



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 01:12 PM GMT

PDB ID : 1P8V  
Title : CRYSTAL STRUCTURE OF THE COMPLEX OF PLATELET RECEPTOR  
GPIB-ALPHA AND ALPHA-THROMBIN AT 2.6A  
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Deposited on : 2003-05-07  
Resolution : 2.60 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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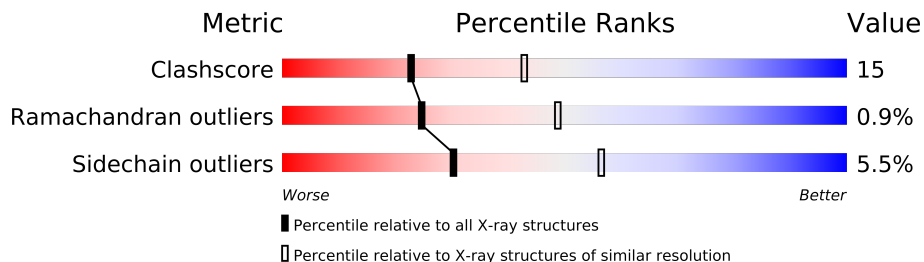
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 21963  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.60 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	79885	2154 (2.60-2.60)
Ramachandran outliers	78287	2113 (2.60-2.60)
Sidechain outliers	78261	2113 (2.60-2.60)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	279	
2	B	29	
3	C	259	

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4702 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Platelet glycoprotein Ib alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	279	Total	C	N	O	S	0	0	0
			2192	1403	357	421	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	ASP	ASN	ENGINEERED	UNP P07359
A	276	TYS	TYR	MODIFIED RESIDUE	UNP P07359
A	279	TYS	-	CLONING ARTIFACT	UNP P07359

- Molecule 2 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	29	Total	C	N	O	S	0	0	0
			239	149	38	51	1			

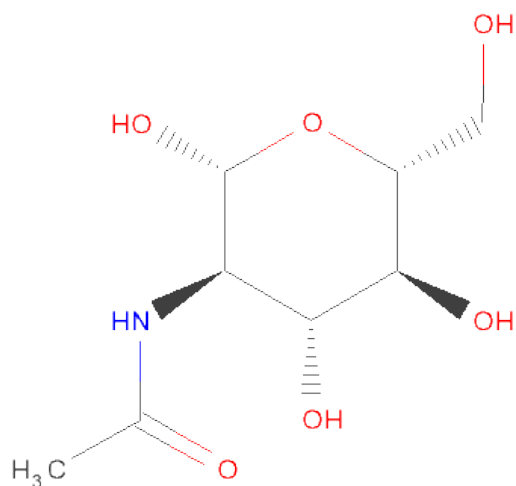
- Molecule 3 is a protein called Prothrombin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	250	Total	C	N	O	S	0	0	0
			2018	1287	357	360	14			

There is a discrepancy between the modelled and reference sequences:

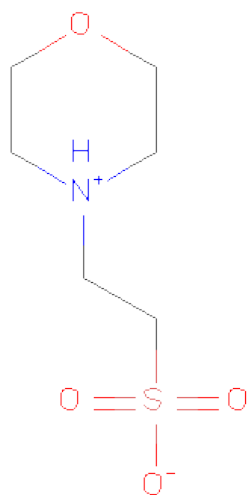
Chain	Residue	Modelled	Actual	Comment	Reference
C	259	GLU	-	CLONING ARTIFACT	UNP P00734

- Molecule 4 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



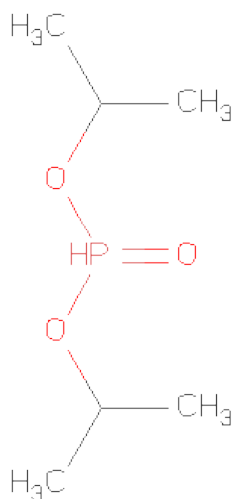
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula:  $C_6H_{13}NO_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 6 is DIISOPROPYL PHOSPHONATE (three-letter code: DFP) (formula:  $C_6H_{15}O_3P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	O	P	0	0
			10	6	3	1		

- Molecule 7 is water.

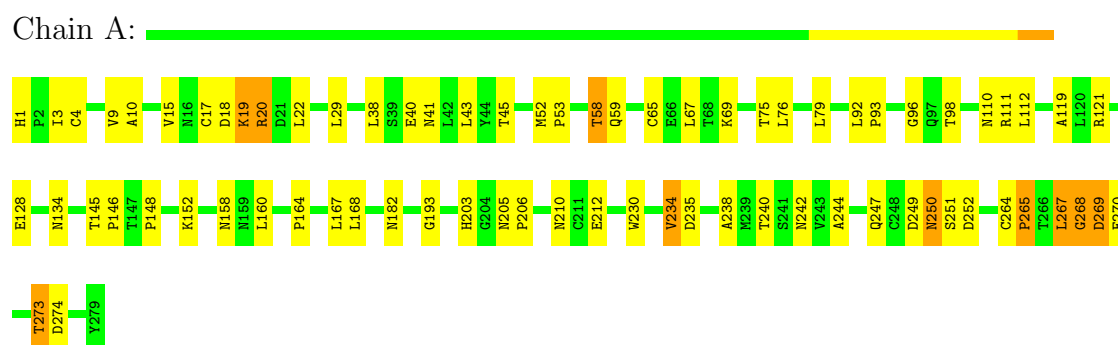
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	135	Total	O	0	0
			135	135		
7	B	3	Total	O	0	0
			3	3		
7	C	79	Total	O	0	0
			79	79		

### 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.

Note EDS was not executed.

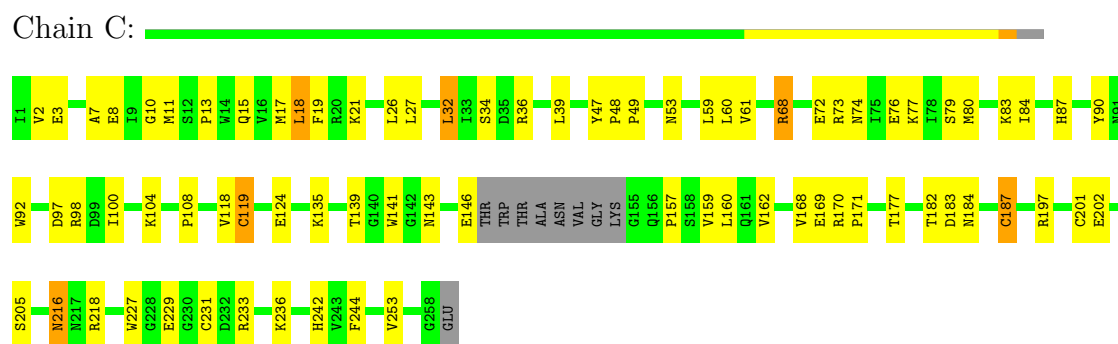
- Molecule 1: Platelet glycoprotein Ib alpha chain



- Molecule 2: Prothrombin



- Molecule 3: Prothrombin



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	47.09Å 111.77Å 176.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.60	Depositor
% Data completeness (in resolution range)	97.7 (30.00-2.60)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.207 , 0.238	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4702	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	43.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: DFP, NAG, MES, 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	A	0.34	0/2206	0.62	0/3012
2	B	0.44	0/241	0.78	0/321
3	C	0.35	0/2070	0.61	0/2797
All	All	0.35	0/4517	0.63	0/6130

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2192	0	2194	50	0
2	B	239	0	235	15	0
3	C	2018	0	1987	67	0
4	C	14	0	13	3	0
5	A	12	0	13	3	0
6	C	10	0	14	3	0
7	A	135	0	0	5	0
7	B	3	0	0	0	0
7	C	79	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	4702	0	4456	130	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 15.

All (130) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:1:HIS:HD2	1:A:4:CYS:H	1.17	0.90
3:C:139:THR:HG22	3:C:162:VAL:HG22	1.63	0.81
3:C:53:ASN:CG	4:C:300:NAG:C1	2.50	0.80
1:A:58:THR:HG22	1:A:59:GLN:HG3	1.65	0.79
1:A:158:ASN:HB2	1:A:182:ASN:HD21	1.51	0.76
3:C:8:GLU:H	3:C:11:MET:CE	2.01	0.73
3:C:8:GLU:H	3:C:11:MET:HE3	1.52	0.73
1:A:242:ASN:HD21	1:A:244:ALA:HB3	1.53	0.73
3:C:87:HIS:CE1	3:C:98:ARG:HD3	2.26	0.69
3:C:36:ARG:NH1	3:C:108:PRO:HD3	2.08	0.69
1:A:18:ASP:O	1:A:20:ARG:HG2	1.93	0.69
3:C:3:GLU:HG3	3:C:197:ARG:HB2	1.75	0.67
2:B:17:ASP:HB2	2:B:20:GLU:HG2	1.77	0.66
2:B:8:PRO:HA	2:B:12:LYS:HD2	1.77	0.66
1:A:110:ASN:HB2	1:A:134:ASN:HD21	1.60	0.65
2:B:17:ASP:HB2	2:B:20:GLU:CG	2.28	0.64
3:C:170:ARG:HB2	3:C:171:PRO:HD3	1.79	0.63
3:C:36:ARG:HE	3:C:104:LYS:CE	2.11	0.63
3:C:182:THR:HG22	3:C:183:ASP:N	2.13	0.63
1:A:168:LEU:HB2	5:A:400:MES:H22	1.82	0.62
1:A:112:LEU:H	1:A:134:ASN:HD22	1.46	0.61
3:C:182:THR:HG22	3:C:184:ASN:H	1.67	0.60
3:C:18:LEU:HD21	3:C:59:LEU:HD13	1.84	0.60
1:A:164:PRO:HG2	1:A:167:LEU:HB2	1.84	0.59
3:C:73:ARG:O	3:C:74:ASN:HB2	2.01	0.59
3:C:7:ALA:HB2	3:C:162:VAL:HG23	1.84	0.58
3:C:90:TYR:CZ	3:C:92:TRP:HB3	2.39	0.58
3:C:61:VAL:CG2	3:C:79:SER:HB2	2.34	0.58
1:A:45:THR:HG22	1:A:69:LYS:HB3	1.85	0.58
2:B:13:LYS:O	2:B:15:LEU:HD13	2.04	0.58
1:A:1:HIS:CD2	1:A:4:CYS:H	2.09	0.57
1:A:146:PRO:C	1:A:148:PRO:HD3	2.24	0.57
1:A:267:LEU:O	1:A:269:ASP:N	2.37	0.57
1:A:1:HIS:CD2	1:A:3:ILE:H	2.23	0.56
3:C:168:VAL:HB	3:C:187:CYS:SG	2.44	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:36:ARG:HE	3:C:104:LYS:HE2	1.70	0.56
1:A:128:GLU:HG2	1:A:152:LYS:HB2	1.87	0.56
2:B:18:LYS:HB2	3:C:8:GLU:OE1	2.06	0.56
1:A:273:THR:HG23	5:A:400:MES:O1S	2.06	0.55
1:A:268:GLY:O	1:A:269:ASP:CB	2.55	0.55
3:C:32:LEU:HD22	3:C:34:SER:O	2.07	0.54
1:A:52:MET:CE	1:A:75:THR:H	2.20	0.54
3:C:242:HIS:HE1	3:C:244:PHE:HB3	1.71	0.54
3:C:8:GLU:HB2	3:C:11:MET:HE2	1.89	0.54
1:A:268:GLY:O	1:A:269:ASP:HB2	2.07	0.54
1:A:160:LEU:H	1:A:182:ASN:HD22	1.55	0.54
2:B:17:ASP:HB3	2:B:20:GLU:H	1.71	0.54
3:C:61:VAL:HG22	3:C:79:SER:HB2	1.90	0.53
3:C:36:ARG:HH12	3:C:108:PRO:HD3	1.72	0.53
1:A:203:HIS:CE1	1:A:230:TRP:H	2.26	0.53
2:B:17:ASP:HB2	2:B:20:GLU:HB3	1.89	0.53
3:C:242:HIS:CE1	3:C:244:PHE:HB3	2.43	0.53
2:B:13:LYS:CD	2:B:15:LEU:HD22	2.39	0.53
3:C:47:TYR:CE2	3:C:49:PRO:HB2	2.43	0.53
1:A:75:THR:HG22	1:A:98:THR:HA	1.91	0.52
3:C:76:GLU:O	3:C:77:LYS:HD2	2.08	0.52
3:C:141:TRP:CZ2	3:C:160:LEU:HD13	2.45	0.51
3:C:118:VAL:HG22	3:C:119:CYS:N	2.26	0.51
2:B:6:LEU:HD13	3:C:218:ARG:HG2	1.93	0.50
2:B:17:ASP:O	2:B:21:ARG:HD3	2.11	0.50
3:C:39:LEU:HD11	3:C:100:ILE:HD11	1.93	0.50
3:C:68:ARG:HD3	3:C:157:PRO:O	2.11	0.50
3:C:143:ASN:HD22	3:C:202:GLU:HB3	1.75	0.50
1:A:96:GLY:HA3	1:A:121:ARG:O	2.11	0.50
1:A:20:ARG:HB2	1:A:22:LEU:HG	1.95	0.49
3:C:216:ASN:HD22	3:C:216:ASN:C	2.15	0.49
2:B:17:ASP:HB2	2:B:20:GLU:CB	2.43	0.49
1:A:111:ARG:HG2	1:A:111:ARG:HH11	1.76	0.49
3:C:53:ASN:ND2	4:C:300:NAG:O5	2.42	0.49
2:B:13:LYS:HD3	2:B:15:LEU:HD22	1.95	0.48
3:C:118:VAL:HG22	3:C:119:CYS:H	1.78	0.48
1:A:210:ASN:HB2	7:A:462:HOH:O	2.12	0.48
3:C:182:THR:CG2	3:C:183:ASP:N	2.76	0.48
3:C:97:ASP:OD2	3:C:98:ARG:NH1	2.46	0.48
3:C:146:GLU:OE2	3:C:233:ARG:HD3	2.14	0.48
3:C:216:ASN:ND2	3:C:218:ARG:H	2.11	0.48
3:C:143:ASN:ND2	3:C:202:GLU:HB3	2.29	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:234:VAL:CG2	1:A:238:ALA:HB3	2.44	0.48
3:C:83:LYS:HD3	3:C:84:ILE:N	2.29	0.47
3:C:36:ARG:HE	3:C:104:LYS:HE3	1.79	0.47
1:A:43:LEU:O	1:A:67:LEU:HD23	2.15	0.47
3:C:15:GLN:NE2	3:C:139:THR:OG1	2.48	0.47
3:C:139:THR:CG2	3:C:162:VAL:HG22	2.39	0.46
3:C:182:THR:HG22	3:C:183:ASP:H	1.80	0.46
3:C:146:GLU:HB3	3:C:231:CYS:HB2	1.96	0.46
1:A:17:CYS:HB2	1:A:38:LEU:HD23	1.96	0.46
3:C:227:TRP:HA	6:C:500:DFP:H2'3	1.97	0.46
1:A:145:THR:N	1:A:146:PRO:HD2	2.30	0.46
3:C:21:LYS:NZ	3:C:80:MET:HE2	2.31	0.46
3:C:233:ARG:O	3:C:236:LYS:HB2	2.17	0.45
1:A:250:ASN:ND2	7:A:435:HOH:O	2.48	0.45
3:C:48:PRO:HG2	3:C:92:TRP:CZ2	2.52	0.45
3:C:8:GLU:N	3:C:11:MET:HE3	2.24	0.44
2:B:18:LYS:HE2	2:B:18:LYS:HB3	1.76	0.44
1:A:112:LEU:HG	1:A:134:ASN:ND2	2.33	0.44
3:C:10:GLY:O	3:C:13:PRO:HD3	2.16	0.44
3:C:141:TRP:CE2	3:C:160:LEU:HD13	2.52	0.44
3:C:27:LEU:HD12	3:C:59:LEU:CD2	2.47	0.44
3:C:8:GLU:H	3:C:11:MET:HE2	1.83	0.43
1:A:92:LEU:HD23	1:A:119:ALA:HB1	2.00	0.43
3:C:72:GLU:O	3:C:76:GLU:HG2	2.18	0.43
1:A:76:LEU:HD12	1:A:79:LEU:HD22	2.00	0.43
1:A:205:ASN:HA	1:A:206:PRO:HD3	1.81	0.43
3:C:80:MET:HE3	3:C:80:MET:HB3	1.82	0.43
7:A:484:HOH:O	3:C:124:GLU:HG3	2.17	0.43
1:A:9:VAL:O	1:A:10:ALA:HB3	2.17	0.43
2:B:22:GLU:HG2	3:C:135:LYS:HD2	2.01	0.43
1:A:247:GLN:HG2	1:A:247:GLN:H	1.66	0.43
1:A:267:LEU:O	1:A:268:GLY:C	2.57	0.42
1:A:52:MET:N	1:A:53:PRO:CD	2.81	0.42
1:A:193:GLY:HA3	5:A:400:MES:H52	2.01	0.42
1:A:52:MET:HE3	1:A:75:THR:H	1.84	0.42
3:C:17:MET:HG3	3:C:26:LEU:CD1	2.50	0.42
3:C:229:GLU:CD	3:C:236:LYS:HZ2	2.23	0.42
1:A:242:ASN:ND2	1:A:244:ALA:HB3	2.28	0.42
3:C:83:LYS:HD3	3:C:84:ILE:H	1.83	0.42
1:A:264:CYS:O	1:A:265:PRO:O	2.37	0.42
1:A:92:LEU:HA	1:A:93:PRO:HD3	1.93	0.41
1:A:41:ASN:O	1:A:65:CYS:HA	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
3:C:53:ASN:OD1	4:C:300:NAG:C1	2.69	0.41
1:A:19:LYS:C	1:A:20:ARG:HG2	2.40	0.41
1:A:15:VAL:HG11	1:A:29:LEU:HD22	2.03	0.41
3:C:19:PHE:HB3	3:C:60:LEU:CD1	2.51	0.41
6:C:500:DFP:H2'1	7:C:567:HOH:O	2.19	0.40
1:A:110:ASN:HB3	1:A:111:ARG:H	1.78	0.40
3:C:2:VAL:O	3:C:3:GLU:HB2	2.22	0.40
3:C:201:CYS:C	6:C:500:DFP:H3'1	2.42	0.40
1:A:251:SER:HA	7:A:433:HOH:O	2.21	0.40
1:A:273:THR:HG22	7:A:523:HOH:O	2.20	0.40
2:B:29:ASP:N	2:B:29:ASP:OD2	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

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	276/279 (99%)	252 (91%)	19 (7%)	5 (2%)	13	25
2	B	27/29 (93%)	22 (82%)	5 (18%)	0	100	100
3	C	246/259 (95%)	229 (93%)	17 (7%)	0	100	100
All	All	549/567 (97%)	503 (92%)	41 (8%)	5 (1%)	25	49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	265	PRO
1	A	268	GLY
1	A	269	ASP
1	A	19	LYS
1	A	252	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	247/248 (100%)	234 (95%)	13 (5%)	32	58
2	B	27/27 (100%)	24 (89%)	3 (11%)	9	16
3	C	217/225 (96%)	206 (95%)	11 (5%)	33	60
All	All	491/500 (98%)	464 (94%)	27 (6%)	30	56

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	ARG
1	A	40	GLU
1	A	58	THR
1	A	212	GLU
1	A	234	VAL
1	A	235	ASP
1	A	240	THR
1	A	249	ASP
1	A	250	ASN
1	A	267	LEU
1	A	270	GLU
1	A	273	THR
1	A	274	ASP
2	B	4	CYS
2	B	6	LEU
2	B	21	ARG
3	C	18	LEU
3	C	32	LEU
3	C	68	ARG
3	C	119	CYS
3	C	159	VAL
3	C	169	GLU
3	C	177	THR
3	C	187	CYS
3	C	205	SER
3	C	216	ASN
3	C	253	VAL

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

Mol	Chain	Res	Type
1	A	1	HIS
1	A	97	GLN
1	A	134	ASN
1	A	173	ASN
1	A	182	ASN
1	A	203	HIS
1	A	226	ASN
1	A	242	ASN
1	A	250	ASN
3	C	15	GLN
3	C	66	HIS
3	C	74	ASN
3	C	143	ASN
3	C	216	ASN
3	C	251	GLN
3	C	256	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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$
1	TYS	A	276	1	16,16,17	4.49	3 (18%)	20,22,24	1.55	2 (10%)
1	TYS	A	279	1	17,17,17	1.46	4 (23%)	24,24,24	1.69	4 (16%)

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	TYS	A	276	1	-	0/9/11/13	0/1/1/1
1	TYS	A	279	1	-	0/13/13/13	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	276	TYS	O-C	16.84	1.23	1.11
1	A	276	TYS	OH-CZ	-3.35	1.38	1.42
1	A	279	TYS	OH-CZ	-2.90	1.38	1.42
1	A	279	TYS	OH-S	-2.28	1.59	1.63
1	A	276	TYS	CA-C	2.27	1.52	1.48
1	A	279	TYS	CD2-CG	2.13	1.43	1.38
1	A	279	TYS	CE1-CZ	2.05	1.42	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	279	TYS	C-CA-N	6.00	119.30	109.36
1	A	276	TYS	C-CA-N	-5.28	108.56	113.83
1	A	279	TYS	CB-CG-CD1	-3.08	114.85	120.90
1	A	276	TYS	OH-CZ-CE2	2.76	123.29	118.70
1	A	279	TYS	CG-CB-CA	-2.51	108.43	114.34
1	A	279	TYS	CB-CG-CD2	2.23	125.28	120.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates

There are no carbohydrates in this entry.

## 5.6 Ligand geometry

3 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$
5	MES	A	400	-	12,12,12	9.60	8 (66%)	16,16,16	2.46	7 (43%)
4	NAG	C	300	3	12,14,15	0.88	1 (8%)	15,19,21	0.72	0
6	DFP	C	500	3	9,9,9	1.27	1 (11%)	11,11,11	0.61	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	MES	A	400	-	-	0/6/14/14	0/1/1/1
4	NAG	C	300	3	-	0/6/23/26	0/1/1/1
6	DFP	C	500	3	-	0/8/8/8	0/0/0/0

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	400	MES	C8-S	-19.46	1.43	1.78
5	A	400	MES	O3S-S	15.09	1.80	1.45
5	A	400	MES	O1S-S	14.97	1.80	1.45
5	A	400	MES	O2S-S	14.34	1.78	1.45
5	A	400	MES	C3-C2	-5.27	1.40	1.51
5	A	400	MES	C5-C6	-4.28	1.42	1.51
5	A	400	MES	C7-N4	-3.09	1.42	1.50
6	C	500	DFP	P-O2P	2.25	1.62	1.58
5	A	400	MES	C5-N4	-2.23	1.44	1.49
4	C	300	NAG	C3-C2	2.03	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	400	MES	C7-C8-S	4.42	124.52	112.49
5	A	400	MES	C8-C7-N4	3.78	118.91	112.44
5	A	400	MES	O3S-S-O2S	-3.53	103.40	112.48
5	A	400	MES	O3S-S-C8	3.38	114.72	105.99
5	A	400	MES	O1-C2-C3	-2.96	107.82	111.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	400	MES	O3S-S-O1S	-2.52	106.01	112.48
5	A	400	MES	O2S-S-O1S	-2.44	107.74	112.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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 ⓘ

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.