



Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 06:32 am BST

PDB ID : 2TGD
Title : LACK OF THE TRANSITION STATE STABILIZATION SITE IS A FACTOR IN THE INACTIVITY OF TRYPSINOGEN, A SERINE PROTEASE ZYMOGEN. STRUCTURE OF DFP INHIBITED BOVINE TRYPSINOGEN AT 2.1 ANGSTROMS RESOLUTION
Authors : Jones, M.O.; Stroud, R.M.
Deposited on : 1986-03-17
Resolution : 2.10 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 : 1.8.5 (274361), CSD as541be (2020)
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

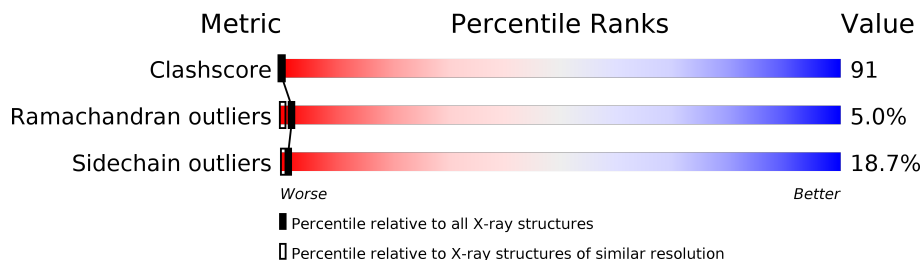
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)

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 respectively. 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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	229	

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
3	DFP	A	248	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 1700 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.

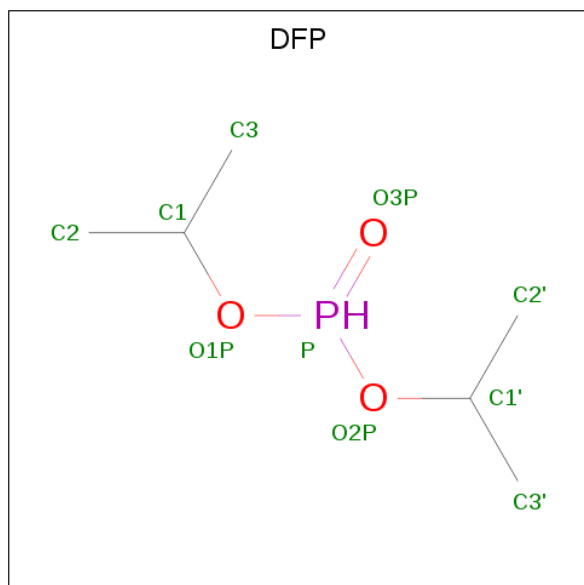
- Molecule 1 is a protein called TRYPSINOGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	222	1616	1002	277	323	14	0	0	0

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is DIISOPROPYL PHOSPHONATE (three-letter code: DFP) (formula: C₆H₁₅O₃P).



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

- Molecule 4 is water.

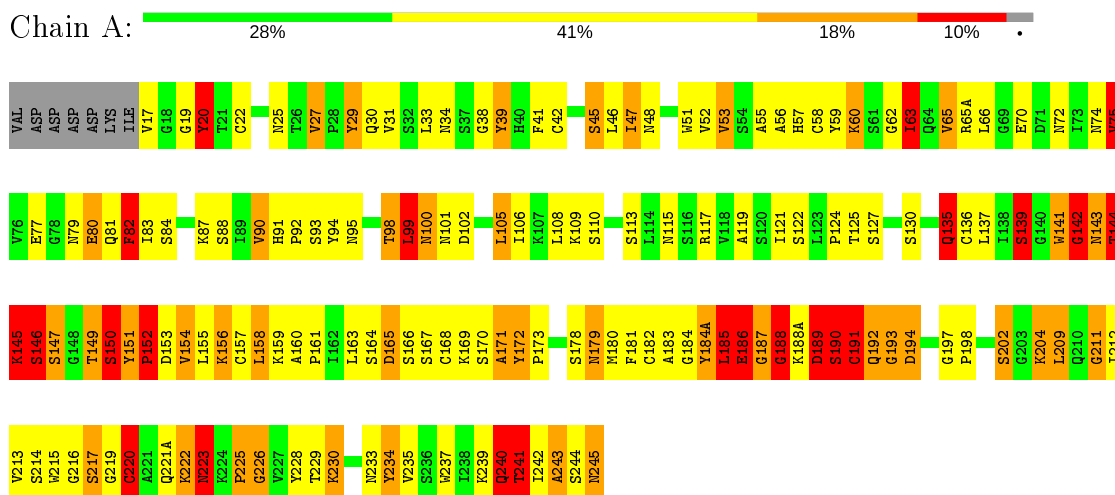
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total	O	0	0
			73	73		

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. 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. 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: TRYPSINOGEN



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	55.15Å 55.15Å 109.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	0.182 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	1700	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: CA, DFP

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	1.77	19/1647 (1.2%)	2.21	71/2233 (3.2%)

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	3	23

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	51	TRP	CD1-NE1	7.63	1.50	1.38
1	A	237	TRP	CD2-CE2	-7.58	1.32	1.41
1	A	51	TRP	CB-CG	7.18	1.63	1.50
1	A	171	ALA	CA-CB	7.08	1.67	1.52
1	A	240	GLN	CD-OE1	6.68	1.38	1.24
1	A	29	TYR	CZ-OH	-6.60	1.26	1.37
1	A	237	TRP	NE1-CE2	-6.16	1.29	1.37
1	A	139	SER	CB-OG	-6.05	1.34	1.42
1	A	82	PHE	CB-CG	-5.95	1.41	1.51
1	A	214	SER	CB-OG	-5.79	1.34	1.42
1	A	29	TYR	CE1-CZ	5.77	1.46	1.38
1	A	197	GLY	CA-C	5.75	1.61	1.51
1	A	234	TYR	CB-CG	-5.66	1.43	1.51
1	A	226	GLY	C-O	5.53	1.32	1.23
1	A	179	ASN	N-CA	-5.32	1.35	1.46
1	A	80	GLU	CD-OE1	5.32	1.31	1.25
1	A	240	GLN	CG-CD	5.30	1.63	1.51
1	A	220	CYS	CB-SG	5.08	1.90	1.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	154	VAL	N-CA	-5.01	1.36	1.46

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	151	TYR	CB-CG-CD1	-24.40	106.36	121.00
1	A	151	TYR	CB-CG-CD2	22.51	134.50	121.00
1	A	65(A)	ARG	NE-CZ-NH2	-13.87	113.36	120.30
1	A	221(A)	GLN	C-N-CA	-9.86	97.04	121.70
1	A	65(A)	ARG	NE-CZ-NH1	9.64	125.12	120.30
1	A	242	ILE	CA-CB-CG2	9.64	130.19	110.90
1	A	242	ILE	CA-CB-CG1	9.10	128.30	111.00
1	A	151	TYR	N-CA-CB	8.85	126.53	110.60
1	A	188	GLY	CA-C-N	8.80	136.56	117.20
1	A	20	TYR	CB-CG-CD1	-8.77	115.74	121.00
1	A	234	TYR	CB-CG-CD2	-8.29	116.03	121.00
1	A	243	ALA	C-N-CA	-8.07	101.53	121.70
1	A	180	MET	CG-SD-CE	7.94	112.90	100.20
1	A	39	TYR	CB-CG-CD1	-7.55	116.47	121.00
1	A	102	ASP	CB-CG-OD2	-7.52	111.53	118.30
1	A	223	ASN	N-CA-CB	-7.34	97.39	110.60
1	A	29	TYR	CB-CG-CD2	-7.30	116.62	121.00
1	A	20	TYR	CA-CB-CG	-7.29	99.55	113.40
1	A	181	PHE	CB-CG-CD2	-7.26	115.72	120.80
1	A	223	ASN	CA-CB-CG	-7.24	97.46	113.40
1	A	157	CYS	N-CA-CB	-7.10	97.81	110.60
1	A	172	TYR	CG-CD1-CE1	-7.06	115.66	121.30
1	A	150	SER	CB-CA-C	7.02	123.45	110.10
1	A	193	GLY	C-N-CA	-6.89	104.46	121.70
1	A	237	TRP	CG-CD2-CE3	-6.83	127.75	133.90
1	A	190	SER	CB-CA-C	-6.71	97.36	110.10
1	A	188	GLY	O-C-N	-6.66	112.04	122.70
1	A	230	LYS	CD-CE-NZ	-6.61	96.49	111.70
1	A	172	TYR	CD1-CE1-CZ	6.48	125.63	119.80
1	A	178	SER	CA-CB-OG	-6.46	93.76	111.20
1	A	188	GLY	CA-C-O	-6.43	109.03	120.60
1	A	130	SER	N-CA-CB	-6.42	100.87	110.50
1	A	98	THR	CA-CB-CG2	-6.31	103.57	112.40
1	A	245	ASN	CB-CA-C	6.27	122.94	110.40
1	A	221(A)	GLN	CA-C-N	6.17	130.78	117.20
1	A	241	THR	N-CA-CB	-6.10	98.71	110.30
1	A	59	TYR	CB-CG-CD2	6.09	124.65	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	27	VAL	CA-CB-CG1	6.09	120.03	110.90
1	A	75	VAL	CA-CB-CG1	5.97	119.86	110.90
1	A	82	PHE	CB-CG-CD1	-5.93	116.65	120.80
1	A	165	ASP	CB-CG-OD1	-5.83	113.05	118.30
1	A	99	LEU	CB-CG-CD2	5.81	120.88	111.00
1	A	65	VAL	CB-CA-C	-5.76	100.46	111.40
1	A	189	ASP	N-CA-C	5.73	126.47	111.00
1	A	190	SER	C-N-CA	-5.72	107.41	121.70
1	A	225	PRO	C-N-CA	-5.71	110.31	122.30
1	A	194	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	A	149	THR	C-N-CA	-5.69	107.48	121.70
1	A	235	VAL	CA-CB-CG1	5.63	119.34	110.90
1	A	240	GLN	CA-CB-CG	5.62	125.78	113.40
1	A	239	LYS	CD-CE-NZ	5.55	124.46	111.70
1	A	188	GLY	C-N-CA	-5.52	107.89	121.70
1	A	45	SER	CB-CA-C	-5.52	99.61	110.10
1	A	88	SER	O-C-N	5.49	131.48	122.70
1	A	90	VAL	CA-CB-CG1	5.42	119.04	110.90
1	A	51	TRP	CG-CD2-CE3	-5.34	129.10	133.90
1	A	149	THR	CA-CB-CG2	-5.33	104.94	112.40
1	A	184(A)	TYR	CG-CD2-CE2	-5.33	117.04	121.30
1	A	63	ILE	CG1-CB-CG2	5.31	123.08	111.40
1	A	82	PHE	CB-CA-C	-5.31	99.79	110.40
1	A	187	GLY	C-N-CA	5.30	133.43	122.30
1	A	184(A)	TYR	CG-CD1-CE1	-5.28	117.08	121.30
1	A	20	TYR	CG-CD2-CE2	-5.24	117.11	121.30
1	A	181	PHE	CD1-CG-CD2	5.20	125.05	118.30
1	A	98	THR	CA-CB-OG1	-5.17	98.15	109.00
1	A	172	TYR	CA-CB-CG	5.14	123.17	113.40
1	A	70	GLU	CG-CD-OE1	-5.12	108.05	118.30
1	A	93	SER	CB-CA-C	-5.11	100.39	110.10
1	A	152	PRO	N-CA-C	-5.08	98.88	112.10
1	A	135	GLN	N-CA-CB	-5.02	101.56	110.60
1	A	184(A)	TYR	CB-CG-CD1	-5.01	117.99	121.00

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	63	ILE	CB
1	A	150	SER	CA
1	A	242	ILE	CB

All (23) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	124	PRO	Mainchain
1	A	141	TRP	Mainchain
1	A	142	GLY	Mainchain,Peptide
1	A	143	ASN	Mainchain
1	A	144	THR	Mainchain
1	A	188	GLY	Mainchain
1	A	189	ASP	Mainchain
1	A	190	SER	Mainchain
1	A	191	CYS	Mainchain
1	A	198	PRO	Mainchain
1	A	211	GLY	Mainchain
1	A	215	TRP	Mainchain
1	A	225	PRO	Mainchain
1	A	233	ASN	Mainchain
1	A	241	THR	Mainchain
1	A	243	ALA	Mainchain
1	A	60	LYS	Mainchain
1	A	62	GLY	Mainchain
1	A	75	VAL	Mainchain
1	A	79	ASN	Mainchain
1	A	80	GLU	Mainchain
1	A	82	PHE	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	A	1616	0	1564	291	3
2	A	1	0	0	0	0
3	A	10	0	14	10	0
4	A	73	0	0	8	6
All	All	1700	0	1578	292	6

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 91.

All (292) 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:A:184(A):TYR:HB2	1:A:188:GLY:CA	1.43	1.47
1:A:222:LYS:HD3	1:A:223:ASN:ND2	1.25	1.45
1:A:184(A):TYR:CB	1:A:188:GLY:HA3	1.45	1.44
1:A:222:LYS:CD	1:A:223:ASN:HD21	1.32	1.42
1:A:17:VAL:CG1	1:A:143:ASN:ND2	1.80	1.40
1:A:17:VAL:CG1	1:A:143:ASN:HD21	1.35	1.35
1:A:222:LYS:CE	1:A:223:ASN:HD21	1.40	1.34
1:A:158:LEU:C	1:A:158:LEU:HD12	1.30	1.32
1:A:222:LYS:CD	1:A:223:ASN:ND2	1.87	1.32
1:A:25:ASN:HD22	1:A:117:ARG:NH2	1.26	1.32
1:A:189:ASP:HB3	1:A:220:CYS:CA	1.59	1.31
1:A:17:VAL:HG11	1:A:143:ASN:ND2	0.96	1.29
1:A:17:VAL:HG22	1:A:189:ASP:O	1.24	1.27
1:A:25:ASN:ND2	1:A:117:ARG:NH2	1.83	1.25
1:A:184(A):TYR:HD1	1:A:188(A):LYS:N	1.35	1.23
1:A:185:LEU:O	1:A:186:GLU:CB	1.71	1.23
1:A:47:ILE:HD13	1:A:47:ILE:N	1.48	1.21
1:A:20:TYR:N	1:A:20:TYR:CD1	1.94	1.21
1:A:158:LEU:HD12	1:A:159:LYS:N	1.54	1.19
1:A:163:LEU:CD2	1:A:183:ALA:HA	1.72	1.19
1:A:189:ASP:HB3	1:A:220:CYS:N	1.55	1.19
1:A:25:ASN:HD22	1:A:117:ARG:CZ	1.57	1.17
1:A:45:SER:O	1:A:47:ILE:HD11	1.44	1.17
1:A:222:LYS:CE	1:A:223:ASN:ND2	2.07	1.17
1:A:158:LEU:CD1	1:A:158:LEU:C	2.07	1.16
1:A:189:ASP:CB	1:A:220:CYS:HA	1.76	1.16
1:A:45:SER:O	1:A:47:ILE:CD1	1.94	1.13
1:A:143:ASN:HB3	1:A:191:CYS:HB2	1.24	1.13
1:A:141:TRP:O	1:A:194:ASP:OD1	1.63	1.13
1:A:158:LEU:CD1	1:A:159:LYS:N	2.12	1.13
1:A:223:ASN:H	1:A:223:ASN:ND2	1.05	1.12
1:A:65:VAL:HG12	1:A:83:ILE:O	1.49	1.09
1:A:189:ASP:O	1:A:220:CYS:CB	2.00	1.09
1:A:190:SER:O	1:A:220:CYS:HB3	1.53	1.09
1:A:184(A):TYR:CD1	1:A:188(A):LYS:N	2.21	1.08
1:A:189:ASP:O	1:A:220:CYS:HA	1.53	1.08
1:A:47:ILE:N	1:A:47:ILE:CD1	2.10	1.07
1:A:17:VAL:HG21	1:A:143:ASN:HD22	1.14	1.06
1:A:17:VAL:CG2	1:A:189:ASP:O	2.02	1.06
1:A:143:ASN:O	1:A:192:GLN:N	1.89	1.05
1:A:189:ASP:HB3	1:A:220:CYS:HA	1.28	1.04
1:A:222:LYS:HE2	1:A:223:ASN:HD21	1.18	1.04

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LYS:HE2	1:A:223:ASN:ND2	1.71	1.04
1:A:151:TYR:C	1:A:153:ASP:N	2.03	1.04
1:A:163:LEU:HD23	1:A:183:ALA:CA	1.87	1.04
1:A:151:TYR:O	1:A:153:ASP:N	1.90	1.03
1:A:163:LEU:HD23	1:A:183:ALA:HA	1.09	1.03
1:A:223:ASN:N	1:A:223:ASN:ND2	1.89	1.03
1:A:151:TYR:CG	1:A:152:PRO:HD2	1.93	1.03
1:A:143:ASN:O	1:A:144:THR:HB	1.57	1.03
1:A:33:LEU:HD22	1:A:63:ILE:HD11	1.44	1.00
1:A:141:TRP:O	1:A:142:GLY:O	1.80	1.00
1:A:223:ASN:N	1:A:223:ASN:HD22	1.52	0.99
1:A:84:SER:OG	1:A:109:LYS:CE	2.12	0.98
1:A:17:VAL:CG2	1:A:190:SER:C	2.32	0.98
1:A:184(A):TYR:HB2	1:A:188:GLY:C	1.84	0.98
1:A:84:SER:OG	1:A:109:LYS:HE2	1.61	0.98
1:A:151:TYR:C	1:A:153:ASP:H	1.44	0.97
1:A:150:SER:O	1:A:151:TYR:CD1	2.18	0.96
1:A:189:ASP:O	1:A:220:CYS:CA	2.12	0.96
1:A:17:VAL:HG22	1:A:189:ASP:C	1.84	0.96
1:A:17:VAL:CG2	1:A:143:ASN:HD22	1.78	0.96
1:A:77:GLU:OE2	4:A:263:HOH:O	1.83	0.95
1:A:193:GLY:HA2	3:A:248:DFP:H2'2	1.46	0.94
1:A:20:TYR:N	1:A:20:TYR:HD1	1.56	0.94
1:A:222:LYS:HD3	1:A:223:ASN:HD22	1.33	0.94
1:A:158:LEU:O	1:A:158:LEU:HD12	1.69	0.93
1:A:144:THR:CG2	1:A:145:LYS:N	2.31	0.93
1:A:184(A):TYR:HD1	1:A:188(A):LYS:H	1.16	0.93
1:A:186:GLU:HA	1:A:223:ASN:HA	1.49	0.93
1:A:151:TYR:CB	1:A:152:PRO:HD2	1.98	0.92
1:A:189:ASP:O	1:A:190:SER:O	1.88	0.92
1:A:47:ILE:HD13	1:A:47:ILE:H	1.14	0.91
1:A:189:ASP:CA	1:A:220:CYS:HA	2.02	0.90
1:A:190:SER:OG	1:A:191:CYS:N	2.02	0.90
1:A:189:ASP:HB3	1:A:220:CYS:H	1.33	0.90
1:A:17:VAL:HG21	1:A:190:SER:C	1.91	0.90
1:A:25:ASN:ND2	1:A:117:ARG:HH21	1.63	0.89
1:A:184(A):TYR:HB3	1:A:188:GLY:HA3	1.51	0.89
1:A:189:ASP:C	1:A:220:CYS:HA	1.91	0.89
1:A:189:ASP:CB	1:A:220:CYS:H	1.85	0.89
1:A:145:LYS:O	1:A:146:SER:HB3	1.69	0.89
1:A:17:VAL:CB	1:A:143:ASN:ND2	2.34	0.89

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ASP:CB	1:A:220:CYS:CA	2.40	0.88
1:A:143:ASN:C	1:A:192:GLN:H	1.74	0.88
1:A:184(A):TYR:O	1:A:186:GLU:N	2.05	0.88
1:A:17:VAL:HG23	1:A:191:CYS:SG	2.15	0.87
1:A:189:ASP:CB	1:A:220:CYS:N	2.36	0.86
1:A:65:VAL:HG13	1:A:65:VAL:O	1.73	0.86
1:A:17:VAL:HG21	1:A:143:ASN:ND2	1.89	0.86
1:A:193:GLY:CA	3:A:248:DFP:H2'2	2.06	0.86
1:A:144:THR:HG22	1:A:145:LYS:N	1.90	0.86
1:A:184(A):TYR:CB	1:A:188:GLY:CA	2.23	0.86
1:A:17:VAL:HG22	1:A:190:SER:O	1.75	0.85
1:A:185:LEU:O	1:A:186:GLU:HB2	0.79	0.84
1:A:17:VAL:HG23	1:A:220:CYS:HB2	1.60	0.84
1:A:17:VAL:HG11	1:A:143:ASN:CG	1.97	0.84
1:A:17:VAL:HG21	1:A:191:CYS:HB2	1.60	0.83
1:A:193:GLY:O	4:A:273:HOH:O	1.95	0.83
1:A:163:LEU:HD21	1:A:184:GLY:N	1.94	0.83
1:A:142:GLY:O	1:A:192:GLN:O	1.97	0.83
1:A:17:VAL:HG22	1:A:190:SER:C	1.96	0.83
1:A:135:GLN:OE1	1:A:135:GLN:C	2.17	0.83
1:A:222:LYS:HD3	1:A:223:ASN:H	1.40	0.82
1:A:184(A):TYR:C	1:A:186:GLU:H	1.75	0.81
1:A:184(A):TYR:HB2	1:A:188:GLY:HA3	0.83	0.81
1:A:143:ASN:HB3	1:A:191:CYS:CB	2.10	0.80
1:A:25:ASN:ND2	1:A:117:ARG:CZ	2.35	0.80
1:A:151:TYR:CG	1:A:152:PRO:CD	2.64	0.79
1:A:158:LEU:HD13	1:A:159:LYS:N	1.97	0.79
1:A:185:LEU:C	1:A:185:LEU:HD13	2.03	0.78
1:A:151:TYR:CD1	1:A:152:PRO:HD3	2.19	0.78
1:A:163:LEU:CD2	1:A:183:ALA:CA	2.53	0.78
1:A:189:ASP:O	1:A:220:CYS:HB2	1.82	0.77
1:A:17:VAL:CG2	1:A:190:SER:O	2.31	0.77
1:A:57:HIS:CG	3:A:248:DFP:H31	2.19	0.76
1:A:143:ASN:O	1:A:192:GLN:HG3	1.83	0.76
1:A:142:GLY:O	1:A:194:ASP:OD1	2.03	0.76
3:A:248:DFP:H3'1	3:A:248:DFP:H21	1.67	0.76
1:A:17:VAL:CG2	1:A:143:ASN:ND2	2.44	0.75
1:A:186:GLU:CA	1:A:223:ASN:HA	2.17	0.75
1:A:223:ASN:HD22	1:A:223:ASN:H	0.77	0.74
1:A:151:TYR:CD1	1:A:152:PRO:CD	2.70	0.74
1:A:190:SER:OG	4:A:316:HOH:O	2.05	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ASN:HD21	1:A:179:ASN:HD22	1.32	0.74
1:A:141:TRP:O	1:A:142:GLY:C	2.26	0.74
1:A:84:SER:OG	1:A:109:LYS:HE3	1.87	0.73
1:A:25:ASN:HD21	1:A:117:ARG:HH21	1.37	0.73
1:A:151:TYR:HB3	1:A:152:PRO:HD2	1.69	0.72
1:A:151:TYR:O	1:A:152:PRO:C	2.27	0.72
1:A:188(A):LYS:O	4:A:297:HOH:O	2.07	0.71
1:A:72:ASN:CG	1:A:75:VAL:HG23	2.11	0.71
1:A:189:ASP:O	1:A:220:CYS:HB3	1.89	0.71
1:A:185:LEU:CD1	1:A:185:LEU:C	2.58	0.70
1:A:17:VAL:CG2	1:A:191:CYS:HB2	2.21	0.70
1:A:46:LEU:C	1:A:47:ILE:HD13	2.10	0.70
1:A:151:TYR:CB	1:A:152:PRO:CD	2.69	0.70
1:A:222:LYS:HD3	1:A:223:ASN:N	2.06	0.70
1:A:72:ASN:OD1	1:A:74:ASN:N	2.23	0.70
1:A:185:LEU:O	1:A:185:LEU:HD13	1.91	0.69
1:A:192:GLN:O	1:A:194:ASP:OD1	2.10	0.69
1:A:65:VAL:CG1	1:A:65:VAL:O	2.41	0.69
1:A:72:ASN:OD1	1:A:75:VAL:HG23	1.94	0.68
1:A:87:LYS:NZ	1:A:245:ASN:HD22	1.91	0.68
1:A:190:SER:O	1:A:220:CYS:CB	2.39	0.68
1:A:189:ASP:CG	4:A:274:HOH:O	2.33	0.67
1:A:143:ASN:O	1:A:144:THR:CB	2.31	0.67
1:A:151:TYR:HB3	1:A:153:ASP:H	1.57	0.67
1:A:121:ILE:HG12	1:A:122:SER:N	2.09	0.66
1:A:33:LEU:HB3	1:A:63:ILE:CD1	2.25	0.66
1:A:145:LYS:O	1:A:146:SER:CB	2.40	0.66
1:A:158:LEU:HD12	1:A:159:LYS:CA	2.24	0.66
1:A:151:TYR:H	1:A:154:VAL:HG22	1.61	0.66
1:A:81:GLN:HE22	1:A:113:SER:H	1.41	0.65
1:A:39:TYR:N	1:A:39:TYR:CD1	2.65	0.65
1:A:150:SER:O	1:A:151:TYR:CE1	2.49	0.65
1:A:151:TYR:CA	1:A:153:ASP:H	2.10	0.64
1:A:163:LEU:HD21	1:A:184:GLY:H	1.62	0.64
1:A:184(A):TYR:CD1	1:A:188:GLY:C	2.72	0.63
1:A:186:GLU:C	1:A:188:GLY:H	2.00	0.63
1:A:57:HIS:CG	3:A:248:DFP:C3	2.82	0.63
1:A:184(A):TYR:C	1:A:186:GLU:N	2.43	0.63
1:A:34:ASN:ND2	1:A:38:GLY:H	1.98	0.62
1:A:17:VAL:CG2	1:A:220:CYS:HB2	2.29	0.61
1:A:189:ASP:CG	1:A:220:CYS:H	2.03	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:VAL:HG22	1:A:190:SER:CA	2.30	0.61
1:A:193:GLY:HA2	3:A:248:DFP:C2'	2.25	0.60
1:A:150:SER:O	1:A:151:TYR:HD1	1.64	0.60
1:A:151:TYR:CB	1:A:153:ASP:H	2.13	0.60
1:A:121:ILE:HG12	1:A:122:SER:H	1.63	0.60
1:A:47:ILE:HD11	1:A:53:VAL:H	1.67	0.60
1:A:151:TYR:HB3	1:A:153:ASP:HB2	1.82	0.60
1:A:17:VAL:CG2	1:A:191:CYS:CB	2.81	0.59
1:A:17:VAL:HG21	1:A:143:ASN:HB3	1.85	0.59
1:A:222:LYS:HB2	1:A:223:ASN:HD22	1.67	0.58
1:A:150:SER:HB3	1:A:154:VAL:HG21	1.85	0.58
1:A:186:GLU:C	1:A:188:GLY:N	2.57	0.58
1:A:144:THR:HG23	1:A:145:LYS:N	2.13	0.58
1:A:172:TYR:N	1:A:173:PRO:HD3	2.18	0.58
1:A:30:GLN:OE1	1:A:139:SER:HB3	2.03	0.58
1:A:55:ALA:O	1:A:58:CYS:HB2	2.03	0.58
1:A:154:VAL:O	1:A:156:LYS:HD2	2.03	0.58
1:A:57:HIS:ND1	3:A:248:DFP:H31	2.19	0.57
1:A:17:VAL:HG21	1:A:191:CYS:CB	2.34	0.57
1:A:158:LEU:CD1	1:A:159:LYS:C	2.72	0.57
1:A:209:LEU:CD2	1:A:209:LEU:C	2.73	0.57
1:A:45:SER:O	1:A:47:ILE:HD13	1.96	0.57
1:A:190:SER:HB3	4:A:266:HOH:O	2.04	0.56
1:A:17:VAL:HG22	1:A:190:SER:N	2.18	0.56
1:A:100:ASN:ND2	1:A:179:ASN:HD22	2.02	0.56
1:A:108:LEU:HB3	1:A:110:SER:O	2.05	0.56
1:A:241:THR:C	1:A:244:SER:H	2.09	0.56
1:A:163:LEU:CD2	1:A:184:GLY:N	2.66	0.55
1:A:151:TYR:HB3	1:A:153:ASP:CB	2.36	0.55
1:A:151:TYR:CB	1:A:153:ASP:HB2	2.36	0.55
1:A:46:LEU:CA	1:A:47:ILE:HD13	2.36	0.55
1:A:222:LYS:CB	1:A:223:ASN:HD22	2.20	0.55
1:A:158:LEU:CD1	1:A:159:LYS:CA	2.84	0.54
1:A:87:LYS:CE	1:A:245:ASN:HD22	2.20	0.54
1:A:186:GLU:HG3	1:A:223:ASN:N	2.23	0.54
1:A:105:LEU:N	1:A:105:LEU:CD2	2.69	0.54
1:A:151:TYR:HB3	1:A:153:ASP:N	2.22	0.54
1:A:150:SER:HB3	1:A:154:VAL:CG2	2.38	0.53
1:A:163:LEU:HD22	1:A:163:LEU:N	2.22	0.53
1:A:223:ASN:OD1	1:A:223:ASN:O	2.27	0.53
1:A:222:LYS:CD	1:A:223:ASN:HD22	1.97	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:33:LEU:CD2	1:A:63:ILE:HD11	2.29	0.52
1:A:184(A):TYR:HB2	1:A:188(A):LYS:N	2.23	0.52
1:A:143:ASN:ND2	1:A:190:SER:HA	2.25	0.52
1:A:27:VAL:HG11	1:A:139:SER:OG	2.10	0.52
1:A:17:VAL:CG2	1:A:190:SER:CA	2.88	0.51
1:A:95:ASN:OD1	1:A:95:ASN:C	2.48	0.51
1:A:53:VAL:HG23	1:A:105:LEU:HD22	1.93	0.51
1:A:143:ASN:HD22	1:A:190:SER:C	2.13	0.51
1:A:19:GLY:C	1:A:20:TYR:HD1	2.08	0.51
1:A:22:CYS:SG	1:A:156:LYS:C	2.89	0.51
1:A:101:ASN:ND2	1:A:234:TYR:OH	2.43	0.51
1:A:184(A):TYR:CD1	1:A:184(A):TYR:N	2.78	0.51
1:A:186:GLU:O	1:A:188:GLY:N	2.44	0.51
1:A:57:HIS:CE1	3:A:248:DFP:H33	2.46	0.50
1:A:219:GLY:O	1:A:220:CYS:SG	2.69	0.50
1:A:144:THR:HG23	1:A:145:LYS:HA	1.92	0.50
1:A:161:PRO:O	1:A:163:LEU:HD22	2.11	0.50
1:A:189:ASP:C	1:A:190:SER:O	2.44	0.50
1:A:41:PHE:O	1:A:42:CYS:SG	2.70	0.50
1:A:135:GLN:OE1	1:A:136:CYS:N	2.44	0.50
1:A:186:GLU:HA	1:A:222:LYS:O	2.11	0.50
1:A:17:VAL:CG2	1:A:191:CYS:SG	2.94	0.50
1:A:216:GLY:O	1:A:217:SER:HB3	2.11	0.50
1:A:87:LYS:HE2	1:A:245:ASN:HD22	1.75	0.49
1:A:193:GLY:HA2	4:A:253:HOH:O	2.12	0.49
1:A:209:LEU:HD21	1:A:211:GLY:O	2.12	0.49
1:A:87:LYS:HE2	1:A:245:ASN:ND2	2.28	0.49
1:A:115:ASN:C	1:A:115:ASN:OD1	2.52	0.48
1:A:189:ASP:OD1	1:A:190:SER:O	2.31	0.48
1:A:143:ASN:CA	1:A:192:GLN:H	2.26	0.48
1:A:57:HIS:CD2	3:A:248:DFP:C3	2.96	0.48
1:A:48:ASN:C	1:A:48:ASN:OD1	2.51	0.48
1:A:25:ASN:HD21	1:A:117:ARG:NH2	1.92	0.48
1:A:33:LEU:HB3	1:A:63:ILE:HD12	1.95	0.48
1:A:209:LEU:HD22	1:A:209:LEU:C	2.35	0.47
1:A:25:ASN:ND2	1:A:117:ARG:HD3	2.30	0.47
1:A:146:SER:OG	1:A:147:SER:N	2.47	0.47
1:A:182:CYS:HA	1:A:226:GLY:O	2.14	0.47
1:A:223:ASN:O	1:A:223:ASN:CG	2.46	0.47
1:A:212:ILE:HB	1:A:229:THR:HB	1.96	0.47
1:A:163:LEU:CD2	1:A:183:ALA:C	2.82	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:VAL:HG12	1:A:66:LEU:HD23	1.96	0.47
1:A:29:TYR:HA	1:A:119:ALA:O	2.16	0.46
1:A:185:LEU:O	1:A:186:GLU:CG	2.59	0.46
1:A:240:GLN:O	1:A:241:THR:C	2.50	0.45
1:A:164:SER:OG	1:A:167:SER:OG	2.23	0.45
1:A:165:ASP:O	1:A:169:LYS:HD3	2.16	0.45
1:A:190:SER:CB	4:A:266:HOH:O	2.64	0.45
1:A:189:ASP:OD1	1:A:220:CYS:N	2.50	0.44
1:A:99:LEU:HA	1:A:99:LEU:HD12	1.88	0.44
1:A:75:VAL:O	1:A:77:GLU:HG3	2.18	0.44
1:A:144:THR:O	1:A:144:THR:HG23	2.12	0.44
1:A:217:SER:OG	1:A:217:SER:O	2.24	0.44
1:A:46:LEU:C	1:A:47:ILE:CD1	2.77	0.44
1:A:185:LEU:HD13	1:A:186:GLU:HB2	1.99	0.44
1:A:82:PHE:C	1:A:83:ILE:HG13	2.36	0.44
1:A:186:GLU:HA	1:A:223:ASN:CA	2.34	0.44
1:A:17:VAL:HG23	1:A:191:CYS:CB	2.47	0.43
1:A:52:VAL:HB	1:A:106:ILE:HB	2.00	0.43
1:A:143:ASN:N	1:A:143:ASN:OD1	2.51	0.43
1:A:160:ALA:HB1	1:A:184:GLY:HA2	2.00	0.43
1:A:202:SER:O	1:A:204:LYS:HE2	2.19	0.43
1:A:230:LYS:CG	1:A:230:LYS:O	2.67	0.43
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.54	0.43
1:A:168:CYS:O	1:A:171:ALA:HB3	2.20	0.42
1:A:163:LEU:HD22	1:A:183:ALA:HA	1.84	0.42
1:A:151:TYR:O	1:A:156:LYS:CE	2.68	0.42
1:A:154:VAL:O	1:A:156:LYS:CD	2.67	0.42
1:A:151:TYR:O	1:A:156:LYS:HE3	2.20	0.42
1:A:56:ALA:HB3	1:A:94:TYR:CE2	2.54	0.42
1:A:165:ASP:O	1:A:166:SER:C	2.56	0.41
1:A:193:GLY:C	3:A:248:DFP:H2'2	2.40	0.41
1:A:46:LEU:HA	1:A:46:LEU:HD12	1.89	0.41
1:A:94:TYR:HA	1:A:101:ASN:HB2	2.02	0.41
1:A:150:SER:C	1:A:151:TYR:HD1	2.21	0.41
1:A:158:LEU:HD11	1:A:159:LYS:C	2.41	0.41
1:A:143:ASN:HD22	1:A:190:SER:CA	2.33	0.41
1:A:163:LEU:CD2	1:A:163:LEU:N	2.82	0.41
1:A:213:VAL:HA	1:A:228:TYR:HD1	1.85	0.41
1:A:98:THR:HG23	1:A:98:THR:H	1.64	0.41
1:A:185:LEU:O	1:A:186:GLU:CD	2.58	0.41
1:A:84:SER:HG	1:A:109:LYS:HE2	1.76	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:ILE:HD11	1:A:53:VAL:N	2.35	0.41
1:A:144:THR:HG23	1:A:145:LYS:CA	2.51	0.40
1:A:101:ASN:HA	1:A:234:TYR:OH	2.21	0.40
1:A:213:VAL:HA	1:A:228:TYR:CD1	2.56	0.40

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:271:HOH:O	4:A:277:HOH:O[6_665]	1.04	1.16
4:A:287:HOH:O	4:A:310:HOH:O[6_665]	1.94	0.26
1:A:98:THR:CG2	4:A:309:HOH:O[5_565]	1.95	0.25
1:A:147:SER:OG	4:A:269:HOH:O[5_675]	2.10	0.10
1:A:146:SER:O	4:A:272:HOH:O[5_675]	2.18	0.02
4:A:284:HOH:O	4:A:315:HOH:O[2_765]	2.18	0.02

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	A	220/229 (96%)	187 (85%)	22 (10%)	11 (5%)	2 0

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	142	GLY
1	A	145	LYS
1	A	146	SER
1	A	185	LEU
1	A	186	GLU
1	A	190	SER
1	A	217	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	144	THR
1	A	187	GLY
1	A	152	PRO
1	A	220	CYS

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	182/190 (96%)	148 (81%)	34 (19%)	1 0

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	20	TYR
1	A	47	ILE
1	A	53	VAL
1	A	60	LYS
1	A	63	ILE
1	A	90	VAL
1	A	99	LEU
1	A	100	ASN
1	A	105	LEU
1	A	125	THR
1	A	127	SER
1	A	135	GLN
1	A	137	LEU
1	A	139	SER
1	A	145	LYS
1	A	146	SER
1	A	147	SER
1	A	149	THR
1	A	150	SER
1	A	155	LEU
1	A	156	LYS
1	A	158	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	170	SER
1	A	185	LEU
1	A	186	GLU
1	A	190	SER
1	A	191	CYS
1	A	192	GLN
1	A	202	SER
1	A	204	LYS
1	A	209	LEU
1	A	222	LYS
1	A	223	ASN
1	A	240	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	34	ASN
1	A	81	GLN
1	A	100	ASN
1	A	101	ASN
1	A	143	ASN
1	A	223	ASN
1	A	233	ASN
1	A	245	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is 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
3	DFP	A	248	1	6,9,9	1.05	0	6,11,11	1.15	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	DFP	A	248	1	-	0/4/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	248	DFP	10	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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.