



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:55 AM UTC

PDB ID : 1DCE / pdb_00001dce
Title : CRYSTAL STRUCTURE OF RAB GERANYLGERANYLTRANSFERASE FROM RAT BRAIN
Authors : Zhang, H.; Seabra, M.C.; Deisenhofer, H.
Deposited on : 1999-11-04
Resolution : 2.00 Å (reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

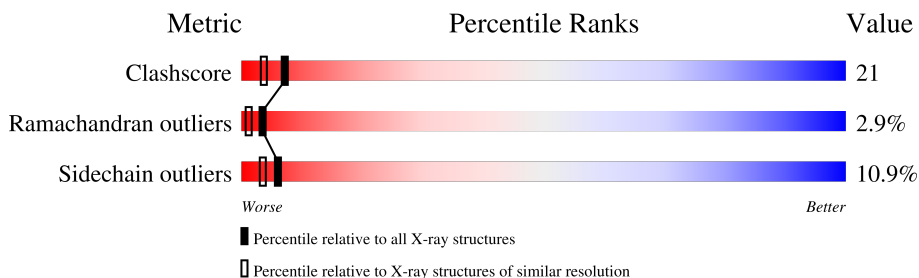
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	567	44% (green), 35% (yellow), 15% (orange), 5% (red)
1	C	567	53% (green), 34% (yellow), 10% (orange), 3% (red)
2	B	331	52% (green), 36% (yellow), 9% (orange), 3% (red)
2	D	331	54% (green), 34% (yellow), 7% (orange), 5% (red)

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 14982 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 PROTEIN (RAB GERANYLGERANYLTRANSFERASE ALPHA SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	567	4494	2833	794	838	29	0	0	0
1	C	567	4509	2845	797	838	29	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	FME	MET	modified residue	UNP Q08602
C	1	FME	MET	modified residue	UNP Q08602

- Molecule 2 is a protein called PROTEIN (RAB GERANYLGERANYLTRANSFERASE BETA SUBUNIT).

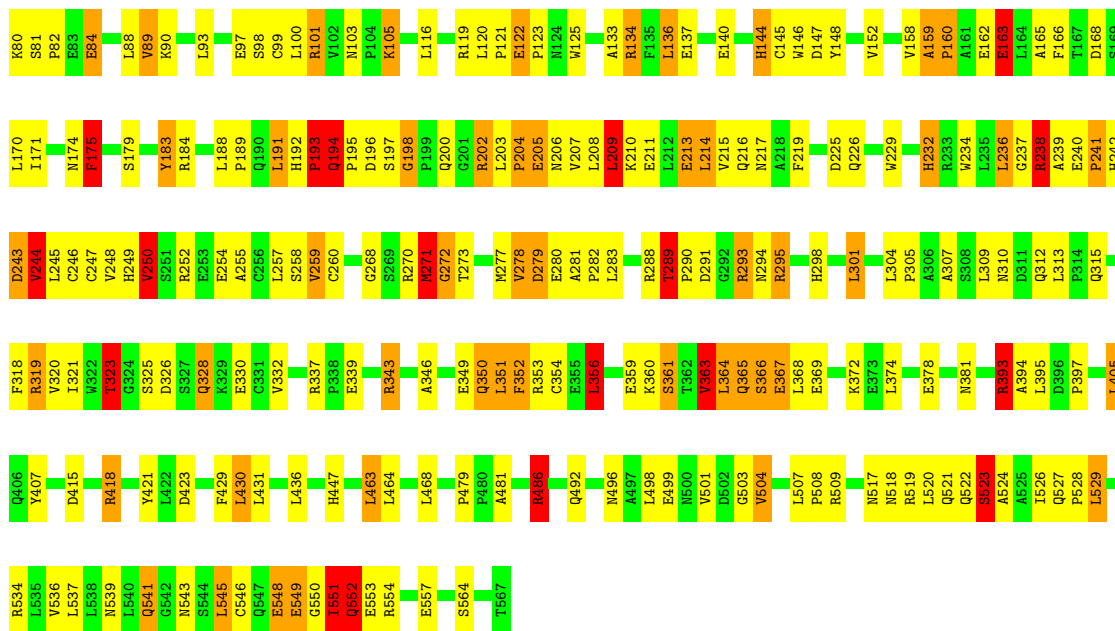
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	329	2574	1642	426	486	20	0	0	0
2	D	329	2574	1642	426	486	20	0	0	0

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

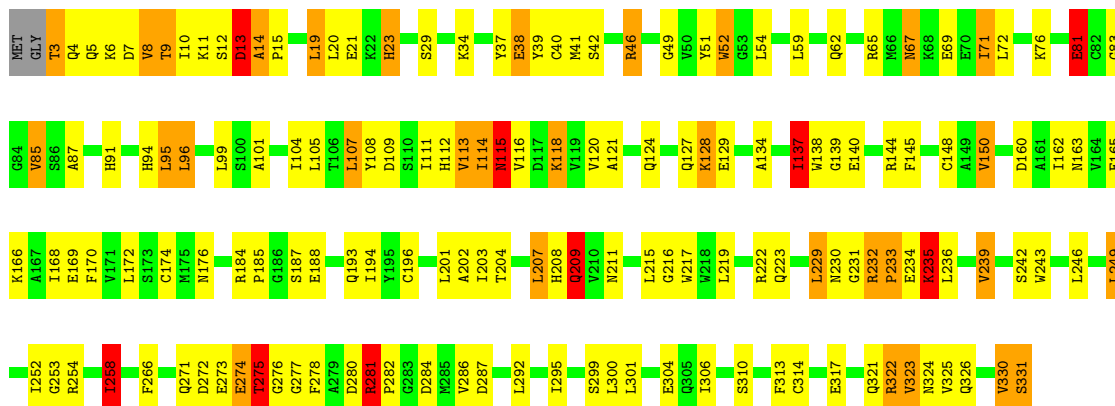
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is water.

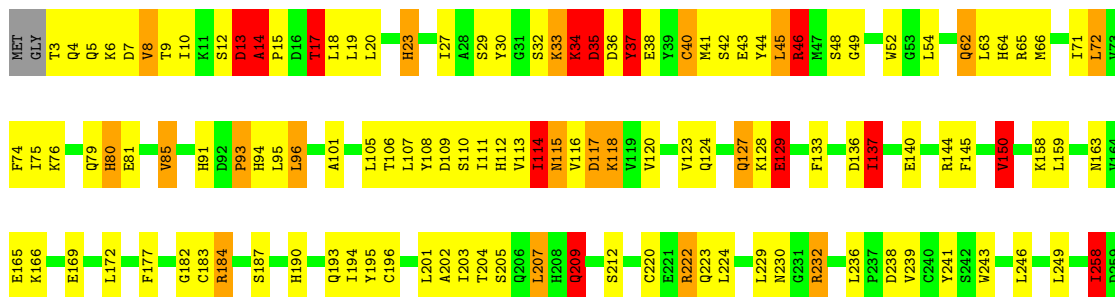
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	280	Total 280	O 280	0	0
4	B	165	Total 165	O 165	0	0
4	C	239	Total 239	O 239	0	0
4	D	145	Total 145	O 145	0	0



• Molecule 2: PROTEIN (RAB GERANYLGERANYLTRANSFERASE BETA SUBUNIT)



• Molecule 2: PROTEIN (RAB GERANYLGERANYLTRANSFERASE BETA SUBUNIT)





4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	57.86Å 77.44Å 121.78Å 74.60° 79.91° 67.89°	Depositor
Resolution (Å)	20.00 – 2.00	Depositor
% Data completeness (in resolution range)	93.4 (20.00-2.00)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.215 , 0.263	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	14982	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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: FME, ZN

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	1.06	1/4581 (0.0%)	2.31	266/6235 (4.3%)
1	C	0.94	1/4596 (0.0%)	2.10	166/6251 (2.7%)
2	B	1.02	0/2633	1.97	82/3568 (2.3%)
2	D	0.98	0/2633	1.98	67/3568 (1.9%)
All	All	1.00	2/14443 (0.0%)	2.13	581/19622 (3.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	9
1	C	0	8
2	B	0	5
2	D	0	4
All	All	0	26

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	294	ASN	N-CA	6.51	1.54	1.46
1	C	319	ARG	CD-NE	-5.03	1.39	1.46

All (581) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	ARG	CD-NE-CZ	33.75	171.65	124.40
1	A	177	ASN	OD1-CG-ND2	19.37	141.97	122.60
1	C	243	ASP	CA-CB-CG	16.40	129.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	184	ARG	CD-NE-CZ	16.37	147.31	124.40
1	C	295	ARG	CD-NE-CZ	15.59	146.23	124.40
1	A	295	ARG	CD-NE-CZ	14.59	144.82	124.40
1	A	442	ASP	CA-CB-CG	14.25	126.85	112.60
1	A	289	THR	N-CA-CB	-14.17	92.89	110.03
1	C	393	ARG	NE-CZ-NH2	-13.98	106.62	119.20
1	A	244	VAL	CA-C-O	13.65	137.85	120.78
2	D	222	ARG	CD-NE-CZ	13.48	143.28	124.40
1	A	347	THR	N-CA-C	12.85	124.82	111.07
1	A	293	ARG	CA-C-O	-12.45	107.16	121.47
1	A	346	ALA	CA-C-N	12.24	136.36	120.44
1	A	346	ALA	C-N-CA	12.24	136.36	120.44
1	C	337	ARG	NE-CZ-NH1	11.77	133.27	121.50
1	C	289	THR	N-CA-CB	-11.57	93.45	109.88
1	C	175	PHE	CA-C-O	11.47	132.45	120.40
1	A	393	ARG	NE-CZ-NH2	-11.29	109.04	119.20
1	A	325	SER	CA-C-O	-11.18	107.35	121.88
1	C	293	ARG	O-C-N	-11.10	109.91	123.01
1	A	226	GLN	OE1-CD-NE2	-11.01	111.59	122.60
2	D	144	ARG	CD-NE-CZ	10.95	139.73	124.40
1	C	492	GLN	OE1-CD-NE2	-10.83	111.77	122.60
2	D	129	GLU	CB-CG-CD	10.63	130.67	112.60
1	C	486	ARG	CD-NE-CZ	10.55	139.17	124.40
1	C	289	THR	CB-CA-C	10.41	124.82	109.09
1	C	486	ARG	NE-CZ-NH2	-10.39	109.85	119.20
1	C	175	PHE	CA-CB-CG	-10.29	103.51	113.80
1	A	62	PHE	CA-CB-CG	10.24	124.04	113.80
1	A	278	VAL	CB-CA-C	-10.21	98.96	111.32
1	C	62	PHE	CA-CB-CG	10.19	123.99	113.80
1	A	295	ARG	CB-CG-CD	10.13	134.59	111.30
1	A	328	GLN	CA-C-O	10.02	131.19	120.36
1	C	244	VAL	CA-C-O	10.01	133.30	120.78
1	C	293	ARG	CA-C-N	-9.98	107.67	122.24
1	C	293	ARG	C-N-CA	-9.98	107.67	122.24
1	A	364	LEU	N-CA-CB	9.96	124.76	110.12
1	A	486	ARG	NE-CZ-NH2	-9.93	110.26	119.20
2	D	190	HIS	CA-CB-CG	9.67	123.47	113.80
1	A	161	ALA	CA-C-O	-9.62	108.91	119.97
1	A	367	GLU	N-CA-CB	9.56	127.13	110.39
1	C	289	THR	CA-CB-OG1	9.41	123.71	109.60
1	C	134	ARG	NE-CZ-NH2	9.24	127.52	119.20
1	A	400	TYR	CA-CB-CG	9.19	130.45	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	LEU	CA-C-O	-9.18	110.82	120.55
1	A	397	PRO	N-CA-C	-9.16	100.37	113.47
1	C	229	TRP	CA-C-O	-9.14	110.73	120.42
2	D	177	PHE	CA-CB-CG	8.88	122.68	113.80
1	C	352	PHE	CA-CB-CG	8.81	122.61	113.80
1	C	272	GLY	N-CA-C	8.80	123.25	111.72
2	D	258	ILE	CA-CB-CG2	8.74	125.35	110.50
1	A	312	GLN	CB-CG-CD	8.66	127.33	112.60
1	A	319	ARG	NH1-CZ-NH2	8.57	130.44	119.30
1	C	289	THR	N-CA-C	-8.56	99.18	110.40
2	B	160	ASP	CA-CB-CG	-8.54	104.06	112.60
2	D	7	ASP	CA-C-O	-8.49	109.64	119.24
2	D	62	GLN	CA-C-O	8.47	127.80	119.08
2	D	281	ARG	CD-NE-CZ	8.46	136.24	124.40
1	C	517	ASN	OD1-CG-ND2	-8.40	114.20	122.60
1	A	396	ASP	CA-CB-CG	-8.37	104.23	112.60
1	A	328	GLN	O-C-N	-8.32	113.40	123.30
1	C	363	VAL	CA-C-O	-8.30	112.41	121.05
2	D	321	GLN	CB-CG-CD	8.30	126.72	112.60
1	A	403	GLU	CB-CG-CD	8.26	126.64	112.60
2	B	281	ARG	NE-CZ-NH2	8.25	126.62	119.20
1	C	163	GLU	CB-CG-CD	8.22	126.58	112.60
1	A	226	GLN	CG-CD-NE2	8.21	128.71	116.40
1	A	344	ASP	CA-CB-CG	-8.20	104.40	112.60
1	A	218	ALA	CA-C-O	-8.14	111.79	120.42
1	A	175	PHE	CA-C-O	8.14	130.37	121.26
1	A	289	THR	CB-CA-C	8.12	120.56	108.86
1	A	397	PRO	O-C-N	8.12	131.35	122.17
1	A	319	ARG	NE-CZ-NH2	-8.12	111.90	119.20
1	A	319	ARG	CD-NE-CZ	8.11	135.75	124.40
1	A	398	LEU	CB-CA-C	8.08	123.77	110.92
1	A	293	ARG	O-C-N	-8.02	113.90	122.96
1	A	219	PHE	CA-CB-CG	8.01	121.81	113.80
2	D	114	ILE	N-CA-CB	-7.97	102.32	112.60
1	A	345	SER	CA-C-O	7.96	130.63	121.47
1	A	2	HIS	CA-CB-CG	-7.95	105.85	113.80
2	B	23	HIS	CA-CB-CG	-7.92	105.88	113.80
2	B	81	GLU	CB-CG-CD	7.89	126.01	112.60
1	A	294	ASN	OD1-CG-ND2	-7.87	114.73	122.60
1	C	121	PRO	CA-C-N	-7.87	113.61	122.26
1	C	121	PRO	C-N-CA	-7.87	113.61	122.26
1	C	418	ARG	CD-NE-CZ	-7.85	113.41	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	281	ARG	CD-NE-CZ	7.84	135.38	124.40
1	A	179	SER	CA-CB-OG	-7.83	95.43	111.10
1	C	122	GLU	O-C-N	7.82	125.96	121.27
1	C	205	GLU	CA-C-N	7.82	131.09	120.38
1	C	205	GLU	C-N-CA	7.82	131.09	120.38
2	D	150	VAL	N-CA-CB	-7.81	98.86	110.58
2	B	209	GLN	CA-C-N	7.76	131.70	120.91
2	B	209	GLN	C-N-CA	7.76	131.70	120.91
1	C	103	ASN	OD1-CG-ND2	-7.72	114.88	122.60
1	C	174	ASN	CA-C-N	-7.69	111.84	123.07
1	C	174	ASN	C-N-CA	-7.69	111.84	123.07
1	A	279	ASP	N-CA-C	-7.69	101.62	111.92
1	C	407	TYR	CA-C-O	-7.58	112.44	120.63
1	C	84	GLU	CA-C-O	7.55	128.65	119.97
1	A	141	ARG	NE-CZ-NH2	7.51	125.96	119.20
1	A	245	LEU	CA-C-O	-7.46	112.12	120.70
2	D	266	PHE	N-CA-C	-7.46	103.23	111.36
2	B	216	GLY	N-CA-C	-7.44	103.40	113.37
1	A	523	SER	CA-C-O	-7.43	109.89	120.51
2	D	137	ILE	CB-CA-C	-7.41	101.23	112.05
1	A	101	ARG	CD-NE-CZ	7.41	134.77	124.40
1	A	518	ASN	CA-C-O	-7.40	112.59	121.32
1	C	301	LEU	CA-CB-CG	7.36	142.07	116.30
1	A	159	ALA	CB-CA-C	7.34	119.43	108.86
2	B	211	ASN	OD1-CG-ND2	-7.34	115.26	122.60
1	A	440	TYR	O-C-N	7.33	129.62	122.07
2	B	91	HIS	CA-C-O	-7.32	113.61	121.88
1	A	175	PHE	CA-C-N	7.31	135.51	121.54
1	A	175	PHE	C-N-CA	7.31	135.51	121.54
1	C	323	THR	N-CA-CB	-7.31	98.25	110.39
1	A	75	HIS	CA-CB-CG	-7.31	106.49	113.80
1	C	332	VAL	CB-CA-C	-7.27	99.71	110.33
1	A	340	CYS	O-C-N	-7.25	116.28	123.46
2	B	313	PHE	CA-CB-CG	-7.25	106.55	113.80
1	C	134	ARG	NE-CZ-NH1	-7.25	114.25	121.50
1	A	440	TYR	N-CA-C	-7.22	103.34	111.07
1	C	365	GLN	OE1-CD-NE2	-7.22	115.38	122.60
2	D	13	ASP	CA-CB-CG	7.21	119.81	112.60
2	B	168	ILE	CA-C-O	7.18	128.42	120.95
2	D	65	ARG	NE-CZ-NH2	7.18	125.66	119.20
1	A	328	GLN	N-CA-C	7.14	120.55	108.90
2	D	46	ARG	CD-NE-CZ	7.13	134.38	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	127	ARG	NE-CZ-NH2	7.05	125.55	119.20
1	C	183	TYR	CA-C-O	-7.03	113.38	120.90
2	B	208	HIS	CA-C-O	7.01	128.17	119.05
1	A	461	GLN	CG-CD-NE2	7.01	126.92	116.40
2	D	230	ASN	CA-CB-CG	7.01	119.61	112.60
1	A	177	ASN	CB-CG-ND2	-6.98	105.94	116.40
1	A	107	TYR	CA-C-O	-6.96	113.69	121.00
1	A	328	GLN	OE1-CD-NE2	-6.95	115.65	122.60
1	A	319	ARG	CA-C-N	6.94	131.80	123.19
1	A	319	ARG	C-N-CA	6.94	131.80	123.19
1	C	101	ARG	NE-CZ-NH1	-6.90	114.60	121.50
1	A	158	VAL	CA-C-O	6.90	129.40	120.78
1	A	206	ASN	OD1-CG-ND2	-6.90	115.70	122.60
2	B	239	VAL	CA-C-O	-6.90	113.78	120.95
1	A	294	ASN	CB-CG-ND2	6.89	126.74	116.40
2	D	140	GLU	CA-C-O	-6.89	113.07	120.92
1	A	349	GLU	CB-CG-CD	6.88	124.30	112.60
2	D	289	PHE	CA-CB-CG	6.88	120.69	113.80
1	A	496	ASN	CB-CG-ND2	6.88	126.72	116.40
1	C	301	LEU	O-C-N	6.87	131.08	123.25
2	B	235	LYS	CB-CG-CD	6.86	127.08	111.30
2	D	91	HIS	CA-CB-CG	6.86	120.66	113.80
1	A	204	PRO	CB-CA-C	6.84	122.84	111.56
1	C	193	PRO	O-C-N	-6.83	113.42	122.64
1	A	374	LEU	CA-C-N	-6.82	111.14	120.28
1	A	374	LEU	C-N-CA	-6.82	111.14	120.28
1	A	192	HIS	CA-C-N	6.79	126.75	119.76
1	A	192	HIS	C-N-CA	6.79	126.75	119.76
1	A	558	MET	CA-C-O	6.79	127.80	119.79
1	A	339	GLU	O-C-N	6.79	130.90	123.10
1	A	315	GLN	O-C-N	6.78	130.99	123.33
1	A	202	ARG	NE-CZ-NH1	6.77	128.27	121.50
2	D	144	ARG	NE-CZ-NH2	-6.77	113.11	119.20
1	C	363	VAL	N-CA-CB	6.77	118.93	110.47
2	D	184	ARG	CA-C-O	-6.76	114.83	120.71
1	A	398	LEU	CA-C-N	6.75	132.16	120.68
1	A	398	LEU	C-N-CA	6.75	132.16	120.68
2	B	193	GLN	OE1-CD-NE2	6.75	129.35	122.60
1	C	245	LEU	CA-C-O	-6.74	113.53	120.80
2	D	27	ILE	CA-C-O	-6.72	113.97	120.95
1	A	433	ASN	OD1-CG-ND2	-6.69	115.91	122.60
1	C	271	MET	N-CA-CB	6.69	119.60	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	219	PHE	CA-CB-CG	6.67	120.47	113.80
1	C	193	PRO	CA-C-N	6.67	138.08	121.80
1	C	193	PRO	C-N-CA	6.67	138.08	121.80
1	C	283	LEU	CA-C-O	-6.65	113.19	120.24
1	C	320	VAL	CA-C-N	-6.65	114.43	123.14
1	C	320	VAL	C-N-CA	-6.65	114.43	123.14
1	C	343	ARG	NE-CZ-NH1	-6.63	114.87	121.50
2	B	252	ILE	CA-C-O	-6.63	112.50	120.78
2	B	208	HIS	O-C-N	-6.62	113.32	122.46
1	C	2	HIS	CA-CB-CG	-6.62	107.18	113.80
1	A	22	GLU	N-CA-C	-6.61	105.03	113.23
1	A	222	ASP	CA-CB-CG	6.60	119.20	112.60
1	A	365	GLN	OE1-CD-NE2	-6.60	116.00	122.60
1	A	36	PHE	CA-CB-CG	6.59	120.39	113.80
1	A	137	GLU	CB-CG-CD	6.59	123.80	112.60
1	C	232	HIS	CA-C-O	-6.58	113.58	120.55
1	A	436	LEU	CB-CA-C	6.57	121.70	110.79
2	B	150	VAL	N-CA-CB	-6.56	98.89	110.77
2	D	6	LYS	N-CA-C	-6.54	104.24	111.36
1	A	398	LEU	O-C-N	-6.53	115.09	122.08
1	A	393	ARG	CD-NE-CZ	-6.53	115.26	124.40
1	C	294	ASN	CB-CA-C	6.51	120.66	111.74
1	A	330	GLU	CA-C-O	-6.50	113.40	120.36
2	B	322	ARG	CA-C-O	-6.50	113.64	120.92
2	B	194	ILE	CA-C-O	-6.50	113.75	120.71
1	A	332	VAL	N-CA-C	6.49	117.23	107.75
1	A	305	PRO	CB-CA-C	6.49	119.56	110.60
2	D	17	THR	CA-C-O	-6.48	113.54	121.06
1	A	286	GLU	CA-CB-CG	-6.48	101.14	114.10
1	C	337	ARG	CD-NE-CZ	6.48	133.47	124.40
2	B	23	HIS	O-C-N	6.47	129.53	122.15
1	C	356	LEU	O-C-N	-6.46	115.66	123.16
1	A	177	ASN	CB-CA-C	6.44	123.23	110.42
1	C	56	LEU	CA-C-O	-6.41	113.62	120.42
2	B	209	GLN	O-C-N	-6.41	113.61	122.46
1	C	204	PRO	CA-C-O	-6.41	114.33	121.32
2	B	230	ASN	OD1-CG-ND2	-6.41	116.19	122.60
1	C	350	GLN	OE1-CD-NE2	-6.40	116.20	122.60
2	D	196	CYS	CA-C-O	-6.40	113.76	120.55
1	A	346	ALA	N-CA-CB	-6.40	100.72	110.12
2	B	184	ARG	CD-NE-CZ	6.38	133.34	124.40
1	A	293	ARG	CA-C-N	-6.37	109.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ARG	C-N-CA	-6.37	109.37	121.54
1	C	194	GLN	N-CA-C	6.37	123.88	109.81
2	B	67	ASN	OD1-CG-ND2	6.37	128.97	122.60
2	B	239	VAL	N-CA-CB	6.35	119.18	110.54
1	C	337	ARG	NE-CZ-NH2	-6.35	113.49	119.20
1	A	368	LEU	N-CA-CB	6.34	119.45	110.12
1	C	217	ASN	OD1-CG-ND2	6.34	128.94	122.60
1	A	96	LEU	N-CA-C	6.33	118.18	111.28
1	C	278	VAL	O-C-N	-6.33	116.22	122.93
1	A	127	ARG	NE-CZ-NH1	-6.32	115.18	121.50
1	A	388	ILE	O-C-N	6.32	128.10	121.91
2	B	204	THR	CA-CB-OG1	-6.31	100.13	109.60
2	B	23	HIS	N-CA-CB	6.31	119.50	110.16
1	C	237	GLY	CA-C-O	-6.31	117.54	122.52
2	B	287	ASP	O-C-N	6.30	127.80	121.56
1	C	381	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	317	THR	CA-C-N	6.29	131.90	122.47
1	A	317	THR	C-N-CA	6.29	131.90	122.47
2	B	148	CYS	CA-C-N	6.28	128.94	120.65
2	B	148	CYS	C-N-CA	6.28	128.94	120.65
1	C	193	PRO	N-CA-C	6.28	125.41	112.47
2	B	209	GLN	CA-C-O	6.26	127.08	119.31
1	C	144	HIS	CA-CB-CG	6.26	120.06	113.80
1	A	512	GLU	CA-C-O	-6.26	113.60	120.30
1	A	318	PHE	CA-C-N	6.26	131.09	122.77
1	A	318	PHE	C-N-CA	6.26	131.09	122.77
1	A	308	SER	CA-CB-OG	-6.24	98.62	111.10
1	A	406	GLN	OE1-CD-NE2	-6.23	116.37	122.60
1	A	218	ALA	CA-C-N	-6.23	110.48	122.06
1	A	218	ALA	C-N-CA	-6.23	110.48	122.06
1	C	250	VAL	N-CA-CB	6.23	120.61	111.52
1	C	519	ARG	CA-CB-CG	-6.22	101.65	114.10
1	A	145	CYS	N-CA-CB	6.21	120.13	110.44
2	D	274	GLU	CA-C-O	-6.21	114.48	121.81
1	A	216	GLN	CG-CD-NE2	-6.21	107.09	116.40
1	A	234	TRP	CA-C-N	6.21	129.44	120.38
1	A	234	TRP	C-N-CA	6.21	129.44	120.38
1	A	238	ARG	N-CA-C	6.20	119.62	109.76
1	C	364	LEU	O-C-N	-6.20	115.08	122.15
1	A	343	ARG	CA-C-O	6.18	127.76	120.66
2	B	150	VAL	O-C-N	-6.17	114.82	121.80
2	D	65	ARG	CD-NE-CZ	-6.17	115.77	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	511	GLN	OE1-CD-NE2	-6.16	116.44	122.60
2	B	137	ILE	CB-CA-C	-6.16	100.02	111.79
2	B	278	PHE	CA-CB-CG	6.16	119.96	113.80
1	C	260	CYS	O-C-N	6.15	131.23	123.23
1	C	271	MET	CA-C-O	-6.15	115.30	122.37
1	A	334	LEU	N-CA-CB	6.14	120.43	110.41
1	C	209	LEU	CA-C-O	-6.14	114.05	120.55
1	A	47	SER	CA-CB-OG	6.13	123.36	111.10
1	C	62	PHE	CA-C-N	6.12	128.99	120.29
1	C	62	PHE	C-N-CA	6.12	128.99	120.29
1	A	325	SER	N-CA-C	-6.12	100.92	110.17
1	A	288	ARG	CA-C-O	6.10	128.34	121.51
1	A	193	PRO	N-CA-C	6.08	120.63	111.14
1	A	414	VAL	CA-C-N	-6.08	115.79	123.15
1	A	414	VAL	C-N-CA	-6.08	115.79	123.15
1	A	150	ARG	N-CA-C	-6.07	104.78	111.82
1	C	328	GLN	CA-C-O	-6.07	113.32	120.60
2	B	115	ASN	CA-CB-CG	6.06	118.66	112.60
1	A	527	GLN	OE1-CD-NE2	-6.06	116.54	122.60
1	C	243	ASP	CA-C-O	6.06	128.84	119.21
1	A	165	ALA	O-C-N	6.05	129.52	122.20
1	C	415	ASP	CA-CB-CG	6.04	118.64	112.60
2	D	264	ARG	NE-CZ-NH2	-6.03	113.77	119.20
1	A	447	HIS	CA-CB-CG	6.03	119.83	113.80
1	A	486	ARG	NH1-CZ-NH2	6.02	127.13	119.30
1	A	170	LEU	CA-C-O	-6.02	112.49	119.59
2	B	170	PHE	CA-CB-CG	-6.02	107.78	113.80
1	A	144	HIS	CA-CB-CG	6.02	119.82	113.80
2	D	128	LYS	CA-C-N	6.02	128.66	120.54
2	D	128	LYS	C-N-CA	6.02	128.66	120.54
1	A	176	SER	CA-CB-OG	6.02	123.13	111.10
2	B	114	ILE	CA-C-O	-5.99	114.68	121.75
2	B	310	SER	CA-C-O	-5.99	114.12	120.23
1	A	280	GLU	O-C-N	5.98	129.76	122.58
1	A	331	CYS	O-C-N	-5.97	115.64	123.16
2	B	144	ARG	NE-CZ-NH2	-5.96	113.84	119.20
2	D	106	THR	CA-CB-OG1	-5.96	100.66	109.60
2	D	212	SER	N-CA-CB	-5.95	101.13	110.06
2	D	241	TYR	CA-C-O	-5.95	113.38	120.10
1	A	536	VAL	N-CA-CB	-5.94	102.42	111.57
2	D	209	GLN	CB-CG-CD	5.93	122.69	112.60
1	A	327	SER	CA-C-O	5.92	127.73	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	28	TYR	CA-C-N	5.92	128.21	120.28
1	A	28	TYR	C-N-CA	5.92	128.21	120.28
1	A	235	LEU	N-CA-C	5.92	119.32	111.75
2	D	80	HIS	CA-CB-CG	-5.92	107.88	113.80
1	A	372	LYS	CB-CG-CD	5.91	124.90	111.30
1	A	434	SER	CA-CB-OG	-5.91	99.27	111.10
2	D	112	HIS	O-C-N	-5.91	114.76	122.39
1	C	250	VAL	CA-CB-CG1	5.91	120.44	110.40
2	D	238	ASP	OD1-CG-OD2	-5.91	108.73	122.90
1	A	145	CYS	N-CA-C	-5.90	105.92	113.23
1	C	519	ARG	CD-NE-CZ	-5.89	116.15	124.40
1	A	478	LEU	CA-C-O	-5.89	114.94	119.71
1	C	301	LEU	CA-C-N	-5.88	112.95	122.36
1	C	301	LEU	C-N-CA	-5.88	112.95	122.36
1	A	384	CYS	O-C-N	-5.87	115.90	122.12
1	C	298	HIS	CA-CB-CG	5.85	119.65	113.80
1	C	309	LEU	CA-C-O	-5.84	113.47	120.65
1	A	242	HIS	N-CA-CB	5.83	120.34	110.49
1	A	374	LEU	CB-CA-C	-5.82	101.07	110.74
1	A	393	ARG	NH1-CZ-NH2	5.82	126.87	119.30
1	A	173	ARG	CA-C-O	5.82	126.47	119.43
1	A	146	TRP	CA-C-O	-5.79	113.81	120.24
1	C	252	ARG	NE-CZ-NH2	5.79	124.41	119.20
1	A	373	GLU	CA-C-N	5.78	129.50	120.82
1	A	373	GLU	C-N-CA	5.78	129.50	120.82
1	A	404	THR	CA-C-O	5.78	127.09	120.90
1	C	517	ASN	CA-CB-CG	5.78	118.38	112.60
2	D	66	MET	CA-C-O	-5.78	114.56	121.56
1	C	293	ARG	NE-CZ-NH2	-5.77	114.00	119.20
1	A	244	VAL	O-C-N	-5.77	115.36	122.57
1	A	426	ARG	CA-C-O	-5.76	114.32	120.42
1	A	8	LYS	CA-C-O	-5.75	112.62	119.35
1	A	224	ASN	CA-C-N	5.75	131.78	122.29
1	A	224	ASN	C-N-CA	5.75	131.78	122.29
1	A	437	LYS	CG-CD-CE	5.75	124.53	111.30
2	B	99	LEU	O-C-N	-5.75	116.03	122.12
1	C	393	ARG	NH1-CZ-NH2	5.75	126.77	119.30
2	B	274	GLU	CA-C-O	-5.74	115.54	122.03
1	A	313	LEU	CA-C-N	5.74	125.84	119.87
1	A	313	LEU	C-N-CA	5.74	125.84	119.87
2	B	258	ILE	CA-CB-CG2	5.74	120.26	110.50
1	A	141	ARG	NE-CZ-NH1	-5.73	115.77	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	294	ASN	CA-CB-CG	-5.73	106.87	112.60
1	C	146	TRP	CA-C-O	-5.73	114.81	120.82
2	D	48	SER	CA-C-O	5.73	126.49	120.42
2	D	23	HIS	CA-CB-CG	-5.72	108.08	113.80
1	A	344	ASP	N-CA-C	5.71	117.37	109.15
1	A	374	LEU	O-C-N	5.71	128.67	122.11
1	A	407	TYR	CA-C-O	-5.70	114.47	120.63
2	B	232	ARG	NE-CZ-NH1	-5.69	115.81	121.50
2	D	223	GLN	OE1-CD-NE2	5.67	128.27	122.60
1	A	514	LEU	CA-C-O	5.67	126.43	120.54
1	C	279	ASP	CA-CB-CG	-5.66	106.94	112.60
2	B	204	THR	CA-C-N	5.66	130.20	122.34
2	B	204	THR	C-N-CA	5.66	130.20	122.34
2	B	184	ARG	NH1-CZ-NH2	-5.65	111.95	119.30
1	A	65	LEU	CA-C-O	-5.65	113.47	119.97
2	B	203	ILE	CB-CG1-CD1	5.64	125.65	113.80
2	D	281	ARG	NE-CZ-NH1	5.64	127.14	121.50
2	D	123	VAL	CA-C-O	-5.63	115.20	121.17
1	A	352	PHE	CA-CB-CG	5.62	119.42	113.80
2	B	215	LEU	CA-C-O	5.62	126.43	119.97
1	A	5	LEU	N-CA-CB	5.61	118.21	109.97
2	D	34	LYS	CA-C-N	5.59	132.22	121.54
2	D	34	LYS	C-N-CA	5.59	132.22	121.54
2	B	295	ILE	N-CA-C	5.59	115.78	110.53
2	B	211	ASN	CB-CG-ND2	5.58	124.78	116.40
1	A	245	LEU	N-CA-C	-5.58	101.64	109.96
1	A	454	THR	N-CA-C	-5.58	106.37	114.12
1	A	341	TRP	CA-C-O	5.57	127.24	121.28
2	B	62	GLN	OE1-CD-NE2	-5.57	117.03	122.60
1	A	202	ARG	CD-NE-CZ	5.57	132.19	124.40
1	A	308	SER	O-C-N	5.57	129.89	122.43
2	B	169	GLU	N-CA-CB	-5.55	101.96	110.12
1	A	384	CYS	CA-C-O	5.54	126.42	120.55
1	A	450	HIS	CA-C-N	-5.54	113.96	122.60
1	A	450	HIS	C-N-CA	-5.54	113.96	122.60
1	A	455	VAL	CA-C-O	-5.54	115.91	121.45
1	C	202	ARG	CD-NE-CZ	5.53	132.15	124.40
1	C	159	ALA	CA-C-O	5.53	127.74	120.16
1	A	369	GLU	CA-C-N	5.53	132.99	122.60
1	A	369	GLU	C-N-CA	5.53	132.99	122.60
2	B	67	ASN	CA-CB-CG	5.52	118.12	112.60
1	A	315	GLN	OE1-CD-NE2	5.51	128.12	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	316	HIS	CA-C-O	5.51	127.91	121.46
1	C	507	LEU	CA-C-O	5.51	122.87	119.29
1	C	367	GLU	CA-C-O	-5.51	114.71	120.55
1	A	159	ALA	CA-C-O	5.51	125.56	120.60
2	B	139	GLY	N-CA-C	5.51	122.08	114.92
1	C	216	GLN	CB-CA-C	-5.49	102.02	110.81
1	C	277	MET	CA-C-O	-5.49	114.39	120.38
2	D	93	PRO	CA-C-O	5.49	127.58	121.43
1	C	365	GLN	CA-C-O	5.48	126.28	119.97
1	A	225	ASP	CB-CG-OD1	5.48	131.01	118.40
1	C	305	PRO	CB-CA-C	5.48	118.47	110.63
1	A	473	ASN	OD1-CG-ND2	-5.47	117.13	122.60
1	A	461	GLN	OE1-CD-NE2	-5.47	117.13	122.60
1	C	47	SER	CA-CB-OG	5.47	122.04	111.10
2	B	196	CYS	O-C-N	-5.47	116.44	122.07
1	A	280	GLU	CA-C-N	5.46	135.12	121.80
1	A	280	GLU	C-N-CA	5.46	135.12	121.80
1	C	90	LYS	CA-C-O	-5.46	115.09	120.82
1	C	421	TYR	CA-C-O	5.45	126.55	120.82
1	C	140	GLU	N-CA-C	-5.45	106.47	113.01
2	B	284	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	67	ASN	O-C-N	5.44	127.67	122.07
1	C	523	SER	CA-CB-OG	5.44	121.98	111.10
2	B	324	ASN	CA-CB-CG	5.43	118.03	112.60
2	B	287	ASP	CA-C-O	-5.42	115.62	120.56
1	A	550	GLY	CA-C-N	5.42	131.72	121.97
1	A	550	GLY	C-N-CA	5.42	131.72	121.97
1	C	369	GLU	O-C-N	-5.42	116.46	122.09
1	C	521	GLN	CG-CD-NE2	5.41	124.52	116.40
1	C	51	LEU	O-C-N	-5.41	116.50	122.07
1	A	487	CYS	CA-C-O	-5.41	113.02	119.35
2	D	35	ASP	N-CA-C	5.40	122.31	110.80
1	C	147	ASP	CA-CB-CG	-5.40	107.20	112.60
2	B	19	LEU	CA-C-N	5.40	127.52	120.28
2	B	19	LEU	C-N-CA	5.40	127.52	120.28
2	B	71	ILE	CA-C-O	5.40	126.57	120.95
1	C	553	GLU	CA-CB-CG	5.39	124.89	114.10
1	A	312	GLN	OE1-CD-NE2	-5.39	117.21	122.60
1	C	272	GLY	CA-C-O	5.39	126.41	121.77
1	C	101	ARG	CA-C-O	-5.38	114.71	120.42
1	C	249	HIS	CA-C-N	-5.38	115.51	122.99
1	C	249	HIS	C-N-CA	-5.38	115.51	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	336	ASP	CA-CB-CG	-5.38	107.22	112.60
1	C	486	ARG	NH1-CZ-NH2	5.38	126.29	119.30
1	C	564	SER	N-CA-C	5.37	117.58	108.02
2	B	323	VAL	O-C-N	-5.37	115.86	122.57
2	D	64	HIS	CA-CB-CG	-5.37	108.43	113.80
1	A	500	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	A	500	ASN	CA-CB-CG	5.36	117.96	112.60
1	A	249	HIS	O-C-N	5.36	129.68	123.41
1	A	427	SER	CA-CB-OG	-5.35	100.40	111.10
1	C	99	CYS	O-C-N	-5.35	116.05	122.15
1	C	84	GLU	O-C-N	-5.34	115.70	122.27
2	B	217	TRP	CB-CA-C	-5.34	102.49	110.88
1	A	472	HIS	CA-CB-CG	-5.32	108.48	113.80
2	B	266	PHE	N-CA-C	-5.32	105.48	111.28
2	D	46	ARG	NE-CZ-NH1	-5.32	116.18	121.50
2	B	46	ARG	CD-NE-CZ	5.32	131.84	124.40
1	C	98	SER	CA-CB-OG	-5.32	100.46	111.10
1	A	77	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	400	TYR	CA-C-N	5.31	127.66	120.38
1	A	400	TYR	C-N-CA	5.31	127.66	120.38
1	A	109	THR	O-C-N	-5.31	116.10	122.15
2	D	14	ALA	CB-CA-C	5.31	120.63	110.17
2	D	194	ILE	CA-C-N	5.30	127.33	120.44
2	D	194	ILE	C-N-CA	5.30	127.33	120.44
1	A	163	GLU	CG-CD-OE1	5.30	130.59	118.40
2	D	232	ARG	CA-CB-CG	5.30	124.70	114.10
1	C	339	GLU	CA-C-O	-5.29	115.42	121.40
1	A	440	TYR	CA-C-O	-5.28	115.27	120.82
2	D	195	TYR	CA-C-O	-5.28	115.28	120.82
1	A	98	SER	O-C-N	5.28	127.72	122.12
1	C	468	LEU	CA-C-N	-5.28	115.98	122.84
1	C	468	LEU	C-N-CA	-5.28	115.98	122.84
1	C	103	ASN	CB-CG-ND2	5.27	124.30	116.40
1	C	196	ASP	N-CA-C	5.27	117.18	108.49
1	A	146	TRP	N-CA-CB	5.25	118.03	110.20
1	A	54	GLN	CA-C-O	5.25	126.11	120.70
1	A	239	ALA	CA-C-O	5.25	127.11	121.44
1	C	423	ASP	O-C-N	5.25	127.47	122.07
1	C	481	ALA	CA-C-O	5.25	125.83	119.11
1	A	477	ALA	O-C-N	-5.25	117.40	123.33
1	C	54	GLN	CA-C-N	5.24	127.27	120.56
1	C	54	GLN	C-N-CA	5.24	127.27	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	GLN	CA-C-O	-5.24	114.18	120.10
1	C	378	GLU	CA-C-N	5.24	124.90	119.56
1	C	378	GLU	C-N-CA	5.24	124.90	119.56
2	D	35	ASP	CA-CB-CG	-5.24	107.36	112.60
1	C	293	ARG	CA-C-O	-5.23	115.08	121.05
1	C	436	LEU	CA-C-O	-5.23	115.30	120.90
1	A	179	SER	CB-CA-C	5.23	121.05	110.38
1	A	116	LEU	O-C-N	-5.23	116.68	122.07
1	A	316	HIS	CA-CB-CG	5.23	119.03	113.80
1	A	436	LEU	CA-C-N	-5.22	112.76	120.28
1	A	436	LEU	C-N-CA	-5.22	112.76	120.28
1	C	205	GLU	CA-C-O	5.22	126.08	120.55
1	A	179	SER	O-C-N	-5.22	115.34	122.33
1	A	473	ASN	CA-C-O	-5.21	114.54	121.47
1	A	312	GLN	N-CA-C	-5.21	107.05	113.41
1	A	327	SER	N-CA-C	5.21	118.71	109.96
1	C	148	TYR	CA-CB-CG	-5.20	104.53	113.90
1	C	105	LYS	CA-CB-CG	-5.20	103.70	114.10
2	D	14	ALA	CA-C-O	-5.20	113.03	120.16
1	A	262	SER	CB-CA-C	-5.20	102.16	110.79
1	A	210	LYS	CA-CB-CG	5.19	124.49	114.10
1	C	553	GLU	N-CA-C	-5.19	106.07	112.72
1	A	439	GLU	CA-CB-CG	5.18	124.46	114.10
2	B	59	LEU	CA-C-O	5.18	125.96	120.10
1	C	184	ARG	NE-CZ-NH2	-5.18	114.54	119.20
1	A	157	ALA	CA-C-O	-5.17	113.11	120.51
1	C	77	GLU	OE1-CD-OE2	-5.17	110.48	122.90
1	C	160	PRO	N-CD-CG	-5.17	95.44	103.20
1	A	279	ASP	CB-CG-OD1	-5.17	106.51	118.40
2	D	137	ILE	N-CA-C	5.17	118.30	111.17
2	B	266	PHE	CA-C-O	-5.16	115.08	120.55
2	D	150	VAL	CB-CA-C	5.16	119.34	112.22
2	B	121	ALA	N-CA-C	-5.16	105.84	111.82
1	A	334	LEU	CA-C-N	5.15	131.38	121.54
1	A	334	LEU	C-N-CA	5.15	131.38	121.54
1	A	263	ARG	O-C-N	5.15	125.57	121.55
2	B	23	HIS	CA-C-O	-5.15	114.96	120.42
1	C	175	PHE	N-CA-C	5.14	117.02	108.02
1	C	343	ARG	O-C-N	-5.14	117.18	123.30
1	A	134	ARG	CB-CA-C	-5.14	103.04	110.96
1	A	149	ARG	O-C-N	5.14	127.56	122.12
1	A	149	ARG	CA-C-N	-5.13	112.51	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	ARG	C-N-CA	-5.13	112.51	120.31
2	D	224	LEU	CA-C-N	5.13	125.42	119.47
2	D	224	LEU	C-N-CA	5.13	125.42	119.47
2	D	241	TYR	O-C-N	5.12	128.21	122.22
2	B	209	GLN	N-CA-CB	-5.12	102.06	110.40
1	A	372	LYS	O-C-N	-5.11	116.61	122.08
1	C	323	THR	CA-C-O	5.11	125.67	119.38
1	C	564	SER	CA-C-N	5.11	130.06	123.11
1	C	564	SER	C-N-CA	5.11	130.06	123.11
1	A	308	SER	CA-C-O	-5.11	113.10	119.38
1	A	84	GLU	CA-CB-CG	5.10	124.31	114.10
1	A	205	GLU	CA-C-N	5.10	129.30	121.19
1	A	205	GLU	C-N-CA	5.10	129.30	121.19
1	C	318	PHE	CA-C-O	-5.10	114.66	120.32
1	A	468	LEU	CA-C-N	-5.10	115.99	122.77
1	A	468	LEU	C-N-CA	-5.10	115.99	122.77
1	A	149	ARG	N-CA-CB	5.09	117.61	110.12
1	A	279	ASP	OD1-CG-OD2	5.09	135.13	122.90
1	A	432	GLU	CA-C-N	-5.09	113.45	120.28
1	A	432	GLU	C-N-CA	-5.09	113.45	120.28
1	A	298	HIS	CA-CB-CG	5.09	118.89	113.80
1	A	259	VAL	N-CA-CB	-5.09	102.52	111.93
1	C	447	HIS	CA-C-O	-5.09	115.25	120.54
1	C	250	VAL	CA-C-N	-5.08	115.93	123.05
1	C	250	VAL	C-N-CA	-5.08	115.93	123.05
1	A	146	TRP	N-CA-C	-5.08	105.44	111.69
1	C	100	LEU	CA-C-N	5.08	127.51	120.29
1	C	100	LEU	C-N-CA	5.08	127.51	120.29
1	A	340	CYS	CA-C-O	5.08	126.69	121.10
1	A	364	LEU	O-C-N	5.08	127.50	122.12
1	A	536	VAL	CA-CB-CG1	5.08	119.03	110.40
2	B	95	LEU	O-C-N	-5.08	116.74	122.12
2	B	275	THR	CA-C-O	-5.08	113.25	120.51
1	A	321	ILE	N-CA-CB	-5.07	105.05	111.64
2	B	184	ARG	NE-CZ-NH1	5.07	126.57	121.50
1	C	393	ARG	NE-CZ-NH1	5.07	126.57	121.50
2	B	232	ARG	CD-NE-CZ	-5.07	117.30	124.40
1	A	437	LYS	CB-CA-C	5.07	120.01	110.63
1	A	519	ARG	CD-NE-CZ	-5.07	117.31	124.40
1	C	89	VAL	CB-CA-C	-5.07	105.23	112.22
1	C	508	PRO	O-C-N	-5.07	115.68	122.22
2	B	128	LYS	CA-C-N	5.06	127.37	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	128	LYS	C-N-CA	5.06	127.37	120.54
1	A	343	ARG	NH1-CZ-NH2	-5.06	112.72	119.30
1	A	349	GLU	CB-CA-C	5.05	118.90	111.17
2	B	258	ILE	CA-C-O	-5.05	115.06	121.48
1	A	376	GLU	O-C-N	-5.05	116.06	122.27
2	D	127	GLN	CA-C-O	5.05	126.80	121.05
1	A	317	THR	N-CA-C	-5.04	99.40	108.48
2	B	232	ARG	NE-CZ-NH2	5.04	123.74	119.20
1	A	188	LEU	CB-CA-C	5.04	120.10	110.17
2	D	136	ASP	CA-C-O	-5.04	115.76	121.25
2	B	29	SER	O-C-N	5.04	128.55	122.35
1	A	442	ASP	N-CA-CB	-5.04	104.48	112.08
2	B	67	ASN	CB-CA-C	-5.03	103.22	111.68
1	C	365	GLN	O-C-N	-5.03	116.08	122.27
1	A	187	LEU	N-CA-C	5.03	116.61	111.03
1	A	368	LEU	CA-C-O	5.03	125.88	120.55
1	C	326	ASP	CA-CB-CG	-5.03	107.57	112.60
2	D	144	ARG	NH1-CZ-NH2	5.03	125.84	119.30
1	C	288	ARG	CA-C-O	5.03	126.83	121.45
2	D	65	ARG	NE-CZ-NH1	-5.03	116.47	121.50
1	A	305	PRO	O-C-N	-5.03	117.01	123.14
1	A	371	CYS	N-CA-C	5.02	116.44	111.07
1	A	316	HIS	CB-CA-C	5.02	119.40	109.66
1	A	489	GLU	O-C-N	5.02	129.53	122.20
1	C	537	LEU	CA-C-N	5.02	130.07	123.00
1	C	537	LEU	C-N-CA	5.02	130.07	123.00
1	A	439	GLU	CA-C-N	-5.01	113.92	120.44
1	A	439	GLU	C-N-CA	-5.01	113.92	120.44
1	A	439	GLU	N-CA-C	-5.01	105.52	111.69
1	C	179	SER	CA-C-O	-5.01	115.24	120.55
1	C	77	GLU	CA-CB-CG	5.00	124.10	114.10
1	C	260	CYS	CA-C-O	-5.00	115.30	120.70

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	161	ALA	Mainchain
1	A	176	SER	Peptide
1	A	211	GLU	Mainchain
1	A	215	VAL	Mainchain
1	A	238	ARG	Peptide

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Mol	Chain	Res	Type	Group
1	A	244	VAL	Peptide
1	A	271	MET	Peptide
1	A	317	THR	Mainchain
1	A	335	LYS	Mainchain
2	B	107	LEU	Mainchain
2	B	174	CYS	Mainchain
2	B	330	VAL	Peptide
2	B	52	TRP	Mainchain
2	B	87	ALA	Mainchain
1	C	158	VAL	Mainchain
1	C	244	VAL	Peptide
1	C	246	CYS	Mainchain
1	C	356	LEU	Mainchain
1	C	393	ARG	Mainchain
1	C	463	LEU	Mainchain
1	C	486	ARG	Mainchain
1	C	541	GLN	Mainchain
2	D	117	ASP	Mainchain
2	D	14	ALA	Peptide
2	D	33	LYS	Peptide
2	D	81	GLU	Mainchain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4494	0	4406	229	0
1	C	4509	0	4448	161	0
2	B	2574	0	2521	104	0
2	D	2574	0	2521	103	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
4	A	280	0	0	35	0
4	B	165	0	0	13	0
4	C	239	0	0	20	0
4	D	145	0	0	14	0
All	All	14982	0	13896	583	0

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 21.

All (583) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:272:GLY:HA2	1:C:323:THR:HG22	1.40	1.00
1:A:203:LEU:HB3	1:A:207:VAL:HG13	1.48	0.93
1:A:242:HIS:HA	1:A:263:ARG:HH22	1.28	0.93
2:D:94:HIS:HD2	2:D:96:LEU:H	1.17	0.93
1:A:498:LEU:H	1:A:518:ASN:HD22	1.17	0.92
2:D:75:ILE:HG22	2:D:114:ILE:HD12	1.49	0.92
1:A:189:PRO:HA	1:A:193:PRO:HG2	1.52	0.89
1:A:5:LEU:HD23	1:A:7:VAL:HG22	1.54	0.89
2:B:5:GLN:HG2	2:B:7:ASP:H	1.37	0.88
2:B:94:HIS:HD2	2:B:96:LEU:H	1.19	0.87
1:A:248:VAL:HG12	1:A:259:VAL:HG22	1.54	0.87
1:C:45:ASP:OD2	1:C:47:SER:HB3	1.75	0.87
1:A:176:SER:HB2	1:A:225:ASP:OD2	1.76	0.86
1:A:203:LEU:HB2	1:A:208:LEU:HB2	1.58	0.85
2:B:8:VAL:HG22	2:B:9:THR:H	1.40	0.85
2:B:23:HIS:HD1	2:B:277:GLY:H	1.26	0.82
2:B:281:ARG:NH1	4:B:1044:HOH:O	2.11	0.81
1:C:248:VAL:HG12	1:C:259:VAL:HG22	1.60	0.81
1:A:294:ASN:OD1	4:A:580:HOH:O	1.97	0.81
1:C:321:ILE:HG13	1:C:328:GLN:HG2	1.61	0.81
2:D:5:GLN:HB3	2:D:8:VAL:H	1.45	0.80
2:B:202:ALA:HA	2:B:207:LEU:CD2	2.11	0.80
2:D:30:TYR:HA	2:D:33:LYS:HE2	1.63	0.80
1:C:551:ILE:O	1:C:552:GLN:HB2	1.81	0.80
1:A:176:SER:O	1:A:177:ASN:HB3	1.80	0.80
2:D:321:GLN:HG2	2:D:326:GLN:NE2	1.96	0.80
1:C:498:LEU:H	1:C:518:ASN:HD22	1.26	0.79
2:D:54:LEU:HD11	2:D:71:ILE:HD13	1.65	0.79
2:B:14:ALA:HB1	2:B:15:PRO:CD	2.14	0.78
2:B:14:ALA:HB1	2:B:15:PRO:HD3	1.65	0.78
1:A:141:ARG:NH1	2:B:234:GLU:HB2	1.99	0.77
1:A:412:LYS:HD3	4:A:816:HOH:O	1.85	0.76
2:B:94:HIS:CD2	2:B:96:LEU:H	2.02	0.76
1:A:347:THR:OG1	1:A:440:TYR:HE1	1.68	0.76
2:D:75:ILE:HG22	2:D:114:ILE:CD1	2.17	0.75
2:B:127:GLN:HE22	2:B:163:ASN:H	1.34	0.74
1:C:81:SER:HB2	1:C:82:PRO:HD2	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:42:SER:O	2:D:45:LEU:HD23	1.89	0.72
2:B:281:ARG:HG3	2:B:281:ARG:HH11	1.54	0.72
1:A:289:THR:HG21	1:A:293:ARG:O	1.89	0.72
1:C:240:GLU:HB2	1:C:241:PRO:HD3	1.71	0.72
2:B:202:ALA:HA	2:B:207:LEU:HD21	1.72	0.72
2:B:116:VAL:HG12	4:B:940:HOH:O	1.90	0.72
2:D:23:HIS:HD1	2:D:277:GLY:H	1.37	0.71
1:C:163:GLU:HG2	1:C:183:TYR:OH	1.90	0.71
2:D:19:LEU:H	2:D:271:GLN:HE22	1.37	0.71
1:A:197:SER:OG	1:A:198:GLY:N	2.21	0.71
1:A:498:LEU:H	1:A:518:ASN:ND2	1.87	0.71
1:C:310:ASN:ND2	1:C:312:GLN:NE2	2.38	0.71
1:C:405:LEU:HD11	1:C:430:LEU:HD11	1.72	0.70
1:A:162:GLU:O	1:A:165:ALA:HB3	1.91	0.70
1:A:523:SER:O	1:A:525:ALA:N	2.25	0.70
1:C:168:ASP:O	1:C:171:ILE:HG12	1.90	0.70
1:A:347:THR:HG1	1:A:440:TYR:HE1	1.37	0.70
1:C:353:ARG:HB2	4:C:801:HOH:O	1.92	0.69
2:B:275:THR:HG23	2:B:276:GLY:O	1.92	0.69
1:C:539:ASN:HD21	1:C:541:GLN:HG3	1.58	0.69
1:C:520:LEU:H	1:C:543:ASN:HD22	1.38	0.69
1:A:232:HIS:O	1:A:236:LEU:HD13	1.93	0.69
1:A:393:ARG:O	1:A:394:ALA:C	2.36	0.69
2:D:202:ALA:HA	2:D:207:LEU:CD2	2.22	0.69
1:C:289:THR:HG21	1:C:293:ARG:O	1.93	0.69
1:C:360:LYS:HA	1:C:363:VAL:HG13	1.72	0.69
1:A:203:LEU:HB3	1:A:207:VAL:CG1	2.22	0.68
1:A:520:LEU:H	1:A:543:ASN:HD22	1.41	0.68
2:B:11:LYS:HB2	4:B:1050:HOH:O	1.93	0.68
2:D:202:ALA:HA	2:D:207:LEU:HD21	1.75	0.68
1:A:288:ARG:O	1:A:301:LEU:HD13	1.93	0.67
1:A:520:LEU:HB3	1:A:545:LEU:HD13	1.73	0.67
2:D:4:GLN:HG3	2:D:236:LEU:HD21	1.74	0.67
1:A:176:SER:HA	4:A:688:HOH:O	1.94	0.67
1:A:168:ASP:OD2	1:A:184:ARG:NH1	2.28	0.67
2:B:37:TYR:HD1	2:B:38:GLU:H	1.41	0.67
1:A:315:GLN:OE1	4:A:815:HOH:O	2.12	0.67
1:A:28:TYR:CE1	1:A:55:ILE:HG23	2.29	0.66
1:A:346:ALA:HA	1:A:351:LEU:HB2	1.76	0.66
1:C:291:ASP:OD2	4:C:777:HOH:O	2.14	0.66
1:A:208:LEU:HD21	4:A:846:HOH:O	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:HIS:HA	1:A:263:ARG:NH2	2.08	0.66
2:B:128:LYS:HB3	2:B:129:GLU:OE1	1.94	0.66
1:A:402:LYS:N	4:A:704:HOH:O	2.28	0.66
2:D:42:SER:OG	2:D:45:LEU:HD21	1.95	0.66
1:A:203:LEU:H	1:A:208:LEU:HD22	1.60	0.66
1:A:393:ARG:O	1:A:395:LEU:N	2.29	0.65
2:B:3:THR:HB	2:B:9:THR:HA	1.76	0.65
2:D:129:GLU:CD	2:D:129:GLU:H	2.05	0.65
1:C:165:ALA:HA	1:C:168:ASP:OD2	1.96	0.65
1:C:518:ASN:HB2	1:C:543:ASN:HD21	1.62	0.65
1:A:210:LYS:HG3	4:A:814:HOH:O	1.97	0.65
4:A:810:HOH:O	2:B:187:SER:HB3	1.97	0.65
1:C:545:LEU:HD23	1:C:546:CYS:N	2.12	0.65
2:D:17:THR:HB	4:D:1038:HOH:O	1.95	0.65
2:D:36:ASP:O	2:D:37:TYR:HB2	1.97	0.65
1:A:263:ARG:HG2	1:A:263:ARG:HH21	1.62	0.65
1:C:498:LEU:H	1:C:518:ASN:ND2	1.95	0.64
2:D:115:ASN:HD22	2:D:115:ASN:C	2.05	0.64
1:A:463:LEU:HD12	1:A:486:ARG:HB2	1.78	0.64
1:A:351:LEU:HD11	1:A:461:GLN:NE2	2.13	0.64
2:B:19:LEU:H	2:B:271:GLN:HE22	1.44	0.64
1:C:523:SER:HB3	1:C:548:GLU:OE1	1.98	0.64
1:A:278:VAL:O	1:A:279:ASP:HB2	1.97	0.64
1:A:16:ALA:O	1:A:17:LYS:C	2.40	0.64
1:C:522:GLN:O	1:C:524:ALA:N	2.29	0.64
1:C:539:ASN:ND2	1:C:541:GLN:HG3	2.13	0.64
2:B:243:TRP:CZ3	2:B:300:LEU:HD22	2.33	0.63
1:C:192:HIS:HB3	1:C:204:PRO:HG2	1.80	0.63
1:C:208:LEU:CD2	1:C:360:LYS:HE3	2.28	0.63
2:B:14:ALA:CB	2:B:15:PRO:CD	2.77	0.63
1:A:313:LEU:HB3	1:A:314:PRO:HD2	1.80	0.63
2:D:127:GLN:HE22	2:D:163:ASN:H	1.47	0.63
2:B:120:VAL:HG12	2:B:124:GLN:HE21	1.64	0.63
2:D:23:HIS:NE2	2:D:271:GLN:NE2	2.45	0.63
1:C:393:ARG:HD3	4:C:588:HOH:O	1.99	0.62
2:D:187:SER:HB3	4:D:1076:HOH:O	1.98	0.62
2:D:9:THR:OG1	2:D:10:ILE:N	2.31	0.62
2:B:232:ARG:HH12	2:B:235:LYS:HZ2	1.47	0.62
2:D:33:LYS:O	2:D:34:LYS:HB2	1.99	0.62
2:B:3:THR:HG22	2:B:4:GLN:H	1.64	0.62
2:B:15:PRO:HG3	2:B:273:GLU:HG3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:80:LYS:HD2	1:C:84:GLU:HG2	1.83	0.61
1:C:250:VAL:HG12	1:C:257:LEU:HD13	1.82	0.61
1:A:288:ARG:HB2	4:A:580:HOH:O	2.00	0.61
1:A:334:LEU:HD12	1:A:337:ARG:HE	1.65	0.61
1:A:372:LYS:NZ	1:A:403:GLU:OE1	2.32	0.61
1:C:193:PRO:HB2	1:C:194:GLN:HG3	1.82	0.61
2:D:32:SER:O	2:D:33:LYS:C	2.44	0.61
1:C:243:ASP:OD1	1:C:244:VAL:HG23	2.01	0.61
1:A:170:LEU:HD22	1:A:174:ASN:ND2	2.15	0.61
2:D:232:ARG:NH2	4:D:1025:HOH:O	2.33	0.61
1:A:393:ARG:HH22	1:A:433:ASN:ND2	1.98	0.61
1:A:531:SER:O	1:A:533:PRO:HD3	2.01	0.61
1:A:215:VAL:HG11	1:A:231:TYR:HD2	1.66	0.60
1:C:144:HIS:HE1	4:C:778:HOH:O	1.84	0.60
1:C:238:ARG:NH1	1:C:353:ARG:H	1.99	0.60
1:C:496:ASN:HB2	1:C:518:ASN:HD21	1.66	0.60
1:C:509:ARG:NH1	1:C:534:ARG:HH12	2.00	0.60
2:D:14:ALA:CB	2:D:15:PRO:HD3	2.31	0.60
1:A:353:ARG:NH2	1:A:356:LEU:HG	2.17	0.60
1:A:518:ASN:HB2	1:A:543:ASN:HD21	1.67	0.60
2:B:330:VAL:O	2:B:331:SER:HB2	2.00	0.60
1:A:244:VAL:HG12	1:A:262:SER:OG	2.01	0.60
1:C:29:GLN:O	1:C:33:GLN:HG3	2.02	0.60
2:B:4:GLN:HG3	2:B:236:LEU:HD11	1.83	0.60
2:D:246:LEU:HD21	2:D:301:LEU:HG	1.82	0.60
1:A:277:MET:HG3	1:A:319:ARG:NH2	2.17	0.59
2:D:330:VAL:O	2:D:331:SER:HB2	1.99	0.59
1:C:289:THR:CG2	1:C:291:ASP:OD1	2.50	0.59
1:A:211:GLU:O	1:A:215:VAL:HG13	2.03	0.59
1:A:310:ASN:OD1	1:A:312:GLN:HG2	2.02	0.59
2:B:321:GLN:HG2	2:B:326:GLN:NE2	2.18	0.59
2:D:109:ASP:CG	2:D:322:ARG:HH21	2.10	0.59
1:C:271:MET:HB2	4:D:1006:HOH:O	2.02	0.59
1:A:74:GLN:HE21	1:A:115:TRP:HZ2	1.51	0.59
1:A:192:HIS:HB2	1:A:193:PRO:HD3	1.84	0.59
2:D:184:ARG:NH2	4:D:971:HOH:O	2.30	0.59
1:A:39:ARG:HA	4:A:813:HOH:O	2.02	0.59
2:B:69:GLU:HG3	4:B:1051:HOH:O	2.02	0.59
1:C:312:GLN:C	1:C:313:LEU:HD12	2.28	0.59
1:A:189:PRO:HA	1:A:193:PRO:CG	2.26	0.59
1:A:204:PRO:O	1:A:205:GLU:C	2.45	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:O	1:A:373:GLU:HG3	2.01	0.59
1:C:273:THR:H	1:C:323:THR:HB	1.68	0.59
1:A:215:VAL:HG11	1:A:231:TYR:CD2	2.38	0.58
1:A:243:ASP:O	1:A:244:VAL:HG23	2.03	0.58
1:C:203:LEU:HB3	1:C:207:VAL:HG13	1.85	0.58
1:A:237:GLY:HA3	4:A:841:HOH:O	2.03	0.58
1:A:347:THR:HG22	1:A:348:ASP:CG	2.28	0.58
2:B:172:LEU:CD1	2:B:209:GLN:HG2	2.32	0.58
2:D:46:ARG:HG2	2:D:74:PHE:CZ	2.38	0.58
1:C:4:ARG:O	2:D:285:MET:HG3	2.04	0.58
1:A:247:CYS:SG	1:A:463:LEU:HD23	2.44	0.58
1:A:397:PRO:HD2	4:A:632:HOH:O	2.02	0.58
1:A:33:GLN:O	1:A:37:GLN:HG2	2.03	0.58
1:A:345:SER:HB2	1:A:347:THR:HB	1.86	0.58
2:D:317:GLU:O	2:D:321:GLN:HG3	2.04	0.58
1:A:496:ASN:HB2	1:A:518:ASN:HD21	1.67	0.57
1:C:200:GLN:HG3	1:C:354:CYS:SG	2.44	0.57
1:A:394:ALA:HB1	4:A:729:HOH:O	2.04	0.57
1:A:393:ARG:HH22	1:A:433:ASN:CG	2.12	0.57
2:B:54:LEU:HD12	2:B:104:ILE:HG23	1.86	0.57
2:B:8:VAL:CG2	2:B:9:THR:H	2.14	0.57
2:B:108:TYR:O	2:B:109:ASP:C	2.46	0.57
1:A:203:LEU:CB	1:A:208:LEU:HB2	2.34	0.57
1:C:105:LYS:HD3	4:C:781:HOH:O	2.04	0.57
2:B:202:ALA:HA	2:B:207:LEU:HD22	1.84	0.57
1:A:233:ARG:HG3	1:A:390:LEU:HD13	1.85	0.57
2:B:81:GLU:HG2	4:B:1056:HOH:O	2.03	0.57
1:A:188:LEU:HB2	1:A:189:PRO:HD3	1.86	0.57
1:A:263:ARG:NH2	1:A:263:ARG:HG2	2.20	0.57
2:B:232:ARG:HH12	2:B:235:LYS:NZ	2.03	0.57
1:A:238:ARG:CZ	1:A:352:PHE:HA	2.35	0.56
1:A:319:ARG:HG2	1:A:330:GLU:HB2	1.87	0.56
2:B:232:ARG:HB2	2:B:233:PRO:HD2	1.88	0.56
1:A:334:LEU:CD1	1:A:337:ARG:HE	2.17	0.56
1:A:393:ARG:HH22	1:A:433:ASN:HD21	1.54	0.56
2:B:272:ASP:OD1	2:B:274:GLU:O	2.23	0.56
1:C:346:ALA:HA	1:C:351:LEU:CB	2.34	0.56
2:D:5:GLN:N	2:D:8:VAL:O	2.38	0.56
1:A:549:GLU:OE2	1:A:554:ARG:HD2	2.06	0.56
1:C:523:SER:OG	1:C:554:ARG:NH1	2.38	0.56
1:A:398:LEU:HD13	4:A:617:HOH:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:GLU:O	2:B:42:SER:N	2.38	0.56
1:A:141:ARG:HH12	2:B:234:GLU:HB2	1.67	0.55
1:C:133:ALA:O	1:C:137:GLU:HG2	2.07	0.55
1:C:546:CYS:HA	1:C:551:ILE:HD13	1.87	0.55
1:A:216:GLN:NE2	4:A:633:HOH:O	2.40	0.55
1:A:141:ARG:HG3	4:A:812:HOH:O	2.05	0.55
1:C:518:ASN:CB	1:C:543:ASN:HD21	2.19	0.55
1:A:468:LEU:HD23	1:A:491:LEU:HD13	1.88	0.55
2:D:4:GLN:HE21	2:D:236:LEU:HD11	1.71	0.55
1:A:396:ASP:OD1	4:A:632:HOH:O	2.18	0.55
1:C:23:GLN:O	1:C:27:LEU:HD13	2.07	0.55
2:D:150:VAL:HG13	2:D:203:ILE:HG21	1.89	0.55
1:A:156:ALA:O	1:A:157:ALA:HB3	2.07	0.55
1:A:167:THR:HA	1:A:170:LEU:HD12	1.87	0.55
1:A:163:GLU:HG2	1:A:183:TYR:OH	2.07	0.55
1:C:203:LEU:CB	1:C:207:VAL:HG13	2.37	0.55
2:B:111:ILE:HG13	2:B:112:HIS:N	2.23	0.54
1:A:105:LYS:NZ	4:A:840:HOH:O	2.36	0.54
1:A:277:MET:HG3	1:A:319:ARG:HH21	1.73	0.54
1:C:97:GLU:OE1	1:C:134:ARG:NH1	2.40	0.54
2:D:127:GLN:HB2	2:D:133:PHE:CE2	2.42	0.54
1:A:522:GLN:O	1:A:523:SER:C	2.48	0.54
2:D:44:TYR:CZ	2:D:45:LEU:HD22	2.42	0.54
2:B:23:HIS:HD1	2:B:277:GLY:N	2.02	0.54
1:C:4:ARG:HB3	2:D:285:MET:SD	2.48	0.54
1:C:551:ILE:O	1:C:552:GLN:CB	2.55	0.54
1:C:74:GLN:NE2	1:C:119:ARG:HH12	2.05	0.54
1:A:518:ASN:CB	1:A:543:ASN:HD21	2.21	0.53
1:C:166:PHE:O	1:C:170:LEU:HB2	2.08	0.53
1:C:208:LEU:HD23	1:C:360:LYS:HE3	1.89	0.53
2:D:94:HIS:CD2	2:D:96:LEU:H	2.09	0.53
1:A:263:ARG:HB2	1:A:264:PRO:HD2	1.89	0.53
1:A:393:ARG:NH2	1:A:433:ASN:HD21	2.07	0.53
2:D:95:LEU:HD23	2:D:145:PHE:HB3	1.91	0.53
2:B:49:GLY:HA2	2:B:52:TRP:CE3	2.43	0.53
1:A:216:GLN:HE21	1:A:220:PHE:HE1	1.55	0.53
1:A:463:LEU:CD1	1:A:486:ARG:HB2	2.39	0.53
2:B:19:LEU:H	2:B:271:GLN:NE2	2.06	0.53
2:D:12:SER:O	2:D:13:ASP:C	2.51	0.53
2:B:299:SER:HB2	2:B:306:ILE:CG2	2.38	0.53
1:C:509:ARG:NH1	1:C:534:ARG:NH1	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:VAL:HG22	2:B:9:THR:N	2.19	0.53
1:C:353:ARG:NE	1:C:394:ALA:O	2.42	0.53
1:C:418:ARG:HA	4:D:1072:HOH:O	2.08	0.53
2:D:115:ASN:HD22	2:D:116:VAL:N	2.07	0.53
1:A:160:PRO:HB2	1:A:191:LEU:HD21	1.91	0.52
1:A:232:HIS:NE2	1:A:236:LEU:HD11	2.24	0.52
1:C:203:LEU:HB3	1:C:204:PRO:HD2	1.91	0.52
2:D:4:GLN:NE2	2:D:236:LEU:HD11	2.24	0.52
2:D:49:GLY:HA2	2:D:52:TRP:CE3	2.44	0.52
1:A:134:ARG:NE	4:A:723:HOH:O	2.30	0.52
1:A:160:PRO:C	1:A:191:LEU:HD21	2.35	0.52
1:A:523:SER:H	1:A:545:LEU:HB2	1.75	0.52
1:A:192:HIS:H	1:A:193:PRO:CD	2.22	0.52
2:D:272:ASP:OD1	2:D:274:GLU:O	2.27	0.52
1:C:226:GLN:NE2	4:C:789:HOH:O	2.41	0.52
1:A:242:HIS:ND1	1:A:325:SER:OG	2.42	0.52
1:A:543:ASN:HB2	1:A:545:LEU:HD22	1.91	0.52
2:D:120:VAL:HG12	2:D:124:GLN:NE2	2.25	0.52
1:A:215:VAL:CG2	1:A:232:HIS:HB2	2.39	0.52
1:A:550:GLY:O	1:A:552:GLN:N	2.43	0.52
2:D:137:ILE:HD11	4:D:1088:HOH:O	2.09	0.52
1:A:476:ARG:HD2	4:A:689:HOH:O	2.10	0.52
2:B:246:LEU:HD21	2:B:301:LEU:HG	1.91	0.52
2:B:281:ARG:HB3	2:B:282:PRO:CD	2.40	0.52
1:C:136:LEU:HD22	1:C:145:CYS:SG	2.50	0.52
2:D:45:LEU:HD23	2:D:45:LEU:H	1.73	0.52
2:D:183:CYS:HB3	4:D:1071:HOH:O	2.09	0.52
1:C:188:LEU:HB2	1:C:189:PRO:HD3	1.93	0.51
1:C:162:GLU:HG2	4:C:798:HOH:O	2.10	0.51
2:D:36:ASP:O	2:D:37:TYR:CB	2.57	0.51
2:B:322:ARG:HG3	2:B:322:ARG:HH11	1.75	0.51
1:A:13:GLN:O	1:A:15:GLU:N	2.43	0.51
2:B:232:ARG:HB2	2:B:233:PRO:CD	2.41	0.51
1:C:346:ALA:HA	1:C:351:LEU:HB2	1.92	0.51
2:D:150:VAL:HG22	2:D:159:LEU:CD1	2.40	0.51
1:A:179:SER:HB2	2:B:188:GLU:OE2	2.11	0.51
1:A:349:GLU:O	1:A:350:GLN:C	2.52	0.51
1:A:447:HIS:HB3	4:A:641:HOH:O	2.10	0.51
2:B:172:LEU:HD11	2:B:209:GLN:HG2	1.93	0.51
2:D:115:ASN:HD21	2:D:117:ASP:HB2	1.75	0.51
1:C:20:GLU:O	1:C:21:ARG:CB	2.58	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:ILE:HG23	4:A:830:HOH:O	2.10	0.51
2:B:12:SER:O	2:B:13:ASP:C	2.51	0.51
1:C:160:PRO:HB2	1:C:191:LEU:HD12	1.92	0.51
1:C:539:ASN:HD22	1:C:539:ASN:C	2.19	0.51
1:C:549:GLU:HB2	4:C:717:HOH:O	2.11	0.51
1:A:318:PHE:O	1:A:330:GLU:HA	2.11	0.51
2:D:85:VAL:HG21	2:D:101:ALA:HB2	1.92	0.50
2:D:324:ASN:ND2	4:D:1069:HOH:O	2.44	0.50
1:A:333:LEU:HB2	1:A:340:CYS:SG	2.52	0.50
2:D:62:GLN:O	2:D:63:LEU:C	2.54	0.50
1:A:289:THR:CG2	1:A:293:ARG:O	2.59	0.50
1:A:549:GLU:C	1:A:551:ILE:H	2.19	0.50
1:C:240:GLU:HB2	1:C:241:PRO:CD	2.41	0.50
1:C:499:GLU:HB3	4:C:794:HOH:O	2.10	0.50
1:A:176:SER:OG	1:A:177:ASN:N	2.42	0.50
1:A:319:ARG:CG	1:A:330:GLU:HG3	2.42	0.50
1:A:282:PRO:HD2	4:A:822:HOH:O	2.11	0.50
2:B:163:ASN:ND2	2:B:166:LYS:H	2.08	0.50
2:B:39:TYR:O	2:B:46:ARG:NH2	2.44	0.50
2:B:3:THR:N	4:B:955:HOH:O	2.44	0.50
1:C:170:LEU:O	1:C:175:PHE:O	2.30	0.50
1:C:49:LEU:HD13	1:C:72:VAL:HG11	1.94	0.49
1:C:281:ALA:HB1	1:C:282:PRO:HD2	1.94	0.49
2:B:85:VAL:HG21	2:B:101:ALA:HB2	1.94	0.49
1:C:211:GLU:O	1:C:215:VAL:HG13	2.12	0.49
1:A:337:ARG:HG3	4:A:732:HOH:O	2.11	0.49
1:C:397:PRO:HD2	4:C:673:HOH:O	2.11	0.49
1:A:215:VAL:HG21	1:A:232:HIS:HB2	1.94	0.49
1:A:246:CYS:HA	1:A:344:ASP:OD2	2.13	0.49
1:C:554:ARG:HD2	4:C:717:HOH:O	2.11	0.49
1:C:248:VAL:HG12	1:C:259:VAL:CG2	2.37	0.49
1:C:295:ARG:HG2	4:C:780:HOH:O	2.12	0.49
2:D:243:TRP:CZ3	2:D:300:LEU:HD22	2.48	0.49
1:A:232:HIS:CE1	1:A:236:LEU:HD11	2.47	0.49
2:D:172:LEU:CD1	2:D:209:GLN:HG2	2.42	0.49
2:B:94:HIS:HD2	2:B:96:LEU:N	1.97	0.49
1:A:418:ARG:HA	4:B:994:HOH:O	2.12	0.49
2:B:281:ARG:NH1	2:B:281:ARG:HG3	2.22	0.49
1:C:93:LEU:CD2	1:C:116:LEU:HD23	2.43	0.48
1:A:242:HIS:O	1:A:244:VAL:N	2.44	0.48
1:A:314:PRO:HB2	1:A:335:LYS:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:15:PRO:HG3	2:B:273:GLU:CG	2.42	0.48
1:C:504:VAL:CG1	1:C:529:LEU:HD22	2.44	0.48
2:D:105:LEU:HB3	2:D:111:ILE:HA	1.96	0.48
1:C:258:SER:OG	1:C:486:ARG:HD3	2.13	0.48
1:C:270:ARG:HG2	2:D:165:GLU:OE2	2.13	0.48
1:C:529:LEU:N	1:C:529:LEU:HD23	2.28	0.48
1:A:431:LEU:HD23	1:A:431:LEU:C	2.38	0.48
1:A:164:LEU:HD12	1:A:184:ARG:NH1	2.27	0.48
2:B:137:ILE:HD13	2:B:137:ILE:H	1.77	0.48
2:B:202:ALA:CA	2:B:207:LEU:HD21	2.43	0.48
2:B:272:ASP:HB2	2:B:286:VAL:HG11	1.96	0.48
1:C:504:VAL:HG12	1:C:529:LEU:HD22	1.95	0.48
2:D:109:ASP:OD2	2:D:322:ARG:NH2	2.47	0.48
2:D:202:ALA:HA	2:D:207:LEU:HD22	1.95	0.48
1:A:141:ARG:NH1	2:B:233:PRO:O	2.42	0.48
1:A:270:ARG:NH2	2:B:165:GLU:HG3	2.29	0.48
2:B:231:GLY:HA3	4:B:1033:HOH:O	2.12	0.48
1:A:174:ASN:OD1	1:A:175:PHE:N	2.47	0.48
1:A:310:ASN:OD1	1:A:310:ASN:C	2.55	0.48
1:A:371:CYS:HB3	1:A:388:ILE:HG13	1.96	0.48
1:A:529:LEU:HD12	1:A:538:LEU:HD22	1.96	0.48
1:C:526:ILE:O	1:C:529:LEU:HG	2.12	0.48
2:D:115:ASN:C	2:D:115:ASN:ND2	2.71	0.48
2:D:120:VAL:HG21	2:D:158:LYS:HD2	1.94	0.48
1:A:192:HIS:CB	1:A:193:PRO:HD3	2.44	0.48
2:D:43:GLU:OE2	2:D:46:ARG:NH2	2.44	0.48
1:A:211:GLU:OE1	1:A:214:LEU:HD12	2.14	0.47
1:C:15:GLU:O	1:C:16:ALA:HB3	2.13	0.47
2:D:34:LYS:O	2:D:36:ASP:N	2.47	0.47
1:A:262:SER:HB3	4:A:780:HOH:O	2.14	0.47
1:C:232:HIS:HE1	1:C:367:GLU:OE1	1.97	0.47
1:A:319:ARG:HG2	1:A:330:GLU:HG3	1.95	0.47
1:A:347:THR:HG22	1:A:348:ASP:N	2.28	0.47
2:B:134:ALA:HA	2:B:140:GLU:O	2.14	0.47
1:A:141:ARG:O	2:B:232:ARG:NH2	2.43	0.47
1:A:398:LEU:HD11	1:A:440:TYR:CE2	2.49	0.47
1:C:162:GLU:O	1:C:165:ALA:HB3	2.14	0.47
1:C:268:GLY:HA2	1:C:273:THR:HB	1.95	0.47
2:D:182:GLY:C	2:D:193:GLN:HG2	2.40	0.47
2:D:274:GLU:O	2:D:276:GLY:N	2.46	0.47
1:A:365:GLN:NE2	1:A:400:TYR:OH	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:THR:CB	2:B:10:ILE:H	2.27	0.47
2:B:12:SER:O	2:B:14:ALA:N	2.48	0.47
1:C:232:HIS:HD2	4:C:649:HOH:O	1.97	0.47
1:C:346:ALA:HA	1:C:351:LEU:HB3	1.94	0.47
1:A:254:GLU:OE2	1:A:509:ARG:NH1	2.42	0.47
1:A:295:ARG:CB	1:A:296:PRO:CD	2.93	0.47
2:B:272:ASP:CG	2:B:275:THR:HG22	2.39	0.47
1:A:205:GLU:O	1:A:209:LEU:HG	2.15	0.47
1:C:43:GLU:HG3	4:C:737:HOH:O	2.15	0.47
2:D:80:HIS:CE1	2:D:93:PRO:HD3	2.50	0.47
1:A:74:GLN:HE22	2:B:138:TRP:HZ3	1.63	0.47
1:A:146:TRP:NE1	1:A:179:SER:OG	2.48	0.47
1:A:398:LEU:CD1	1:A:440:TYR:CE2	2.98	0.47
1:A:466:THR:OG1	1:A:467:HIS:HD2	1.97	0.47
1:C:93:LEU:HD21	1:C:116:LEU:HD23	1.97	0.47
1:C:486:ARG:NH2	4:C:805:HOH:O	2.34	0.47
1:A:348:ASP:HB2	1:A:349:GLU:OE1	2.15	0.47
2:B:120:VAL:HG12	2:B:124:GLN:NE2	2.28	0.47
1:A:47:SER:O	1:A:50:GLU:HG2	2.15	0.46
1:A:346:ALA:HA	1:A:351:LEU:CB	2.43	0.46
2:B:172:LEU:CD2	2:B:209:GLN:HG2	2.45	0.46
2:B:323:VAL:HG23	2:B:325:VAL:HG23	1.98	0.46
1:A:353:ARG:NH1	1:A:355:GLU:HA	2.30	0.46
1:C:210:LYS:HA	1:C:213:GLU:OE2	2.15	0.46
2:D:44:TYR:CE2	2:D:45:LEU:HD22	2.50	0.46
1:A:146:TRP:CE2	1:A:179:SER:OG	2.69	0.46
1:A:289:THR:CG2	1:A:291:ASP:OD1	2.63	0.46
2:D:120:VAL:HG12	2:D:124:GLN:HE21	1.80	0.46
1:A:223:PRO:HG2	1:A:378:GLU:OE2	2.15	0.46
1:C:353:ARG:NH2	1:C:395:LEU:O	2.46	0.46
1:A:443:VAL:CG2	1:A:445:VAL:HG22	2.45	0.46
1:C:159:ALA:HA	1:C:160:PRO:HD2	1.76	0.46
1:C:368:LEU:HD11	1:C:372:LYS:HE3	1.97	0.46
2:D:166:LYS:HE2	2:D:169:GLU:OE1	2.16	0.46
1:A:17:LYS:O	1:A:18:ARG:C	2.59	0.46
1:A:140:GLU:OE2	1:A:175:PHE:HD2	1.99	0.46
1:A:243:ASP:HB3	1:A:325:SER:HB3	1.98	0.46
1:A:263:ARG:CZ	4:A:780:HOH:O	2.64	0.46
1:A:319:ARG:HG2	1:A:330:GLU:CB	2.46	0.46
1:C:312:GLN:O	1:C:313:LEU:HD12	2.15	0.46
1:A:310:ASN:CG	1:A:312:GLN:HG2	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:396:ASP:O	1:A:397:PRO:C	2.60	0.45
2:B:317:GLU:O	2:B:321:GLN:HG3	2.15	0.45
1:C:134:ARG:HH11	1:C:134:ARG:HD2	1.51	0.45
1:C:353:ARG:HG3	1:C:393:ARG:O	2.16	0.45
1:C:557:GLU:HG3	4:C:755:HOH:O	2.17	0.45
1:A:164:LEU:CD1	1:A:184:ARG:NH1	2.79	0.45
1:A:367:GLU:OE1	1:A:391:LEU:HD11	2.16	0.45
1:A:539:ASN:C	1:A:539:ASN:HD22	2.22	0.45
1:A:81:SER:HB2	1:A:82:PRO:HD2	1.98	0.45
1:C:101:ARG:HD2	4:C:779:HOH:O	2.16	0.45
1:A:244:VAL:CG1	1:A:262:SER:OG	2.63	0.45
2:B:137:ILE:HG22	4:B:1059:HOH:O	2.16	0.45
1:C:520:LEU:H	1:C:543:ASN:ND2	2.12	0.45
1:A:13:GLN:O	1:A:14:ALA:C	2.59	0.45
1:A:545:LEU:HD23	1:A:546:CYS:N	2.31	0.45
1:C:89:VAL:HG13	1:C:116:LEU:HD21	1.99	0.45
1:C:10:SER:O	1:C:11:GLU:C	2.60	0.45
1:C:74:GLN:NE2	1:C:119:ARG:NH1	2.64	0.45
1:A:203:LEU:O	1:A:204:PRO:C	2.59	0.45
1:A:311:ASP:HB3	4:A:701:HOH:O	2.17	0.45
1:A:351:LEU:HD11	1:A:461:GLN:CD	2.41	0.45
1:C:202:ARG:HD3	1:C:234:TRP:O	2.17	0.45
2:D:8:VAL:HG12	2:D:9:THR:H	1.81	0.45
2:D:115:ASN:ND2	2:D:118:LYS:H	2.15	0.45
1:A:81:SER:OG	1:A:84:GLU:HB2	2.17	0.44
1:A:204:PRO:O	1:A:207:VAL:HG12	2.17	0.44
1:A:216:GLN:O	1:A:217:ASN:C	2.58	0.44
1:C:242:HIS:O	1:C:244:VAL:HB	2.17	0.44
2:D:18:LEU:HD12	2:D:271:GLN:HE22	1.80	0.44
2:D:220:CYS:HA	2:D:258:ILE:CD1	2.47	0.44
1:A:334:LEU:HG	1:A:337:ARG:HG3	1.99	0.44
1:C:25:LEU:HD21	2:D:40:CYS:SG	2.57	0.44
1:C:356:LEU:HD23	1:C:361:SER:OG	2.18	0.44
1:A:80:LYS:HD2	1:A:84:GLU:HG2	2.00	0.44
2:B:67:ASN:O	2:B:71:ILE:HG13	2.18	0.44
2:B:83:GLY:HA3	2:B:118:LYS:HG3	1.99	0.44
2:B:253:GLY:O	2:B:254:ARG:HD3	2.17	0.44
1:C:393:ARG:HD2	1:C:429:PHE:CG	2.52	0.44
2:D:150:VAL:HG13	2:D:203:ILE:CG2	2.47	0.44
1:A:440:TYR:HB3	4:A:825:HOH:O	2.16	0.44
2:B:176:ASN:ND2	4:B:1018:HOH:O	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:VAL:O	1:C:210:LYS:HG3	2.17	0.44
1:C:343:ARG:HD2	1:C:464:LEU:HD12	2.00	0.44
1:C:360:LYS:CA	1:C:363:VAL:HG13	2.45	0.44
1:A:122:GLU:HG3	4:A:817:HOH:O	2.16	0.44
2:B:76:LYS:HG3	2:B:113:VAL:O	2.17	0.44
1:C:205:GLU:O	1:C:209:LEU:HG	2.18	0.44
1:A:333:LEU:HD12	1:A:337:ARG:HB2	2.00	0.44
1:A:517:ASN:HD22	1:A:542:GLY:HA3	1.82	0.44
2:D:108:TYR:O	2:D:109:ASP:C	2.61	0.44
1:A:161:ALA:N	1:A:191:LEU:HD21	2.33	0.44
1:A:217:ASN:HB2	4:A:649:HOH:O	2.16	0.44
1:A:393:ARG:C	1:A:395:LEU:N	2.74	0.44
1:C:46:GLU:CD	1:C:46:GLU:H	2.25	0.44
1:C:89:VAL:HG11	1:C:120:LEU:HD21	2.00	0.44
2:B:52:TRP:HA	2:B:292:LEU:HD22	1.99	0.44
2:B:229:LEU:HB2	2:B:242:SER:OG	2.18	0.44
1:C:289:THR:HG23	1:C:291:ASP:OD1	2.17	0.44
1:C:319:ARG:HG3	1:C:330:GLU:HG2	2.00	0.44
1:A:242:HIS:ND1	1:A:242:HIS:C	2.74	0.43
2:B:5:GLN:HG2	2:B:6:LYS:N	2.32	0.43
1:C:193:PRO:HB2	1:C:194:GLN:H	1.51	0.43
1:A:363:VAL:HG23	4:A:831:HOH:O	2.18	0.43
2:B:105:LEU:HB3	2:B:111:ILE:HA	2.00	0.43
1:C:350:GLN:OE1	1:C:354:CYS:HB3	2.17	0.43
1:A:498:LEU:N	1:A:518:ASN:HD22	1.99	0.43
1:C:243:ASP:CB	1:C:325:SER:OG	2.66	0.43
2:D:3:THR:N	2:D:10:ILE:H	2.15	0.43
2:D:275:THR:HG22	2:D:276:GLY:O	2.18	0.43
1:A:46:GLU:CD	1:A:46:GLU:H	2.24	0.43
1:A:82:PRO:HG3	4:A:594:HOH:O	2.18	0.43
2:B:21:GLU:HG3	2:D:305:GLN:NE2	2.33	0.43
1:C:123:PRO:HG2	1:C:125:TRP:CZ2	2.53	0.43
2:D:34:LYS:HA	4:D:1074:HOH:O	2.18	0.43
2:D:45:LEU:HD23	2:D:45:LEU:N	2.32	0.43
2:D:118:LYS:HB2	2:D:118:LYS:NZ	2.33	0.43
2:B:65:ARG:NH1	4:B:1004:HOH:O	2.46	0.43
1:C:501:VAL:HG23	1:C:529:LEU:HD21	2.00	0.43
1:A:164:LEU:O	1:A:165:ALA:C	2.61	0.43
1:A:208:LEU:HD13	1:A:235:LEU:HD22	2.01	0.43
1:A:343:ARG:HH21	1:A:461:GLN:HB3	1.84	0.43
1:C:195:PRO:HG3	4:C:782:HOH:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HD3	1:A:234:TRP:O	2.18	0.43
1:A:479:PRO:O	1:A:503:GLY:HA3	2.19	0.43
2:B:5:GLN:HG2	2:B:7:ASP:N	2.19	0.43
1:C:171:ILE:HD11	1:C:214:LEU:HD11	2.01	0.43
1:C:243:ASP:HB2	1:C:325:SER:OG	2.18	0.43
1:C:247:CYS:SG	1:C:463:LEU:HD23	2.59	0.43
1:C:321:ILE:HG13	1:C:328:GLN:CG	2.41	0.43
1:A:319:ARG:HG2	1:A:330:GLU:CG	2.49	0.42
1:C:203:LEU:HB3	1:C:207:VAL:CG1	2.47	0.42
2:D:94:HIS:HE1	4:D:970:HOH:O	2.01	0.42
1:C:238:ARG:HA	1:C:238:ARG:HD3	1.80	0.42
2:D:204:THR:O	2:D:205:SER:HB2	2.18	0.42
1:C:160:PRO:HB2	1:C:191:LEU:CD1	2.50	0.42
1:C:240:GLU:O	1:C:241:PRO:C	2.62	0.42
1:C:278:VAL:O	1:C:279:ASP:C	2.62	0.42
1:C:479:PRO:O	1:C:503:GLY:HA3	2.19	0.42
1:C:527:GLN:HB3	1:C:528:PRO:HD3	2.01	0.42
2:D:14:ALA:HB3	2:D:15:PRO:HD3	2.00	0.42
1:A:214:LEU:HD23	1:A:214:LEU:HA	1.83	0.42
1:C:289:THR:CG2	1:C:293:ARG:O	2.64	0.42
1:A:412:LYS:HB2	4:A:816:HOH:O	2.19	0.42
1:C:37:GLN:O	1:C:38:LYS:C	2.62	0.42
1:A:34:ALA:HA	1:A:37:GLN:CG	2.49	0.42
2:B:94:HIS:HE1	4:B:936:HOH:O	2.02	0.42
2:B:115:ASN:C	2:B:115:ASN:HD22	2.27	0.42
1:C:197:SER:OG	1:C:198:GLY:N	2.52	0.42
1:C:7:VAL:O	1:C:8:LYS:HG3	2.19	0.42
1:C:16:ALA:O	1:C:17:LYS:CB	2.67	0.42
1:C:125:TRP:CE3	1:C:152:VAL:HG13	2.55	0.42
1:A:141:ARG:HH11	2:B:234:GLU:HB2	1.79	0.42
2:B:258:ILE:HD12	2:B:258:ILE:HA	1.81	0.42
1:C:238:ARG:O	1:C:239:ALA:HB3	2.20	0.42
1:A:313:LEU:CB	1:A:314:PRO:HD2	2.45	0.42
1:C:431:LEU:C	1:C:431:LEU:HD23	2.44	0.42
2:D:14:ALA:CB	2:D:15:PRO:CD	2.98	0.42
2:D:320:LEU:HB3	2:D:325:VAL:O	2.20	0.42
1:A:45:ASP:OD2	1:A:47:SER:HB3	2.20	0.41
1:A:216:GLN:O	1:A:219:PHE:N	2.53	0.41
1:A:167:THR:HB	1:A:184:ARG:HD2	2.02	0.41
1:A:334:LEU:HD12	1:A:337:ARG:NE	2.34	0.41
1:A:555:LEU:HD23	1:A:555:LEU:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:232:ARG:NH1	2:B:235:LYS:NZ	2.67	0.41
2:D:72:LEU:HG	2:D:113:VAL:HG21	2.02	0.41
1:A:240:GLU:H	1:A:240:GLU:HG2	1.40	0.41
1:A:181:TRP:CH2	1:A:215:VAL:HG12	2.56	0.41
1:A:181:TRP:CZ3	1:A:215:VAL:HG12	2.55	0.41
1:A:257:LEU:HD23	1:A:276:LEU:HD22	2.01	0.41
2:B:317:GLU:OE2	2:B:326:GLN:OE1	2.38	0.41
2:D:29:SER:O	2:D:30:TYR:C	2.63	0.41
1:A:225:ASP:OD1	1:A:226:GLN:N	2.53	0.41
1:C:28:TYR:CZ	2:D:41:MET:HG2	2.56	0.41
1:C:41:ALA:HB1	4:C:737:HOH:O	2.20	0.41
1:C:194:GLN:HG3	1:C:194:GLN:H	1.38	0.41
2:B:95:LEU:O	2:B:96:LEU:C	2.64	0.41
2:B:280:ASP:OD2	2:B:281:ARG:NH1	2.54	0.41
1:C:550:GLY:O	1:C:551:ILE:C	2.64	0.41
2:D:8:VAL:HG12	2:D:9:THR:N	2.36	0.41
1:A:157:ALA:O	1:A:158:VAL:C	2.63	0.41
1:A:527:GLN:HB3	1:A:528:PRO:HD3	2.03	0.41
1:C:307:ALA:HB3	4:C:768:HOH:O	2.19	0.41
2:D:18:LEU:HD12	2:D:271:GLN:NE2	2.35	0.41
2:D:137:ILE:HD13	4:D:1007:HOH:O	2.20	0.41
1:A:191:LEU:HB3	1:A:192:HIS:CE1	2.55	0.41
1:A:211:GLU:HG2	4:A:814:HOH:O	2.21	0.41
1:A:238:ARG:NH1	1:A:351:LEU:O	2.54	0.41
1:A:402:LYS:HG3	4:A:755:HOH:O	2.19	0.41
1:C:254:GLU:O	1:C:255:ALA:C	2.64	0.41
2:D:19:LEU:H	2:D:271:GLN:NE2	2.10	0.41
2:D:262:LYS:HE2	2:D:262:LYS:HB3	1.91	0.41
1:A:80:LYS:HD3	1:A:80:LYS:HA	1.85	0.41
1:A:181:TRP:HB3	1:A:231:TYR:CD1	2.56	0.41
1:A:471:SER:HB3	1:A:492:GLN:HG3	2.03	0.41
2:B:116:VAL:HG13	4:B:1064:HOH:O	2.20	0.41
1:C:144:HIS:HD2	4:D:952:HOH:O	2.02	0.41
2:D:14:ALA:HB1	2:D:15:PRO:HD3	2.02	0.41
2:D:111:ILE:HG21	4:D:1042:HOH:O	2.21	0.41
2:B:95:LEU:HD23	2:B:145:PHE:HB3	2.03	0.40
2:B:219:LEU:CD1	2:B:249:LEU:HD13	2.51	0.40
1:C:365:GLN:O	1:C:366:SER:C	2.61	0.40
2:D:38:GLU:O	2:D:42:SER:HB3	2.21	0.40
1:C:9:THR:O	1:C:10:SER:C	2.64	0.40
1:C:207:VAL:HG23	1:C:210:LYS:HE3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:291:ASP:OD1	1:C:291:ASP:C	2.64	0.40
1:A:171:ILE:O	1:A:171:ILE:HG22	2.20	0.40
1:A:225:ASP:O	1:A:229:TRP:CD1	2.74	0.40
1:C:279:ASP:O	1:C:280:GLU:HB2	2.20	0.40
2:D:79:GLN:OE1	2:D:114:ILE:HG23	2.21	0.40
1:A:22:GLU:O	1:A:26:LYS:N	2.45	0.40
1:A:295:ARG:O	1:A:296:PRO:C	2.64	0.40
1:A:559:LEU:N	1:A:560:PRO:CD	2.84	0.40
2:B:51:TYR:OH	2:B:314:CYS:HB3	2.22	0.40
2:B:223:GLN:HA	2:B:229:LEU:HD12	2.04	0.40
1:C:545:LEU:HD23	1:C:545:LEU:C	2.45	0.40
1:A:553:GLU:O	1:A:557:GLU:HG3	2.22	0.40
2:D:23:HIS:HD1	2:D:277:GLY:N	2.11	0.40

There are no symmetry-related clashes.

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	565/567 (100%)	492 (87%)	48 (8%)	25 (4%)	2 0
1	C	565/567 (100%)	503 (89%)	45 (8%)	17 (3%)	3 1
2	B	327/331 (99%)	310 (95%)	12 (4%)	5 (2%)	8 4
2	D	327/331 (99%)	309 (94%)	13 (4%)	5 (2%)	8 4
All	All	1784/1796 (99%)	1614 (90%)	118 (7%)	52 (3%)	3 1

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	17	LYS
1	A	158	VAL

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Mol	Chain	Res	Type
1	A	174	ASN
1	A	176	SER
1	A	197	SER
1	A	243	ASP
1	A	394	ALA
1	A	524	ALA
1	A	548	GLU
1	A	551	ILE
1	A	552	GLN
2	B	13	ASP
2	B	14	ALA
1	C	11	GLU
1	C	12	GLU
1	C	17	LYS
1	C	238	ARG
1	C	523	SER
1	C	549	GLU
1	C	551	ILE
2	D	13	ASP
2	D	14	ALA
2	D	35	ASP
2	D	37	TYR
1	A	12	GLU
1	A	177	ASN
2	B	34	LYS
1	C	21	ARG
1	C	548	GLU
1	C	552	GLN
2	D	34	LYS
1	A	18	ARG
1	A	192	HIS
1	A	241	PRO
1	A	242	HIS
1	A	244	VAL
1	A	270	ARG
1	A	549	GLU
2	B	8	VAL
1	C	193	PRO
1	C	198	GLY
1	A	335	LYS
1	C	236	LEU
1	A	169	SER

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Mol	Chain	Res	Type
1	C	359	GLU
2	B	275	THR
1	C	225	ASP
1	C	244	VAL
1	C	241	PRO
1	A	188	LEU
1	A	195	PRO
1	A	204	PRO

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	490/507 (97%)	433 (88%)	57 (12%)	5	3
1	C	494/507 (97%)	449 (91%)	45 (9%)	9	6
2	B	283/284 (100%)	250 (88%)	33 (12%)	5	3
2	D	283/284 (100%)	249 (88%)	34 (12%)	5	3
All	All	1550/1582 (98%)	1381 (89%)	169 (11%)	6	3

All (169) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	27	LEU
1	A	37	GLN
1	A	46	GLU
1	A	47	SER
1	A	49	LEU
1	A	73	LEU
1	A	83	GLU
1	A	88	LEU
1	A	122	GLU
1	A	136	LEU
1	A	171	ILE
1	A	173	ARG

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Mol	Chain	Res	Type
1	A	176	SER
1	A	179	SER
1	A	197	SER
1	A	202	ARG
1	A	204	PRO
1	A	215	VAL
1	A	221	THR
1	A	243	ASP
1	A	244	VAL
1	A	250	VAL
1	A	257	LEU
1	A	259	VAL
1	A	270	ARG
1	A	289	THR
1	A	295	ARG
1	A	301	LEU
1	A	304	LEU
1	A	309	LEU
1	A	313	LEU
1	A	315	GLN
1	A	317	THR
1	A	319	ARG
1	A	326	ASP
1	A	334	LEU
1	A	347	THR
1	A	351	LEU
1	A	363	VAL
1	A	364	LEU
1	A	367	GLU
1	A	374	LEU
1	A	393	ARG
1	A	403	GLU
1	A	405	LEU
1	A	430	LEU
1	A	436	LEU
1	A	476	ARG
1	A	486	ARG
1	A	504	VAL
1	A	520	LEU
1	A	521	GLN
1	A	536	VAL
1	A	544	SER

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Mol	Chain	Res	Type
1	A	545	LEU
1	A	553	GLU
2	B	3	THR
2	B	9	THR
2	B	13	ASP
2	B	20	LEU
2	B	38	GLU
2	B	40	CYS
2	B	41	MET
2	B	72	LEU
2	B	81	GLU
2	B	85	VAL
2	B	96	LEU
2	B	107	LEU
2	B	113	VAL
2	B	114	ILE
2	B	115	ASN
2	B	118	LYS
2	B	137	ILE
2	B	150	VAL
2	B	162	ILE
2	B	185	PRO
2	B	201	LEU
2	B	207	LEU
2	B	209	GLN
2	B	222	ARG
2	B	229	LEU
2	B	233	PRO
2	B	235	LYS
2	B	239	VAL
2	B	249	LEU
2	B	258	ILE
2	B	281	ARG
2	B	304	GLU
2	B	331	SER
1	C	30	SER
1	C	46	GLU
1	C	49	LEU
1	C	73	LEU
1	C	76	LEU
1	C	88	LEU
1	C	122	GLU

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Mol	Chain	Res	Type
1	C	136	LEU
1	C	163	GLU
1	C	175	PHE
1	C	191	LEU
1	C	194	GLN
1	C	206	ASN
1	C	209	LEU
1	C	213	GLU
1	C	214	LEU
1	C	236	LEU
1	C	238	ARG
1	C	244	VAL
1	C	250	VAL
1	C	259	VAL
1	C	271	MET
1	C	289	THR
1	C	290	PRO
1	C	301	LEU
1	C	304	LEU
1	C	315	GLN
1	C	323	THR
1	C	349	GLU
1	C	351	LEU
1	C	352	PHE
1	C	356	LEU
1	C	361	SER
1	C	363	VAL
1	C	364	LEU
1	C	366	SER
1	C	374	LEU
1	C	405	LEU
1	C	430	LEU
1	C	504	VAL
1	C	529	LEU
1	C	536	VAL
1	C	545	LEU
1	C	551	ILE
1	C	552	GLN
2	D	8	VAL
2	D	13	ASP
2	D	17	THR
2	D	20	LEU

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Mol	Chain	Res	Type
2	D	34	LYS
2	D	35	ASP
2	D	37	TYR
2	D	40	CYS
2	D	45	LEU
2	D	46	ARG
2	D	72	LEU
2	D	76	LYS
2	D	85	VAL
2	D	96	LEU
2	D	107	LEU
2	D	110	SER
2	D	114	ILE
2	D	115	ASN
2	D	118	LYS
2	D	129	GLU
2	D	137	ILE
2	D	150	VAL
2	D	201	LEU
2	D	207	LEU
2	D	209	GLN
2	D	222	ARG
2	D	229	LEU
2	D	239	VAL
2	D	249	LEU
2	D	258	ILE
2	D	260	ARG
2	D	275	THR
2	D	322	ARG
2	D	331	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (51) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	74	GLN
1	A	75	HIS
1	A	124	ASN
1	A	200	GLN
1	A	216	GLN
1	A	232	HIS
1	A	249	HIS

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Mol	Chain	Res	Type
1	A	315	GLN
1	A	328	GLN
1	A	406	GLN
1	A	467	HIS
1	A	517	ASN
1	A	518	ASN
1	A	539	ASN
1	A	543	ASN
2	B	67	ASN
2	B	94	HIS
2	B	124	GLN
2	B	127	GLN
2	B	163	ASN
2	B	176	ASN
2	B	209	GLN
2	B	271	GLN
2	B	321	GLN
2	B	326	GLN
1	C	74	GLN
1	C	144	HIS
1	C	155	GLN
1	C	232	HIS
1	C	294	ASN
1	C	312	GLN
1	C	315	GLN
1	C	365	GLN
1	C	447	HIS
1	C	517	ASN
1	C	518	ASN
1	C	539	ASN
1	C	543	ASN
2	D	4	GLN
2	D	5	GLN
2	D	67	ASN
2	D	94	HIS
2	D	115	ASN
2	D	127	GLN
2	D	163	ASN
2	D	176	ASN
2	D	206	GLN
2	D	271	GLN
2	D	305	GLN

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Mol	Chain	Res	Type
2	D	326	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	FME	A	1	1	8,9,10	0.77	0	8,9,11	1.95	2 (25%)
1	FME	C	1	1	8,9,10	0.85	0	8,9,11	2.01	3 (37%)

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
1	FME	A	1	1	-	2/7/9/11	-
1	FME	C	1	1	-	4/7/9/11	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	O-C-CA	-4.71	112.65	124.77
1	C	1	FME	O-C-CA	-4.03	114.39	124.77
1	C	1	FME	CA-N-CN	-3.15	117.98	122.82
1	A	1	FME	CA-N-CN	-2.26	119.34	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	FME	O1-CN-N	-2.03	120.07	125.32

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	1	FME	O1-CN-N-CA
1	C	1	FME	O1-CN-N-CA
1	C	1	FME	CA-CB-CG-SD
1	A	1	FME	CA-CB-CG-SD
1	C	1	FME	CB-CA-N-CN
1	C	1	FME	CB-CG-SD-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

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.