



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:57 PM UTC

PDB ID : 6CHA / pdb_00006cha
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 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

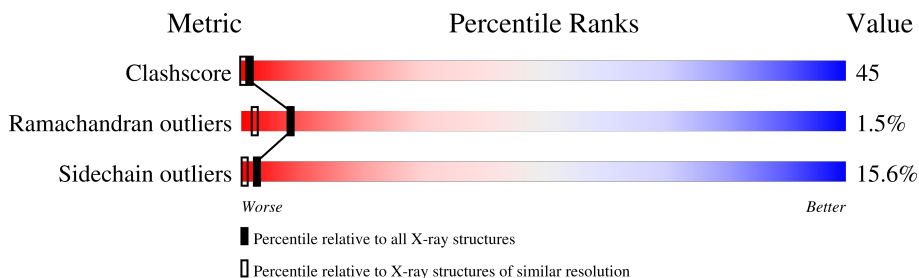
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (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 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	15% 31% 23% 31%
1	E	13	31% 15% 15% 8% 31%
2	B	131	14% 44% 34% 9%
2	F	131	20% 44% 27% 10%
3	C	97	21% 37% 33% 9%
3	G	97	12% 49% 32% 6%

2 Entry composition [i](#)

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
			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			

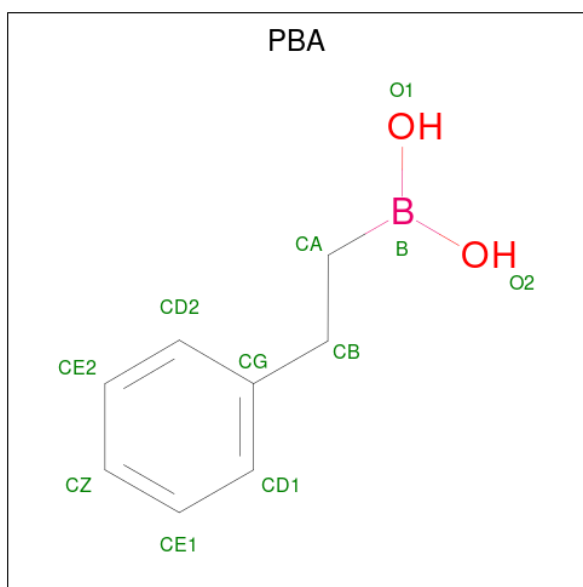
- Molecule 2 is a protein called ALPHA-CHYMOTRYPSIN A.

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 PHENYLETHANE BORONIC ACID (CCD ID: PBA) (formula: C₈H₁₁BO₂).



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

- Molecule 5 is water.


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

3 Residue-property plots [i](#)

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.

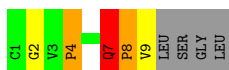
- Molecule 1: ALPHA-CHYMOTRYPSIN A

Chain A: 



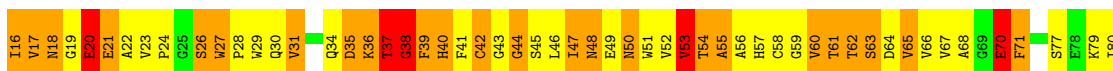
- Molecule 1: ALPHA-CHYMOTRYPSIN A

Chain E: 

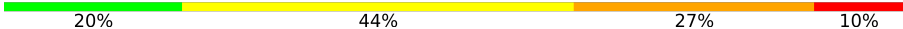


- Molecule 2: ALPHA-CHYMOTRYPSIN A

Chain B: 

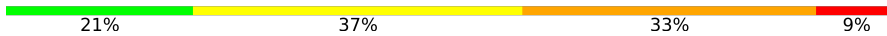


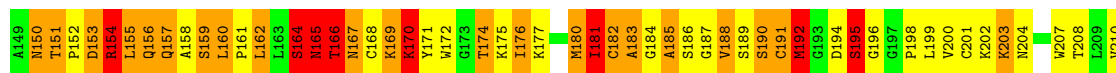
- Molecule 2: ALPHA-CHYMOTRYPSIN A

Chain F: 



- Molecule 3: ALPHA-CHYMOTRYPSIN A

Chain C:  21% 37% 33% 9%



- Molecule 3: ALPHA-CHYMOTRYPSIN A

Chain G:  12% 49% 32% 6%



4 Data and refinement statistics

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 i

5.1 Standard geometry i

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	1.90	3/55 (5.5%)	2.20	1/76 (1.3%)
1	E	1.97	1/55 (1.8%)	2.70	5/76 (6.6%)
2	B	2.22	40/1000 (4.0%)	3.25	162/1361 (11.9%)
2	F	2.18	35/1000 (3.5%)	3.07	133/1361 (9.8%)
3	C	2.39	37/715 (5.2%)	3.26	117/973 (12.0%)
3	G	2.76	59/715 (8.3%)	3.44	150/973 (15.4%)
All	All	2.35	175/3540 (4.9%)	3.22	568/4820 (11.8%)

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 (175) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	215	TRP	C-O	14.18	1.39	1.23
3	G	236	ASN	C-N	12.23	1.50	1.33
2	F	32	SER	N-CA	11.04	1.60	1.46
3	C	200	VAL	N-CA	10.34	1.57	1.46
3	G	216	GLY	CA-C	9.82	1.63	1.51
3	G	225	PRO	C-O	9.70	1.34	1.23
2	B	140	GLY	CA-C	9.63	1.62	1.51
3	G	210	VAL	CA-C	9.60	1.65	1.52
2	F	71	PHE	CA-C	9.43	1.60	1.52
2	B	142	GLY	C-N	9.30	1.46	1.33
3	G	161	PRO	C-O	9.28	1.34	1.23
3	C	182	CYS	CA-CB	9.07	1.67	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	33	LEU	CA-C	8.81	1.63	1.52
3	G	217	SER	CB-OG	8.79	1.59	1.42
3	G	199	LEU	CA-C	8.65	1.62	1.52
2	B	22	ALA	N-CA	8.53	1.55	1.45
3	C	215	TRP	N-CA	8.51	1.57	1.46
2	F	66	VAL	CA-CB	8.40	1.64	1.54
3	G	212	ILE	CA-C	8.38	1.63	1.52
2	B	34	GLN	N-CA	8.22	1.55	1.45
2	B	53	VAL	CA-C	8.20	1.62	1.52
3	G	232	THR	CB-OG1	8.20	1.56	1.43
3	G	157	GLN	C-O	8.11	1.33	1.23
3	C	216	GLY	CA-C	8.10	1.60	1.51
3	G	182	CYS	N-CA	8.08	1.55	1.45
3	G	228	TYR	N-CA	8.04	1.55	1.45
2	F	93	LYS	CD-CE	8.03	1.76	1.52
3	G	191	CYS	C-N	7.89	1.44	1.33
3	G	200	VAL	C-O	7.87	1.32	1.24
2	B	27	TRP	C-O	7.80	1.32	1.23
3	G	159	SER	N-CA	7.78	1.55	1.45
3	G	215	TRP	N-CA	7.78	1.55	1.46
3	C	215	TRP	C-O	7.76	1.33	1.23
3	C	176	ILE	CB-CG1	7.74	1.69	1.53
2	F	65	VAL	N-CA	7.66	1.54	1.46
2	F	47	ILE	N-CA	7.55	1.56	1.46
2	F	88	VAL	CA-CB	7.51	1.64	1.54
3	C	229	ALA	N-CA	7.46	1.55	1.46
2	B	43	GLY	CA-C	7.43	1.60	1.52
2	B	110	THR	CA-CB	7.33	1.65	1.53
3	C	207	TRP	N-CA	7.31	1.55	1.46
2	B	123	LEU	C-O	7.30	1.35	1.24
3	C	182	CYS	C-O	7.26	1.32	1.23
3	G	218	SER	N-CA	7.13	1.55	1.46
2	F	131	ALA	CA-C	7.03	1.62	1.52
2	B	56	ALA	CA-C	7.02	1.62	1.52
3	G	215	TRP	C-N	-6.98	1.25	1.33
3	G	180	MET	N-CA	6.98	1.54	1.46
3	C	188	VAL	C-O	6.92	1.33	1.23
3	C	230	ARG	N-CA	6.91	1.55	1.46
1	A	8	PRO	C-N	-6.88	1.23	1.33
3	G	190	SER	CA-C	6.74	1.62	1.53
3	G	192	MET	N-CA	6.72	1.54	1.46
2	B	97	LEU	C-N	6.71	1.43	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	110	THR	CB-OG1	6.68	1.54	1.43
2	F	100	ASN	C-N	-6.68	1.24	1.33
3	G	231	VAL	N-CA	6.66	1.54	1.46
3	C	196	GLY	N-CA	6.66	1.55	1.45
2	B	42	CYS	C-N	6.65	1.40	1.33
2	B	30	GLN	CA-CB	6.62	1.63	1.53
2	B	45	SER	N-CA	6.61	1.54	1.46
2	F	101	ASN	N-CA	6.59	1.56	1.46
2	F	119	SER	C-O	6.58	1.31	1.23
3	C	211	GLY	N-CA	6.57	1.52	1.45
2	F	96	SER	CB-OG	6.57	1.55	1.42
3	G	174	THR	CB-OG1	6.57	1.54	1.43
3	G	204	ASN	N-CA	6.55	1.54	1.46
2	F	64	ASP	C-O	6.55	1.32	1.23
2	F	120	ALA	CA-CB	6.53	1.63	1.53
3	G	243	ALA	N-CA	6.52	1.54	1.46
2	B	54	THR	C-N	6.48	1.42	1.33
3	C	170	LYS	CE-NZ	6.47	1.68	1.49
3	G	241	THR	CA-CB	6.47	1.63	1.53
2	B	144	THR	CB-OG1	6.46	1.54	1.43
3	C	212	ILE	CB-CG1	6.42	1.66	1.53
3	G	230	ARG	N-CA	6.42	1.54	1.46
2	B	84	LYS	CB-CG	6.42	1.71	1.52
3	C	169	LYS	CG-CD	6.41	1.71	1.52
3	C	241	THR	CA-CB	6.41	1.63	1.53
2	B	44	GLY	CA-C	6.41	1.58	1.51
3	G	154	ARG	CD-NE	6.39	1.55	1.46
3	C	219	THR	CA-CB	6.35	1.63	1.53
2	F	56	ALA	CA-C	6.31	1.61	1.52
2	B	106	LEU	CA-C	6.24	1.59	1.52
3	G	239	GLN	N-CA	6.24	1.53	1.46
3	G	219	THR	C-N	-6.19	1.25	1.33
2	F	97	LEU	C-N	-6.18	1.24	1.33
3	G	156	GLN	CA-C	6.17	1.60	1.52
2	B	27	TRP	CA-CB	6.17	1.60	1.53
3	G	154	ARG	N-CA	6.13	1.53	1.45
3	G	221	SER	CA-C	6.12	1.60	1.52
3	C	194	ASP	C-O	6.11	1.32	1.24
3	C	219	THR	CB-OG1	6.10	1.53	1.43
3	C	169	LYS	CB-CG	6.09	1.70	1.52
3	C	181	ILE	C-O	6.08	1.30	1.24
2	F	140	GLY	N-CA	6.05	1.51	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	122	CYS	C-O	6.04	1.31	1.23
3	G	196	GLY	C-O	6.03	1.32	1.24
2	B	118	VAL	CA-C	5.95	1.60	1.52
2	F	100	ASN	CA-C	5.93	1.60	1.52
2	B	94	TYR	CA-C	5.92	1.60	1.52
2	F	22	ALA	N-CA	5.91	1.52	1.45
3	G	208	THR	CB-OG1	5.91	1.53	1.43
3	G	195	SER	C-O	5.91	1.31	1.24
2	F	40	HIS	C-O	5.87	1.31	1.23
3	G	201	CYS	N-CA	5.87	1.53	1.45
2	F	144	THR	CB-CG2	5.85	1.71	1.52
1	A	5	ALA	C-N	5.85	1.40	1.33
2	F	32	SER	C-O	5.83	1.30	1.23
3	G	201	CYS	CA-C	5.83	1.59	1.52
2	B	54	THR	CA-CB	5.79	1.62	1.53
1	E	8	PRO	C-N	-5.79	1.25	1.33
3	G	210	VAL	N-CA	5.78	1.53	1.46
3	G	211	GLY	N-CA	5.77	1.51	1.45
3	C	224	THR	CB-OG1	5.75	1.52	1.43
2	B	65	VAL	C-O	5.73	1.29	1.24
2	B	143	LEU	N-CA	-5.67	1.38	1.46
2	B	90	LYS	C-O	5.66	1.30	1.23
2	B	134	THR	C-O	-5.66	1.17	1.23
2	F	44	GLY	CA-C	5.64	1.57	1.51
3	G	230	ARG	C-N	-5.63	1.26	1.34
3	G	215	TRP	CD2-CE3	-5.62	1.31	1.40
2	F	43	GLY	N-CA	5.62	1.50	1.44
3	C	154	ARG	CA-CB	5.60	1.61	1.53
3	G	181	ILE	CA-CB	5.60	1.62	1.54
3	C	236	ASN	N-CA	5.60	1.53	1.46
3	G	178	ASP	N-CA	5.59	1.52	1.46
3	G	220	CYS	N-CA	5.58	1.54	1.46
1	A	6	ILE	CA-CB	5.58	1.60	1.53
3	G	208	THR	C-N	-5.55	1.25	1.33
3	C	198	PRO	N-CA	-5.55	1.41	1.46
2	B	22	ALA	CA-CB	5.55	1.62	1.53
2	F	53	VAL	C-N	5.54	1.39	1.33
3	G	189	SER	CA-CB	-5.54	1.44	1.53
2	B	47	ILE	N-CA	5.53	1.52	1.46
3	G	215	TRP	CZ2-CH2	5.53	1.47	1.37
3	C	232	THR	N-CA	5.51	1.53	1.46
2	B	100	ASN	N-CA	5.50	1.52	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	53	VAL	N-CA	5.48	1.52	1.46
3	G	230	ARG	CD-NE	5.47	1.53	1.46
3	C	191	CYS	N-CA	5.46	1.52	1.46
3	G	207	TRP	N-CA	5.45	1.53	1.46
2	F	135	THR	CA-CB	5.43	1.59	1.52
2	F	65	VAL	C-O	5.42	1.29	1.24
2	B	143	LEU	CA-CB	5.40	1.62	1.53
3	G	154	ARG	NE-CZ	5.39	1.39	1.33
3	G	211	GLY	C-N	-5.38	1.26	1.33
2	F	91	ASN	C-N	-5.35	1.26	1.33
2	F	27	TRP	C-O	5.34	1.30	1.24
3	C	207	TRP	NE1-CE2	5.34	1.43	1.37
3	C	234	LEU	CA-CB	5.34	1.61	1.54
3	C	195	SER	C-O	5.32	1.30	1.23
2	F	46	LEU	CA-C	5.31	1.59	1.52
3	C	238	VAL	N-CA	5.26	1.52	1.46
3	G	209	LEU	N-CA	5.26	1.53	1.46
3	C	180	MET	C-N	-5.26	1.26	1.33
2	B	102	ASP	C-N	-5.21	1.27	1.33
2	F	66	VAL	C-O	5.20	1.30	1.24
3	G	177	LYS	CA-C	5.19	1.60	1.53
2	B	145	ARG	NE-CZ	5.18	1.38	1.33
2	F	122	CYS	N-CA	5.17	1.52	1.45
2	B	143	LEU	C-N	-5.17	1.25	1.33
2	B	109	SER	N-CA	5.13	1.52	1.46
3	G	219	THR	CB-OG1	5.12	1.51	1.43
3	C	218	SER	CA-CB	5.11	1.62	1.53
3	G	190	SER	CB-OG	5.11	1.52	1.42
3	G	165	ASN	C-O	5.10	1.30	1.24
2	B	54	THR	C-O	5.10	1.30	1.24
3	C	161	PRO	C-O	5.08	1.29	1.23
3	C	235	VAL	N-CA	5.06	1.52	1.46
2	B	20	GLU	C-O	5.05	1.29	1.23
2	F	145	ARG	CB-CG	5.04	1.67	1.52
2	B	98	THR	CA-CB	5.02	1.61	1.53
3	C	153	ASP	C-O	5.02	1.30	1.24
3	G	164	SER	N-CA	5.02	1.52	1.46

All (568) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	39	PHE	CA-CB-CG	19.59	133.39	113.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	167	ASN	OD1-CG-ND2	16.74	139.34	122.60
3	G	153	ASP	CA-CB-CG	-14.66	97.94	112.60
2	B	47	ILE	CA-C-N	13.50	144.89	121.80
2	B	47	ILE	C-N-CA	13.50	144.89	121.80
3	C	224	THR	O-C-N	13.42	134.88	121.72
2	F	48	ASN	CA-CB-CG	13.31	125.91	112.60
2	B	70	GLU	CB-CG-CD	13.00	134.70	112.60
2	B	128	ASP	CA-CB-CG	12.82	125.42	112.60
2	F	35	ASP	CA-CB-CG	-12.72	99.88	112.60
2	B	60	VAL	O-C-N	12.29	135.65	122.63
2	B	48	ASN	CB-CA-C	-12.02	87.61	111.17
2	B	20	GLU	CG-CD-OE2	-11.88	91.06	118.40
2	F	81	GLN	OE1-CD-NE2	11.75	134.35	122.60
2	B	48	ASN	CA-CB-CG	-11.36	101.24	112.60
3	C	190	SER	N-CA-C	-11.32	95.92	110.53
3	C	167	ASN	CA-CB-CG	-11.23	101.36	112.60
2	B	21	GLU	CA-C-O	-11.17	109.71	121.55
2	B	59	GLY	O-C-N	-11.09	113.53	122.51
3	G	156	GLN	OE1-CD-NE2	-10.96	111.64	122.60
2	F	115	SER	CA-C-O	-10.65	109.86	120.94
3	C	219	THR	N-CA-CB	-10.65	94.94	110.80
3	G	162	LEU	CA-C-O	-10.58	109.33	121.81
2	F	130	PHE	CB-CA-C	10.47	127.53	110.78
2	B	110	THR	CB-CA-C	10.44	126.39	110.62
2	B	88	VAL	CA-C-O	-10.19	108.46	121.40
2	B	17	VAL	CA-C-O	-10.12	109.76	120.48
2	F	46	LEU	CA-C-N	-10.01	107.35	121.77
2	F	46	LEU	C-N-CA	-10.01	107.35	121.77
3	C	219	THR	CA-CB-OG1	-10.01	94.59	109.60
3	G	197	GLY	O-C-N	9.99	131.76	121.77
2	F	141	TRP	CA-C-O	-9.98	108.47	120.55
2	B	30	GLN	OE1-CD-NE2	-9.94	112.67	122.60
3	C	156	GLN	OE1-CD-NE2	-9.88	112.72	122.60
3	G	223	SER	CA-CB-OG	-9.77	91.55	111.10
2	F	95	ASN	OD1-CG-ND2	9.77	132.37	122.60
2	F	137	VAL	CA-C-O	9.76	131.50	120.76
3	G	190	SER	N-CA-C	-9.76	97.94	110.53
3	C	208	THR	CA-CB-OG1	-9.74	94.99	109.60
2	B	64	ASP	CA-CB-CG	-9.72	102.88	112.60
2	B	20	GLU	O-C-N	9.63	134.23	123.25
3	C	181	ILE	CA-C-O	9.62	130.56	120.36
2	B	20	GLU	OE1-CD-OE2	9.50	145.70	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	17	VAL	CA-C-O	-9.49	109.99	120.71
2	F	145	ARG	NE-CZ-NH1	-9.48	112.02	121.50
2	F	70	GLU	CA-CB-CG	9.47	133.04	114.10
2	F	80	ILE	O-C-N	9.44	132.27	122.54
2	B	110	THR	CA-CB-CG2	9.38	126.44	110.50
3	G	160	LEU	N-CA-CB	-9.31	101.33	111.10
3	C	157	GLN	O-C-N	9.28	133.77	123.10
3	G	189	SER	CA-C-O	-9.27	110.69	120.89
3	G	170	LYS	CA-C-N	9.24	133.41	120.29
3	G	170	LYS	C-N-CA	9.24	133.41	120.29
3	G	219	THR	CA-CB-OG1	-9.23	95.75	109.60
2	B	116	GLN	OE1-CD-NE2	-9.23	113.37	122.60
2	F	21	GLU	CA-C-O	-9.18	110.88	121.16
2	B	109	SER	CA-C-O	9.15	129.98	119.27
3	C	151	THR	CA-C-O	9.09	128.65	120.19
2	F	119	SER	O-C-N	-9.05	114.24	123.29
3	G	236	ASN	CA-C-N	-9.03	108.17	120.28
3	G	236	ASN	C-N-CA	-9.03	108.17	120.28
3	G	218	SER	CA-C-N	8.97	136.59	122.60
3	G	218	SER	C-N-CA	8.97	136.59	122.60
2	B	45	SER	O-C-N	8.92	134.70	123.28
3	G	177	LYS	CA-C-O	8.90	133.75	121.73
2	F	109	SER	N-CA-C	-8.89	101.56	111.07
2	B	109	SER	CA-CB-OG	-8.89	93.32	111.10
2	B	125	SER	O-C-N	8.85	133.03	123.03
2	F	102	ASP	CA-CB-CG	8.84	121.44	112.60
2	B	134	THR	CA-C-O	-8.82	111.28	121.16
2	F	82	LYS	CA-C-O	-8.78	111.41	120.54
2	F	71	PHE	O-C-N	8.76	133.31	121.92
3	C	232	THR	OG1-CB-CG2	8.74	126.79	109.30
3	C	200	VAL	CA-C-O	8.73	131.41	121.28
2	F	46	LEU	O-C-N	8.70	133.72	123.02
3	C	162	LEU	O-C-N	8.68	132.77	122.96
3	G	228	TYR	CA-C-O	-8.62	111.37	121.11
2	F	129	ASP	CA-CB-CG	-8.62	103.98	112.60
3	G	232	THR	CA-CB-OG1	-8.61	96.69	109.60
2	B	92	SER	CA-C-O	-8.61	108.26	119.10
3	C	182	CYS	N-CA-CB	-8.53	96.45	110.52
2	F	23	VAL	N-CA-C	-8.51	100.61	108.95
3	C	208	THR	OG1-CB-CG2	8.45	126.20	109.30
3	C	170	LYS	N-CA-C	-8.44	102.08	111.28
2	F	34	GLN	CG-CD-NE2	-8.44	103.74	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	180	MET	CA-C-N	8.37	134.62	122.99
3	C	180	MET	C-N-CA	8.37	134.62	122.99
3	C	166	THR	O-C-N	8.35	130.72	122.03
3	C	239	GLN	CB-CG-CD	8.25	126.62	112.60
3	G	174	THR	CA-CB-OG1	-8.24	97.23	109.60
3	G	215	TRP	CA-C-N	8.23	130.55	120.51
3	G	215	TRP	C-N-CA	8.23	130.55	120.51
2	F	79	LYS	CB-CA-C	8.19	121.29	111.22
2	B	17	VAL	O-C-N	8.14	131.73	123.18
3	G	217	SER	CA-C-O	-8.14	112.08	120.96
2	B	116	GLN	CB-CG-CD	8.14	126.43	112.60
3	C	176	ILE	O-C-N	8.13	132.86	122.77
3	G	185	ALA	N-CA-C	-8.08	103.00	112.86
2	B	125	SER	N-CA-CB	8.01	123.06	110.56
3	G	236	ASN	N-CA-C	-8.01	102.63	111.36
3	C	231	VAL	O-C-N	7.99	129.62	121.87
2	B	106	LEU	O-C-N	7.97	132.51	123.27
3	G	191	CYS	CA-C-N	-7.93	109.50	121.31
3	G	191	CYS	C-N-CA	-7.93	109.50	121.31
2	B	37	THR	CA-CB-OG1	-7.92	97.72	109.60
2	F	38	GLY	CA-C-O	-7.92	110.18	118.97
2	F	95	ASN	CA-C-O	-7.91	112.31	120.54
3	G	169	LYS	CA-C-N	7.89	131.07	120.65
3	G	169	LYS	C-N-CA	7.89	131.07	120.65
3	G	229	ALA	CA-C-N	-7.89	110.23	121.99
3	G	229	ALA	C-N-CA	-7.89	110.23	121.99
3	G	215	TRP	CA-C-O	-7.88	112.85	121.28
2	B	93	LYS	CA-C-N	7.86	131.90	120.82
2	B	93	LYS	C-N-CA	7.86	131.90	120.82
3	C	165	ASN	CA-C-N	7.83	130.98	120.65
3	C	165	ASN	C-N-CA	7.83	130.98	120.65
3	G	214	SER	CB-CA-C	7.83	123.20	110.37
3	G	154	ARG	NE-CZ-NH2	-7.82	112.17	119.20
2	F	41	PHE	CA-C-O	7.81	127.44	118.77
2	B	37	THR	N-CA-CB	7.79	121.31	110.01
3	G	190	SER	CA-C-O	-7.77	113.00	121.94
3	C	187	GLY	O-C-N	-7.77	112.60	122.70
2	F	29	TRP	O-C-N	7.75	133.42	122.41
3	G	165	ASN	CA-C-O	-7.74	110.47	119.61
2	F	46	LEU	CA-C-O	-7.74	111.51	120.49
2	B	18	ASN	CA-CB-CG	7.74	120.33	112.60
2	B	23	VAL	N-CA-C	-7.67	102.03	108.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	151	THR	CA-CB-OG1	-7.67	98.09	109.60
2	B	120	ALA	N-CA-C	7.67	122.31	110.42
3	G	159	SER	CA-C-O	-7.63	112.20	121.36
2	F	133	GLY	CA-C-O	-7.58	111.79	119.37
3	G	211	GLY	CA-C-N	7.58	133.19	123.10
3	G	211	GLY	C-N-CA	7.58	133.19	123.10
3	C	169	LYS	CB-CG-CD	-7.58	93.86	111.30
2	F	91	ASN	OD1-CG-ND2	-7.57	115.03	122.60
2	F	34	GLN	OE1-CD-NE2	7.56	130.16	122.60
3	G	181	ILE	CA-CB-CG2	7.56	123.35	110.50
2	B	125	SER	CB-CA-C	-7.55	97.34	109.80
2	F	116	GLN	OE1-CD-NE2	-7.54	115.06	122.60
2	B	134	THR	O-C-N	7.51	132.06	122.89
3	G	230	ARG	CA-C-O	-7.51	112.11	120.60
3	C	216	GLY	CA-C-O	7.50	129.26	121.38
2	F	38	GLY	CA-C-N	-7.49	110.47	122.53
2	F	38	GLY	C-N-CA	-7.49	110.47	122.53
2	F	133	GLY	N-CA-C	-7.49	105.57	114.48
2	F	129	ASP	CA-C-N	-7.43	113.18	122.84
2	F	129	ASP	C-N-CA	-7.43	113.18	122.84
2	B	108	LEU	CA-C-N	-7.42	108.60	121.66
2	B	108	LEU	C-N-CA	-7.42	108.60	121.66
2	B	93	LYS	N-CA-CB	7.41	121.77	110.44
3	C	162	LEU	CA-C-O	-7.40	112.97	121.47
3	G	178	ASP	N-CA-CB	-7.37	97.19	109.72
3	G	153	ASP	OD1-CG-OD2	7.36	140.57	122.90
3	G	186	SER	N-CA-CB	-7.35	100.88	111.54
2	B	101	ASN	CA-C-O	7.34	130.24	121.65
3	C	204	ASN	OD1-CG-ND2	-7.34	115.26	122.60
3	C	224	THR	CA-C-O	-7.34	111.35	120.23
2	B	135	THR	CA-CB-OG1	-7.33	98.60	109.60
2	F	80	ILE	CA-C-O	-7.33	114.00	122.13
3	C	153	ASP	N-CA-C	-7.32	103.01	112.23
3	G	210	VAL	CA-C-N	-7.31	113.82	121.35
3	G	210	VAL	C-N-CA	-7.31	113.82	121.35
3	C	208	THR	O-C-N	7.27	132.68	123.23
2	F	40	HIS	N-CA-C	7.25	121.18	110.30
2	B	54	THR	CA-CB-OG1	-7.25	98.73	109.60
2	B	48	ASN	O-C-N	7.20	130.82	123.26
2	B	121	VAL	CA-C-N	7.19	132.73	122.09
2	B	121	VAL	C-N-CA	7.19	132.73	122.09
3	C	164	SER	CA-CB-OG	-7.17	96.75	111.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	224	THR	CA-CB-CG2	7.17	122.68	110.50
2	B	115	SER	CA-C-O	-7.16	110.27	120.51
3	G	181	ILE	CA-CB-CG1	-7.15	98.25	110.40
3	C	199	LEU	N-CA-C	-7.12	96.67	108.34
2	F	48	ASN	N-CA-C	-7.10	99.50	108.45
3	G	229	ALA	CA-C-O	-7.10	112.83	120.92
2	F	137	VAL	CA-CB-CG2	7.08	122.44	110.40
3	C	157	GLN	CA-C-O	-7.08	113.88	121.45
3	C	191	CYS	O-C-N	-7.07	115.83	123.26
2	F	19	GLY	O-C-N	7.07	129.35	122.92
2	F	105	LEU	O-C-N	7.07	132.42	123.23
2	B	61	THR	CA-CB-OG1	-7.06	99.00	109.60
2	B	125	SER	CA-CB-OG	-7.06	96.98	111.10
2	F	37	THR	N-CA-C	-7.05	104.55	113.01
3	G	236	ASN	N-CA-CB	7.05	120.59	110.16
3	G	170	LYS	N-CA-C	-7.02	103.32	110.97
2	F	100	ASN	O-C-N	7.01	130.88	122.96
3	C	181	ILE	O-C-N	-7.00	115.64	123.20
2	F	110	THR	N-CA-CB	7.00	122.90	110.80
3	G	239	GLN	CB-CG-CD	6.98	124.47	112.60
2	F	38	GLY	N-CA-C	6.97	125.04	115.00
3	G	176	ILE	CB-CG1-CD1	6.96	128.42	113.80
2	F	130	PHE	CA-CB-CG	6.96	120.75	113.80
3	G	240	GLN	CB-CG-CD	6.94	124.41	112.60
2	B	138	THR	CA-C-O	6.93	128.63	120.66
2	B	20	GLU	CB-CG-CD	-6.93	100.81	112.60
2	B	26	SER	N-CA-C	6.93	121.19	112.87
3	G	178	ASP	CB-CA-C	6.92	122.32	110.84
3	G	219	THR	N-CA-CB	-6.92	100.01	110.73
3	C	203	LYS	CA-C-O	-6.90	111.78	120.20
3	G	199	LEU	CA-C-O	-6.90	112.92	120.30
3	G	179	ALA	O-C-N	6.88	131.27	122.06
3	C	236	ASN	CB-CG-ND2	6.87	126.70	116.40
2	B	112	ALA	CA-C-N	-6.85	113.00	123.14
2	B	112	ALA	C-N-CA	-6.85	113.00	123.14
2	B	38	GLY	CA-C-N	-6.85	110.64	121.87
2	B	38	GLY	C-N-CA	-6.85	110.64	121.87
2	F	93	LYS	CA-C-O	6.84	127.35	119.35
2	B	30	GLN	O-C-N	-6.83	113.92	123.01
2	B	50	ASN	OD1-CG-ND2	6.82	129.42	122.60
2	F	110	THR	O-C-N	6.80	131.27	123.31
3	G	240	GLN	CG-CD-NE2	6.79	126.59	116.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	236	ASN	OD1-CG-ND2	-6.79	115.81	122.60
3	C	239	GLN	CA-C-N	6.79	129.27	120.44
3	C	239	GLN	C-N-CA	6.79	129.27	120.44
2	F	145	ARG	CD-NE-CZ	-6.79	114.89	124.40
3	C	219	THR	OG1-CB-CG2	6.79	122.87	109.30
2	F	131	ALA	CA-C-O	6.79	128.96	121.56
2	B	19	GLY	CA-C-O	-6.78	114.80	122.33
3	G	214	SER	N-CA-CB	-6.77	98.66	110.44
3	G	207	TRP	CA-C-O	-6.77	113.33	121.05
3	G	232	THR	OG1-CB-CG2	6.77	122.83	109.30
3	G	244	ALA	N-CA-C	6.75	121.35	113.18
2	B	110	THR	CA-CB-OG1	-6.74	99.50	109.60
2	F	137	VAL	O-C-N	-6.73	115.58	123.05
3	G	224	THR	CA-CB-OG1	-6.73	99.51	109.60
3	G	233	ALA	CA-C-N	-6.72	111.69	121.98
3	G	233	ALA	C-N-CA	-6.72	111.69	121.98
2	B	71	PHE	CA-C-O	-6.72	111.95	119.81
2	B	124	PRO	CB-CA-C	-6.71	100.49	111.56
3	G	152	PRO	CB-CA-C	-6.71	101.04	110.63
3	G	218	SER	CA-CB-OG	-6.70	97.70	111.10
2	F	101	ASN	N-CA-C	-6.68	102.97	111.92
2	B	62	THR	CB-CA-C	6.66	123.67	110.42
3	C	222	THR	CA-C-N	6.66	132.99	122.60
3	C	222	THR	C-N-CA	6.66	132.99	122.60
3	G	198	PRO	CB-CA-C	-6.66	99.76	110.21
3	C	228	TYR	CA-C-O	-6.65	113.51	120.70
2	F	70	GLU	N-CA-CB	-6.65	99.46	110.23
2	B	123	LEU	N-CA-CB	-6.64	99.16	110.11
3	G	161	PRO	CB-CA-C	-6.63	101.15	110.63
3	G	223	SER	CA-C-O	-6.62	111.36	119.18
3	G	240	GLN	OE1-CD-NE2	-6.60	116.00	122.60
3	C	202	LYS	N-CA-CB	6.54	120.96	110.16
2	B	58	CYS	N-CA-C	-6.52	105.19	113.01
2	B	111	ALA	O-C-N	6.50	130.80	122.81
2	B	119	SER	O-C-N	6.49	129.78	123.29
2	F	93	LYS	CD-CE-NZ	-6.47	91.20	111.90
2	B	35	ASP	CA-CB-CG	6.46	119.06	112.60
2	B	116	GLN	CG-CD-OE1	6.46	133.72	120.80
2	B	118	VAL	CA-C-O	6.46	126.79	120.27
2	F	115	SER	N-CA-CB	-6.45	101.48	111.35
2	B	60	VAL	CA-C-O	-6.45	114.27	121.36
2	B	114	PHE	O-C-N	6.44	130.74	122.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	145	ARG	N-CA-CB	6.44	122.38	110.99
3	C	180	MET	O-C-N	-6.42	115.34	123.24
2	B	63	SER	CA-C-N	-6.42	110.12	121.29
2	B	63	SER	C-N-CA	-6.42	110.12	121.29
3	G	186	SER	N-CA-C	6.42	120.42	111.56
3	G	225	PRO	CA-C-O	-6.41	113.62	121.31
3	G	162	LEU	O-C-N	6.40	130.15	122.85
3	G	231	VAL	O-C-N	6.39	128.15	121.89
3	C	185	ALA	N-CA-CB	-6.39	101.56	113.89
3	G	228	TYR	N-CA-CB	-6.38	100.16	111.08
3	G	223	SER	O-C-N	6.37	129.72	122.20
2	B	30	GLN	CG-CD-NE2	6.36	125.95	116.40
2	B	114	PHE	CA-C-O	-6.35	114.81	121.55
2	B	84	LYS	CA-C-O	-6.35	114.17	121.47
3	C	221	SER	CA-C-O	-6.35	114.16	121.15
2	B	110	THR	N-CA-CB	-6.35	101.19	110.84
2	F	82	LYS	CA-C-N	-6.34	113.74	122.93
2	F	82	LYS	C-N-CA	-6.34	113.74	122.93
3	C	245	ASN	N-CA-C	6.32	128.69	111.00
2	F	54	THR	CA-C-O	-6.31	114.64	121.14
3	C	167	ASN	CB-CG-OD1	-6.31	108.18	120.80
3	G	154	ARG	O-C-N	-6.30	116.00	123.06
3	C	153	ASP	CA-C-N	6.29	131.40	122.72
3	C	153	ASP	C-N-CA	6.29	131.40	122.72
3	C	215	TRP	CG-CD2-CE3	-6.28	127.62	133.90
3	G	179	ALA	CA-C-O	-6.28	111.39	119.80
3	G	219	THR	CA-CB-CG2	6.28	121.17	110.50
3	C	200	VAL	O-C-N	-6.27	116.29	123.00
3	C	211	GLY	O-C-N	-6.27	117.74	123.57
3	C	156	GLN	CA-C-O	-6.26	113.98	121.56
1	E	4	PRO	CA-C-N	6.26	129.82	120.31
1	E	4	PRO	C-N-CA	6.26	129.82	120.31
2	F	36	LYS	CA-CB-CG	-6.26	101.58	114.10
2	F	63	SER	N-CA-C	-6.26	105.47	113.23
3	C	191	CYS	CA-C-O	6.26	128.01	121.38
2	B	16	ILE	CA-C-N	-6.26	115.43	123.19
2	B	16	ILE	C-N-CA	-6.26	115.43	123.19
3	C	168	CYS	O-C-N	6.25	129.96	122.27
2	B	104	THR	O-C-N	6.24	130.88	123.33
1	E	7	GLN	N-CA-C	6.24	118.65	109.42
2	B	125	SER	CA-C-O	-6.23	114.06	121.66
3	C	158	ALA	O-C-N	6.23	130.37	123.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	21	GLU	O-C-N	6.22	130.47	122.81
1	E	2	GLY	CA-C-O	-6.22	111.49	119.58
3	C	150	ASN	CB-CG-ND2	-6.22	107.07	116.40
2	F	32	SER	O-C-N	-6.22	115.77	123.36
3	C	171	TYR	CA-C-N	6.22	132.80	122.54
3	C	171	TYR	C-N-CA	6.22	132.80	122.54
3	G	179	ALA	CA-C-N	-6.21	112.66	122.73
3	G	179	ALA	C-N-CA	-6.21	112.66	122.73
3	C	150	ASN	OD1-CG-ND2	6.21	128.81	122.60
2	B	120	ALA	O-C-N	6.20	130.03	123.03
3	C	170	LYS	N-CA-CB	6.19	119.22	110.12
2	F	98	THR	CA-CB-OG1	-6.18	100.33	109.60
2	B	83	LEU	N-CA-CB	-6.18	100.35	110.43
2	F	109	SER	O-C-N	6.18	128.44	122.07
2	B	54	THR	O-C-N	6.18	131.00	122.78
2	F	95	ASN	O-C-N	6.18	130.40	123.05
3	G	215	TRP	N-CA-C	-6.17	98.75	108.14
2	B	39	PHE	CA-C-N	6.17	133.32	121.54
2	B	39	PHE	C-N-CA	6.17	133.32	121.54
2	F	31	VAL	O-C-N	6.15	129.76	123.00
2	B	24	PRO	CA-C-N	-6.14	112.91	122.86
2	B	24	PRO	C-N-CA	-6.14	112.91	122.86
3	C	208	THR	CA-C-O	-6.14	114.06	120.70
2	F	95	ASN	CA-CB-CG	-6.14	106.46	112.60
2	F	131	ALA	CB-CA-C	-6.13	98.26	109.54
3	G	232	THR	CB-CA-C	6.13	120.61	110.81
3	G	195	SER	O-C-N	6.12	130.74	122.59
2	B	119	SER	CA-C-O	-6.11	114.74	121.28
3	G	198	PRO	N-CA-C	6.10	123.24	112.01
3	G	173	GLY	CA-C-O	6.09	131.17	120.57
2	F	23	VAL	CA-C-O	6.09	125.37	119.71
3	G	231	VAL	N-CA-C	6.08	117.55	110.62
3	C	151	THR	CB-CA-C	6.07	117.11	108.68
3	G	229	ALA	O-C-N	6.07	130.47	122.95
3	G	217	SER	O-C-N	6.06	130.33	123.06
2	B	45	SER	CA-C-N	-6.06	112.47	120.95
2	B	45	SER	C-N-CA	-6.06	112.47	120.95
2	B	145	ARG	NH1-CZ-NH2	6.06	127.17	119.30
2	B	27	TRP	CA-C-O	6.05	127.47	121.29
3	G	165	ASN	N-CA-CB	6.05	121.07	110.18
3	G	210	VAL	CA-C-O	6.03	128.32	120.78
3	C	218	SER	CA-C-N	6.01	131.67	122.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	218	SER	C-N-CA	6.01	131.67	122.29
3	G	181	ILE	O-C-N	6.01	129.53	123.10
3	G	241	THR	N-CA-CB	6.00	118.70	110.01
3	G	178	ASP	CA-CB-CG	-5.99	106.61	112.60
3	G	235	VAL	O-C-N	-5.99	115.23	122.06
3	G	169	LYS	N-CA-CB	5.99	120.33	110.39
3	G	236	ASN	O-C-N	5.99	128.97	122.15
3	C	181	ILE	CB-CG1-CD1	-5.98	101.23	113.80
3	C	171	TYR	O-C-N	-5.98	114.22	122.30
3	C	196	GLY	CA-C-O	-5.98	112.70	119.04
2	F	101	ASN	CA-CB-CG	-5.98	106.62	112.60
3	G	229	ALA	CB-CA-C	-5.98	100.58	109.90
3	C	191	CYS	N-CA-CB	-5.97	102.26	111.46
3	G	190	SER	O-C-N	5.97	129.99	122.65
2	B	95	ASN	CA-CB-CG	-5.96	106.64	112.60
2	F	134	THR	CA-C-O	-5.96	114.47	120.96
2	B	123	LEU	CB-CA-C	5.95	116.95	108.68
2	B	132	ALA	CB-CA-C	5.93	119.16	109.90
3	G	167	ASN	CA-CB-CG	5.93	118.53	112.60
2	B	89	PHE	CA-C-N	-5.90	113.35	122.09
2	B	89	PHE	C-N-CA	-5.90	113.35	122.09
2	F	120	ALA	N-CA-C	5.90	119.67	110.17
2	F	133	GLY	O-C-N	5.90	128.83	122.22
2	F	56	ALA	O-C-N	5.89	129.52	122.27
3	C	232	THR	CA-CB-OG1	-5.88	100.77	109.60
2	F	29	TRP	CA-C-O	-5.88	112.19	119.18
3	G	159	SER	O-C-N	5.87	129.63	123.06
3	G	225	PRO	CB-CA-C	-5.86	103.42	111.21
3	C	153	ASP	CB-CA-C	5.85	122.32	110.38
3	G	226	GLY	N-CA-C	-5.85	104.75	112.82
2	F	101	ASN	CA-C-O	-5.84	113.74	120.98
2	B	83	LEU	N-CA-C	5.83	118.74	109.24
3	C	218	SER	CB-CA-C	-5.82	97.47	110.21
2	F	57	HIS	CB-CG-ND1	5.82	131.43	122.70
2	F	91	ASN	CB-CG-ND2	5.81	125.11	116.40
3	C	154	ARG	N-CA-C	5.80	118.70	109.24
3	G	167	ASN	CA-C-O	5.80	126.64	119.79
1	A	4	PRO	CA-C-O	-5.79	114.85	121.56
2	B	41	PHE	N-CA-CB	5.78	118.58	110.90
2	B	141	TRP	CA-C-O	-5.77	112.92	119.78
2	F	28	PRO	CA-C-O	-5.76	110.91	118.86
2	F	125	SER	N-CA-C	-5.76	100.79	109.95

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	105	LEU	CA-C-O	-5.76	114.41	120.80
3	G	153	ASP	CB-CG-OD2	-5.75	105.18	118.40
3	C	154	ARG	NE-CZ-NH2	-5.73	114.04	119.20
2	F	83	LEU	CA-C-N	5.72	130.89	121.39
2	F	83	LEU	C-N-CA	5.72	130.89	121.39
2	B	63	SER	CA-CB-OG	-5.71	99.69	111.10
2	B	131	ALA	CA-C-O	5.70	128.02	121.47
2	B	117	THR	CA-C-N	5.69	131.06	122.98
2	B	117	THR	C-N-CA	5.69	131.06	122.98
3	C	210	VAL	N-CA-CB	-5.68	101.38	112.75
2	F	96	SER	CA-C-O	-5.68	111.66	119.05
3	G	230	ARG	CA-C-N	5.68	128.54	120.53
3	G	230	ARG	C-N-CA	5.68	128.54	120.53
2	B	21	GLU	OE1-CD-OE2	5.67	136.52	122.90
2	F	124	PRO	CB-CA-C	-5.67	101.55	110.96
2	B	55	ALA	N-CA-CB	5.66	119.52	110.46
2	F	20	GLU	CG-CD-OE2	-5.66	105.39	118.40
2	B	132	ALA	CA-C-O	5.66	127.37	120.92
2	F	58	CYS	CA-C-O	-5.66	112.65	119.49
2	B	31	VAL	O-C-N	5.65	129.02	122.97
2	B	113	SER	CB-CA-C	5.64	120.93	111.22
3	C	198	PRO	CB-CA-C	-5.64	101.99	110.17
3	C	199	LEU	CA-C-O	-5.64	114.26	120.24
2	B	71	PHE	CA-C-N	5.64	130.27	122.77
2	B	71	PHE	C-N-CA	5.64	130.27	122.77
3	G	154	ARG	CD-NE-CZ	-5.64	116.51	124.40
2	F	90	LYS	CA-CB-CG	-5.62	102.85	114.10
2	B	90	LYS	CA-C-O	-5.62	114.46	120.92
3	G	203	LYS	O-C-N	5.61	130.44	123.14
2	F	73	GLN	CB-CG-CD	-5.61	103.06	112.60
2	B	41	PHE	CA-C-O	5.61	124.99	118.77
2	B	54	THR	CA-C-N	-5.60	110.81	122.07
2	B	54	THR	C-N-CA	-5.60	110.81	122.07
2	F	30	GLN	OE1-CD-NE2	-5.59	117.00	122.60
2	F	20	GLU	CG-CD-OE1	5.59	131.26	118.40
3	G	235	VAL	N-CA-CB	-5.59	99.71	110.78
3	C	236	ASN	CA-CB-CG	-5.58	107.02	112.60
2	F	129	ASP	CB-CA-C	-5.58	101.75	110.74
3	G	174	THR	N-CA-C	5.58	119.71	113.01
3	G	206	ALA	O-C-N	-5.58	116.38	123.24
2	F	19	GLY	CA-C-O	-5.57	115.63	122.03
3	G	183	ALA	CA-C-O	-5.57	115.28	121.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	85	ILE	CA-CB-CG2	5.56	119.95	110.50
3	C	223	SER	N-CA-CB	5.56	119.35	110.73
3	C	240	GLN	CA-C-O	-5.56	114.98	120.82
2	F	91	ASN	CA-C-N	5.55	131.31	120.99
2	F	91	ASN	C-N-CA	5.55	131.31	120.99
2	B	112	ALA	O-C-N	5.55	129.41	122.86
2	B	137	VAL	CA-CB-CG2	5.55	119.83	110.40
2	F	142	GLY	O-C-N	-5.54	115.52	122.84
2	B	141	TRP	N-CA-CB	-5.54	102.45	110.70
3	G	219	THR	N-CA-C	5.52	120.01	112.88
3	C	202	LYS	CB-CA-C	-5.52	100.75	109.80
3	C	165	ASN	CA-CB-CG	-5.52	107.08	112.60
2	B	88	VAL	N-CA-C	-5.52	100.50	108.89
3	C	222	THR	CA-CB-OG1	5.52	117.88	109.60
2	B	130	PHE	N-CA-C	-5.51	98.21	108.02
2	B	130	PHE	CA-C-O	-5.50	114.39	120.33
2	B	105	LEU	O-C-N	5.50	129.62	123.19
2	F	30	GLN	O-C-N	-5.50	116.14	122.95
3	G	159	SER	N-CA-C	-5.50	101.58	110.32
2	B	66	VAL	CA-C-O	-5.49	114.66	120.48
2	B	138	THR	CA-CB-CG2	-5.48	101.18	110.50
2	F	64	ASP	CA-C-N	-5.48	113.98	122.69
2	F	64	ASP	C-N-CA	-5.48	113.98	122.69
3	C	200	VAL	CA-CB-CG1	5.47	119.70	110.40
3	G	212	ILE	CA-CB-CG1	5.47	119.70	110.40
3	G	199	LEU	CB-CA-C	5.46	119.22	110.16
3	G	149	ALA	O-C-N	-5.46	114.27	123.00
2	F	102	ASP	O-C-N	-5.45	115.34	122.59
2	B	18	ASN	OD1-CG-ND2	5.45	128.05	122.60
3	G	178	ASP	OD1-CG-OD2	-5.44	109.85	122.90
2	B	132	ALA	CA-C-N	-5.44	114.05	122.69
2	B	132	ALA	C-N-CA	-5.44	114.05	122.69
2	F	23	VAL	N-CA-CB	5.43	115.13	110.08
3	C	170	LYS	CB-CG-CD	5.41	123.74	111.30
3	G	169	LYS	O-C-N	5.40	129.67	122.43
2	B	100	ASN	CA-CB-CG	-5.40	107.20	112.60
2	F	48	ASN	CB-CG-ND2	5.40	124.49	116.40
3	C	182	CYS	CA-CB-SG	-5.39	102.00	114.40
3	G	245	ASN	CA-CB-CG	5.39	117.99	112.60
3	C	194	ASP	CA-C-N	5.38	128.49	120.90
3	C	194	ASP	C-N-CA	5.38	128.49	120.90
3	G	194	ASP	CA-CB-CG	-5.38	107.22	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	104	THR	CA-CB-CG2	5.38	119.64	110.50
2	B	111	ALA	N-CA-CB	5.38	117.94	110.04
2	B	114	PHE	N-CA-CB	5.38	117.94	110.04
3	G	186	SER	CA-CB-OG	-5.37	100.36	111.10
2	F	28	PRO	N-CA-CB	5.37	108.46	103.41
3	C	195	SER	CA-C-N	-5.37	113.02	122.09
3	C	195	SER	C-N-CA	-5.37	113.02	122.09
2	F	105	LEU	CA-C-O	-5.34	114.93	120.70
3	G	218	SER	O-C-N	-5.34	115.44	122.39
2	F	29	TRP	N-CA-C	-5.33	106.77	113.28
3	G	207	TRP	CA-C-N	-5.33	114.31	122.62
3	G	207	TRP	C-N-CA	-5.33	114.31	122.62
2	F	44	GLY	CA-C-O	-5.33	115.86	121.56
3	C	221	SER	CB-CA-C	5.33	118.27	109.70
3	C	231	VAL	CA-C-O	-5.32	115.42	120.95
2	B	95	ASN	CB-CA-C	5.32	119.45	110.79
3	G	224	THR	CA-C-N	-5.32	114.44	119.76
3	G	224	THR	C-N-CA	-5.32	114.44	119.76
2	F	104	THR	CA-C-N	-5.31	114.97	122.94
2	F	104	THR	C-N-CA	-5.31	114.97	122.94
2	B	136	CYS	CB-CA-C	5.31	121.62	111.48
2	F	119	SER	N-CA-CB	-5.31	102.65	111.57
2	B	26	SER	CA-C-N	5.30	128.48	122.59
2	B	26	SER	C-N-CA	5.30	128.48	122.59
3	C	183	ALA	CA-C-O	-5.30	115.41	121.40
3	C	245	ASN	CA-CB-CG	-5.30	107.30	112.60
3	C	190	SER	CA-CB-OG	-5.30	100.50	111.10
3	G	207	TRP	O-C-N	5.29	129.26	123.01
2	F	119	SER	CB-CA-C	5.29	120.47	110.95
2	F	20	GLU	CA-CB-CG	5.29	124.67	114.10
3	C	160	LEU	N-CA-CB	-5.28	103.43	110.77
3	C	160	LEU	N-CA-C	5.28	114.92	108.11
3	G	208	THR	CA-CB-OG1	-5.27	101.70	109.60
2	B	88	VAL	O-C-N	5.26	128.45	122.98
2	B	20	GLU	CA-C-O	-5.25	115.66	121.33
3	C	153	ASP	CA-C-O	5.25	125.99	119.79
2	B	91	ASN	CB-CG-OD1	-5.25	110.30	120.80
2	B	40	HIS	O-C-N	5.24	129.56	122.59
2	B	27	TRP	CE3-CZ3-CH2	5.24	127.91	121.10
3	G	232	THR	N-CA-CB	-5.23	102.15	109.94
3	C	201	CYS	CA-C-N	5.22	129.55	122.19
3	C	201	CYS	C-N-CA	5.22	129.55	122.19

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	234	LEU	N-CA-CB	-5.22	104.09	110.98
2	F	92	SER	CA-C-O	-5.20	112.54	119.10
2	B	103	ILE	CA-C-O	-5.20	115.83	121.19
3	G	202	LYS	CA-C-N	-5.20	114.90	122.44
3	G	202	LYS	C-N-CA	-5.20	114.90	122.44
2	B	81	GLN	CB-CG-CD	-5.20	103.77	112.60
2	F	27	TRP	N-CA-C	-5.19	99.93	108.75
2	B	81	GLN	N-CA-C	5.19	116.78	107.80
2	F	33	LEU	O-C-N	5.19	129.26	123.19
2	B	128	ASP	N-CA-CB	5.19	117.78	110.36
2	F	94	TYR	CA-CB-CG	-5.19	104.56	113.90
2	B	104	THR	CA-CB-OG1	-5.18	101.83	109.60
2	F	94	TYR	CA-C-N	-5.18	116.11	122.84
2	F	94	TYR	C-N-CA	-5.18	116.11	122.84
2	F	87	LYS	CA-C-O	-5.17	114.18	120.54
3	C	154	ARG	CA-C-O	5.17	126.06	120.43
2	F	61	THR	CA-C-O	-5.16	115.75	121.33
2	F	29	TRP	CB-CG-CD1	-5.16	119.16	126.90
1	E	7	GLN	CG-CD-NE2	5.16	124.14	116.40
3	G	221	SER	CB-CA-C	5.15	117.94	109.90
2	B	141	TRP	O-C-N	5.15	128.69	122.35
2	B	140	GLY	CA-C-O	5.15	127.12	121.87
2	F	144	THR	OG1-CB-CG2	5.14	119.58	109.30
3	C	201	CYS	N-CA-C	-5.13	101.39	109.50
3	C	188	VAL	CA-C-O	-5.12	116.32	121.49
2	F	40	HIS	CB-CG-CD2	-5.12	124.54	131.20
3	C	154	ARG	NH1-CZ-NH2	5.11	125.94	119.30
3	C	240	GLN	N-CA-CB	5.10	117.41	110.01
2	B	138	THR	OG1-CB-CG2	5.10	119.50	109.30
2	B	145	ARG	CD-NE-CZ	-5.09	117.27	124.40
3	G	199	LEU	N-CA-C	-5.09	100.11	108.41
2	F	105	LEU	CA-C-N	-5.09	115.82	123.00
2	F	105	LEU	C-N-CA	-5.09	115.82	123.00
2	B	39	PHE	CB-CA-C	5.09	122.64	111.09
3	G	230	ARG	CD-NE-CZ	-5.09	117.28	124.40
3	C	235	VAL	CB-CA-C	5.08	118.48	111.97
3	C	192	MET	O-C-N	5.08	129.19	122.89
2	B	86	ALA	O-C-N	5.08	129.74	122.28
3	G	236	ASN	OD1-CG-ND2	5.07	127.67	122.60
3	G	237	TRP	O-C-N	-5.07	116.75	122.12
3	C	159	SER	CA-CB-OG	-5.07	100.97	111.10
3	G	186	SER	CA-C-O	-5.06	114.56	120.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	101	ASN	O-C-N	5.05	129.14	122.47
2	F	61	THR	O-C-N	5.05	129.01	123.25
3	C	161	PRO	CB-CA-C	-5.05	102.28	110.21
3	G	243	ALA	N-CA-CB	5.04	117.62	110.06
2	F	100	ASN	CA-C-O	-5.04	115.68	121.47
3	C	155	LEU	N-CA-CB	5.03	117.28	109.48
3	G	231	VAL	CA-CB-CG1	5.03	118.95	110.40
3	G	181	ILE	CA-C-O	-5.03	115.04	120.67
3	G	231	VAL	CA-C-N	5.02	127.32	120.54
3	G	231	VAL	C-N-CA	5.02	127.32	120.54
2	F	107	LYS	CA-C-N	5.02	128.45	121.02
2	F	107	LYS	C-N-CA	5.02	128.45	121.02
3	G	150	ASN	OD1-CG-ND2	5.02	127.62	122.60
2	B	31	VAL	CA-CB-CG2	5.01	118.92	110.40
3	G	206	ALA	CA-C-O	5.01	126.98	121.11
2	B	128	ASP	OD1-CG-OD2	-5.01	110.87	122.90
2	B	92	SER	N-CA-CB	5.01	119.44	110.32
3	G	169	LYS	CA-CB-CG	-5.01	104.08	114.10
3	G	210	VAL	CA-CB-CG1	5.01	118.91	110.40
2	B	134	THR	CA-C-N	5.00	129.45	121.99
2	B	134	THR	C-N-CA	5.00	129.45	121.99

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
1	E	54	0	56	9	4
2	B	980	0	951	105	7
2	F	980	0	951	97	0
3	C	702	0	698	73	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	702	0	698	54	0
4	C	11	0	11	2	0
4	G	11	0	11	1	0
5	A	6	0	0	4	0
5	B	43	0	0	29	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	3432	307	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 45.

All (307) 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:CD	2:F:93:LYS:CE	1.76	1.61
3:C:170:LYS:CE	3:C:170:LYS:NZ	1.68	1.56
1:E:7:GLN:H	1:E:7:GLN:NE2	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
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
1:A:1:CYS:N	5:A:671:HOH:O	1.94	1.00
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
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
2:B:27:TRP:C	5:B:637:HOH:O	2.10	0.95
3:C:195:SER:HB2	4:C:1:PBA:O1	1.67	0.94

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:9:VAL:N	5:E:584:HOH:O	1.99	0.94
2:F:97:LEU:C	5:F:560:HOH:O	2.09	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
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:68:ALA:HA	2:B:70:GLU:OE1	1.71	0.91
1:E:7:GLN:NE2	1:E:7:GLN:N	2.17	0.91
2:B:29:TRP:N	5:B:637:HOH:O	1.74	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:HD3	2:B:36:LYS:O	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:CD	2:F:93:LYS:NZ	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
1:E:7:GLN:H	1:E:7:GLN:CD	1.89	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:91:ASN:HD22	2:F:91:ASN:C	1.99	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:CE	2:F:93:LYS:CG	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
1:E:7:GLN:N	1:E:7:GLN:CD	2.47	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:HG3	3:C:154:ARG:HH11	1.60	0.66
2:F:40:HIS:CE1	2:F:42:CYS:O	2.49	0.66
2:B:98:THR:HG22	2:B:100:ASN:H	1.59	0.66
2:B:123:LEU:HD23	3:C:239:GLN:HE22	1.59	0.66
2:B:128:ASP:OD2	5:B:523:HOH:O	2.14	0.66
2:B:28:PRO:N	5:B:637:HOH:O	2.24	0.66
2:B:50:ASN:OD1	2:B:107:LYS:NZ	2.29	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
2:B:36:LYS:HD3	2:B:36:LYS:C	2.19	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:17:VAL:HG22	5:B:695:HOH:O	1.98	0.63
3:C:154:ARG:HG3	3:C:154:ARG:NH1	2.15	0.62
2:F:86:ALA:HB2	2:F:109:SER:HA	1.81	0.61
2:B:103:ILE:HG23	2:B:103:ILE:O	1.98	0.61
2:F:72:ASP:OD2	3:G:153:ASP:HB3	2.00	0.61
2:F:87:LYS:HG2	2:F:89:PHE:CE1	2.36	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:98:THR:CG2	5:B:625:HOH:O	2.33	0.61
2:B:107:LYS:HD3	5:B:643:HOH:O	2.01	0.61
2:F:74:GLY:O	2:F:75:SER:C	2.44	0.61
2:B:21:GLU:CD	3:C:154:ARG:HD2	2.26	0.60
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:C:233:ALA:C	5:C:503:HOH:O	2.45	0.59
3:G:178:ASP:N	3:G:178:ASP:OD2	2.34	0.59
2:B:26:SER:C	2:B:28:PRO:HD3	2.27	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
2:B:103:ILE:HD13	2:B:103:ILE:C	2.25	0.57
3:C:160:LEU:HD13	5:C:691:HOH:O	2.04	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
1:A:1:CYS:C	2:B:122:CYS:SG	2.88	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
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
3:C:184:GLY:O	3:C:185:ALA:CB	2.54	0.56
2:B:28:PRO:HB3	2:B:117:THR:O	2.06	0.55
2:B:29:TRP:CG	5:B:637:HOH:O	2.56	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:170:LYS:NZ	3:C:170:LYS:CD	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
2:B:61:THR:C	2:B:63:SER:N	2.65	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:B:103:ILE:CD1	2:B:103:ILE:C	2.81	0.54
2:F:139:THR:HA	3:G:156:GLN:O	2.08	0.54
2:F:72:ASP:C	2:F:74:GLY:H	2.15	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
3:C:164:SER:HB2	3:C:167:ASN:OD1	2.09	0.52
2:F:36:LYS:HZ2	2:F:36:LYS:HA	1.75	0.52
3:G:191:CYS:O	3:G:192:MET:C	2.53	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
3:C:191:CYS:O	3:C:192:MET:C	2.54	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
2:B:61:THR:C	2:B:63:SER:H	2.17	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:160:LEU:HD12	3:C:183:ALA:HB1	1.92	0.51
3:C:167:ASN:OD1	3:C:167:ASN:N	2.43	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:G:190:SER:C	5:G:629:HOH:O	2.52	0.50
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:7:GLN:O	1:E:8:PRO:C	2.50	0.50
2:B:48:ASN:N	2:B:48:ASN:HD22	2.02	0.50
2:B:47:ILE:C	2:B:48:ASN:ND2	2.70	0.49
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
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
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
2:F:82:LYS:O	2:F:84:LYS:NZ	2.44	0.47
3:G:151:THR:O	3:G:151:THR:OG1	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
2:F:91:ASN:ND2	2:F:91:ASN:C	2.65	0.47
2:B:31:VAL:HG22	2:B:44:GLY:C	2.40	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:99:ILE:CG1	5:F:560:HOH:O	2.57	0.46
2:F:60:VAL:HG12	2:F:61:THR:N	2.30	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
1:E:7:GLN:C	1:E:8:PRO:O	2.55	0.46
2:F:36:LYS:C	2:F:38:GLY:N	2.71	0.46
2:F:72:ASP:C	2:F:74:GLY:N	2.73	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:TRP:N	2:F:28:PRO:HD3	2.31	0.45
2:F:47:ILE:O	5:F:538:HOH:O	2.20	0.45
2:B:90:LYS:H	2:B:90:LYS:CD	2.29	0.45
2:B:131:ALA:O	2:B:134:THR:OG1	2.33	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
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:O	2:B:36:LYS:CD	2.55	0.44
2:F:84:LYS:HE3	2:F:84:LYS:H	1.82	0.44
2:F:84:LYS:N	2:F:84:LYS:CE	2.81	0.44
2:B:39:PHE:CE2	2:B:40:HIS:HB3	2.52	0.44
3:C:232:THR:HG22	3:C:233:ALA:N	2.31	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:70:GLU:CD	2:B:70:GLU:H	2.26	0.43
2:F:26:SER:C	2:F:28:PRO:HD3	2.43	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:28:PRO:HB3	2:B:117:THR:C	2.44	0.43
2:B:60:VAL:CG1	2:B:61:THR:N	2.81	0.43
2:B:105:LEU:HD12	3:C:241:THR:HG21	2.01	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:F:135:THR:O	2:F:135:THR:HG22	2.18	0.42
2:B:47:ILE:C	2:B:48:ASN:HD22	2.27	0.42
3:C:160:LEU:N	3:C:160:LEU:CD2	2.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:108:LEU:O	2:F:109:SER:C	2.61	0.42
2:B:103:ILE:HG12	3:C:212:ILE:HD13	2.01	0.42
2:B:126:ALA:HA	3:C:232:THR:O	2.19	0.42
2:B:145:ARG:CD	3:C:150:ASN:CG	2.92	0.42
3:G:209:LEU:HG	3:G:231:VAL:HG21	2.02	0.42
2:F:53:VAL:HG22	2:F:105:LEU:CD2	2.48	0.42
3:C:235:VAL:O	3:C:236:ASN:C	2.62	0.42
2:F:36:LYS:HA	2:F:36:LYS:NZ	2.35	0.41
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:HG21	3:C:181:ILE:HD12	1.44	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: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
2:F:36:LYS:HG2	2:F:36:LYS:HZ3	1.77	0.41
2:F:142:GLY:O	2:F:143:LEU:C	2.62	0.41
3:G:231:VAL:O	3:G:235:VAL:N	2.48	0.41
3:G:242:LEU:O	3:G:243:ALA:C	2.63	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
3:C:164:SER:C	3:C:166:THR:N	2.78	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: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
2:F:121:VAL:HG22	2:F:122:CYS:N	2.37	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
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 [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%)	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%)	5	1
2	F	129/131 (98%)	119 (92%)	7 (5%)	3 (2%)	5	1
3	C	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	11	3
3	G	95/97 (98%)	91 (96%)	4 (4%)	0	100	100
All	All	462/482 (96%)	430 (93%)	25 (5%)	7 (2%)	8	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%)	5 (83%)	1 (17%)	2	0
1	E	6/10 (60%)	5 (83%)	1 (17%)	2	0
2	B	109/109 (100%)	89 (82%)	20 (18%)	2	0
2	F	109/109 (100%)	92 (84%)	17 (16%)	2	0
3	C	77/77 (100%)	65 (84%)	12 (16%)	2	0
3	G	77/77 (100%)	68 (88%)	9 (12%)	5	1
All	All	384/392 (98%)	324 (84%)	60 (16%)	2	0

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
2	B	20	GLU
2	B	36	LYS
2	B	37	THR
2	B	42	CYS
2	B	53	VAL
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	104	THR
2	B	107	LYS
2	B	110	THR
2	B	113	SER
2	B	116	GLN
2	B	123	LEU
2	B	145	ARG
3	C	154	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	164	SER
3	C	165	ASN
3	C	166	THR
3	C	170	LYS
3	C	175	LYS
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	32	SER
2	F	35	ASP
2	F	36	LYS
2	F	37	THR
2	F	46	LEU
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	103	ILE
2	F	107	LYS
2	F	125	SER
2	F	135	THR
3	G	167	ASN
3	G	170	LYS
3	G	174	THR
3	G	177	LYS
3	G	178	ASP
3	G	189	SER
3	G	192	MET
3	G	203	LYS
3	G	232	THR

Sometimes 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
3	C	240	GLN
1	E	7	GLN
2	F	48	ASN
2	F	50	ASN
2	F	91	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	PBA	G	1	-	11,11,11	1.24	1 (9%)	11,13,13	1.59	2 (18%)
4	PBA	C	1	3	11,11,11	2.31	3 (27%)	11,13,13	1.68	3 (27%)

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	G	1	-	-	3/3/5/5	0/1/1/1
4	PBA	C	1	3	-	1/3/5/5	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	6.39	1.67	1.56
4	C	1	PBA	CD2-CG	2.44	1.43	1.38
4	C	1	PBA	CB-CG	2.15	1.57	1.51
4	G	1	PBA	B-CA	-2.07	1.53	1.56

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	1	PBA	O1-B-CA	-3.89	112.43	121.06
4	C	1	PBA	O2-B-CA	-2.98	114.45	121.06
4	C	1	PBA	O1-B-CA	-2.48	115.55	121.06
4	C	1	PBA	CD2-CG-CD1	2.21	121.51	118.23
4	G	1	PBA	CA-CB-CG	-2.09	108.45	113.47

There are no chirality outliers.

All (4) torsion outliers are listed below:

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

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	1	PBA	1	0
4	C	1	PBA	2	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section is therefore empty.

6.4 Ligands [i](#)

EDS was not executed - this section is therefore empty.

6.5 Other polymers [i](#)

EDS was not executed - this section is therefore empty.