21	1.45	0.97
1:C:72:GLN:HB3	1:C:77:LEU:HD21	1.47	0.96
1:A:153:GLN:HE22	1:A:170:ASN:H	1.10	0.96
1:A:253:ARG:HH21	1:B:253:ARG:HH21	1.08	0.93
1:C:253:ARG:HH21	1:D:253:ARG:HH21	0.92	0.92
1:D:711:VAL:HG13	1:D:740:HIS:CE1	2.04	0.91
1:A:325:MET:HE1	1:A:327:ILE:HD11	1.52	0.89
1:A:72:GLN:O	1:A:74:ASN:N	2.05	0.87
1:D:193:ILE:HG22	1:D:194:ILE:HD12	1.57	0.87
1:C:660:GLU:OE2	1:C:684:ARG:NH2	2.07	0.87
1:B:435:GLN:NE2	1:B:437:SER:OG	2.08	0.87
1:B:599:GLY:N	1:B:602:GLU:OE2	2.07	0.86
3:B:2192:NAG:O3	3:B:2192:NAG:O7	1.93	0.86
1:C:72:GLN:HB3	1:C:77:LEU:CD2	2.06	0.85
1:D:486:VAL:HG12	1:D:487:ASN:ND2	1.95	0.82
1:C:253:ARG:HH21	1:D:253:ARG:NH2	1.75	0.82
1:C:327:ILE:HD13	1:C:389:ILE:HD12	1.62	0.81
1:B:78:VAL:HG13	2:B:851:NAG:H81	1.64	0.80
1:B:471:ARG:HG3	1:B:480:TYR:CE1	2.17	0.80
1:C:731:GLN:HE22	1:D:731:GLN:HE21	1.29	0.79
2:A:2191:NAG:O3	2:A:2191:NAG:H82	1.82	0.79
1:C:290:PRO:HG3	1:C:326:ASP:OD1	1.82	0.78
1:A:78:VAL:HG22	1:A:89:PHE:HB2	1.63	0.78
1:D:82:GLU:HG2	1:D:467:TYR:OH	1.84	0.78
1:D:343:ARG:HD2	1:D:389:ILE:HG23	1.65	0.78
1:A:660:GLU:OE2	1:A:684:ARG:NH2	2.15	0.77
1:A:153:GLN:NE2	1:A:170:ASN:H	1.82	0.77
1:C:253:ARG:NH2	1:D:253:ARG:HH21	1.77	0.76
1:B:173:TYR:CE1	1:B:184:ARG:HG3	2.21	0.76
1:C:153:GLN:NE2	1:C:170:ASN:H	1.83	0.76
1:A:325:MET:CE	1:A:327:ILE:HD11	2.16	0.75
1:C:190:LYS:HE2	1:C:193:ILE:HD12	1.68	0.74
1:C:157:TRP:CE3	1:C:164:LEU:HD13	2.24	0.73
1:C:184:ARG:HD3	1:C:186:THR:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:153:GLN:HE22	1:C:170:ASN:N	1.84	0.73
1:A:146:GLU:O	1:A:175:LYS:NZ	2.17	0.72
1:D:140:ARG:O	1:D:141:GLN:HG3	1.89	0.72
1:C:726:VAL:HG23	1:C:728:VAL:HG12	1.72	0.72
1:A:153:GLN:HE22	1:A:170:ASN:N	1.86	0.72
1:C:327:ILE:HD13	1:C:389:ILE:CD1	2.19	0.71
1:C:183:TYR:CD2	1:C:276:LEU:HD23	2.24	0.71
1:D:726:VAL:HG23	1:D:728:VAL:HG12	1.71	0.71
1:A:351:THR:OG1	1:A:592:HIS:HD2	1.74	0.71
1:B:711:VAL:HG13	1:B:740:HIS:CE1	2.25	0.71
1:B:75:ASN:HD22	1:B:92:ASN:H	1.38	0.70
1:D:711:VAL:CG1	1:D:740:HIS:CE1	2.75	0.70
1:C:190:LYS:HE2	1:C:193:ILE:CD1	2.21	0.70
1:C:173:TYR:CE1	1:C:184:ARG:HG3	2.26	0.70
1:B:658:ARG:HG2	1:B:661:TYR:CE2	2.26	0.70
1:B:184:ARG:HD3	1:B:186:THR:O	1.92	0.70
1:A:115:LEU:HD21	1:A:155:VAL:HG21	1.74	0.69
1:B:157:TRP:CE3	1:B:164:LEU:HD13	2.27	0.69
1:C:193:ILE:HG22	1:C:194:ILE:HD12	1.73	0.69
1:B:370:SER:OG	1:B:386:TYR:CE2	2.47	0.68
1:C:55:LEU:HD23	1:C:500:LEU:CD2	2.23	0.68
1:D:82:GLU:CG	1:D:467:TYR:OH	2.43	0.67
1:A:194:ILE:HD12	4:A:2291:NAG:H82	1.75	0.67
1:C:385:CYS:HB3	1:C:387:PHE:CE2	2.30	0.67
1:C:224:ALA:HB1	1:C:268:PHE:CZ	2.29	0.67
1:C:81:ALA:O	1:C:492:ARG:NH1	2.28	0.66
1:B:177:GLU:HB2	1:B:180:LEU:HD22	1.78	0.66
1:A:726:VAL:HG23	1:A:728:VAL:HG23	1.76	0.66
1:D:214:LEU:HD23	1:D:225:TYR:HB3	1.78	0.66
1:A:327:ILE:CD1	1:A:389:ILE:CD1	2.68	0.65
1:D:643:GLY:HA2	1:D:697:GLN:HE22	1.60	0.65
1:A:82:GLU:HG2	1:A:467:TYR:OH	1.96	0.64
1:A:129:THR:HG23	1:A:151:ASN:HA	1.78	0.64
2:B:1501:NAG:O6	5:B:1502:FUC:O5	2.11	0.64
1:B:761:GLN:HG3	1:B:762:CYS:N	2.13	0.64
1:C:502:LYS:HA	1:C:505:GLN:HE21	1.63	0.63
1:A:162:HIS:NE2	1:A:177:GLU:OE1	2.31	0.63
1:C:214:LEU:HD23	1:C:225:TYR:HB3	1.80	0.63
1:D:146:GLU:O	1:D:175:LYS:HE2	1.99	0.63
1:B:35:HIS:CD2	1:B:35:HIS:H	2.17	0.63
1:C:72:GLN:CB	1:C:77:LEU:HD21	2.26	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:500:LEU:HG	1:A:504:LEU:HD22	1.79	0.62
1:D:85:ASN:C	1:D:85:ASN:OD1	2.38	0.62
1:B:206:GLU:OE2	1:B:663:ASP:OD2	2.16	0.62
1:C:756:SER:O	1:C:760:LYS:HG3	2.00	0.62
1:C:60:LEU:HD12	1:C:60:LEU:O	2.00	0.61
1:B:726:VAL:HG23	1:B:728:VAL:HG12	1.80	0.61
2:A:6851:NAG:O7	2:A:6851:NAG:O3	2.17	0.61
1:D:193:ILE:HG22	1:D:194:ILE:CD1	2.29	0.61
1:A:346:ILE:H	1:A:392:LYS:NZ	1.99	0.61
1:A:105:TYR:HB2	1:A:114:ILE:HD11	1.82	0.61
1:C:598:LEU:HG	1:C:631:TYR:OH	2.01	0.61
1:A:510:PRO:HD3	1:A:569:SER:HB2	1.83	0.61
1:C:246:LEU:HD13	1:C:248:TYR:O	2.01	0.61
1:B:302:ASP:HB3	1:B:314:GLN:HB2	1.83	0.61
1:A:157:TRP:CE3	1:A:164:LEU:HD13	2.36	0.60
1:B:76:ILE:HD12	1:B:90:LEU:HD23	1.82	0.60
1:D:640:LEU:HD11	1:D:650:GLY:HA3	1.83	0.60
1:C:82:GLU:HB2	1:C:467:TYR:OH	2.01	0.60
1:C:60:LEU:HD12	1:C:60:LEU:C	2.22	0.60
1:B:711:VAL:CG1	1:B:740:HIS:CE1	2.85	0.59
1:A:87:SER:OG	2:A:851:NAG:H83	2.02	0.59
1:C:414:TYR:CE2	1:C:433:LYS:HE2	2.38	0.59
1:C:136:ASP:O	1:C:140:ARG:HA	2.03	0.59
1:A:253:ARG:NH2	1:B:253:ARG:HH21	1.89	0.59
1:D:135:TYR:CZ	1:D:140:ARG:HA	2.37	0.59
1:B:364:PHE:HE2	1:B:389:ILE:HD11	1.68	0.58
1:C:129:THR:HG23	1:C:151:ASN:HA	1.84	0.58
1:B:597:ARG:NH1	1:B:679:ASN:OD1	2.36	0.58
1:C:114:ILE:HG22	1:C:135:TYR:HB2	1.86	0.58
1:A:343:ARG:HD2	1:A:389:ILE:HG23	1.84	0.58
1:C:340:LEU:HB2	1:C:343:ARG:HG3	1.84	0.58
1:A:155:VAL:HG12	1:A:166:TYR:HB3	1.85	0.58
1:C:157:TRP:CZ3	1:C:164:LEU:HD13	2.38	0.58
1:A:117:GLU:HB2	1:A:132:TYR:CE2	2.39	0.58
1:C:581:ARG:CZ	2:C:5201:NAG:H5	2.34	0.58
1:D:214:LEU:HD23	1:D:225:TYR:CB	2.34	0.57
1:D:206:GLU:HB3	1:D:665:VAL:HG22	1.87	0.57
1:A:81:ALA:O	1:A:492:ARG:NH1	2.35	0.57
1:A:581:ARG:NH2	2:A:5201:NAG:H3	2.19	0.57
1:A:693:GLU:OE1	1:A:696:LYS:NZ	2.29	0.57
1:B:597:ARG:HG2	7:B:7141:HOH:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:179:ASN:HD22	1:C:179:ASN:H	1.52	0.57
1:B:82:GLU:CG	1:B:467:TYR:OH	2.46	0.57
1:A:640:LEU:HD11	1:A:650:GLY:HA3	1.86	0.57
1:C:731:GLN:HE21	1:D:731:GLN:HE22	1.44	0.57
1:C:343:ARG:HD2	1:C:389:ILE:CG2	2.34	0.56
1:A:83:TYR:HB2	1:A:85:ASN:OD1	2.04	0.56
1:B:89:PHE:CE1	1:B:107:ILE:HD13	2.40	0.56
1:D:214:LEU:CD2	1:D:225:TYR:HB3	2.35	0.56
1:B:397:ILE:HG13	1:B:398:THR:HG23	1.87	0.56
1:A:305:TRP:CE2	1:A:311:ILE:HD12	2.41	0.56
1:B:658:ARG:HG2	1:B:661:TYR:CD2	2.40	0.56
1:C:80:ASN:HD22	1:C:81:ALA:N	2.02	0.56
1:A:87:SER:OG	2:A:851:NAG:C8	2.53	0.56
1:B:453:ARG:HG3	1:B:454:CYS:SG	2.45	0.56
1:D:710:ASN:C	1:D:710:ASN:HD22	2.09	0.56
1:B:65:ASP:OD2	1:B:464:GLU:N	2.34	0.56
1:B:433:LYS:NZ	1:B:488:ASP:OD1	2.37	0.56
1:D:520:ASN:O	1:D:521:GLU:HB2	2.05	0.56
1:B:136:ASP:HB2	1:B:143:ILE:HD11	1.88	0.56
1:A:415:LEU:HB3	1:A:434:ILE:HG23	1.87	0.56
1:D:55:LEU:HD12	1:D:500:LEU:HD22	1.88	0.56
1:B:56:LYS:HE3	1:B:495:GLU:OE2	2.05	0.56
1:C:95:PHE:O	1:C:98:PHE:HB2	2.06	0.55
1:A:657:SER:HA	1:A:688:VAL:HG13	1.88	0.55
1:D:726:VAL:HG23	1:D:728:VAL:CG1	2.36	0.55
1:B:710:ASN:C	1:B:710:ASN:HD22	2.09	0.55
1:C:69:LEU:HD23	1:C:78:VAL:HA	1.87	0.55
1:C:723:LEU:HB3	1:C:728:VAL:HG13	1.88	0.55
1:D:581:ARG:HD3	2:D:5201:NAG:H5	1.87	0.55
1:A:55:LEU:HD23	1:A:500:LEU:HD22	1.87	0.55
1:A:273:THR:O	1:A:276:LEU:HD22	2.07	0.55
1:A:598:LEU:HD22	1:A:671:MET:HG2	1.89	0.55
1:B:351:THR:OG1	1:B:592:HIS:HD2	1.88	0.55
1:C:169:ASN:O	1:C:170:ASN:HB2	2.07	0.55
1:C:94:THR:O	1:C:94:THR:HG22	2.06	0.55
1:D:135:TYR:OH	1:D:140:ARG:HA	2.05	0.54
1:A:72:GLN:HG3	1:A:77:LEU:HD23	1.87	0.54
1:D:42:THR:HB	1:D:569:SER:OG	2.06	0.54
1:D:364:PHE:HE2	1:D:389:ILE:HD11	1.72	0.54
1:A:696:LYS:HG3	1:A:728:VAL:HG22	1.87	0.54
1:B:80:ASN:HB3	1:B:85:ASN:OD1	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLU:HG3	1:A:179:ASN:HB2	1.90	0.54
1:D:206:GLU:CB	1:D:665:VAL:HG22	2.37	0.54
1:A:253:ARG:HH21	1:B:253:ARG:NH2	1.91	0.54
1:A:200:ASP:OD1	1:A:230:ASP:OD2	2.26	0.54
4:A:2292:NAG:H81	7:A:7174:HOH:O	2.08	0.54
1:D:131:SER:OG	1:D:150:ASN:OD1	2.24	0.54
1:A:214:LEU:HD23	1:A:225:TYR:HB3	1.89	0.54
1:C:598:LEU:HD22	1:C:671:MET:HG2	1.89	0.53
1:C:114:ILE:CG2	1:C:135:TYR:HB2	2.37	0.53
1:C:95:PHE:O	1:C:98:PHE:CB	2.56	0.53
1:A:155:VAL:HG12	1:A:166:TYR:CB	2.38	0.53
1:C:385:CYS:HB3	1:C:387:PHE:HE2	1.71	0.53
1:C:760:LYS:NZ	1:C:766:PRO:O	2.42	0.53
1:D:172:ILE:HD13	1:D:214:LEU:HD21	1.90	0.53
1:A:500:LEU:HA	1:A:503:MET:CE	2.39	0.53
1:C:710:ASN:C	1:C:710:ASN:HD22	2.10	0.53
1:A:461:PHE:CD2	1:A:468:TYR:HB3	2.43	0.53
1:B:39:SER:OG	1:B:506:ASN:HA	2.08	0.53
1:B:208:PHE:O	1:B:209:SER:HB2	2.08	0.53
1:B:75:ASN:ND2	1:B:92:ASN:H	2.06	0.53
1:C:414:TYR:CE2	1:C:435:GLN:HG3	2.44	0.53
1:B:446:SER:HB2	1:B:457:TYR:CE2	2.44	0.53
1:B:69:LEU:CD1	1:B:107:ILE:HD12	2.39	0.53
1:B:134:ILE:HD13	1:B:178:PRO:HB3	1.91	0.53
1:D:109:PRO:HD2	1:D:161:GLY:O	2.08	0.53
1:C:248:TYR:CZ	1:D:234:PRO:HB2	2.43	0.52
1:A:72:GLN:CG	1:A:77:LEU:CD2	2.79	0.52
1:A:302:ASP:HB3	1:A:314:GLN:HB2	1.91	0.52
1:A:177:GLU:HB2	1:A:180:LEU:HD12	1.91	0.52
1:B:340:LEU:HB2	1:B:343:ARG:HG3	1.91	0.52
1:D:430:ASN:ND2	1:D:446:SER:OG	2.29	0.52
2:C:2191:NAG:O7	2:C:2191:NAG:H3	2.09	0.52
1:D:756:SER:O	1:D:760:LYS:HG3	2.10	0.52
1:D:477:LEU:HD12	1:D:501:ASP:HB2	1.92	0.52
1:A:60:LEU:C	1:A:60:LEU:HD12	2.30	0.52
1:C:90:LEU:HD11	1:C:95:PHE:CZ	2.46	0.51
1:A:72:GLN:C	1:A:74:ASN:N	2.53	0.51
1:C:384:ILE:HG13	1:C:404:VAL:HG21	1.92	0.51
1:A:681:ASP:HB3	2:A:6851:NAG:H2	1.91	0.51
1:B:402:TRP:CD2	1:B:421:GLU:HB2	2.45	0.51
1:B:105:TYR:HB2	1:B:114:ILE:HD11	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:154:TRP:CE2	1:D:212:SER:HB2	2.46	0.51
1:B:465:ALA:O	1:B:485:SER:OG	2.26	0.51
1:D:435:GLN:NE2	1:D:437:SER:OG	2.36	0.51
1:B:657:SER:HA	1:B:688:VAL:CG1	2.40	0.51
1:A:169:ASN:O	1:A:170:ASN:HB2	2.11	0.51
1:B:71:LYS:H	1:B:71:LYS:HD2	1.76	0.51
1:C:159:PRO:HD3	1:C:216:TRP:CB	2.41	0.51
1:A:207:VAL:HG12	1:A:208:PHE:CD1	2.46	0.51
1:B:385:CYS:HB3	1:B:387:PHE:CE2	2.46	0.51
1:D:114:ILE:HG23	1:D:135:TYR:HB3	1.93	0.51
1:D:113:PHE:CZ	1:D:178:PRO:HG2	2.46	0.51
1:B:378:GLU:H	1:B:378:GLU:CD	2.13	0.51
1:B:602:GLU:HG3	1:B:603:VAL:H	1.75	0.51
1:B:78:VAL:HG13	2:B:851:NAG:C8	2.39	0.50
1:D:500:LEU:HG	1:D:504:LEU:HD22	1.92	0.50
1:B:684:ARG:HB3	2:B:6851:NAG:C8	2.42	0.50
1:A:55:LEU:HD23	1:A:500:LEU:CD2	2.42	0.50
1:A:410:LEU:O	1:A:410:LEU:HD23	2.12	0.50
1:A:87:SER:CB	2:A:851:NAG:H83	2.41	0.50
1:A:72:GLN:O	1:A:75:ASN:HB2	2.12	0.50
1:C:372:TYR:OH	1:C:436:LEU:HG	2.12	0.50
1:B:658:ARG:HG3	1:B:658:ARG:O	2.11	0.50
2:D:5201:NAG:O7	2:D:5201:NAG:H3	2.12	0.50
1:B:684:ARG:HB3	2:B:6851:NAG:H81	1.93	0.50
1:A:366:LEU:HD12	1:A:366:LEU:O	2.11	0.50
1:C:410:LEU:HD11	1:C:436:LEU:HD21	1.94	0.50
1:D:596:ARG:O	1:D:597:ARG:NE	2.35	0.50
1:C:154:TRP:CE2	1:C:212:SER:HB3	2.46	0.49
1:B:173:TYR:CZ	1:B:184:ARG:HG3	2.47	0.49
1:D:142:LEU:HD12	1:D:143:ILE:O	2.12	0.49
1:C:134:ILE:HD11	1:C:148:ILE:HD11	1.94	0.49
1:B:415:LEU:HD23	1:B:415:LEU:C	2.32	0.49
1:D:140:ARG:HH11	1:D:140:ARG:HG2	1.78	0.49
1:B:675:THR:HB	1:B:677:GLU:OE1	2.12	0.49
1:B:55:LEU:HD12	1:B:500:LEU:CD2	2.43	0.49
3:B:2192:NAG:HO3	3:B:2192:NAG:C7	2.16	0.48
1:A:500:LEU:HA	1:A:503:MET:HE3	1.95	0.48
1:C:179:ASN:HD22	1:C:179:ASN:N	2.10	0.48
1:B:114:ILE:HG23	1:B:135:TYR:HB3	1.95	0.48
1:C:516:PHE:CE1	1:C:518:ILE:HD11	2.48	0.48
1:C:177:GLU:HB2	1:C:180:LEU:HG	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:757:HIS:HD2	7:A:7143:HOH:O	1.96	0.48
1:C:658:ARG:HG2	1:C:661:TYR:CE2	2.47	0.48
1:B:330:TYR:HB2	1:B:337:TRP:CH2	2.48	0.48
1:A:491:LEU:O	1:A:492:ARG:HB3	2.13	0.48
1:B:327:ILE:HD13	1:B:389:ILE:HG13	1.95	0.48
1:C:372:TYR:CE1	1:C:386:TYR:CD2	3.02	0.48
1:C:414:TYR:CZ	1:C:433:LYS:HE2	2.48	0.48
1:A:597:ARG:HH11	1:A:682:HIS:HB2	1.78	0.48
1:B:92:ASN:OD1	1:B:92:ASN:C	2.51	0.48
1:D:688:VAL:HG22	1:D:719:ILE:HG12	1.96	0.48
1:D:71:LYS:HD2	1:D:71:LYS:H	1.79	0.48
1:A:433:LYS:HG2	1:A:433:LYS:O	2.13	0.48
1:B:206:GLU:HB3	1:B:665:VAL:HG22	1.95	0.48
1:D:643:GLY:HA2	1:D:697:GLN:NE2	2.29	0.47
1:A:54:ARG:HE	1:D:40:ARG:NH1	2.13	0.47
1:C:448:GLU:HA	1:C:451:PRO:HG3	1.96	0.47
1:C:67:GLU:HA	1:C:79:PHE:O	2.14	0.47
1:D:295:ILE:HD13	1:D:295:ILE:O	2.14	0.47
1:C:514:LEU:HD23	1:C:526:TYR:O	2.14	0.47
1:C:246:LEU:CD1	1:C:248:TYR:O	2.63	0.47
1:C:278:SER:HB3	1:C:279:VAL:HG23	1.97	0.47
1:C:343:ARG:HD2	1:C:389:ILE:HG22	1.97	0.47
1:A:129:THR:CG2	1:A:151:ASN:HA	2.44	0.47
1:D:403:GLU:OE2	1:D:585:TYR:HA	2.15	0.47
1:A:80:ASN:HD22	1:A:81:ALA:N	2.13	0.46
1:D:453:ARG:HG3	1:D:453:ARG:O	2.07	0.46
1:D:457:TYR:HA	1:D:471:ARG:O	2.15	0.46
1:C:487:ASN:O	1:C:488:ASP:HB2	2.15	0.46
1:C:741:GLY:O	1:C:742:ILE:C	2.53	0.46
1:B:643:GLY:HA2	1:B:697:GLN:HE22	1.80	0.46
1:D:74:ASN:O	1:D:92:ASN:HB2	2.16	0.46
1:D:107:ILE:HG22	1:D:108:SER:O	2.15	0.46
1:C:374:ILE:CD1	1:C:406:GLY:HA2	2.46	0.46
1:A:598:LEU:HB2	1:A:671:MET:SD	2.56	0.46
1:C:159:PRO:HD3	1:C:216:TRP:HB3	1.97	0.46
1:D:594:ILE:C	1:D:594:ILE:HD12	2.36	0.46
1:D:472:CYS:O	1:D:478:PRO:HA	2.14	0.46
1:D:157:TRP:CZ3	1:D:164:LEU:CD2	2.99	0.46
1:A:741:GLY:O	1:A:742:ILE:C	2.53	0.46
1:C:98:PHE:CD2	1:C:135:TYR:OH	2.69	0.46
1:D:658:ARG:HG2	1:D:661:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:358:ARG:HB2	1:C:359:PRO:HD2	1.96	0.45
1:D:741:GLY:O	1:D:742:ILE:C	2.53	0.45
1:A:206:GLU:OE2	1:A:663:ASP:OD2	2.34	0.45
1:D:158:SER:HB3	1:D:163:LYS:HB2	1.97	0.45
1:D:486:VAL:CG1	1:D:487:ASN:ND2	2.72	0.45
1:C:94:THR:O	1:C:95:PHE:CD1	2.70	0.45
1:B:65:ASP:OD1	1:B:466:LYS:HB2	2.16	0.45
1:A:306:ALA:HB3	1:A:310:ARG:HG2	1.98	0.45
1:D:114:ILE:CG2	1:D:135:TYR:HB3	2.47	0.45
1:D:657:SER:HA	1:D:688:VAL:HG13	1.99	0.45
1:D:453:ARG:HG3	1:D:454:CYS:SG	2.57	0.45
1:C:470:LEU:HD23	1:C:470:LEU:HA	1.79	0.45
1:D:485:SER:O	1:D:486:VAL:C	2.53	0.45
1:A:180:LEU:O	1:A:181:PRO:C	2.54	0.45
1:B:59:SER:HB3	1:B:71:LYS:HE3	1.99	0.45
1:A:90:LEU:HD12	1:A:90:LEU:HA	1.69	0.45
1:B:614:SER:HA	1:B:619:VAL:HB	1.98	0.45
1:C:660:GLU:CD	1:C:684:ARG:HH21	2.09	0.45
1:C:364:PHE:HE2	1:C:389:ILE:HD11	1.81	0.45
1:D:202:VAL:CG2	1:D:665:VAL:HG13	2.47	0.45
1:B:516:PHE:CD1	1:B:523:LYS:HG2	2.52	0.45
1:A:562:ASN:HB2	7:A:6872:HOH:O	2.17	0.45
1:D:78:VAL:O	1:D:86:SER:HB2	2.17	0.44
1:A:710:ASN:C	1:A:710:ASN:HD22	2.20	0.44
1:A:193:ILE:HG22	1:A:194:ILE:HG12	1.98	0.44
1:C:214:LEU:HD23	1:C:225:TYR:CB	2.45	0.44
1:A:512:LYS:HG2	1:A:529:ILE:HD13	1.99	0.44
1:B:310:ARG:NH2	1:B:368:GLY:O	2.48	0.44
1:A:107:ILE:HG22	1:A:108:SER:O	2.17	0.44
1:A:248:TYR:CZ	1:B:234:PRO:HB2	2.53	0.44
1:C:464:GLU:O	1:C:465:ALA:HB3	2.18	0.44
1:C:55:LEU:HD23	1:C:500:LEU:HD22	2.00	0.44
1:A:60:LEU:HD12	1:A:60:LEU:O	2.17	0.44
1:A:234:PRO:HB2	1:B:248:TYR:CZ	2.53	0.44
1:C:640:LEU:HD11	1:C:650:GLY:HA3	1.98	0.44
1:A:115:LEU:HD21	1:A:155:VAL:CG2	2.45	0.44
1:C:510:PRO:HD3	1:C:569:SER:HB2	2.00	0.44
1:A:458:SER:OG	1:A:471:ARG:HB3	2.18	0.44
1:A:688:VAL:HG22	1:A:719:ILE:HG12	1.99	0.44
1:D:65:ASP:HB3	1:D:66:HIS:CE1	2.53	0.44
1:D:121:VAL:HB	1:D:129:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:373:LYS:HE2	7:B:7148:HOH:O	2.18	0.44
1:B:594:ILE:CD1	1:B:594:ILE:H	2.30	0.44
1:C:516:PHE:HE1	1:C:518:ILE:HD11	1.82	0.43
1:C:626:ILE:O	1:C:650:GLY:HA2	2.18	0.43
1:D:415:LEU:C	1:D:415:LEU:CD1	2.87	0.43
1:C:193:ILE:HG22	1:C:194:ILE:CD1	2.45	0.43
1:C:157:TRP:CE3	1:C:164:LEU:CD1	3.00	0.43
1:A:80:ASN:HD22	1:A:82:GLU:H	1.66	0.43
1:A:87:SER:HB3	2:A:851:NAG:H83	1.99	0.43
1:A:134:ILE:HG21	1:A:178:PRO:HB3	1.99	0.43
1:C:471:ARG:HG3	1:C:480:TYR:CE1	2.54	0.43
1:D:626:ILE:O	1:D:650:GLY:HA2	2.19	0.43
1:A:596:ARG:NH2	1:A:678:ASP:OD2	2.41	0.43
1:C:106:SER:HB3	1:C:115:LEU:HB3	2.01	0.43
2:C:2191:NAG:O7	2:C:2191:NAG:C3	2.67	0.43
1:B:677:GLU:CD	1:B:677:GLU:H	2.22	0.43
1:C:415:LEU:HB3	1:C:434:ILE:HG23	2.00	0.43
1:C:55:LEU:HD23	1:C:500:LEU:HD21	2.00	0.43
1:C:80:ASN:HD22	1:C:80:ASN:C	2.22	0.43
1:D:597:ARG:NH2	1:D:679:ASN:OD1	2.52	0.43
1:C:74:ASN:HD22	1:C:74:ASN:HA	1.76	0.43
3:A:3212:NAG:C1	3:A:3212:NAG:O7	2.66	0.43
1:A:516:PHE:CD1	1:A:523:LYS:HG2	2.53	0.43
1:A:174:VAL:HG23	1:A:185:ILE:CD1	2.49	0.43
1:B:544:LEU:HG	1:B:546:VAL:CG1	2.49	0.43
1:A:229:ASN:HB3	1:A:265:THR:OG1	2.19	0.43
1:B:214:LEU:HD23	1:B:225:TYR:HB3	2.00	0.43
1:A:329:ASP:OD2	1:A:343:ARG:NH1	2.52	0.43
1:D:541:PRO:HG3	1:D:623:ARG:CZ	2.48	0.43
1:D:627:TRP:HB2	1:D:651:ILE:HB	2.01	0.43
1:C:94:THR:C	1:C:95:PHE:CD1	2.92	0.42
1:C:72:GLN:CB	1:C:77:LEU:CD2	2.87	0.42
1:B:658:ARG:HD2	1:B:661:TYR:CE1	2.54	0.42
1:C:96:ASP:OD2	1:C:97:GLU:N	2.53	0.42
1:C:273:THR:HA	1:C:276:LEU:HD13	2.01	0.42
1:B:397:ILE:HD12	1:B:434:ILE:HD13	2.00	0.42
1:A:598:LEU:HG	1:A:631:TYR:OH	2.20	0.42
1:C:600:THR:OG1	1:C:601:PHE:N	2.46	0.42
1:B:290:PRO:HG3	1:B:326:ASP:OD1	2.20	0.42
1:D:273:THR:HA	1:D:276:LEU:HD22	1.99	0.42
1:C:482:LEU:HA	1:C:482:LEU:HD23	1.89	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:631:TYR:O	1:B:634:TYR:HB3	2.19	0.42
1:A:389:ILE:HD13	1:A:389:ILE:HA	1.81	0.42
2:A:5201:NAG:H3	2:A:5201:NAG:O7	2.19	0.42
1:A:201:TRP:CZ2	1:A:710:ASN:HA	2.54	0.42
1:C:403:GLU:OE2	1:C:585:TYR:HA	2.19	0.42
1:D:179:ASN:N	1:D:179:ASN:OD1	2.52	0.42
1:B:117:GLU:HG3	1:B:132:TYR:CE2	2.55	0.42
1:B:206:GLU:CB	1:B:665:VAL:HG22	2.49	0.42
1:B:109:PRO:HG2	1:B:158:SER:O	2.20	0.42
1:D:711:VAL:HG13	1:D:740:HIS:ND1	2.33	0.42
1:D:486:VAL:HG12	1:D:487:ASN:HD21	1.80	0.42
1:A:54:ARG:NE	1:D:40:ARG:NH1	2.67	0.42
1:D:320:GLN:O	1:D:354:VAL:HG12	2.20	0.42
1:A:325:MET:CE	1:A:327:ILE:CD1	2.93	0.41
1:D:202:VAL:HG22	1:D:665:VAL:HG13	2.02	0.41
1:B:461:PHE:CD2	1:B:468:TYR:HB3	2.55	0.41
1:B:405:ILE:HG12	1:B:419:SER:HA	2.02	0.41
1:D:387:PHE:CE1	1:D:394:CYS:HB3	2.55	0.41
1:C:248:TYR:HA	1:C:249:PRO:HD3	1.95	0.41
1:B:482:LEU:HA	1:B:482:LEU:HD23	1.83	0.41
1:B:366:LEU:C	1:B:366:LEU:HD13	2.41	0.41
1:D:70:TYR:CG	1:D:71:LYS:N	2.87	0.41
1:D:157:TRP:CZ3	1:D:164:LEU:HD21	2.55	0.41
1:B:110:ASP:OD2	1:B:162:HIS:ND1	2.36	0.41
1:D:172:ILE:CD1	1:D:214:LEU:HD21	2.50	0.41
1:B:588:ASP:O	1:B:592:HIS:HB2	2.20	0.41
1:D:254:VAL:HA	1:D:255:PRO:HD3	1.95	0.41
1:D:379:GLU:HB3	1:D:381:TYR:HD1	1.85	0.41
1:A:325:MET:HE1	1:A:371:PHE:CE2	2.55	0.41
3:B:2192:NAG:C7	3:B:2192:NAG:O3	2.65	0.41
1:B:69:LEU:HD13	1:B:107:ILE:HD12	2.02	0.41
1:D:658:ARG:HB2	1:D:687:THR:HG22	2.01	0.41
1:B:214:LEU:HD23	1:B:214:LEU:HA	1.75	0.41
1:C:588:ASP:O	1:C:592:HIS:HB2	2.21	0.41
1:B:520:ASN:OD1	2:B:5201:NAG:H2	2.08	0.41
1:C:167:VAL:HA	1:C:171:ASP:O	2.21	0.41
1:B:741:GLY:O	1:B:742:ILE:C	2.58	0.41
1:B:237:GLU:HG2	1:B:253:ARG:HG2	2.01	0.41
1:D:520:ASN:HB2	2:D:5201:NAG:H61	2.02	0.41
1:B:366:LEU:HD22	1:B:366:LEU:HA	1.87	0.41
1:C:720:SER:O	1:C:724:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:487:ASN:N	1:A:487:ASN:OD1	2.54	0.41
1:D:622:LYS:HE2	1:D:622:LYS:HB2	1.60	0.41
1:B:435:GLN:HE21	1:B:437:SER:HG	1.54	0.41
1:C:765:LEU:HA	1:C:766:PRO:HD3	1.80	0.41
6:C:2292:NAG:H82	6:C:2292:NAG:H2	1.92	0.41
1:B:149:PRO:HA	2:B:1501:NAG:H83	2.02	0.41
1:A:731:GLN:NE2	1:B:731:GLN:HE22	2.19	0.41
2:B:1501:NAG:HO6	5:B:1502:FUC:C1	2.04	0.40
1:B:92:ASN:ND2	7:B:7058:HOH:O	2.52	0.40
1:B:657:SER:HA	1:B:688:VAL:HG13	2.02	0.40
1:B:513:LYS:O	1:B:527:GLN:HA	2.22	0.40
1:A:531:PRO:HA	1:A:532:PRO:HD3	1.94	0.40
1:C:530:LEU:HA	1:C:531:PRO:HD3	1.96	0.40
1:A:87:SER:CB	2:A:851:NAG:C8	2.99	0.40
1:B:172:ILE:HD13	1:B:214:LEU:HD21	2.03	0.40
1:B:472:CYS:O	1:B:478:PRO:HA	2.21	0.40
1:C:598:LEU:HB2	1:C:671:MET:SD	2.60	0.40
1:D:581:ARG:NH2	2:D:5201:NAG:O7	2.54	0.40
1:D:157:TRP:CZ3	1:D:164:LEU:HD22	2.57	0.40
1:A:95:PHE:CZ	1:A:116:LEU:HD11	2.57	0.40
1:A:765:LEU:HA	1:A:766:PRO:HD3	1.83	0.40
1:A:309:GLU:HB3	1:A:330:TYR:HB3	2.03	0.40
1:D:695:PHE:HB3	1:D:728:VAL:HG21	2.02	0.40
1:A:174:VAL:HG23	1:A:185:ILE:HD11	2.03	0.40
1:B:214:LEU:CD2	1:B:225:TYR:HB3	2.52	0.40
1:B:654:ALA:N	1:B:655:PRO:CD	2.84	0.40
1:B:660:GLU:HG3	1:B:683:TYR:CD1	2.56	0.40
1:B:221:THR:HG23	1:B:274:ASP:OD2	2.22	0.40
1:A:425:MET:HA	1:A:426:PRO:HD3	1.94	0.40
1:D:345:HIS:HE1	1:D:391:LYS:O	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:36:HIS:ND1	1:D:388:GLN:OE1[2_645]	1.96	0.24

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	725/733 (99%)	693 (96%)	29 (4%)	3 (0%)	39	37
1	B	731/733 (100%)	703 (96%)	28 (4%)	0	100	100
1	C	725/733 (99%)	691 (95%)	33 (5%)	1 (0%)	56	58
1	D	725/733 (99%)	693 (96%)	30 (4%)	2 (0%)	46	45
All	All	2906/2932 (99%)	2780 (96%)	120 (4%)	6 (0%)	52	53

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	73	GLU
1	D	486	VAL
1	C	73	GLU
1	A	140	ARG
1	D	621	ASN
1	A	181	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	651/658 (99%)	584 (90%)	67 (10%)	9	5
1	B	658/658 (100%)	611 (93%)	47 (7%)	18	14
1	C	651/658 (99%)	601 (92%)	50 (8%)	16	12
1	D	652/658 (99%)	601 (92%)	51 (8%)	16	11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	2612/2632 (99%)	2397 (92%)	215 (8%)	14 10

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	61	ARG
1	A	66	HIS
1	A	73	GLU
1	A	74	ASN
1	A	77	LEU
1	A	78	VAL
1	A	80	ASN
1	A	96	ASP
1	A	129	THR
1	A	142	LEU
1	A	145	GLU
1	A	156	THR
1	A	170	ASN
1	A	179	ASN
1	A	246	LEU
1	A	276	LEU
1	A	278	SER
1	A	279	VAL
1	A	283	THR
1	A	313	LEU
1	A	316	LEU
1	A	326	ASP
1	A	332	GLU
1	A	336	ARG
1	A	340	LEU
1	A	354	VAL
1	A	358	ARG
1	A	360	SER
1	A	366	LEU
1	A	370	SER
1	A	376	SER
1	A	379	GLU
1	A	385	CYS
1	A	388	GLN
1	A	389	ILE
1	A	392	LYS

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Mol	Chain	Res	Type
1	A	395	THR
1	A	410	LEU
1	A	415	LEU
1	A	436	LEU
1	A	440	THR
1	A	448	GLU
1	A	453	ARG
1	A	464	GLU
1	A	472	CYS
1	A	477	LEU
1	A	482	LEU
1	A	485	SER
1	A	489	LYS
1	A	492	ARG
1	A	498	SER
1	A	502	LYS
1	A	504	LEU
1	A	506	ASN
1	A	507	VAL
1	A	512	LYS
1	A	514	LEU
1	A	519	LEU
1	A	538	LYS
1	A	566	TYR
1	A	598	LEU
1	A	658	ARG
1	A	673	LEU
1	A	677	GLU
1	A	685	ASN
1	A	710	ASN
1	B	34	HIS
1	B	40	ARG
1	B	51	ASN
1	B	55	LEU
1	B	71	LYS
1	B	72	GLN
1	B	73	GLU
1	B	142	LEU
1	B	164	LEU
1	B	180	LEU
1	B	184	ARG
1	B	202	VAL

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Mol	Chain	Res	Type
1	B	230	ASP
1	B	262	VAL
1	B	276	LEU
1	B	280	THR
1	B	313	LEU
1	B	316	LEU
1	B	354	VAL
1	B	373	LYS
1	B	376	SER
1	B	385	CYS
1	B	388	GLN
1	B	389	ILE
1	B	390	ASP
1	B	392	LYS
1	B	395	THR
1	B	436	LEU
1	B	448	GLU
1	B	471	ARG
1	B	472	CYS
1	B	482	LEU
1	B	504	LEU
1	B	514	LEU
1	B	566	TYR
1	B	589	LYS
1	B	594	ILE
1	B	597	ARG
1	B	615	LYS
1	B	658	ARG
1	B	673	LEU
1	B	685	ASN
1	B	688	VAL
1	B	710	ASN
1	B	711	VAL
1	B	728	VAL
1	B	761	GLN
1	C	71	LYS
1	C	74	ASN
1	C	75	ASN
1	C	77	LEU
1	C	80	ASN
1	C	95	PHE
1	C	129	THR

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Mol	Chain	Res	Type
1	C	164	LEU
1	C	170	ASN
1	C	179	ASN
1	C	202	VAL
1	C	230	ASP
1	C	235	LEU
1	C	245	SER
1	C	246	LEU
1	C	256	TYR
1	C	276	LEU
1	C	278	SER
1	C	280	THR
1	C	283	THR
1	C	313	LEU
1	C	316	LEU
1	C	354	VAL
1	C	358	ARG
1	C	360	SER
1	C	373	LYS
1	C	385	CYS
1	C	395	THR
1	C	415	LEU
1	C	436	LEU
1	C	440	THR
1	C	464	GLU
1	C	477	LEU
1	C	482	LEU
1	C	492	ARG
1	C	502	LYS
1	C	506	ASN
1	C	511	SER
1	C	514	LEU
1	C	536	LYS
1	C	566	TYR
1	C	597	ARG
1	C	598	LEU
1	C	614	SER
1	C	658	ARG
1	C	673	LEU
1	C	685	ASN
1	C	699	GLU
1	C	710	ASN

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Mol	Chain	Res	Type
1	C	728	VAL
1	D	41	LYS
1	D	51	ASN
1	D	66	HIS
1	D	71	LYS
1	D	76	ILE
1	D	77	LEU
1	D	85	ASN
1	D	101	SER
1	D	129	THR
1	D	142	LEU
1	D	164	LEU
1	D	177	GLU
1	D	179	ASN
1	D	180	LEU
1	D	184	ARG
1	D	276	LEU
1	D	280	THR
1	D	283	THR
1	D	295	ILE
1	D	316	LEU
1	D	326	ASP
1	D	336	ARG
1	D	348	MET
1	D	354	VAL
1	D	366	LEU
1	D	395	THR
1	D	410	LEU
1	D	413	ASP
1	D	415	LEU
1	D	436	LEU
1	D	450	ASN
1	D	453	ARG
1	D	464	GLU
1	D	470	LEU
1	D	472	CYS
1	D	482	LEU
1	D	492	ARG
1	D	504	LEU
1	D	513	LYS
1	D	514	LEU
1	D	519	LEU

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Mol	Chain	Res	Type
1	D	521	GLU
1	D	575	VAL
1	D	658	ARG
1	D	673	LEU
1	D	685	ASN
1	D	710	ASN
1	D	711	VAL
1	D	728	VAL
1	D	761	GLN
1	D	762	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
1	A	100	HIS
1	A	153	GLN
1	A	169	ASN
1	A	170	ASN
1	A	179	ASN
1	A	338	ASN
1	A	344	GLN
1	A	455	GLN
1	A	508	GLN
1	A	572	ASN
1	A	592	HIS
1	A	710	ASN
1	B	35	HIS
1	B	75	ASN
1	B	169	ASN
1	B	196	ASN
1	B	227	GLN
1	B	344	GLN
1	B	430	ASN
1	B	508	GLN
1	B	572	ASN
1	B	592	HIS
1	B	697	GLN
1	B	710	ASN
1	B	731	GLN
1	C	74	ASN
1	C	80	ASN

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Mol	Chain	Res	Type
1	C	100	HIS
1	C	141	GLN
1	C	153	GLN
1	C	169	ASN
1	C	170	ASN
1	C	179	ASN
1	C	344	GLN
1	C	430	ASN
1	C	455	GLN
1	C	505	GLN
1	C	572	ASN
1	C	592	HIS
1	C	697	GLN
1	C	710	ASN
1	C	731	GLN
1	D	75	ASN
1	D	100	HIS
1	D	169	ASN
1	D	196	ASN
1	D	227	GLN
1	D	345	HIS
1	D	430	ASN
1	D	487	ASN
1	D	595	ASN
1	D	697	GLN
1	D	710	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

19 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	$\#\|Z\| > 2$
3	NAG	A	1501	1,3	14,14,15	0.63	0	15,19,21	2.41	6 (40%)
3	NAG	A	1502	3	14,14,15	0.50	0	15,19,21	1.76	2 (13%)
4	NAG	A	2291	1,4	14,14,15	0.37	0	15,19,21	1.27	1 (6%)
4	NAG	A	2292	4	14,14,15	0.25	0	15,19,21	0.59	0
4	MAN	A	2293	4	11,11,12	0.32	0	14,15,17	1.01	2 (14%)
3	NAG	A	2811	1,3	14,14,15	0.58	0	15,19,21	3.47	6 (40%)
3	NAG	A	2812	3	14,14,15	0.38	0	15,19,21	1.19	2 (13%)
3	NAG	A	3211	1,3	14,14,15	0.44	0	15,19,21	0.85	0
3	NAG	A	3212	3	14,14,15	0.50	0	15,19,21	0.77	0
3	NAG	B	2191	1,3	14,14,15	0.82	1 (7%)	15,19,21	1.27	2 (13%)
3	NAG	B	2192	3	14,14,15	1.04	1 (7%)	15,19,21	1.79	3 (20%)
3	NAG	B	2291	1,3	14,14,15	0.32	0	15,19,21	1.03	1 (6%)
3	NAG	B	2292	3	14,14,15	0.26	0	15,19,21	0.59	0
6	NAG	C	2291	1,6	14,14,15	0.37	0	15,19,21	1.10	1 (6%)
6	NAG	C	2292	6	14,14,15	0.20	0	15,19,21	0.89	2 (13%)
6	MAN	C	2293	6	11,11,12	0.42	0	14,15,17	2.17	5 (35%)
6	MAN	C	2294	6	11,11,12	0.31	0	14,15,17	1.84	3 (21%)
3	NAG	D	2291	1,3	14,14,15	0.28	0	15,19,21	0.88	0
3	NAG	D	2292	3	14,14,15	0.34	0	15,19,21	1.18	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	A	1501	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	1502	3	-	0/6/23/26	0/1/1/1
4	NAG	A	2291	1,4	-	0/6/23/26	0/1/1/1
4	NAG	A	2292	4	-	0/6/23/26	0/1/1/1
4	MAN	A	2293	4	-	0/2/19/22	0/1/1/1
3	NAG	A	2811	1,3	-	0/6/23/26	0/1/1/1
3	NAG	A	2812	3	-	0/6/23/26	0/1/1/1
3	NAG	A	3211	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	3212	3	-	0/6/23/26	0/1/1/1
3	NAG	B	2191	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2192	3	1/1/5/7	0/6/23/26	0/1/1/1
3	NAG	B	2291	1,3	-	0/6/23/26	0/1/1/1
3	NAG	B	2292	3	-	0/6/23/26	0/1/1/1
6	NAG	C	2291	1,6	-	0/6/23/26	0/1/1/1
6	NAG	C	2292	6	-	0/6/23/26	0/1/1/1
6	MAN	C	2293	6	-	0/2/19/22	0/1/1/1
6	MAN	C	2294	6	1/1/4/5	0/2/19/22	0/1/1/1
3	NAG	D	2291	1,3	-	0/6/23/26	0/1/1/1
3	NAG	D	2292	3	-	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2191	NAG	O4-C4	2.30	1.48	1.43
3	B	2192	NAG	C1-C2	3.56	1.57	1.52

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	2811	NAG	C4-C3-C2	-9.22	96.89	111.23
3	A	1501	NAG	C4-C3-C2	-5.04	103.39	111.23
6	C	2293	MAN	C6-C5-C4	-4.63	101.58	113.02
6	C	2294	MAN	O5-C1-C2	-4.36	103.78	110.86
4	A	2291	NAG	C2-N2-C7	-4.12	117.75	123.04
3	A	1502	NAG	C2-N2-C7	-3.66	118.34	123.04
3	D	2292	NAG	C1-O5-C5	-3.19	108.20	112.25
3	A	1501	NAG	C3-C4-C5	-3.18	104.66	110.20
6	C	2293	MAN	C1-O5-C5	-2.99	108.45	112.25
3	B	2192	NAG	C4-C3-C2	-2.92	106.69	111.23
6	C	2293	MAN	O6-C6-C5	-2.87	101.86	111.33
3	B	2291	NAG	C2-N2-C7	-2.53	119.79	123.04
3	A	2811	NAG	C8-C7-N2	-2.15	111.99	116.11
6	C	2292	NAG	C4-C3-C2	-2.12	107.94	111.23
4	A	2293	MAN	O5-C1-C2	-2.09	107.47	110.86
6	C	2294	MAN	C2-C3-C4	-2.02	107.61	111.04
3	B	2191	NAG	C1-O5-C5	2.01	114.81	112.25
3	A	2811	NAG	O5-C5-C6	2.04	111.77	107.35
6	C	2292	NAG	O5-C5-C6	2.06	111.81	107.35
3	A	2811	NAG	O4-C4-C5	2.12	114.86	109.24
3	A	1501	NAG	O3-C3-C2	2.14	113.36	109.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2293	MAN	C3-C4-C5	2.16	113.96	110.20
6	C	2293	MAN	C3-C4-C5	2.19	114.01	110.20
6	C	2291	NAG	O5-C5-C6	2.23	112.17	107.35
3	B	2192	NAG	C1-O5-C5	2.36	115.24	112.25
3	A	2812	NAG	C1-O5-C5	2.36	115.24	112.25
3	A	2812	NAG	C2-N2-C7	2.49	126.24	123.04
6	C	2294	MAN	C1-O5-C5	3.00	116.06	112.25
3	B	2191	NAG	O4-C4-C3	3.26	117.67	110.34
3	A	1501	NAG	C2-N2-C7	3.28	127.25	123.04
3	A	2811	NAG	C1-O5-C5	3.46	116.64	112.25
3	A	1501	NAG	O4-C4-C3	3.57	118.37	110.34
3	A	1501	NAG	C3-C2-N2	3.84	119.77	110.56
6	C	2293	MAN	C1-C2-C3	3.90	114.16	109.54
3	B	2192	NAG	C2-N2-C7	4.15	128.37	123.04
3	A	1502	NAG	C1-O5-C5	4.52	117.99	112.25
3	A	2811	NAG	C2-N2-C7	7.86	133.14	123.04

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	C	2294	MAN	C1
3	B	2192	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2291	NAG	1	0
4	A	2292	NAG	1	0
3	A	3212	NAG	1	0
3	B	2192	NAG	3	0
6	C	2292	NAG	1	0

5.6 Ligand geometry (i)

22 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	$\#\|Z\| > 2$
2	NAG	A	2191	1	14,14,15	0.28	0	15,19,21	1.84	2 (13%)
2	NAG	A	5201	1	14,14,15	0.35	0	15,19,21	2.05	5 (33%)
2	NAG	A	6851	1	14,14,15	0.35	0	15,19,21	1.60	4 (26%)
2	NAG	A	851	1	14,14,15	0.28	0	15,19,21	2.05	3 (20%)
2	NAG	B	1501	1	14,14,15	0.39	0	15,19,21	1.41	2 (13%)
5	FUC	B	1502	-	10,10,11	0.40	0	14,14,16	1.37	1 (7%)
2	NAG	B	2811	1	14,14,15	0.33	0	15,19,21	0.95	0
2	NAG	B	3211	1	14,14,15	0.32	0	15,19,21	0.99	1 (6%)
2	NAG	B	5201	1	14,14,15	0.48	0	15,19,21	4.45	6 (40%)
2	NAG	B	6851	1	14,14,15	0.29	0	15,19,21	1.05	2 (13%)
2	NAG	B	851	1	14,14,15	0.31	0	15,19,21	1.17	1 (6%)
2	NAG	C	1501	1	14,14,15	0.35	0	15,19,21	0.99	1 (6%)
2	NAG	C	2191	1	14,14,15	0.28	0	15,19,21	0.71	0
2	NAG	C	2811	1	14,14,15	0.35	0	15,19,21	1.09	1 (6%)
2	NAG	C	3211	1	14,14,15	0.40	0	15,19,21	0.79	0
2	NAG	C	5201	1	14,14,15	0.50	0	15,19,21	1.47	2 (13%)
2	NAG	D	1501	1	14,14,15	0.33	0	15,19,21	1.12	1 (6%)
2	NAG	D	2191	1	14,14,15	0.32	0	15,19,21	0.59	0
2	NAG	D	2811	1	14,14,15	0.33	0	15,19,21	0.68	0
2	NAG	D	3211	1	14,14,15	0.26	0	15,19,21	1.28	2 (13%)
2	NAG	D	5201	1	14,14,15	0.31	0	15,19,21	1.59	2 (13%)
2	NAG	D	6851	1	14,14,15	0.40	0	15,19,21	1.48	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
2	NAG	A	2191	1	-	0/6/23/26	0/1/1/1
2	NAG	A	5201	1	-	0/6/23/26	0/1/1/1
2	NAG	A	6851	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	851	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1501	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FUC	B	1502	-	-	0/0/17/20	0/1/1/1
2	NAG	B	2811	1	-	0/6/23/26	0/1/1/1
2	NAG	B	3211	1	-	0/6/23/26	0/1/1/1
2	NAG	B	5201	1	-	0/6/23/26	0/1/1/1
2	NAG	B	6851	1	-	0/6/23/26	0/1/1/1
2	NAG	B	851	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1501	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	C	2191	1	-	0/6/23/26	0/1/1/1
2	NAG	C	2811	1	-	0/6/23/26	0/1/1/1
2	NAG	C	3211	1	-	0/6/23/26	0/1/1/1
2	NAG	C	5201	1	-	0/6/23/26	0/1/1/1
2	NAG	D	1501	1	-	0/6/23/26	0/1/1/1
2	NAG	D	2191	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	2811	1	-	0/6/23/26	0/1/1/1
2	NAG	D	3211	1	-	0/6/23/26	0/1/1/1
2	NAG	D	5201	1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	6851	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	5201	NAG	C3-C2-N2	-8.89	89.26	110.56
2	A	2191	NAG	C4-C3-C2	-5.53	102.63	111.23
2	A	851	NAG	C4-C3-C2	-5.52	102.64	111.23
2	B	5201	NAG	C8-C7-N2	-4.40	107.68	116.11
2	D	3211	NAG	C2-N2-C7	-3.52	118.52	123.04
2	B	1501	NAG	C4-C3-C2	-3.48	105.82	111.23
2	B	3211	NAG	C2-N2-C7	-3.31	118.78	123.04
2	A	6851	NAG	C4-C3-C2	-3.13	106.37	111.23
2	C	1501	NAG	C4-C3-C2	-2.87	106.76	111.23
2	A	5201	NAG	C4-C3-C2	-2.86	106.78	111.23
2	C	2811	NAG	C2-N2-C7	-2.85	119.37	123.04
2	B	6851	NAG	C4-C3-C2	-2.58	107.22	111.23
2	D	3211	NAG	C4-C3-C2	-2.14	107.91	111.23
2	B	6851	NAG	O3-C3-C2	2.02	113.12	109.11
2	A	6851	NAG	O3-C3-C2	2.11	113.30	109.11
2	B	851	NAG	C2-N2-C7	2.27	125.95	123.04
2	A	5201	NAG	C3-C2-N2	2.29	116.06	110.56
2	D	1501	NAG	C3-C4-C5	2.34	114.27	110.20
2	A	6851	NAG	C3-C2-N2	2.36	116.21	110.56
2	D	5201	NAG	C3-C2-N2	2.54	116.64	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	5201	NAG	C2-N2-C7	2.72	126.53	123.04
2	B	1501	NAG	O3-C3-C2	2.73	114.53	109.11
2	B	5201	NAG	C1-O5-C5	2.80	115.80	112.25
2	B	5201	NAG	C4-C3-C2	2.86	115.67	111.23
2	A	6851	NAG	C2-N2-C7	2.87	126.73	123.04
2	A	5201	NAG	O5-C5-C6	3.02	113.89	107.35
2	A	2191	NAG	C3-C2-N2	3.07	117.92	110.56
2	A	851	NAG	C2-N2-C7	3.35	127.34	123.04
2	B	5201	NAG	O7-C7-N2	3.47	128.94	121.86
2	A	851	NAG	C1-O5-C5	3.49	116.68	112.25
2	D	6851	NAG	C1-O5-C5	3.56	116.76	112.25
5	B	1502	FUC	C1-C2-C3	3.59	113.79	109.54
2	C	5201	NAG	C1-O5-C5	3.62	116.84	112.25
2	A	5201	NAG	C1-O5-C5	3.70	116.95	112.25
2	A	5201	NAG	C2-N2-C7	4.62	128.98	123.04
2	D	5201	NAG	C2-N2-C7	4.69	129.07	123.04
2	B	5201	NAG	C2-N2-C7	12.71	139.37	123.04

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	D	5201	NAG	C1
2	D	2191	NAG	C1
2	D	6851	NAG	C1
2	C	1501	NAG	C1
2	A	6851	NAG	C1

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2191	NAG	1	0
2	A	5201	NAG	2	0
2	A	6851	NAG	2	0
2	A	851	NAG	5	0
2	B	1501	NAG	4	0
5	B	1502	FUC	3	0
2	B	5201	NAG	1	0
2	B	6851	NAG	2	0
2	B	851	NAG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	2191	NAG	2	0
2	C	5201	NAG	1	0
2	D	5201	NAG	4	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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.