



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:08 PM UTC

PDB ID : 2CHA / pdb_00002cha
Title : THE STRUCTURE OF CRYSTALLINE ALPHA-CHYMOTRYPSIN,
\$V.THE ATOMIC STRUCTURE OF TOSYL-ALPHA-CHYMOTRYPSIN
AT 2 ANGSTROMS RESOLUTION
Authors : Birktoft, J.J.; Blow, D.M.
Deposited on : 1975-01-01
Resolution : 2.00 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)
Xtrriage (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

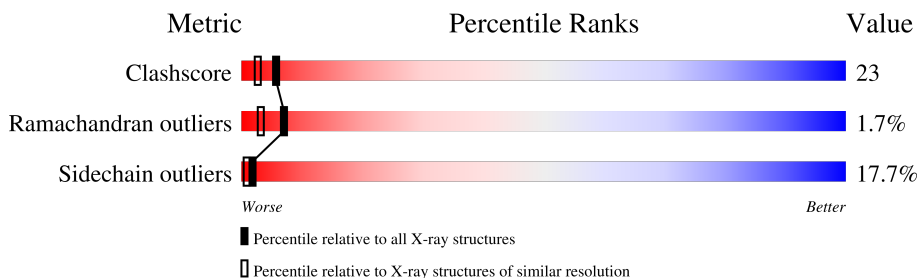
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (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 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	13	8% 23% 31% 8% 31%
1	E	13	8% 23% 31% 8% 31%
2	B	131	24% 36% 26% 15%
2	F	131	24% 36% 27% 13%
3	C	97	29% 35% 30% 6%
3	G	97	27% 37% 30% 6%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 3542 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 ALPHA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	9	Total	C	N	O	S	0	0	1
			54	34	10	9	1			
1	E	9	Total	C	N	O	S	0	0	1
			54	34	10	9	1			

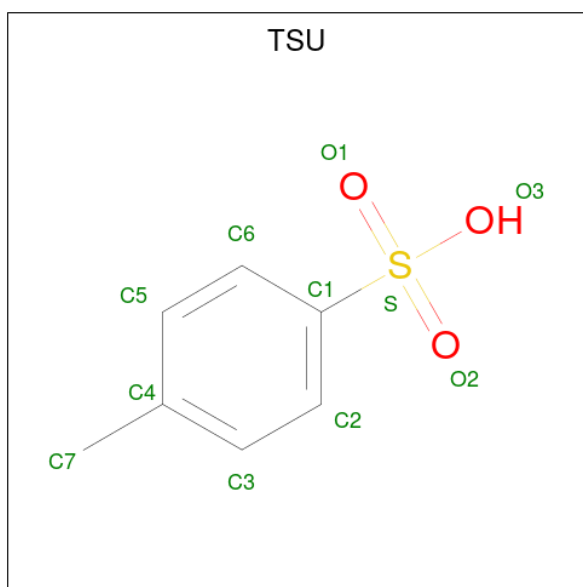
- Molecule 2 is a protein called ALPHA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	131	Total	C	N	O	S	0	0	0
			980	618	162	196	4			
2	F	131	Total	C	N	O	S	0	0	0
			980	618	162	196	4			

- Molecule 3 is a protein called ALPHA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	97	Total	C	N	O	S	0	0	0
			702	436	123	136	7			
3	G	97	Total	C	N	O	S	0	0	0
			702	436	123	136	7			

- Molecule 4 is PARA-TOLUENE SULFONATE (CCD ID: TSU) (formula: C₇H₈O₃S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	O	S	0	0
			10	7	2	1		
4	G	1	Total	C	O	S	0	0
			10	7	2	1		

- Molecule 5 is water.

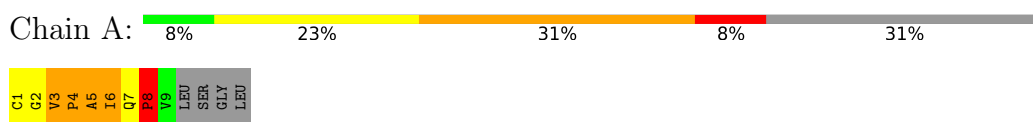
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	33	Total	O	0	0
			33	33		
5	C	14	Total	O	0	0
			14	14		
5	F	1	Total	O	0	0
			1	1		
5	G	1	Total	O	0	0
			1	1		

3 Residue-property plots

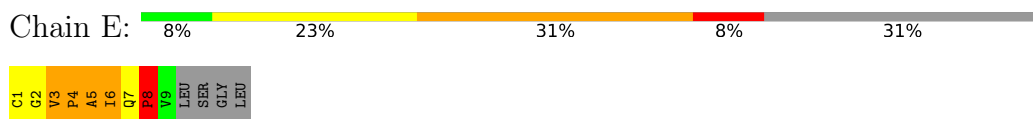
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

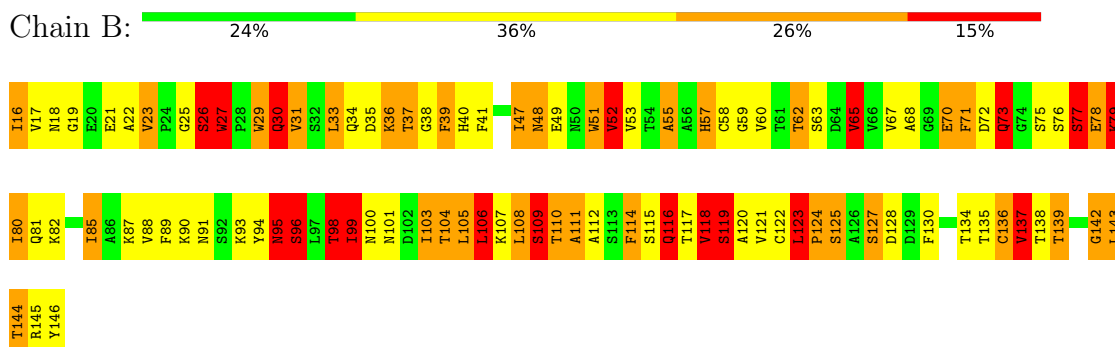
- Molecule 1: ALPHA-CHYMOTRYPSIN A



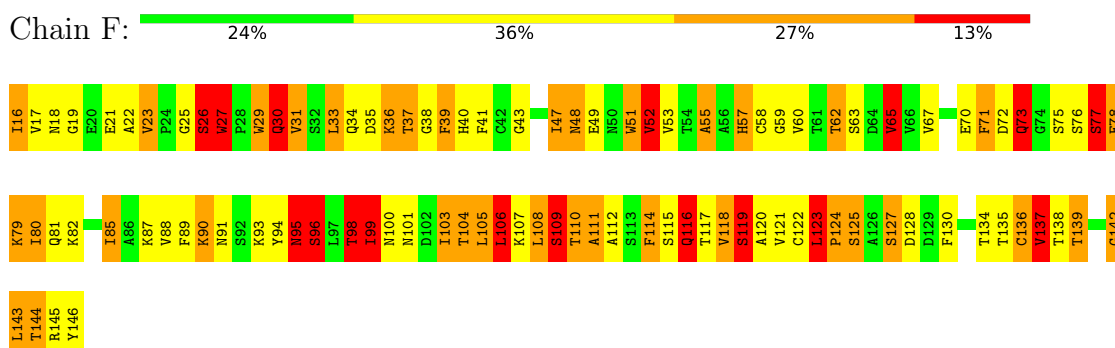
- Molecule 1: ALPHA-CHYMOTRYPSIN A



- Molecule 2: ALPHA-CHYMOTRYPSIN A

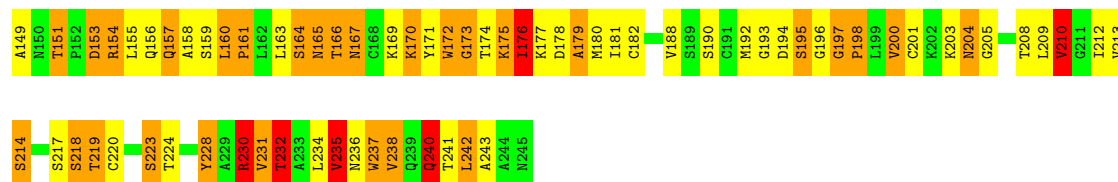


- Molecule 2: ALPHA-CHYMOTRYPSIN A



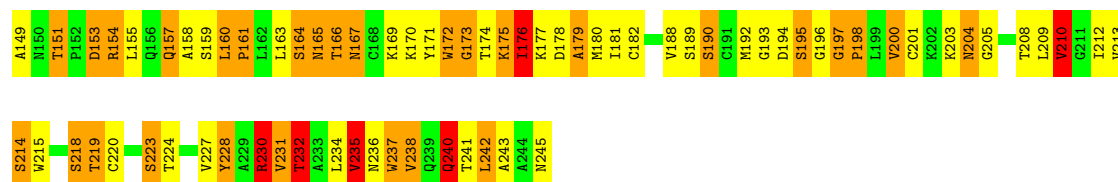
- Molecule 3: ALPHA-CHYMOTRYPSIN A

Chain C:  29% 35% 30% 6%



- Molecule 3: ALPHA-CHYMOTRYPSIN A

Chain G:  27% 37% 30% 6%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	49.10Å 67.40Å 65.90Å 90.00° 101.70° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	unknown	Depositor
R, R_{free}	(Not available) , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	3542	wwPDB-VP
Average B, all atoms (Å ²)	0.0	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: TSU

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	1.39	1/55 (1.8%)	2.67	6/76 (7.9%)
1	E	1.40	1/55 (1.8%)	2.67	6/76 (7.9%)
2	B	0.88	0/1000	2.12	47/1361 (3.5%)
2	F	0.88	0/1000	2.11	47/1361 (3.5%)
3	C	0.90	0/715	2.22	35/973 (3.6%)
3	G	0.90	0/715	2.22	35/973 (3.6%)
All	All	0.91	2/3540 (0.1%)	2.18	176/4820 (3.7%)

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	4
1	E	0	4
2	B	0	61
2	F	0	62
3	C	0	35
3	G	0	35
All	All	0	201

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	8	PRO	C-N	-7.08	1.23	1.33
1	A	8	PRO	C-N	-7.04	1.23	1.33

All (176) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	160	LEU	N-CA-C	11.69	121.81	108.25
3	G	160	LEU	N-CA-C	11.68	121.80	108.25
2	F	76	SER	N-CA-C	-11.14	99.08	112.89
2	B	76	SER	N-CA-C	-11.12	99.10	112.89
3	C	151	THR	CA-C-O	-10.50	112.47	119.29
3	G	151	THR	CA-C-O	-10.46	112.49	119.29
2	B	65	VAL	CA-CB-CG1	8.70	125.19	110.40
2	F	65	VAL	CA-CB-CG1	8.69	125.17	110.40
2	F	123	LEU	CA-C-O	-8.68	112.12	120.19
2	B	123	LEU	CA-C-O	-8.61	112.18	120.19
3	G	232	THR	CA-CB-CG2	8.32	124.65	110.50
3	C	232	THR	CA-CB-CG2	8.32	124.64	110.50
2	F	118	VAL	CA-CB-CG1	8.21	124.36	110.40
2	B	118	VAL	CA-CB-CG1	8.19	124.32	110.40
3	C	224	THR	CA-C-O	-7.93	113.16	119.66
3	G	224	THR	CA-C-O	-7.91	113.17	119.66
2	F	62	THR	CA-CB-CG2	7.77	123.71	110.50
2	B	62	THR	CA-CB-CG2	7.76	123.69	110.50
3	C	196	GLY	N-CA-C	-7.64	105.28	115.21
3	G	196	GLY	N-CA-C	-7.63	105.29	115.21
2	B	23	VAL	CB-CA-C	7.62	119.12	110.89
2	F	23	VAL	CB-CA-C	7.62	119.12	110.89
3	G	224	THR	CB-CA-C	7.62	120.44	109.08
3	G	235	VAL	N-CA-C	7.62	118.39	110.62
3	C	235	VAL	N-CA-C	7.62	118.39	110.62
3	C	195	SER	CA-C-O	7.61	129.52	121.15
3	C	224	THR	CB-CA-C	7.60	120.41	109.08
1	E	6	ILE	N-CA-CB	7.58	120.19	111.39
3	G	195	SER	CA-C-O	7.57	129.48	121.15
2	B	104	THR	CA-CB-CG2	7.56	123.36	110.50
3	G	160	LEU	CA-C-O	-7.55	113.39	120.34
1	A	6	ILE	N-CA-CB	7.55	120.14	111.39
2	F	104	THR	CA-CB-CG2	7.54	123.32	110.50
3	C	160	LEU	CA-C-O	-7.49	113.45	120.34
3	C	210	VAL	CA-CB-CG1	7.11	122.48	110.40
3	G	210	VAL	CA-CB-CG1	7.11	122.48	110.40
3	C	235	VAL	CA-CB-CG2	7.03	122.35	110.40
3	G	235	VAL	CA-CB-CG2	7.02	122.34	110.40
2	B	137	VAL	CA-CB-CG1	6.93	122.18	110.40
2	F	137	VAL	CA-CB-CG1	6.91	122.14	110.40
3	C	179	ALA	N-CA-C	6.80	121.59	113.16
3	G	179	ALA	N-CA-C	6.77	121.56	113.16
3	C	240	GLN	CA-C-N	6.51	129.48	120.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	240	GLN	C-N-CA	6.51	129.48	120.63
3	G	240	GLN	CA-C-N	6.50	129.47	120.63
3	G	240	GLN	C-N-CA	6.50	129.47	120.63
3	C	176	ILE	CA-CB-CG2	6.40	121.38	110.50
3	G	176	ILE	CA-CB-CG2	6.38	121.34	110.50
2	B	99	ILE	CA-CB-CG1	6.35	121.19	110.40
2	F	99	ILE	CA-CB-CG1	6.35	121.19	110.40
2	B	27	TRP	CA-C-O	-6.26	111.58	120.16
2	F	123	LEU	N-CA-C	6.26	118.96	110.31
2	F	27	TRP	CA-C-O	-6.26	111.58	120.16
2	B	123	LEU	N-CA-C	6.25	118.93	110.31
2	B	52	VAL	CA-CB-CG1	6.22	120.97	110.40
1	A	7	GLN	CA-C-O	-6.22	113.58	119.80
2	F	52	VAL	CA-CB-CG1	6.21	120.95	110.40
1	E	7	GLN	CA-C-O	-6.20	113.60	119.80
1	A	5	ALA	N-CA-C	-6.17	104.47	111.07
1	E	5	ALA	N-CA-C	-6.14	104.50	111.07
3	G	237	TRP	CA-C-O	-6.14	113.43	120.24
3	C	237	TRP	CA-C-O	-6.13	113.43	120.24
3	G	193	GLY	N-CA-C	-6.09	106.66	113.79
2	B	25	GLY	N-CA-C	-6.04	106.60	115.30
3	C	193	GLY	N-CA-C	-6.04	106.72	113.79
2	F	25	GLY	N-CA-C	-6.04	106.60	115.30
3	C	235	VAL	CB-CA-C	6.03	120.28	112.14
2	F	114	PHE	CA-CB-CG	6.01	119.81	113.80
2	B	121	VAL	CA-CB-CG1	6.01	120.62	110.40
2	B	114	PHE	CA-CB-CG	6.01	119.81	113.80
2	F	121	VAL	CA-CB-CG1	6.01	120.61	110.40
3	G	235	VAL	CB-CA-C	6.00	120.24	112.14
2	B	109	SER	N-CA-C	-5.99	103.92	111.11
2	F	109	SER	N-CA-C	-5.98	103.93	111.11
3	G	172	TRP	N-CA-C	5.96	120.71	112.90
2	B	51	TRP	N-CA-C	5.95	119.26	110.46
2	F	51	TRP	N-CA-C	5.93	119.24	110.46
3	C	172	TRP	N-CA-C	5.90	120.63	112.90
2	F	134	THR	CA-CB-CG2	5.87	120.48	110.50
2	B	96	SER	N-CA-C	5.86	119.91	112.87
2	B	134	THR	CA-CB-CG2	5.86	120.46	110.50
2	F	96	SER	N-CA-C	5.84	119.88	112.87
2	F	60	VAL	CA-CB-CG1	5.79	120.25	110.40
2	B	60	VAL	CA-CB-CG1	5.78	120.23	110.40
2	F	48	ASN	CA-CB-CG	-5.76	106.84	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	48	ASN	CA-CB-CG	-5.76	106.84	112.60
2	F	31	VAL	CA-CB-CG2	5.69	120.07	110.40
2	B	29	TRP	N-CA-C	5.66	119.91	112.89
2	B	116	GLN	CA-C-O	-5.66	113.70	120.10
2	F	29	TRP	N-CA-C	5.66	119.90	112.89
2	B	31	VAL	CA-CB-CG2	5.65	120.00	110.40
2	B	65	VAL	CB-CA-C	5.64	119.51	110.82
2	F	65	VAL	CB-CA-C	5.64	119.50	110.82
2	B	47	ILE	CB-CA-C	5.63	118.03	111.55
2	F	47	ILE	CB-CA-C	5.63	118.03	111.55
2	B	99	ILE	CA-CB-CG2	5.62	120.05	110.50
2	F	116	GLN	CA-C-O	-5.61	113.76	120.10
2	F	99	ILE	CA-CB-CG2	5.61	120.03	110.50
3	C	195	SER	O-C-N	-5.57	116.17	122.97
3	G	241	THR	CA-CB-CG2	5.57	119.97	110.50
3	C	241	THR	CA-CB-CG2	5.57	119.96	110.50
2	B	110	THR	CA-CB-CG2	5.56	119.95	110.50
2	B	135	THR	CA-CB-CG2	5.54	119.93	110.50
2	F	110	THR	CA-CB-CG2	5.54	119.92	110.50
2	F	135	THR	CA-CB-CG2	5.54	119.92	110.50
3	G	195	SER	O-C-N	-5.52	116.23	122.97
2	F	85	ILE	CA-C-O	-5.51	114.82	121.54
2	F	93	LYS	N-CA-C	5.50	119.68	112.92
2	F	118	VAL	CA-C-O	-5.47	114.07	121.02
2	B	93	LYS	N-CA-C	5.47	119.65	112.92
1	A	3	VAL	CB-CA-C	5.47	121.31	111.36
3	G	175	LYS	N-CA-C	5.46	118.16	111.82
3	G	197	GLY	CA-C-O	-5.46	113.71	121.52
3	C	223	SER	N-CA-C	-5.46	106.62	113.72
1	E	3	VAL	CB-CA-C	5.46	121.30	111.36
3	G	223	SER	N-CA-C	-5.46	106.62	113.72
2	B	85	ILE	CA-C-O	-5.45	114.89	121.54
3	C	197	GLY	CA-C-O	-5.45	113.73	121.52
3	G	224	THR	CA-CB-CG2	5.45	119.76	110.50
3	G	161	PRO	CA-N-CD	-5.44	104.38	112.00
3	C	175	LYS	N-CA-C	5.44	118.12	111.82
3	C	224	THR	CA-CB-CG2	5.43	119.74	110.50
2	B	79	LYS	CA-C-O	-5.43	116.12	122.37
2	F	79	LYS	CA-C-O	-5.43	116.13	122.37
2	F	88	VAL	CA-CB-CG1	5.43	119.63	110.40
2	B	118	VAL	CA-C-O	-5.43	114.13	121.02
2	B	88	VAL	CA-CB-CG1	5.41	119.60	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	161	PRO	CA-N-CD	-5.41	104.43	112.00
3	G	166	THR	CA-CB-CG2	5.40	119.69	110.50
3	C	166	THR	CA-CB-CG2	5.40	119.67	110.50
3	G	161	PRO	N-CD-CG	5.31	111.16	103.20
2	B	95	ASN	CA-C-O	-5.30	115.03	120.54
2	B	119	SER	N-CA-CB	5.29	119.43	110.49
3	C	161	PRO	N-CD-CG	5.29	111.13	103.20
2	F	119	SER	N-CA-CB	5.28	119.41	110.49
3	C	230	ARG	NE-CZ-NH2	5.28	123.95	119.20
3	G	231	VAL	CA-CB-CG1	5.28	119.37	110.40
3	C	231	VAL	CA-CB-CG1	5.27	119.36	110.40
2	F	95	ASN	CA-C-O	-5.27	115.06	120.54
3	C	166	THR	CA-C-O	-5.26	115.30	120.82
2	F	80	ILE	CB-CG1-CD1	5.25	124.83	113.80
3	G	230	ARG	NE-CZ-NH2	5.25	123.92	119.20
2	B	80	ILE	CB-CG1-CD1	5.24	124.81	113.80
3	G	166	THR	CA-C-O	-5.24	115.32	120.82
2	B	37	THR	CA-C-N	5.19	131.64	121.06
2	B	37	THR	C-N-CA	5.19	131.64	121.06
2	F	37	THR	CA-C-N	5.19	131.64	121.06
2	F	37	THR	C-N-CA	5.19	131.64	121.06
2	F	138	THR	CA-CB-CG2	5.18	119.31	110.50
2	B	138	THR	CA-CB-CG2	5.18	119.30	110.50
3	C	173	GLY	CA-C-N	5.17	131.42	121.54
3	C	173	GLY	C-N-CA	5.17	131.42	121.54
2	F	125	SER	O-C-N	-5.16	116.44	123.15
3	G	173	GLY	CA-C-N	5.16	131.39	121.54
3	G	173	GLY	C-N-CA	5.16	131.39	121.54
2	B	125	SER	O-C-N	-5.15	116.45	123.15
1	A	3	VAL	CA-C-O	-5.12	113.09	119.95
1	E	3	VAL	CA-C-O	-5.10	113.12	119.95
2	B	108	LEU	CA-C-O	-5.08	115.32	120.71
2	F	103	ILE	CB-CG1-CD1	5.08	124.46	113.80
2	F	108	LEU	CA-C-O	-5.07	115.33	120.71
2	F	76	SER	CA-C-N	5.07	131.22	121.54
2	F	76	SER	C-N-CA	5.07	131.22	121.54
2	B	103	ILE	CB-CG1-CD1	5.07	124.44	113.80
2	B	76	SER	CA-C-N	5.06	131.20	121.54
2	B	76	SER	C-N-CA	5.06	131.20	121.54
3	C	176	ILE	N-CA-CB	5.05	116.04	110.53
3	G	231	VAL	CG1-CB-CG2	-5.02	99.75	110.80
1	E	4	PRO	CB-CA-C	-5.02	104.99	111.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	231	VAL	CG1-CB-CG2	-5.02	99.76	110.80
3	G	176	ILE	N-CA-CB	5.02	116.00	110.53
2	B	98	THR	CA-C-N	5.01	130.99	121.97
2	B	98	THR	C-N-CA	5.01	130.99	121.97
1	A	4	PRO	CB-CA-C	-5.00	105.01	111.46
2	F	98	THR	CA-C-N	5.00	130.97	121.97
2	F	98	THR	C-N-CA	5.00	130.97	121.97

There are no chirality outliers.

All (201) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	2	GLY	Mainchain
1	A	3	VAL	Mainchain
1	A	5	ALA	Mainchain
1	A	8	PRO	Mainchain
2	B	101	ASN	Mainchain
2	B	103	ILE	Mainchain
2	B	104	THR	Mainchain
2	B	105	LEU	Mainchain
2	B	106	LEU	Mainchain
2	B	108	LEU	Mainchain
2	B	109	SER	Mainchain
2	B	110	THR	Mainchain
2	B	111	ALA	Mainchain
2	B	114	PHE	Mainchain
2	B	116	GLN	Mainchain
2	B	117	THR	Mainchain
2	B	118	VAL	Mainchain
2	B	119	SER	Mainchain
2	B	120	ALA	Mainchain
2	B	124	PRO	Mainchain
2	B	127	SER	Mainchain
2	B	128	ASP	Mainchain
2	B	130	PHE	Mainchain
2	B	136	CYS	Mainchain
2	B	137	VAL	Mainchain
2	B	142	GLY	Mainchain
2	B	143	LEU	Mainchain
2	B	144	THR	Mainchain
2	B	16	ILE	Mainchain
2	B	17	VAL	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	B	18	ASN	Sidechain
2	B	19	GLY	Mainchain
2	B	21	GLU	Mainchain
2	B	26	SER	Mainchain
2	B	27	TRP	Mainchain
2	B	30	GLN	Mainchain
2	B	31	VAL	Mainchain
2	B	33	LEU	Mainchain
2	B	36	LYS	Mainchain
2	B	37	THR	Mainchain
2	B	39	PHE	Mainchain
2	B	47	ILE	Mainchain
2	B	52	VAL	Mainchain
2	B	53	VAL	Mainchain
2	B	55	ALA	Mainchain
2	B	57	HIS	Mainchain
2	B	63	SER	Mainchain
2	B	65	VAL	Mainchain
2	B	70	GLU	Mainchain
2	B	71	PHE	Mainchain
2	B	73	GLN	Mainchain
2	B	77	SER	Mainchain
2	B	79	LYS	Mainchain
2	B	80	ILE	Mainchain
2	B	81	GLN	Mainchain
2	B	82	LYS	Mainchain
2	B	85	ILE	Mainchain
2	B	87	LYS	Mainchain
2	B	89	PHE	Mainchain
2	B	91	ASN	Mainchain
2	B	94	TYR	Mainchain,Sidechain
2	B	95	ASN	Mainchain
2	B	96	SER	Mainchain
2	B	98	THR	Mainchain
3	C	151	THR	Mainchain
3	C	153	ASP	Mainchain
3	C	154	ARG	Mainchain
3	C	155	LEU	Mainchain
3	C	157	GLN	Mainchain
3	C	161	PRO	Mainchain
3	C	163	LEU	Mainchain
3	C	165	ASN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	C	166	THR	Mainchain
3	C	167	ASN	Mainchain
3	C	170	LYS	Mainchain
3	C	171	TYR	Mainchain
3	C	172	TRP	Mainchain
3	C	176	ILE	Mainchain
3	C	178	ASP	Mainchain
3	C	188	VAL	Mainchain
3	C	190	SER	Mainchain
3	C	198	PRO	Mainchain
3	C	200	VAL	Mainchain
3	C	204	ASN	Mainchain
3	C	205	GLY	Mainchain
3	C	208	THR	Mainchain
3	C	210	VAL	Mainchain
3	C	212	ILE	Mainchain
3	C	214	SER	Mainchain
3	C	218	SER	Mainchain
3	C	220	CYS	Mainchain
3	C	228	TYR	Mainchain
3	C	230	ARG	Mainchain
3	C	232	THR	Mainchain
3	C	235	VAL	Mainchain
3	C	237	TRP	Mainchain
3	C	238	VAL	Mainchain
3	C	240	GLN	Mainchain
3	C	242	LEU	Mainchain
1	E	2	GLY	Mainchain
1	E	3	VAL	Mainchain
1	E	5	ALA	Mainchain
1	E	8	PRO	Mainchain
2	F	101	ASN	Mainchain
2	F	103	ILE	Mainchain
2	F	104	THR	Mainchain
2	F	105	LEU	Mainchain
2	F	106	LEU	Mainchain
2	F	108	LEU	Mainchain
2	F	109	SER	Mainchain
2	F	110	THR	Mainchain
2	F	111	ALA	Mainchain
2	F	114	PHE	Mainchain
2	F	116	GLN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	F	117	THR	Mainchain
2	F	118	VAL	Mainchain
2	F	119	SER	Mainchain
2	F	120	ALA	Mainchain
2	F	124	PRO	Mainchain
2	F	127	SER	Mainchain
2	F	128	ASP	Mainchain
2	F	130	PHE	Mainchain
2	F	136	CYS	Mainchain
2	F	137	VAL	Mainchain
2	F	142	GLY	Mainchain
2	F	143	LEU	Mainchain
2	F	144	THR	Mainchain
2	F	16	ILE	Mainchain
2	F	17	VAL	Mainchain
2	F	18	ASN	Sidechain
2	F	19	GLY	Mainchain
2	F	21	GLU	Mainchain
2	F	26	SER	Mainchain
2	F	27	TRP	Mainchain
2	F	30	GLN	Mainchain
2	F	31	VAL	Mainchain
2	F	33	LEU	Mainchain
2	F	36	LYS	Mainchain
2	F	37	THR	Mainchain
2	F	39	PHE	Mainchain
2	F	43	GLY	Mainchain
2	F	47	ILE	Mainchain
2	F	52	VAL	Mainchain
2	F	53	VAL	Mainchain
2	F	55	ALA	Mainchain
2	F	57	HIS	Mainchain
2	F	63	SER	Mainchain
2	F	65	VAL	Mainchain
2	F	70	GLU	Mainchain
2	F	71	PHE	Mainchain
2	F	73	GLN	Mainchain
2	F	77	SER	Mainchain
2	F	79	LYS	Mainchain
2	F	80	ILE	Mainchain
2	F	81	GLN	Mainchain
2	F	82	LYS	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	F	85	ILE	Mainchain
2	F	87	LYS	Mainchain
2	F	89	PHE	Mainchain
2	F	91	ASN	Mainchain
2	F	94	TYR	Mainchain,Sidechain
2	F	95	ASN	Mainchain
2	F	96	SER	Mainchain
2	F	98	THR	Mainchain
3	G	151	THR	Mainchain
3	G	153	ASP	Mainchain
3	G	154	ARG	Mainchain
3	G	155	LEU	Mainchain
3	G	157	GLN	Mainchain
3	G	161	PRO	Mainchain
3	G	163	LEU	Mainchain
3	G	165	ASN	Mainchain
3	G	166	THR	Mainchain
3	G	167	ASN	Mainchain
3	G	170	LYS	Mainchain
3	G	171	TYR	Mainchain
3	G	172	TRP	Mainchain
3	G	176	ILE	Mainchain
3	G	178	ASP	Mainchain
3	G	188	VAL	Mainchain
3	G	190	SER	Mainchain
3	G	198	PRO	Mainchain
3	G	200	VAL	Mainchain
3	G	204	ASN	Mainchain
3	G	205	GLY	Mainchain
3	G	208	THR	Mainchain
3	G	210	VAL	Mainchain
3	G	212	ILE	Mainchain
3	G	214	SER	Mainchain
3	G	218	SER	Mainchain
3	G	220	CYS	Mainchain
3	G	228	TYR	Mainchain
3	G	230	ARG	Mainchain
3	G	232	THR	Mainchain
3	G	235	VAL	Mainchain
3	G	237	TRP	Mainchain
3	G	238	VAL	Mainchain
3	G	240	GLN	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	G	242	LEU	Mainchain

5.2 Too-close contacts [i](#)

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	54	0	56	4	0
1	E	54	0	56	4	0
2	B	980	0	951	62	6
2	F	980	0	951	62	3
3	C	702	0	696	44	7
3	G	702	0	696	43	5
4	C	10	0	7	0	0
4	G	10	0	7	0	0
5	A	1	0	0	1	0
5	B	33	0	0	5	0
5	C	14	0	0	1	1
5	F	1	0	0	2	0
5	G	1	0	0	0	0
All	All	3542	0	3420	161	11

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 23.

All (161) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:THR:CG2	2:F:99:ILE:HD11	1.51	1.41
2:B:99:ILE:HD11	3:G:219:THR:CG2	1.51	1.37
3:C:219:THR:HG21	2:F:99:ILE:CD1	1.73	1.19
2:B:99:ILE:CD1	3:G:219:THR:HG21	1.73	1.17
2:B:99:ILE:CD1	3:G:219:THR:CG2	2.28	1.11
3:C:219:THR:CG2	2:F:99:ILE:CD1	2.28	1.08
2:B:34:GLN:HE21	2:B:67:VAL:HG21	1.42	0.84
2:F:34:GLN:HE21	2:F:67:VAL:HG21	1.42	0.83
2:F:49:GLU:HG3	2:F:112:ALA:O	1.80	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:219:THR:HG21	2:F:99:ILE:HD11	0.83	0.81
2:B:99:ILE:HD11	3:G:219:THR:HG21	0.83	0.81
2:F:23:VAL:O	2:F:26:SER:HB3	1.82	0.80
2:B:49:GLU:HG3	2:B:112:ALA:O	1.80	0.80
2:B:23:VAL:O	2:B:26:SER:HB3	1.82	0.80
2:B:100:ASN:OD1	3:C:179:ALA:HB3	1.84	0.77
2:F:146:TYR:OXT	5:F:4:HOH:O	2.02	0.77
2:F:100:ASN:OD1	3:G:179:ALA:HB3	1.84	0.77
2:B:39:PHE:CD2	2:F:39:PHE:CD1	2.64	0.76
2:B:33:LEU:O	2:B:40:HIS:HA	1.86	0.75
2:F:33:LEU:O	2:F:40:HIS:HA	1.86	0.75
2:B:39:PHE:CG	2:F:39:PHE:CD2	2.75	0.72
2:B:39:PHE:CD2	2:F:39:PHE:CG	2.75	0.71
1:A:4:PRO:HB2	1:A:6:ILE:O	1.91	0.70
2:B:39:PHE:CD2	2:F:39:PHE:CD2	2.35	0.70
1:E:4:PRO:HB2	1:E:6:ILE:O	1.91	0.70
2:B:39:PHE:CD1	2:F:39:PHE:CD2	2.64	0.69
2:B:136:CYS:HB3	3:C:200:VAL:O	1.94	0.68
2:F:34:GLN:NE2	2:F:67:VAL:HG21	2.09	0.68
2:F:136:CYS:HB3	3:G:200:VAL:O	1.94	0.68
2:B:34:GLN:NE2	2:B:67:VAL:HG21	2.09	0.68
3:C:240:GLN:O	3:C:243:ALA:HB3	1.95	0.66
3:G:240:GLN:O	3:G:243:ALA:HB3	1.95	0.65
2:B:55:ALA:O	2:B:58:CYS:HB2	1.98	0.64
2:F:16:ILE:HG21	3:G:158:ALA:HB2	1.79	0.64
2:F:55:ALA:O	2:F:58:CYS:HB2	1.98	0.64
2:B:16:ILE:HG21	3:C:158:ALA:HB2	1.79	0.63
3:C:165:ASN:HD21	3:C:230:ARG:NH1	1.97	0.63
3:G:165:ASN:HD21	3:G:230:ARG:NH1	1.97	0.63
3:C:192:MET:HG2	3:G:192:MET:SD	2.40	0.62
3:C:192:MET:SD	3:G:192:MET:HG2	2.40	0.61
2:F:16:ILE:O	2:F:144:THR:HA	2.01	0.60
2:B:98:THR:HG22	2:B:100:ASN:HB2	1.84	0.60
2:B:16:ILE:O	2:B:144:THR:HA	2.01	0.60
2:B:57:HIS:HD2	2:F:146:TYR:O	1.85	0.60
2:F:145:ARG:HB3	5:F:4:HOH:O	2.00	0.59
2:F:98:THR:HG22	2:F:100:ASN:HB2	1.84	0.59
2:B:146:TYR:O	2:F:57:HIS:HD2	1.85	0.59
2:B:124:PRO:HD3	3:C:209:LEU:O	2.02	0.59
2:F:124:PRO:HD3	3:G:209:LEU:O	2.02	0.58
3:C:231:VAL:O	3:C:235:VAL:HG12	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:231:VAL:O	3:G:235:VAL:HG12	2.03	0.58
3:G:230:ARG:O	3:G:234:LEU:HD22	2.04	0.57
3:C:230:ARG:O	3:C:234:LEU:HD22	2.04	0.57
3:G:165:ASN:HD21	3:G:230:ARG:HH12	1.53	0.56
3:G:176:ILE:HD12	3:G:182:CYS:SG	2.46	0.55
3:C:176:ILE:HD12	3:C:182:CYS:SG	2.46	0.55
3:C:165:ASN:HD21	3:C:230:ARG:HH12	1.53	0.55
3:C:217:SER:HB3	5:C:5:HOH:O	2.07	0.54
3:C:181:ILE:HG23	3:C:228:TYR:HB2	1.90	0.54
3:G:181:ILE:HG23	3:G:228:TYR:HB2	1.90	0.54
2:F:123:LEU:HD23	2:F:124:PRO:HD2	1.91	0.53
2:B:72:ASP:OD2	3:C:153:ASP:HB3	2.09	0.53
1:E:4:PRO:HG2	1:E:8:PRO:HD3	1.91	0.53
2:B:30:GLN:HE22	3:C:198:PRO:HD3	1.73	0.53
2:F:30:GLN:HE22	3:G:198:PRO:HD3	1.73	0.53
2:F:72:ASP:OD2	3:G:153:ASP:HB3	2.09	0.53
2:B:146:TYR:OXT	2:F:57:HIS:O	2.27	0.53
2:B:123:LEU:HD23	2:B:124:PRO:HD2	1.91	0.52
2:B:57:HIS:O	2:F:146:TYR:OXT	2.27	0.52
3:C:219:THR:HG22	2:F:99:ILE:HD11	1.74	0.52
3:G:177:LYS:HB2	3:G:180:MET:HE3	1.91	0.52
2:B:137:VAL:HG13	3:C:158:ALA:O	2.10	0.52
2:B:68:ALA:HB1	5:B:155:HOH:O	2.09	0.52
2:F:137:VAL:HG13	3:G:158:ALA:O	2.10	0.52
3:C:177:LYS:HB2	3:C:180:MET:HE3	1.91	0.51
1:A:4:PRO:HG2	1:A:8:PRO:HD3	1.91	0.51
3:G:169:LYS:HA	3:G:173:GLY:H	1.75	0.51
3:C:169:LYS:HA	3:C:173:GLY:H	1.75	0.51
2:B:36:LYS:C	2:B:38:GLY:H	2.19	0.51
5:A:38:HOH:O	2:B:119:SER:HB2	2.10	0.50
3:C:165:ASN:ND2	3:C:230:ARG:HH12	2.09	0.50
2:F:27:TRP:CD1	2:F:139:THR:HG21	2.46	0.50
2:F:48:ASN:HB2	2:F:51:TRP:H	1.77	0.50
3:C:164:SER:CB	3:C:167:ASN:OD1	2.60	0.49
2:B:27:TRP:CD1	2:B:139:THR:HG21	2.46	0.49
2:B:48:ASN:HB2	2:B:51:TRP:H	1.77	0.49
3:G:164:SER:CB	3:G:167:ASN:OD1	2.60	0.49
3:G:165:ASN:ND2	3:G:230:ARG:HH12	2.09	0.49
2:B:99:ILE:HD11	3:G:219:THR:HG22	1.73	0.48
2:F:36:LYS:C	2:F:38:GLY:H	2.19	0.48
2:B:26:SER:HG	2:B:27:TRP:CD1	2.32	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:34:GLN:O	2:F:41:PHE:HE2	1.97	0.48
2:F:26:SER:HG	2:F:27:TRP:CD1	2.32	0.47
3:G:197:GLY:O	3:G:213:VAL:HG23	2.15	0.47
3:C:197:GLY:O	3:C:213:VAL:HG23	2.14	0.47
1:E:8:PRO:HA	2:F:26:SER:HB2	1.96	0.47
2:B:39:PHE:CD1	2:B:40:HIS:N	2.83	0.47
2:B:59:GLY:O	3:G:149:ALA:N	2.48	0.47
2:B:99:ILE:CG1	3:G:219:THR:CG2	2.93	0.47
2:B:99:ILE:CG1	3:G:219:THR:HG21	2.41	0.47
3:C:219:THR:HG21	2:F:99:ILE:CG1	2.41	0.47
1:E:4:PRO:CB	1:E:6:ILE:O	2.63	0.47
2:F:49:GLU:HG2	2:F:111:ALA:HB1	1.96	0.47
3:G:195:SER:C	3:G:197:GLY:H	2.23	0.47
2:B:34:GLN:O	2:B:41:PHE:HE2	1.97	0.47
2:B:49:GLU:HG2	2:B:111:ALA:HB1	1.96	0.46
3:C:195:SER:C	3:C:197:GLY:H	2.23	0.46
1:A:8:PRO:HA	2:B:26:SER:HB2	1.97	0.46
2:B:52:VAL:O	2:B:105:LEU:HD13	2.15	0.46
2:F:52:VAL:O	2:F:105:LEU:HD13	2.15	0.46
2:B:98:THR:O	2:B:99:ILE:HG12	2.16	0.46
3:C:219:THR:CG2	2:F:99:ILE:CG1	2.93	0.46
2:F:98:THR:O	2:F:99:ILE:HG12	2.16	0.46
2:F:29:TRP:HA	2:F:119:SER:O	2.16	0.46
2:F:39:PHE:CD1	2:F:40:HIS:N	2.83	0.46
2:B:29:TRP:HA	2:B:119:SER:O	2.15	0.46
2:B:143:LEU:HB3	2:B:145:ARG:O	2.16	0.46
2:F:143:LEU:HB3	2:F:145:ARG:O	2.16	0.45
3:C:192:MET:HG2	3:G:192:MET:HG2	1.99	0.45
3:C:149:ALA:N	2:F:59:GLY:O	2.48	0.45
2:B:48:ASN:HB2	2:B:51:TRP:HB2	1.98	0.45
2:B:105:LEU:O	2:B:106:LEU:HD23	2.17	0.45
2:F:48:ASN:HB2	2:F:51:TRP:HB2	1.98	0.44
3:C:201:CYS:SG	3:C:210:VAL:HG21	2.57	0.44
2:B:70:GLU:HB3	5:B:157:HOH:O	2.17	0.44
2:B:36:LYS:HB2	5:B:177:HOH:O	2.17	0.44
2:B:71:PHE:HB3	2:B:78:GLU:OE2	2.18	0.43
2:F:105:LEU:O	2:F:106:LEU:HD23	2.17	0.43
2:F:71:PHE:HB3	2:F:78:GLU:OE2	2.18	0.43
3:G:201:CYS:SG	3:G:210:VAL:HG21	2.57	0.43
1:A:4:PRO:CB	1:A:6:ILE:O	2.63	0.43
2:B:51:TRP:CZ2	2:B:107:LYS:HD2	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:142:GLY:HA3	3:G:194:ASP:OD2	2.18	0.43
2:B:105:LEU:HD21	3:C:238:VAL:HG13	2.01	0.42
2:B:118:VAL:HG22	5:B:155:HOH:O	2.19	0.42
2:B:142:GLY:HA3	3:C:194:ASP:OD2	2.18	0.42
2:F:51:TRP:CZ2	2:F:107:LYS:HD2	2.54	0.42
3:C:165:ASN:O	3:C:169:LYS:HG3	2.19	0.42
3:G:164:SER:HB2	3:G:167:ASN:OD1	2.20	0.42
3:C:164:SER:HB2	3:C:167:ASN:OD1	2.20	0.41
2:B:146:TYR:O	2:F:57:HIS:CD2	2.69	0.41
2:F:95:ASN:HB3	2:F:98:THR:HB	2.02	0.41
2:F:124:PRO:O	3:G:235:VAL:HG21	2.20	0.41
3:G:165:ASN:O	3:G:169:LYS:HG3	2.19	0.41
2:B:73:GLN:HG3	3:C:153:ASP:HA	2.03	0.41
2:B:72:ASP:OD1	3:C:154:ARG:HG3	2.20	0.41
2:F:22:ALA:HB2	3:G:157:GLN:HB2	2.03	0.41
2:F:51:TRP:HZ2	3:G:245:ASN:HB2	1.86	0.41
2:B:22:ALA:HB2	3:C:157:GLN:HB2	2.03	0.41
2:B:124:PRO:O	3:C:235:VAL:HG21	2.20	0.41
2:F:72:ASP:OD1	3:G:154:ARG:HG3	2.20	0.41
3:C:165:ASN:ND2	3:C:230:ARG:NH1	2.68	0.41
2:F:73:GLN:HG3	3:G:153:ASP:HA	2.03	0.41
3:C:167:ASN:O	3:C:170:LYS:HB2	2.21	0.41
2:F:36:LYS:C	2:F:38:GLY:N	2.79	0.40
2:B:95:ASN:HB3	2:B:98:THR:HB	2.01	0.40
2:F:90:LYS:H	2:F:90:LYS:HG3	1.64	0.40
2:F:105:LEU:HD21	3:G:238:VAL:HG13	2.02	0.40
3:G:215:TRP:CZ2	3:G:227:VAL:HG21	2.57	0.40
5:B:153:HOH:O	3:C:156:GLN:HB2	2.21	0.40
3:G:189:SER:C	3:G:190:SER:O	2.65	0.40

All (11) 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)
2:B:127:SER:OG	2:F:127:SER:OG[1_554]	0.92	1.28
2:B:79:LYS:CE	3:C:170:LYS:CD[1_655]	1.06	1.14
2:B:79:LYS:CD	3:C:170:LYS:CD[1_655]	2.07	0.13
3:C:204:ASN:ND2	3:G:236:ASN:CA[1_554]	2.11	0.09
3:C:236:ASN:CA	3:G:204:ASN:ND2[1_554]	2.11	0.09
2:B:79:LYS:CE	3:C:170:LYS:CE[1_655]	2.12	0.08

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:127:SER:CB	2:F:127:SER:OG[1_554]	2.14	0.06
2:B:127:SER:OG	2:F:127:SER:CB[1_554]	2.14	0.06
3:G:243:ALA:O	5:C:43:HOH:O[1_556]	2.16	0.04
3:C:204:ASN:ND2	3:G:236:ASN:O[1_554]	2.18	0.02
3:C:236:ASN:O	3:G:204:ASN:ND2[1_554]	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	7/13 (54%)	6 (86%)	1 (14%)	0	100	100
1	E	7/13 (54%)	6 (86%)	1 (14%)	0	100	100
2	B	129/131 (98%)	117 (91%)	8 (6%)	4 (3%)	3	1
2	F	129/131 (98%)	117 (91%)	8 (6%)	4 (3%)	3	1
3	C	95/97 (98%)	86 (90%)	9 (10%)	0	100	100
3	G	95/97 (98%)	86 (90%)	9 (10%)	0	100	100
All	All	462/482 (96%)	418 (90%)	36 (8%)	8 (2%)	7	3

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	99	ILE
2	F	99	ILE
2	B	77	SER
2	F	77	SER
2	B	75	SER
2	F	75	SER
2	B	35	ASP
2	F	35	ASP

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	6/10 (60%)	5 (83%)	1 (17%)	2	1
1	E	6/10 (60%)	5 (83%)	1 (17%)	2	1
2	B	109/109 (100%)	90 (83%)	19 (17%)	2	1
2	F	109/109 (100%)	90 (83%)	19 (17%)	2	1
3	C	77/77 (100%)	63 (82%)	14 (18%)	2	1
3	G	77/77 (100%)	63 (82%)	14 (18%)	2	1
All	All	384/392 (98%)	316 (82%)	68 (18%)	2	1

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	CYS
2	B	26	SER
2	B	30	GLN
2	B	62	THR
2	B	65	VAL
2	B	73	GLN
2	B	77	SER
2	B	78	GLU
2	B	90	LYS
2	B	96	SER
2	B	99	ILE
2	B	106	LEU
2	B	109	SER
2	B	115	SER
2	B	116	GLN
2	B	119	SER
2	B	122	CYS
2	B	123	LEU
2	B	125	SER
2	B	139	THR
3	C	159	SER
3	C	160	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	164	SER
3	C	174	THR
3	C	175	LYS
3	C	176	ILE
3	C	203	LYS
3	C	214	SER
3	C	218	SER
3	C	219	THR
3	C	223	SER
3	C	232	THR
3	C	235	VAL
3	C	242	LEU
1	E	1	CYS
2	F	26	SER
2	F	30	GLN
2	F	62	THR
2	F	65	VAL
2	F	73	GLN
2	F	77	SER
2	F	78	GLU
2	F	90	LYS
2	F	96	SER
2	F	99	ILE
2	F	106	LEU
2	F	109	SER
2	F	115	SER
2	F	116	GLN
2	F	119	SER
2	F	122	CYS
2	F	123	LEU
2	F	125	SER
2	F	139	THR
3	G	159	SER
3	G	160	LEU
3	G	164	SER
3	G	174	THR
3	G	175	LYS
3	G	176	ILE
3	G	203	LYS
3	G	214	SER
3	G	218	SER
3	G	219	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	G	223	SER
3	G	232	THR
3	G	235	VAL
3	G	242	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	34	GLN
2	B	57	HIS
2	B	73	GLN
3	C	165	ASN
3	C	245	ASN
2	F	34	GLN
2	F	48	ASN
2	F	57	HIS
3	G	157	GLN
3	G	165	ASN
3	G	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](#)

2 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
4	TSU	G	51	-	9,10,11	0.85	1 (11%)	11,13,16	1.28	1 (9%)
4	TSU	C	51	-	9,10,11	0.83	1 (11%)	11,13,16	1.28	1 (9%)

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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TSU	G	51	-	-	2/2/4/6	0/1/1/1
4	TSU	C	51	-	-	2/2/4/6	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	51	TSU	C1-S	-2.04	1.75	1.80
4	C	51	TSU	C1-S	-2.02	1.76	1.80

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	51	TSU	O2-S-C1	2.44	110.10	105.05
4	G	51	TSU	O2-S-C1	2.43	110.07	105.05

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	51	TSU	C2-C1-S-O2
4	C	51	TSU	C6-C1-S-O2
4	G	51	TSU	C2-C1-S-O2
4	G	51	TSU	C6-C1-S-O2

There are no ring outliers.

No monomer is involved in short contacts.

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.