



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 11:38 pm GMT

PDB ID : 1SR5  
Title : ANTITHROMBIN-ANHYDROTHROMBIN-HEPARIN TERNARY COMPLEX STRUCTURE  
Authors : Dementiev, A.; Petitou, M.; Gettins, P.G.  
Deposited on : 2004-03-22  
Resolution : 3.10 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)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

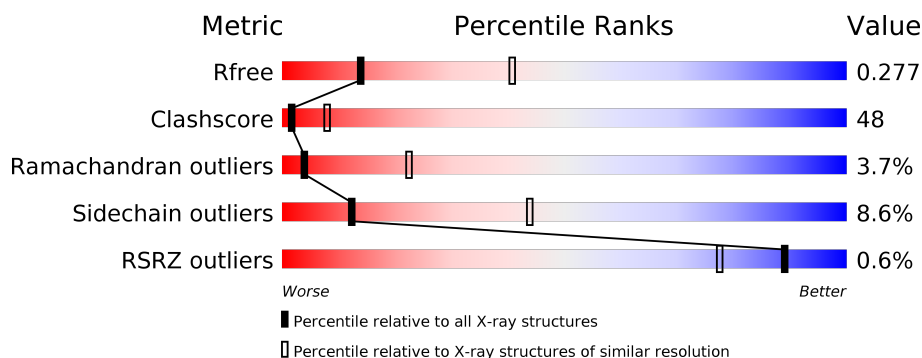
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
$R_{free}$	100719	1001 (3.12-3.08)
Clashscore	112137	1099 (3.12-3.08)
Ramachandran outliers	110173	1057 (3.12-3.08)
Sidechain outliers	110143	1057 (3.12-3.08)
RSRZ outliers	101464	1006 (3.12-3.08)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	432	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 37%, green 50%, grey 7%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>%</span> <span>37%</span> <span>50%</span> <span>7%</span> <span>5%</span> </div> </div>
2	B	36	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 44%, yellow 44%, grey 11%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>44%</span> <span>44%</span> <span>11%</span> </div> </div>
3	C	259	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, green 34%, yellow 51%, orange 11%, grey 5%);"></div> <div style="display: flex; justify-content: space-between; width: 100%;"> <span>34%</span> <span>51%</span> <span>11%</span> <span>•</span> </div> </div>

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 5534 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 Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	409	Total	C	N	O	S	0	0	0
			3085	1974	523	571	17			

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	32	Total	C	N	O	S	0	0	0
			248	156	40	51	1			

- Molecule 3 is a protein called Prothrombin.

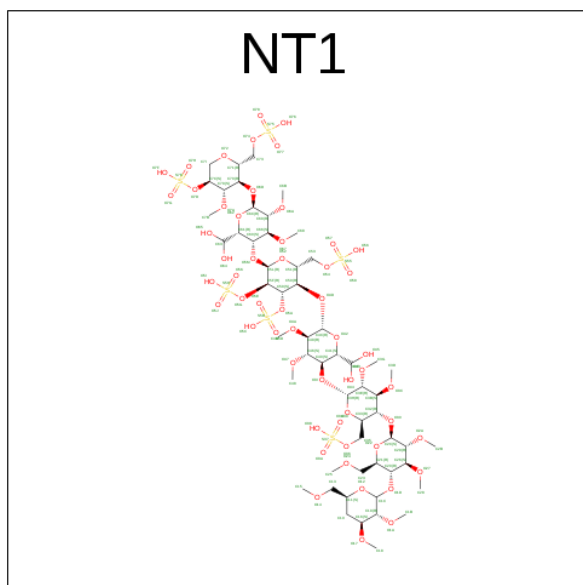
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	248	Total	C	N	O	S	0	0	0
			1960	1251	341	354	14			

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



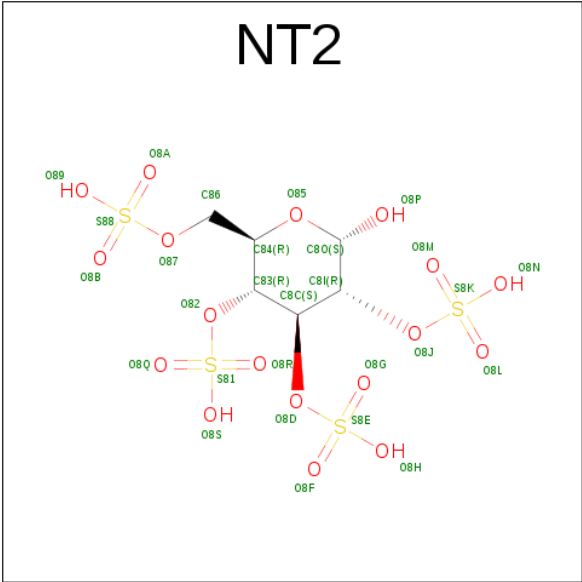
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SUGAR (HEPARIN HEPTASACCHARIDE) (three-letter code: NT1) (formula:  $C_{55}H_{98}O_{54}S_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	O	S	0	0
			111	53	52	6		

- Molecule 6 is SUGAR (2,3,4,6-TETRA-O-SULFOHEXOPYRANOSE) (three-letter code: NT2) (formula:  $C_6H_{12}O_{18}S_4$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	O	S	0	0
			13	6	6	1		

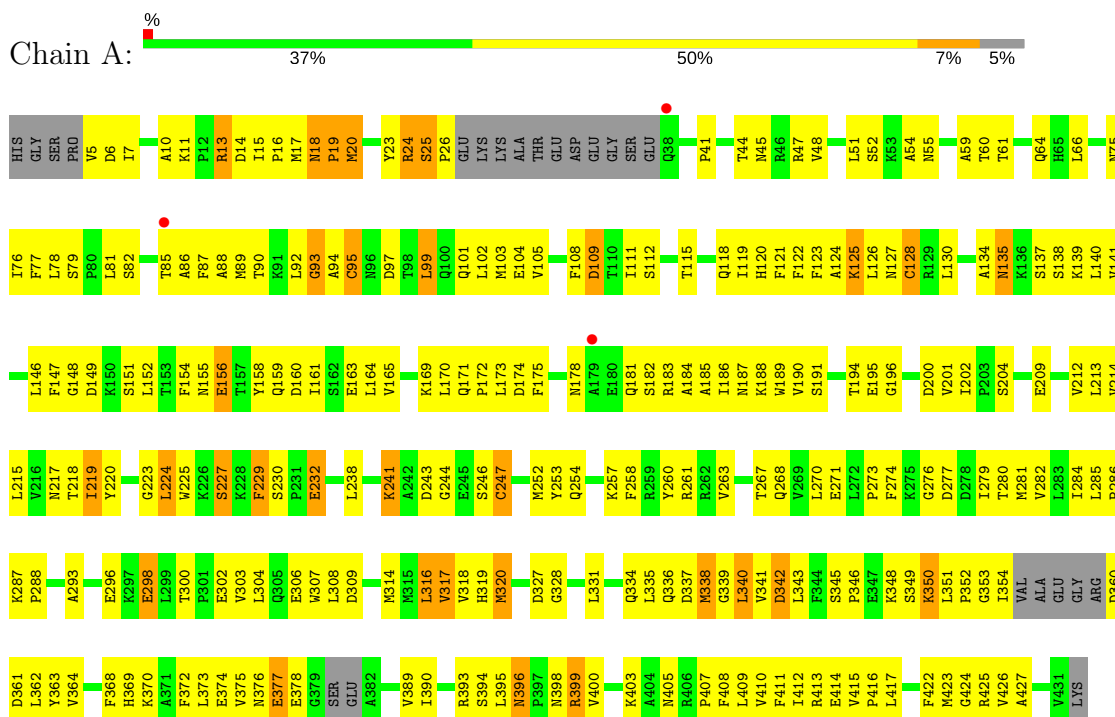
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	37	Total	O	0	0
			37	37		
7	B	4	Total	O	0	0
			4	4		
7	C	34	Total	O	0	0
			34	34		

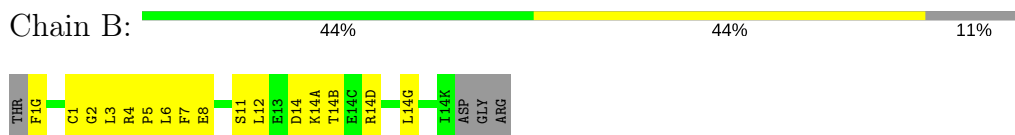
### 3 Residue-property plots

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.

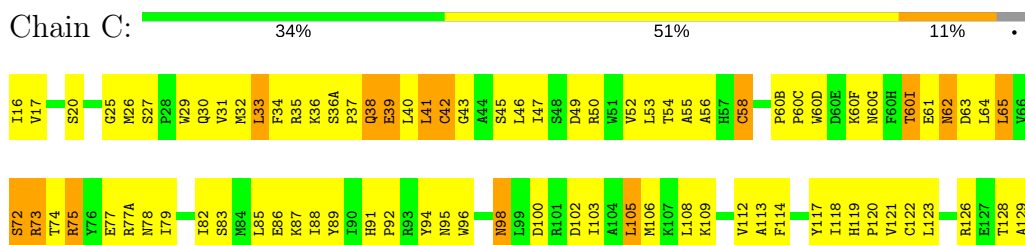
#### • Molecule 1: Antithrombin-III

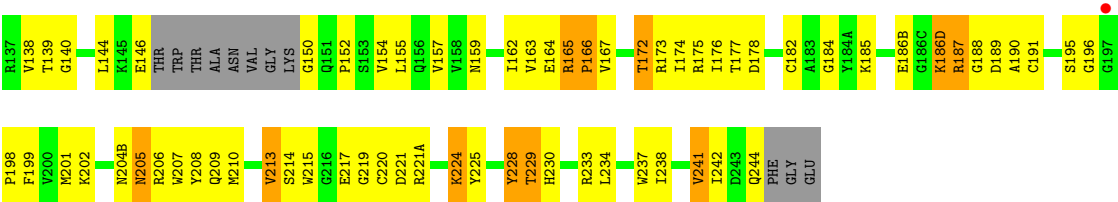


#### • Molecule 2: Prothrombin



#### • Molecule 3: Prothrombin





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.04Å 90.70Å 159.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 3.10 28.66 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.6 (30.00-3.10) 99.7 (28.66-3.10)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.20 (at 3.11Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.227 , 0.278 0.238 , 0.277	Depositor DCC
$R_{free}$ test set	1206 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	66.0	Xtriage
Anisotropy	0.879	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.25 , 56.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.027 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	5534	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.17% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NT1, NT2, NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.45	0/3149	0.83	10/4286 (0.2%)
2	B	0.46	0/251	0.69	0/335
3	C	0.46	0/2011	0.72	1/2728 (0.0%)
All	All	0.45	0/5411	0.78	11/7349 (0.1%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	342	ASP	CB-CG-OD1	-13.24	106.39	118.30
1	A	342	ASP	CB-CG-OD2	11.43	128.59	118.30
1	A	229	PHE	O-C-N	-10.33	106.17	122.70
1	A	94	ALA	N-CA-CB	9.60	123.54	110.10
1	A	128	CYS	CA-CB-SG	7.95	128.31	114.00
1	A	93	GLY	N-CA-C	-7.38	94.65	113.10
1	A	18	ASN	C-N-CD	6.77	142.62	128.40
1	A	94	ALA	N-CA-C	-6.68	92.96	111.00
1	A	229	PHE	CA-C-N	6.37	131.21	117.20
1	A	317	VAL	N-CA-C	-5.61	95.85	111.00
3	C	75	ARG	CD-NE-CZ	-5.07	116.50	123.60

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3085	0	2922	320	1
2	B	248	0	236	16	1
3	C	1960	0	1884	177	0
4	A	28	0	26	6	0
4	C	14	0	13	3	0
5	A	111	0	76	13	0
6	C	13	0	8	4	0
7	A	37	0	0	2	0
7	B	4	0	0	0	0
7	C	34	0	0	1	0
All	All	5534	0	5165	508	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 48.

All (508) 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)
5:A:601:NT1:C2B	5:A:601:NT1:O2A	1.63	1.43
5:A:601:NT1:C6B	5:A:601:NT1:O6A	1.63	1.41
5:A:601:NT1:O3F	5:A:601:NT1:C3G	1.65	1.39
5:A:601:NT1:O27	5:A:601:NT1:C28	1.67	1.39
1:A:95:CYS:O	1:A:99:LEU:HB3	1.29	1.24
1:A:5:VAL:HG11	1:A:15:ILE:HD11	1.24	1.16
1:A:7:ILE:CD1	1:A:164:LEU:O	1.94	1.15
1:A:15:ILE:HG23	1:A:16:PRO:HD2	1.25	1.13
1:A:23:TYR:HB2	1:A:99:LEU:HD21	1.11	1.10
1:A:95:CYS:O	1:A:99:LEU:CB	2.01	1.09
1:A:298:GLU:O	1:A:298:GLU:HG2	1.55	1.05
1:A:23:TYR:OH	1:A:25:SER:HB3	1.54	1.05
3:C:41:LEU:O	3:C:42:CYS:SG	2.15	1.04
1:A:254:GLN:NE2	1:A:258:PHE:HZ	1.58	1.01
1:A:7:ILE:HD11	1:A:164:LEU:O	1.57	1.01
1:A:90:THR:O	1:A:93:GLY:O	1.79	1.00
3:C:50:ARG:HA	3:C:108:LEU:HD12	1.42	0.99
1:A:23:TYR:O	1:A:24:ARG:HG3	1.62	0.98
1:A:7:ILE:HD13	1:A:164:LEU:O	1.61	0.98
3:C:61:GLU:HG2	3:C:87:LYS:HA	1.45	0.98
1:A:25:SER:HB2	1:A:26:PRO:HD2	1.47	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:GLN:HE21	1:A:258:PHE:HZ	0.97	0.95
1:A:23:TYR:HB2	1:A:99:LEU:CD2	1.94	0.95
3:C:62:ASN:HD22	3:C:62:ASN:H	1.06	0.94
1:A:15:ILE:CG2	1:A:16:PRO:HD2	1.98	0.93
3:C:62:ASN:H	3:C:62:ASN:ND2	1.67	0.93
1:A:334:GLN:O	1:A:337:ASP:OD1	1.87	0.93
3:C:72:SER:O	3:C:154:VAL:HA	1.69	0.91
1:A:170:LEU:HD23	1:A:171:GLN:N	1.87	0.90
1:A:229:PHE:HB2	1:A:377:GLU:HA	1.53	0.89
1:A:238:LEU:HD22	1:A:246:SER:HB3	1.52	0.89
2:B:1(G):PHE:HD1	3:C:242:ILE:HG21	1.38	0.87
1:A:81:LEU:HD21	1:A:127:ASN:HD21	1.40	0.86
1:A:23:TYR:CB	1:A:99:LEU:HD21	2.03	0.85
3:C:165:ARG:HH11	3:C:178:ASP:HA	1.40	0.84
5:A:601:NT1:C6B	5:A:601:NT1:C69	2.55	0.84
1:A:18:ASN:O	4:A:502:NAG:H61	1.75	0.84
1:A:102:LEU:HD23	1:A:340:LEU:HD11	1.60	0.83
2:B:6:LEU:HD12	3:C:25:GLY:HA3	1.61	0.83
3:C:36(A):SER:HA	3:C:38:GLN:N	1.96	0.81
1:A:229:PHE:CD2	1:A:252:MET:HB3	2.16	0.80
1:A:19:PRO:HB3	1:A:92:LEU:HD12	1.61	0.80
3:C:72:SER:O	3:C:73:ARG:HB2	1.82	0.80
1:A:282:VAL:HG21	1:A:308:LEU:HD21	1.64	0.80
1:A:316:LEU:HD23	1:A:400:VAL:HG13	1.63	0.80
1:A:412:ILE:HD12	1:A:422:PHE:CD2	2.16	0.80
1:A:20:MET:SD	1:A:353:GLY:HA2	2.22	0.79
1:A:284:ILE:HD13	1:A:307:TRP:CZ3	2.16	0.79
1:A:155:ASN:O	1:A:156:GLU:HB2	1.82	0.79
3:C:94:TYR:CZ	3:C:96:TRP:HB3	2.17	0.79
1:A:414:GLU:OE1	1:A:417:LEU:HB2	1.84	0.78
3:C:36(A):SER:HA	3:C:38:GLN:H	1.49	0.78
3:C:62:ASN:N	3:C:62:ASN:HD22	1.70	0.78
3:C:70:LYS:HG2	3:C:77:GLU:OE1	1.83	0.78
1:A:5:VAL:CG1	1:A:15:ILE:HD11	2.11	0.78
3:C:103:ILE:HD11	3:C:238:ILE:HD11	1.65	0.77
1:A:55:ASN:ND2	1:A:81:LEU:HA	2.00	0.77
1:A:23:TYR:OH	1:A:25:SER:CB	2.31	0.76
3:C:41:LEU:O	3:C:41:LEU:HD12	1.84	0.76
1:A:95:CYS:HB2	1:A:352:PRO:CG	2.15	0.76
1:A:187:ASN:ND2	1:A:200:ASP:HA	1.99	0.76
1:A:328:GLY:HA3	1:A:370:LYS:HD3	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:601:NT1:C2B	5:A:601:NT1:C29	2.65	0.75
1:A:335:LEU:HB3	1:A:340:LEU:HD23	1.67	0.75
1:A:75:ASN:HB3	1:A:427:ALA:H	1.51	0.75
1:A:108:PHE:O	1:A:111:ILE:HG12	1.86	0.75
3:C:35:ARG:O	3:C:38:GLN:HA	1.87	0.74
3:C:62:ASN:N	3:C:62:ASN:ND2	2.32	0.74
3:C:31:VAL:HG22	3:C:68:ILE:HG23	1.67	0.74
3:C:29:TRP:CD2	3:C:121:VAL:HB	2.23	0.74
1:A:175:PHE:O	1:A:209:GLU:HA	1.88	0.73
1:A:258:PHE:HB2	1:A:316:LEU:CD1	2.18	0.73
3:C:60(G):ASN:HD21	4:C:503:NAG:C1	2.01	0.73
5:A:601:NT1:C3E	5:A:601:NT1:C3G	2.67	0.72
1:A:78:LEU:HD23	1:A:78:LEU:N	2.04	0.72
1:A:229:PHE:HD2	1:A:252:MET:HB3	1.54	0.72
3:C:72:SER:OG	3:C:73:ARG:N	2.21	0.72
1:A:66:LEU:HA	1:A:334:GLN:NE2	2.05	0.71
1:A:253:TYR:HE2	1:A:317:VAL:HG12	1.55	0.71
1:A:66:LEU:HA	1:A:334:GLN:HE21	1.55	0.71
1:A:101:GLN:OE1	1:A:341:VAL:HG22	1.90	0.71
1:A:319:HIS:CD2	1:A:403:LYS:HG3	2.25	0.71
1:A:229:PHE:HB3	1:A:377:GLU:CG	2.21	0.70
1:A:284:ILE:CD1	1:A:307:TRP:CZ3	2.74	0.70
5:A:601:NT1:C26	5:A:601:NT1:C28	2.69	0.70
1:A:146:LEU:HD21	1:A:215:LEU:HG	1.74	0.70
1:A:101:GLN:HE22	1:A:342:ASP:H	1.38	0.69
1:A:328:GLY:CA	1:A:370:LYS:HD3	2.22	0.69
3:C:105:LEU:H	3:C:105:LEU:HD12	1.57	0.69
1:A:147:PHE:O	1:A:213:LEU:HD12	1.92	0.69
1:A:227:SER:HB3	1:A:254:GLN:HE22	1.55	0.69
1:A:190:VAL:HG21	1:A:201:VAL:HG21	1.75	0.69
1:A:317:VAL:CG2	1:A:399:ARG:HD2	2.22	0.69
1:A:51:LEU:O	1:A:54:ALA:HB3	1.92	0.69
1:A:23:TYR:O	1:A:24:ARG:CG	2.40	0.68
1:A:253:TYR:HE2	1:A:317:VAL:CG1	2.06	0.68
1:A:95:CYS:HB2	1:A:352:PRO:HG3	1.76	0.68
1:A:155:ASN:HD21	4:A:502:NAG:HN2	1.41	0.68
2:B:14(B):THR:HB	3:C:159:ASN:HD21	1.59	0.68
1:A:336:GLN:HA	1:A:340:LEU:O	1.94	0.68
3:C:32:MET:HE1	3:C:70:LYS:HD3	1.76	0.68
3:C:87:LYS:HE2	7:C:632:HOH:O	1.94	0.68
3:C:35:ARG:HG2	3:C:39:GLU:H	1.57	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:237:TRP:O	3:C:241:VAL:HG13	1.94	0.67
3:C:55:ALA:O	3:C:58:CYS:HB2	1.94	0.67
1:A:229:PHE:HB2	1:A:377:GLU:CA	2.25	0.67
1:A:213:LEU:HD23	1:A:364:VAL:HG22	1.78	0.66
3:C:86:GLU:HB2	3:C:109:LYS:HA	1.78	0.66
3:C:36(A):SER:CA	3:C:38:GLN:H	2.09	0.66
3:C:204(B):ASN:C	3:C:205:ASN:HD22	1.98	0.65
1:A:190:VAL:HG13	1:A:191:SER:N	2.12	0.65
3:C:98:ASN:H	3:C:98:ASN:HD22	1.42	0.65
1:A:351:LEU:HD12	1:A:362:LEU:HG	1.77	0.65
3:C:204(B):ASN:O	3:C:205:ASN:ND2	2.27	0.65
1:A:23:TYR:CZ	1:A:25:SER:HB3	2.30	0.65
1:A:15:ILE:CG2	1:A:16:PRO:CD	2.72	0.65
1:A:227:SER:CB	1:A:254:GLN:HE22	2.10	0.65
3:C:119:HIS:CD2	3:C:120:PRO:HD2	2.32	0.65
1:A:267:THR:HB	1:A:286:PRO:HA	1.79	0.65
2:B:1:CYS:C	3:C:122:CYS:SG	2.75	0.65
1:A:254:GLN:NE2	1:A:258:PHE:CZ	2.47	0.65
1:A:300:THR:O	1:A:303:VAL:HG12	1.97	0.65
3:C:60(I):THR:OG1	3:C:63:ASP:OD1	2.14	0.64
2:B:1(G):PHE:CD1	3:C:242:ILE:HG21	2.26	0.64
1:A:23:TYR:HH	1:A:25:SER:HB3	1.62	0.64
1:A:345:SER:O	1:A:349:SER:HB2	1.97	0.64
1:A:85:THR:HG22	1:A:123:PHE:CD1	2.32	0.64
1:A:339:GLY:O	1:A:341:VAL:HG13	1.98	0.64
1:A:336:GLN:O	1:A:339:GLY:O	2.15	0.64
1:A:119:ILE:HG23	1:A:120:HIS:N	2.13	0.64
1:A:149:ASP:HA	1:A:173:LEU:O	1.98	0.63
1:A:213:LEU:HB3	1:A:363:TYR:O	1.97	0.63
1:A:5:VAL:HG11	1:A:15:ILE:CD1	2.16	0.63
1:A:257:LYS:HA	1:A:314:MET:O	1.99	0.63
1:A:18:ASN:CB	4:A:502:NAG:O6	2.47	0.63
3:C:144:LEU:HD11	3:C:152:PRO:HB3	1.80	0.63
3:C:34:PHE:HB2	3:C:65:LEU:CD1	2.28	0.62
1:A:202:ILE:HG23	1:A:368:PHE:CE2	2.35	0.62
3:C:56:ALA:HB3	3:C:102:ASP:OD1	1.98	0.62
1:A:306:GLU:O	1:A:309:ASP:HB2	1.99	0.62
1:A:339:GLY:O	1:A:340:LEU:C	2.37	0.62
1:A:163:GLU:HB2	1:A:169:LYS:HG2	1.82	0.62
1:A:258:PHE:HB2	1:A:316:LEU:HD11	1.82	0.62
3:C:228:TYR:N	3:C:228:TYR:CD1	2.68	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:98:ASN:N	3:C:98:ASN:HD22	1.97	0.61
1:A:25:SER:HB2	1:A:26:PRO:CD	2.25	0.61
3:C:61:GLU:CG	3:C:87:LYS:HA	2.26	0.61
3:C:32:MET:CE	3:C:70:LYS:HD3	2.30	0.61
1:A:78:LEU:HD23	1:A:78:LEU:H	1.65	0.60
1:A:85:THR:O	1:A:88:ALA:HB3	2.01	0.60
3:C:112:VAL:HG22	3:C:113:ALA:H	1.65	0.60
2:B:1(G):PHE:HA	3:C:242:ILE:CG2	2.32	0.60
3:C:233:ARG:HG3	3:C:233:ARG:HH21	1.67	0.60
1:A:376:ASN:OD1	1:A:376:ASN:C	2.39	0.60
3:C:165:ARG:HG2	6:C:602:NT2:H8C	1.84	0.60
1:A:112:SER:OG	1:A:115:THR:CB	2.49	0.59
2:B:14(B):THR:HB	3:C:159:ASN:ND2	2.16	0.59
1:A:229:PHE:HB3	1:A:377:GLU:CB	2.32	0.59
3:C:165:ARG:HG2	3:C:165:ARG:HH21	1.67	0.59
3:C:34:PHE:HB2	3:C:65:LEU:HD12	1.84	0.59
1:A:395:LEU:HG	1:A:396:ASN:N	2.17	0.59
1:A:95:CYS:O	1:A:99:LEU:HB2	2.00	0.59
1:A:155:ASN:HB3	1:A:158:TYR:HB3	1.85	0.59
3:C:60(B):PRO:HG2	3:C:96:TRP:CZ2	2.38	0.59
1:A:119:ILE:CG2	1:A:120:HIS:N	2.64	0.59
1:A:190:VAL:HG11	1:A:201:VAL:CG2	2.33	0.59
1:A:139:LYS:HA	4:A:501:NAG:H83	1.85	0.58
3:C:46:LEU:O	3:C:120:PRO:HA	2.03	0.58
1:A:126:LEU:HD23	1:A:126:LEU:C	2.24	0.58
1:A:151:SER:O	1:A:152:LEU:HG	2.02	0.58
1:A:182:SER:C	1:A:184:ALA:H	2.06	0.58
1:A:246:SER:O	1:A:247:CYS:HB2	2.02	0.58
3:C:112:VAL:HG22	3:C:113:ALA:N	2.18	0.58
1:A:134:ALA:HA	1:A:279:ILE:HD12	1.86	0.57
3:C:17:VAL:HG21	3:C:220:CYS:HB3	1.86	0.57
3:C:53:LEU:HD23	3:C:209:GLN:NE2	2.20	0.57
1:A:148:GLY:O	1:A:172:PRO:HA	2.03	0.57
1:A:159:GLN:O	1:A:169:LYS:HD2	2.04	0.57
3:C:163:VAL:HB	3:C:182:CYS:SG	2.45	0.57
3:C:202:LYS:NZ	3:C:205:ASN:HB2	2.19	0.57
1:A:190:VAL:HG21	1:A:218:THR:HG21	1.86	0.57
3:C:43:GLY:O	3:C:196:GLY:HA3	2.04	0.57
1:A:346:PRO:HG3	1:A:363:TYR:CE2	2.39	0.57
3:C:176:ILE:HG22	3:C:177:THR:N	2.20	0.56
1:A:187:ASN:HD22	1:A:200:ASP:HA	1.66	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:35:ARG:HG2	3:C:39:GLU:N	2.19	0.56
2:B:2:GLY:O	2:B:3:LEU:HD23	2.06	0.56
1:A:17:MET:CB	1:A:118:GLN:NE2	2.69	0.56
1:A:317:VAL:HG22	1:A:399:ARG:HD2	1.86	0.56
1:A:13:ARG:CZ	5:A:601:NT1:O5K	2.53	0.56
3:C:69:GLY:HA3	3:C:118:ILE:HD13	1.87	0.56
1:A:190:VAL:HG13	1:A:191:SER:H	1.71	0.56
1:A:18:ASN:O	4:A:502:NAG:C6	2.51	0.56
3:C:129(C):LEU:HB2	3:C:210:MET:HE1	1.86	0.56
1:A:229:PHE:CB	1:A:377:GLU:HB3	2.36	0.56
1:A:337:ASP:OD1	1:A:337:ASP:N	2.32	0.56
1:A:229:PHE:CB	1:A:377:GLU:CB	2.84	0.56
1:A:13:ARG:HG2	1:A:14:ASP:N	2.20	0.55
1:A:171:GLN:NE2	1:A:172:PRO:HD2	2.22	0.55
1:A:230:SER:HB2	1:A:232:GLU:OE1	2.07	0.55
3:C:67:ARG:HH21	3:C:70:LYS:HZ1	1.55	0.55
1:A:253:TYR:CE2	1:A:317:VAL:HG12	2.40	0.55
1:A:202:ILE:HG12	1:A:368:PHE:CD2	2.41	0.55
3:C:165:ARG:HG2	3:C:165:ARG:NH2	2.22	0.55
3:C:98:ASN:N	3:C:98:ASN:ND2	2.54	0.55
1:A:102:LEU:HD23	1:A:340:LEU:CD1	2.34	0.55
1:A:147:PHE:CE1	1:A:171:GLN:HB3	2.42	0.55
1:A:229:PHE:CE2	1:A:252:MET:HB3	2.41	0.55
1:A:219:ILE:HD13	1:A:422:PHE:CE1	2.42	0.55
3:C:186(D):LYS:HB2	3:C:186(D):LYS:NZ	2.22	0.55
1:A:48:VAL:HG21	1:A:125:LYS:CE	2.37	0.55
3:C:41:LEU:O	3:C:42:CYS:CB	2.55	0.55
3:C:20:SER:O	3:C:157:VAL:HG12	2.06	0.54
1:A:147:PHE:HB2	1:A:214:VAL:HG23	1.89	0.54
1:A:48:VAL:HG21	1:A:125:LYS:HE3	1.90	0.54
3:C:40:LEU:HG	3:C:41:LEU:N	2.23	0.54
3:C:67:ARG:HH21	3:C:70:LYS:NZ	2.05	0.54
3:C:138:VAL:HG11	3:C:190:ALA:HB2	1.90	0.54
1:A:284:ILE:CD1	1:A:307:TRP:HZ3	2.20	0.54
1:A:350:LYS:C	1:A:352:PRO:HD3	2.29	0.54
1:A:135:ASN:OD1	1:A:140:LEU:HB3	2.08	0.53
1:A:146:LEU:HD23	1:A:215:LEU:HA	1.90	0.53
1:A:147:PHE:CD1	1:A:171:GLN:HB3	2.44	0.53
1:A:155:ASN:O	1:A:156:GLU:CB	2.55	0.53
3:C:202:LYS:HD2	3:C:207:TRP:CZ2	2.43	0.53
1:A:352:PRO:C	1:A:354:ILE:H	2.12	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:PHE:HB2	1:A:316:LEU:HD12	1.91	0.53
1:A:407:PRO:HA	1:A:426:VAL:O	2.07	0.53
1:A:44:THR:HG21	1:A:417:LEU:HD21	1.90	0.53
3:C:172:THR:HB	3:C:217:GLU:OE1	2.08	0.53
3:C:177:THR:HG22	3:C:178:ASP:N	2.23	0.53
3:C:201:MET:SD	3:C:210:MET:HG3	2.49	0.53
3:C:165:ARG:CG	6:C:602:NT2:H8C	2.39	0.53
1:A:389:VAL:HG23	1:A:390:ILE:HG23	1.91	0.53
3:C:29:TRP:O	3:C:31:VAL:HG23	2.08	0.53
3:C:91:HIS:CG	3:C:92:PRO:HD2	2.44	0.53
1:A:47:ARG:HD2	1:A:122:PHE:CZ	2.43	0.53
3:C:45:SER:O	3:C:52:VAL:HG13	2.09	0.52
3:C:87:LYS:HB3	3:C:89:TYR:CE2	2.44	0.52
1:A:41:PRO:HG3	1:A:417:LEU:HD23	1.91	0.52
1:A:335:LEU:HB3	1:A:340:LEU:CD2	2.37	0.52
1:A:93:GLY:CA	1:A:353:GLY:HA3	2.39	0.52
3:C:67:ARG:NH2	3:C:70:LYS:NZ	2.57	0.52
1:A:335:LEU:O	1:A:338:MET:HG3	2.10	0.52
2:B:6:LEU:CD1	3:C:25:GLY:HA3	2.38	0.52
3:C:36:LYS:HB2	3:C:63:ASP:O	2.10	0.52
1:A:78:LEU:HD23	1:A:423:MET:O	2.09	0.51
3:C:188:GLY:O	3:C:189:ASP:HB2	2.10	0.51
1:A:273:PRO:HA	1:A:280:THR:HA	1.90	0.51
3:C:47:ILE:HG21	3:C:123:LEU:HD21	1.92	0.51
1:A:76:ILE:HG22	1:A:77:PHE:N	2.24	0.51
1:A:78:LEU:CD2	1:A:78:LEU:N	2.73	0.51
1:A:112:SER:OG	1:A:115:THR:OG1	1.93	0.51
1:A:287:LYS:HG2	1:A:288:PRO:HD2	1.92	0.51
3:C:144:LEU:CD1	3:C:152:PRO:HD3	2.40	0.51
1:A:17:MET:CB	1:A:118:GLN:HE22	2.23	0.51
1:A:335:LEU:HD13	1:A:340:LEU:CD2	2.40	0.51
3:C:65:LEU:HD12	3:C:65:LEU:C	2.31	0.51
1:A:190:VAL:HG21	1:A:201:VAL:CG2	2.40	0.51
1:A:146:LEU:HD21	1:A:215:LEU:CG	2.40	0.51
1:A:81:LEU:HD21	1:A:127:ASN:ND2	2.18	0.51
3:C:187:ARG:NH1	3:C:221:ASP:OD2	2.44	0.51
3:C:37:PRO:O	3:C:38:GLN:O	2.29	0.51
3:C:67:ARG:NH2	3:C:70:LYS:HZ1	2.07	0.51
1:A:331:LEU:HD11	1:A:369:HIS:HB2	1.92	0.51
1:A:181:GLN:O	1:A:185:ALA:HB2	2.10	0.50
1:A:61:THR:O	1:A:64:GLN:HB2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:73:ARG:HD3	3:C:152:PRO:O	2.12	0.50
1:A:393:ARG:NH2	3:C:189:ASP:OD2	2.38	0.50
3:C:129:ALA:HA	3:C:210:MET:HE3	1.93	0.50
1:A:126:LEU:HD21	1:A:130:LEU:HD11	1.94	0.50
1:A:186:ILE:HG21	1:A:202:ILE:CD1	2.42	0.50
1:A:319:HIS:HB2	1:A:403:LYS:HA	1.91	0.50
1:A:66:LEU:CD2	1:A:78:LEU:HD13	2.42	0.50
3:C:36:LYS:H	3:C:64:LEU:HA	1.77	0.50
2:B:1:CYS:O	3:C:122:CYS:SG	2.69	0.50
3:C:174:ILE:HD12	3:C:215:TRP:CZ3	2.46	0.50
1:A:161:ILE:HG22	1:A:165:VAL:HG12	1.94	0.50
1:A:45:ASN:CB	1:A:125:LYS:HZ3	2.25	0.50
1:A:48:VAL:HG21	5:A:601:NT1:O3A	2.11	0.50
1:A:412:ILE:HD12	1:A:422:PHE:CG	2.45	0.50
3:C:102:ASP:HB3	3:C:229:THR:HG23	1.93	0.50
3:C:91:HIS:ND1	3:C:92:PRO:HD2	2.26	0.50
1:A:352:PRO:O	1:A:354:ILE:N	2.45	0.50
2:B:4:ARG:NH2	2:B:8:GLU:OE2	2.41	0.50
1:A:55:ASN:HD21	1:A:81:LEU:HA	1.72	0.50
2:B:3:LEU:HD21	3:C:206:ARG:HG2	1.92	0.50
3:C:17:VAL:HG11	3:C:221:ASP:CB	2.42	0.50
1:A:41:PRO:O	1:A:44:THR:HB	2.12	0.49
3:C:60(G):ASN:ND2	4:C:503:NAG:H83	2.26	0.49
3:C:165:ARG:CB	3:C:166:PRO:HD3	2.41	0.49
3:C:33:LEU:HD21	3:C:64:LEU:HD22	1.93	0.49
1:A:101:GLN:NE2	1:A:342:ASP:OD1	2.45	0.49
1:A:66:LEU:HD12	1:A:334:GLN:HE21	1.76	0.49
1:A:343:LEU:HG	1:A:364:VAL:CG2	2.42	0.49
1:A:263:VAL:HG11	1:A:307:TRP:CD1	2.47	0.49
3:C:146:GLU:OE2	3:C:219:GLY:HA3	2.12	0.49
3:C:128:THR:HG21	3:C:208:TYR:CD2	2.47	0.49
1:A:394:SER:OG	3:C:60(F):LYS:NZ	2.45	0.49
3:C:88:ILE:HG22	3:C:89:TYR:N	2.26	0.49
1:A:115:THR:HA	1:A:122:PHE:CE2	2.47	0.49
1:A:182:SER:O	1:A:184:ALA:N	2.46	0.49
1:A:90:THR:O	1:A:93:GLY:C	2.49	0.49
3:C:49:ASP:O	3:C:112:VAL:HG12	2.13	0.49
3:C:129(C):LEU:HB2	3:C:210:MET:CE	2.42	0.49
2:B:14:ASP:HB2	3:C:26:MET:HE3	1.93	0.49
1:A:154:PHE:HD1	1:A:354:ILE:HG22	1.77	0.49
1:A:18:ASN:CB	4:A:502:NAG:C6	2.90	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:ASN:O	1:A:369:HIS:HA	2.13	0.49
1:A:327:ASP:O	1:A:370:LYS:HA	2.13	0.49
3:C:60(B):PRO:HG2	3:C:96:TRP:CE2	2.47	0.49
1:A:118:GLN:HA	1:A:118:GLN:HE21	1.77	0.49
1:A:229:PHE:CD2	1:A:252:MET:SD	3.06	0.49
3:C:195:SER:HA	3:C:213:VAL:HB	1.94	0.49
1:A:351:LEU:CD1	1:A:362:LEU:HG	2.42	0.49
1:A:412:ILE:HB	1:A:422:PHE:HB2	1.95	0.49
3:C:100:ASP:OD1	3:C:177:THR:HG21	2.13	0.49
1:A:19:PRO:O	1:A:20:MET:HB2	2.13	0.48
1:A:194:THR:O	1:A:196:GLY:N	2.46	0.48
1:A:81:LEU:HD23	1:A:81:LEU:C	2.34	0.48
3:C:16:ILE:HD11	3:C:139:THR:C	2.33	0.48
1:A:190:VAL:HG11	1:A:201:VAL:HG23	1.94	0.48
1:A:75:ASN:HB2	1:A:425:ARG:O	2.14	0.48
1:A:101:GLN:NE2	1:A:342:ASP:HB2	2.27	0.48
1:A:270:LEU:HD12	1:A:271:GLU:H	1.78	0.48
1:A:298:GLU:CG	1:A:298:GLU:O	2.38	0.48
3:C:88:ILE:HD13	3:C:106:MET:HB3	1.96	0.48
1:A:393:ARG:HB2	3:C:214:SER:O	2.13	0.48
1:A:270:LEU:HD12	1:A:271:GLU:N	2.29	0.48
1:A:346:PRO:HG3	1:A:363:TYR:CZ	2.49	0.48
1:A:396:ASN:ND2	1:A:398:ASN:H	2.12	0.48
1:A:316:LEU:HD23	1:A:400:VAL:CG1	2.40	0.47
3:C:136:GLY:HA3	3:C:199:PHE:CZ	2.48	0.47
6:C:602:NT2:S81	6:C:602:NT2:O8D	2.72	0.47
1:A:212:VAL:HG23	1:A:213:LEU:N	2.28	0.47
1:A:258:PHE:CD2	1:A:316:LEU:HD12	2.49	0.47
1:A:118:GLN:HA	1:A:118:GLN:NE2	2.29	0.47
1:A:45:ASN:HB2	1:A:125:LYS:NZ	2.29	0.47
3:C:34:PHE:HB2	3:C:65:LEU:HD11	1.95	0.47
1:A:182:SER:C	1:A:184:ALA:N	2.67	0.47
1:A:335:LEU:CB	1:A:340:LEU:HD23	2.42	0.47
1:A:229:PHE:CB	1:A:377:GLU:HA	2.35	0.47
1:A:174:ASP:OD2	1:A:178:ASN:ND2	2.47	0.47
1:A:190:VAL:CG1	1:A:191:SER:N	2.78	0.47
3:C:114:PHE:HA	3:C:118:ILE:HB	1.96	0.47
1:A:252:MET:HE2	1:A:320:MET:HG2	1.97	0.47
1:A:146:LEU:HD21	1:A:215:LEU:CD1	2.45	0.47
1:A:229:PHE:HB3	1:A:377:GLU:HB3	1.97	0.47
1:A:394:SER:HB2	3:C:42:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ARG:HG2	1:A:47:ARG:HH11	1.78	0.47
3:C:60(B):PRO:HB2	3:C:60(C):PRO:HD3	1.96	0.47
1:A:121:PHE:O	1:A:124:ALA:HB3	2.14	0.47
1:A:141:VAL:HG13	1:A:220:TYR:HB3	1.98	0.46
1:A:241:LYS:HE3	1:A:243:ASP:OD2	2.15	0.46
1:A:102:LEU:CD2	1:A:340:LEU:HD11	2.38	0.46
1:A:352:PRO:C	1:A:354:ILE:N	2.67	0.46
3:C:174:ILE:HG22	3:C:175:ARG:N	2.30	0.46
3:C:186(D):LYS:CB	3:C:186(D):LYS:NZ	2.78	0.46
1:A:190:VAL:HG11	1:A:201:VAL:HG21	1.96	0.46
3:C:144:LEU:HD11	3:C:152:PRO:CB	2.45	0.46
3:C:29:TRP:CG	3:C:121:VAL:HB	2.50	0.46
1:A:138:SER:HB3	1:A:224:LEU:H	1.79	0.46
1:A:412:ILE:CD1	1:A:422:PHE:CD2	2.93	0.46
3:C:184:GLY:HA3	3:C:225:TYR:HD2	1.79	0.46
3:C:30:GLN:HG2	3:C:155:LEU:CD1	2.46	0.46
1:A:349:SER:OG	1:A:350:LYS:N	2.48	0.46
1:A:373:LEU:HD12	1:A:374:GLU:H	1.80	0.46
1:A:77:PHE:CE2	1:A:373:LEU:HB2	2.51	0.46
1:A:276:GLY:O	1:A:277:ASP:HB2	2.14	0.46
1:A:45:ASN:CB	1:A:125:LYS:NZ	2.79	0.46
5:A:601:NT1:C6B	5:A:601:NT1:H69	2.42	0.46
1:A:118:GLN:O	1:A:119:ILE:C	2.54	0.46
3:C:130:LEU:HD12	3:C:162:ILE:HD13	1.96	0.46
1:A:15:ILE:HG22	1:A:16:PRO:N	2.31	0.46
3:C:204(B):ASN:C	3:C:205:ASN:ND2	2.67	0.46
3:C:195:SER:HA	3:C:213:VAL:CG1	2.46	0.46
1:A:303:VAL:HG13	1:A:304:LEU:N	2.31	0.45
1:A:303:VAL:CG1	1:A:304:LEU:N	2.79	0.45
1:A:45:ASN:ND2	1:A:125:LYS:HZ3	2.13	0.45
1:A:260:TYR:HE1	1:A:268:GLN:HB3	1.80	0.45
1:A:284:ILE:HD11	1:A:307:TRP:CZ3	2.51	0.45
1:A:86:ALA:O	1:A:89:MET:HB2	2.15	0.45
3:C:103:ILE:CG2	3:C:234:LEU:HD23	2.47	0.45
1:A:410:VAL:N	1:A:424:GLY:O	2.46	0.45
5:A:601:NT1:H3G2	5:A:601:NT1:O3I	2.16	0.45
1:A:48:VAL:CG2	1:A:125:LYS:CE	2.95	0.45
3:C:98:ASN:H	3:C:98:ASN:ND2	2.12	0.45
1:A:119:ILE:CG2	1:A:120:HIS:H	2.28	0.45
1:A:81:LEU:HD11	1:A:126:LEU:CD2	2.47	0.45
1:A:335:LEU:O	1:A:336:GLN:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLY:HA3	1:A:353:GLY:HA3	1.98	0.45
3:C:114:PHE:N	3:C:114:PHE:CD1	2.85	0.45
1:A:319:HIS:CG	1:A:403:LYS:HG3	2.52	0.45
1:A:59:ALA:O	1:A:60:THR:C	2.54	0.45
1:A:258:PHE:HD2	1:A:316:LEU:HD12	1.80	0.45
1:A:93:GLY:HA2	1:A:353:GLY:HA3	1.99	0.45
3:C:186(B):GLU:O	3:C:186(D):LYS:N	2.48	0.45
3:C:202:LYS:HD2	3:C:207:TRP:CE2	2.52	0.44
3:C:105:LEU:HD12	3:C:105:LEU:N	2.28	0.44
3:C:30:GLN:HG2	3:C:155:LEU:HD13	1.97	0.44
3:C:103:ILE:CD1	3:C:238:ILE:HD11	2.43	0.44
1:A:204:SER:HA	7:A:605:HOH:O	2.16	0.44
3:C:35:ARG:HG3	3:C:35:ARG:O	2.18	0.44
1:A:82:SER:HA	7:A:616:HOH:O	2.17	0.44
3:C:56:ALA:HB3	3:C:102:ASP:HA	1.99	0.44
1:A:284:ILE:O	1:A:408:PHE:HB2	2.17	0.44
3:C:103:ILE:HG21	3:C:234:LEU:HD23	2.00	0.44
1:A:137:SER:OG	1:A:138:SER:N	2.51	0.44
1:A:229:PHE:CE2	1:A:252:MET:CB	3.01	0.44
1:A:105:VAL:HG22	1:A:338:MET:O	2.18	0.44
1:A:229:PHE:O	1:A:377:GLU:HB3	2.17	0.43
1:A:253:TYR:HA	1:A:318:VAL:O	2.18	0.43
1:A:52:SER:C	1:A:54:ALA:N	2.71	0.43
3:C:176:ILE:CG2	3:C:177:THR:N	2.81	0.43
3:C:54:THR:OG1	3:C:55:ALA:N	2.51	0.43
1:A:81:LEU:HD11	1:A:126:LEU:HD21	2.01	0.43
1:A:170:LEU:C	1:A:170:LEU:HD23	2.35	0.43
1:A:241:LYS:HB2	1:A:241:LYS:HE3	1.88	0.43
1:A:350:LYS:C	1:A:352:PRO:CD	2.87	0.43
1:A:345:SER:HA	1:A:346:PRO:HD3	1.86	0.43
3:C:60(G):ASN:HD22	4:C:503:NAG:H83	1.84	0.43
6:C:602:NT2:S81	6:C:602:NT2:H861	2.58	0.43
1:A:112:SER:OG	1:A:115:THR:HB	2.17	0.43
1:A:341:VAL:HG23	1:A:342:ASP:N	2.32	0.43
1:A:6:ASP:O	1:A:10:ALA:HB2	2.19	0.43
3:C:166:PRO:O	3:C:167:VAL:C	2.56	0.43
3:C:98:ASN:ND2	3:C:100:ASP:HB2	2.34	0.43
1:A:11:LYS:O	1:A:14:ASP:N	2.52	0.43
1:A:260:TYR:CG	1:A:261:ARG:N	2.87	0.43
1:A:101:GLN:O	1:A:102:LEU:C	2.55	0.43
2:B:4:ARG:HB2	2:B:7:PHE:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:72:SER:C	3:C:154:VAL:HA	2.38	0.43
3:C:72:SER:O	3:C:154:VAL:CA	2.55	0.43
1:A:223:GLY:HA3	1:A:274:PHE:CE1	2.54	0.42
1:A:304:LEU:O	1:A:304:LEU:HD12	2.19	0.42
1:A:186:ILE:HG21	1:A:202:ILE:HD12	2.01	0.42
1:A:252:MET:CE	1:A:320:MET:HG2	2.50	0.42
1:A:158:TYR:C	1:A:160:ASP:H	2.22	0.42
1:A:360:ASP:CG	1:A:361:ASP:H	2.21	0.42
1:A:274:PHE:HD2	1:A:279:ILE:HG22	1.85	0.42
3:C:74:THR:O	3:C:75:ARG:C	2.58	0.42
1:A:171:GLN:HA	1:A:172:PRO:HD3	1.75	0.42
1:A:87:PHE:CZ	1:A:335:LEU:CD1	3.03	0.42
3:C:17:VAL:HG11	3:C:221:ASP:HB3	2.01	0.42
1:A:350:LYS:O	1:A:352:PRO:HD2	2.19	0.42
3:C:102:ASP:HB3	3:C:229:THR:CG2	2.50	0.42
3:C:202:LYS:HZ1	3:C:205:ASN:HB2	1.83	0.42
1:A:412:ILE:HD12	1:A:422:PHE:HB2	2.01	0.42
3:C:221:ASP:CG	3:C:221:ASP:O	2.58	0.42
3:C:88:ILE:CG2	3:C:89:TYR:N	2.83	0.42
1:A:15:ILE:CG2	1:A:16:PRO:N	2.83	0.42
1:A:293:ALA:HA	1:A:296:GLU:OE1	2.19	0.42
1:A:79:SER:OG	1:A:82:SER:HB2	2.20	0.42
1:A:101:GLN:O	1:A:104:GLU:N	2.52	0.42
1:A:218:THR:O	1:A:219:ILE:HB	2.20	0.42
1:A:343:LEU:HD12	1:A:351:LEU:HD21	2.02	0.41
1:A:154:PHE:HD1	1:A:354:ILE:CG2	2.33	0.41
1:A:405:ASN:OD1	1:A:405:ASN:N	2.53	0.41
3:C:144:LEU:HD13	3:C:150:GLY:O	2.20	0.41
3:C:36:LYS:N	3:C:64:LEU:HA	2.35	0.41
3:C:79:ILE:HG23	3:C:117:TYR:CD2	2.55	0.41
1:A:285:LEU:HA	1:A:286:PRO:HD2	1.93	0.41
1:A:189:TRP:O	1:A:190:VAL:C	2.59	0.41
1:A:342:ASP:OD2	1:A:348:LYS:O	2.38	0.41
1:A:411:PHE:HE1	1:A:423:MET:HE3	1.86	0.41
1:A:186:ILE:C	1:A:188:LYS:N	2.73	0.41
1:A:66:LEU:HD22	1:A:78:LEU:HD13	2.00	0.41
3:C:172:THR:OG1	3:C:173:ARG:N	2.53	0.41
1:A:118:GLN:HA	1:A:120:HIS:CE1	2.55	0.41
1:A:51:LEU:HD11	1:A:119:ILE:HG13	2.02	0.41
1:A:284:ILE:HB	1:A:409:LEU:HB2	2.02	0.41
1:A:412:ILE:HD12	1:A:422:PHE:CB	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:415:VAL:HB	1:A:416:PRO:HD3	2.03	0.41
1:A:425:ARG:HD3	1:A:427:ALA:HB2	2.01	0.41
1:A:66:LEU:HA	1:A:66:LEU:HD12	1.89	0.41
3:C:178:ASP:HB3	3:C:233:ARG:NH1	2.36	0.41
2:B:2:GLY:O	3:C:206:ARG:HA	2.21	0.41
3:C:16:ILE:HD11	3:C:140:GLY:N	2.36	0.41
3:C:230:HIS:CG	3:C:233:ARG:HB2	2.56	0.41
1:A:252:MET:HE1	1:A:375:VAL:HG12	2.01	0.41
1:A:281:MET:CE	1:A:410:VAL:HG13	2.51	0.41
1:A:343:LEU:HG	1:A:364:VAL:HG23	2.03	0.41
1:A:229:PHE:HB3	1:A:377:GLU:HG3	2.01	0.41
3:C:77(A):ARG:O	3:C:78:ASN:HB2	2.21	0.41
1:A:47:ARG:HG2	1:A:47:ARG:NH1	2.36	0.41
1:A:393:ARG:HD3	3:C:191:CYS:O	2.20	0.41
3:C:82:ILE:CG2	3:C:83:SER:N	2.84	0.41
1:A:161:ILE:HG22	1:A:165:VAL:CG1	2.51	0.41
3:C:60(D):TRP:CD1	3:C:60(D):TRP:N	2.88	0.41
3:C:65:LEU:C	3:C:65:LEU:CD1	2.89	0.41
1:A:300:THR:H	1:A:303:VAL:HG12	1.85	0.40
1:A:95:CYS:CB	1:A:352:PRO:HG3	2.49	0.40
3:C:164:GLU:OE2	3:C:164:GLU:N	2.30	0.40
3:C:17:VAL:HG23	3:C:191:CYS:HB2	2.03	0.40
3:C:224:LYS:HB3	3:C:224:LYS:NZ	2.36	0.40
1:A:160:ASP:O	1:A:163:GLU:HB3	2.21	0.40
3:C:185:LYS:HG3	3:C:225:TYR:OH	2.22	0.40
3:C:64:LEU:C	3:C:64:LEU:HD12	2.42	0.40
1:A:103:MET:O	1:A:109:ASP:HB3	2.21	0.40
1:A:115:THR:O	1:A:119:ILE:N	2.55	0.40
2:B:4:ARG:HA	2:B:5:PRO:HD3	1.83	0.40
3:C:85:LEU:HD13	3:C:106:MET:HB3	2.04	0.40
1:A:186:ILE:HG21	1:A:202:ILE:HD11	2.03	0.40
1:A:353:GLY:C	1:A:354:ILE:HG13	2.40	0.40
1:A:125:LYS:NZ	5:A:601:NT1:O3A	2.52	0.40
1:A:147:PHE:HB2	1:A:214:VAL:CG2	2.51	0.40
1:A:229:PHE:HB2	1:A:377:GLU:CB	2.51	0.40
3:C:165:ARG:NH1	3:C:178:ASP:HA	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:378:GLU:O	2:B:11:SER:OG[4_445]	1.94	0.26

## 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	401/432 (93%)	310 (77%)	74 (18%)	17 (4%)	3	19
2	B	30/36 (83%)	25 (83%)	4 (13%)	1 (3%)	4	25
3	C	244/259 (94%)	197 (81%)	40 (16%)	7 (3%)	5	28
All	All	675/727 (93%)	532 (79%)	118 (18%)	25 (4%)	4	22

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	PRO
3	C	38	GLN
1	A	20	MET
1	A	25	SER
1	A	183	ARG
1	A	195	GLU
1	A	219	ILE
1	A	350	LYS
1	A	377	GLU
3	C	73	ARG
1	A	24	ARG
1	A	225	TRP
1	A	298	GLU
3	C	126	ARG
1	A	241	LYS
1	A	247	CYS
1	A	340	LEU
2	B	14(A)	LYS
3	C	41	LEU

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Mol	Chain	Res	Type
3	C	42	CYS
1	A	109	ASP
1	A	232	GLU
3	C	213	VAL
1	A	244	GLY
3	C	166	PRO

### 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	316/383 (82%)	298 (94%)	18 (6%)	24	60
2	B	26/31 (84%)	23 (88%)	3 (12%)	6	27
3	C	206/225 (92%)	180 (87%)	26 (13%)	5	22
All	All	548/639 (86%)	501 (91%)	47 (9%)	12	44

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ARG
1	A	95	CYS
1	A	97	ASP
1	A	99	LEU
1	A	125	LYS
1	A	128	CYS
1	A	135	ASN
1	A	156	GLU
1	A	224	LEU
1	A	227	SER
1	A	302	GLU
1	A	316	LEU
1	A	320	MET
1	A	338	MET
1	A	372	PHE
1	A	396	ASN

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Mol	Chain	Res	Type
1	A	399	ARG
1	A	413	ARG
2	B	12	LEU
2	B	14(D)	ARG
2	B	14(G)	LEU
3	C	27	SER
3	C	33	LEU
3	C	39	GLU
3	C	58	CYS
3	C	60(I)	THR
3	C	62	ASN
3	C	65	LEU
3	C	67	ARG
3	C	70	LYS
3	C	72	SER
3	C	95	ASN
3	C	98	ASN
3	C	105	LEU
3	C	130	LEU
3	C	165	ARG
3	C	172	THR
3	C	186(D)	LYS
3	C	187	ARG
3	C	198	PRO
3	C	205	ASN
3	C	221(A)	ARG
3	C	224	LYS
3	C	228	TYR
3	C	229	THR
3	C	241	VAL
3	C	244	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	101	GLN
1	A	118	GLN
1	A	127	ASN
1	A	171	GLN
1	A	178	ASN
1	A	254	GLN

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Mol	Chain	Res	Type
1	A	319	HIS
1	A	334	GLN
1	A	396	ASN
3	C	38	GLN
3	C	60(G)	ASN
3	C	62	ASN
3	C	78	ASN
3	C	95	ASN
3	C	98	ASN
3	C	143	ASN
3	C	205	ASN
3	C	244	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	NAG	A	501	1	14,14,15	2.60	6 (42%)	15,19,21	2.99	7 (46%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	NAG	A	502	-	14,14,15	3.04	8 (57%)	15,19,21	2.58	6 (40%)
5	NT1	A	601	-	115,117,121	3.11	48 (41%)	150,176,180	2.41	33 (22%)
4	NAG	C	503	-	14,14,15	2.68	8 (57%)	15,19,21	3.08	7 (46%)
6	NT2	C	602	-	11,13,28	2.25	4 (36%)	15,18,45	4.22	9 (60%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	501	1	-	0/6/23/26	0/1/1/1
4	NAG	A	502	-	-	0/6/23/26	0/1/1/1
5	NT1	A	601	-	-	0/87/220/226	0/7/7/7
4	NAG	C	503	-	-	0/6/23/26	0/1/1/1
6	NT2	C	602	-	-	0/2/24/41	0/1/1/1

All (74) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NT1	O64-C63	-6.07	1.26	1.40
5	A	601	NT1	O65-C63	-5.10	1.28	1.40
5	A	601	NT1	O44-C43	-4.68	1.29	1.40
5	A	601	NT1	O45-C43	-4.51	1.30	1.40
5	A	601	NT1	O5G-C5F	-3.76	1.38	1.46
5	A	601	NT1	O5D-S5B	-2.88	1.33	1.45
5	A	601	NT1	O5A-C59	-2.39	1.41	1.46
5	A	601	NT1	O74-C73	-2.24	1.37	1.46
4	C	503	NAG	O4-C4	2.07	1.47	1.43
5	A	601	NT1	O52-C51	2.07	1.49	1.44
5	A	601	NT1	C32-C33	2.10	1.58	1.52
4	A	502	NAG	O3-C3	2.10	1.47	1.43
5	A	601	NT1	C7I-C7C	2.13	1.55	1.51
4	A	502	NAG	C8-C7	2.14	1.55	1.50
5	A	601	NT1	O22-C21	2.16	1.49	1.44
5	A	601	NT1	C23-C21	2.18	1.56	1.51
6	C	602	NT2	C86-C84	2.22	1.59	1.51
6	C	602	NT2	C83-C84	2.24	1.59	1.52
5	A	601	NT1	O34-C33	2.28	1.49	1.44
5	A	601	NT1	C3H-C3E	2.30	1.58	1.52
5	A	601	NT1	O5M-C5L	2.32	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NT1	O7A-C79	2.36	1.49	1.42
4	A	501	NAG	O5-C5	2.38	1.48	1.43
4	A	501	NAG	O5-C1	2.44	1.47	1.43
4	A	502	NAG	O4-C4	2.48	1.48	1.43
4	C	503	NAG	C8-C7	2.49	1.55	1.50
4	C	503	NAG	O5-C1	2.53	1.47	1.43
5	A	601	NT1	C19-C16	2.55	1.59	1.52
4	A	501	NAG	C8-C7	2.60	1.56	1.50
5	A	601	NT1	O12-C11	2.62	1.49	1.44
4	A	502	NAG	C2-N2	2.62	1.50	1.46
4	C	503	NAG	O5-C5	2.74	1.49	1.43
5	A	601	NT1	O52-C5L	2.79	1.48	1.41
5	A	601	NT1	O3I-C40	2.81	1.50	1.43
5	A	601	NT1	O3I-C3H	2.82	1.49	1.41
4	A	502	NAG	O5-C5	2.91	1.49	1.43
5	A	601	NT1	C26-C20	3.02	1.58	1.52
4	A	501	NAG	C4-C3	3.10	1.60	1.52
5	A	601	NT1	O47-C46	3.11	1.51	1.42
5	A	601	NT1	O12-C1C	3.12	1.49	1.41
5	A	601	NT1	O1D-C20	3.13	1.51	1.43
5	A	601	NT1	C50-C51	3.25	1.61	1.52
4	A	501	NAG	C3-C2	3.44	1.60	1.52
4	C	503	NAG	C4-C3	3.51	1.61	1.52
5	A	601	NT1	C2C-C29	3.55	1.61	1.52
5	A	601	NT1	O1A-C1B	3.61	1.55	1.42
4	C	503	NAG	C3-C2	3.70	1.60	1.52
4	C	503	NAG	C1-C2	3.77	1.57	1.52
5	A	601	NT1	C5F-C59	3.94	1.60	1.52
5	A	601	NT1	C49-C46	3.98	1.60	1.52
5	A	601	NT1	C66-C60	4.21	1.61	1.52
6	C	602	NT2	C8O-C8I	4.27	1.61	1.52
6	C	602	NT2	O85-C8O	4.50	1.51	1.43
5	A	601	NT1	O1D-C1C	4.53	1.53	1.41
5	A	601	NT1	C61-C60	4.65	1.62	1.52
4	A	502	NAG	C4-C3	5.05	1.65	1.52
5	A	601	NT1	C10-C11	5.22	1.61	1.51
4	C	503	NAG	C4-C5	5.33	1.64	1.53
5	A	601	NT1	O17-C18	5.41	1.62	1.42
4	A	502	NAG	C4-C5	5.61	1.64	1.53
5	A	601	NT1	C3B-C32	5.79	1.64	1.52
5	A	601	NT1	O2A-C2B	5.88	1.63	1.42
4	A	502	NAG	C1-C2	5.92	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	NT1	O6A-C6B	5.92	1.63	1.42
5	A	601	NT1	O22-C2C	6.35	1.57	1.41
5	A	601	NT1	O3F-C3G	6.42	1.65	1.42
4	A	501	NAG	C4-C5	6.51	1.66	1.53
5	A	601	NT1	C41-C40	6.58	1.66	1.52
5	A	601	NT1	O30-C32	6.69	1.60	1.43
5	A	601	NT1	C46-C40	6.89	1.67	1.52
5	A	601	NT1	O27-C28	7.02	1.67	1.42
5	A	601	NT1	C3E-C3B	7.32	1.67	1.52
5	A	601	NT1	C20-C21	8.47	1.68	1.52
5	A	601	NT1	C29-C26	9.79	1.73	1.52

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	602	NT2	O8D-C8C-C83	-9.76	87.65	109.87
5	A	601	NT1	O30-C2C-C29	-9.19	90.19	109.07
5	A	601	NT1	C23-C21-C20	-7.91	101.17	113.36
5	A	601	NT1	O22-C21-C20	-7.28	95.39	109.14
5	A	601	NT1	O1D-C20-C26	-6.55	90.66	107.50
4	C	503	NAG	O5-C1-C2	-5.84	103.34	111.47
5	A	601	NT1	O22-C2C-C29	-5.81	97.81	109.50
4	A	501	NAG	O5-C1-C2	-5.61	103.66	111.47
5	A	601	NT1	O30-C2C-O22	-5.46	97.44	110.70
6	C	602	NT2	C86-C84-C83	-5.09	99.36	113.24
6	C	602	NT2	C8I-C8C-C83	-3.75	101.84	109.61
5	A	601	NT1	C35-C33-C32	-3.35	104.97	113.30
4	C	503	NAG	O7-C7-C8	-3.28	116.09	122.06
4	A	501	NAG	O7-C7-C8	-3.15	116.33	122.06
5	A	601	NT1	O5M-C5L-C5F	-3.04	102.81	109.07
4	A	502	NAG	O7-C7-C8	-3.04	116.53	122.06
4	A	502	NAG	C3-C4-C5	-2.80	105.28	110.22
5	A	601	NT1	C2C-O30-C32	-2.78	111.23	118.00
4	A	502	NAG	O4-C4-C3	-2.78	104.32	110.36
5	A	601	NT1	C2C-C29-C26	-2.50	105.61	110.74
4	A	501	NAG	O4-C4-C3	-2.48	104.96	110.36
4	C	503	NAG	O4-C4-C3	-2.27	105.41	110.36
5	A	601	NT1	C6C-O6D-C70	-2.15	112.76	118.00
5	A	601	NT1	O36-C35-C33	-2.14	103.57	107.67
5	A	601	NT1	O2A-C29-C26	-2.01	104.10	108.94
5	A	601	NT1	C3H-O3I-C40	2.10	123.11	118.00
4	C	503	NAG	C4-C3-C2	2.18	114.22	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	601	NT1	O47-C46-C40	2.20	114.23	108.94
5	A	601	NT1	C7B-O7A-C79	2.23	120.63	114.54
4	A	501	NAG	C4-C3-C2	2.29	114.38	111.02
5	A	601	NT1	C3D-O3C-C3B	2.43	121.18	114.54
5	A	601	NT1	O5I-S5H-O5K	2.53	117.75	108.79
4	A	501	NAG	C2-N2-C7	2.65	126.81	122.94
6	C	602	NT2	O85-C84-C86	2.81	113.15	106.41
5	A	601	NT1	C48-O47-C46	3.00	122.75	114.54
5	A	601	NT1	O3F-C3E-C3B	3.02	116.22	108.94
4	C	503	NAG	C2-N2-C7	3.07	127.43	122.94
4	A	502	NAG	C8-C7-N2	3.20	121.88	116.11
5	A	601	NT1	O42-C4C-C49	3.21	115.96	109.50
6	C	602	NT2	C8O-C8I-C8C	3.30	116.61	110.65
5	A	601	NT1	C6C-O62-C61	3.34	118.46	113.15
5	A	601	NT1	C26-C20-C21	3.44	115.28	110.36
5	A	601	NT1	O30-C32-C3B	3.59	116.73	107.50
4	A	501	NAG	C8-C7-N2	3.62	122.65	116.11
5	A	601	NT1	O62-C6C-C69	3.64	116.82	109.50
5	A	601	NT1	O34-C33-C35	3.72	114.07	106.64
5	A	601	NT1	O45-C43-O44	3.79	118.26	111.28
4	C	503	NAG	C8-C7-N2	3.79	122.96	116.11
5	A	601	NT1	C3H-O34-C33	4.00	121.26	113.72
5	A	601	NT1	O7D-C7C-C79	4.01	111.27	106.55
6	C	602	NT2	C8O-O85-C84	4.12	120.83	113.39
6	C	602	NT2	C8C-C83-C84	4.53	120.50	110.88
5	A	601	NT1	O22-C21-C23	4.73	116.70	106.69
5	A	601	NT1	O65-C63-O64	5.00	120.48	111.28
4	A	502	NAG	C1-O5-C5	5.25	119.41	112.17
4	A	502	NAG	C2-N2-C7	5.54	131.03	122.94
6	C	602	NT2	O8J-C8I-C8C	5.76	122.89	110.36
6	C	602	NT2	O85-C8O-C8I	6.30	120.49	110.04
5	A	601	NT1	O1D-C20-C21	6.37	123.94	106.72
4	A	501	NAG	C1-O5-C5	7.43	122.40	112.17
4	C	503	NAG	C1-O5-C5	7.62	122.66	112.17
5	A	601	NT1	O1D-C1C-O12	11.93	139.66	110.70

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 26 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	501	NAG	1	0
4	A	502	NAG	5	0
5	A	601	NT1	13	0
4	C	503	NAG	3	0
6	C	602	NT2	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	409/432 (94%)	-0.38	3 (0%) 87 75	34, 67, 98, 116	0
2	B	32/36 (88%)	-0.61	0 100 100	37, 50, 74, 76	0
3	C	248/259 (95%)	-0.47	1 (0%) 92 84	15, 50, 69, 86	0
All	All	689/727 (94%)	-0.43	4 (0%) 89 77	15, 59, 95, 116	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	GLN	2.5
1	A	179	ALA	2.1
3	C	197	GLY	2.0
1	A	85	THR	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

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



Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	NT2	C	602	13/28	0.88	0.23	1.37	115,118,119,120	0
5	NT1	A	601	111/115	0.92	0.18	-0.21	67,82,114,116	0
4	NAG	A	502	14/15	0.77	0.21	-	125,127,128,129	0
4	NAG	A	501	14/15	0.83	0.32	-	103,105,105,105	0
4	NAG	C	503	14/15	0.83	0.26	-	101,104,105,105	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.