



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 10:07 AM GMT

PDB ID : 1D6W
Title : STRUCTURE OF THROMBIN COMPLEXED WITH SELECTIVE NON-ELECTROPHILIC INHIBITORS HAVING CYCLOHEXYL MOIETIES AT P1
Authors : Mochalkin, I.; Tulinsky, A.
Deposited on : 1999-10-15
Resolution : 2.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

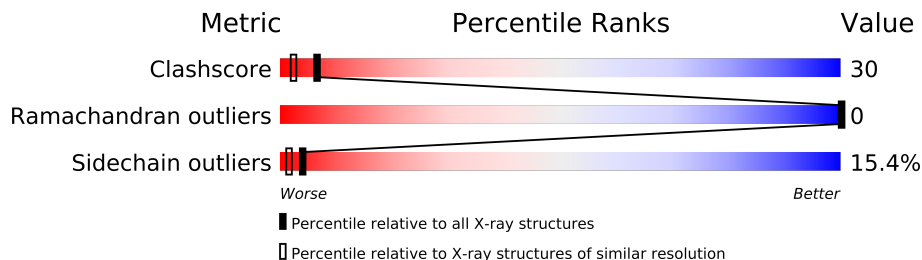
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.00 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	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)

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. 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	287	
2	I	10	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2516 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 THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	278	Total	C	N	O	S	0	0	0
			2255	1436	395	409	15			

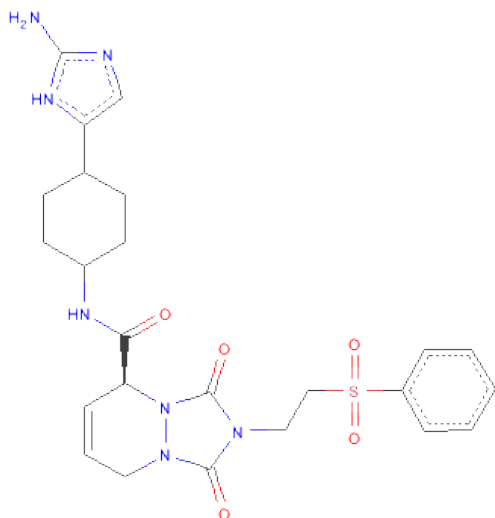
- Molecule 2 is a protein called DECAPEPTIDE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	10	Total	C	N	O	S	0	0	0
			89	56	10	22	1			

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Na	0	0
			2	2		

- Molecule 4 is (5S)-N-[TRANS-4-(2-AMINO-1H-IMIDAZOL-5-YL)CYCLOHEXYL]-1,3-DI OXO-2-[2-(PHENYLSULFONYL)ETHYL]-2,3,5,8-TETRAHYDRO-1H-[1,2,4]TRIAZOLO[1,2-A]PYRIDAZINE-5-CARBOXAMIDE (three-letter code: 00R) (formula: C₂₄H₂₉N₇O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	37	24	7	5	1	0	0

- Molecule 5 is water.

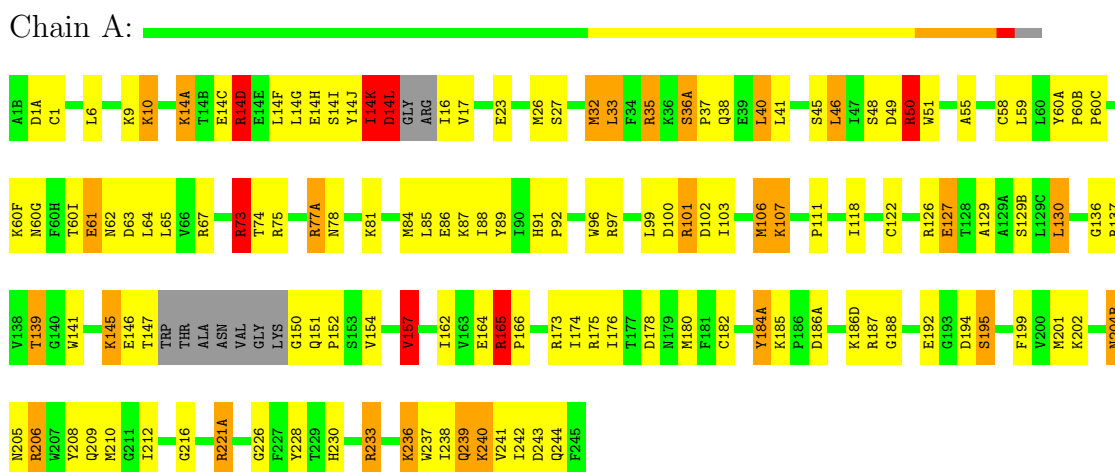
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	I	2	Total	O	0	0
			2	2		
5	A	131	Total	O	0	0
			131	131		

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: THROMBIN



- Molecule 2: DECAPEPTIDE INHIBITOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	71.43Å 71.67Å 72.45Å 90.00° 101.00° 90.00°	Depositor
Resolution (Å)	9.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (9.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.174 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2516	wwPDB-VP
Average B, all atoms (Å ²)	28.0	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: NA, 00R, 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	0.99	0/2309	1.66	38/3115 (1.2%)
2	I	0.87	0/73	1.62	1/96 (1.0%)
All	All	0.99	0/2382	1.66	39/3211 (1.2%)

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	A	0	2

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	ARG	NE-CZ-NH1	22.12	131.36	120.30
1	A	14(D)	ARG	NE-CZ-NH1	20.32	130.46	120.30
1	A	233	ARG	NE-CZ-NH2	-16.15	112.23	120.30
1	A	173	ARG	NE-CZ-NH2	-12.82	113.89	120.30
1	A	35	ARG	NE-CZ-NH2	-9.83	115.38	120.30
1	A	14(D)	ARG	NE-CZ-NH2	-9.30	115.65	120.30
1	A	184(A)	TYR	CB-CG-CD2	-8.17	116.10	121.00
1	A	75	ARG	NE-CZ-NH2	8.00	124.30	120.30
1	A	233	ARG	CD-NE-CZ	7.53	134.15	123.60
1	A	50	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	A	187	ARG	NE-CZ-NH2	7.33	123.96	120.30
1	A	67	ARG	NE-CZ-NH2	7.08	123.84	120.30
1	A	14(L)	ASP	CB-CG-OD1	6.82	124.44	118.30
1	A	137	ARG	NE-CZ-NH2	6.82	123.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	165	ARG	NE-CZ-NH2	6.72	123.66	120.30
1	A	1(A)	ASP	CB-CG-OD2	-6.71	112.26	118.30
1	A	14(K)	ILE	CB-CA-C	6.70	125.00	111.60
1	A	175	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	A	126	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	A	77(A)	ARG	NE-CZ-NH2	6.52	123.56	120.30
1	A	14(C)	GLU	CG-CD-OE2	-6.38	105.55	118.30
1	A	97	ARG	NE-CZ-NH2	6.33	123.46	120.30
1	A	14(D)	ARG	CD-NE-CZ	6.26	132.37	123.60
1	A	26	MET	CG-SD-CE	6.24	110.18	100.20
2	I	364	LEU	CA-C-O	6.19	133.09	120.10
1	A	101	ARG	NE-CZ-NH2	6.17	123.39	120.30
1	A	14(K)	ILE	C-N-CA	6.14	137.06	121.70
1	A	84	MET	CG-SD-CE	6.10	109.96	100.20
1	A	206	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	A	32	MET	CG-SD-CE	5.88	109.61	100.20
1	A	106	MET	CG-SD-CE	5.68	109.28	100.20
1	A	10	LYS	CA-CB-CG	5.60	125.72	113.40
1	A	73	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	A	14(D)	ARG	NH1-CZ-NH2	-5.40	113.46	119.40
1	A	1(A)	ASP	OD1-CG-OD2	5.30	133.37	123.30
1	A	1(A)	ASP	CA-CB-CG	-5.28	101.79	113.40
1	A	184(A)	TYR	CB-CG-CD1	5.16	124.10	121.00
1	A	173	ARG	CB-CA-C	-5.11	100.18	110.40
1	A	157	VAL	CB-CA-C	-5.00	101.90	111.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	165	ARG	Sidechain
1	A	73	ARG	Sidechain

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	2255	0	2229	134	0
2	I	89	0	69	5	0
3	A	2	0	0	0	0
4	A	37	0	29	11	0
5	A	131	0	0	11	0
5	I	2	0	0	0	0
All	All	2516	0	2327	139	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 30.

All (139) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:50:ARG:NH1	1:A:107:LYS:HE2	1.65	1.11
1:A:81:LYS:HD3	1:A:118:ILE:CD1	1.80	1.11
1:A:60(F):LYS:HE3	5:A:567:HOH:O	1.48	1.10
1:A:81:LYS:HD3	1:A:118:ILE:HD12	1.36	1.08
1:A:240:LYS:CE	1:A:244:GLN:NE2	2.18	1.07
2:I:360:PRO:HG2	2:I:363:TYS:HE2	1.36	1.07
1:A:33:LEU:O	5:A:521:HOH:O	1.76	1.03
1:A:240:LYS:HE3	1:A:244:GLN:NE2	1.72	1.03
1:A:240:LYS:CE	1:A:244:GLN:HE22	1.76	0.98
1:A:14(J):TYR:C	1:A:14(K):ILE:HG13	1.82	0.97
1:A:240:LYS:HE2	1:A:244:GLN:NE2	1.85	0.89
1:A:32:MET:HG3	1:A:40:LEU:HD12	1.59	0.83
1:A:50:ARG:HH11	1:A:107:LYS:HE2	1.41	0.80
2:I:360:PRO:HG2	2:I:363:TYS:CE2	2.11	0.80
1:A:14(I):SER:C	1:A:14(K):ILE:H	1.84	0.79
1:A:81:LYS:HD3	1:A:118:ILE:HD11	1.63	0.78
1:A:41:LEU:CD1	1:A:64:LEU:HD22	2.14	0.78
1:A:14(A):LYS:HG2	1:A:23:GLU:OE2	1.85	0.76
1:A:216:GLY:HA3	4:A:380:00R:C24	2.18	0.73
1:A:216:GLY:HA3	4:A:380:00R:N23	2.03	0.73
1:A:59:LEU:HD13	1:A:88:ILE:HD13	1.69	0.72
1:A:41:LEU:HD11	1:A:64:LEU:CD2	2.21	0.71
1:A:50:ARG:HH12	1:A:107:LYS:HE2	1.54	0.71
1:A:40:LEU:HD12	5:A:521:HOH:O	1.91	0.71
1:A:14(A):LYS:HE2	5:A:414:HOH:O	1.91	0.70
1:A:41:LEU:HD12	1:A:64:LEU:HD22	1.74	0.70
1:A:240:LYS:CE	1:A:244:GLN:HE21	2.06	0.69
1:A:73:ARG:HG3	1:A:141:TRP:HB3	1.73	0.68
1:A:240:LYS:O	1:A:244:GLN:HB2	1.94	0.67
1:A:174:ILE:HD12	4:A:380:00R:C37	2.24	0.67

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:ILE:CD1	4:A:380:00R:C37	2.72	0.67
1:A:73:ARG:NH1	1:A:152:PRO:O	2.23	0.67
1:A:184(A):TYR:CZ	1:A:186(D):LYS:HE3	2.30	0.66
1:A:50:ARG:HH11	1:A:50:ARG:HG2	1.60	0.66
2:I:362:GLU:CD	2:I:362:GLU:H	2.00	0.65
1:A:87:LYS:HB3	1:A:89:TYR:CE1	2.33	0.63
1:A:73:ARG:HD3	1:A:152:PRO:O	1.98	0.63
1:A:46:LEU:HD22	1:A:48:SER:O	1.99	0.63
1:A:81:LYS:CD	1:A:118:ILE:HD11	2.28	0.62
1:A:146:GLU:OE2	1:A:221(A):ARG:HD3	1.98	0.62
1:A:174:ILE:CD1	4:A:380:00R:C36	2.78	0.62
1:A:60(F):LYS:CE	5:A:567:HOH:O	2.26	0.61
1:A:55:ALA:O	1:A:58:CYS:HB2	2.02	0.60
1:A:129:ALA:O	1:A:130:LEU:HB2	2.01	0.59
1:A:41:LEU:CD1	1:A:64:LEU:CD2	2.78	0.59
1:A:145:LYS:CE	1:A:150:GLY:N	2.66	0.59
1:A:60(B):PRO:HG2	1:A:96:TRP:CD2	2.38	0.58
1:A:178:ASP:O	1:A:233:ARG:HD2	2.03	0.58
1:A:17:VAL:O	1:A:188:GLY:HA2	2.03	0.58
1:A:60(A):TYR:CZ	1:A:60(C):PRO:HG2	2.38	0.58
1:A:240:LYS:HE3	1:A:244:GLN:HE22	1.43	0.58
1:A:99:LEU:HD11	4:A:380:00R:C16	2.34	0.58
1:A:14(A):LYS:CG	5:A:428:HOH:O	2.52	0.58
1:A:14(J):TYR:O	1:A:14(K):ILE:HG13	2.03	0.57
1:A:164:GLU:CD	1:A:164:GLU:H	2.09	0.56
1:A:51:TRP:CZ3	1:A:107:LYS:HB3	2.41	0.55
1:A:147:THR:O	1:A:147:THR:HG22	2.07	0.55
1:A:85:LEU:HD13	1:A:106:MET:HE2	1.87	0.54
1:A:59:LEU:HD13	1:A:88:ILE:CG2	2.37	0.54
1:A:60(B):PRO:HG2	1:A:96:TRP:CE3	2.43	0.54
1:A:145:LYS:HE3	1:A:150:GLY:N	2.23	0.53
1:A:41:LEU:HD11	1:A:64:LEU:HD21	1.88	0.53
1:A:81:LYS:CD	1:A:118:ILE:CD1	2.69	0.53
1:A:49:ASP:O	1:A:111:PRO:HA	2.08	0.53
1:A:85:LEU:HD11	1:A:106:MET:HE1	1.90	0.53
1:A:239:GLN:HG3	5:A:543:HOH:O	2.07	0.53
1:A:127:GLU:CD	1:A:127:GLU:H	2.11	0.53
1:A:86:GLU:OE2	1:A:107:LYS:HD3	2.10	0.52
1:A:165:ARG:HH12	1:A:176:ILE:HG22	1.73	0.52
1:A:41:LEU:HD11	1:A:64:LEU:HD22	1.83	0.52
1:A:236:LYS:HE2	5:A:528:HOH:O	2.09	0.51
1:A:35:ARG:O	1:A:38:GLN:HA	2.10	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14(D):ARG:NE	5:A:529:HOH:O	2.42	0.51
1:A:59:LEU:HD13	1:A:88:ILE:HG21	1.91	0.51
1:A:240:LYS:HE2	1:A:244:GLN:HE21	1.68	0.50
1:A:87:LYS:HD3	1:A:88:ILE:H	1.76	0.50
1:A:239:GLN:CG	5:A:543:HOH:O	2.59	0.50
1:A:165:ARG:N	1:A:166:PRO:HD2	2.26	0.50
1:A:77(A):ARG:O	1:A:78:ASN:HB2	2.11	0.50
1:A:162:ILE:HD11	1:A:199:PHE:CZ	2.45	0.50
1:A:136:GLY:HA3	1:A:199:PHE:CZ	2.47	0.50
1:A:145:LYS:HE2	1:A:150:GLY:N	2.27	0.50
1:A:216:GLY:CA	4:A:380:00R:N23	2.75	0.50
1:A:146:GLU:OE1	1:A:221(A):ARG:NH1	2.45	0.50
2:I:359:ILE:HD12	2:I:363:TYR:HB3	1.94	0.49
1:A:85:LEU:HD13	1:A:106:MET:CE	2.42	0.49
1:A:208:TYR:HB2	1:A:210:MET:HE2	1.94	0.49
1:A:61:GLU:OE2	1:A:87:LYS:HA	2.12	0.49
1:A:99:LEU:O	1:A:102:ASP:HB2	2.12	0.49
1:A:85:LEU:CD1	1:A:106:MET:HE1	2.43	0.49
1:A:50:ARG:HH11	1:A:107:LYS:CE	2.18	0.49
1:A:184(A):TYR:OH	1:A:186(D):LYS:HE3	2.12	0.48
1:A:165:ARG:N	1:A:166:PRO:CD	2.76	0.48
1:A:91:HIS:ND1	1:A:92:PRO:HD2	2.29	0.48
1:A:35:ARG:HD2	1:A:41:LEU:HD21	1.97	0.47
1:A:174:ILE:HD11	4:A:380:00R:C36	2.44	0.47
1:A:45:SER:OG	1:A:209:GLN:NE2	2.40	0.46
1:A:1:CYS:C	1:A:122:CYS:SG	2.94	0.46
1:A:139:THR:CG2	1:A:157:VAL:HG13	2.45	0.46
1:A:195:SER:OG	4:A:380:00R:H01A	2.16	0.46
1:A:50:ARG:HE	1:A:111:PRO:HD3	1.81	0.45
1:A:14(H):GLU:HA	1:A:14(L):ASP:HA	1.98	0.45
1:A:107:LYS:HE3	1:A:107:LYS:HB2	1.69	0.45
1:A:201:MET:SD	1:A:210:MET:HG3	2.56	0.45
1:A:14(G):LEU:HD21	1:A:202:LYS:HD2	1.99	0.45
1:A:174:ILE:HD12	4:A:380:00R:H37	1.97	0.45
1:A:237:TRP:O	1:A:241:VAL:HG13	2.15	0.45
1:A:165:ARG:HH12	1:A:176:ILE:CG2	2.30	0.45
1:A:86:GLU:HB3	1:A:107:LYS:HG3	1.98	0.44
1:A:60(A):TYR:CE2	1:A:60(C):PRO:HG2	2.52	0.44
1:A:60(B):PRO:HG2	1:A:96:TRP:CE2	2.52	0.44
1:A:182:CYS:HA	1:A:226:GLY:O	2.18	0.44
1:A:85:LEU:CD1	1:A:106:MET:CE	2.95	0.44
1:A:145:LYS:HE2	1:A:150:GLY:CA	2.49	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:174:ILE:HD11	4:A:380:00R:O35	2.18	0.43
1:A:36(A):SER:HA	1:A:37:PRO:C	2.38	0.43
1:A:204(B):ASN:O	1:A:205:ASN:HB2	2.19	0.43
1:A:60(I):THR:O	1:A:63:ASP:HB2	2.19	0.43
1:A:127:GLU:N	1:A:127:GLU:CD	2.72	0.43
2:I:360:PRO:CG	2:I:363:TYR:HE2	2.26	0.42
1:A:14(J):TYR:C	1:A:14(K):ILE:CG1	2.71	0.42
1:A:14(G):LEU:HD21	1:A:202:LYS:HB3	2.00	0.42
1:A:130:LEU:HA	1:A:130:LEU:HD23	1.73	0.41
1:A:73:ARG:HG3	1:A:141:TRP:CB	2.48	0.41
1:A:87:LYS:HD3	1:A:88:ILE:N	2.35	0.41
1:A:59:LEU:CD1	1:A:88:ILE:HG23	2.50	0.41
1:A:87:LYS:HB3	1:A:89:TYR:HE1	1.85	0.41
1:A:87:LYS:HD3	1:A:87:LYS:HA	1.85	0.41
1:A:16:ILE:HD13	1:A:194:ASP:OD1	2.21	0.41
1:A:178:ASP:C	1:A:180:MET:H	2.24	0.41
1:A:204(B):ASN:ND2	1:A:206:ARG:H	2.18	0.41
1:A:100:ASP:O	1:A:101:ARG:HB2	2.21	0.41
1:A:14(A):LYS:HG3	5:A:428:HOH:O	2.17	0.41
1:A:151:GLN:HA	1:A:152:PRO:HD3	1.90	0.41
1:A:230:HIS:CG	1:A:233:ARG:HG3	2.56	0.41
1:A:73:ARG:NH2	1:A:74:THR:CG2	2.84	0.41
1:A:14(I):SER:C	1:A:14(K):ILE:N	2.59	0.40
1:A:103:ILE:HD11	1:A:238:ILE:HD11	2.03	0.40
1:A:212:ILE:O	1:A:228:TYR:HA	2.21	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	272/287 (95%)	254 (93%)	18 (7%)	0	100	100
2	I	7/10 (70%)	7 (100%)	0	0	100	100
All	All	279/297 (94%)	261 (94%)	18 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	245/251 (98%)	207 (84%)	38 (16%)	4	1
2	I	8/9 (89%)	7 (88%)	1 (12%)	7	3
All	All	253/260 (97%)	214 (85%)	39 (15%)	4	1

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	9	LYS
1	A	10	LYS
1	A	14(A)	LYS
1	A	14(D)	ARG
1	A	14(F)	LEU
1	A	14(K)	ILE
1	A	14(L)	ASP
1	A	27	SER
1	A	33	LEU
1	A	36(A)	SER
1	A	40	LEU
1	A	46	LEU
1	A	50	ARG
1	A	60(G)	ASN
1	A	61	GLU
1	A	62	ASN
1	A	65	LEU
1	A	107	LYS
1	A	127	GLU
1	A	129(B)	SER
1	A	130	LEU
1	A	139	THR
1	A	145	LYS
1	A	154	VAL
1	A	157	VAL

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Mol	Chain	Res	Type
1	A	165	ARG
1	A	185	LYS
1	A	186(A)	ASP
1	A	192	GLU
1	A	195	SER
1	A	204(B)	ASN
1	A	221(A)	ARG
1	A	236	LYS
1	A	239	GLN
1	A	240	LYS
1	A	242	ILE
1	A	243	ASP
2	I	362	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	60(G)	ASN
1	A	62	ASN
1	A	78	ASN
1	A	156	GLN
1	A	204(B)	ASN
1	A	209	GLN
1	A	244	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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
2	TYS	I	363	2	16,16,17	5.29	3 (18%)	20,22,24	1.43	2 (10%)

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
2	TYS	I	363	2	-	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)
2	I	363	TYS	O-C	20.47	1.25	1.11
2	I	363	TYS	OH-CZ	-4.32	1.37	1.42
2	I	363	TYS	CA-C	2.13	1.52	1.48

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	363	TYS	CG-CB-CA	-2.94	107.49	114.42
2	I	363	TYS	OH-S-O2	-2.72	99.77	107.64

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 ⓘ

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 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	$\# Z > 2$
4	00R	A	380	-	41,41,41	3.88	12 (29%)	49,60,60	2.16	15 (30%)

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	00R	A	380	-	-	0/23/44/44	0/3/5/5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	380	00R	O19-C18	11.60	1.46	1.23
4	A	380	00R	C22-C05	-11.53	1.24	1.50
4	A	380	00R	C18-N20	11.29	1.60	1.34
4	A	380	00R	C26-N25	8.65	1.48	1.36
4	A	380	00R	C06-C01	5.11	1.66	1.52
4	A	380	00R	C04-C03	5.07	1.66	1.52
4	A	380	00R	C01-C02	4.97	1.64	1.51
4	A	380	00R	C04-C05	4.00	1.64	1.53
4	A	380	00R	O34-S33	2.55	1.48	1.44
4	A	380	00R	C08-N10	2.45	1.39	1.35
4	A	380	00R	C26-C22	-2.44	1.32	1.37
4	A	380	00R	C12-N11	2.09	1.39	1.35

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	380	00R	C05-C22-N23	5.78	127.72	121.54
4	A	380	00R	N27-C24-N25	5.48	130.76	123.28
4	A	380	00R	C02-N20-C18	-5.19	114.80	123.18
4	A	380	00R	C14-N10-N11	4.22	122.67	119.03
4	A	380	00R	O35-S33-C36	3.93	112.55	108.39
4	A	380	00R	N23-C24-N25	-3.87	109.48	111.08
4	A	380	00R	C04-C05-C22	-3.20	107.71	112.45
4	A	380	00R	N27-C24-N23	-2.66	119.74	124.65
4	A	380	00R	C04-C03-C02	2.34	114.71	111.47
4	A	380	00R	O35-S33-O34	-2.33	115.20	118.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	380	00R	C06-C01-C02	-2.24	108.37	111.47
4	A	380	00R	C17-C18-N20	2.17	118.23	115.09
4	A	380	00R	O19-C18-N20	-2.13	118.83	122.93
4	A	380	00R	C18-C17-N11	-2.10	107.08	110.81
4	A	380	00R	C40-C41-C36	2.09	121.28	118.95

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.