



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 04:46 pm GMT

PDB ID : 1JMO
Title : Crystal Structure of the Heparin Cofactor II-S195A Thrombin Complex
Authors : Baglin, T.P.; Carrell, R.W.; Esmon, C.T.; Huntington, J.A.
Deposited on : 2001-07-19
Resolution : 2.20 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

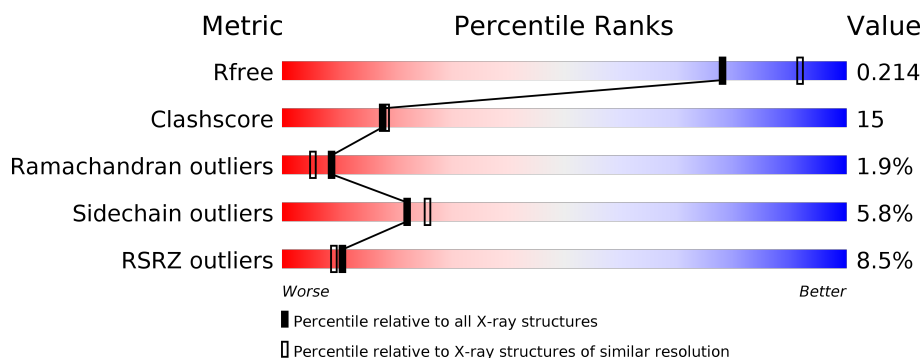
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	111664	4343 (2.20-2.20)
Clashscore	122126	5027 (2.20-2.20)
Ramachandran outliers	120053	4952 (2.20-2.20)
Sidechain outliers	120020	4953 (2.20-2.20)
RSRZ outliers	108989	4245 (2.20-2.20)

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 $\leq 5\%$. 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	L	48	<div> <div>8%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>•••</div> </div> </div>
2	H	260	<div> <div>7%</div> <div> <div></div> <div>77%</div> <div>21%</div> <div>•</div> </div> </div>
3	A	480	<div> <div>8%</div> <div> <div></div> <div>58%</div> <div>25%</div> <div>5%</div> <div>11%</div> </div> </div>

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	NDG	A	482	-	-	-	X
4	NDG	H	1	-	-	-	X
5	NAG	A	481	-	-	-	X
5	NAG	H	2	-	-	-	X
7	MPD	H	2004	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 6235 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, light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	47	Total	C	N	O	S	0	0	0
			378	237	61	79	1			

- Molecule 2 is a protein called Thrombin, heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	259	Total	C	N	O	S	2	0	0
			2092	1334	370	374	14			

There is a discrepancy between the modelled and reference sequences:

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

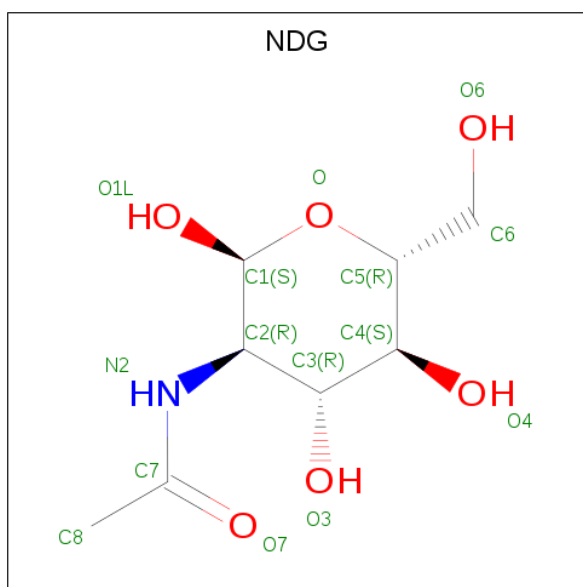
- Molecule 3 is a protein called HEPARIN COFACTOR II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	427	Total	C	N	O	S	81	0	0
			3460	2203	591	644	22			

There are 2 discrepancies between the modelled and reference sequences:

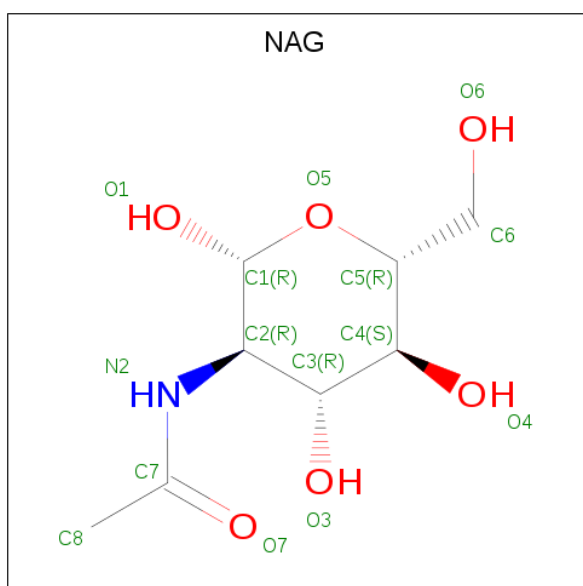
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	TYS	TYR	MODIFIED RESIDUE	UNP P05546
A	73	TYS	TYR	MODIFIED RESIDUE	UNP P05546

- Molecule 4 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).

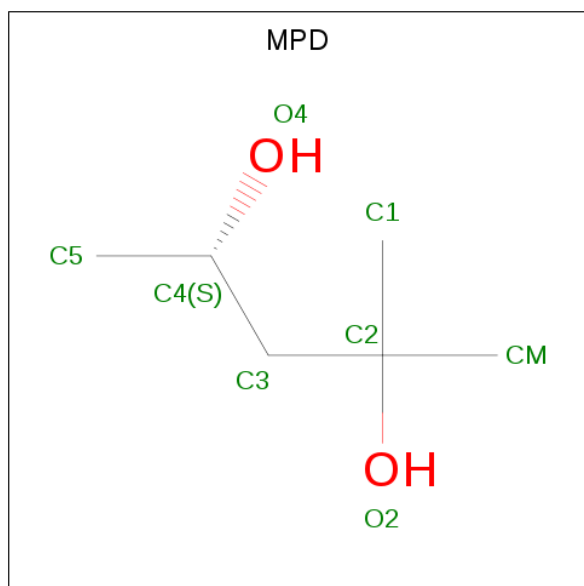


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	A	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	1	Total	Na	0	0
			1	1		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	H	1	Total	C	O	0	0
			8	6	2		
7	H	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		
7	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	39	Total	O	0	0
			39	39		
8	H	83	Total	O	0	0
			83	83		

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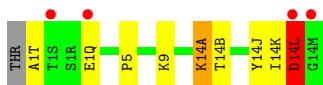
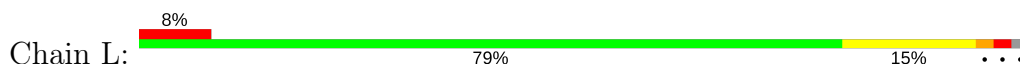
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	86	Total	O	0	0
			86	86		

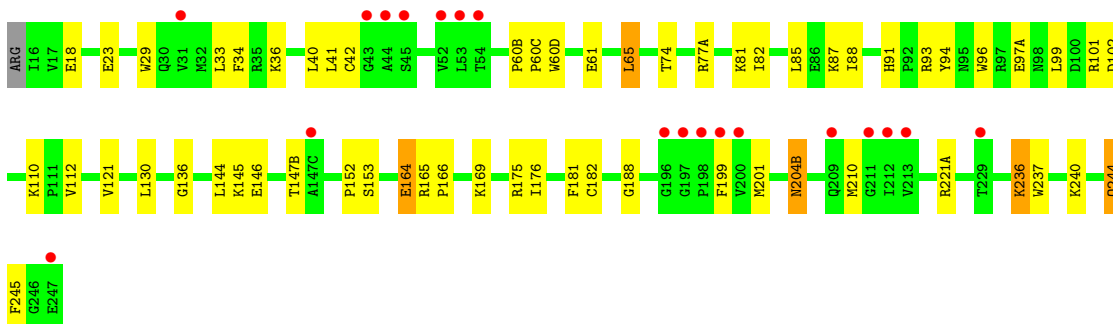
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

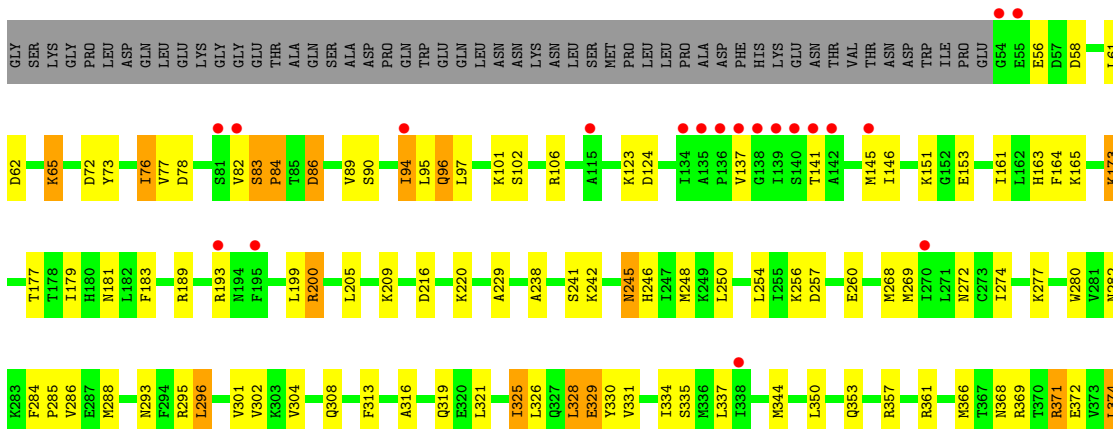
- Molecule 1: Thrombin, light chain

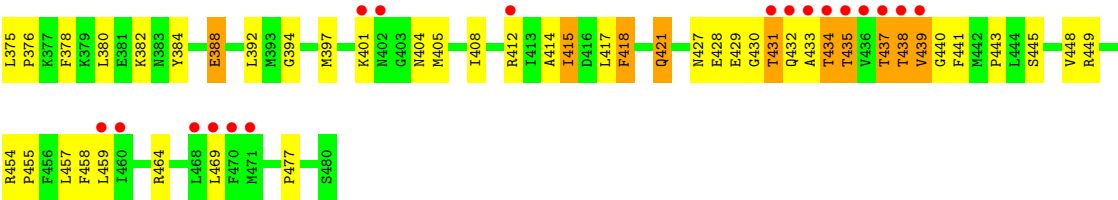


- Molecule 2: Thrombin, heavy chain



- Molecule 3: HEPARIN COFACTOR II





4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	152.31Å 152.31Å 126.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.44 – 2.20 29.43 – 2.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (29.44-2.20) 91.2 (29.43-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.20Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.205 , 0.211 0.205 , 0.214	Depositor DCC
R_{free} test set	983 reflections (1.28%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 40.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.035 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6235	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MPD, NAG, NDG, TYS

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	L	0.40	0/385	0.77	1/516 (0.2%)
2	H	0.35	0/2147	0.65	0/2902
3	A	0.34	0/3491	0.63	1/4704 (0.0%)
All	All	0.35	0/6023	0.64	2/8122 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	14(L)	ASP	N-CA-C	7.17	130.36	111.00
3	A	229	ALA	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	378	0	356	6	0
2	H	2092	0	2063	43	0
3	A	3460	0	3464	132	0
4	A	14	0	13	6	0
4	H	14	0	12	1	0
5	A	14	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	H	14	0	13	1	0
6	H	1	0	0	0	0
7	A	24	0	42	1	0
7	H	16	0	28	4	0
8	A	86	0	0	5	0
8	H	83	0	0	1	0
8	L	39	0	0	0	0
All	All	6235	0	6004	173	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 15.

All (173) 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)
3:A:96:GLN:HE21	3:A:357:ARG:HH22	1.03	0.99
2:H:61:GLU:HG2	2:H:87:LYS:HA	1.51	0.92
2:H:181:PHE:HA	7:H:2003:MPD:H53	1.52	0.89
3:A:96:GLN:HE21	3:A:357:ARG:NH2	1.75	0.84
3:A:151:LYS:HB2	3:A:404:ASN:ND2	1.93	0.83
4:H:1:NDG:H6C2	5:H:2:NAG:O5	1.83	0.79
3:A:448:VAL:HG12	8:A:2057:HOH:O	1.84	0.78
3:A:439:VAL:HG12	3:A:440:GLY:H	1.52	0.75
1:L:14(A):LYS:HG3	2:H:23:GLU:OE2	1.87	0.75
3:A:321:LEU:HD22	3:A:353:GLN:NE2	2.01	0.75
3:A:372:GLU:HB2	3:A:449:ARG:HG2	1.70	0.74
3:A:325:ILE:HD13	3:A:326:LEU:N	2.03	0.73
1:L:14(J):TYR:O	1:L:14(L):ASP:N	2.21	0.73
3:A:76:ILE:HD13	3:A:77:VAL:N	2.03	0.73
3:A:368:ASN:HB2	4:A:482:NDG:HA	1.54	0.72
2:H:77(A):ARG:HH11	2:H:77(A):ARG:HG3	1.55	0.71
3:A:448:VAL:HG11	8:A:2072:HOH:O	1.92	0.70
3:A:151:LYS:HB2	3:A:404:ASN:HD21	1.58	0.69
3:A:248:MET:SD	3:A:256:LYS:HB3	2.33	0.69
3:A:325:ILE:HD11	3:A:337:LEU:CD1	2.23	0.68
3:A:439:VAL:HG12	3:A:440:GLY:N	2.09	0.67
3:A:401:LYS:HG2	3:A:414:ALA:HB2	1.77	0.66
2:H:61:GLU:CG	2:H:87:LYS:HA	2.25	0.66
2:H:81:LYS:HG2	2:H:112:VAL:HG23	1.80	0.64
1:L:1(T):ALA:O	1:L:1(Q):GLU:HG2	1.98	0.64
3:A:137:VAL:O	3:A:141:THR:HG23	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:96:GLN:NE2	3:A:357:ARG:HH22	1.87	0.64
2:H:85:LEU:HD13	2:H:88:ILE:HD11	1.80	0.63
3:A:295:ARG:HG2	3:A:344:MET:CE	2.28	0.63
3:A:454:ARG:HG3	3:A:454:ARG:HH11	1.64	0.63
3:A:368:ASN:CB	4:A:482:NDG:HA	2.12	0.63
3:A:268:MET:HE2	3:A:415:ILE:HB	1.82	0.61
3:A:62:ASP:OD2	3:A:65:LYS:HB2	2.01	0.61
3:A:329:GLU:OE2	3:A:335:SER:HB3	2.00	0.60
3:A:293:ASN:HB3	3:A:301:VAL:HG21	1.83	0.60
2:H:42:CYS:SG	3:A:445:SER:HB2	2.42	0.60
3:A:200:ARG:HH11	3:A:200:ARG:HG3	1.66	0.59
3:A:308:GLN:HG3	3:A:374:LEU:HD22	1.82	0.59
3:A:295:ARG:O	3:A:455:PRO:HD3	2.03	0.59
3:A:153:GLU:HB3	3:A:397:MET:SD	2.42	0.59
3:A:325:ILE:HD11	3:A:337:LEU:HD11	1.84	0.58
3:A:321:LEU:HD22	3:A:353:GLN:HE21	1.68	0.58
2:H:97(A):GLU:OE2	2:H:175:ARG:HD3	2.03	0.58
2:H:169:LYS:HA	2:H:176:ILE:HD12	1.85	0.57
3:A:330:TYR:HB2	3:A:334:ILE:HG13	1.86	0.57
3:A:325:ILE:C	3:A:325:ILE:HD13	2.24	0.57
3:A:173:LYS:NZ	3:A:173:LYS:HB3	2.20	0.57
3:A:285:PRO:HG2	3:A:288:MET:CG	2.35	0.57
3:A:435:THR:HG22	3:A:437:THR:HG22	1.87	0.56
3:A:368:ASN:CG	4:A:482:NDG:HA	2.09	0.56
3:A:96:GLN:NE2	3:A:357:ARG:NH2	2.51	0.56
2:H:77(A):ARG:HG3	2:H:77(A):ARG:NH1	2.21	0.56
3:A:433:ALA:O	3:A:434:THR:OG1	2.18	0.55
2:H:36:LYS:HG3	2:H:65:LEU:CD2	2.36	0.55
2:H:153:SER:HB2	3:A:56:GLU:HG3	1.89	0.55
3:A:285:PRO:HG2	3:A:288:MET:HG3	1.89	0.54
2:H:36:LYS:HG3	2:H:65:LEU:HD22	1.91	0.53
3:A:304:VAL:HG11	3:A:477:PRO:HG2	1.91	0.53
3:A:293:ASN:HB3	3:A:301:VAL:CG2	2.39	0.53
3:A:193:ARG:HH11	3:A:193:ARG:HG2	1.74	0.53
1:L:14(A):LYS:HD2	1:L:14(B):THR:HG23	1.91	0.53
3:A:286:VAL:HG12	3:A:428:GLU:HG3	1.90	0.53
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.91	0.53
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.44	0.53
3:A:382:LYS:O	3:A:421:GLN:HG2	2.09	0.52
2:H:99:LEU:HG	3:A:441:PHE:HZ	1.73	0.52
3:A:163:HIS:HA	8:A:2078:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:58:ASP:O	3:A:295:ARG:NH1	2.43	0.52
3:A:331:VAL:HG21	3:A:431:THR:HG23	1.92	0.52
3:A:325:ILE:HD11	3:A:337:LEU:HG	1.92	0.52
3:A:368:ASN:HB2	4:A:482:NDG:N2	2.23	0.52
3:A:435:THR:CG2	3:A:437:THR:HG22	2.39	0.52
3:A:200:ARG:HG3	3:A:200:ARG:NH1	2.25	0.52
2:H:240:LYS:HD2	7:H:2004:MPD:HM2	1.92	0.52
2:H:82:ILE:HD13	3:A:61:LEU:HD13	1.92	0.52
3:A:432:GLN:HG2	3:A:433:ALA:H	1.75	0.52
3:A:369:ARG:O	3:A:371:ARG:HD2	2.10	0.51
3:A:238:ALA:O	3:A:242:LYS:HG3	2.11	0.51
3:A:141:THR:HG22	3:A:183:PHE:CD1	2.46	0.51
2:H:99:LEU:O	2:H:102:ASP:HB2	2.11	0.50
3:A:439:VAL:CG1	3:A:440:GLY:H	2.17	0.50
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.46	0.50
3:A:257:ASP:HB3	3:A:260:GLU:HG3	1.94	0.49
2:H:144:LEU:HD21	2:H:152:PRO:HB3	1.93	0.49
3:A:401:LYS:CG	3:A:414:ALA:HB2	2.42	0.49
3:A:209:LYS:HE2	8:A:2063:HOH:O	2.11	0.49
3:A:350:LEU:CD1	3:A:457:LEU:HD12	2.43	0.49
2:H:204(B):ASN:HD22	2:H:204(B):ASN:C	2.15	0.48
3:A:325:ILE:HD11	3:A:337:LEU:CG	2.43	0.48
2:H:99:LEU:HD11	3:A:443:PRO:HB3	1.95	0.48
3:A:325:ILE:HD12	3:A:366:MET:SD	2.52	0.48
2:H:165:ARG:HB2	2:H:166:PRO:HD3	1.94	0.48
2:H:201:MET:SD	2:H:210:MET:HG3	2.54	0.47
3:A:164:PHE:HB3	3:A:179:ILE:CD1	2.44	0.47
2:H:164:GLU:CD	2:H:164:GLU:H	2.17	0.47
3:A:269:MET:HA	3:A:415:ILE:HD13	1.97	0.47
3:A:189:ARG:NH1	3:A:464:ARG:HD3	2.30	0.47
3:A:177:THR:HG22	3:A:181:ASN:ND2	2.29	0.47
3:A:295:ARG:HG2	3:A:344:MET:SD	2.55	0.47
3:A:418:PHE:C	3:A:418:PHE:CD2	2.87	0.47
3:A:418:PHE:C	3:A:418:PHE:HD2	2.18	0.47
3:A:62:ASP:CG	3:A:65:LYS:HB2	2.35	0.47
3:A:284:PHE:O	3:A:428:GLU:HB2	2.14	0.46
1:L:5:PRO:HA	1:L:9:LYS:HG3	1.97	0.46
3:A:76:ILE:HD12	3:A:78:ASP:OD1	2.15	0.46
3:A:384:TYR:HD2	7:A:2002:MPD:HM1	1.81	0.46
3:A:141:THR:HG22	3:A:183:PHE:CE1	2.51	0.46
3:A:295:ARG:HG2	3:A:344:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:438:THR:HG23	3:A:438:THR:O	2.16	0.45
3:A:280:TRP:CZ3	3:A:328:LEU:HB3	2.52	0.45
2:H:237:TRP:HB2	7:H:2004:MPD:H53	1.97	0.45
3:A:164:PHE:HB3	3:A:179:ILE:HD13	1.98	0.45
3:A:246:HIS:O	3:A:250:LEU:HG	2.17	0.45
3:A:295:ARG:HB3	3:A:454:ARG:HG2	1.97	0.45
3:A:73:TYS:O2	3:A:73:TYS:HE2	2.15	0.45
3:A:350:LEU:C	3:A:350:LEU:HD13	2.37	0.45
3:A:405:MET:HE1	3:A:408:ILE:HD12	1.99	0.45
3:A:454:ARG:HG3	3:A:454:ARG:NH1	2.31	0.45
2:H:29:TRP:CG	2:H:121:VAL:HB	2.52	0.45
3:A:375:LEU:HD12	3:A:376:PRO:HD2	1.98	0.45
3:A:434:THR:O	3:A:435:THR:O	2.35	0.45
2:H:60(B):PRO:HB2	2:H:60(C):PRO:HD3	1.99	0.45
3:A:216:ASP:O	3:A:220:LYS:HD3	2.16	0.44
2:H:244:GLN:HG3	2:H:245:PHE:CD2	2.53	0.44
3:A:102:SER:O	3:A:106:ARG:HG3	2.17	0.44
3:A:296:LEU:HD13	3:A:302:VAL:HG12	1.99	0.44
2:H:145:LYS:NZ	2:H:147(B):THR:OG1	2.48	0.44
3:A:440:GLY:O	3:A:441:PHE:C	2.56	0.44
3:A:412:ARG:HG2	3:A:412:ARG:HH11	1.83	0.44
3:A:161:ILE:HD11	3:A:394:GLY:HA3	2.00	0.44
3:A:321:LEU:HG	3:A:361:ARG:HH22	1.83	0.44
3:A:427:ASN:HB2	3:A:428:GLU:OE1	2.18	0.44
3:A:388:GLU:HB2	8:A:2036:HOH:O	2.18	0.43
3:A:412:ARG:HG2	3:A:412:ARG:NH1	2.33	0.43
2:H:145:LYS:HE3	2:H:145:LYS:HB2	1.74	0.43
3:A:368:ASN:CG	4:A:482:NDG:N2	2.67	0.43
3:A:428:GLU:H	3:A:428:GLU:CD	2.22	0.43
2:H:91:HIS:CE1	2:H:101:ARG:HD3	2.54	0.43
2:H:74:THR:HB	3:A:58:ASP:HA	2.00	0.43
3:A:388:GLU:HA	3:A:388:GLU:OE1	2.18	0.43
3:A:282:ASN:HD22	3:A:313:PHE:HE1	1.66	0.43
2:H:240:LYS:HB2	7:H:2004:MPD:HM2	2.01	0.43
2:H:93:ARG:HB2	2:H:101:ARG:HD2	2.01	0.42
3:A:193:ARG:NH1	3:A:193:ARG:HG2	2.35	0.42
3:A:316:ALA:HB2	3:A:366:MET:HA	2.02	0.42
2:H:61:GLU:H	2:H:61:GLU:CD	2.22	0.42
3:A:316:ALA:HB2	3:A:366:MET:HG2	2.01	0.42
3:A:337:LEU:O	3:A:458:PHE:HA	2.19	0.42
3:A:145:MET:HE1	3:A:205:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:241:SER:O	3:A:245:ASN:HB2	2.19	0.42
3:A:94:ILE:C	3:A:95:LEU:HD22	2.40	0.42
3:A:368:ASN:CB	4:A:482:NDG:N2	2.82	0.42
2:H:40:LEU:HD12	2:H:41:LEU:N	2.35	0.42
3:A:378:PHE:HD1	3:A:380:LEU:HD13	1.85	0.41
2:H:236:LYS:HB2	8:H:2042:HOH:O	2.19	0.41
3:A:274:ILE:N	3:A:274:ILE:HD12	2.34	0.41
3:A:415:ILE:HD12	3:A:417:LEU:H	1.86	0.41
2:H:110:LYS:NZ	3:A:72:ASP:OD1	2.54	0.41
3:A:97:LEU:O	3:A:101:LYS:HG3	2.21	0.41
3:A:123:LYS:HG3	3:A:124:ASP:N	2.35	0.41
3:A:257:ASP:HB3	3:A:260:GLU:CG	2.50	0.41
3:A:350:LEU:HD12	3:A:457:LEU:CD1	2.51	0.41
3:A:430:GLY:O	3:A:431:THR:O	2.39	0.41
2:H:60(D):TRP:CH2	3:A:443:PRO:HG2	2.56	0.41
1:L:14(A):LYS:H	1:L:14(A):LYS:HG3	1.71	0.41
3:A:277:LYS:NZ	3:A:429:GLU:OE2	2.52	0.41
2:H:146:GLU:OE2	2:H:221(A):ARG:NH2	2.54	0.41
3:A:401:LYS:O	3:A:412:ARG:NH1	2.54	0.41
3:A:165:LYS:HE2	3:A:165:LYS:HB3	1.82	0.40
3:A:448:VAL:HG13	3:A:448:VAL:O	2.20	0.40
3:A:405:MET:CE	3:A:408:ILE:HD12	2.51	0.40
3:A:94:ILE:HG22	3:A:95:LEU:N	2.35	0.40
3:A:95:LEU:C	3:A:97:LEU:H	2.24	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	L	45/48 (94%)	42 (93%)	1 (2%)	2 (4%)	3 1

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	257/260 (99%)	245 (95%)	12 (5%)	0	100	100
3	A	423/480 (88%)	394 (93%)	17 (4%)	12 (3%)	5	2
All	All	725/788 (92%)	681 (94%)	30 (4%)	14 (2%)	9	5

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	14(L)	ASP
3	A	82	VAL
3	A	84	PRO
3	A	431	THR
3	A	434	THR
3	A	435	THR
3	A	438	THR
1	L	14(K)	ILE
3	A	94	ILE
3	A	83	SER
3	A	86	ASP
3	A	90	SER
3	A	439	VAL
3	A	89	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	L	41/42 (98%)	40 (98%)	1 (2%)	52	65
2	H	224/225 (100%)	215 (96%)	9 (4%)	34	43
3	A	385/431 (89%)	357 (93%)	28 (7%)	15	16
All	All	650/698 (93%)	612 (94%)	38 (6%)	22	26

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	14(A)	LYS
2	H	33	LEU
2	H	34	PHE
2	H	65	LEU
2	H	130	LEU
2	H	164	GLU
2	H	182	CYS
2	H	204(B)	ASN
2	H	236	LYS
2	H	244	GLN
3	A	65	LYS
3	A	76	ILE
3	A	83	SER
3	A	84	PRO
3	A	86	ASP
3	A	96	GLN
3	A	146	ILE
3	A	173	LYS
3	A	199	LEU
3	A	200	ARG
3	A	245	ASN
3	A	254	LEU
3	A	272	ASN
3	A	296	LEU
3	A	319	GLN
3	A	325	ILE
3	A	328	LEU
3	A	329	GLU
3	A	371	ARG
3	A	374	LEU
3	A	388	GLU
3	A	392	LEU
3	A	415	ILE
3	A	418	PHE
3	A	421	GLN
3	A	437	THR
3	A	459	LEU
3	A	469	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	1(O)	GLN

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Mol	Chain	Res	Type
2	H	71	HIS
2	H	156	GLN
2	H	204(B)	ASN
2	H	239	GLN
2	H	244	GLN
3	A	96	GLN
3	A	181	ASN
3	A	353	GLN
3	A	363	GLN
3	A	404	ASN
3	A	411	GLN
3	A	447	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	TYS	A	60	3	15,16,17	2.66	1 (6%)	19,22,24	0.83	1 (5%)
3	TYS	A	73	3	15,16,17	2.77	2 (13%)	19,22,24	0.74	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	TYS	A	60	3	-	0/9/11/13	0/1/1/1
3	TYS	A	73	3	-	0/9/11/13	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	73	TYS	OH-CZ	-10.24	1.26	1.42
3	A	60	TYS	OH-CZ	-9.74	1.27	1.42
3	A	73	TYS	CA-C	2.07	1.53	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	60	TYS	OH-S-O2	2.08	113.47	107.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	73	TYS	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 1 is monoatomic - leaving 9 for Mogul analysis.

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	$\# Z > 2$
7	MPD	A	2001	-	7,7,7	0.50	0	9,10,10	0.58	0
7	MPD	A	2002	-	7,7,7	0.56	0	9,10,10	0.46	0
7	MPD	A	2005	-	7,7,7	0.47	0	9,10,10	0.49	0
5	NAG	A	481	3	14,14,15	0.52	0	17,19,21	0.87	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NDG	A	482	3	14,14,15	0.75	1 (7%)	17,19,21	0.83	1 (5%)
4	NDG	H	1	2,5	14,14,15	0.90	0	17,19,21	0.89	1 (5%)
5	NAG	H	2	4	14,14,15	0.61	0	17,19,21	1.11	2 (11%)
7	MPD	H	2003	-	7,7,7	0.39	0	9,10,10	0.47	0
7	MPD	H	2004	-	7,7,7	0.39	0	9,10,10	0.50	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
7	MPD	A	2001	-	-	0/5/5/5	0/0/0/0
7	MPD	A	2002	-	-	0/5/5/5	0/0/0/0
7	MPD	A	2005	-	-	0/5/5/5	0/0/0/0
5	NAG	A	481	3	-	0/6/23/26	0/1/1/1
4	NDG	A	482	3	-	0/6/23/26	0/1/1/1
4	NDG	H	1	2,5	-	0/6/23/26	0/1/1/1
5	NAG	H	2	4	-	0/6/23/26	0/1/1/1
7	MPD	H	2003	-	-	0/5/5/5	0/0/0/0
7	MPD	H	2004	-	-	0/5/5/5	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	482	NDG	C1-C2	2.07	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	H	2	NAG	O5-C1-C2	-2.80	107.66	111.52
5	H	2	NAG	C2-N2-C7	-2.08	119.92	122.94
5	A	481	NAG	C2-N2-C7	-2.05	119.95	122.94
4	A	482	NDG	C2-N2-C7	-2.05	119.96	122.94
4	H	1	NDG	O4-C4-C5	2.16	114.70	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	2002	MPD	1	0
4	A	482	NDG	6	0
4	H	1	NDG	1	0
5	H	2	NAG	1	0
7	H	2003	MPD	1	0
7	H	2004	MPD	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95th 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	L	47/48 (97%)	-0.14	4 (8%)	11 9	36, 46, 78, 100	0
2	H	259/260 (99%)	-0.02	19 (7%)	15 13	32, 45, 63, 76	1 (0%)
3	A	414/480 (86%)	0.18	38 (9%)	9 7	40, 54, 85, 123	6 (1%)
All	All	720/788 (91%)	0.09	61 (8%)	11 9	32, 51, 79, 123	7 (0%)

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	82	VAL	8.6
1	L	14(M)	GLY	7.2
3	A	81	SER	6.9
3	A	434	THR	6.7
3	A	436	VAL	5.7
3	A	435	THR	5.4
3	A	437	THR	5.1
3	A	401	LYS	5.0
3	A	54	GLY	4.9
3	A	433	ALA	4.7
3	A	94	ILE	4.3
2	H	53	LEU	4.1
2	H	212	ILE	4.0
3	A	439	VAL	3.8
3	A	438	THR	3.8
3	A	139	ILE	3.5
3	A	468	LEU	3.4
3	A	134	ILE	3.4
3	A	460	ILE	3.4
3	A	402	ASN	3.3
2	H	247	GLU	3.2
3	A	195	PHE	3.2
3	A	137	VAL	3.2

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Mol	Chain	Res	Type	RSRZ
2	H	198	PRO	3.2
3	A	142	ALA	3.1
2	H	44	ALA	3.1
2	H	197	GLY	3.1
3	A	55	GLU	3.1
3	A	135	ALA	3.0
1	L	1(Q)	GLU	2.9
2	H	200	VAL	2.9
2	H	213	VAL	2.9
2	H	147(C)	ALA	2.8
2	H	229	THR	2.8
2	H	45	SER	2.7
3	A	136	PRO	2.7
1	L	1(S)	THR	2.7
3	A	115	ALA	2.6
3	A	470	PHE	2.6
3	A	432	GLN	2.5
3	A	431	THR	2.5
2	H	196	GLY	2.5
3	A	141	THR	2.5
3	A	412	ARG	2.5
2	H	43	GLY	2.5
3	A	138	GLY	2.4
2	H	31	VAL	2.4
2	H	199	PHE	2.4
3	A	193	ARG	2.4
2	H	54	THR	2.4
3	A	338	ILE	2.3
2	H	211	GLY	2.3
3	A	469	LEU	2.3
3	A	459	LEU	2.3
1	L	14(L)	ASP	2.2
3	A	140	SER	2.2
3	A	145	MET	2.1
3	A	270	ILE	2.1
2	H	52	VAL	2.1
3	A	471	MET	2.1
2	H	209	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å ²)	Q<0.9
3	TYS	A	60	16/17	0.91	0.11	46,49,73,75	0
3	TYS	A	73	16/17	0.96	0.11	65,74,83,84	0

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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	B-factors(Å ²)	Q<0.9
5	NAG	A	481	14/15	0.40	0.54	103,107,111,111	0
4	NDG	A	482	14/15	0.63	0.50	101,104,105,105	0
7	MPD	A	2002	8/8	0.70	0.36	117,118,118,119	0
4	NDG	H	1	14/15	0.71	0.45	99,105,109,115	0
5	NAG	H	2	14/15	0.71	0.56	119,123,124,125	0
7	MPD	H	2003	8/8	0.72	0.37	80,82,82,83	0
7	MPD	A	2005	8/8	0.78	0.39	116,117,117,117	0
7	MPD	H	2004	8/8	0.79	0.63	129,130,131,131	0
7	MPD	A	2001	8/8	0.88	0.33	110,111,111,111	0
6	NA	H	501	1/1	0.96	0.10	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.