



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:05 PM GMT

PDB ID : 1DZH  
Title : P14-FLUORESCCEIN-N135Q-S380C-ANTITHROMBIN-III  
Authors : Mccoy, A.J.; Huntington, J.A.; Carrell, R.W.  
Deposited on : 2000-02-28  
Resolution : 2.85 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 (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

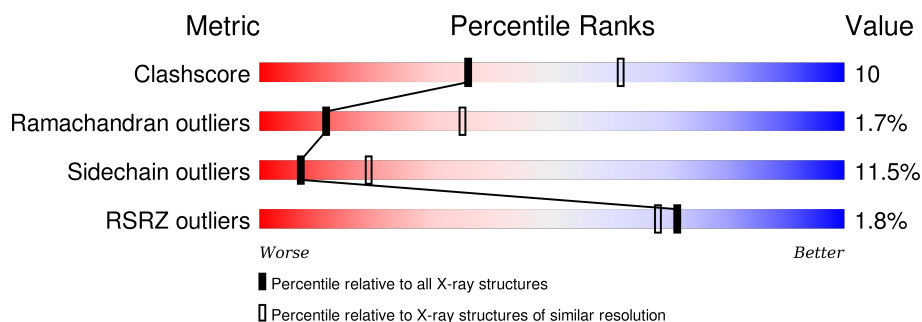
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.85 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	2499 (2.90-2.82)
Ramachandran outliers	100387	2439 (2.90-2.82)
Sidechain outliers	100360	2442 (2.90-2.82)
RSRZ outliers	91569	2236 (2.90-2.82)

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	I	432	
2	L	432	

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
1	CYF	I	380	X	-	-	-
5	GOL	I	901	-	-	-	X

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 6609 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
			Total	C	N	O	S			
1	I	418	3302	2108	551	625	18	0	0	0

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	CYF	SER	ENGINEERED MUTATION	UNP P01008

- Molecule 2 is a protein called ANTITHROMBIN-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	L	407	3110	1988	522	583	17	0	0	1

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

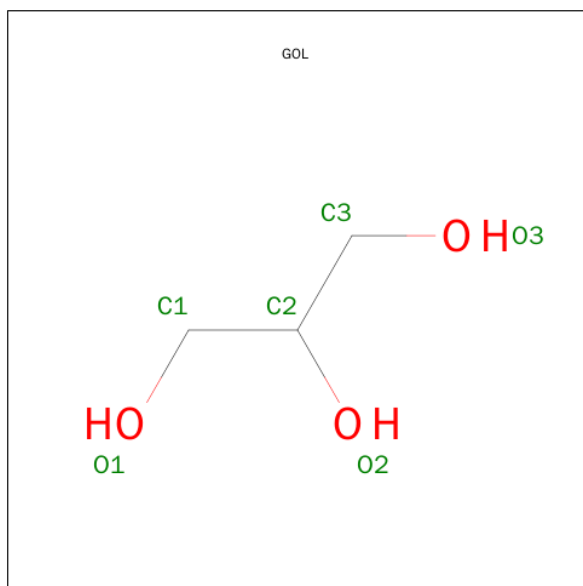


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	I	1	Total	C	N	O	0	0
			14	8	1	5		
3	L	1	Total	C	N	O	0	0
			14	8	1	5		

- 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	0	0
			28	16	2	10		
4	L	2	Total	C	N	O	0	0
			28	16	2	10		

- 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	0	0
			6	3	3		
5	L	1	Total	C	O	0	0
			6	3	3		

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

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

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	28	Total	O	0	0
			28	28		
7	L	9	Total	O	0	0
			9	9		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.17Å 99.86Å 89.42Å 90.00° 105.63° 90.00°	Depositor
Resolution (Å)	20.00 – 2.85 20.01 – 2.85	Depositor EDS
% Data completeness (in resolution range)	99.7 (20.00-2.85) 100.0 (20.01-2.85)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.47 (at 2.83Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.207 , 0.258 0.206 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	63.4	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 67.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 27289 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6609	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.99% 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, 0.375 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, CYF

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	0.51	0/3332	1.00	2/4507 (0.0%)
2	L	0.50	0/3173	1.00	4/4305 (0.1%)
All	All	0.51	0/6505	1.00	6/8812 (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
1	I	1	8
2	L	0	10
All	All	1	18

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	322	ARG	NE-CZ-NH1	9.84	125.22	120.30
2	L	322	ARG	CD-NE-CZ	5.66	131.52	123.60
1	I	132	ARG	NE-CZ-NH1	5.57	123.09	120.30
2	L	316	LEU	CA-CB-CG	5.35	127.60	115.30
2	L	322	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	I	158	TYR	CB-CG-CD1	5.17	124.10	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	I	380	CYF	C10



All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	107	LYS	Mainchain
1	I	155	ASN	Mainchain
1	I	180	GLU	Mainchain
1	I	189	TRP	Mainchain
1	I	257	LYS	Mainchain
1	I	328	GLY	Mainchain
1	I	406	ARG	Mainchain
1	I	71	ASN	Mainchain
2	L	107	LYS	Mainchain
2	L	157	THR	Mainchain
2	L	182	SER	Mainchain
2	L	231	PRO	Mainchain
2	L	300	THR	Mainchain
2	L	322	ARG	Mainchain
2	L	367	ALA	Mainchain
2	L	428	ASN	Mainchain
2	L	80	PRO	Mainchain
2	L	98	THR	Mainchain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	3302	0	3213	66	0
2	L	3110	0	2984	59	0
3	I	28	0	26	0	0
3	L	14	0	13	0	0
4	I	28	0	25	2	0
4	L	28	0	25	1	0
5	I	6	0	8	0	0
5	L	6	0	8	0	0
6	L	50	0	43	1	0
7	I	28	0	0	1	0
7	L	9	0	0	0	0
All	All	6609	0	6345	125	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 10.

All (125) 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:105:VAL:HG21	1:I:340:LEU:HB2	1.61	0.83
2:L:222:LYS:HE2	2:L:381:GLU:HG3	1.62	0.81
1:I:213:LEU:HD11	1:I:354:ILE:HD13	1.65	0.78
1:I:91:LYS:HB2	1:I:102:LEU:HD13	1.67	0.76
2:L:331:LEU:HD21	2:L:369:HIS:HB2	1.71	0.73
1:I:284:ILE:HB	1:I:409:LEU:HB2	1.72	0.71
1:I:300:THR:HB	1:I:303:VAL:HB	1.72	0.70
2:L:102:LEU:HD23	2:L:340:LEU:HD21	1.75	0.69
2:L:428:ASN:HD22	2:L:430:CYS:H	1.44	0.66
2:L:183:ARG:HH11	2:L:204:SER:HA	1.60	0.66
2:L:102:LEU:HD21	2:L:343:LEU:HD22	1.79	0.65
1:I:19:PRO:HG2	1:I:21:CYS:HB2	1.78	0.65
1:I:300:THR:HG22	1:I:303:VAL:H	1.63	0.63
1:I:376:ASN:ND2	1:I:378:GLU:H	1.96	0.62
2:L:85:THR:HG22	2:L:89:MET:HE2	1.83	0.60
1:I:291:SER:HB3	1:I:294:LYS:HG3	1.83	0.60
1:I:252:MET:SD	1:I:377:GLU:HG3	2.41	0.60
1:I:276:GLY:O	1:I:277:ASP:HB2	2.01	0.60
2:L:276:GLY:O	2:L:277:ASP:HB2	2.02	0.59
1:I:376:ASN:HD22	1:I:378:GLU:H	1.51	0.59
1:I:71:ASN:HD21	1:I:73:ASN:HD22	1.50	0.57
1:I:94:ALA:HA	1:I:351:LEU:HD23	1.88	0.56
1:I:380:CYF:OL	1:I:380:CYF:H16	2.06	0.56
2:L:82:SER:HA	2:L:217:ASN:ND2	2.22	0.55
2:L:157:THR:HG21	4:L:842:NAG:H82	1.89	0.55
2:L:63:TYR:HE2	2:L:296:GLU:HG2	1.72	0.55
1:I:380:CYF:O4	1:I:380:CYF:C11	2.55	0.54
1:I:152:LEU:HD13	1:I:354:ILE:HG21	1.89	0.54
1:I:373:LEU:HG	1:I:375:VAL:HG23	1.90	0.54
2:L:79:SER:H	2:L:369:HIS:CE1	2.27	0.53
1:I:292:LEU:HD21	1:I:425:ARG:HG3	1.91	0.52
2:L:183:ARG:NH1	2:L:204:SER:HA	2.25	0.52
2:L:79:SER:H	2:L:369:HIS:HE1	1.58	0.51
2:L:358:GLY:O	2:L:359:ARG:C	2.49	0.51
1:I:292:LEU:HD11	1:I:409:LEU:HG	1.92	0.50
2:L:263:VAL:HG12	2:L:264:ALA:H	1.76	0.50
2:L:183:ARG:HA	2:L:207:ILE:HD12	1.94	0.49
1:I:380:CYF:C15	1:I:380:CYF:H8	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:201:VAL:HG12	1:I:370:LYS:HB2	1.94	0.49
2:L:70:LYS:HE3	2:L:76:ILE:HG12	1.95	0.49
2:L:355:VAL:HG21	2:L:359:ARG:HB2	1.94	0.49
1:I:198:ILE:HG12	1:I:370:LYS:HD3	1.94	0.49
2:L:428:ASN:ND2	2:L:430:CYS:H	2.10	0.48
2:L:410:VAL:HG22	2:L:426:VAL:HG23	1.94	0.48
1:I:77:PHE:CE1	1:I:373:LEU:HD22	2.49	0.48
1:I:374:GLU:HB3	1:I:380:CYF:H16	1.96	0.47
1:I:376:ASN:HD22	1:I:376:ASN:C	2.17	0.47
2:L:120:HIS:HB3	2:L:165:VAL:HG11	1.96	0.47
6:L:862:NAG:H62	6:L:863:BMA:H2	1.97	0.47
1:I:270:LEU:HD21	1:I:272:LEU:HD21	1.96	0.47
1:I:388:VAL:HG22	2:L:317:VAL:HB	1.95	0.47
1:I:328:GLY:HA2	1:I:370:LYS:HG3	1.97	0.47
1:I:152:LEU:HA	1:I:356:ALA:HB2	1.96	0.47
1:I:7:ILE:HG13	1:I:8:CYS:N	2.28	0.47
1:I:290:LYS:HE2	1:I:295:VAL:HG23	1.95	0.47
2:L:85:THR:HB	2:L:217:ASN:ND2	2.30	0.47
2:L:154:PHE:HA	2:L:355:VAL:HA	1.98	0.46
2:L:23:TYR:HB3	2:L:116:SER:HB3	1.97	0.46
2:L:124:ALA:HB2	2:L:165:VAL:HG13	1.97	0.46
4:I:841:NAG:H61	4:I:842:NAG:H82	1.97	0.46
1:I:198:ILE:HG23	1:I:370:LYS:HD3	1.97	0.46
2:L:273:PRO:HA	2:L:280:THR:HG22	1.96	0.46
2:L:147:PHE:HB3	2:L:173:LEU:HD12	1.98	0.46
1:I:320:MET:HA	1:I:321:PRO:HD3	1.86	0.45
1:I:332:LYS:O	1:I:336:GLN:HB2	2.15	0.45
2:L:173:LEU:HB3	2:L:182:SER:OG	2.16	0.45
1:I:173:LEU:HD13	1:I:182:SER:HB3	1.97	0.45
1:I:411:PHE:CE2	1:I:423:MET:HE3	2.51	0.45
1:I:407:PRO:HA	1:I:426:VAL:O	2.17	0.45
1:I:248:SER:O	1:I:430:CYS:HB3	2.17	0.45
1:I:201:VAL:HG22	7:I:2011:HOH:O	2.16	0.45
1:I:285:LEU:HD12	1:I:286:PRO:HD2	1.98	0.44
2:L:239:PHE:O	2:L:246:SER:HA	2.17	0.44
1:I:390:ILE:HG12	2:L:319:HIS:CD2	2.53	0.44
1:I:294:LYS:O	1:I:298:GLU:HG3	2.16	0.44
1:I:101:GLN:HG2	1:I:339:GLY:O	2.17	0.44
1:I:114:LYS:HZ3	1:I:118:GLN:HE22	1.65	0.44
2:L:200:ASP:O	2:L:201:VAL:C	2.56	0.44
2:L:202:ILE:HA	2:L:203:PRO:HD2	1.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:148:GLY:O	1:I:172:PRO:HA	2.18	0.44
1:I:380:CYF:O4	1:I:380:CYF:C12	2.66	0.44
1:I:79:SER:OG	1:I:219:ILE:HG13	2.18	0.44
1:I:390:ILE:HG12	2:L:319:HIS:HD2	1.83	0.43
1:I:396:ASN:OD1	1:I:397:PRO:HD2	2.19	0.43
1:I:374:GLU:HB3	1:I:380:CYF:OL	2.18	0.43
2:L:190:VAL:HG21	2:L:201:VAL:HG21	2.00	0.43
1:I:155:ASN:HB3	1:I:158:TYR:HB2	2.00	0.43
2:L:60:THR:O	2:L:64:GLN:HG3	2.19	0.43
2:L:95:CYS:HB3	2:L:96:ASN:OD1	2.18	0.43
2:L:410:VAL:CG2	2:L:426:VAL:HG23	2.48	0.43
1:I:281:MET:HE3	1:I:283:LEU:HD21	2.01	0.43
2:L:24:ARG:HA	2:L:114:LYS:O	2.18	0.43
2:L:57:ARG:HB2	2:L:57:ARG:HE	1.57	0.43
2:L:157:THR:O	2:L:158:TYR:C	2.55	0.43
2:L:261:ARG:HG2	2:L:310:GLU:HG2	2.01	0.42
2:L:65:HIS:CE1	2:L:338:MET:HG2	2.54	0.42
1:I:60:THR:O	1:I:64:GLN:HG3	2.19	0.42
1:I:202:ILE:HA	1:I:203:PRO:HD2	1.92	0.42
2:L:154:PHE:O	2:L:155:ASN:C	2.57	0.42
1:I:287:LYS:HG3	1:I:290:LYS:H	1.84	0.42
1:I:123:PHE:O	1:I:124:ALA:C	2.58	0.42
2:L:331:LEU:HB2	2:L:335:LEU:HD12	2.02	0.42
1:I:324:ARG:HE	1:I:374:GLU:CD	2.23	0.42
2:L:89:MET:SD	2:L:144:ASN:HB3	2.59	0.41
2:L:77:PHE:CZ	2:L:422:PHE:HB3	2.55	0.41
2:L:365:SER:OG	2:L:389:VAL:HG22	2.19	0.41
1:I:198:ILE:HG21	1:I:201:VAL:HG13	2.02	0.41
2:L:23:TYR:CZ	2:L:100:GLN:HG3	2.56	0.41
2:L:257:LYS:HA	2:L:314:MET:O	2.20	0.41
2:L:415:VAL:HB	2:L:416:PRO:HD3	2.02	0.41
1:I:16:PRO:HD2	1:I:161:ILE:HD11	2.01	0.41
1:I:361:ASP:O	1:I:362:LEU:C	2.59	0.41
1:I:81:LEU:O	1:I:82:SER:C	2.59	0.41
1:I:380:CYF:OL	1:I:380:CYF:C16	2.67	0.41
2:L:60:THR:HG21	2:L:300:THR:HA	2.03	0.41
2:L:415:VAL:N	2:L:416:PRO:HD2	2.36	0.41
2:L:270:LEU:HD21	2:L:272:LEU:HD21	2.03	0.41
2:L:107:LYS:O	2:L:110:THR:HB	2.21	0.41
2:L:230:SER:HA	2:L:231:PRO:HD3	1.84	0.41
4:I:841:NAG:H61	4:I:842:NAG:N2	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:230:SER:HB3	1:I:233:ASN:ND2	2.36	0.40
1:I:331:LEU:O	1:I:332:LYS:C	2.60	0.40
2:L:143:ALA:O	2:L:218:THR:HB	2.21	0.40
2:L:257:LYS:HD2	2:L:315:MET:HG2	2.02	0.40
1:I:417:LEU:HB2	1:I:419:THR:HG23	2.04	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	413/432 (96%)	364 (88%)	40 (10%)	9 (2%)	8	27
2	L	403/432 (93%)	349 (87%)	49 (12%)	5 (1%)	16	44
All	All	816/864 (94%)	713 (87%)	89 (11%)	14 (2%)	11	35

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	174	ASP
1	I	362	LEU
1	I	19	PRO
1	I	159	GLN
2	L	418	ASN
1	I	26	PRO
1	I	365	SER
1	I	137	SER
1	I	332	LYS
2	L	19	PRO
2	L	400	VAL
2	L	352	PRO
1	I	83	ILE

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Mol	Chain	Res	Type
2	L	355	VAL

### 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	I	353/382 (92%)	320 (91%)	33 (9%)	11	29
2	L	323/383 (84%)	278 (86%)	45 (14%)	4	11
All	All	676/765 (88%)	598 (88%)	78 (12%)	7	19

All (78) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	I	17	MET
1	I	22	ILE
1	I	24	ARG
1	I	69	SER
1	I	73	ASN
1	I	91	LYS
1	I	101	GLN
1	I	125	LYS
1	I	128	CYS
1	I	132	ARG
1	I	138	SER
1	I	153	THR
1	I	158	TYR
1	I	197	ARG
1	I	199	THR
1	I	201	VAL
1	I	216	VAL
1	I	219	ILE
1	I	230	SER
1	I	235	ARG
1	I	316	LEU
1	I	322	ARG

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Mol	Chain	Res	Type
1	I	324	ARG
1	I	327	ASP
1	I	330	SER
1	I	337	ASP
1	I	345	SER
1	I	359	ARG
1	I	376	ASN
1	I	381	GLU
1	I	385	SER
1	I	419	THR
1	I	430	CYS
2	L	9	THR
2	L	22	ILE
2	L	44	THR
2	L	47	ARG
2	L	57	ARG
2	L	78	LEU
2	L	84	SER
2	L	95	CYS
2	L	97	ASP
2	L	107	LYS
2	L	115	THR
2	L	116	SER
2	L	120	HIS
2	L	123	PHE
2	L	129	ARG
2	L	150	LYS
2	L	152	LEU
2	L	155	ASN
2	L	182	SER
2	L	183	ARG
2	L	188	LYS
2	L	199	THR
2	L	210	LEU
2	L	218	THR
2	L	238	LEU
2	L	257	LYS
2	L	262	ARG
2	L	263	VAL
2	L	265	GLU
2	L	285	LEU
2	L	310	GLU

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Mol	Chain	Res	Type
2	L	314	MET
2	L	316	LEU
2	L	330	SER
2	L	331	LEU
2	L	341	VAL
2	L	342	ASP
2	L	352	PRO
2	L	380	SER
2	L	389	VAL
2	L	395	LEU
2	L	410	VAL
2	L	418	ASN
2	L	423	MET
2	L	428	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	I	71	ASN
1	I	118	GLN
1	I	233	ASN
1	I	254	GLN
1	I	268	GLN
1	I	305	GLN
1	I	376	ASN
1	I	418	ASN
2	L	71	ASN
2	L	100	GLN
2	L	254	GLN
2	L	319	HIS
2	L	336	GLN
2	L	369	HIS
2	L	418	ASN
2	L	428	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.



## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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$
1	CYF	I	380	1	34,38,39	3.03	9 (26%)	42,54,56	2.45	12 (28%)

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
1	CYF	I	380	1	1/1/4/6	0/14/32/34	0/4/4/4

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	380	CYF	C14-C10	-9.11	1.41	1.53
1	I	380	CYF	C9-C10	-8.85	1.38	1.52
1	I	380	CYF	C11-C10	-7.04	1.41	1.52
1	I	380	CYF	O1-C1	-5.29	1.24	1.37
1	I	380	CYF	O3-C6	-5.15	1.24	1.37
1	I	380	CYF	C18-C19	2.15	1.43	1.39
1	I	380	CYF	CAL-SG	2.20	1.86	1.81
1	I	380	CYF	C19-C14	2.38	1.44	1.40
1	I	380	CYF	O2-C3	4.01	1.44	1.38

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	380	CYF	OL-CL-CAL	-3.90	114.45	121.46
1	I	380	CYF	C4-O2-C3	-3.39	110.58	118.53
1	I	380	CYF	C8-C9-C10	-2.54	122.08	126.02
1	I	380	CYF	C12-C11-C10	-2.52	122.11	126.02
1	I	380	CYF	O2-C4-C5	-2.34	111.54	115.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	380	CYF	C18-C17-NL	2.15	127.06	120.13
1	I	380	CYF	C14-C10-C11	2.65	117.97	112.71
1	I	380	CYF	O2-C3-C11	3.06	124.90	122.54
1	I	380	CYF	CAL-CL-NL	4.18	120.15	114.52
1	I	380	CYF	C14-C10-C9	4.83	122.29	112.71
1	I	380	CYF	O2-C4-C9	6.16	127.31	122.54
1	I	380	CYF	C11-C10-C9	8.97	119.20	105.87

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	I	380	CYF	C10

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	I	380	CYF	7	0

## 5.5 Carbohydrates ⓘ

8 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	1.20	1 (7%)	15,19,21	0.64	0
4	NAG	I	842	4	14,14,15	1.17	1 (7%)	15,19,21	0.67	0
4	NAG	L	841	2,4	14,14,15	1.44	3 (21%)	15,19,21	1.40	1 (6%)
4	NAG	L	842	4	14,14,15	1.43	2 (14%)	15,19,21	1.66	3 (20%)
6	NAG	L	861	2,6	14,14,15	1.29	1 (7%)	15,19,21	0.89	1 (6%)
6	NAG	L	862	6	14,14,15	1.29	1 (7%)	15,19,21	1.92	2 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	BMA	L	863	6	11,11,12	0.95	1 (9%)	14,15,17	1.88	2 (14%)
6	BMA	L	864	6	11,11,12	1.36	2 (18%)	14,15,17	3.74	2 (14%)

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	841	2,4	-	0/6/23/26	0/1/1/1
4	NAG	L	842	4	-	0/6/23/26	0/1/1/1
6	NAG	L	861	2,6	-	0/6/23/26	0/1/1/1
6	NAG	L	862	6	-	0/6/23/26	0/1/1/1
6	BMA	L	863	6	-	0/2/19/22	0/1/1/1
6	BMA	L	864	6	-	0/2/19/22	0/1/1/1

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	861	NAG	O7-C7	-3.65	1.14	1.23
6	L	862	NAG	O7-C7	-3.64	1.14	1.23
4	L	841	NAG	O7-C7	-3.64	1.14	1.23
4	L	842	NAG	O7-C7	-3.56	1.15	1.23
4	I	842	NAG	O7-C7	-3.55	1.15	1.23
6	L	864	BMA	O5-C1	-3.50	1.37	1.43
4	I	841	NAG	O7-C7	-3.41	1.15	1.23
6	L	864	BMA	O5-C5	-2.19	1.38	1.43
6	L	863	BMA	O5-C1	-2.02	1.40	1.43
4	L	841	NAG	C2-N2	2.06	1.50	1.46
4	L	841	NAG	C4-C3	2.14	1.58	1.52
4	L	842	NAG	C1-C2	2.76	1.56	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	L	842	NAG	C4-C3-C2	-4.32	104.51	111.23
4	L	841	NAG	O4-C4-C3	-3.81	101.77	110.34
6	L	863	BMA	O3-C3-C2	-3.27	104.09	110.00
6	L	861	NAG	C4-C3-C2	2.50	115.11	111.23
4	L	842	NAG	C3-C2-N2	2.64	116.87	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	862	NAG	C2-N2-C7	2.79	126.63	123.04
6	L	864	BMA	O5-C1-C2	3.21	116.07	110.86
4	L	842	NAG	C1-O5-C5	3.30	116.44	112.25
6	L	863	BMA	C1-O5-C5	5.30	118.98	112.25
6	L	862	NAG	C1-O5-C5	5.79	119.59	112.25
6	L	864	BMA	C1-O5-C5	13.08	128.85	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	I	841	NAG	2	0
4	I	842	NAG	2	0
4	L	842	NAG	1	0
6	L	862	NAG	1	0
6	L	863	BMA	1	0

## 5.6 Ligand geometry

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	1.16	1 (7%)	15,19,21	1.03	1 (6%)
3	NAG	I	861	1	14,14,15	1.20	1 (7%)	15,19,21	1.66	1 (6%)
5	GOL	I	901	-	5,5,5	0.65	0	5,5,5	0.55	0
3	NAG	L	801	2	14,14,15	1.27	2 (14%)	15,19,21	1.07	1 (6%)
5	GOL	L	901	-	5,5,5	0.72	0	5,5,5	0.71	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	801	2	-	0/6/23/26	0/1/1/1
5	GOL	L	901	-	-	0/4/4/4	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	801	NAG	O7-C7	-3.65	1.14	1.23
3	I	801	NAG	O7-C7	-3.57	1.14	1.23
3	I	861	NAG	O7-C7	-3.54	1.15	1.23
3	L	801	NAG	C1-C2	-2.12	1.49	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	801	NAG	C1-O5-C5	2.37	115.26	112.25
3	L	801	NAG	C2-N2-C7	2.82	126.66	123.04
3	I	861	NAG	C1-O5-C5	5.41	119.12	112.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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	I	417/432 (96%)	-0.43	4 (0%) 84 81	27, 57, 100, 148	0
2	L	407/432 (94%)	-0.28	11 (2%) 58 52	28, 59, 123, 148	0
All	All	824/864 (95%)	-0.36	15 (1%) 71 68	27, 58, 115, 148	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	L	135	ASN	4.2
2	L	398	ASN	3.9
2	L	402	PHE	3.9
2	L	242	ALA	3.4
2	L	400	VAL	3.2
1	I	18	ASN	3.0
2	L	396	ASN	2.6
2	L	18	ASN	2.5
2	L	49	TRP	2.5
1	I	134	ALA	2.4
2	L	397	PRO	2.3
1	I	40	ILE	2.2
2	L	243	ASP	2.2
1	I	41	PRO	2.2
2	L	399	ARG	2.1

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

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
1	CYF	I	380	35/36	0.89	0.21	-	36,65,77,82	0

### 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<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
4	NAG	I	841	14/15	0.93	0.21	1.03	78,82,92,100	0
4	NAG	L	841	14/15	0.93	0.21	0.15	70,88,103,109	0
4	NAG	I	842	14/15	0.70	0.45	-	107,118,125,125	0
6	NAG	L	862	14/15	0.86	0.45	-	124,128,133,135	0
4	NAG	L	842	14/15	0.76	0.35	-	120,126,132,133	0
6	BMA	L	864	11/12	0.77	0.33	-	140,141,143,143	0
6	BMA	L	863	11/12	0.79	0.44	-	137,139,145,148	0
6	NAG	L	861	14/15	0.84	0.32	-	93,101,109,116	0

### 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
5	GOL	I	901	6/6	0.92	0.21	2.56	50,52,56,58	0
5	GOL	L	901	6/6	0.94	0.15	0.17	61,65,69,70	0
3	NAG	I	801	14/15	0.79	0.41	-	121,128,135,138	0
3	NAG	I	861	14/15	0.80	0.43	-	112,118,121,124	0
3	NAG	L	801	14/15	0.73	0.29	-	110,115,122,123	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.