Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:02 am BST

PDB ID	:	6CHA
Title	:	STRUCTURE OF A TETRAHEDRAL TRANSITION STATE COMPLEX OF ALPHA-*CHYMOTRYPSIN AT 1.8-*ANGSTROMS RESOLUTION
Authors	:	Tulinsky, A.; Blevins, R.A.
Deposited on	:	1987-02-06
Resolution	:	1.80 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:

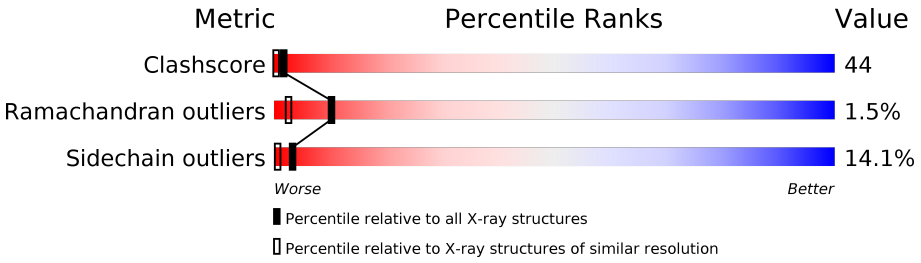
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	13	23% 46% 31%
1	E	13	31% 31% 8% 31%
2	B	131	27% 49% 18% 6%
2	F	131	34% 45% 17% .
3	C	97	33% 39% 23% 5%
3	G	97	33% 44% 21% .

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3679 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
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			

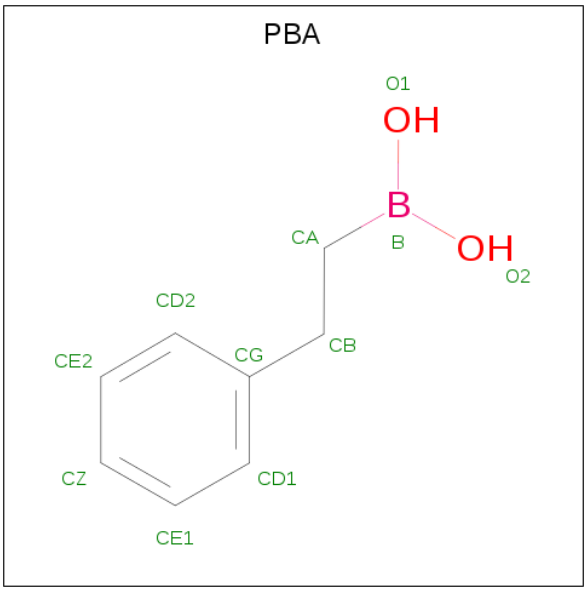
- Molecule 2 is a protein called ALPHA-CHYMOTRYPSIN A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
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
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 PHENYLETHANE BORONIC ACID (three-letter code: PBA) (formula: $C_8H_{11}BO_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total B C O 11 1 8 2	0	0
4	G	1	Total B C O 11 1 8 2	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	6	Total O 6 6	0	0
5	B	43	Total O 43 43	0	0
5	C	39	Total O 39 39	0	0
5	E	2	Total O 2 2	0	0
5	F	55	Total O 55 55	0	0
5	G	40	Total O 40 40	0	0

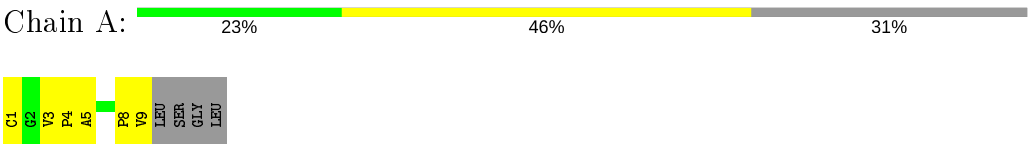
3 Residue-property plots (i)

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.

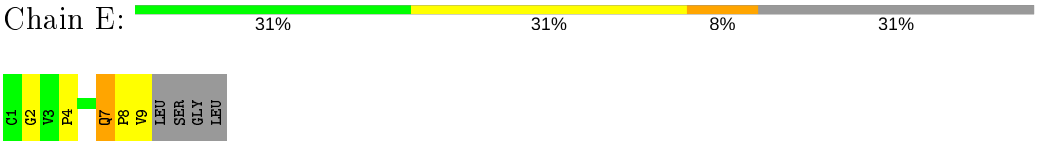
- Molecule 1: ALPHA-CHYMOTRYPSIN A

Chain A:



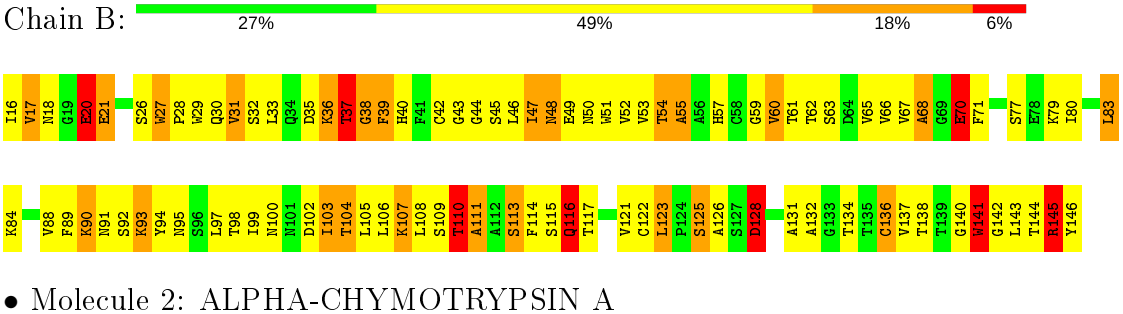
- Molecule 1: ALPHA-CHYMOTRYPSIN A

Chain E:



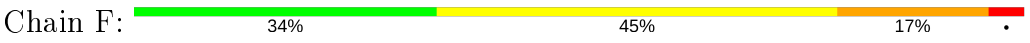
- Molecule 2: ALPHA-CHYMOTRYPSIN A

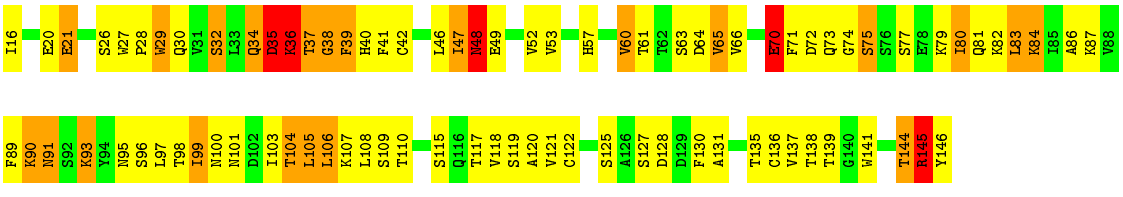
Chain B:



- Molecule 2: ALPHA-CHYMOTRYPSIN A

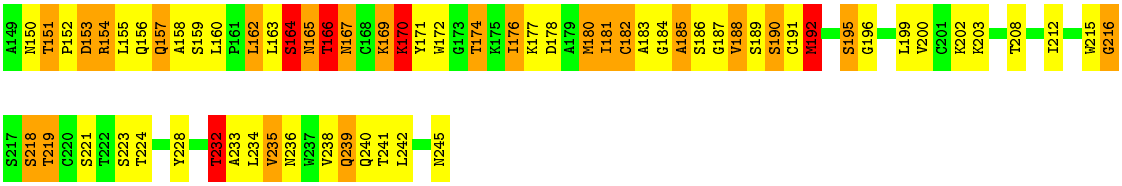
Chain F:





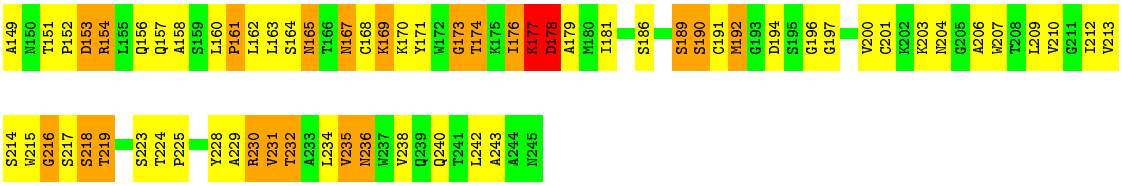
- Molecule 3: ALPHA-CHYMOTRYPSIN A

Chain C:



- Molecule 3: ALPHA-CHYMOTRYPSIN A

Chain G:



4 Data and refinement statistics (i)

Xtriage (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	49.27Å 67.16Å 65.91Å 90.00° 101.68° 90.00°	Depositor
Resolution (Å)	5.00 – 1.80	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-1.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3679	wwPDB-VP
Average B, all atoms (Å^2)	17.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	1.40	0/55	1.78	1/76 (1.3%)
1	E	1.50	0/55	1.89	1/76 (1.3%)
2	B	1.73	13/1000 (1.3%)	2.59	75/1361 (5.5%)
2	F	1.71	13/1000 (1.3%)	2.32	49/1361 (3.6%)
3	C	1.84	15/715 (2.1%)	2.45	48/973 (4.9%)
3	G	2.08	18/715 (2.5%)	2.63	52/973 (5.3%)
All	All	1.81	59/3540 (1.7%)	2.48	226/4820 (4.7%)

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
2	F	0	1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	217	SER	CB-OG	13.45	1.59	1.42
2	F	93	LYS	CD-CE	10.11	1.76	1.51
2	F	96	SER	CB-OG	10.03	1.55	1.42
3	G	215	TRP	C-O	8.39	1.39	1.23
3	C	170	LYS	CE-NZ	7.88	1.68	1.49
3	G	190	SER	CB-OG	7.78	1.52	1.42
3	G	216	GLY	CA-C	7.12	1.63	1.51
2	B	84	LYS	CB-CG	7.09	1.71	1.52
3	G	236	ASN	C-N	6.92	1.50	1.34
2	B	115	SER	CB-OG	6.91	1.51	1.42
2	B	140	GLY	CA-C	6.85	1.62	1.51
2	F	32	SER	N-CA	6.84	1.60	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	232	THR	CB-OG1	6.81	1.56	1.43
3	C	228	TYR	CG-CD1	6.76	1.48	1.39
3	C	169	LYS	CB-CG	6.73	1.70	1.52
3	C	218	SER	CA-CB	6.68	1.62	1.52
3	C	215	TRP	CD2-CE2	-6.54	1.33	1.41
2	B	123	LEU	C-O	6.38	1.35	1.23
3	C	196	GLY	N-CA	6.37	1.55	1.46
2	B	20	GLU	CD-OE2	6.33	1.32	1.25
3	C	182	CYS	CA-CB	6.17	1.67	1.53
2	B	94	TYR	CE1-CZ	6.14	1.46	1.38
3	G	215	TRP	CD2-CE3	-6.06	1.31	1.40
3	G	215	TRP	CD2-CE2	6.05	1.48	1.41
2	F	127	SER	CB-OG	5.99	1.50	1.42
2	F	26	SER	CB-OG	5.91	1.50	1.42
2	F	144	THR	CB-CG2	5.91	1.71	1.52
2	F	20	GLU	CD-OE2	5.88	1.32	1.25
3	G	214	SER	CA-CB	5.85	1.61	1.52
3	G	196	GLY	C-O	5.84	1.32	1.23
3	C	200	VAL	N-CA	5.77	1.57	1.46
3	G	189	SER	CB-OG	5.71	1.49	1.42
2	B	43	GLY	CA-C	5.71	1.60	1.51
2	B	146	TYR	CE1-CZ	5.69	1.46	1.38
3	C	169	LYS	CG-CD	5.66	1.71	1.52
3	C	216	GLY	CA-C	5.63	1.60	1.51
3	G	225	PRO	C-O	5.60	1.34	1.23
2	B	110	THR	CB-OG1	5.59	1.54	1.43
3	G	189	SER	CA-CB	-5.58	1.44	1.52
2	F	145	ARG	CB-CG	5.56	1.67	1.52
2	F	137	VAL	CB-CG1	5.53	1.64	1.52
3	G	174	THR	CB-OG1	5.50	1.54	1.43
3	G	215	TRP	CZ2-CH2	5.47	1.47	1.37
3	G	161	PRO	C-O	5.45	1.34	1.23
3	C	215	TRP	N-CA	5.43	1.57	1.46
2	B	68	ALA	CA-CB	5.42	1.63	1.52
2	B	144	THR	CB-OG1	5.42	1.54	1.43
2	F	120	ALA	CA-CB	5.41	1.63	1.52
2	B	142	GLY	C-N	5.38	1.46	1.34
3	C	176	ILE	CB-CG1	5.31	1.69	1.54
3	G	157	GLN	C-O	5.31	1.33	1.23
2	B	141	TRP	CE3-CZ3	5.24	1.47	1.38
2	F	118	VAL	CB-CG2	5.23	1.63	1.52
3	C	215	TRP	C-O	5.18	1.33	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	70	GLU	CD-OE1	-5.17	1.20	1.25
3	G	154	ARG	CD-NE	5.15	1.55	1.46
3	C	219	THR	CB-OG1	5.13	1.53	1.43
3	C	188	VAL	C-O	5.12	1.33	1.23
2	F	101	ASN	N-CA	5.07	1.56	1.46

All (226) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	20	GLU	OE1-CD-OE2	18.66	145.70	123.30
2	F	145	ARG	NE-CZ-NH1	-16.57	112.02	120.30
3	G	154	ARG	NE-CZ-NH2	-16.27	112.17	120.30
3	G	153	ASP	CB-CG-OD2	-14.58	105.18	118.30
2	B	20	GLU	CG-CD-OE2	-13.62	91.06	118.30
3	C	154	ARG	NE-CZ-NH2	-12.52	114.04	120.30
3	G	178	ASP	CB-CG-OD1	11.70	128.83	118.30
2	B	146	TYR	CB-CG-CD1	-11.61	114.04	121.00
2	B	48	ASN	CB-CA-C	-11.39	87.61	110.40
2	B	21	GLU	OE1-CD-OE2	11.02	136.52	123.30
2	B	110	THR	CA-CB-CG2	10.03	126.44	112.40
2	B	145	ARG	NE-CZ-NH2	-9.60	115.50	120.30
2	B	128	ASP	CB-CG-OD1	9.37	126.73	118.30
2	B	47	ILE	C-N-CA	9.27	144.89	121.70
3	G	153	ASP	OD1-CG-OD2	9.09	140.57	123.30
3	G	228	TYR	CD1-CE1-CZ	-9.07	111.64	119.80
2	F	70	GLU	CA-CB-CG	8.93	133.04	113.40
2	F	93	LYS	CD-CE-NZ	-8.91	91.20	111.70
3	C	153	ASP	CB-CG-OD2	8.59	126.03	118.30
2	F	130	PHE	CB-CA-C	8.56	127.53	110.40
2	B	125	SER	N-CA-CB	8.37	123.06	110.50
2	B	146	TYR	CG-CD2-CE2	-8.27	114.68	121.30
2	F	39	PHE	CA-CB-CG	8.12	133.39	113.90
2	B	60	VAL	O-C-N	8.10	135.65	122.70
3	C	219	THR	N-CA-CB	-8.09	94.94	110.30
2	B	138	THR	CA-CB-CG2	-8.02	101.18	112.40
2	F	131	ALA	CB-CA-C	-7.89	98.26	110.10
3	G	214	SER	N-CA-CB	-7.89	98.66	110.50
3	C	182	CYS	N-CA-CB	-7.86	96.45	110.60
3	C	163	LEU	CB-CG-CD2	-7.76	97.81	111.00
2	F	137	VAL	CA-CB-CG2	7.69	122.44	110.90
2	B	70	GLU	CB-CG-CD	7.59	134.70	114.20
3	C	167	ASN	OD1-CG-ND2	7.58	139.34	121.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	45	SER	O-C-N	7.50	134.70	122.70
3	G	178	ASP	N-CA-CB	-7.45	97.19	110.60
3	G	224	THR	CA-CB-CG2	7.34	122.68	112.40
3	C	232	THR	OG1-CB-CG2	7.30	126.79	110.00
3	G	223	SER	CA-CB-OG	-7.28	91.55	111.20
3	C	224	THR	O-C-N	7.25	134.88	121.10
2	B	20	GLU	O-C-N	7.21	134.23	122.70
2	B	70	GLU	OE1-CD-OE2	-7.21	114.65	123.30
3	G	154	ARG	NE-CZ-NH1	7.15	123.88	120.30
2	F	70	GLU	OE1-CD-OE2	7.14	131.87	123.30
2	F	21	GLU	OE1-CD-OE2	7.12	131.84	123.30
3	G	178	ASP	OD1-CG-OD2	-7.08	109.85	123.30
2	B	145	ARG	NH1-CZ-NH2	7.07	127.17	119.40
3	C	208	THR	OG1-CB-CG2	7.04	126.20	110.00
2	F	128	ASP	CB-CG-OD1	7.03	124.63	118.30
3	G	153	ASP	CA-CB-CG	-7.03	97.94	113.40
3	C	215	TRP	CG-CD2-CE3	-6.98	127.62	133.90
3	C	157	GLN	O-C-N	6.92	133.77	122.70
3	G	214	SER	CB-CA-C	6.90	123.20	110.10
2	F	46	LEU	O-C-N	6.89	133.72	122.70
3	C	219	THR	CA-CB-OG1	-6.86	94.59	109.00
3	C	169	LYS	CB-CG-CD	-6.82	93.86	111.60
2	B	55	ALA	N-CA-CB	6.73	119.52	110.10
2	B	125	SER	CB-CA-C	-6.72	97.34	110.10
3	G	181	ILE	CA-CB-CG1	-6.71	98.25	111.00
3	C	167	ASN	CB-CG-OD1	-6.71	108.18	121.60
2	F	29	TRP	O-C-N	6.70	133.42	122.70
2	B	17	VAL	CG1-CB-CG2	-6.69	100.20	110.90
3	C	208	THR	CA-CB-OG1	-6.67	94.99	109.00
3	C	182	CYS	CA-CB-SG	-6.67	102.00	114.00
3	C	218	SER	CB-CA-C	-6.65	97.47	110.10
2	B	94	TYR	CB-CG-CD1	-6.63	117.02	121.00
2	F	110	THR	N-CA-CB	6.63	122.90	110.30
2	F	71	PHE	O-C-N	6.63	133.31	122.70
2	B	109	SER	CA-CB-OG	-6.62	93.32	111.20
3	C	245	ASN	N-CA-C	6.55	128.69	111.00
2	B	145	ARG	N-CA-CB	6.54	122.38	110.60
2	B	128	ASP	OD1-CG-OD2	-6.54	110.87	123.30
2	F	39	PHE	CB-CA-C	6.53	123.47	110.40
3	G	177	LYS	CA-C-O	6.50	133.75	120.10
2	F	20	GLU	CG-CD-OE1	6.48	131.26	118.30
2	B	125	SER	O-C-N	6.46	133.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	20	GLU	CG-CD-OE2	-6.46	105.39	118.30
2	F	41	PHE	CB-CG-CD1	-6.45	116.28	120.80
3	G	186	SER	N-CA-CB	-6.41	100.88	110.50
3	G	229	ALA	CB-CA-C	-6.35	100.58	110.10
3	C	176	ILE	O-C-N	6.35	132.86	122.70
2	F	145	ARG	NE-CZ-NH2	6.32	123.46	120.30
3	C	187	GLY	O-C-N	-6.31	112.60	122.70
3	G	219	THR	CA-CB-OG1	-6.31	95.75	109.00
3	C	162	LEU	O-C-N	6.29	132.77	122.70
3	G	219	THR	CA-CB-CG2	6.26	121.17	112.40
3	C	208	THR	O-C-N	6.24	132.68	122.70
2	B	39	PHE	CB-CG-CD2	-6.23	116.44	120.80
3	G	181	ILE	CA-CB-CG2	6.22	123.35	110.90
2	F	145	ARG	CD-NE-CZ	-6.22	114.89	123.60
2	B	93	LYS	N-CA-CB	6.21	121.77	110.60
2	B	102	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	F	70	GLU	N-CA-CB	-6.19	99.46	110.60
3	G	201	CYS	CA-CB-SG	6.19	125.14	114.00
2	F	35	ASP	CA-CB-CG	-6.15	99.88	113.40
2	B	106	LEU	O-C-N	6.13	132.51	122.70
2	B	39	PHE	CB-CA-C	6.12	122.64	110.40
3	C	185	ALA	N-CA-CB	-6.10	101.56	110.10
2	B	27	TRP	CE3-CZ3-CH2	6.10	127.91	121.20
2	F	105	LEU	O-C-N	6.08	132.42	122.70
2	B	116	GLN	CG-CD-OE1	6.06	133.72	121.60
3	C	171	TYR	CB-CG-CD1	6.06	124.63	121.00
2	B	132	ALA	CB-CA-C	6.04	119.16	110.10
2	F	29	TRP	CB-CG-CD1	-6.03	119.16	127.00
2	B	145	ARG	NE-CZ-NH1	-6.02	117.29	120.30
2	F	115	SER	N-CA-CB	-6.01	101.48	110.50
2	F	80	ILE	O-C-N	5.98	132.27	122.70
3	G	228	TYR	CB-CG-CD1	-5.97	117.42	121.00
3	C	153	ASP	CB-CA-C	5.96	122.32	110.40
3	G	178	ASP	CB-CA-C	5.96	122.32	110.40
2	B	92	SER	N-CA-CB	5.96	119.44	110.50
2	B	137	VAL	CA-CB-CG2	5.96	119.83	110.90
3	G	218	SER	C-N-CA	5.96	136.59	121.70
3	C	154	ARG	NH1-CZ-NH2	5.95	125.94	119.40
2	B	94	TYR	CD1-CE1-CZ	-5.91	114.48	119.80
3	C	223	SER	N-CA-CB	5.90	119.35	110.50
3	C	208	THR	CA-CB-CG2	-5.89	104.15	112.40
3	G	173	GLY	CA-C-O	5.87	131.17	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	192	MET	CG-SD-CE	5.87	109.59	100.20
3	C	200	VAL	CA-CB-CG1	5.87	119.70	110.90
3	G	232	THR	CA-CB-OG1	-5.86	96.69	109.00
2	B	134	THR	O-C-N	5.85	132.06	122.70
3	G	165	ASN	N-CA-CB	5.82	121.07	110.60
3	G	228	TYR	N-CA-CB	-5.80	100.16	110.60
2	B	37	THR	N-CA-CB	5.80	121.31	110.30
2	F	38	GLY	CA-C-O	-5.79	110.18	120.60
3	C	239	GLN	CB-CG-CD	5.78	126.62	111.60
3	C	202	LYS	N-CA-CB	5.75	120.96	110.60
2	F	46	LEU	C-N-CA	-5.74	107.35	121.70
2	B	59	GLY	O-C-N	-5.73	113.53	122.70
2	B	116	GLN	CB-CG-CD	5.70	126.43	111.60
2	B	113	SER	CB-CA-C	5.70	120.93	110.10
3	G	230	ARG	NE-CZ-NH2	5.70	123.15	120.30
2	F	48	ASN	CA-CB-CG	5.69	125.91	113.40
2	B	91	ASN	CB-CG-OD1	-5.65	110.30	121.60
2	B	17	VAL	O-C-N	5.64	131.73	122.70
2	B	92	SER	CA-C-O	-5.64	108.26	120.10
2	B	123	LEU	N-CA-CB	-5.62	99.16	110.40
2	B	136	CYS	CB-CA-C	5.61	121.62	110.40
3	G	197	GLY	O-C-N	5.61	131.76	121.10
3	G	174	THR	CA-CB-OG1	-5.60	97.23	109.00
2	B	111	ALA	N-CA-CB	5.60	117.94	110.10
3	C	219	THR	OG1-CB-CG2	5.60	122.87	110.00
3	G	242	LEU	CA-CB-CG	5.59	128.17	115.30
2	B	33	LEU	CB-CG-CD1	-5.59	101.50	111.00
3	C	190	SER	N-CA-C	-5.58	95.92	111.00
3	G	228	TYR	CG-CD2-CE2	-5.58	116.83	121.30
3	G	232	THR	OG1-CB-CG2	5.58	122.83	110.00
3	C	235	VAL	CG1-CB-CG2	5.57	119.81	110.90
3	G	236	ASN	N-CA-CB	5.55	120.59	110.60
2	B	60	VAL	CA-CB-CG1	-5.54	102.58	110.90
2	B	88	VAL	CA-C-O	-5.54	108.46	120.10
2	B	21	GLU	CG-CD-OE2	-5.54	107.22	118.30
2	F	141	TRP	CA-C-O	-5.54	108.47	120.10
2	B	48	ASN	CA-CB-CG	-5.53	101.24	113.40
3	G	194	ASP	CB-CG-OD1	5.50	123.25	118.30
2	B	30	GLN	O-C-N	-5.49	113.92	122.70
2	B	110	THR	CB-CA-C	5.48	126.39	111.60
3	C	167	ASN	CA-CB-CG	-5.47	101.36	113.40
2	B	128	ASP	CA-CB-CG	5.47	125.42	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	119	SER	CB-CA-C	5.46	120.47	110.10
3	G	206	ALA	CB-CA-C	5.46	118.28	110.10
2	F	79	LYS	CB-CA-C	5.45	121.29	110.40
2	B	27	TRP	CD1-CG-CD2	-5.44	101.94	106.30
2	F	137	VAL	CA-C-O	5.43	131.50	120.10
3	G	219	THR	N-CA-CB	-5.42	100.01	110.30
2	F	81	GLN	OE1-CD-NE2	5.41	134.35	121.90
3	G	236	ASN	C-N-CA	-5.41	108.17	121.70
3	G	169	LYS	N-CA-CB	5.41	120.33	110.60
2	F	34	GLN	CG-CD-NE2	-5.40	103.74	116.70
3	C	200	VAL	CA-C-O	5.38	131.41	120.10
2	B	37	THR	CA-CB-OG1	-5.37	97.72	109.00
3	G	243	ALA	N-CA-CB	5.37	117.62	110.10
2	F	36	LYS	CA-CB-CG	-5.37	101.58	113.40
3	G	231	VAL	CA-CB-CG1	5.37	118.95	110.90
2	F	106	LEU	CA-CB-CG	5.36	127.63	115.30
3	G	235	VAL	N-CA-CB	-5.36	99.71	111.50
3	G	179	ALA	O-C-N	5.36	131.27	122.70
2	F	110	THR	O-C-N	5.36	131.27	122.70
3	C	164	SER	CA-CB-OG	-5.35	96.75	111.20
2	B	31	VAL	CA-CB-CG1	-5.35	102.88	110.90
2	B	31	VAL	CA-CB-CG2	5.35	118.92	110.90
3	G	210	VAL	CA-CB-CG1	5.34	118.91	110.90
3	C	158	ALA	N-CA-CB	5.31	117.54	110.10
3	C	199	LEU	N-CA-C	-5.31	96.67	111.00
3	C	171	TYR	O-C-N	-5.30	114.22	122.70
2	F	119	SER	O-C-N	-5.29	114.24	122.70
2	B	125	SER	CA-CB-OG	-5.27	96.98	111.20
3	G	149	ALA	O-C-N	-5.27	114.27	122.70
2	B	131	ALA	CA-C-N	-5.26	105.62	117.20
1	A	3	VAL	CG1-CB-CG2	-5.26	102.49	110.90
3	G	169	LYS	CD-CE-NZ	-5.25	99.62	111.70
2	B	108	LEU	C-N-CA	-5.24	108.60	121.70
2	F	119	SER	N-CA-CB	-5.23	102.65	110.50
2	F	60	VAL	CA-CB-CG2	5.21	118.72	110.90
2	F	29	TRP	CB-CG-CD2	5.20	133.36	126.60
2	B	140	GLY	CA-C-N	-5.19	105.78	117.20
3	C	151	THR	CA-CB-OG1	-5.19	98.09	109.00
3	C	245	ASN	CA-C-O	5.19	131.00	120.10
2	B	54	THR	O-C-N	5.19	131.00	122.70
3	G	176	ILE	CB-CG1-CD1	5.18	128.42	113.90
2	F	104	THR	CA-CB-CG2	5.17	119.64	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	66	VAL	CG1-CB-CG2	5.17	119.17	110.90
3	C	180	MET	C-N-CA	5.17	134.62	121.70
3	G	171	TYR	CB-CG-CD2	5.17	124.10	121.00
3	G	162	LEU	CA-C-O	-5.13	109.33	120.10
2	F	20	GLU	CA-CB-CG	5.12	124.67	113.40
3	C	221	SER	N-CA-CB	-5.11	102.83	110.50
2	F	100	ASN	O-C-N	5.11	130.88	122.70
2	B	104	THR	O-C-N	5.11	130.88	122.70
3	C	228	TYR	CB-CG-CD1	-5.11	117.93	121.00
2	F	29	TRP	NE1-CE2-CZ2	-5.11	124.78	130.40
2	B	146	TYR	CD1-CG-CD2	5.09	123.50	117.90
2	F	21	GLU	CG-CD-OE2	-5.08	108.13	118.30
2	B	66	VAL	CA-CB-CG1	-5.08	103.28	110.90
2	B	48	ASN	O-C-N	5.08	130.82	122.70
2	B	111	ALA	O-C-N	5.07	130.80	122.70
3	G	154	ARG	CD-NE-CZ	-5.06	116.51	123.60
1	E	2	GLY	CA-C-O	-5.06	111.49	120.60
3	C	215	TRP	CD2-CE3-CZ3	-5.05	112.23	118.80
2	F	71	PHE	CB-CG-CD2	-5.05	117.27	120.80
3	G	194	ASP	CB-CG-OD2	-5.04	113.76	118.30
2	B	83	LEU	N-CA-CB	-5.02	100.35	110.40
2	B	114	PHE	O-C-N	5.02	130.74	122.70
2	F	146	TYR	CA-C-O	-5.02	109.57	120.10
2	B	95	ASN	CB-CG-OD1	-5.01	111.58	121.60
3	C	166	THR	O-C-N	5.01	130.72	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	F	145	ARG	Sidechain

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	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	54	0	56	9	4
2	B	980	0	950	101	7
2	F	980	0	951	91	0
3	C	702	0	697	71	2
3	G	702	0	698	53	0
4	C	11	0	11	3	0
4	G	11	0	11	3	0
5	A	6	0	0	4	0
5	B	43	0	0	30	0
5	C	39	0	0	12	0
5	E	2	0	0	1	0
5	F	55	0	0	24	1
5	G	40	0	0	24	0
All	All	3679	0	3430	297	7

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 44.

All (297) 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)
2:F:93:LYS:CE	2:F:93:LYS:CD	1.76	1.61
3:C:170:LYS:CE	3:C:170:LYS:NZ	1.68	1.56
1:E:7:GLN:NE2	1:E:7:GLN:H	1.34	1.24
2:F:91:ASN:ND2	2:F:93:LYS:H	1.36	1.21
2:F:104:THR:HG21	5:F:698:HOH:O	1.40	1.18
2:F:52:VAL:HB	5:F:606:HOH:O	1.01	1.17
4:G:1:PBA:HD1	4:G:1:PBA:O2	1.43	1.15
3:G:176:ILE:HG12	5:G:693:HOH:O	1.47	1.12
3:G:176:ILE:CG1	5:G:693:HOH:O	1.95	1.12
2:B:103:ILE:HD13	2:B:104:THR:N	1.64	1.10
2:F:104:THR:CB	5:F:698:HOH:O	1.99	1.09
3:G:163:LEU:HD23	5:G:596:HOH:O	1.54	1.06
2:F:104:THR:CG2	5:F:698:HOH:O	1.97	1.05
2:F:39:PHE:HD1	5:F:667:HOH:O	1.42	1.01
2:F:106:LEU:HB2	5:F:606:HOH:O	1.60	1.01
2:F:47:ILE:HD13	2:F:53:VAL:HG23	1.41	0.99
2:B:63:SER:HB2	5:B:561:HOH:O	1.60	0.99
2:F:39:PHE:CD1	5:F:667:HOH:O	2.14	0.99
2:F:70:GLU:HB2	5:F:581:HOH:O	1.63	0.98
2:B:98:THR:HG23	5:B:625:HOH:O	1.61	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:236:ASN:O	3:C:240:GLN:HG3	1.64	0.97
2:B:21:GLU:OE2	3:C:154:ARG:HD2	1.65	0.97
3:C:195:SER:HB2	4:C:1:PBA:O1	1.67	0.94
1:E:9:VAL:N	5:E:584:HOH:O	1.99	0.94
2:F:47:ILE:HD13	2:F:53:VAL:CG2	1.99	0.93
2:F:91:ASN:HD22	2:F:93:LYS:N	1.65	0.92
1:A:1:CYS:N	5:A:671:HOH:O	1.94	0.92
3:G:163:LEU:CD2	5:G:596:HOH:O	2.12	0.92
3:G:191:CYS:HB2	5:G:629:HOH:O	1.68	0.92
2:B:27:TRP:C	5:B:637:HOH:O	2.10	0.91
2:B:68:ALA:HA	2:B:70:GLU:OE1	1.71	0.91
1:E:7:GLN:N	1:E:7:GLN:NE2	2.17	0.91
2:B:29:TRP:N	5:B:637:HOH:O	1.74	0.90
2:F:97:LEU:C	5:F:560:HOH:O	2.09	0.90
2:B:103:ILE:HD13	2:B:104:THR:H	1.35	0.89
2:F:91:ASN:ND2	2:F:93:LYS:N	2.19	0.89
2:F:34:GLN:NE2	5:F:545:HOH:O	2.05	0.89
2:F:135:THR:O	5:F:608:HOH:O	1.92	0.88
2:B:71:PHE:HA	5:B:553:HOH:O	1.75	0.86
5:B:514:HOH:O	3:G:219:THR:HG22	1.77	0.85
2:B:36:LYS:O	2:B:36:LYS:HD3	1.77	0.85
5:B:625:HOH:O	3:C:177:LYS:HD2	1.76	0.84
5:B:514:HOH:O	3:G:219:THR:CG2	2.25	0.84
2:F:93:LYS:NZ	2:F:93:LYS:CD	2.40	0.83
3:C:216:GLY:O	3:G:218:SER:HB2	1.77	0.83
2:F:91:ASN:HD22	2:F:93:LYS:H	0.83	0.82
2:B:128:ASP:OD2	3:C:203:LYS:NZ	2.12	0.82
2:F:145:ARG:NE	5:F:571:HOH:O	2.05	0.82
3:C:169:LYS:HE3	5:C:659:HOH:O	1.81	0.81
3:C:184:GLY:O	3:C:185:ALA:HB3	1.80	0.81
3:G:168:CYS:HA	5:G:596:HOH:O	1.80	0.81
2:F:60:VAL:O	5:F:509:HOH:O	1.98	0.80
1:E:7:GLN:H	1:E:7:GLN:HE21	1.26	0.80
2:B:125:SER:N	2:B:128:ASP:OD1	2.14	0.80
3:G:165:ASN:ND2	5:G:569:HOH:O	2.07	0.79
3:G:176:ILE:HB	5:G:693:HOH:O	1.82	0.79
2:B:145:ARG:HD2	3:C:150:ASN:OD1	1.83	0.79
3:C:165:ASN:ND2	5:C:502:HOH:O	2.17	0.78
2:B:21:GLU:OE2	3:C:154:ARG:CD	2.32	0.78
3:C:195:SER:CB	4:C:1:PBA:O1	2.35	0.74
2:B:71:PHE:O	5:B:553:HOH:O	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:GLN:H	1:E:7:GLN:CD	1.89	0.74
2:B:103:ILE:CD1	2:B:104:THR:N	2.50	0.74
2:B:17:VAL:O	2:B:18:ASN:HB2	1.87	0.73
3:G:191:CYS:N	5:G:629:HOH:O	2.20	0.73
5:C:690:HOH:O	2:F:37:THR:HG22	1.88	0.73
2:B:67:VAL:O	2:B:70:GLU:OE1	2.07	0.73
3:C:239:GLN:NE2	5:C:521:HOH:O	2.22	0.73
2:F:103:ILE:HD12	3:G:212:ILE:HD11	1.69	0.73
3:G:191:CYS:CB	5:G:629:HOH:O	2.32	0.72
2:F:98:THR:O	2:F:99:ILE:HB	1.89	0.71
3:G:230:ARG:NH2	5:G:628:HOH:O	2.23	0.70
2:F:99:ILE:HG12	5:F:560:HOH:O	1.90	0.70
2:B:83:LEU:HD22	2:B:110:THR:O	1.91	0.69
2:B:98:THR:CG2	2:B:100:ASN:HB2	2.22	0.69
2:B:143:LEU:HD23	3:C:151:THR:HG22	1.73	0.69
2:B:53:VAL:HG23	2:B:103:ILE:HD11	1.73	0.69
2:F:93:LYS:CG	2:F:93:LYS:CE	2.71	0.69
2:B:83:LEU:CD2	2:B:110:THR:O	2.40	0.68
3:C:153:ASP:OD1	5:C:690:HOH:O	2.12	0.68
3:C:169:LYS:HE2	5:C:652:HOH:O	1.94	0.68
2:B:18:ASN:HB3	3:C:188:VAL:HG12	1.75	0.67
2:F:21:GLU:OE1	3:G:154:ARG:NH2	2.26	0.67
2:B:49:GLU:O	2:B:111:ALA:HB1	1.95	0.67
2:B:98:THR:HG22	2:B:100:ASN:HB2	1.76	0.67
3:G:154:ARG:NH1	5:G:547:HOH:O	2.26	0.67
3:C:154:ARG:HH11	3:C:154:ARG:HG3	1.60	0.66
2:F:40:HIS:CE1	2:F:42:CYS:O	2.49	0.66
2:B:123:LEU:HD23	3:C:239:GLN:HE22	1.59	0.66
2:B:98:THR:HG22	2:B:100:ASN:H	1.59	0.66
2:B:128:ASP:OD2	5:B:523:HOH:O	2.14	0.66
2:B:50:ASN:OD1	2:B:107:LYS:NZ	2.29	0.66
2:B:28:PRO:N	5:B:637:HOH:O	2.24	0.66
2:F:91:ASN:C	2:F:91:ASN:HD22	1.99	0.66
2:F:104:THR:HB	5:F:698:HOH:O	1.81	0.66
3:G:230:ARG:HG3	5:G:628:HOH:O	1.95	0.65
2:B:17:VAL:CG2	5:B:695:HOH:O	2.44	0.65
3:G:168:CYS:CA	5:G:596:HOH:O	2.42	0.65
3:G:168:CYS:CB	5:G:596:HOH:O	2.44	0.65
2:B:39:PHE:CZ	2:B:40:HIS:HB3	2.32	0.65
5:B:625:HOH:O	3:C:180:MET:CE	2.45	0.65
2:F:136:CYS:HB3	3:G:200:VAL:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:ARG:CD	3:C:150:ASN:OD1	2.46	0.64
2:B:70:GLU:OE2	2:B:141:TRP:HH2	1.82	0.63
5:B:553:HOH:O	3:C:155:LEU:HB2	1.98	0.63
2:B:17:VAL:HG22	5:B:695:HOH:O	1.98	0.63
1:E:7:GLN:N	1:E:7:GLN:CD	2.47	0.62
3:C:154:ARG:NH1	3:C:154:ARG:HG3	2.15	0.62
2:F:86:ALA:HB2	2:F:109:SER:HA	1.81	0.61
2:B:103:ILE:O	2:B:103:ILE:HG23	1.98	0.61
2:F:87:LYS:HG2	2:F:89:PHE:CE1	2.36	0.61
2:F:72:ASP:OD2	3:G:153:ASP:HB3	2.00	0.61
2:F:57:HIS:CD2	5:F:635:HOH:O	2.52	0.61
3:G:177:LYS:HE3	5:G:570:HOH:O	1.99	0.61
2:B:107:LYS:HD3	5:B:643:HOH:O	2.01	0.61
2:B:98:THR:CG2	5:B:625:HOH:O	2.33	0.61
2:B:38:GLY:O	2:B:39:PHE:HB2	2.01	0.60
3:G:153:ASP:HB2	5:G:520:HOH:O	2.01	0.60
3:C:166:THR:HG22	3:C:167:ASN:OD1	2.00	0.60
1:A:4:PRO:HG2	1:A:8:PRO:CD	2.32	0.60
2:B:105:LEU:HD21	3:C:238:VAL:HG13	1.83	0.60
3:C:160:LEU:N	3:C:160:LEU:HD23	2.17	0.60
3:G:178:ASP:N	3:G:178:ASP:OD2	2.34	0.59
5:B:625:HOH:O	3:C:180:MET:HE1	2.02	0.58
2:B:35:ASP:OD2	2:B:37:THR:HG23	2.04	0.58
2:B:60:VAL:HG12	2:B:61:THR:N	2.18	0.58
2:F:103:ILE:HD12	3:G:212:ILE:CD1	2.34	0.58
2:F:21:GLU:OE1	3:G:154:ARG:HD2	2.04	0.57
2:F:84:LYS:HE3	2:F:84:LYS:N	2.18	0.57
3:C:160:LEU:HD13	5:C:691:HOH:O	2.04	0.57
4:G:1:PBA:HD1	4:G:1:PBA:HO2	1.66	0.57
2:B:27:TRP:N	2:B:28:PRO:HD3	2.19	0.57
2:F:87:LYS:HG2	2:F:89:PHE:CZ	2.40	0.57
2:B:71:PHE:CA	5:B:553:HOH:O	2.44	0.56
3:C:169:LYS:CE	5:C:652:HOH:O	2.51	0.56
2:F:91:ASN:HD21	2:F:93:LYS:HB2	1.69	0.56
2:F:74:GLY:O	2:F:75:SER:C	2.44	0.56
3:C:174:THR:HA	5:C:659:HOH:O	2.05	0.56
2:F:107:LYS:CE	5:G:580:HOH:O	2.52	0.56
1:A:4:PRO:HG2	1:A:8:PRO:HD3	1.87	0.56
2:B:21:GLU:CD	3:C:154:ARG:HD2	2.26	0.56
2:F:36:LYS:HZ2	2:F:36:LYS:HA	1.71	0.56
3:C:184:GLY:O	3:C:185:ALA:CB	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:PRO:HB3	2:B:117:THR:O	2.06	0.55
3:C:170:LYS:CD	3:C:170:LYS:NZ	2.64	0.55
2:B:141:TRP:HZ2	5:B:553:HOH:O	1.88	0.55
2:F:95:ASN:O	2:F:99:ILE:N	2.36	0.55
3:C:233:ALA:C	5:C:503:HOH:O	2.45	0.55
2:B:26:SER:C	2:B:28:PRO:HD3	2.27	0.54
3:C:154:ARG:O	3:C:156:GLN:HG2	2.07	0.54
3:G:167:ASN:O	3:G:170:LYS:HB2	2.06	0.54
2:B:143:LEU:O	5:B:695:HOH:O	2.18	0.54
3:C:189:SER:OG	3:C:190:SER:O	2.21	0.54
2:F:139:THR:HA	3:G:156:GLN:O	2.08	0.54
2:B:47:ILE:O	2:B:48:ASN:ND2	2.41	0.53
2:F:49:GLU:O	2:F:108:LEU:HD12	2.08	0.53
2:F:90:LYS:HB2	5:F:602:HOH:O	2.08	0.53
2:F:36:LYS:CG	2:F:63:SER:O	2.57	0.53
3:G:169:LYS:O	3:G:173:GLY:HA2	2.08	0.53
2:B:39:PHE:CG	2:B:40:HIS:N	2.67	0.53
2:F:107:LYS:HE3	5:G:580:HOH:O	2.10	0.52
2:B:103:ILE:C	2:B:103:ILE:HD13	2.25	0.52
3:C:164:SER:HB2	3:C:167:ASN:OD1	2.09	0.52
1:A:1:CYS:C	2:B:122:CYS:SG	2.88	0.52
2:B:48:ASN:ND2	2:B:48:ASN:N	2.51	0.52
2:F:47:ILE:HG13	2:F:48:ASN:HD22	1.75	0.52
2:F:36:LYS:HG2	2:F:63:SER:O	2.10	0.52
2:F:53:VAL:HG22	2:F:105:LEU:HD23	1.92	0.52
2:B:90:LYS:H	2:B:90:LYS:HD3	1.75	0.51
2:F:66:VAL:O	2:F:83:LEU:N	2.26	0.51
2:F:98:THR:O	2:F:99:ILE:CB	2.55	0.51
3:G:230:ARG:CG	5:G:628:HOH:O	2.55	0.51
2:F:63:SER:OG	5:F:684:HOH:O	2.19	0.51
3:C:167:ASN:N	3:C:167:ASN:OD1	2.43	0.51
3:C:160:LEU:HD12	3:C:183:ALA:HB1	1.92	0.51
1:A:9:VAL:N	5:A:511:HOH:O	2.44	0.51
2:B:16:ILE:HA	3:C:189:SER:O	2.11	0.51
5:A:550:HOH:O	2:B:28:PRO:HG3	2.10	0.51
2:B:103:ILE:O	2:B:103:ILE:CG2	2.59	0.51
3:C:160:LEU:CD1	3:C:183:ALA:HB1	2.42	0.50
2:B:68:ALA:CA	2:B:70:GLU:OE1	2.51	0.50
3:C:235:VAL:HG22	3:C:239:GLN:HE21	1.77	0.50
3:C:153:ASP:OD2	2:F:37:THR:HG21	2.12	0.50
1:A:8:PRO:HG3	2:B:26:SER:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:THR:C	2:B:63:SER:N	2.65	0.50
2:B:48:ASN:HD22	2:B:48:ASN:N	2.02	0.50
3:G:163:LEU:HD22	5:G:596:HOH:O	1.96	0.49
2:B:123:LEU:CD2	3:C:239:GLN:HE22	2.26	0.49
2:F:107:LYS:HE2	5:G:580:HOH:O	2.10	0.49
2:B:17:VAL:O	3:C:188:VAL:HA	2.12	0.49
2:F:72:ASP:C	2:F:74:GLY:H	2.15	0.49
1:A:5:ALA:N	5:A:550:HOH:O	2.46	0.49
3:G:164:SER:OG	3:G:167:ASN:HB2	2.12	0.48
3:G:203:LYS:O	3:G:204:ASN:HB2	2.12	0.48
2:B:51:TRP:CE2	3:C:242:LEU:HD23	2.48	0.48
1:A:1:CYS:O	2:B:122:CYS:SG	2.72	0.48
2:F:47:ILE:CD1	2:F:53:VAL:CG2	2.83	0.48
2:F:70:GLU:OE2	2:F:73:GLN:HG3	2.14	0.48
2:B:21:GLU:OE2	3:C:154:ARG:NE	2.47	0.48
3:G:191:CYS:O	3:G:192:MET:C	2.53	0.48
2:F:99:ILE:CD1	5:F:560:HOH:O	2.61	0.47
1:E:4:PRO:HG2	1:E:8:PRO:HD3	1.95	0.47
3:G:151:THR:OG1	3:G:151:THR:O	2.29	0.47
2:F:40:HIS:HE1	2:F:42:CYS:O	1.96	0.47
2:B:63:SER:CB	5:B:561:HOH:O	2.38	0.47
2:B:136:CYS:O	3:C:159:SER:HA	2.15	0.47
3:C:191:CYS:O	3:C:192:MET:C	2.54	0.47
1:E:7:GLN:O	1:E:8:PRO:C	2.50	0.47
2:B:61:THR:C	2:B:63:SER:H	2.17	0.46
3:C:219:THR:CG2	5:C:696:HOH:O	2.63	0.46
2:B:17:VAL:HG23	5:B:695:HOH:O	2.13	0.46
2:F:60:VAL:HG12	2:F:61:THR:N	2.30	0.46
2:F:99:ILE:CG1	5:F:560:HOH:O	2.57	0.46
2:B:103:ILE:C	2:B:103:ILE:CD1	2.81	0.46
3:G:231:VAL:O	3:G:234:LEU:N	2.36	0.46
2:B:48:ASN:HB2	2:B:50:ASN:H	1.80	0.46
3:G:190:SER:C	5:G:629:HOH:O	2.52	0.46
2:B:29:TRP:CD2	5:B:637:HOH:O	2.67	0.46
2:B:46:LEU:HD23	2:B:52:VAL:CG2	2.46	0.46
2:F:103:ILE:HG13	2:F:104:THR:N	2.30	0.46
3:C:192:MET:CG	3:G:192:MET:HG2	2.45	0.46
2:F:16:ILE:HA	5:G:629:HOH:O	2.15	0.45
2:B:49:GLU:O	2:B:111:ALA:CB	2.61	0.45
3:C:232:THR:HG22	3:C:233:ALA:N	2.31	0.45
2:F:27:TRP:N	2:F:28:PRO:HD3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:47:ILE:O	5:F:538:HOH:O	2.20	0.45
2:F:91:ASN:C	2:F:91:ASN:ND2	2.65	0.45
2:B:90:LYS:H	2:B:90:LYS:CD	2.29	0.45
3:C:195:SER:HB2	4:C:1:PBA:HO1	1.78	0.45
2:F:108:LEU:O	5:F:636:HOH:O	2.21	0.45
2:B:27:TRP:N	2:B:28:PRO:CD	2.80	0.45
2:B:47:ILE:C	2:B:48:ASN:ND2	2.70	0.45
3:C:164:SER:CB	3:C:167:ASN:OD1	2.65	0.45
3:G:209:LEU:HA	3:G:209:LEU:HD12	1.75	0.45
3:C:218:SER:HB3	3:G:216:GLY:O	2.16	0.45
3:C:160:LEU:HD23	3:C:160:LEU:H	1.82	0.44
2:F:47:ILE:HG13	2:F:48:ASN:ND2	2.32	0.44
2:F:36:LYS:HG3	2:F:63:SER:HB3	1.99	0.44
3:C:182:CYS:HB2	5:C:502:HOH:O	2.16	0.44
2:B:36:LYS:HD3	2:B:36:LYS:HA	1.70	0.44
2:B:36:LYS:CD	2:B:36:LYS:O	2.55	0.44
2:F:84:LYS:HE3	2:F:84:LYS:H	1.82	0.44
2:F:135:THR:O	2:F:135:THR:HG22	2.18	0.44
2:F:84:LYS:CE	2:F:84:LYS:N	2.81	0.44
2:B:39:PHE:CE2	2:B:40:HIS:HB3	2.52	0.44
2:B:89:PHE:HB2	2:B:105:LEU:HB2	1.99	0.44
5:B:625:HOH:O	3:C:180:MET:HE3	2.12	0.43
2:F:21:GLU:OE1	3:G:154:ARG:CZ	2.66	0.43
2:F:93:LYS:NZ	2:F:93:LYS:HD3	2.28	0.43
2:B:48:ASN:CB	2:B:50:ASN:H	2.30	0.43
2:B:37:THR:OG1	2:B:38:GLY:N	2.49	0.43
2:F:80:ILE:HD11	2:F:82:LYS:HE3	1.99	0.43
2:B:57:HIS:HA	5:B:680:HOH:O	2.18	0.43
2:F:28:PRO:HB3	2:F:117:THR:O	2.18	0.43
2:F:144:THR:HG23	3:G:152:PRO:HG3	1.99	0.43
3:G:236:ASN:O	3:G:240:GLN:HG3	2.17	0.43
2:B:98:THR:HG22	2:B:100:ASN:N	2.29	0.43
2:B:105:LEU:HD12	3:C:241:THR:HG21	2.01	0.43
2:B:60:VAL:CG1	2:B:61:THR:N	2.81	0.43
3:G:235:VAL:HA	3:G:238:VAL:HB	2.00	0.43
2:F:35:ASP:HA	2:F:64:ASP:OD2	2.19	0.42
2:B:36:LYS:C	2:B:36:LYS:HD3	2.19	0.42
3:C:160:LEU:N	3:C:160:LEU:CD2	2.83	0.42
2:B:103:ILE:HG12	3:C:212:ILE:HD13	2.01	0.42
2:B:29:TRP:CG	5:B:637:HOH:O	2.56	0.42
2:B:126:ALA:HA	3:C:232:THR:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:GLN:C	1:E:8:PRO:O	2.55	0.42
3:G:209:LEU:HG	3:G:231:VAL:HG21	2.02	0.42
2:B:31:VAL:HG22	2:B:44:GLY:C	2.40	0.42
2:F:53:VAL:HG22	2:F:105:LEU:CD2	2.48	0.42
2:B:39:PHE:CD2	2:B:40:HIS:N	2.88	0.41
2:B:141:TRP:HB2	5:B:586:HOH:O	2.19	0.41
3:C:181:ILE:HD12	3:C:181:ILE:HG21	1.44	0.41
2:F:72:ASP:C	2:F:74:GLY:N	2.73	0.41
3:G:213:VAL:CG1	4:G:1:PBA:HB1	2.49	0.41
2:B:53:VAL:HG23	2:B:103:ILE:CD1	2.48	0.41
3:C:162:LEU:HD23	3:C:162:LEU:HA	1.78	0.41
3:G:160:LEU:HA	3:G:161:PRO:HD3	1.93	0.41
2:F:138:THR:HG22	3:G:160:LEU:CD2	2.51	0.41
2:F:36:LYS:C	2:F:38:GLY:N	2.71	0.41
2:B:54:THR:OG1	2:B:55:ALA:N	2.53	0.41
5:B:514:HOH:O	3:G:219:THR:HG21	2.04	0.41
3:G:231:VAL:O	3:G:235:VAL:N	2.48	0.41
2:B:20:GLU:O	3:C:157:GLN:N	2.49	0.41
3:C:151:THR:HA	3:C:152:PRO:HD3	1.80	0.41
3:G:200:VAL:HG23	3:G:207:TRP:CE3	2.56	0.41
3:C:162:LEU:HD22	3:C:181:ILE:HD11	2.02	0.40
2:F:16:ILE:O	5:F:630:HOH:O	2.22	0.40
2:B:29:TRP:CG	2:B:121:VAL:HB	2.57	0.40
3:C:166:THR:HG22	3:C:167:ASN:N	2.36	0.40
3:C:172:TRP:HB2	3:C:176:ILE:CG1	2.51	0.40
2:F:16:ILE:HG21	3:G:158:ALA:HB2	2.03	0.40
2:F:121:VAL:HG22	2:F:122:CYS:N	2.37	0.40
2:F:27:TRP:O	2:F:30:GLN:HB3	2.22	0.40
2:F:65:VAL:HG21	5:F:624:HOH:O	2.22	0.40
5:B:695:HOH:O	3:C:191:CYS:CB	2.69	0.40
2:F:36:LYS:CD	2:F:63:SER:O	2.70	0.40

All (7) 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:116:GLN:CG	1:E:7:GLN:OE1[2_746]	1.51	0.69
2:B:116:GLN:NE2	1:E:7:GLN:OE1[2_746]	1.71	0.49
2:B:116:GLN:CD	1:E:7:GLN:OE1[2_746]	1.87	0.33
2:B:79:LYS:CE	3:C:170:LYS:CD[1_655]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:LYS:CD	3:C:170:LYS:NZ[1_655]	2.18	0.02
2:B:125:SER:CB	5:F:563:HOH:O[1_554]	2.18	0.02
2:B:116:GLN:CG	1:E:7:GLN:CD[2_746]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	7/13 (54%)	7 (100%)	0	0	100 100
1	E	7/13 (54%)	7 (100%)	0	0	100 100
2	B	129/131 (98%)	119 (92%)	7 (5%)	3 (2%)	6 1
2	F	129/131 (98%)	119 (92%)	7 (5%)	3 (2%)	6 1
3	C	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	14 4
3	G	95/97 (98%)	91 (96%)	4 (4%)	0	100 100
All	All	462/482 (96%)	430 (93%)	25 (5%)	7 (2%)	10 2

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	75	SER
2	F	99	ILE
2	F	77	SER
2	B	99	ILE
2	B	77	SER
3	C	174	THR
2	B	38	GLY

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%)	6 (100%)	0	100	100
1	E	6/10 (60%)	5 (83%)	1 (17%)	2	0
2	B	109/109 (100%)	89 (82%)	20 (18%)	1	0
2	F	109/109 (100%)	94 (86%)	15 (14%)	3	1
3	C	77/77 (100%)	66 (86%)	11 (14%)	3	0
3	G	77/77 (100%)	70 (91%)	7 (9%)	9	2
All	All	384/392 (98%)	330 (86%)	54 (14%)	3	0

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	20	GLU
2	B	32	SER
2	B	36	LYS
2	B	37	THR
2	B	42	CYS
2	B	62	THR
2	B	65	VAL
2	B	70	GLU
2	B	80	ILE
2	B	90	LYS
2	B	93	LYS
2	B	97	LEU
2	B	103	ILE
2	B	107	LYS
2	B	110	THR
2	B	113	SER
2	B	116	GLN
2	B	128	ASP
2	B	141	TRP
2	B	145	ARG
3	C	164	SER
3	C	165	ASN

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Mol	Chain	Res	Type
3	C	166	THR
3	C	170	LYS
3	C	178	ASP
3	C	181	ILE
3	C	186	SER
3	C	192	MET
3	C	195	SER
3	C	232	THR
3	C	234	LEU
1	E	7	GLN
2	F	29	TRP
2	F	32	SER
2	F	35	ASP
2	F	36	LYS
2	F	37	THR
2	F	47	ILE
2	F	48	ASN
2	F	65	VAL
2	F	70	GLU
2	F	83	LEU
2	F	84	LYS
2	F	90	LYS
2	F	91	ASN
2	F	125	SER
2	F	145	ARG
3	G	167	ASN
3	G	174	THR
3	G	177	LYS
3	G	178	ASP
3	G	189	SER
3	G	192	MET
3	G	232	THR

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

Mol	Chain	Res	Type
2	B	18	ASN
2	B	48	ASN
3	C	165	ASN
3	C	239	GLN
1	E	7	GLN
2	F	48	ASN

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Mol	Chain	Res	Type
2	F	50	ASN
2	F	91	ASN
3	G	165	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	PBA	C	1	3	9,11,11	3.58	3 (33%)	11,13,13	1.79	3 (27%)
4	PBA	G	1	-	9,11,11	1.29	1 (11%)	11,13,13	1.66	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PBA	C	1	3	-	2/3/5/5	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PBA	G	1	-	-	3/3/5/5	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1	PBA	B-CA	10.01	1.67	1.56
4	G	1	PBA	B-CA	-2.62	1.53	1.56
4	C	1	PBA	CD2-CG	2.27	1.43	1.38
4	C	1	PBA	CB-CG	2.09	1.57	1.51

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	1	PBA	O1-B-CA	-4.46	112.43	121.20
4	C	1	PBA	O2-B-CA	-3.43	114.45	121.20
4	C	1	PBA	O1-B-CA	-2.87	115.55	121.20
4	C	1	PBA	CD2-CG-CD1	2.13	121.51	118.17

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	G	1	PBA	CA-CB-CG-CD1
4	G	1	PBA	CA-CB-CG-CD2
4	G	1	PBA	B-CA-CB-CG
4	C	1	PBA	CA-CB-CG-CD1
4	C	1	PBA	CA-CB-CG-CD2

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	1	PBA	3	0
4	G	1	PBA	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section 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.