



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 11:02 pm BST

PDB ID : 1DCE  
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](mailto: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.

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

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

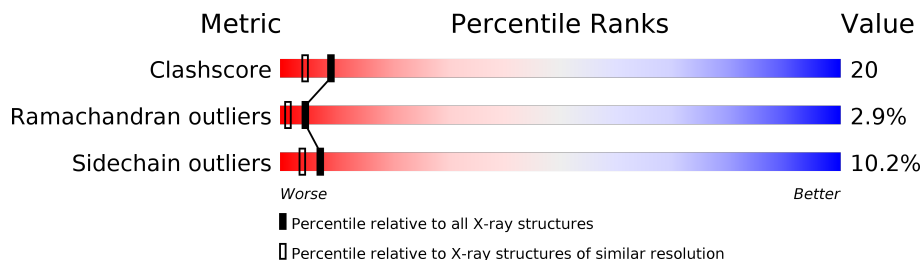
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	51% 33% 11% .
1	C	567	62% 27% 8% .
2	B	331	60% 28% 10% ..
2	D	331	59% 30% 7% ..

## 2 Entry composition i

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 (three-letter code: 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.

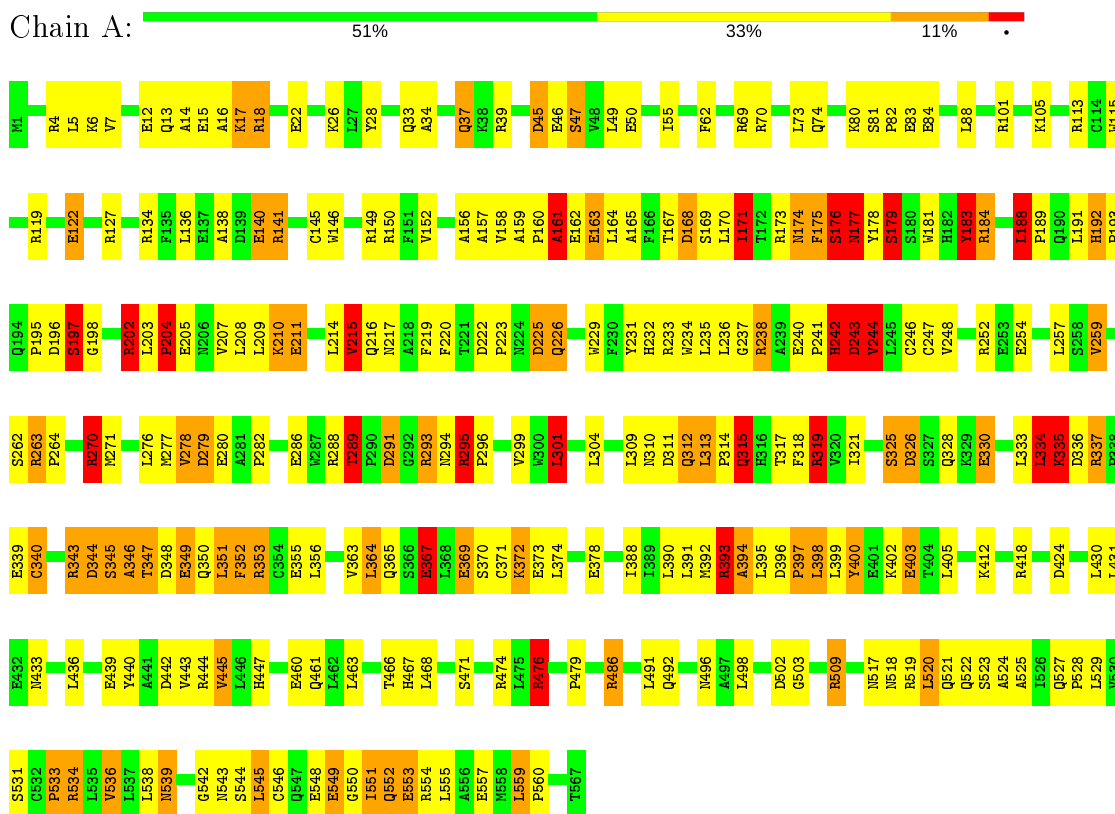
<b>Mol</b>	<b>Chain</b>	<b>Residues</b>	<b>Atoms</b>		<b>ZeroOcc</b>	<b>AltConf</b>
4	A	280	Total 280	O 280	0	0
4	B	165	Total 165	O 165	0	0
4	C	239	Total 239	O 239	0	0
4	D	145	Total 145	O 145	0	0

### 3 Residue-property plots

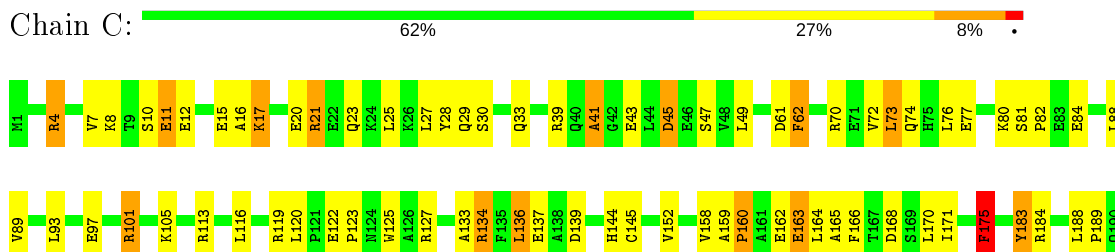
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

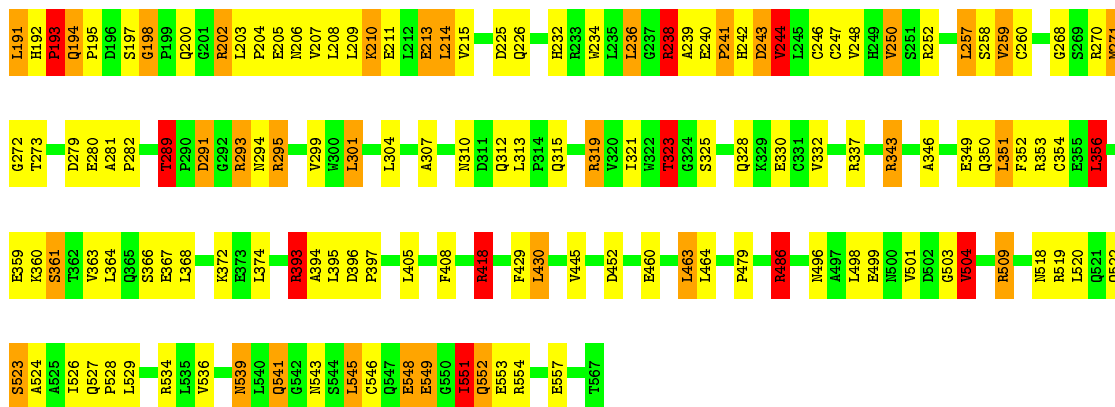
Note EDS was not executed.

- Molecule 1: PROTEIN (RAB GERANYLGERANYLTRANSFERASE ALPHA SUB-UNIT)

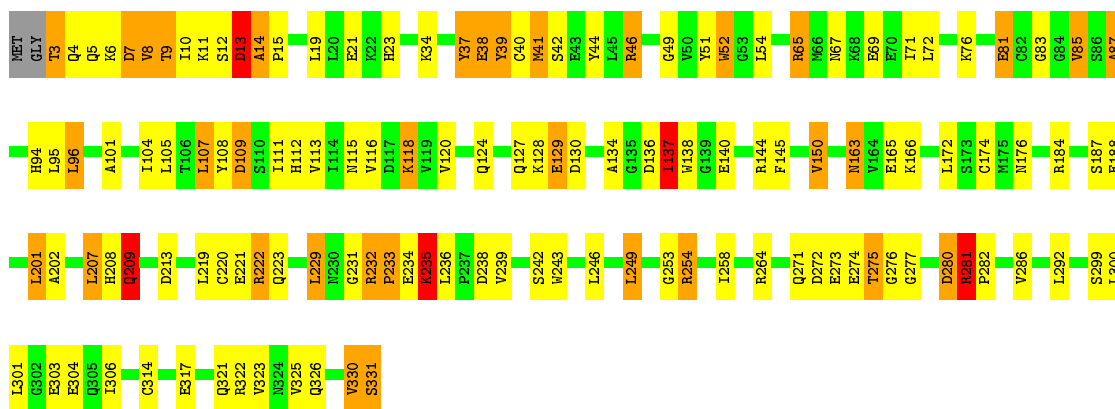


- Molecule 1: PROTEIN (RAB GERANYLGERANYLTRANSFERASE ALPHA SUB-UNIT)

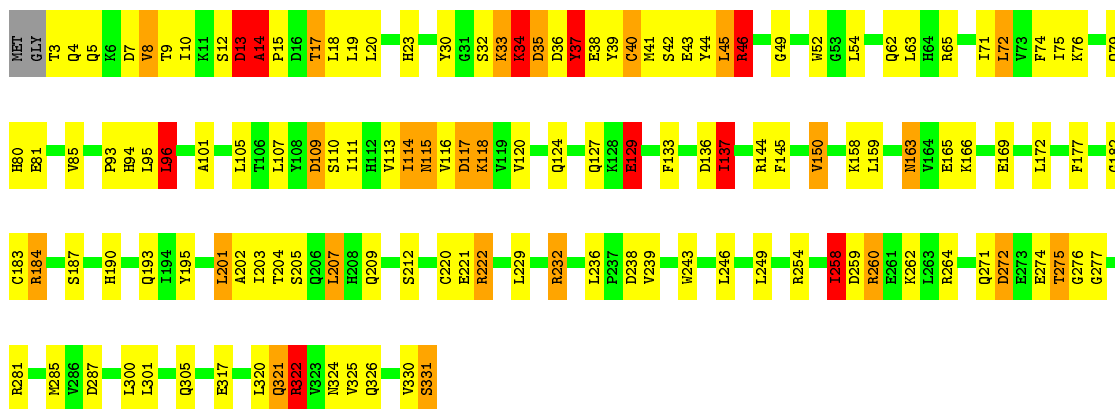




• Molecule 2: PROTEIN (RAB GERANYLGERANYLTRANSFERASE BETA SUBUNIT)



• 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, $\alpha$ , $\beta$ , $\gamma$	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 <sup>2</sup> )	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: ZN, FME

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	0.81	0/4581	1.92	135/6235 (2.2%)
1	C	0.73	0/4596	1.79	78/6251 (1.2%)
2	B	0.81	1/2633 (0.0%)	1.64	38/3568 (1.1%)
2	D	0.77	0/2633	1.69	49/3568 (1.4%)
All	All	0.78	1/14443 (0.0%)	1.79	300/19622 (1.5%)

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 (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	220	CYS	CB-SG	-5.20	1.73	1.81

All (300) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	319	ARG	CD-NE-CZ	34.32	171.65	123.60
1	C	393	ARG	NE-CZ-NH2	-27.36	106.62	120.30
1	C	337	ARG	NE-CZ-NH1	25.95	133.27	120.30
1	A	393	ARG	NE-CZ-NH2	-22.51	109.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	486	ARG	NE-CZ-NH2	-20.90	109.85	120.30
1	A	486	ARG	NE-CZ-NH2	-20.07	110.26	120.30
1	A	184	ARG	CD-NE-CZ	16.94	147.31	123.60
1	A	319	ARG	NE-CZ-NH2	-16.81	111.90	120.30
1	C	295	ARG	CD-NE-CZ	16.17	146.23	123.60
1	A	202	ARG	NE-CZ-NH1	15.95	128.27	120.30
1	A	295	ARG	CD-NE-CZ	15.16	144.82	123.60
1	C	134	ARG	NE-CZ-NH2	14.43	127.52	120.30
2	D	144	ARG	NE-CZ-NH2	-14.39	113.11	120.30
1	A	225	ASP	CB-CG-OD1	14.12	131.01	118.30
2	D	222	ARG	CD-NE-CZ	14.05	143.28	123.60
2	D	281	ARG	NE-CZ-NH1	13.67	127.14	120.30
1	C	337	ARG	NE-CZ-NH2	-13.63	113.49	120.30
1	A	279	ASP	CB-CG-OD1	-13.10	106.51	118.30
2	D	264	ARG	NE-CZ-NH2	-13.06	113.77	120.30
2	B	144	ARG	NE-CZ-NH2	-12.93	113.84	120.30
1	C	45	ASP	CB-CG-OD1	12.72	129.75	118.30
2	B	281	ARG	NE-CZ-NH2	12.64	126.62	120.30
1	C	293	ARG	NE-CZ-NH2	-12.59	114.00	120.30
2	B	184	ARG	NE-CZ-NH1	12.55	126.57	120.30
1	C	393	ARG	NE-CZ-NH1	12.55	126.57	120.30
1	C	134	ARG	NE-CZ-NH1	-12.10	114.25	120.30
2	D	322	ARG	NE-CZ-NH1	11.86	126.23	120.30
1	C	301	LEU	CA-CB-CG	11.64	142.07	115.30
1	C	184	ARG	NE-CZ-NH2	-11.52	114.54	120.30
2	D	144	ARG	CD-NE-CZ	11.52	139.73	123.60
1	A	442	ASP	CB-CG-OD1	11.45	128.60	118.30
1	C	101	ARG	NE-CZ-NH1	-11.40	114.60	120.30
1	A	343	ARG	NE-CZ-NH1	11.34	125.97	120.30
1	A	141	ARG	NE-CZ-NH2	11.32	125.96	120.30
1	C	486	ARG	CD-NE-CZ	11.12	139.17	123.60
1	A	113	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	C	113	ARG	NE-CZ-NH2	-10.95	114.83	120.30
1	C	343	ARG	NE-CZ-NH1	-10.86	114.87	120.30
2	D	65	ARG	NE-CZ-NH2	10.72	125.66	120.30
1	C	77	GLU	OE1-CD-OE2	-10.68	110.48	123.30
2	B	144	ARG	NE-CZ-NH1	10.63	125.61	120.30
1	A	127	ARG	NE-CZ-NH2	10.50	125.55	120.30
2	B	44	TYR	CB-CG-CD1	10.37	127.22	121.00
1	A	127	ARG	NE-CZ-NH1	-10.25	115.18	120.30
1	A	319	ARG	NH1-CZ-NH2	10.04	130.44	119.40
1	C	184	ARG	NE-CZ-NH1	9.99	125.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	293	ARG	CA-C-N	9.76	138.66	117.20
1	A	113	ARG	NE-CZ-NH2	-9.62	115.49	120.30
1	A	403	GLU	OE1-CD-OE2	-9.49	111.91	123.30
2	B	222	ARG	NE-CZ-NH2	-9.49	115.56	120.30
1	A	400	TYR	CB-CG-CD1	9.34	126.60	121.00
1	A	367	GLU	N-CA-CB	9.18	127.13	110.60
1	A	289	THR	N-CA-CB	-9.16	92.89	110.30
1	A	141	ARG	NE-CZ-NH1	-9.07	115.77	120.30
2	D	238	ASP	CB-CG-OD2	9.07	126.46	118.30
2	D	281	ARG	NE-CZ-NH2	-9.06	115.77	120.30
2	D	281	ARG	CD-NE-CZ	9.03	136.24	123.60
2	B	232	ARG	NE-CZ-NH1	-8.99	115.81	120.30
1	A	400	TYR	CA-CB-CG	8.97	130.45	113.40
2	B	130	ASP	CB-CG-OD2	-8.93	110.26	118.30
1	C	289	THR	N-CA-CB	-8.87	93.45	110.30
1	A	295	ARG	CB-CG-CD	8.84	134.59	111.60
2	B	130	ASP	CB-CG-OD1	8.80	126.22	118.30
1	A	177	ASN	OD1-CG-ND2	8.73	141.97	121.90
1	A	319	ARG	CD-NE-CZ	8.68	135.75	123.60
2	D	184	ARG	NE-CZ-NH2	-8.61	115.99	120.30
1	C	396	ASP	CB-CG-OD1	8.59	126.03	118.30
1	A	202	ARG	NE-CZ-NH2	-8.49	116.06	120.30
1	A	244	VAL	CA-C-O	8.45	137.85	120.10
1	C	452	ASP	CB-CG-OD2	8.42	125.88	118.30
2	B	281	ARG	CD-NE-CZ	8.41	135.38	123.60
2	D	46	ARG	NE-CZ-NH1	-8.24	116.18	120.30
1	C	252	ARG	NE-CZ-NH2	8.22	124.41	120.30
2	D	136	ASP	CB-CG-OD1	8.16	125.64	118.30
1	C	293	ARG	CA-C-N	8.09	135.00	117.20
2	D	221	GLU	OE1-CD-OE2	-8.01	113.69	123.30
1	A	183	TYR	CB-CG-CD1	8.00	125.80	121.00
1	C	293	ARG	O-C-N	-7.99	109.91	122.70
1	A	101	ARG	CD-NE-CZ	7.98	134.77	123.60
1	A	263	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	39	ARG	NE-CZ-NH2	-7.76	116.42	120.30
2	B	264	ARG	NE-CZ-NH1	7.71	124.15	120.30
2	D	46	ARG	CD-NE-CZ	7.70	134.38	123.60
2	D	238	ASP	OD1-CG-OD2	-7.67	108.73	123.30
2	D	65	ARG	NE-CZ-NH1	-7.66	116.47	120.30
2	D	260	ARG	NE-CZ-NH2	-7.64	116.48	120.30
2	B	109	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	A	178	TYR	CB-CG-CD2	-7.62	116.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	393	ARG	NE-CZ-NH1	7.57	124.09	120.30
2	B	254	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	A	444	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	A	369	GLU	OE1-CD-OE2	7.49	132.28	123.30
1	A	168	ASP	CB-CG-OD1	7.43	124.99	118.30
2	B	44	TYR	CB-CG-CD2	-7.34	116.60	121.00
1	A	291	ASP	CB-CG-OD1	7.29	124.86	118.30
1	C	418	ARG	CD-NE-CZ	-7.28	113.41	123.60
2	D	258	ILE	CA-CB-CG2	7.23	125.35	110.90
1	A	168	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	330	GLU	OE1-CD-OE2	-7.20	114.67	123.30
1	A	364	LEU	N-CA-CB	7.18	124.76	110.40
1	A	398	LEU	CB-CA-C	7.14	123.77	110.20
1	A	519	ARG	NE-CZ-NH1	-7.11	116.74	120.30
1	C	243	ASP	CA-CB-CG	7.09	129.00	113.40
2	D	238	ASP	CB-CG-OD1	7.08	124.67	118.30
1	C	337	ARG	CD-NE-CZ	7.05	133.47	123.60
1	A	344	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	A	486	ARG	NH1-CZ-NH2	7.03	127.13	119.40
2	D	14	ALA	CB-CA-C	7.02	120.63	110.10
1	C	289	THR	CA-CB-OG1	7.00	123.71	109.00
2	B	184	ARG	CD-NE-CZ	6.96	133.34	123.60
2	D	264	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	A	399	LEU	CA-CB-CG	6.93	131.23	115.30
2	B	232	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	A	183	TYR	CB-CG-CD2	-6.82	116.91	121.00
1	C	291	ASP	CB-CG-OD2	6.80	124.42	118.30
1	A	393	ARG	NH1-CZ-NH2	6.79	126.87	119.40
1	C	61	ASP	CB-CG-OD1	6.79	124.41	118.30
2	D	287	ASP	CB-CG-OD1	6.78	124.40	118.30
2	B	184	ARG	NH1-CZ-NH2	-6.77	111.95	119.40
1	A	346	ALA	N-CA-CB	-6.70	100.72	110.10
1	C	393	ARG	NH1-CZ-NH2	6.70	126.77	119.40
1	A	252	ARG	NE-CZ-NH1	-6.69	116.96	120.30
1	A	225	ASP	CB-CG-OD2	-6.66	112.31	118.30
1	C	88	LEU	CA-CB-CG	6.65	130.59	115.30
2	B	65	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	A	534	ARG	NE-CZ-NH2	6.63	123.61	120.30
2	D	254	ARG	NE-CZ-NH1	-6.62	116.99	120.30
2	D	259	ASP	CB-CG-OD1	6.56	124.20	118.30
1	C	193	PRO	C-N-CA	6.55	138.08	121.70
1	A	278	VAL	CB-CA-C	-6.55	98.96	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	291	ASP	CB-CG-OD1	6.54	124.19	118.30
2	D	46	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	C	4	ARG	NE-CZ-NH2	-6.43	117.08	120.30
1	C	486	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	A	177	ASN	CB-CA-C	6.42	123.23	110.40
1	A	367	GLU	OE1-CD-OE2	6.39	130.97	123.30
2	B	264	ARG	NE-CZ-NH2	-6.37	117.11	120.30
1	C	250	VAL	CA-CB-CG1	6.36	120.44	110.90
1	A	442	ASP	CB-CG-OD2	-6.35	112.58	118.30
1	C	323	THR	N-CA-CB	-6.34	98.25	110.30
2	B	129	GLU	OE1-CD-OE2	-6.34	115.70	123.30
2	D	222	ARG	NE-CZ-NH1	6.34	123.47	120.30
1	A	70	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	A	222	ASP	CB-CG-OD1	6.30	123.97	118.30
1	C	244	VAL	CA-C-O	6.28	133.30	120.10
1	C	291	ASP	OD1-CG-OD2	-6.28	111.37	123.30
2	D	195	TYR	CB-CG-CD1	6.27	124.76	121.00
1	C	486	ARG	NH1-CZ-NH2	6.26	126.29	119.40
2	D	212	SER	N-CA-CB	-6.25	101.13	110.50
1	A	45	ASP	CB-CG-OD1	6.23	123.91	118.30
1	A	279	ASP	OD1-CG-OD2	6.22	135.13	123.30
1	A	159	ALA	CB-CA-C	6.22	119.43	110.10
1	A	293	ARG	CA-C-O	-6.16	107.16	120.10
1	C	332	VAL	CB-CA-C	-6.15	99.71	111.40
1	C	101	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	A	163	GLU	CG-CD-OE1	6.14	130.59	118.30
1	A	202	ARG	CD-NE-CZ	6.14	132.19	123.60
2	B	213	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	4	ARG	NE-CZ-NH1	6.11	123.36	120.30
1	A	442	ASP	CA-CB-CG	6.11	126.85	113.40
1	C	202	ARG	CD-NE-CZ	6.10	132.15	123.60
2	D	129	GLU	CB-CG-CD	6.10	130.67	114.20
1	A	325	SER	CA-C-O	-6.07	107.35	120.10
1	A	343	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
1	A	436	LEU	CB-CA-C	6.05	121.70	110.20
1	A	312	GLN	CB-CG-CD	6.05	127.33	111.60
1	C	70	ARG	NE-CZ-NH2	-6.04	117.28	120.30
2	D	109	ASP	CB-CG-OD1	6.01	123.71	118.30
2	D	232	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	C	252	ARG	NH1-CZ-NH2	-5.97	112.83	119.40
1	A	393	ARG	CD-NE-CZ	-5.96	115.26	123.60
2	B	235	LYS	CB-CG-CD	5.95	127.08	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	424	ASP	CB-CG-OD1	5.90	123.61	118.30
2	B	46	ARG	CD-NE-CZ	5.89	131.84	123.60
2	B	280	ASP	CB-CG-OD1	5.88	123.59	118.30
1	A	364	LEU	CA-CB-CG	5.88	128.83	115.30
1	C	175	PHE	CA-C-O	5.88	132.45	120.10
2	D	201	LEU	CB-CG-CD1	5.87	120.98	111.00
1	A	346	ALA	C-N-CA	5.86	136.36	121.70
2	B	208	HIS	O-C-N	-5.86	113.32	122.70
2	D	144	ARG	NH1-CZ-NH2	5.85	125.84	119.40
1	A	439	GLU	OE1-CD-OE2	5.85	130.32	123.30
1	A	69	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	179	SER	CA-CB-OG	-5.84	95.43	111.20
1	A	474	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	A	244	VAL	CG1-CB-CG2	-5.82	101.59	110.90
1	A	328	GLN	O-C-N	-5.82	113.40	122.70
2	D	321	GLN	CB-CG-CD	5.82	126.72	111.60
2	D	190	HIS	CA-CB-CG	5.81	123.47	113.60
1	C	337	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
1	C	193	PRO	O-C-N	-5.80	113.42	122.70
2	B	137	ILE	CB-CA-C	-5.79	100.02	111.60
1	A	179	SER	CB-CA-C	5.76	121.05	110.10
2	B	303	GLU	OE1-CD-OE2	5.76	130.21	123.30
2	D	150	VAL	N-CA-CB	-5.74	98.86	111.50
2	B	150	VAL	N-CA-CB	-5.73	98.89	111.50
1	C	504	VAL	N-CA-CB	-5.71	98.93	111.50
2	B	136	ASP	CB-CG-OD1	5.69	123.42	118.30
2	B	209	GLN	O-C-N	-5.68	113.61	122.70
1	A	286	GLU	OE1-CD-OE2	5.66	130.09	123.30
2	B	221	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	A	476	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	A	69	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	C	319	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	C	164	LEU	CA-CB-CG	5.61	128.21	115.30
1	C	293	ARG	C-N-CA	-5.61	107.67	121.70
1	C	77	GLU	CG-CD-OE1	5.60	129.49	118.30
2	D	65	ARG	CD-NE-CZ	-5.59	115.77	123.60
1	A	270	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	A	286	GLU	CA-CB-CG	-5.57	101.14	113.40
1	C	62	PHE	CB-CG-CD1	-5.57	116.90	120.80
2	B	129	GLU	CG-CD-OE2	5.56	129.42	118.30
1	C	257	LEU	CA-CB-CG	5.56	128.09	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLU	OE1-CD-OE2	5.54	129.95	123.30
1	A	370	SER	N-CA-CB	-5.53	102.21	110.50
1	A	326	ASP	CB-CG-OD2	5.52	123.27	118.30
1	A	175	PHE	C-N-CA	5.52	135.51	121.70
1	A	346	ALA	CB-CA-C	5.51	118.36	110.10
1	A	502	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	140	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	A	293	ARG	O-C-N	-5.50	113.90	122.70
1	C	73	LEU	CA-CB-CG	5.46	127.85	115.30
1	A	445	VAL	CG1-CB-CG2	-5.45	102.19	110.90
1	A	171	ILE	N-CA-CB	5.44	123.31	110.80
2	B	281	ARG	NH1-CZ-NH2	-5.43	113.43	119.40
1	A	559	LEU	CA-CB-CG	5.42	127.77	115.30
1	A	536	VAL	CA-CB-CG1	5.42	119.03	110.90
1	A	242	HIS	N-CA-CB	5.41	120.34	110.60
1	A	397	PRO	O-C-N	5.41	131.35	122.70
1	A	337	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	C	460	GLU	OE1-CD-OE2	-5.38	116.84	123.30
2	D	272	ASP	CB-CG-OD1	5.37	123.14	118.30
1	A	280	GLU	C-N-CA	5.37	135.12	121.70
1	C	41	ALA	CB-CA-C	5.37	118.15	110.10
1	C	519	ARG	CA-CB-CG	-5.34	101.65	113.40
1	A	336	ASP	CB-CG-OD2	-5.34	113.50	118.30
2	D	7	ASP	CA-C-N	5.33	128.94	117.20
1	C	452	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	A	161	ALA	CA-C-O	-5.33	108.91	120.10
1	C	260	CYS	O-C-N	5.33	131.23	122.70
1	A	392	MET	CG-SD-CE	5.32	108.72	100.20
1	C	519	ARG	CD-NE-CZ	-5.32	116.15	123.60
1	A	336	ASP	CB-CG-OD1	5.31	123.08	118.30
1	C	295	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	145	CYS	N-CA-CB	5.29	120.13	110.60
1	C	127	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	C	299	VAL	CA-CB-CG2	5.28	118.82	110.90
1	A	536	VAL	CA-CB-CG2	-5.28	102.98	110.90
2	B	87	ALA	CB-CA-C	-5.28	102.18	110.10
1	A	328	GLN	CA-C-O	5.28	131.19	120.10
2	B	41	MET	CA-CB-CG	-5.28	104.33	113.30
1	A	319	ARG	NE-CZ-NH1	-5.27	117.67	120.30
2	D	7	ASP	CB-CG-OD2	-5.26	113.56	118.30
2	B	222	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	B	201	LEU	CA-CB-CG	5.24	127.35	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	301	LEU	O-C-N	5.24	131.08	122.70
1	C	139	ASP	CB-CG-OD1	5.23	123.01	118.30
1	A	176	SER	N-CA-CB	-5.23	102.65	110.50
1	C	553	GLU	CA-CB-CG	5.22	124.89	113.40
2	D	195	TYR	CB-CG-CD2	-5.22	117.87	121.00
2	D	177	PHE	CB-CG-CD2	5.22	124.45	120.80
1	A	188	LEU	CB-CA-C	5.21	120.10	110.20
1	A	509	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	A	400	TYR	CB-CG-CD2	-5.19	117.89	121.00
2	D	137	ILE	CB-CA-C	-5.19	101.23	111.60
1	A	225	ASP	CB-CA-C	-5.18	100.04	110.40
1	A	315	GLN	O-C-N	5.18	130.99	122.70
1	A	315	GLN	N-CA-CB	5.17	119.91	110.60
1	C	160	PRO	N-CD-CG	-5.17	95.44	103.20
1	A	150	ARG	NE-CZ-NH2	5.17	122.89	120.30
2	D	96	LEU	CB-CG-CD2	5.17	119.79	111.00
1	A	138	ALA	N-CA-CB	5.15	117.31	110.10
1	A	301	LEU	CA-CB-CG	5.15	127.14	115.30
2	D	232	ARG	CA-CB-CG	5.13	124.70	113.40
1	C	294	ASN	CB-CA-C	5.13	120.66	110.40
1	A	339	GLU	O-C-N	5.13	130.90	122.70
1	A	152	VAL	CG1-CB-CG2	-5.12	102.70	110.90
1	A	347	THR	N-CA-C	5.12	124.82	111.00
1	C	193	PRO	N-CA-C	5.12	125.41	112.10
1	A	339	GLU	CB-CA-C	-5.12	100.17	110.40
1	A	372	LYS	CB-CG-CD	5.12	124.90	111.60
2	B	238	ASP	OD1-CG-OD2	-5.10	113.60	123.30
1	A	119	ARG	NE-CZ-NH1	5.09	122.85	120.30
2	D	184	ARG	NH1-CZ-NH2	5.09	125.00	119.40
1	A	149	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	178	TYR	CB-CG-CD1	5.08	124.05	121.00
1	C	408	PHE	CB-CG-CD2	-5.08	117.24	120.80
1	C	127	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	A	460	GLU	CG-CD-OE1	5.05	128.41	118.30
2	D	96	LEU	CA-CB-CG	5.05	126.92	115.30
1	A	280	GLU	CG-CD-OE1	-5.05	108.20	118.30
1	A	299	VAL	CG1-CB-CG2	-5.05	102.83	110.90
1	A	210	LYS	CA-CB-CG	5.04	124.49	113.40
1	A	439	GLU	CA-CB-CG	5.03	124.46	113.40
1	A	345	SER	CA-C-O	5.01	130.63	120.10
1	C	445	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	A	334	LEU	N-CA-CB	5.01	120.43	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	7	ASP	CB-CG-OD1	5.00	122.80	118.30
1	A	226	GLN	CG-CD-NE2	5.00	128.71	116.70

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
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	222	0
1	C	4509	0	4448	150	0
2	B	2574	0	2521	102	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	563	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 20.

All (563) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:347:THR:HG1	1:A:440:TYR:HE1	1.33	0.74
2:B:127:GLN:HE22	2:B:163:ASN:H	1.34	0.74
1:A:197:SER:OG	1:A:198:GLY:N	2.21	0.73
1:C:81:SER:HB2	1:C:82:PRO:HD2	1.69	0.73
2:D:42:SER:O	2:D:45:LEU:HD23	1.89	0.72
2:B:281:ARG:HH11	2:B:281:ARG:HG3	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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:HH21	1:A:263:ARG:HG2	1.62	0.65
1:C:498:LEU:H	1:C:518:ASN:ND2	1.95	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:393:ARG:O	1:A:394:ALA:C	2.36	0.64
1:A:278:VAL:O	1:A:279:ASP:HB2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:C:250:VAL:HG12	1:C:257:LEU:HD13	1.82	0.61
1:C:80:LYS:HD2	1:C:84:GLU:HG2	1.83	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
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
2:D:129:GLU:H	2:D:129:GLU:CD	2.05	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:115:ASN:HD22	2:D:115:ASN:C	2.05	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:MET:HB2	4:D:1006:HOH:O	2.02	0.59
1:A:16:ALA:O	1:A:17:LYS:C	2.40	0.59
1:A:192:HIS:HB2	1:A:193:PRO:HD3	1.84	0.59
1:A:74:GLN:HE21	1:A:115:TRP:HZ2	1.51	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:A:189:PRO:HA	1:A:193:PRO:CG	2.26	0.59
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:105:LYS:NZ	4:A:840:HOH:O	2.36	0.58
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
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
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
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:HG2	1:A:263:ARG:NH2	2.20	0.57
2:B:232:ARG:HH12	2:B:235:LYS:NZ	2.03	0.57
2:D:32:SER:O	2:D:33:LYS:C	2.44	0.56
1:A:319:ARG:HG2	1:A:330:GLU:HB2	1.87	0.56
1:A:238:ARG:CZ	1:A:352:PHE:HA	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:232:ARG:HH12	2:B:235:LYS:HZ2	1.52	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
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:D:109:ASP:CG	2:D:322:ARG:HH21	2.10	0.54
1:C:312:GLN:C	1:C:313:LEU:HD12	2.28	0.54
2:B:111:ILE:HG13	2:B:112:HIS:N	2.23	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:204:PRO:O	1:A:205:GLU:C	2.45	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:A:347:THR:HG22	1:A:348:ASP:CG	2.28	0.54
1:C:551:ILE:O	1:C:552:GLN:CB	2.55	0.54
1:C:4:ARG:HB3	2:D:285:MET:SD	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:393:ARG:HH22	1:A:433:ASN:CG	2.12	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
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
2:B:108:TYR:O	2:B:109:ASP:C	2.46	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:49:GLY:HA2	2:D:52:TRP:CE3	2.44	0.52
2:D:4:GLN:NE2	2:D:236:LEU:HD11	2.24	0.52
1:A:134:ARG:NE	4:A:723:HOH:O	2.30	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
1:C:20:GLU:O	1:C:21:ARG:CB	2.58	0.52
2:D:183:CYS:HB3	4:D:1071:HOH:O	2.09	0.52
2:D:45:LEU:H	2:D:45:LEU:HD23	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:ARG:HH11	2:B:322:ARG:HG3	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:447:HIS:HB3	4:A:641:HOH:O	2.10	0.51
1:A:179:SER:HB2	2:B:188:GLU:OE2	2.11	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:A:321:ILE:HG23	4:A:830:HOH:O	2.10	0.51
1:C:160:PRO:HB2	1:C:191:LEU:HD12	1.92	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
1:A:289:THR:CG2	1:A:293:ARG:O	2.59	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:281:ALA:HB1	1:C:282:PRO:HD2	1.94	0.49
1:C:49:LEU:HD13	1:C:72:VAL:HG11	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:A:522:GLN:O	1:A:523:SER:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:529:LEU:N	1:C:529:LEU:HD23	2.28	0.48
1:C:270:ARG:HG2	2:D:165:GLU:OE2	2.13	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:12:SER:O	2:D:13:ASP:C	2.51	0.48
2:D:202:ALA:HA	2:D:207:LEU:HD22	1.95	0.48
2:D:109:ASP:OD2	2:D:322:ARG:NH2	2.47	0.48
1:A:270:ARG:NH2	2:B:165:GLU:HG3	2.29	0.48
1:A:347:THR:HG22	1:A:348:ASP:N	2.28	0.48
2:B:231:GLY:HA3	4:B:1033:HOH:O	2.12	0.48
1:A:141:ARG:NH1	2:B:233:PRO:O	2.42	0.48
1:A:174:ASN:OD1	1:A:175:PHE:N	2.47	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: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:160:PRO:C	1:A:191:LEU:HD21	2.35	0.47
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:118:LYS:HZ2	2:D:118:LYS:CB	2.27	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
2:B:134:ALA:HA	2:B:140:GLU:O	2.14	0.47
1:A:398:LEU:HD11	1:A:440:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:ARG:O	2:B:232:ARG:NH2	2.43	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: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
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
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: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:A:74:GLN:HE22	2:B:138:TRP:HZ3	1.63	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:C:539:ASN:HD22	1:C:539:ASN:C	2.19	0.47
1:A:346:ALA:HA	1:A:351:LEU:CB	2.43	0.46
1:A:47:SER:O	1:A:50:GLU:HG2	2.15	0.46
2:B:172:LEU:CD2	2:B:209:GLN:HG2	2.45	0.46
1:A:349:GLU:O	1:A:350:GLN:C	2.52	0.46
2:B:12:SER:O	2:B:13:ASP:C	2.51	0.46
1:C:312:GLN:O	1:C:313:LEU:HD12	2.15	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: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:549:GLU:C	1:A:551:ILE:H	2.19	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:GLN:O	2:D:63:LEU:C	2.54	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
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: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: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:A:175:PHE:CG	1:A:176:SER:N	2.83	0.45
1:C:74:GLN:NE2	1:C:119:ARG:NH1	2.64	0.45
1:A:311:ASP:HB3	4:A:701:HOH:O	2.17	0.45
1:C:202:ARG:HD3	1:C:234:TRP:O	2.17	0.45
2:D:115:ASN:ND2	2:D:118:LYS:H	2.15	0.45
2:D:8:VAL:HG12	2:D:9:THR:H	1.81	0.45
1:A:204:PRO:O	1:A:207:VAL:HG12	2.17	0.44
1:A:81:SER:OG	1:A:84:GLU:HB2	2.17	0.44
1:C:242:HIS:O	1:C:244:VAL:HB	2.17	0.44
2:D:220:CYS:HA	2:D:258:ILE:CD1	2.47	0.44
2:D:18:LEU:HD12	2:D:271:GLN:HE22	1.80	0.44
1:A:310:ASN:C	1:A:310:ASN:OD1	2.55	0.44
1:A:334:LEU:HG	1:A:337:ARG:HG3	1.99	0.44
1:C:356:LEU:HD23	1:C:361:SER:OG	2.18	0.44
1:C:25:LEU:HD21	2:D:40:CYS:SG	2.57	0.44
1:A:80:LYS:HD2	1:A:84:GLU:HG2	2.00	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
2:B:67:ASN:O	2:B:71:ILE:HG13	2.18	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
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:C:89:VAL:HG11	1:C:120:LEU:HD21	2.00	0.44
2:B:229:LEU:HB2	2:B:242:SER:OG	2.18	0.44
2:B:52:TRP:HA	2:B:292:LEU:HD22	1.99	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
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
1:A:431:LEU:C	1:A:431:LEU:HD23	2.38	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: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:115:ASN:ND2	2:D:115:ASN:C	2.71	0.43
2:D:118:LYS:NZ	2:D:118:LYS:HB2	2.33	0.43
2:D:34:LYS:HA	4:D:1074:HOH:O	2.18	0.43
2:D:45:LEU:N	2:D:45:LEU:HD23	2.32	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:182:GLY:C	2:D:193:GLN:HG2	2.40	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:A:539:ASN:HD22	1:A:539:ASN:C	2.22	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:HA	1:A:214:LEU:HD23	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
2:B:272:ASP:CG	2:B:275:THR:HG22	2.39	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
1:C:197:SER:OG	1:C:198:GLY:N	2.52	0.42
1:C:125:TRP:CE3	1:C:152:VAL:HG13	2.55	0.42
1:C:16:ALA:O	1:C:17:LYS:CB	2.67	0.42
1:C:7:VAL:O	1:C:8:LYS:HG3	2.19	0.42
1:A:141:ARG:HH11	2:B:234:GLU:HB2	1.79	0.42
2:B:258:ILE:HA	2:B:258:ILE:HD12	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
2:D:118:LYS:HZ2	2:D:118:LYS:HB2	1.85	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:216:GLN:O	1:A:219:PHE:N	2.53	0.41
1:A:45:ASP:OD2	1:A:47:SER:HB3	2.20	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:HA	1:A:555:LEU:HD23	1.91	0.41
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:HG2	1:A:240:GLU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:146:TRP:CE2	1:A:179:SER:OG	2.69	0.41
1:A:225:ASP:OD1	1:A:226:GLN:N	2.53	0.41
1:C:194:GLN:H	1:C:194:GLN:HG3	1.38	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
2:B:280:ASP:OD2	2:B:281:ARG:NH1	2.54	0.41
2:D:8:VAL:HG12	2:D:9:THR:N	2.36	0.41
1:A:17:LYS:O	1:A:18:ARG:C	2.59	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:137:ILE:HD13	4:D:1007:HOH:O	2.20	0.41
2:D:18:LEU:HD12	2:D:271:GLN:NE2	2.35	0.41
1:A:351:LEU:HD11	1:A:461:GLN:CD	2.41	0.41
1:A:191:LEU:HB3	1:A:192:HIS:CE1	2.55	0.41
1:A:196:ASP:O	1:A:197:SER:HB3	2.21	0.41
1:A:238:ARG:NH1	1:A:351:LEU:O	2.54	0.41
1:A:310:ASN:CG	1:A:312:GLN:HG2	2.40	0.41
1:A:396:ASP:O	1:A:397:PRO:C	2.60	0.41
1:A:402:LYS:HG3	4:A:755:HOH:O	2.19	0.41
2:D:262:LYS:HE2	2:D:262:LYS:HB3	1.91	0.41
1:A:211:GLU:HG2	4:A:814:HOH:O	2.21	0.41
2:D:19:LEU:H	2:D:271:GLN:NE2	2.10	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
1:A:80:LYS:HA	1:A:80:LYS:HD3	1.85	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:111:ILE:HG21	4:D:1042:HOH:O	2.21	0.41
2:D:14:ALA:HB1	2:D:15:PRO:HD3	2.02	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
2:D:38:GLU:O	2:D:42:SER:HB3	2.21	0.40
1:C:207:VAL:HG23	1:C:210:LYS:HE3	2.03	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:13:GLN:O	1:A:14:ALA:C	2.59	0.40
1:A:22:GLU:O	1:A:26:LYS:N	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:N	1:A:560:PRO:CD	2.84	0.40
2:B:223:GLN:HA	2:B:229:LEU:HD12	2.04	0.40
2:B:51:TYR:OH	2:B:314:CYS:HB3	2.22	0.40
1:A:553:GLU:O	1:A:557:GLU:HG3	2.22	0.40
1:C:10:SER:O	1:C:11:GLU:C	2.60	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%)	<b>2</b> <b>0</b>
1	C	565/567 (100%)	503 (89%)	45 (8%)	17 (3%)	<b>4</b> <b>1</b>
2	B	327/331 (99%)	310 (95%)	12 (4%)	5 (2%)	<b>10</b> <b>4</b>
2	D	327/331 (99%)	309 (94%)	13 (4%)	5 (2%)	<b>10</b> <b>4</b>
All	All	1784/1796 (99%)	1614 (90%)	118 (7%)	52 (3%)	<b>4</b> <b>1</b>

All (52) Ramachandran outliers are listed below:

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

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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
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

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Mol	Chain	Res	Type
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%)	437 (89%)	53 (11%)	6	3
1	C	494/507 (97%)	453 (92%)	41 (8%)	11	7
2	B	283/284 (100%)	252 (89%)	31 (11%)	6	3
2	D	283/284 (100%)	250 (88%)	33 (12%)	5	3
All	All	1550/1582 (98%)	1392 (90%)	158 (10%)	7	4

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LYS
1	A	37	GLN
1	A	47	SER
1	A	49	LEU
1	A	62	PHE
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
1	A	176	SER
1	A	179	SER
1	A	183	TYR
1	A	197	SER
1	A	202	ARG
1	A	204	PRO
1	A	215	VAL
1	A	243	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
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	319	ARG
1	A	326	ASP
1	A	334	LEU
1	A	340	CYS
1	A	349	GLU
1	A	351	LEU
1	A	352	PHE
1	A	353	ARG
1	A	364	LEU
1	A	367	GLU
1	A	374	LEU
1	A	393	ARG
1	A	405	LEU
1	A	430	LEU
1	A	476	ARG
1	A	520	LEU
1	A	521	GLN
1	A	533	PRO
1	A	534	ARG
1	A	536	VAL
1	A	539	ASN
1	A	544	SER
1	A	545	LEU
1	A	553	GLU
2	B	3	THR
2	B	7	ASP
2	B	9	THR
2	B	13	ASP
2	B	37	TYR
2	B	38	GLU
2	B	39	TYR
2	B	40	CYS
2	B	41	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	B	72	LEU
2	B	81	GLU
2	B	85	VAL
2	B	96	LEU
2	B	107	LEU
2	B	115	ASN
2	B	118	LYS
2	B	137	ILE
2	B	150	VAL
2	B	163	ASN
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	281	ARG
2	B	304	GLU
2	B	331	SER
1	C	30	SER
1	C	62	PHE
1	C	73	LEU
1	C	76	LEU
1	C	122	GLU
1	C	136	LEU
1	C	163	GLU
1	C	175	PHE
1	C	183	TYR
1	C	191	LEU
1	C	194	GLN
1	C	206	ASN
1	C	210	LYS
1	C	213	GLU
1	C	214	LEU
1	C	236	LEU
1	C	238	ARG
1	C	244	VAL
1	C	259	VAL
1	C	271	MET

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	C	289	THR
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	364	LEU
1	C	366	SER
1	C	374	LEU
1	C	418	ARG
1	C	430	LEU
1	C	504	VAL
1	C	509	ARG
1	C	536	VAL
1	C	539	ASN
1	C	545	LEU
1	C	551	ILE
2	D	8	VAL
2	D	13	ASP
2	D	17	THR
2	D	20	LEU
2	D	34	LYS
2	D	35	ASP
2	D	37	TYR
2	D	39	TYR
2	D	40	CYS
2	D	45	LEU
2	D	46	ARG
2	D	72	LEU
2	D	76	LYS
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

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Mol	Chain	Res	Type
2	D	163	ASN
2	D	201	LEU
2	D	207	LEU
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

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	74	GLN
1	A	200	GLN
1	A	216	GLN
1	A	232	HIS
1	A	249	HIS
1	A	315	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	80	HIS
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	29	GLN
1	C	74	GLN
1	C	144	HIS
1	C	155	GLN

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Mol	Chain	Res	Type
1	C	217	ASN
1	C	232	HIS
1	C	298	HIS
1	C	312	GLN
1	C	315	GLN
1	C	467	HIS
1	C	517	ASN
1	C	518	ASN
1	C	539	ASN
1	C	543	ASN
1	C	552	GLN
2	D	4	GLN
2	D	67	ASN
2	D	94	HIS
2	D	124	GLN
2	D	127	GLN
2	D	163	ASN
2	D	176	ASN
2	D	271	GLN
2	D	305	GLN
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	0.83	0	7,9,11	2.05	2 (28%)
1	FME	C	1	1	8,9,10	0.92	0	7,9,11	2.15	2 (28%)

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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	FME	O-C-CA	-4.63	112.65	124.78
1	C	1	FME	O-C-CA	-3.96	114.39	124.78
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

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	CB-CA-N-CN
1	C	1	FME	CA-CB-CG-SD
1	A	1	FME	CA-CB-CG-SD
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 carbohydrates 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

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.