Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:05 PM GMT

PDB ID	:	1DZG
Title	:	N135Q-S380C-ANTITHROMBIN-III
Authors	:	Mccoy, A.J.; Huntington, J.A.; Carrell, R.W.
Deposited on	:	2000-02-28
Resolution	:	2.80 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

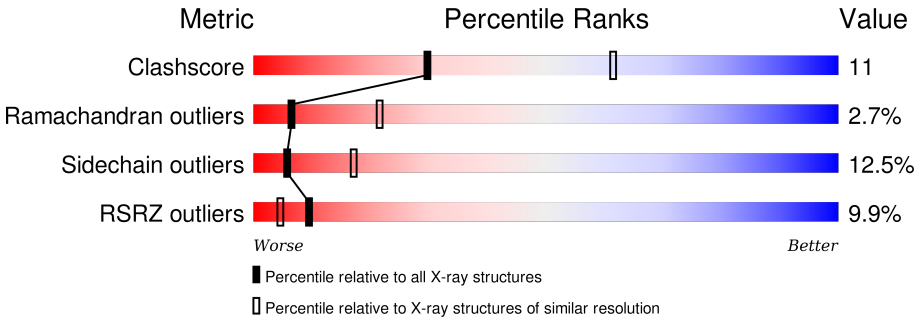
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	I	432	10% 60% 33% 5%
2	L	432	9% 67% 23% 5%

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
5	GOL	I	901	-	-	-	X
5	GOL	L	901	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6593 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	I	422	Total	C	N	O	S	0	0	0
			3271	2088	549	616	18			

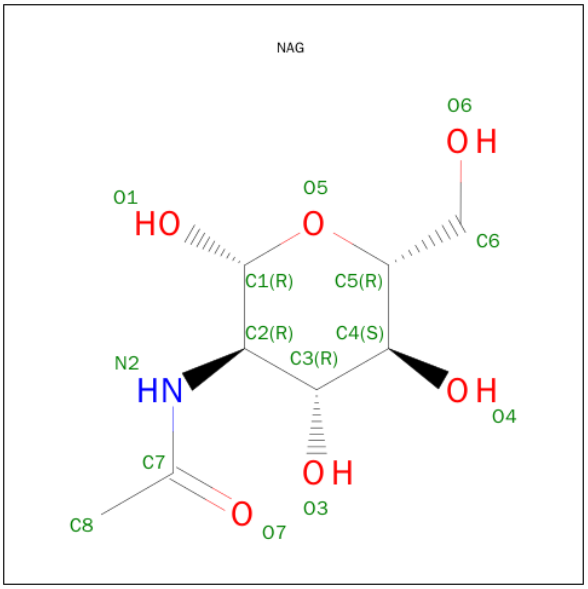
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	135	GLN	ASN	ENGINEERED MUTATION	UNP P01008
I	380	CYS	SER	ENGINEERED MUTATION	UNP P01008

- Molecule 2 is a protein called ANTITHROMBIN-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	409	Total	C	N	O	S	0	0	0
			3180	2031	525	606	18			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

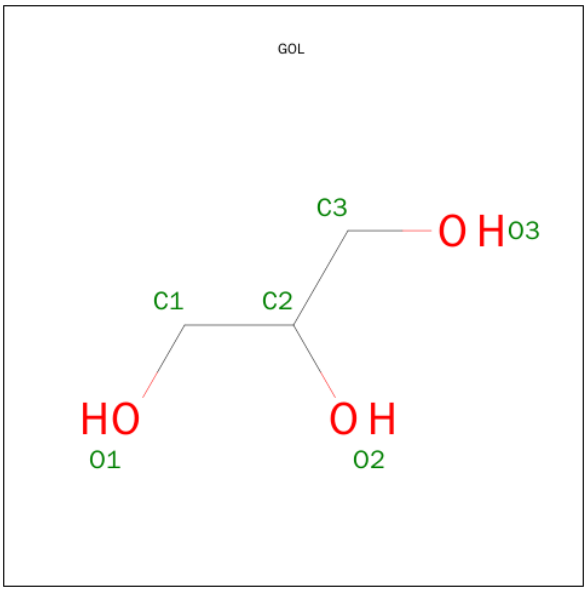


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	I	1	Total C N O 14 8 1 5	0	0
3	I	1	Total C N O 14 8 1 5	0	0
3	L	1	Total C N O 14 8 1 5	0	0

- Molecule 4 is a polymer of unknown type called SUGAR (2-MER).

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	I	1	Total C O 6 3 3	0	0
5	L	1	Total C O 6 3 3	0	0

- Molecule 6 is water.

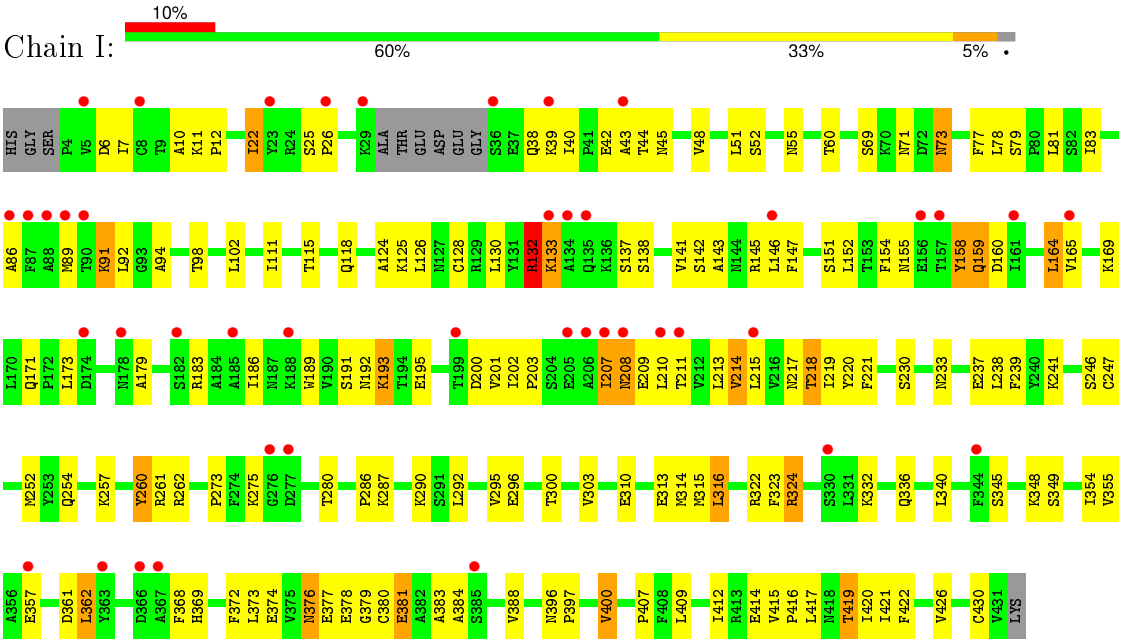
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	I	2	Total O 2 2	0	0
6	L	2	Total O 2 2	0	0

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.

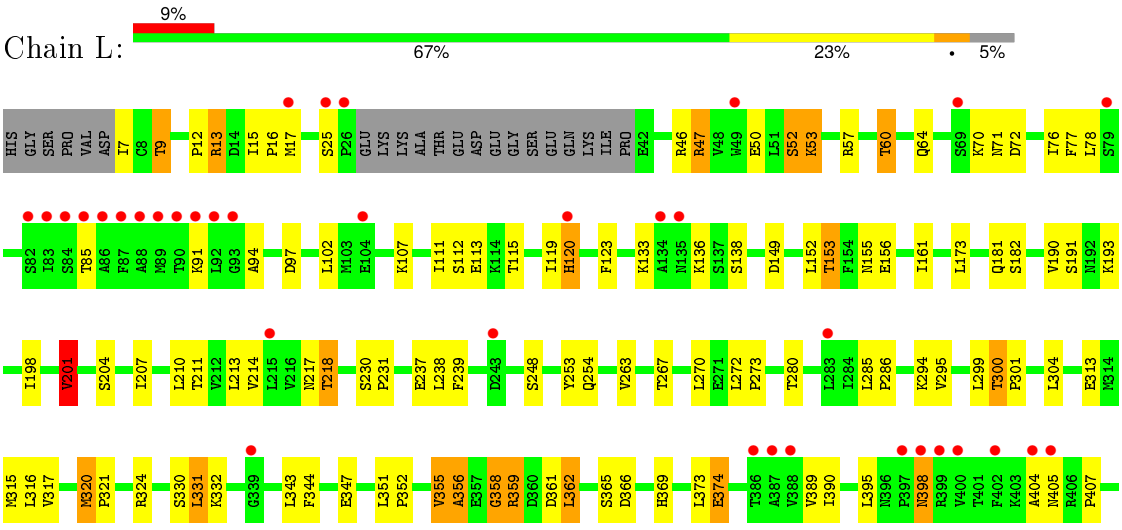
- Molecule 1: ANTITHROMBIN-III

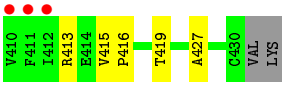
Chain I:



- Molecule 2: ANTITHROMBIN-III

Chain L:




V410
F411
I412
R413
E414
V415
P416
T419
A427
C430
VAL
LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	68.61Å 99.54Å 88.69Å 90.00° 104.79° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80 26.24 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (20.00-2.80) 97.9 (26.24-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.228 , 0.297 0.247 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	72.6	Xtriage
Anisotropy	0.336	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 65.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 27915 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	6593	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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, 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	I	0.45	0/3337	1.00	4/4524 (0.1%)
2	L	0.43	0/3245	0.92	1/4398 (0.0%)
All	All	0.44	0/6582	0.96	5/8922 (0.1%)

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
2	L	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	324	ARG	CD-NE-CZ	6.28	132.39	123.60
1	I	260	TYR	CA-CB-CG	6.01	124.81	113.40
1	I	132	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	I	6	ASP	N-CA-CB	5.62	120.71	110.60
2	L	405	ASN	N-CA-C	5.03	124.58	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	L	300	THR	Mainchain

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	I	3271	0	3182	85	0
2	L	3180	0	3094	59	0
3	I	28	0	26	0	0
3	L	14	0	13	0	0
4	I	28	0	25	0	0
4	L	56	0	50	2	0
5	I	6	0	8	2	0
5	L	6	0	8	1	0
6	I	2	0	0	0	0
6	L	2	0	0	0	0
All	All	6593	0	6406	145	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 11.

All (145) 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:I:81:LEU:HD21	1:I:130:LEU:HD21	1.58	0.86
1:I:378:GLU:HG3	1:I:384:ALA:HB3	1.64	0.79
1:I:324:ARG:HE	1:I:372:PHE:HZ	1.36	0.74
2:L:214:VAL:HG22	2:L:389:VAL:HG23	1.70	0.73
1:I:388:VAL:HG22	2:L:317:VAL:HB	1.72	0.72
1:I:91:LYS:HB2	1:I:102:LEU:HD13	1.70	0.72
2:L:13:ARG:HH11	2:L:13:ARG:HB2	1.58	0.69
2:L:111:ILE:HD12	2:L:119:ILE:HD12	1.75	0.68
2:L:331:LEU:HD21	2:L:369:HIS:HB2	1.76	0.67
2:L:300:THR:HB	2:L:301:PRO:HD2	1.79	0.63
1:I:45:ASN:HD21	1:I:125:LYS:HD3	1.64	0.62
2:L:17:MET:SD	2:L:120:HIS:HB2	2.39	0.62
1:I:415:VAL:HB	1:I:416:PRO:HD3	1.80	0.62
1:I:7:ILE:HD11	1:I:132:ARG:HE	1.63	0.61
2:L:239:PHE:HE2	2:L:404:ALA:HB1	1.65	0.61
1:I:217:ASN:O	1:I:218:THR:HB	1.99	0.61
2:L:60:THR:HG21	2:L:300:THR:HA	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:261:ARG:HG2	1:I:310:GLU:HB3	1.83	0.60
1:I:126:LEU:HD11	1:I:419:THR:HG21	1.85	0.59
2:L:85:THR:HB	2:L:217:ASN:ND2	2.17	0.59
1:I:186:ILE:HG21	1:I:202:ILE:HD11	1.85	0.58
2:L:47:ARG:HD2	2:L:112:SER:HB2	1.85	0.58
2:L:415:VAL:HB	2:L:416:PRO:HD3	1.85	0.58
1:I:164:LEU:HD23	1:I:165:VAL:HG23	1.86	0.57
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.85	0.57
1:I:86:ALA:HB1	1:I:215:LEU:HD21	1.87	0.57
1:I:147:PHE:HB2	1:I:214:VAL:HG23	1.87	0.57
1:I:102:LEU:HG	1:I:340:LEU:HD11	1.87	0.56
1:I:324:ARG:HG3	1:I:374:GLU:HG3	1.88	0.55
2:L:213:LEU:HB3	2:L:390:ILE:HD12	1.88	0.55
1:I:40:ILE:HG23	1:I:44:THR:HB	1.89	0.55
2:L:153:THR:HB	2:L:356:ALA:HB2	1.88	0.54
1:I:86:ALA:HB2	1:I:217:ASN:HB3	1.89	0.54
2:L:213:LEU:HD23	2:L:390:ILE:HD12	1.89	0.54
2:L:355:VAL:HG13	2:L:362:LEU:HD11	1.89	0.54
1:I:361:ASP:O	1:I:362:LEU:C	2.46	0.54
2:L:91:LYS:HG3	2:L:102:LEU:HD13	1.89	0.53
1:I:257:LYS:HE2	1:I:313:GLU:HB3	1.90	0.53
1:I:273:PRO:HB3	1:I:280:THR:HG22	1.91	0.53
1:I:115:THR:HB	1:I:118:GLN:HG3	1.92	0.52
1:I:414:GLU:HB2	1:I:421:ILE:HD11	1.90	0.52
1:I:195:GLU:HG2	1:I:220:TYR:CE2	2.45	0.52
4:L:841:NAG:H62	4:L:842:NAG:C7	2.40	0.52
1:I:316:LEU:HB3	1:I:400:VAL:HG12	1.91	0.52
1:I:11:LYS:HB3	1:I:12:PRO:HD2	1.91	0.51
1:I:146:LEU:HG	1:I:213:LEU:HD22	1.92	0.51
2:L:70:LYS:HD3	2:L:76:ILE:HG12	1.93	0.51
2:L:7:ILE:HG22	2:L:9:THR:HG23	1.94	0.50
1:I:45:ASN:HB3	1:I:48:VAL:HB	1.93	0.50
2:L:304:LEU:HD12	5:L:901:GOL:H12	1.95	0.49
1:I:412:ILE:HB	1:I:422:PHE:HB2	1.93	0.49
1:I:287:LYS:HG3	1:I:290:LYS:H	1.78	0.48
1:I:252:MET:SD	1:I:377:GLU:HG3	2.52	0.48
2:L:207:ILE:HG23	2:L:211:THR:HG21	1.96	0.48
2:L:193:LYS:HB3	2:L:218:THR:HG21	1.94	0.48
2:L:358:GLY:O	2:L:359:ARG:C	2.51	0.48
2:L:355:VAL:CG2	2:L:359:ARG:HB2	2.43	0.48
2:L:190:VAL:HG21	2:L:201:VAL:HG21	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:195:GLU:HG2	1:I:220:TYR:HE2	1.78	0.48
1:I:345:SER:HB3	1:I:348:LYS:HD2	1.95	0.48
1:I:132:ARG:O	1:I:133:LYS:C	2.51	0.48
2:L:270:LEU:HD21	2:L:272:LEU:HD21	1.95	0.47
1:I:83:ILE:HA	1:I:217:ASN:ND2	2.28	0.47
2:L:253:TYR:O	2:L:254:GLN:HB3	2.14	0.47
1:I:179:ALA:HB1	1:I:208:ASN:HA	1.97	0.47
1:I:207:ILE:HD12	1:I:207:ILE:H	1.80	0.47
1:I:207:ILE:HG23	1:I:211:THR:HG21	1.96	0.47
2:L:300:THR:HB	2:L:301:PRO:CD	2.45	0.46
2:L:191:SER:HA	2:L:198:ILE:O	2.16	0.46
1:I:7:ILE:CD1	1:I:132:ARG:HH21	2.29	0.46
2:L:324:ARG:HB2	2:L:374:GLU:OE1	2.15	0.46
1:I:42:GLU:O	1:I:43:ALA:HB3	2.16	0.46
1:I:420:ILE:HD11	5:I:901:GOL:H2	1.97	0.46
2:L:407:PRO:HB3	2:L:427:ALA:HB2	1.96	0.46
2:L:155:ASN:OD1	2:L:156:GLU:N	2.49	0.46
1:I:376:ASN:ND2	1:I:379:GLY:H	2.14	0.46
2:L:173:LEU:HD13	2:L:182:SER:HB3	1.97	0.45
2:L:77:PHE:CE2	2:L:373:LEU:HB2	2.51	0.45
1:I:323:PHE:HE1	1:I:373:LEU:HD23	1.80	0.45
1:I:237:GLU:HG2	1:I:238:LEU:H	1.81	0.45
1:I:145:ARG:HG3	1:I:169:LYS:O	2.16	0.45
1:I:217:ASN:OD1	1:I:369:HIS:HB2	2.16	0.45
1:I:152:LEU:HD13	1:I:354:ILE:HG21	1.97	0.45
2:L:365:SER:OG	2:L:389:VAL:HG13	2.16	0.45
1:I:300:THR:H	1:I:303:VAL:HB	1.81	0.45
1:I:239:PHE:HB3	1:I:247:CYS:HB3	1.98	0.45
2:L:111:ILE:HG22	2:L:112:SER:H	1.82	0.45
2:L:415:VAL:HB	2:L:416:PRO:CD	2.45	0.45
2:L:153:THR:CB	2:L:356:ALA:HB2	2.47	0.45
2:L:359:ARG:HG2	2:L:361:ASP:OD2	2.16	0.45
1:I:92:LEU:HB3	1:I:158:TYR:HE1	1.81	0.45
1:I:51:LEU:HG	1:I:55:ASN:ND2	2.31	0.44
1:I:407:PRO:HA	1:I:426:VAL:O	2.17	0.44
1:I:51:LEU:HA	1:I:111:ILE:HD11	2.00	0.44
2:L:267:THR:HA	2:L:286:PRO:HA	1.99	0.44
1:I:130:LEU:HD13	1:I:417:LEU:HD12	2.00	0.44
1:I:77:PHE:CE1	1:I:373:LEU:HD22	2.53	0.44
1:I:154:PHE:O	1:I:155:ASN:C	2.56	0.44
1:I:25:SER:HB2	1:I:26:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:94:ALA:HA	2:L:351:LEU:HD23	1.98	0.44
2:L:398:ASN:H	2:L:398:ASN:HD22	1.66	0.44
1:I:208:ASN:HB2	1:I:209:GLU:H	1.71	0.44
1:I:202:ILE:HG23	1:I:368:PHE:CE2	2.53	0.43
2:L:152:LEU:HD11	2:L:359:ARG:NH1	2.33	0.43
2:L:71:ASN:ND2	2:L:72:ASP:H	2.16	0.43
1:I:336:GLN:HA	1:I:340:LEU:O	2.18	0.43
1:I:171:GLN:HG3	1:I:173:LEU:HG	2.01	0.43
1:I:189:TRP:O	1:I:193:LYS:HG2	2.19	0.43
1:I:124:ALA:HA	1:I:165:VAL:HG13	2.01	0.43
2:L:207:ILE:HG12	2:L:389:VAL:HG21	2.00	0.43
2:L:332:LYS:HG3	2:L:344:PHE:CD2	2.53	0.43
1:I:230:SER:HB3	1:I:233:ASN:ND2	2.33	0.43
2:L:53:LYS:HG3	2:L:57:ARG:HH21	1.82	0.43
1:I:143:ALA:HB3	1:I:218:THR:HG22	2.01	0.42
4:L:801:NAG:H62	4:L:802:NAG:O7	2.20	0.42
1:I:132:ARG:HA	1:I:132:ARG:HD3	1.46	0.42
1:I:290:LYS:HE2	1:I:295:VAL:HG22	2.01	0.42
1:I:7:ILE:HD11	1:I:132:ARG:NE	2.32	0.42
1:I:261:ARG:HG2	1:I:310:GLU:CB	2.49	0.42
1:I:22:ILE:HG12	1:I:115:THR:CG2	2.50	0.42
2:L:46:ARG:O	2:L:50:GLU:HG3	2.20	0.42
2:L:230:SER:HA	2:L:231:PRO:HD3	1.83	0.42
1:I:396:ASN:OD1	1:I:397:PRO:HD2	2.19	0.42
2:L:273:PRO:HA	2:L:280:THR:HG22	2.02	0.42
1:I:221:PHE:HD2	1:I:380:CYS:HG	1.67	0.41
1:I:48:VAL:HG13	1:I:126:LEU:HD13	2.03	0.41
2:L:355:VAL:HG22	2:L:359:ARG:HB2	2.02	0.41
1:I:380:CYS:O	1:I:381:GLU:HB2	2.20	0.41
1:I:45:ASN:ND2	1:I:48:VAL:HG23	2.36	0.41
2:L:320:MET:HA	2:L:321:PRO:HD3	1.92	0.41
2:L:17:MET:HG3	2:L:161:ILE:HG23	2.01	0.41
1:I:79:SER:OG	1:I:219:ILE:HD12	2.20	0.41
1:I:261:ARG:HG2	1:I:310:GLU:CG	2.51	0.41
2:L:149:ASP:HB3	2:L:152:LEU:HD12	2.03	0.41
2:L:52:SER:HB2	2:L:419:THR:HG23	2.03	0.41
2:L:60:THR:O	2:L:64:GLN:HG3	2.21	0.41
1:I:420:ILE:HG13	5:I:901:GOL:H12	2.03	0.41
1:I:159:GLN:O	1:I:160:ASP:C	2.59	0.41
1:I:207:ILE:HA	1:I:211:THR:OG1	2.22	0.40
1:I:383:ALA:O	1:I:384:ALA:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:366:ASP:O	2:L:389:VAL:HG12	2.22	0.40
1:I:292:LEU:O	1:I:296:GLU:HG3	2.21	0.40
2:L:111:ILE:HG13	2:L:111:ILE:H	1.69	0.40
1:I:286:PRO:HB3	1:I:295:VAL:HG21	2.03	0.40
2:L:15:ILE:HA	2:L:16:PRO:HD3	1.98	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	I	418/432 (97%)	346 (83%)	58 (14%)	14 (3%)	5	16
2	L	405/432 (94%)	357 (88%)	40 (10%)	8 (2%)	9	30
All	All	823/864 (95%)	703 (85%)	98 (12%)	22 (3%)	6	21

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	203	PRO
1	I	332	LYS
2	L	356	ALA
1	I	164	LEU
1	I	362	LEU
2	L	201	VAL
1	I	94	ALA
1	I	133	LYS
1	I	349	SER
2	L	107	LYS
2	L	358	GLY
1	I	218	THR
1	I	357	GLU

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Mol	Chain	Res	Type
1	I	381	GLU
2	L	362	LEU
1	I	10	ALA
1	I	73	ASN
1	I	159	GLN
2	L	12	PRO
2	L	113	GLU
2	L	352	PRO
1	I	207	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	I	350/383 (91%)	306 (87%)	44 (13%)	5 17
2	L	344/383 (90%)	301 (88%)	43 (12%)	6 17
All	All	694/766 (91%)	607 (88%)	87 (12%)	6 17

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

Mol	Chain	Res	Type
1	I	22	ILE
1	I	38	GLN
1	I	39	LYS
1	I	52	SER
1	I	60	THR
1	I	69	SER
1	I	71	ASN
1	I	73	ASN
1	I	78	LEU
1	I	89	MET
1	I	91	LYS
1	I	98	THR
1	I	128	CYS
1	I	132	ARG

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Mol	Chain	Res	Type
1	I	137	SER
1	I	138	SER
1	I	141	VAL
1	I	142	SER
1	I	151	SER
1	I	158	TYR
1	I	183	ARG
1	I	191	SER
1	I	192	ASN
1	I	193	LYS
1	I	200	ASP
1	I	201	VAL
1	I	208	ASN
1	I	210	LEU
1	I	214	VAL
1	I	241	LYS
1	I	246	SER
1	I	254	GLN
1	I	260	TYR
1	I	262	ARG
1	I	275	LYS
1	I	314	MET
1	I	315	MET
1	I	316	LEU
1	I	322	ARG
1	I	355	VAL
1	I	376	ASN
1	I	400	VAL
1	I	419	THR
1	I	430	CYS
2	L	9	THR
2	L	13	ARG
2	L	25	SER
2	L	47	ARG
2	L	52	SER
2	L	53	LYS
2	L	60	THR
2	L	78	LEU
2	L	97	ASP
2	L	115	THR
2	L	120	HIS
2	L	123	PHE

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Mol	Chain	Res	Type
2	L	133	LYS
2	L	136	LYS
2	L	138	SER
2	L	153	THR
2	L	181	GLN
2	L	201	VAL
2	L	204	SER
2	L	210	LEU
2	L	218	THR
2	L	237	GLU
2	L	238	LEU
2	L	248	SER
2	L	263	VAL
2	L	285	LEU
2	L	294	LYS
2	L	295	VAL
2	L	299	LEU
2	L	313	GLU
2	L	315	MET
2	L	316	LEU
2	L	320	MET
2	L	330	SER
2	L	331	LEU
2	L	343	LEU
2	L	347	GLU
2	L	355	VAL
2	L	359	ARG
2	L	374	GLU
2	L	395	LEU
2	L	398	ASN
2	L	413	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	45	ASN
1	I	159	GLN
1	I	178	ASN
1	I	233	ASN
1	I	254	GLN
1	I	305	GLN
1	I	319	HIS

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Mol	Chain	Res	Type
1	I	376	ASN
1	I	418	ASN
2	L	71	ASN
2	L	171	GLN
2	L	181	GLN
2	L	233	ASN
2	L	254	GLN
2	L	334	GLN
2	L	398	ASN
2	L	418	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

6 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	$\#\|Z\| > 2$
4	NAG	I	841	1,4	14,14,15	1.19	1 (7%)	15,19,21	1.53	2 (13%)
4	NAG	I	842	4	14,14,15	1.25	1 (7%)	15,19,21	0.85	0
4	NAG	L	801	2,4	14,14,15	1.26	1 (7%)	15,19,21	1.82	2 (13%)
4	NAG	L	802	4	14,14,15	1.16	1 (7%)	15,19,21	1.29	2 (13%)
4	NAG	L	841	2,4	14,14,15	1.40	2 (14%)	15,19,21	1.36	2 (13%)
4	NAG	L	842	4	14,14,15	1.26	1 (7%)	15,19,21	1.30	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
4	NAG	I	841	1,4	-	0/6/23/26	0/1/1/1
4	NAG	I	842	4	-	0/6/23/26	0/1/1/1
4	NAG	L	801	2,4	-	0/6/23/26	0/1/1/1
4	NAG	L	802	4	-	0/6/23/26	0/1/1/1
4	NAG	L	841	2,4	-	0/6/23/26	0/1/1/1
4	NAG	L	842	4	-	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	842	NAG	O7-C7	-3.70	1.14	1.23
4	L	801	NAG	O7-C7	-3.69	1.14	1.23
4	I	842	NAG	O7-C7	-3.69	1.14	1.23
4	L	802	NAG	O7-C7	-3.68	1.14	1.23
4	L	841	NAG	O7-C7	-3.66	1.14	1.23
4	I	841	NAG	O7-C7	-3.64	1.14	1.23
4	L	841	NAG	C2-N2	2.08	1.50	1.46

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	I	841	NAG	C4-C3-C2	-3.09	106.42	111.23
4	L	802	NAG	C4-C3-C2	-2.19	107.82	111.23
4	L	841	NAG	O4-C4-C3	-2.00	105.83	110.34
4	L	841	NAG	C4-C3-C2	2.73	115.47	111.23
4	L	801	NAG	C1-O5-C5	3.25	116.37	112.25
4	L	802	NAG	C2-N2-C7	3.60	127.66	123.04
4	L	842	NAG	C1-O5-C5	3.67	116.90	112.25
4	I	841	NAG	C1-O5-C5	4.33	117.75	112.25
4	L	801	NAG	C2-N2-C7	5.05	129.53	123.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	L	801	NAG	1	0
4	L	802	NAG	1	0
4	L	841	NAG	1	0
4	L	842	NAG	1	0

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	$\#\|Z\| > 2$
3	NAG	I	801	1	14,14,15	1.31	1 (7%)	15,19,21	2.02	2 (13%)
3	NAG	I	861	1	14,14,15	1.17	1 (7%)	15,19,21	0.76	0
5	GOL	I	901	-	5,5,5	0.59	0	5,5,5	0.79	0
3	NAG	L	861	2	14,14,15	1.17	1 (7%)	15,19,21	0.77	0
5	GOL	L	901	-	5,5,5	0.67	0	5,5,5	0.58	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
3	NAG	I	801	1	-	0/6/23/26	0/1/1/1
3	NAG	I	861	1	-	0/6/23/26	0/1/1/1
5	GOL	I	901	-	-	0/4/4/4	0/0/0/0
3	NAG	L	861	2	-	0/6/23/26	0/1/1/1
5	GOL	L	901	-	-	0/4/4/4	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	801	NAG	O7-C7	-3.81	1.14	1.23
3	I	861	NAG	O7-C7	-3.65	1.14	1.23
3	L	861	NAG	O7-C7	-3.62	1.14	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	801	NAG	C2-N2-C7	5.12	129.62	123.04
3	I	801	NAG	C1-O5-C5	5.15	118.78	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	901	GOL	2	0
5	L	901	GOL	1	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	I	422/432 (97%)	0.50	43 (10%) 9 4	39, 82, 125, 145	0
2	L	409/432 (94%)	0.36	39 (9%) 10 5	35, 68, 116, 156	0
All	All	831/864 (96%)	0.43	82 (9%) 9 4	35, 75, 122, 156	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	207	ILE	10.2
2	L	400	VAL	7.5
1	I	174	ASP	7.2
2	L	398	ASN	5.6
2	L	90	THR	4.9
1	I	36	SER	4.7
1	I	90	THR	4.1
1	I	135	GLN	4.1
2	L	399	ARG	4.0
1	I	206	ALA	3.9
1	I	133	LYS	3.8
1	I	363	TYR	3.7
1	I	43	ALA	3.6
2	L	397	PRO	3.4
1	I	134	ALA	3.4
1	I	8	CYS	3.4
1	I	357	GLU	3.3
1	I	161	ILE	3.2
2	L	402	PHE	3.1
2	L	88	ALA	3.1
1	I	5	VAL	3.0
2	L	26	PRO	2.9
2	L	404	ALA	2.9
2	L	86	ALA	2.9

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Mol	Chain	Res	Type	RSRZ
2	L	339	GLY	2.8
2	L	412	ILE	2.8
1	I	208	ASN	2.8
1	I	210	LEU	2.7
1	I	385	SER	2.7
1	I	146	LEU	2.7
2	L	85	THR	2.7
2	L	135	ASN	2.7
1	I	199	THR	2.7
2	L	243	ASP	2.7
1	I	277	ASP	2.6
2	L	84	SER	2.6
2	L	388	VAL	2.6
1	I	367	ALA	2.6
2	L	92	LEU	2.6
1	I	26	PRO	2.6
1	I	156	GLU	2.6
2	L	386	THR	2.6
2	L	134	ALA	2.6
2	L	93	GLY	2.5
1	I	88	ALA	2.5
1	I	87	PHE	2.5
2	L	25	SER	2.5
1	I	182	SER	2.5
2	L	82	SER	2.5
1	I	185	ALA	2.4
2	L	91	LYS	2.4
1	I	29	LYS	2.4
2	L	17	MET	2.4
1	I	157	THR	2.4
1	I	89	MET	2.3
1	I	215	LEU	2.3
1	I	165	VAL	2.3
1	I	205	GLU	2.3
1	I	344	PHE	2.3
1	I	330	SER	2.3
2	L	120	HIS	2.3
1	I	211	THR	2.3
1	I	366	ASP	2.3
2	L	283	LEU	2.3
1	I	86	ALA	2.3
1	I	276	GLY	2.3

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Mol	Chain	Res	Type	RSRZ
2	L	69	SER	2.2
1	I	188	LYS	2.2
1	I	178	ASN	2.2
2	L	410	VAL	2.2
2	L	83	ILE	2.2
2	L	387	ALA	2.2
2	L	405	ASN	2.1
2	L	87	PHE	2.1
2	L	79	SER	2.1
2	L	215	LEU	2.1
2	L	411	PHE	2.1
2	L	89	MET	2.0
1	I	23	TYR	2.0
1	I	39	LYS	2.0
2	L	49	TRP	2.0
2	L	104	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
4	NAG	I	841	14/15	0.70	0.38	1.44	124,126,130,135	0
4	NAG	L	841	14/15	0.89	0.15	-0.90	87,94,101,108	0
4	NAG	L	842	14/15	0.81	0.46	-	118,125,127,128	0
4	NAG	L	802	14/15	0.88	0.59	-	144,148,156,157	0
4	NAG	L	801	14/15	0.75	0.33	-	120,123,130,137	0
4	NAG	I	842	14/15	0.76	0.63	-	139,142,145,146	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, 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
5	GOL	I	901	6/6	0.75	0.60	9.88	91,93,94,94	0
5	GOL	L	901	6/6	0.60	0.41	4.29	76,81,85,88	0
3	NAG	I	861	14/15	0.66	0.41	-	147,150,154,154	0
3	NAG	L	861	14/15	0.58	0.36	-	118,120,124,126	0
3	NAG	I	801	14/15	0.87	0.39	-	128,132,139,139	0

6.5 Other polymers

There are no such residues in this entry.