Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:38 AM GMT

PDB ID	:	2B5T
Title	:	2.1 Angstrom structure of a nonproductive complex between antithrombin, synthetic heparin mimetic SR123781 and two S195A thrombin molecules
Authors	:	Johnson, D.J.; Li, W.; Luis, S.A.; Carrell, R.W.; Huntington, J.A.
Deposited on	:	2005-09-29
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 ①) were used in the production of this report:

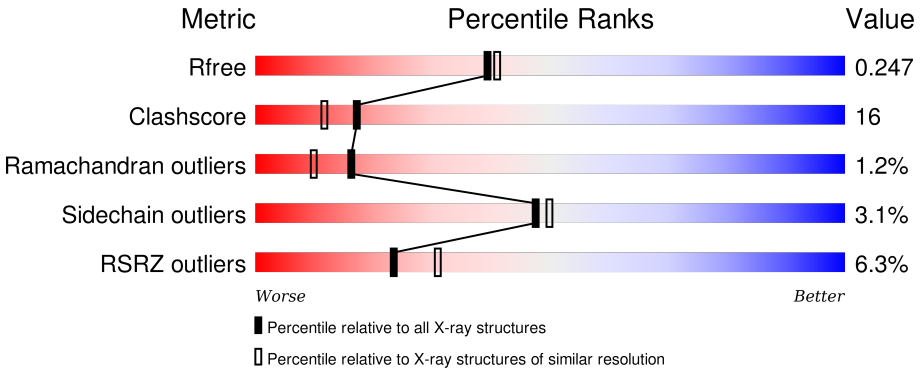
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (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))
R_{free}	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (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.

Mol	Chain	Length	Quality of chain
1	A	49	4% 65% 31% ·
1	C	49	6% 80% 14% 6%
2	B	259	3% 75% 20% · ·
2	D	259	5% 78% 19% ·
3	I	432	8% 60% 33% · ·

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
4	GOL	A	1102	-	-	X	X
4	GOL	A	1108	-	-	-	X
4	GOL	B	1101	-	-	-	X
4	GOL	B	1103	-	-	X	X
4	GOL	B	1105	-	-	-	X
4	GOL	B	1109	-	-	-	X
4	GOL	D	1110	-	-	-	X
4	GOL	D	1111	-	-	-	X
4	GOL	I	1112	-	-	-	X
5	NAG	B	501	-	-	X	-
5	FUC	B	602	-	-	X	-
6	SO4	B	2003	-	-	-	X
7	NDG	D	501	-	-	-	X
8	GU6	I	434	X	-	-	-
8	GU8	I	437	-	-	X	-
9	NDG	I	501	-	-	X	-
9	MAN	I	703	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 9026 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 Thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	47	Total	C	N	O	S	0	1	0
			394	245	65	83	1			
1	C	46	Total	C	N	O	S	0	0	0
			372	233	60	78	1			

- Molecule 2 is a protein called Thrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	252	Total	C	N	O	S	0	3	0
			2065	1317	368	366	14			
2	D	252	Total	C	N	O	S	0	0	0
			2022	1290	353	365	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	195	ALA	SER	ENGINEERED	UNP P00734
D	195	ALA	SER	ENGINEERED	UNP P00734

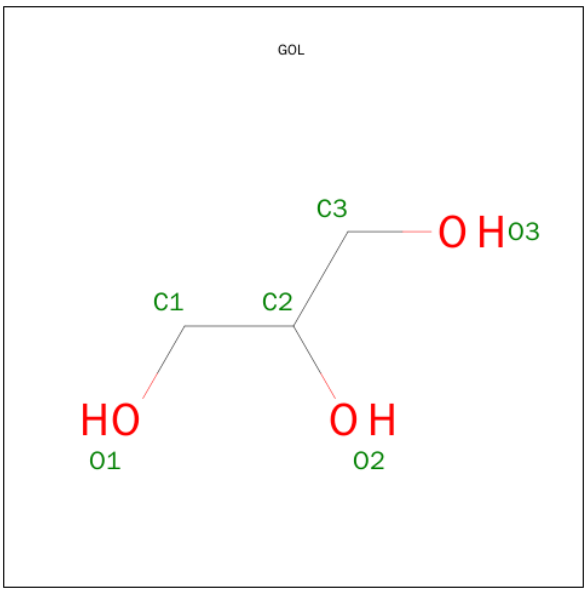
- Molecule 3 is a protein called Antithrombin-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	415	Total	C	N	O	S	0	0	0
			3233	2065	540	609	19			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	137	ALA	SER	ENGINEERED	UNP P01008
I	317	CYS	VAL	ENGINEERED	UNP P01008
I	401	CYS	THR	ENGINEERED	UNP P01008

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

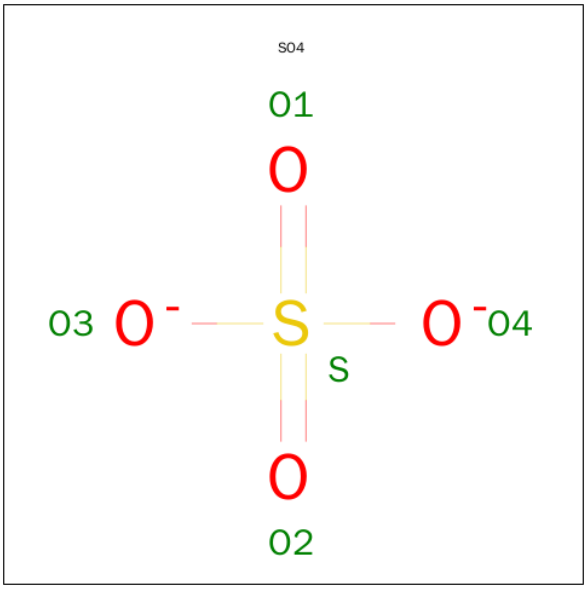


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	D	1	Total C O 6 3 3	0	0
4	I	1	Total C O 6 3 3	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	2	Total C N O 24 14 1 9	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	B	1	Total O S 5 4 1	0	0
6	D	1	Total O S 5 4 1	0	0
6	I	1	Total O S 5 4 1	0	0

- Molecule 7 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	2	Total C N O 24 14 1 9	0	0

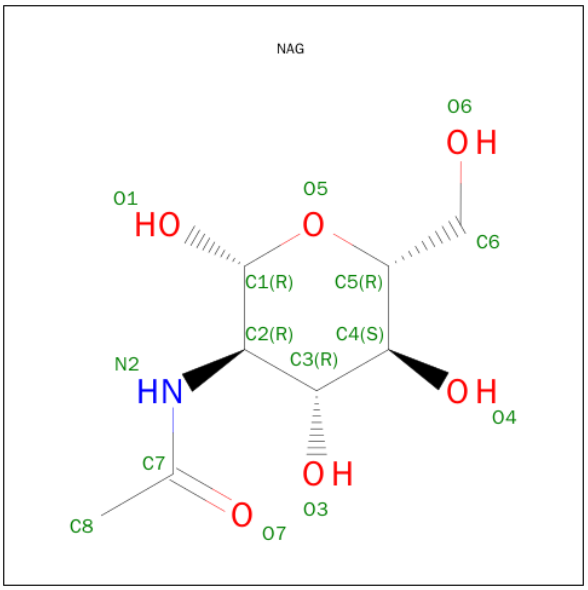
- Molecule 8 is a polymer of unknown type called SUGAR (16-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	I	16	Total	C	O	S	0	0
			278	127	134	17		

- Molecule 9 is a polymer of unknown type called SUGAR (7-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	I	7	Total	C	N	O	0	0
			81	46	2	33		

- Molecule 10 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	I	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 11 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	I	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	29	Total	O	0	0
			29	29		

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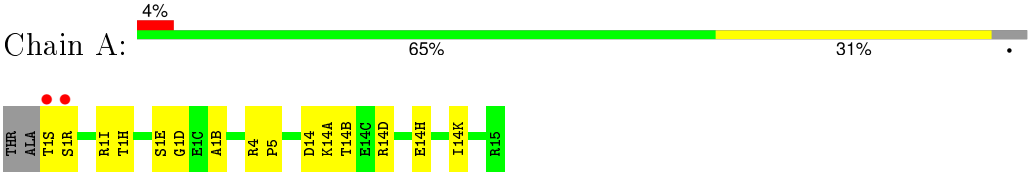
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	B	132	Total O 132 132	0	0
12	C	24	Total O 24 24	0	0
12	D	117	Total O 117 117	0	0
12	I	87	Total O 87 87	0	0

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 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.

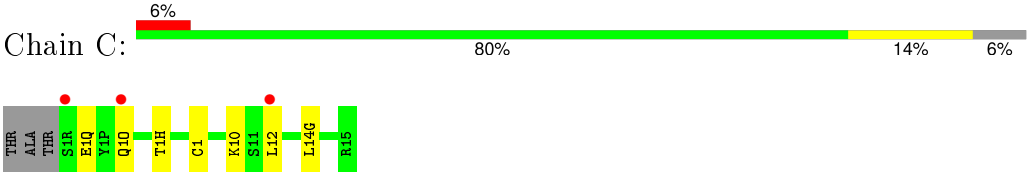
- Molecule 1: Thrombin

Chain A:



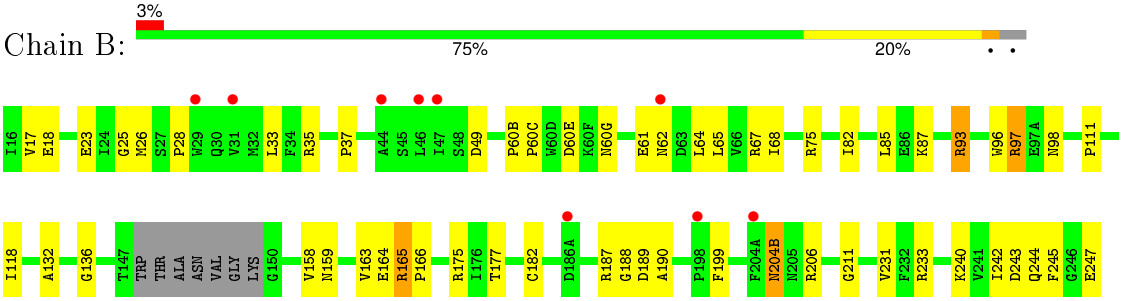
- Molecule 1: Thrombin

Chain C:



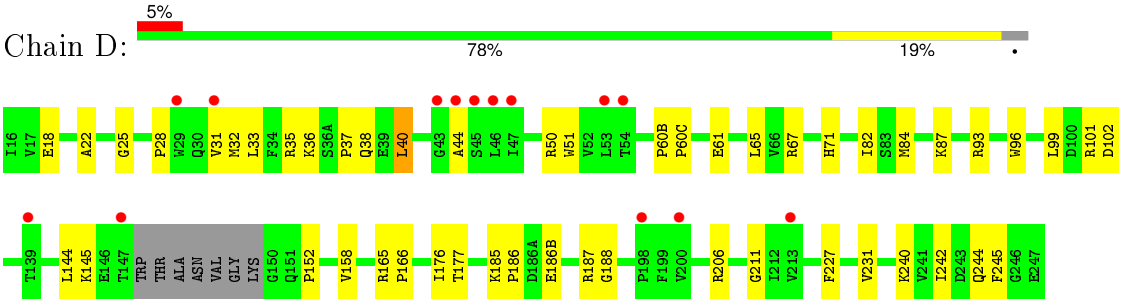
- Molecule 2: Thrombin

Chain B:



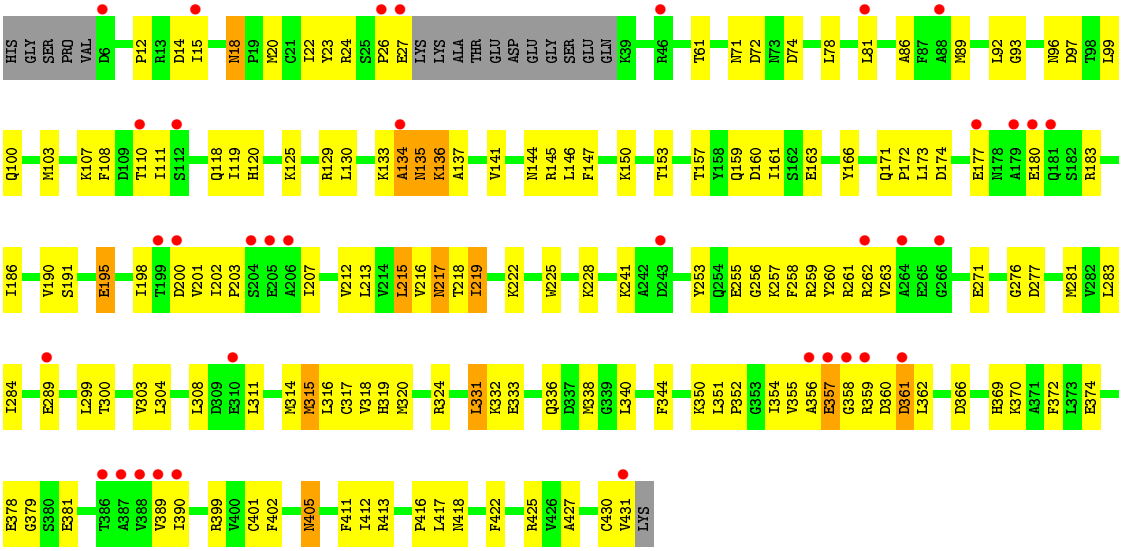
- Molecule 2: Thrombin

Chain D:



- Molecule 3: Antithrombin-III

Chain I:


HIS GLY SER PRO VAL D6 P12 R13 D14 I15 N18 P19 M20 C21 I22 Y23 R24 S25 P26 E27 LYS LYS ALA THR GLU ASP GLU GLY SER GLU GLN K39 R46 T61 N71 D72 N73 D74 L78 L81 A86 F87 A88 M89 L92 G93 N96 D97 T98 L99
Q100 M103 K107 F108 D109 T110 I111 S112 Q118 I119 H120 K125 R129 L130 K133 A134 N135 K136 A137 V141 N144 R145 L146 F147 K150 T153 T157 Y158 Q159 D160 I161 S162 E163 Y166 Q171 P172 L173 D174 E177 N178 A179 E180 Q181 S182 R183
I186 V190 S191 E195 I198 T199 D200 V201 I202 P203 S204 E205 A206 I207 V212 L213 V214 L215 V216 N217 T218 I219 K222 W225 K228 K241 A242 D243 Y253 Q254 E255 G256 K257 F258 R259 Y260 R261 R262 V263 A264 E265 G266 E271 G276 D277 M281 V282 L283
I284 E289 L299 T300 V303 L304 L308 D309 E310 L311 M314 M315 L316 C317 V318 H319 M320 R324 I331 K332 E333 Q336 D337 M338 G339 L340 F344 K350 L351 P352 G353 I354 V355 A356 E357 G358 R359 D360 D361 I362 D366 H369 K370 A371 F372 L373 E374
E378 G379 S380 E381 T386 A387 V388 V389 I390 R399 V400 C401 F402 N405 F411 I412 R413 P416 L417 N418 F422 R425 V426 A427 C430 V431 LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	59.28Å 59.53Å 108.41Å 77.55° 78.94° 68.08°	Depositor
Resolution (Å)	35.70 – 2.10 35.72 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (35.70-2.10) 87.4 (35.72-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.209 , 0.247 0.210 , 0.247	Depositor DCC
R_{free} test set	2937 reflections (4.08%)	DCC
Wilson B-factor (Å^2)	33.6	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 60.9	EDS
Estimated twinning fraction	0.014 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 71924 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9026	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, BMA, NAG, NDG, GU3, GU2, GU1, GU0, SO4, GU5, GU4, GU9, GU8, GU6, FUC, 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	0.40	0/401	0.66	0/535
1	C	0.42	0/379	0.66	0/506
2	B	0.36	0/2118	0.66	0/2859
2	D	0.35	0/2074	0.64	0/2805
3	I	0.39	0/3299	0.65	2/4470 (0.0%)
All	All	0.38	0/8271	0.65	2/11175 (0.0%)

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
8	I	1	0

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	402	PHE	N-CA-C	-5.51	96.14	111.00
3	I	360	ASP	N-CA-C	-5.47	96.24	111.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	I	434	GU6	C5

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	394	0	369	15	0
1	C	372	0	346	5	0
2	B	2065	0	2030	52	0
2	D	2022	0	1965	36	0
3	I	3233	0	3143	124	0
4	A	12	0	16	5	0
4	B	30	0	40	4	0
4	D	24	0	32	4	0
4	I	6	0	8	2	0
5	B	24	0	22	8	0
6	B	20	0	0	2	0
6	D	5	0	0	0	0
6	I	5	0	0	0	0
7	D	24	0	22	4	0
8	I	278	0	193	36	0
9	I	81	0	68	8	0
10	I	14	0	13	0	0
11	I	28	0	25	1	0
12	A	29	0	0	0	0
12	B	132	0	0	0	0
12	C	24	0	0	0	0
12	D	117	0	0	1	0
12	I	87	0	0	4	0
All	All	9026	0	8292	274	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (274) 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)
2:B:93[A]:ARG:HB3	2:B:93[A]:ARG:HH11	1.09	1.14
3:I:129:ARG:HD3	3:I:417:LEU:HD11	1.35	1.03
3:I:358:GLY:HA2	3:I:361:ASP:OD1	1.66	0.94
2:D:18:GLU:HG3	2:D:187:ARG:HG3	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:361:ASP:HB3	12:I:2052:HOH:O	1.68	0.92
3:I:319:HIS:HE1	3:I:399:ARG:HE	1.19	0.90
3:I:283:LEU:HD11	3:I:320:MET:HE1	1.52	0.88
9:I:501:NDG:H6C1	9:I:602:FUC:H5	1.59	0.82
3:I:107:LYS:O	3:I:110:THR:HG22	1.80	0.80
1:A:1(B):ALA:HB3	4:A:1102:GOL:H32	1.63	0.80
2:B:93[A]:ARG:NH1	2:B:93[A]:ARG:HB3	1.94	0.80
3:I:26:PRO:O	3:I:27:GLU:HB2	1.80	0.80
7:D:501:NDG:H6C2	7:D:602:FUC:H3	1.64	0.79
2:B:93[A]:ARG:CB	2:B:93[A]:ARG:HH11	1.94	0.78
5:B:501:NAG:H62	5:B:602:FUC:H3	1.66	0.77
2:D:35:ARG:HD2	2:D:37:PRO:O	1.85	0.76
3:I:355:VAL:HG12	3:I:362:LEU:HD22	1.68	0.75
3:I:129:ARG:CD	3:I:417:LEU:HD11	2.15	0.74
3:I:405:ASN:H	3:I:405:ASN:HD22	1.35	0.74
1:A:1(D):GLY:H	4:A:1102:GOL:H2	1.53	0.74
3:I:134:ALA:C	3:I:136:LYS:H	1.91	0.73
3:I:281:MET:HE3	3:I:283:LEU:HD21	1.70	0.73
3:I:217:ASN:H	3:I:217:ASN:HD22	1.35	0.72
2:D:240:LYS:HE2	4:D:1106:GOL:O1	1.90	0.71
2:D:61:GLU:HG2	2:D:87:LYS:HA	1.71	0.71
3:I:135:ASN:O	3:I:137:ALA:N	2.24	0.70
2:B:159:ASN:H	4:B:1103:GOL:H31	1.58	0.69
3:I:324:ARG:HH22	4:I:1112:GOL:H11	1.58	0.68
2:D:61:GLU:H	2:D:61:GLU:CD	1.97	0.68
3:I:283:LEU:HD11	3:I:320:MET:CE	2.23	0.66
2:D:240:LYS:HD2	8:I:433:GU4:O25	1.94	0.66
2:D:61:GLU:CG	2:D:87:LYS:HA	2.25	0.66
5:B:501:NAG:H62	5:B:602:FUC:H5	1.77	0.65
8:I:438:GU9:H1	8:I:439:GU8:O3	1.97	0.64
3:I:356:ALA:O	3:I:357:GLU:HB2	1.96	0.64
3:I:257:LYS:HA	3:I:314:MET:O	1.98	0.64
3:I:222:LYS:HG2	3:I:381:GLU:HB3	1.79	0.63
2:D:158:VAL:HA	4:D:1110:GOL:H2	1.79	0.63
2:B:60(G):ASN:HD22	5:B:501:NAG:H61	1.64	0.63
2:B:65:LEU:HD21	2:B:82:ILE:HD13	1.80	0.62
11:I:901:NAG:H62	11:I:902:NAG:O7	1.99	0.62
2:B:97:ARG:HH11	2:B:97:ARG:HG3	1.64	0.62
1:A:14(A):LYS:HG3	1:A:14(B):THR:HG23	1.80	0.62
3:I:284:ILE:HD12	3:I:284:ILE:N	2.15	0.62
3:I:300:THR:OG1	3:I:303:VAL:HG23	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:125:LYS:HE2	12:I:2033:HOH:O	2.00	0.62
3:I:96:ASN:ND2	9:I:501:NDG:H8C1	2.15	0.62
3:I:12:PRO:HG2	8:I:446:GU6:O17	1.98	0.62
2:B:158:VAL:HA	4:B:1103:GOL:H31	1.82	0.61
8:I:436:GU5:H5	8:I:437:GU8:H62	1.82	0.61
3:I:198:ILE:HD11	3:I:372:PHE:HE2	1.66	0.61
5:B:501:NAG:H62	5:B:602:FUC:C3	2.30	0.61
3:I:157:THR:O	3:I:161:ILE:HG13	1.99	0.61
3:I:135:ASN:C	3:I:137:ALA:H	2.03	0.61
3:I:174:ASP:OD2	3:I:177:GLU:HB2	2.01	0.61
2:D:177:THR:HA	4:D:1111:GOL:H2	1.83	0.61
8:I:441:GU8:H1	8:I:442:GU9:H92	1.83	0.60
2:B:61:GLU:CD	2:B:61:GLU:H	2.04	0.60
2:D:36:LYS:HE2	2:D:65:LEU:HD13	1.83	0.60
2:B:132:ALA:CB	2:B:164:GLU:HG3	2.31	0.60
8:I:440:GU9:H1	8:I:441:GU8:C8	2.32	0.60
1:A:1(D):GLY:H	4:A:1102:GOL:C2	2.15	0.59
3:I:258:PHE:HB2	3:I:316:LEU:HD21	1.85	0.59
8:I:440:GU9:H1	8:I:441:GU8:H82	1.84	0.58
9:I:501:NDG:C6	9:I:602:FUC:H5	2.32	0.58
2:B:35:ARG:HD2	2:B:37:PRO:O	2.04	0.58
3:I:389:VAL:HG12	3:I:390:ILE:N	2.19	0.58
3:I:217:ASN:N	3:I:217:ASN:HD22	2.00	0.57
9:I:501:NDG:H6C2	9:I:602:FUC:H3	1.86	0.57
7:D:501:NDG:H6C2	7:D:602:FUC:C3	2.34	0.57
2:B:165:ARG:HD2	6:B:2002:SO4:O1	2.04	0.57
3:I:22:ILE:HD12	3:I:24:ARG:NH2	2.19	0.57
2:B:17:VAL:HG12	2:B:18:GLU:HG2	1.87	0.57
2:D:18:GLU:HB2	2:D:188:GLY:HA2	1.87	0.56
8:I:437:GU8:H72	8:I:437:GU8:C8	2.36	0.56
8:I:442:GU9:C4	8:I:442:GU9:H92	2.34	0.56
2:B:165:ARG:NH1	2:B:177:THR:O	2.39	0.56
8:I:448:GU3:O2	8:I:448:GU3:H8A	2.04	0.56
2:B:25:GLY:O	2:B:28:PRO:HD3	2.05	0.56
2:D:65:LEU:HD11	2:D:84:MET:SD	2.45	0.56
8:I:437:GU8:O2	8:I:438:GU9:H62	2.06	0.56
2:D:65:LEU:HD11	2:D:84:MET:CE	2.36	0.56
8:I:441:GU8:H1	8:I:442:GU9:C9	2.36	0.56
8:I:436:GU5:O1	8:I:436:GU5:H72	2.06	0.55
3:I:119:ILE:CG2	3:I:120:HIS:N	2.70	0.55
3:I:153:THR:O	3:I:355:VAL:HG23	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:GLU:CG	2:B:87:LYS:HA	2.38	0.54
1:A:1(S):THR:HG22	1:A:1(R):SER:N	2.21	0.54
3:I:222:LYS:HG2	3:I:381:GLU:CB	2.38	0.54
8:I:445:GU1:O2	8:I:445:GU1:H82	2.08	0.54
2:B:189:ASP:OD1	2:B:190:ALA:N	2.41	0.54
1:A:14(H):GLU:O	1:A:14(K):ILE:HG13	2.07	0.54
3:I:354:ILE:HD12	3:I:354:ILE:N	2.22	0.54
3:I:89:MET:HA	3:I:166:TYR:OH	2.07	0.54
2:D:144:LEU:HD21	2:D:152:PRO:HB3	1.90	0.53
2:B:60(G):ASN:ND2	5:B:501:NAG:H61	2.23	0.53
2:B:240:LYS:NZ	8:I:435:GU0:O3	2.41	0.53
3:I:405:ASN:ND2	3:I:405:ASN:H	2.05	0.53
3:I:324:ARG:NH2	4:I:1112:GOL:H11	2.24	0.53
3:I:350:LYS:C	3:I:352:PRO:HD3	2.29	0.53
9:I:501:NDG:H6C1	9:I:602:FUC:C5	2.34	0.53
2:D:176:ILE:HD12	2:D:227:PHE:CE2	2.42	0.53
3:I:183:ARG:HE	3:I:203:PRO:C	2.13	0.52
8:I:439:GU8:O1	8:I:440:GU9:H83	2.09	0.52
3:I:412:ILE:HB	3:I:422:PHE:HB2	1.90	0.52
2:B:204(B):ASN:ND2	2:B:206:ARG:H	2.07	0.52
8:I:436:GU5:H1	8:I:437:GU8:C8	2.39	0.52
8:I:442:GU9:O1	8:I:442:GU9:H72	2.09	0.52
3:I:99:LEU:O	3:I:103:MET:HG2	2.10	0.52
3:I:89:MET:HE3	3:I:166:TYR:HB3	1.92	0.51
3:I:425:ARG:HD3	3:I:427:ALA:HB2	1.92	0.51
3:I:133:LYS:O	3:I:135:ASN:N	2.43	0.51
2:B:211:GLY:HA2	2:B:231:VAL:HG23	1.92	0.51
3:I:319:HIS:CE1	3:I:399:ARG:HE	2.11	0.51
3:I:201:VAL:HG23	12:I:2040:HOH:O	2.09	0.51
3:I:332:LYS:HG3	3:I:344:PHE:CE1	2.45	0.51
7:D:501:NDG:C6	7:D:602:FUC:H5	2.40	0.51
8:I:442:GU9:H1	8:I:443:GU8:C8	2.40	0.51
3:I:417:LEU:O	3:I:418:ASN:HB2	2.10	0.51
3:I:81:LEU:HD21	3:I:130:LEU:CD1	2.41	0.51
3:I:405:ASN:N	3:I:405:ASN:HD22	1.99	0.50
3:I:261:ARG:HD3	3:I:262:ARG:N	2.27	0.50
8:I:446:GU6:H1	8:I:446:GU6:O14	2.11	0.50
2:B:204(B):ASN:HD22	2:B:204(B):ASN:C	2.15	0.50
2:B:64:LEU:HB2	2:B:85:LEU:HD12	1.93	0.50
5:B:501:NAG:H62	5:B:602:FUC:C5	2.40	0.50
3:I:23:TYR:O	3:I:24:ARG:HD3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:351:LEU:N	3:I:352:PRO:HD3	2.27	0.50
8:I:442:GU9:H1	8:I:443:GU8:H82	1.94	0.50
3:I:190:VAL:HG21	3:I:201:VAL:HG21	1.94	0.50
3:I:430:CYS:O	3:I:431:VAL:HB	2.12	0.50
3:I:93:GLY:HA3	3:I:354:ILE:CD1	2.42	0.49
2:D:60(B):PRO:HD2	2:D:96:TRP:CD2	2.46	0.49
2:B:68:ILE:HG22	2:B:118:ILE:HG12	1.93	0.49
8:I:445:GU1:O1	8:I:445:GU1:H73	2.12	0.49
2:D:31:VAL:HB	2:D:44:ALA:HB3	1.94	0.49
5:B:501:NAG:C6	5:B:602:FUC:H5	2.40	0.49
2:B:165:ARG:HB3	2:B:166:PRO:HD3	1.93	0.49
3:I:253:TYR:HA	3:I:318:VAL:O	2.12	0.49
3:I:271:GLU:OE2	3:I:413:ARG:NH1	2.39	0.49
3:I:89:MET:HG2	3:I:166:TYR:CZ	2.48	0.49
3:I:186:ILE:HG21	3:I:202:ILE:CD1	2.43	0.49
3:I:186:ILE:HD12	3:I:207:ILE:HD11	1.93	0.49
2:B:98:ASN:HD21	2:B:175:ARG:NH2	2.10	0.49
3:I:20:MET:SD	3:I:352:PRO:HB2	2.53	0.48
2:B:247:GLU:OE1	3:I:228:LYS:NZ	2.46	0.48
2:D:67:ARG:HG2	2:D:82:ILE:HG12	1.94	0.48
8:I:436:GU5:H1	8:I:437:GU8:H82	1.94	0.48
2:D:99:LEU:O	2:D:102:ASP:HB2	2.13	0.48
3:I:198:ILE:HD11	3:I:372:PHE:CE2	2.48	0.48
2:D:144:LEU:O	2:D:145:LYS:HG3	2.13	0.48
3:I:134:ALA:C	3:I:136:LYS:N	2.62	0.48
3:I:228:LYS:NZ	3:I:378:GLU:OE1	2.43	0.48
1:A:1(S):THR:HG22	1:A:1(R):SER:H	1.78	0.48
3:I:355:VAL:CG1	3:I:362:LEU:HB2	2.44	0.48
2:D:65:LEU:CD1	2:D:84:MET:SD	3.01	0.48
3:I:332:LYS:HG3	3:I:344:PHE:CD1	2.48	0.48
3:I:134:ALA:O	3:I:136:LYS:N	2.43	0.48
3:I:108:PHE:O	3:I:111:ILE:HG12	2.14	0.48
1:A:14:ASP:HB2	2:B:23:GLU:OE2	2.14	0.47
1:C:1:CYS:O	2:D:206:ARG:HD3	2.14	0.47
2:D:35:ARG:O	2:D:38:GLN:HA	2.15	0.47
3:I:191:SER:O	3:I:195:GLU:HA	2.14	0.47
3:I:319:HIS:HE1	3:I:399:ARG:NE	2.01	0.47
2:D:25:GLY:O	2:D:28:PRO:HD3	2.14	0.47
3:I:276:GLY:O	3:I:277:ASP:HB2	2.15	0.47
1:A:1(E):SER:HB2	4:A:1102:GOL:O2	2.14	0.47
2:D:185:LYS:HB2	2:D:186(B):GLU:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:146:LEU:N	3:I:146:LEU:HD12	2.30	0.47
3:I:283:LEU:C	3:I:284:ILE:HD12	2.35	0.47
3:I:218:THR:HG22	3:I:370:LYS:HB3	1.97	0.47
3:I:259:ARG:HH12	3:I:311:LEU:HB2	1.79	0.46
3:I:260:TYR:CG	3:I:261:ARG:N	2.83	0.46
2:B:65:LEU:HD11	2:B:82:ILE:CG2	2.45	0.46
1:A:1(R):SER:OG	2:B:206:ARG:NE	2.44	0.46
3:I:146:LEU:HG	3:I:215:LEU:HD22	1.98	0.46
5:B:501:NAG:H4	5:B:602:FUC:H3	1.98	0.46
3:I:261:ARG:HG3	3:I:263:VAL:HG13	1.96	0.46
3:I:186:ILE:HG21	3:I:202:ILE:HD11	1.96	0.46
3:I:225:TRP:NE1	3:I:379:GLY:HA2	2.31	0.46
3:I:336:GLN:HA	3:I:340:LEU:O	2.15	0.46
8:I:439:GU8:H1	8:I:440:GU9:C6	2.46	0.46
3:I:86:ALA:O	3:I:89:MET:HB2	2.15	0.46
2:B:61:GLU:HG2	2:B:87:LYS:HA	1.98	0.45
3:I:23:TYR:CE2	3:I:100:GLN:HG3	2.51	0.45
8:I:438:GU9:H72	8:I:438:GU9:O3	2.15	0.45
3:I:331:LEU:HB2	3:I:369:HIS:CD2	2.52	0.45
3:I:93:GLY:HA3	3:I:354:ILE:HD12	1.98	0.45
2:B:60(B):PRO:HB2	2:B:96:TRP:CZ3	2.52	0.45
1:A:1(H):THR:HB	2:B:242:ILE:O	2.16	0.45
1:A:1(D):GLY:N	4:A:1102:GOL:H2	2.27	0.45
2:B:132:ALA:HB2	2:B:164:GLU:HG3	1.97	0.45
3:I:190:VAL:HG11	3:I:201:VAL:CG2	2.47	0.45
3:I:357:GLU:HB3	3:I:358:GLY:H	1.47	0.45
9:I:501:NDG:C6	9:I:602:FUC:C5	2.95	0.45
8:I:437:GU8:H72	8:I:437:GU8:H83	1.99	0.45
8:I:439:GU8:C8	8:I:439:GU8:H72	2.48	0.45
2:D:22:ALA:O	2:D:71:HIS:HE1	2.00	0.45
3:I:389:VAL:CG1	3:I:390:ILE:N	2.80	0.44
2:B:60(C):PRO:HD3	2:B:96:TRP:CZ3	2.51	0.44
3:I:18:ASN:HD22	3:I:118:GLN:HE22	1.66	0.44
1:C:10:LYS:O	1:C:12:LEU:HG	2.17	0.44
7:D:501:NDG:H6C2	7:D:602:FUC:H5	1.99	0.44
9:I:501:NDG:O4	9:I:502:NAG:H82	2.18	0.44
3:I:355:VAL:HG11	3:I:362:LEU:HB2	2.00	0.44
1:C:14(G):LEU:H	1:C:14(G):LEU:HD22	1.82	0.44
8:I:441:GU8:H73	8:I:441:GU8:O1	2.17	0.43
2:D:211:GLY:HA2	2:D:231:VAL:HG23	1.99	0.43
8:I:437:GU8:C7	8:I:437:GU8:H83	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:218:THR:O	3:I:219:ILE:HB	2.18	0.43
3:I:160:ASP:O	3:I:163:GLU:HB3	2.18	0.43
2:D:165:ARG:HB3	2:D:166:PRO:HD3	1.99	0.43
2:D:87:LYS:HD2	12:D:2095:HOH:O	2.17	0.43
2:B:67:ARG:HG2	2:B:82:ILE:HG12	2.01	0.43
3:I:119:ILE:HG23	3:I:120:HIS:N	2.32	0.43
8:I:444:GU5:H82	8:I:444:GU5:O2	2.18	0.43
3:I:256:GLY:HA2	3:I:315:MET:CE	2.49	0.43
8:I:437:GU8:H72	8:I:437:GU8:O3	2.19	0.43
1:A:1(I):ARG:HH12	3:I:228:LYS:HZ3	1.66	0.43
2:D:165:ARG:NH1	4:D:1107:GOL:H12	2.33	0.43
3:I:171:GLN:HA	3:I:172:PRO:HD3	1.85	0.43
2:B:244:GLN:HG3	2:B:245:PHE:CE2	2.54	0.43
3:I:61:THR:HG22	3:I:338:MET:HE3	1.99	0.43
3:I:14:ASP:C	3:I:15:ILE:HG13	2.39	0.43
2:B:18:GLU:HB2	2:B:188:GLY:HA2	2.00	0.43
1:A:14(D):ARG:O	1:A:14(H):GLU:HG2	2.19	0.43
2:B:75:ARG:CZ	6:B:2006:SO4:O3	2.66	0.43
8:I:440:GU9:H5	8:I:441:GU8:H62	2.00	0.43
1:C:1(Q):GLU:H	1:C:1(Q):GLU:HG2	1.68	0.43
3:I:26:PRO:O	3:I:27:GLU:CB	2.60	0.43
3:I:180:GLU:O	3:I:183:ARG:HB3	2.18	0.43
2:B:18:GLU:HG3	2:B:187:ARG:HG3	2.01	0.42
2:B:60(B):PRO:O	2:B:60(E):ASP:N	2.37	0.42
3:I:299:LEU:HD21	3:I:411:PHE:HZ	1.83	0.42
2:B:93[B]:ARG:NH2	8:I:433:GU4:O4	2.52	0.42
2:D:32:MET:CG	2:D:40:LEU:HD22	2.50	0.42
8:I:448:GU3:O2	8:I:448:GU3:H7A	2.19	0.42
3:I:71:ASN:HB3	3:I:74:ASP:OD2	2.20	0.42
3:I:281:MET:HE3	3:I:320:MET:HE1	2.02	0.42
3:I:96:ASN:HD22	9:I:501:NDG:H8C1	1.82	0.42
2:B:204(B):ASN:HD22	2:B:206:ARG:H	1.67	0.42
3:I:399:ARG:HD2	3:I:401:CYS:SG	2.59	0.42
2:B:49:ASP:O	2:B:111:PRO:HA	2.20	0.42
2:B:159:ASN:H	4:B:1103:GOL:C3	2.28	0.41
3:I:89:MET:HG2	3:I:166:TYR:CE1	2.56	0.41
3:I:304:LEU:O	3:I:308:LEU:HG	2.21	0.41
3:I:255:GLU:CG	3:I:317:CYS:HB3	2.50	0.41
3:I:120:HIS:H	3:I:120:HIS:CD2	2.38	0.41
2:D:60(C):PRO:HD3	2:D:96:TRP:CE3	2.56	0.41
3:I:144:ASN:O	3:I:145:ARG:HB2	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:I:444:GU5:H5	8:I:445:GU1:C6	2.50	0.41
2:B:98:ASN:ND2	2:B:175:ARG:NH2	2.68	0.41
3:I:150:LYS:N	3:I:173:LEU:O	2.53	0.41
2:B:97:ARG:HG3	2:B:97:ARG:NH1	2.34	0.41
3:I:144:ASN:HA	3:I:216:VAL:O	2.21	0.41
2:B:136:GLY:HA3	2:B:199:PHE:CE1	2.56	0.41
3:I:405:ASN:ND2	3:I:405:ASN:N	2.67	0.41
3:I:159:GLN:HA	3:I:159:GLN:OE1	2.21	0.41
1:C:1(H):THR:HB	2:D:242:ILE:O	2.20	0.41
3:I:147:PHE:O	3:I:213:LEU:HD12	2.21	0.41
2:B:23:GLU:OE2	2:B:26:MET:HE3	2.20	0.41
2:D:185:LYS:HB3	2:D:186:PRO:HD2	2.03	0.41
2:B:60(B):PRO:HB2	2:B:60(C):PRO:HD3	2.01	0.41
3:I:61:THR:HG22	3:I:338:MET:CE	2.51	0.41
1:A:4:ARG:HA	1:A:5:PRO:HD3	1.92	0.41
8:I:438:GU9:H1	8:I:439:GU8:C8	2.51	0.40
3:I:157:THR:HG22	3:I:161:ILE:HD11	2.02	0.40
2:D:244:GLN:HG3	2:D:245:PHE:CD2	2.56	0.40
3:I:319:HIS:HD2	12:I:2019:HOH:O	2.02	0.40
2:D:50:ARG:HG3	2:D:51:TRP:CD1	2.57	0.40
2:B:159:ASN:N	4:B:1103:GOL:H31	2.32	0.40
3:I:317:CYS:O	3:I:401:CYS:HB3	2.21	0.40
2:B:163:VAL:HB	2:B:182:CYS:SG	2.61	0.40
3:I:324:ARG:HH11	3:I:374:GLU:HB2	1.87	0.40

There are no symmetry-related clashes.

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	46/49 (94%)	45 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	44/49 (90%)	42 (96%)	2 (4%)	0	100	100
2	B	251/259 (97%)	244 (97%)	7 (3%)	0	100	100
2	D	248/259 (96%)	239 (96%)	9 (4%)	0	100	100
3	I	411/432 (95%)	378 (92%)	21 (5%)	12 (3%)	6	2
All	All	1000/1048 (95%)	948 (95%)	40 (4%)	12 (1%)	16	10

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	I	134	ALA
3	I	136	LYS
3	I	195	GLU
3	I	241	LYS
3	I	357	GLU
3	I	359	ARG
3	I	18	ASN
3	I	72	ASP
3	I	289	GLU
3	I	92	LEU
3	I	135	ASN
3	I	219	ILE

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	43/43 (100%)	43 (100%)	0	100	100
1	C	40/43 (93%)	39 (98%)	1 (2%)	55	59
2	B	220/224 (98%)	210 (96%)	10 (4%)	34	32
2	D	214/224 (96%)	210 (98%)	4 (2%)	65	70
3	I	345/382 (90%)	331 (96%)	14 (4%)	37	36
All	All	862/916 (94%)	833 (97%)	29 (3%)	47	45

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	33	LEU
2	B	62	ASN
2	B	93[A]	ARG
2	B	93[B]	ARG
2	B	97	ARG
2	B	165	ARG
2	B	204(B)	ASN
2	B	233[A]	ARG
2	B	233[B]	ARG
2	B	243	ASP
1	C	1(O)	GLN
2	D	33	LEU
2	D	40	LEU
2	D	93	ARG
2	D	101	ARG
3	I	78	LEU
3	I	97	ASP
3	I	141	VAL
3	I	200	ASP
3	I	212	VAL
3	I	215	LEU
3	I	217	ASN
3	I	315	MET
3	I	331	LEU
3	I	333	GLU
3	I	361	ASP
3	I	366	ASP
3	I	405	ASN
3	I	416	PRO

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

Mol	Chain	Res	Type
1	A	1(O)	GLN
2	B	156	GLN
2	B	204(B)	ASN
2	B	205	ASN
2	B	239	GLN
1	C	1(O)	GLN
2	D	71	HIS
2	D	156	GLN

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Mol	Chain	Res	Type
2	D	205	ASN
2	D	239	GLN
2	D	244	GLN
3	I	18	ASN
3	I	120	HIS
3	I	181	GLN
3	I	217	ASN
3	I	268	GLN
3	I	319	HIS
3	I	405	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

29 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	$\#\|Z\| > 2$
5	NAG	B	501	2,5	14,14,15	0.63	0	15,19,21	1.03	2 (13%)
5	FUC	B	602	5	10,10,11	0.59	0	14,14,16	0.88	1 (7%)
7	NDG	D	501	2,7	14,14,15	0.70	0	15,19,21	0.97	1 (6%)
7	FUC	D	602	7	10,10,11	0.56	0	14,14,16	0.90	2 (14%)
8	GU4	I	433	8	27,28,28	1.86	4 (14%)	37,45,45	0.98	1 (2%)
8	GU6	I	434	8	22,23,24	3.30	9 (40%)	25,36,38	2.62	5 (20%)
8	GU0	I	435	8	22,23,24	1.87	4 (18%)	25,36,38	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
8	GU5	I	436	8	16,17,18	1.31	1 (6%)	19,24,26	0.81	0
8	GU8	I	437	8	13,14,15	0.51	0	16,18,20	1.00	1 (6%)
8	GU9	I	438	8	13,14,15	0.61	0	16,18,20	0.97	1 (6%)
8	GU8	I	439	8	13,14,15	0.54	0	16,18,20	0.82	0
8	GU9	I	440	8	13,14,15	0.54	0	16,18,20	0.83	0
8	GU8	I	441	8	13,14,15	0.55	0	16,18,20	0.72	0
8	GU9	I	442	8	13,14,15	0.56	0	16,18,20	0.69	0
8	GU8	I	443	8	13,14,15	0.51	0	16,18,20	0.83	0
8	GU5	I	444	8	16,17,18	1.33	1 (6%)	19,24,26	0.79	0
8	GU1	I	445	8	10,14,15	0.54	0	12,19,21	0.64	0
8	GU6	I	446	8	22,23,24	1.89	4 (18%)	25,36,38	1.00	1 (4%)
8	GU2	I	447	8	10,14,15	0.55	0	12,19,21	0.69	0
8	GU3	I	448	8	21,21,22	1.61	3 (14%)	26,31,33	1.14	1 (3%)
9	NDG	I	501	9,3	14,14,15	0.65	0	15,19,21	0.94	1 (6%)
9	NAG	I	502	9	14,14,15	0.56	0	15,19,21	0.85	1 (6%)
9	FUC	I	602	9	10,10,11	0.54	0	14,14,16	0.90	1 (7%)
9	BMA	I	701	9	11,11,12	0.61	0	14,15,17	0.49	0
9	MAN	I	702	9	11,11,12	0.57	0	14,15,17	0.79	0
9	MAN	I	703	9	11,11,12	0.66	0	14,15,17	0.73	0
9	MAN	I	704	9	10,10,12	0.56	0	12,13,17	0.75	0
11	NAG	I	901	11,3	14,14,15	0.62	0	15,19,21	0.96	1 (6%)
11	NAG	I	902	11	14,14,15	0.54	0	15,19,21	0.66	0

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
5	NAG	B	501	2,5	-	0/6/23/26	0/1/1/1
5	FUC	B	602	5	-	0/0/17/20	0/1/1/1
7	NDG	D	501	2,7	-	0/6/23/26	0/1/1/1
7	FUC	D	602	7	-	0/0/17/20	0/1/1/1
8	GU4	I	433	8	-	0/21/41/41	0/1/1/1
8	GU6	I	434	8	1/1/7/8	0/16/32/36	0/1/1/1
8	GU0	I	435	8	-	0/16/32/36	0/1/1/1
8	GU5	I	436	8	-	0/10/26/30	0/1/1/1
8	GU8	I	437	8	-	0/7/23/27	0/1/1/1
8	GU9	I	438	8	-	0/7/23/27	0/1/1/1
8	GU8	I	439	8	-	0/7/23/27	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	GU9	I	440	8	-	0/7/23/27	0/1/1/1
8	GU8	I	441	8	-	0/7/23/27	0/1/1/1
8	GU9	I	442	8	-	0/7/23/27	0/1/1/1
8	GU8	I	443	8	-	0/7/23/27	0/1/1/1
8	GU5	I	444	8	-	0/10/26/30	0/1/1/1
8	GU1	I	445	8	-	0/4/24/28	0/1/1/1
8	GU6	I	446	8	-	0/16/32/36	0/1/1/1
8	GU2	I	447	8	-	0/4/24/28	1/1/1/1
8	GU3	I	448	8	-	0/15/31/35	0/1/1/1
9	NDG	I	501	9,3	-	0/6/23/26	0/1/1/1
9	NAG	I	502	9	-	0/6/23/26	0/1/1/1
9	FUC	I	602	9	-	0/0/17/20	0/1/1/1
9	BMA	I	701	9	-	0/2/19/22	0/1/1/1
9	MAN	I	702	9	-	0/2/19/22	0/1/1/1
9	MAN	I	703	9	-	0/2/19/22	0/1/1/1
9	MAN	I	704	9	-	0/2/16/22	0/1/1/1
11	NAG	I	901	11,3	-	0/6/23/26	0/1/1/1
11	NAG	I	902	11	-	0/6/23/26	0/1/1/1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	434	GU6	O3-C3	-6.95	1.36	1.47
8	I	434	GU6	C4-C3	-6.38	1.39	1.52
8	I	434	GU6	C2-C3	-4.77	1.39	1.52
8	I	434	GU6	O2-C2	-4.53	1.36	1.46
8	I	434	GU6	C4-C5	-4.48	1.39	1.52
8	I	434	GU6	O6-S6	-4.48	1.43	1.57
8	I	436	GU5	O6-S6	-4.34	1.43	1.57
8	I	448	GU3	O6-S6	-4.34	1.43	1.57
8	I	444	GU5	O6-S6	-4.33	1.43	1.57
8	I	446	GU6	O6-S6	-4.31	1.43	1.57
8	I	433	GU4	O6-S6	-4.28	1.43	1.57
8	I	435	GU0	O6-S6	-4.26	1.43	1.57
8	I	434	GU6	O3-S3	-4.23	1.43	1.57
8	I	434	GU6	O2-S2	-4.19	1.43	1.57
8	I	446	GU6	O3-S3	-4.19	1.43	1.57
8	I	448	GU3	O2-S2	-4.18	1.43	1.57
8	I	446	GU6	O2-S2	-4.18	1.43	1.57
8	I	435	GU0	O2-S2	-4.13	1.43	1.57
8	I	435	GU0	O3-S3	-4.12	1.43	1.57
8	I	433	GU4	O2-S2	-4.09	1.44	1.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	433	GU4	O3-S3	-4.06	1.44	1.57
8	I	433	GU4	O4-S4	-4.05	1.44	1.57
8	I	434	GU6	O5-C5	-3.80	1.37	1.44
8	I	446	GU6	O3-C3	-2.53	1.43	1.47
8	I	435	GU0	O3-C3	-2.50	1.43	1.47
8	I	448	GU3	O1-C1	2.25	1.44	1.40

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	I	448	GU3	C2-O2-S2	-3.73	111.67	118.77
8	I	446	GU6	C2-O2-S2	-3.03	112.99	118.77
8	I	434	GU6	C4-C3-C2	-2.75	104.88	110.60
8	I	438	GU9	C4-C5-C6	-2.65	107.33	112.59
11	I	901	NAG	C2-N2-C7	-2.63	119.66	123.04
9	I	502	NAG	C2-N2-C7	-2.58	119.73	123.04
8	I	437	GU8	C1-C2-C3	-2.51	105.33	110.59
7	D	501	NDG	C2-N2-C7	-2.50	119.82	123.04
9	I	501	NDG	C2-N2-C7	-2.42	119.92	123.04
5	B	501	NAG	C2-N2-C7	-2.24	120.16	123.04
7	D	602	FUC	C1-O5-C5	2.08	115.60	112.38
7	D	602	FUC	C1-C2-C3	2.15	112.09	109.54
5	B	602	FUC	C1-O5-C5	2.18	115.75	112.38
9	I	602	FUC	C1-O5-C5	2.25	115.85	112.38
5	B	501	NAG	C1-O5-C5	2.33	115.20	112.25
8	I	433	GU4	O2-C2-C1	2.76	111.41	107.65
8	I	434	GU6	O5-C5-C4	4.31	117.99	109.97
8	I	434	GU6	O5-C5-C6	5.01	118.31	107.06
8	I	434	GU6	C4-C5-C6	5.57	123.63	112.59
8	I	434	GU6	O2-C2-C1	8.56	119.29	107.65

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	I	434	GU6	C5

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	447	GU2	C1-C2-C3-C4-C5-O5

23 monomers are involved in 57 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	501	NAG	8	0
5	B	602	FUC	6	0
7	D	501	NDG	4	0
7	D	602	FUC	4	0
8	I	433	GU4	2	0
8	I	435	GU0	1	0
8	I	436	GU5	4	0
8	I	437	GU8	8	0
8	I	438	GU9	4	0
8	I	439	GU8	5	0
8	I	440	GU9	5	0
8	I	441	GU8	6	0
8	I	442	GU9	6	0
8	I	443	GU8	2	0
8	I	444	GU5	2	0
8	I	445	GU1	3	0
8	I	446	GU6	2	0
8	I	448	GU3	2	0
9	I	501	NDG	8	0
9	I	502	NAG	1	0
9	I	602	FUC	5	0
11	I	901	NAG	1	0
11	I	902	NAG	1	0

5.6 Ligand geometry (i)

19 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	GOL	A	1102	-	5,5,5	0.69	0	5,5,5	0.51	0
4	GOL	A	1108	-	5,5,5	0.70	0	5,5,5	0.53	0
4	GOL	B	1101	-	5,5,5	0.77	0	5,5,5	0.47	0
4	GOL	B	1103	-	5,5,5	0.72	0	5,5,5	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	GOL	B	1104	-	5,5,5	0.58	0	5,5,5	0.42	0
4	GOL	B	1105	-	5,5,5	0.65	0	5,5,5	0.43	0
4	GOL	B	1109	-	5,5,5	0.67	0	5,5,5	0.45	0
6	SO4	B	2001	-	4,4,4	0.21	0	6,6,6	0.12	0
6	SO4	B	2002	-	4,4,4	0.19	0	6,6,6	0.11	0
6	SO4	B	2003	-	4,4,4	0.15	0	6,6,6	0.13	0
6	SO4	B	2006	-	4,4,4	0.28	0	6,6,6	0.09	0
4	GOL	D	1106	-	5,5,5	0.59	0	5,5,5	0.43	0
4	GOL	D	1107	-	5,5,5	0.58	0	5,5,5	0.36	0
4	GOL	D	1110	-	5,5,5	0.69	0	5,5,5	0.45	0
4	GOL	D	1111	-	5,5,5	0.71	0	5,5,5	0.49	0
6	SO4	D	2004	-	4,4,4	0.15	0	6,6,6	0.11	0
4	GOL	I	1112	-	5,5,5	0.64	0	5,5,5	0.40	0
6	SO4	I	2005	-	4,4,4	0.28	0	6,6,6	0.07	0
10	NAG	I	801	3	14,14,15	0.55	0	15,19,21	0.72	0

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	GOL	A	1102	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1108	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1101	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1103	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1104	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1105	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1109	-	-	0/4/4/4	0/0/0/0
6	SO4	B	2001	-	-	0/0/0/0	0/0/0/0
6	SO4	B	2002	-	-	0/0/0/0	0/0/0/0
6	SO4	B	2003	-	-	0/0/0/0	0/0/0/0
6	SO4	B	2006	-	-	0/0/0/0	0/0/0/0
4	GOL	D	1106	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1107	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1110	-	-	0/4/4/4	0/0/0/0
4	GOL	D	1111	-	-	0/4/4/4	0/0/0/0
6	SO4	D	2004	-	-	0/0/0/0	0/0/0/0
4	GOL	I	1112	-	-	0/4/4/4	0/0/0/0
6	SO4	I	2005	-	-	0/0/0/0	0/0/0/0
10	NAG	I	801	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1102	GOL	5	0
4	B	1103	GOL	4	0
6	B	2002	SO4	1	0
6	B	2006	SO4	1	0
4	D	1106	GOL	1	0
4	D	1107	GOL	1	0
4	D	1110	GOL	1	0
4	D	1111	GOL	1	0
4	I	1112	GOL	2	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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^2)	Q<0.9
1	A	47/49 (95%)	-0.04	2 (4%)	39	48	22, 34, 47, 66	1 (2%)
1	C	46/49 (93%)	0.10	3 (6%)	22	29	28, 38, 51, 58	0
2	B	252/259 (97%)	0.15	9 (3%)	46	55	14, 31, 50, 63	3 (1%)
2	D	252/259 (97%)	0.22	14 (5%)	28	36	18, 33, 47, 64	0
3	I	415/432 (96%)	0.57	36 (8%)	13	17	34, 51, 77, 89	0
All	All	1012/1048 (96%)	0.33	64 (6%)	23	31	14, 41, 68, 89	4 (0%)

All (64) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	388	VAL	7.6
3	I	358	GLY	6.5
3	I	431	VAL	6.0
3	I	386	THR	5.9
3	I	134	ALA	4.8
3	I	199	THR	4.4
3	I	357	GLU	4.1
3	I	179	ALA	4.0
3	I	390	ILE	4.0
3	I	389	VAL	3.9
3	I	356	ALA	3.9
1	A	1(S)	THR	3.9
2	D	29	TRP	3.5
3	I	204	SER	3.4
3	I	15	ILE	3.4
2	D	44	ALA	3.3
3	I	264	ALA	3.0
3	I	266	GLY	2.9
1	C	1(R)	SER	2.9
3	I	359	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	53	LEU	2.9
3	I	387	ALA	2.9
2	B	204(A)[A]	PHE	2.8
2	B	46	LEU	2.8
2	D	198	PRO	2.7
3	I	243	ASP	2.7
3	I	200	ASP	2.6
1	C	1(O)	GLN	2.6
3	I	310	GLU	2.6
2	D	213	VAL	2.6
2	B	29	TRP	2.5
3	I	27	GLU	2.5
2	D	47	ILE	2.5
3	I	206	ALA	2.5
2	D	31	VAL	2.5
3	I	46	ARG	2.5
3	I	205	GLU	2.4
3	I	110	THR	2.4
2	B	198	PRO	2.4
2	B	31	VAL	2.4
3	I	26	PRO	2.3
1	C	12	LEU	2.3
3	I	6	ASP	2.3
3	I	88	ALA	2.3
3	I	177	GLU	2.2
2	D	54	THR	2.2
3	I	112	SER	2.2
2	D	147	THR	2.2
2	B	44	ALA	2.2
2	D	43	GLY	2.2
2	D	200	VAL	2.2
3	I	180	GLU	2.2
2	D	46	LEU	2.2
3	I	181	GLN	2.2
2	B	47	ILE	2.2
3	I	262	ARG	2.1
2	B	62	ASN	2.1
2	D	139	THR	2.1
2	D	45	SER	2.1
3	I	81	LEU	2.1
2	B	186(A)	ASP	2.1
3	I	361	ASP	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1(R)	SER	2.0
3	I	289	GLU	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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(Å^2)	Q<0.9
9	MAN	I	703	11/12	0.71	0.33	5.04	99,101,102,103	0
7	NDG	D	501	14/15	0.74	0.32	3.13	59,66,74,80	0
8	GU6	I	434	23/24	0.98	0.12	0.03	25,30,32,37	0
8	GU5	I	444	17/18	0.96	0.10	-0.39	52,57,59,59	0
8	GU0	I	435	23/24	0.98	0.10	-0.67	28,33,41,43	0
8	GU4	I	433	28/28	0.99	0.09	-0.80	22,26,30,33	0
8	GU6	I	446	23/24	0.95	0.10	-1.04	47,61,65,67	0
5	NAG	B	501	14/15	0.46	0.38	-	73,77,84,88	0
11	NAG	I	902	14/15	0.58	0.45	-	102,104,105,106	0
8	GU8	I	439	14/15	0.79	0.49	-	88,92,93,94	0
5	FUC	B	602	10/11	0.80	0.43	-	90,91,91,91	0
9	NAG	I	502	14/15	0.79	0.42	-	98,100,101,103	0
9	FUC	I	602	10/11	0.84	0.47	-	101,103,104,104	0
8	GU8	I	437	14/15	0.90	0.23	-	54,59,65,70	0
9	MAN	I	702	11/12	0.50	0.66	-	115,116,117,118	0
9	BMA	I	701	11/12	0.71	0.33	-	103,105,110,113	0
11	NAG	I	901	14/15	0.74	0.23	-	92,94,96,99	0
9	NDG	I	501	14/15	0.82	0.30	-	83,88,94,98	0
8	GU3	I	448	21/22	0.94	0.14	-	56,61,66,67	0
8	GU2	I	447	14/15	0.92	0.18	-	61,64,69,70	0
8	GU5	I	436	17/18	0.98	0.09	-	38,42,47,50	0
9	MAN	I	704	10/12	0.65	0.34	-	103,104,105,105	0
7	FUC	D	602	10/11	0.73	0.48	-	83,84,85,85	0
8	GU9	I	438	14/15	0.75	0.37	-	81,86,89,90	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
8	GU8	I	443	14/15	0.94	0.11	-	60,63,69,69	0
8	GU1	I	445	14/15	0.96	0.09	-	51,54,57,57	0
8	GU9	I	440	14/15	0.90	0.23	-	84,84,86,87	0
8	GU8	I	441	14/15	0.91	0.25	-	79,83,84,85	0
8	GU9	I	442	14/15	0.87	0.25	-	69,75,80,81	0

6.4 Ligands

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, 95th 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(Å^2)	Q<0.9
4	GOL	A	1102	6/6	0.89	0.27	8.62	54,57,58,60	0
4	GOL	B	1101	6/6	0.72	0.36	8.27	49,55,57,60	0
4	GOL	A	1108	6/6	0.85	0.26	7.66	73,76,77,78	0
4	GOL	B	1105	6/6	0.85	0.25	6.03	95,95,95,95	0
4	GOL	D	1110	6/6	0.82	0.22	4.98	72,75,76,77	0
6	SO4	B	2003	5/5	0.88	0.21	4.15	85,86,87,88	0
4	GOL	I	1112	6/6	0.78	0.27	3.81	80,81,81,82	0
4	GOL	D	1111	6/6	0.88	0.25	3.53	63,64,64,66	0
4	GOL	B	1103	6/6	0.80	0.20	2.97	63,65,65,66	0
4	GOL	B	1109	6/6	0.86	0.17	2.27	62,62,64,64	0
4	GOL	D	1106	6/6	0.88	0.13	0.87	66,67,67,68	0
4	GOL	D	1107	6/6	0.95	0.13	0.83	32,41,44,45	0
10	NAG	I	801	14/15	0.89	0.21	0.71	66,68,73,74	0
4	GOL	B	1104	6/6	0.95	0.13	0.13	30,35,37,46	0
6	SO4	B	2006	5/5	0.97	0.19	0.08	56,56,58,59	0
6	SO4	B	2001	5/5	0.94	0.12	-0.99	85,85,86,87	0
6	SO4	I	2005	5/5	0.98	0.09	-1.68	63,63,64,64	0
6	SO4	D	2004	5/5	0.98	0.10	-	61,63,64,64	0
6	SO4	B	2002	5/5	0.96	0.13	-	89,89,90,91	0

6.5 Other polymers

There are no such residues in this entry.