



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:04 PM UTC

PDB ID : 2TGD / pdb_00002tgd
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

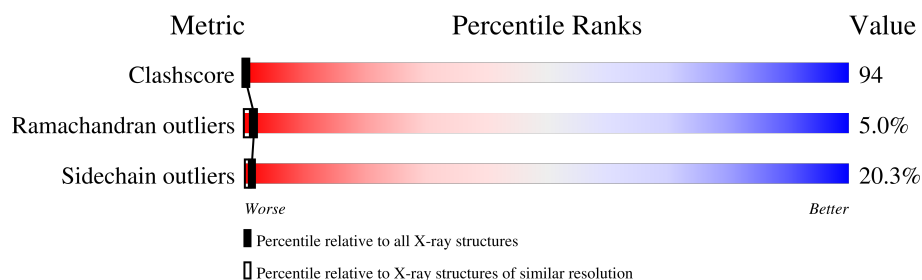
1 Overall quality at a glance

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	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (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 of 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.

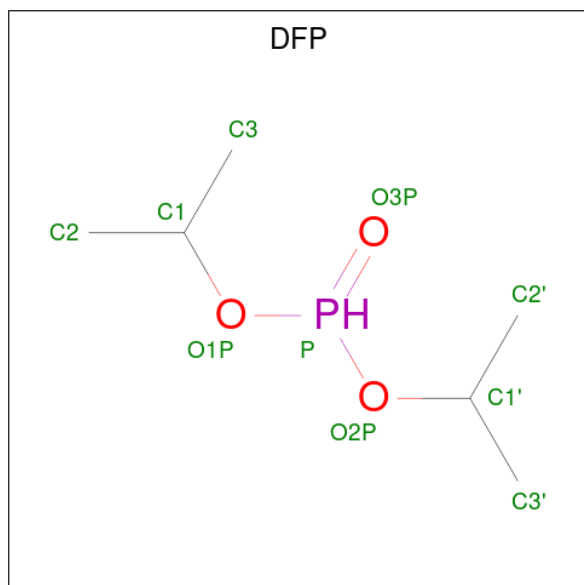
- Molecule 1 is a protein called TRYPSINOGEN.

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

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 3 is DIISOPROPYL PHOSPHONATE (CCD ID: 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.

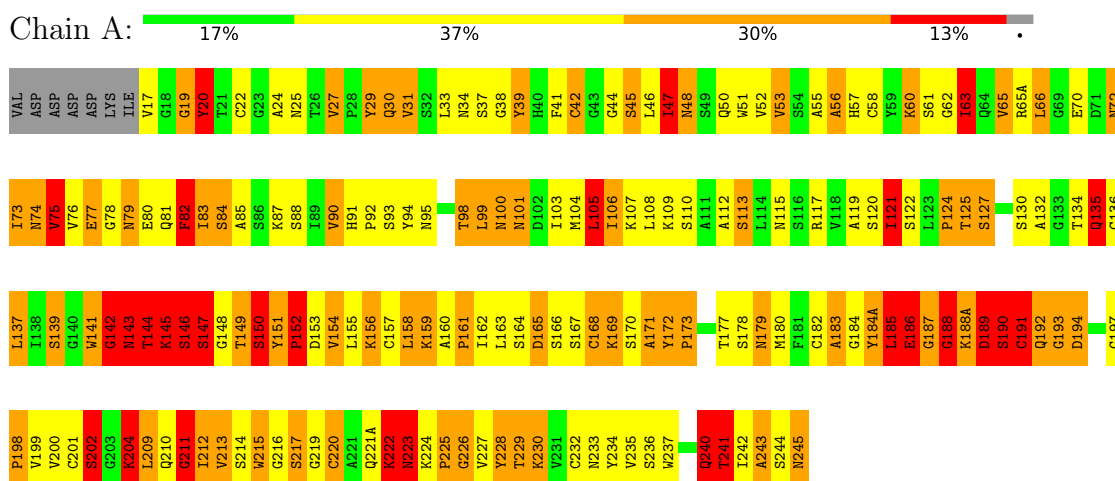
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	73	Total 73	O 73	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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

Xtriage (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.	Xtriage
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: DFP, CA

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	2.35	84/1647 (5.1%)	2.70	144/2233 (6.4%)

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 (84) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	150	SER	N-CA	-13.37	1.37	1.46
1	A	179	ASN	N-CA	-8.75	1.35	1.46
1	A	240	GLN	C-N	-8.73	1.22	1.33
1	A	171	ALA	CA-CB	8.45	1.67	1.53
1	A	179	ASN	CA-CB	-8.18	1.41	1.53
1	A	240	GLN	CD-OE1	7.94	1.38	1.23
1	A	241	THR	N-CA	-7.88	1.36	1.46
1	A	48	ASN	CA-C	-7.72	1.43	1.52
1	A	121	ILE	C-O	-7.48	1.16	1.24
1	A	237	TRP	NE1-CE2	-7.19	1.29	1.37
1	A	75	VAL	C-N	-7.18	1.26	1.33
1	A	63	ILE	CA-CB	-7.14	1.45	1.54
1	A	197	GLY	CA-C	7.13	1.61	1.51
1	A	177	THR	CA-C	-7.12	1.43	1.53
1	A	188(A)	LYS	N-CA	6.93	1.54	1.46
1	A	70	GLU	CA-C	-6.81	1.43	1.53
1	A	188(A)	LYS	C-N	6.75	1.42	1.33
1	A	222	LYS	C-N	-6.56	1.24	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183	ALA	CA-C	-6.54	1.44	1.52
1	A	189	ASP	N-CA	6.54	1.54	1.46
1	A	135	GLN	N-CA	-6.45	1.38	1.46
1	A	73	ILE	N-CA	-6.42	1.38	1.46
1	A	72	ASN	C-O	-6.42	1.16	1.24
1	A	162	ILE	C-O	6.40	1.31	1.24
1	A	242	ILE	CA-C	-6.36	1.44	1.52
1	A	185	LEU	CA-C	-6.29	1.44	1.52
1	A	51	TRP	CD1-NE1	6.23	1.50	1.37
1	A	165	ASP	CA-C	-6.22	1.45	1.52
1	A	121	ILE	CA-CB	-6.22	1.44	1.55
1	A	56	ALA	CA-CB	-6.17	1.43	1.53
1	A	98	THR	CA-CB	-6.15	1.44	1.54
1	A	240	GLN	CA-C	-6.12	1.44	1.52
1	A	20	TYR	CA-CB	-6.07	1.45	1.53
1	A	214	SER	CA-C	-6.04	1.46	1.52
1	A	243	ALA	C-N	-6.00	1.25	1.33
1	A	20	TYR	CA-C	-5.98	1.44	1.52
1	A	236	SER	CA-C	-5.97	1.45	1.52
1	A	223	ASN	CA-CB	-5.97	1.45	1.53
1	A	134	THR	C-N	-5.92	1.25	1.33
1	A	84	SER	C-N	-5.87	1.25	1.33
1	A	137	LEU	CA-C	-5.87	1.45	1.52
1	A	212	ILE	CA-CB	-5.87	1.47	1.54
1	A	226	GLY	C-O	5.80	1.32	1.23
1	A	242	ILE	CG1-CD1	5.78	1.74	1.51
1	A	232	CYS	C-N	-5.76	1.26	1.34
1	A	154	VAL	N-CA	-5.76	1.36	1.45
1	A	221(A)	GLN	C-N	-5.76	1.25	1.33
1	A	83	ILE	CA-CB	-5.70	1.47	1.54
1	A	186	GLU	N-CA	-5.67	1.38	1.46
1	A	103	ILE	C-O	5.63	1.30	1.23
1	A	93	SER	CA-CB	-5.62	1.45	1.53
1	A	79	ASN	CA-C	-5.61	1.45	1.52
1	A	120	SER	CA-C	-5.56	1.45	1.53
1	A	230	LYS	CA-C	5.53	1.59	1.53
1	A	199	VAL	CA-CB	-5.47	1.46	1.54
1	A	77	GLU	CA-CB	-5.45	1.45	1.53
1	A	29	TYR	CZ-OH	-5.44	1.26	1.38
1	A	66	LEU	CB-CG	-5.43	1.42	1.53
1	A	169	LYS	C-N	-5.40	1.26	1.33
1	A	202	SER	CA-C	-5.39	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	200	VAL	N-CA	-5.39	1.40	1.46
1	A	214	SER	N-CA	5.37	1.52	1.46
1	A	143	ASN	CA-CB	-5.36	1.44	1.53
1	A	149	THR	CB-OG1	5.36	1.52	1.43
1	A	237	TRP	CD2-CE2	-5.35	1.32	1.41
1	A	204	LYS	C-O	-5.33	1.17	1.23
1	A	161	PRO	N-CA	5.32	1.52	1.46
1	A	42	CYS	C-N	-5.26	1.27	1.33
1	A	215	TRP	CA-C	-5.25	1.45	1.52
1	A	210	GLN	CD-NE2	-5.23	1.22	1.33
1	A	178	SER	N-CA	-5.22	1.39	1.46
1	A	173	PRO	CA-C	-5.21	1.47	1.52
1	A	229	THR	N-CA	-5.21	1.39	1.46
1	A	106	ILE	CA-CB	-5.21	1.47	1.54
1	A	228	TYR	N-CA	-5.19	1.39	1.45
1	A	90	VAL	CA-CB	-5.17	1.48	1.54
1	A	77	GLU	N-CA	-5.13	1.40	1.46
1	A	51	TRP	NE1-CE2	-5.12	1.31	1.37
1	A	107	LYS	CA-C	-5.10	1.46	1.52
1	A	100	ASN	C-O	-5.09	1.17	1.23
1	A	113	SER	N-CA	-5.08	1.39	1.46
1	A	241	THR	C-N	-5.07	1.27	1.34
1	A	198	PRO	C-N	-5.07	1.27	1.33
1	A	50	GLN	CA-CB	-5.04	1.46	1.53

All (144) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	150	SER	N-CA-C	18.00	123.54	108.78
1	A	223	ASN	CA-CB-CG	-15.14	97.46	112.60
1	A	149	THR	CA-C-N	-14.41	107.48	123.04
1	A	149	THR	C-N-CA	-14.41	107.48	123.04
1	A	243	ALA	CA-C-N	-13.52	101.53	122.49
1	A	243	ALA	C-N-CA	-13.52	101.53	122.49
1	A	221(A)	GLN	CA-C-N	-12.83	97.04	121.54
1	A	221(A)	GLN	C-N-CA	-12.83	97.04	121.54
1	A	150	SER	CA-C-O	11.75	124.75	117.94
1	A	242	ILE	CA-CB-CG2	11.58	130.19	110.50
1	A	193	GLY	CA-C-N	-11.43	104.46	122.29
1	A	193	GLY	C-N-CA	-11.43	104.46	122.29
1	A	189	ASP	N-CA-C	10.79	126.47	107.80
1	A	242	ILE	CA-CB-CG1	10.53	128.30	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	O-C-N	10.24	128.40	121.23
1	A	151	TYR	CB-CG-CD1	-9.63	106.36	120.80
1	A	223	ASN	N-CA-CB	-9.50	97.39	111.25
1	A	151	TYR	CB-CG-CD2	9.14	134.50	120.80
1	A	63	ILE	N-CA-C	9.01	121.25	108.36
1	A	165	ASP	CA-CB-CG	-8.92	103.68	112.60
1	A	188	GLY	CA-C-N	8.80	136.56	117.20
1	A	178	SER	CA-CB-OG	-8.67	93.76	111.10
1	A	151	TYR	N-CA-CB	8.44	126.53	110.49
1	A	31	VAL	CA-C-O	-8.19	113.07	121.67
1	A	240	GLN	CA-C-N	-8.19	109.79	120.44
1	A	240	GLN	C-N-CA	-8.19	109.79	120.44
1	A	20	TYR	CA-CB-CG	-7.97	99.55	113.90
1	A	157	CYS	N-CA-CB	-7.97	97.81	111.69
1	A	241	THR	N-CA-CB	-7.79	98.71	110.01
1	A	98	THR	CA-CB-OG1	-7.63	98.15	109.60
1	A	225	PRO	CA-C-N	-7.63	110.31	121.30
1	A	225	PRO	C-N-CA	-7.63	110.31	121.30
1	A	190	SER	CA-C-N	-7.40	107.41	121.54
1	A	190	SER	C-N-CA	-7.40	107.41	121.54
1	A	213	VAL	N-CA-C	7.37	118.88	108.93
1	A	184(A)	TYR	N-CA-C	7.24	120.99	108.76
1	A	143	ASN	CA-CB-CG	-7.20	105.41	112.60
1	A	171	ALA	CA-C-N	-7.19	114.23	122.00
1	A	171	ALA	C-N-CA	-7.19	114.23	122.00
1	A	172	TYR	CA-C-N	7.07	128.92	120.23
1	A	172	TYR	C-N-CA	7.07	128.92	120.23
1	A	194	ASP	CA-CB-CG	7.05	119.66	112.60
1	A	135	GLN	CB-CG-CD	-7.05	100.61	112.60
1	A	188(A)	LYS	N-CA-C	6.99	120.94	109.06
1	A	88	SER	O-C-N	6.98	131.48	123.31
1	A	124	PRO	CA-C-O	-6.96	113.17	122.08
1	A	65	VAL	CB-CA-C	-6.96	100.46	110.83
1	A	143	ASN	N-CA-C	-6.77	103.70	112.23
1	A	245	ASN	CB-CA-C	6.76	122.94	110.10
1	A	112	ALA	CA-C-O	-6.74	113.72	121.47
1	A	132	ALA	CA-C-N	-6.72	112.76	123.31
1	A	132	ALA	C-N-CA	-6.72	112.76	123.31
1	A	78	GLY	CA-C-N	-6.71	112.09	122.49
1	A	78	GLY	C-N-CA	-6.71	112.09	122.49
1	A	188	GLY	O-C-N	-6.66	112.04	122.70
1	A	188	GLY	CA-C-O	-6.63	109.03	120.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	152	PRO	N-CA-C	-6.60	98.88	112.47
1	A	212	ILE	CB-CG1-CD1	-6.58	99.98	113.80
1	A	93	SER	CB-CA-C	-6.56	100.39	111.02
1	A	190	SER	CB-CA-C	-6.56	97.36	110.42
1	A	221(A)	GLN	CA-C-O	-6.53	111.18	120.51
1	A	222	LYS	CA-C-N	-6.49	113.50	123.17
1	A	222	LYS	C-N-CA	-6.49	113.50	123.17
1	A	65(A)	ARG	NE-CZ-NH2	-6.49	113.36	119.20
1	A	179	ASN	CB-CG-ND2	-6.48	106.68	116.40
1	A	223	ASN	CB-CA-C	-6.37	100.40	111.23
1	A	82	PHE	CB-CA-C	-6.34	99.79	110.19
1	A	44	GLY	CA-C-O	-6.29	115.43	121.41
1	A	227	VAL	O-C-N	6.29	129.83	123.10
1	A	77	GLU	CA-C-N	-6.28	116.04	123.08
1	A	77	GLU	C-N-CA	-6.28	116.04	123.08
1	A	19	GLY	CA-C-N	-6.27	111.85	123.01
1	A	19	GLY	C-N-CA	-6.27	111.85	123.01
1	A	74	ASN	OD1-CG-ND2	6.21	128.81	122.60
1	A	188(A)	LYS	CA-C-O	-6.18	113.18	120.60
1	A	48	ASN	OD1-CG-ND2	6.16	128.76	122.60
1	A	237	TRP	CG-CD2-CE3	-6.15	127.75	133.90
1	A	187	GLY	CA-C-N	6.13	133.43	121.41
1	A	187	GLY	C-N-CA	6.13	133.43	121.41
1	A	213	VAL	CA-C-O	-6.13	113.44	120.98
1	A	88	SER	CA-C-O	-6.05	113.60	120.32
1	A	73	ILE	CB-CG1-CD1	-6.01	101.17	113.80
1	A	85	ALA	CA-C-N	-6.00	112.72	122.26
1	A	85	ALA	C-N-CA	-6.00	112.72	122.26
1	A	240	GLN	OE1-CD-NE2	-5.93	116.67	122.60
1	A	130	SER	N-CA-CB	-5.85	100.87	110.52
1	A	240	GLN	CA-CB-CG	5.84	125.78	114.10
1	A	61	SER	O-C-N	-5.83	116.13	123.01
1	A	105	LEU	CA-C-N	-5.83	115.35	123.10
1	A	105	LEU	C-N-CA	-5.83	115.35	123.10
1	A	39	TYR	CB-CA-C	-5.82	100.47	110.95
1	A	190	SER	CA-C-O	-5.77	112.26	120.51
1	A	79	ASN	N-CA-CB	5.71	119.23	110.61
1	A	27	VAL	CA-CB-CG1	5.67	120.03	110.40
1	A	179	ASN	OD1-CG-ND2	5.66	128.26	122.60
1	A	168	CYS	CA-C-N	5.58	128.32	120.28
1	A	168	CYS	C-N-CA	5.58	128.32	120.28
1	A	177	THR	CB-CA-C	-5.58	100.81	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	CA-CB-CG1	5.57	119.86	110.40
1	A	179	ASN	N-CA-CB	-5.55	102.43	110.70
1	A	188	GLY	C-N-CA	-5.52	107.89	121.70
1	A	134	THR	CA-C-N	-5.49	115.15	122.72
1	A	134	THR	C-N-CA	-5.49	115.15	122.72
1	A	93	SER	N-CA-C	-5.46	105.31	112.41
1	A	240	GLN	N-CA-CB	-5.46	102.07	110.20
1	A	180	MET	CG-SD-CE	5.45	112.90	100.90
1	A	230	LYS	CB-CA-C	-5.45	103.53	112.03
1	A	135	GLN	N-CA-CB	-5.44	101.56	110.43
1	A	47	ILE	CB-CA-C	-5.43	105.09	111.94
1	A	31	VAL	O-C-N	5.41	129.05	123.04
1	A	76	VAL	N-CA-CB	-5.41	105.12	111.39
1	A	24	ALA	CB-CA-C	-5.39	103.16	109.80
1	A	144	THR	CB-CA-C	-5.39	99.70	110.42
1	A	187	GLY	O-C-N	5.36	129.67	122.70
1	A	165	ASP	CB-CA-C	-5.36	102.47	110.88
1	A	37	SER	N-CA-C	-5.32	103.70	111.30
1	A	224	LYS	CA-C-O	5.31	123.82	119.36
1	A	78	GLY	CA-C-O	-5.30	114.07	119.37
1	A	77	GLU	N-CA-CB	-5.29	102.26	110.98
1	A	161	PRO	N-CA-CB	5.27	108.31	102.72
1	A	30	GLN	CA-C-O	-5.27	115.26	121.16
1	A	148	GLY	N-CA-C	-5.26	100.72	113.18
1	A	235	VAL	CA-CB-CG1	5.26	119.34	110.40
1	A	162	ILE	CA-C-O	-5.26	115.05	121.04
1	A	227	VAL	CA-C-O	-5.25	114.79	120.67
1	A	125	THR	CA-C-O	5.24	125.33	119.41
1	A	101	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	185	LEU	CA-C-N	-5.23	111.55	121.54
1	A	185	LEU	C-N-CA	-5.23	111.55	121.54
1	A	177	THR	CA-C-N	5.22	127.79	120.28
1	A	177	THR	C-N-CA	5.22	127.79	120.28
1	A	172	TYR	CA-CB-CG	5.15	123.17	113.90
1	A	143	ASN	N-CA-CB	-5.14	102.39	110.30
1	A	98	THR	N-CA-CB	-5.13	103.11	110.65
1	A	211	GLY	N-CA-C	5.13	118.58	111.10
1	A	90	VAL	N-CA-CB	5.11	120.45	110.95
1	A	127	SER	CA-CB-OG	-5.08	100.93	111.10
1	A	90	VAL	CA-CB-CG1	5.08	119.04	110.40
1	A	50	GLN	CA-CB-CG	-5.07	103.95	114.10
1	A	186	GLU	O-C-N	5.04	129.30	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	ILE	CA-CB-CG1	5.03	118.95	110.40
1	A	147	SER	N-CA-C	5.03	117.47	108.17
1	A	45	SER	CA-C-O	-5.02	114.58	120.60
1	A	48	ASN	N-CA-C	-5.02	101.27	108.60

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	Peptide,Mainchain
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	299	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	300	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 94.

All (300) 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:158:LEU:C	1:A:158:LEU:HD12	1.30	1.37
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: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:CD1	1:A:20:TYR:N	1.94	1.21
1:A:158:LEU:C	1:A:158:LEU:CD1	2.07	1.20
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:141:TRP:O	1:A:194:ASP:OD1	1.63	1.13
1:A:143:ASN:HB3	1:A:191:CYS:HB2	1.24	1.13
1:A:158:LEU:CD1	1:A:159:LYS:N	2.12	1.13
1:A:223:ASN:ND2	1:A:223:ASN:H	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:151:TYR:C	1:A:153:ASP:N	2.03	1.07
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
1:A:222:LYS:HE2	1:A:223:ASN:ND2	1.71	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:ND2	1:A:223:ASN:N	1.89	1.03
1:A:151:TYR:CG	1:A:152:PRO:HD2	1.93	1.03
1:A:17:VAL:CG2	1:A:190:SER:C	2.32	1.03
1:A:143:ASN:O	1:A:144:THR:HB	1.57	1.03
1:A:184(A):TYR:HB2	1:A:188:GLY:C	1.84	1.03
1:A:151:TYR:C	1:A:153:ASP:H	1.44	1.02
1:A:17:VAL:HG22	1:A:189:ASP:C	1.84	1.01
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:84:SER:OG	1:A:109:LYS:HE2	1.61	0.98
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:CG2	1:A:143:ASN:HD22	1.78	0.96
1:A:17:VAL:HG21	1:A:190:SER:C	1.91	0.95
1:A:77:GLU:OE2	4:A:263:HOH:O	1.83	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:189:ASP:C	1:A:220:CYS:HA	1.91	0.94
1:A:222:LYS:HD3	1:A:223:ASN:HD22	1.33	0.94
1:A:158:LEU:HD12	1:A:158:LEU:O	1.69	0.93
1:A:144:THR:CG2	1:A:145:LYS:N	2.31	0.93
1:A:143:ASN:C	1:A:192:GLN:H	1.74	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: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:17:VAL:HG22	1:A:190:SER:C	1.96	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
1:A:17:VAL:HG11	1:A:143:ASN:CG	1.97	0.88
1:A:189:ASP:CB	1:A:220:CYS:CA	2.40	0.88
1:A:184(A):TYR:O	1:A:186:GLU:N	2.05	0.88
1:A:135:GLN:C	1:A:135:GLN:OE1	2.17	0.88
1:A:17:VAL:HG23	1:A:191:CYS:SG	2.15	0.87
1:A:65:VAL:HG13	1:A:65:VAL:O	1.73	0.86
1:A:189:ASP:CB	1:A:220:CYS:N	2.36	0.86
1:A:184(A):TYR:C	1:A:186:GLU:H	1.75	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	0.84
1:A:17:VAL:HG23	1:A:220:CYS:HB2	1.60	0.84
1:A:185:LEU:O	1:A:186:GLU:HB2	0.79	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:142:GLY:O	1:A:192:GLN:O	1.97	0.83
1:A:163:LEU:HD21	1:A:184:GLY:N	1.94	0.83
1:A:222:LYS:HD3	1:A:223:ASN:H	1.40	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HD13	1:A:185:LEU:C	2.03	0.82
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:141:TRP:O	1:A:142:GLY:C	2.26	0.79
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: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:151:TYR:O	1:A:152:PRO:C	2.27	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
1:A:72:ASN:CG	1:A:75:VAL:HG23	2.11	0.76
3:A:248:DFP:H21	3:A:248:DFP:H3'1	1.67	0.76
1:A:17:VAL:CG2	1:A:143:ASN:ND2	2.44	0.75
1:A:46:LEU:C	1:A:47:ILE:HD13	2.10	0.75
1:A:186:GLU:CA	1:A:223:ASN:HA	2.17	0.75
1:A:223:ASN:H	1:A:223:ASN:HD22	0.77	0.74
1:A:151:TYR:CD1	1:A:152:PRO:CD	2.70	0.74
1:A:100:ASN:HD21	1:A:179:ASN:HD22	1.32	0.74
1:A:185:LEU:C	1:A:185:LEU:CD1	2.58	0.74
1:A:104:MET:HE3	1:A:106:ILE:HD11	1.70	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:188(A):LYS:O	4:A:297:HOH:O	2.07	0.71
1:A:189:ASP:O	1:A:220:CYS:HB3	1.89	0.71
1:A:189:ASP:CG	4:A:274:HOH:O	2.33	0.71
1:A:17:VAL:CG2	1:A:191:CYS:HB2	2.21	0.70
1:A:151:TYR:CB	1:A:152:PRO:CD	2.69	0.70
1:A:72:ASN:OD1	1:A:74:ASN:N	2.23	0.70
1:A:222:LYS:HD3	1:A:223:ASN:N	2.06	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:O	1:A:65:VAL:CG1	2.41	0.69
1:A:72:ASN:OD1	1:A:75:VAL:HG23	1.94	0.68
1:A:190:SER:OG	4:A:316:HOH:O	2.05	0.68
1:A:87:LYS:NZ	1:A:245:ASN:HD22	1.91	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184(A):TYR:CD1	1:A:188:GLY:C	2.72	0.68
1:A:190:SER:O	1:A:220:CYS:CB	2.39	0.68
1:A:186:GLU:C	1:A:188:GLY:H	2.00	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:184(A):TYR:C	1:A:186:GLU:N	2.43	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:189:ASP:CG	1:A:220:CYS:H	2.03	0.66
1:A:81:GLN:HE22	1:A:113:SER:H	1.41	0.65
1:A:39:TYR:CD1	1:A:39:TYR:N	2.65	0.65
1:A:150:SER:O	1:A:151:TYR:CE1	2.49	0.65
1:A:163:LEU:HD21	1:A:184:GLY:H	1.62	0.64
1:A:186:GLU:C	1:A:188:GLY:N	2.57	0.63
1:A:57:HIS:CG	3:A:248:DFP:C3	2.82	0.63
1:A:34:ASN:ND2	1:A:38:GLY:H	1.98	0.62
1:A:151:TYR:CA	1:A:153:ASP:H	2.10	0.62
1:A:209:LEU:C	1:A:209:LEU:CD2	2.73	0.62
1:A:158:LEU:CD1	1:A:159:LYS:C	2.72	0.61
1:A:17:VAL:CG2	1:A:220:CYS:HB2	2.29	0.61
1:A:17:VAL:HG22	1:A:190:SER:CA	2.30	0.61
1:A:19:GLY:C	1:A:20:TYR:HD1	2.08	0.60
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:241:THR:C	1:A:244:SER:H	2.09	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:45:SER:O	1:A:47:ILE:HD13	1.96	0.57
1:A:143:ASN:HD22	1:A:190:SER:C	2.13	0.56
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:95:ASN:OD1	1:A:95:ASN:C	2.48	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:22:CYS:SG	1:A:156:LYS:C	2.89	0.56
1:A:184(A):TYR:CB	1:A:188:GLY:C	2.70	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:46:LEU:CA	1:A:47:ILE:HD13	2.36	0.55
1:A:151:TYR:CB	1:A:153:ASP:HB2	2.36	0.55
1:A:189:ASP:C	1:A:190:SER:O	2.44	0.55
1:A:222:LYS:CB	1:A:223:ASN:HD22	2.20	0.55
1:A:87:LYS:CE	1:A:245:ASN:HD22	2.20	0.54
1:A:158:LEU:CD1	1:A:159:LYS:CA	2.84	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:115:ASN:C	1:A:115:ASN:OD1	2.52	0.53
1:A:48:ASN:OD1	1:A:48:ASN:C	2.51	0.53
1:A:163:LEU:N	1:A:163:LEU:HD22	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
1:A:33:LEU:CD2	1:A:63:ILE:HD11	2.29	0.52
1:A:163:LEU:CD2	1:A:183:ALA:C	2.82	0.52
1:A:143:ASN:ND2	1:A:190:SER:HA	2.25	0.52
1:A:184(A):TYR:HB2	1:A:188(A):LYS:N	2.23	0.52
1:A:27:VAL:HG11	1:A:139:SER:OG	2.10	0.52
1:A:223:ASN:O	1:A:223:ASN:CG	2.46	0.52
1:A:209:LEU:C	1:A:209:LEU:HD22	2.35	0.51
1:A:53:VAL:HG23	1:A:105:LEU:HD22	1.93	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:VAL:CG2	1:A:190:SER:CA	2.88	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: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: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:216:GLY:O	1:A:217:SER:HB3	2.11	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:46:LEU:C	1:A:47:ILE:CD1	2.77	0.49
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:82:PHE:C	1:A:83:ILE:HG13	2.36	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: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:212:ILE:HB	1:A:229:THR:HB	1.96	0.47
1:A:31:VAL:HG12	1:A:66:LEU:HD23	1.96	0.47
1:A:217:SER:OG	1:A:217:SER:O	2.24	0.47
1:A:240:GLN:O	1:A:241:THR:C	2.50	0.47
1:A:29:TYR:HA	1:A:119:ALA:O	2.16	0.46
1:A:165:ASP:O	1:A:166:SER:C	2.56	0.46
1:A:193:GLY:C	3:A:248:DFP:H2'2	2.40	0.46
1:A:150:SER:C	1:A:151:TYR:HD1	2.21	0.46
1:A:185:LEU:O	1:A:186:GLU:CD	2.58	0.46
1:A:185:LEU:O	1:A:186:GLU:CG	2.59	0.46
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:158:LEU:HD11	1:A:159:LYS:C	2.41	0.45
1:A:72:ASN:OD1	1:A:72:ASN:C	2.60	0.45
1:A:189:ASP:OD1	1:A:220:CYS:N	2.50	0.44
1:A:99:LEU:HD12	1:A:99:LEU:HA	1.88	0.44
1:A:75:VAL:O	1:A:77:GLU:HG3	2.18	0.44
1:A:144:THR:HG23	1:A:144:THR:O	2.12	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:LEU:HD13	1:A:186:GLU:HB2	1.99	0.44
1:A:29:TYR:C	1:A:29:TYR:CD2	2.96	0.44
1:A:186:GLU:HA	1:A:223:ASN:CA	2.34	0.44
1:A:222:LYS:HE2	1:A:223:ASN:CG	2.38	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:160:ALA:HB1	1:A:184:GLY:HA2	2.00	0.43
1:A:74:ASN:C	1:A:75:VAL:CG2	2.90	0.43
1:A:202:SER:O	1:A:204:LYS:HE2	2.19	0.43
1:A:230:LYS:O	1:A:230:LYS:CG	2.67	0.43
1:A:91:HIS:CG	1:A:92:PRO:HD2	2.54	0.43
1:A:150:SER:C	1:A:151:TYR:CD1	2.93	0.42
1:A:168:CYS:O	1:A:171:ALA:HB3	2.20	0.42
1:A:189:ASP:HB3	1:A:220:CYS:C	2.35	0.42
1:A:192:GLN:O	1:A:194:ASP:CG	2.62	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:56:ALA:HB3	1:A:94:TYR:CE2	2.54	0.42
1:A:151:TYR:O	1:A:156:LYS:HE3	2.20	0.42
1:A:46:LEU:HD12	1:A:46:LEU:HA	1.89	0.41
1:A:94:TYR:HA	1:A:101:ASN:HB2	2.02	0.41
1:A:143:ASN:HD22	1:A:190:SER:CA	2.33	0.41
1:A:98:THR:H	1:A:98:THR:HG23	1.64	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:192:GLN:C	1:A:194:ASP:N	2.77	0.41
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	1 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
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%)	145 (80%)	37 (20%)	1 0

All (37) 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	73	ILE
1	A	90	VAL
1	A	99	LEU
1	A	105	LEU
1	A	121	ILE
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
1	A	159	LYS
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	201	CYS
1	A	202	SER
1	A	204	LYS
1	A	209	LEU
1	A	222	LYS
1	A	223	ASN
1	A	240	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	34	ASN
1	A	57	HIS
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 oligosaccharides 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	0.92	0	6,11,11	1.16	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.