Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 09:00 PM GMT

PDB ID	:	1MT5
Title	:	CRYSTAL STRUCTURE OF FATTY ACID AMIDE HYDROLASE
Authors	:	Bracey, M.H.; Hanson, M.A.; Masuda, K.R.; Stevens, R.C.; Cravatt, B.F.
Deposited on	:	2002-09-20
Resolution	:	2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

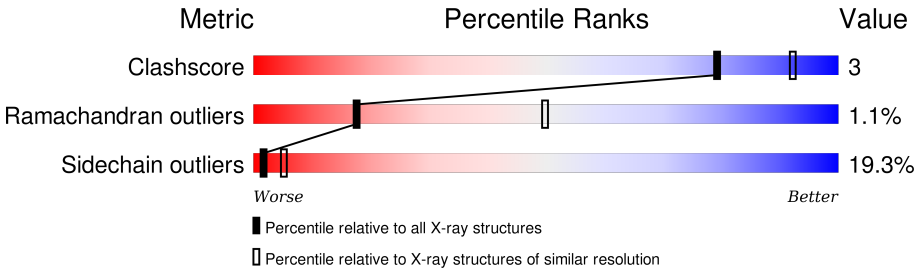
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	537	76% 22% •
1	B	537	76% 20% •
1	C	537	76% 19% •
1	D	537	77% 19% •
1	E	537	75% 21% •
1	F	537	75% 20% 5%
1	G	537	76% 21% • •

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Mol	Chain	Length	Quality of chain
1	H	537	77% 20%
1	I	537	77% 21%
1	J	537	75% 22%
1	K	537	74% 23%
1	L	537	75% 22%
1	M	537	69% 28%
1	N	537	74% 22%
1	O	537	75% 21%
1	P	537	73% 24%

2 Entry composition

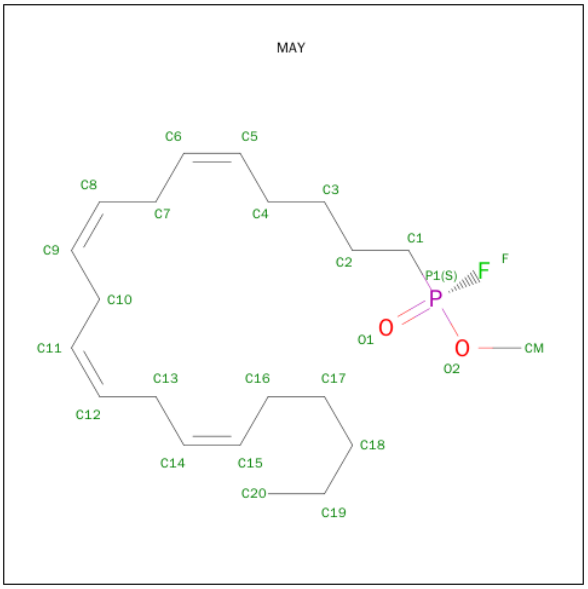
There are 2 unique types of molecules in this entry. The entry contains 64524 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Fatty-acid amide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	B	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	C	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	D	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	E	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	F	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	G	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	H	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	I	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	J	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	K	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	L	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	M	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	N	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			
1	O	537	Total	C	N	O	S	0	0	0
			4010	2568	669	744	29			
1	P	537	Total	C	N	O	S	0	0	0
			4008	2568	669	742	29			

- Molecule 2 is METHYL ARACHIDONYL FLUOROPHOSPHONATE (three-letter code: MAY) (formula: $C_{21}H_{36}FO_2P$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			24	21	2	1		
2	B	1	Total	C	O	P	0	0
			24	21	2	1		
2	C	1	Total	C	O	P	0	0
			24	21	2	1		
2	D	1	Total	C	O	P	0	0
			24	21	2	1		
2	E	1	Total	C	O	P	0	0
			24	21	2	1		
2	F	1	Total	C	O	P	0	0
			24	21	2	1		
2	G	1	Total	C	O	P	0	0
			24	21	2	1		
2	H	1	Total	C	O	P	0	0
			24	21	2	1		
2	I	1	Total	C	O	P	0	0
			24	21	2	1		
2	J	1	Total	C	O	P	0	0
			24	21	2	1		
2	K	1	Total	C	O	P	0	0
			24	21	2	1		
2	L	1	Total	C	O	P	0	0
			24	21	2	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	M	1	Total	C	O	P	0	0
			24	21	2	1		
2	N	1	Total	C	O	P	0	0
			24	21	2	1		
2	O	1	Total	C	O	P	0	0
			24	21	2	1		
2	P	1	Total	C	O	P	0	0
			24	21	2	1		

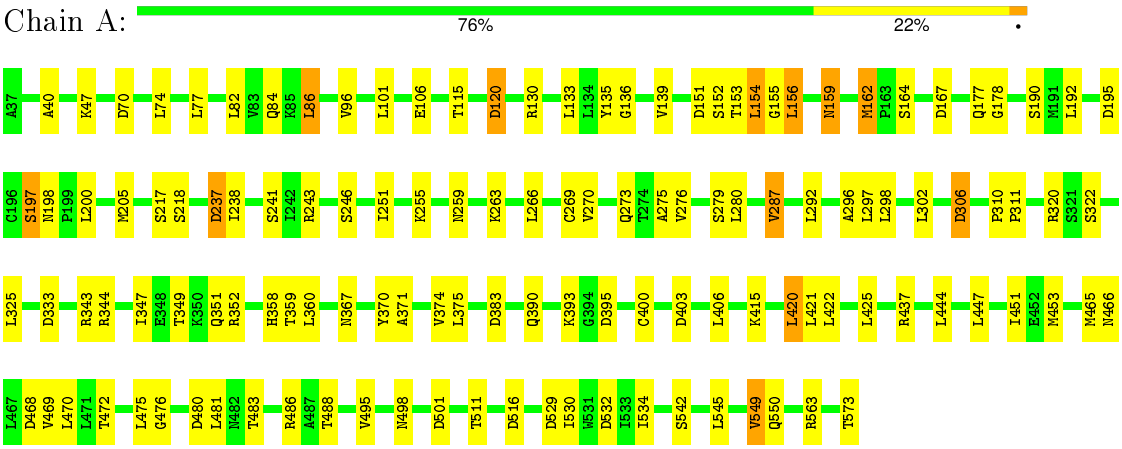
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

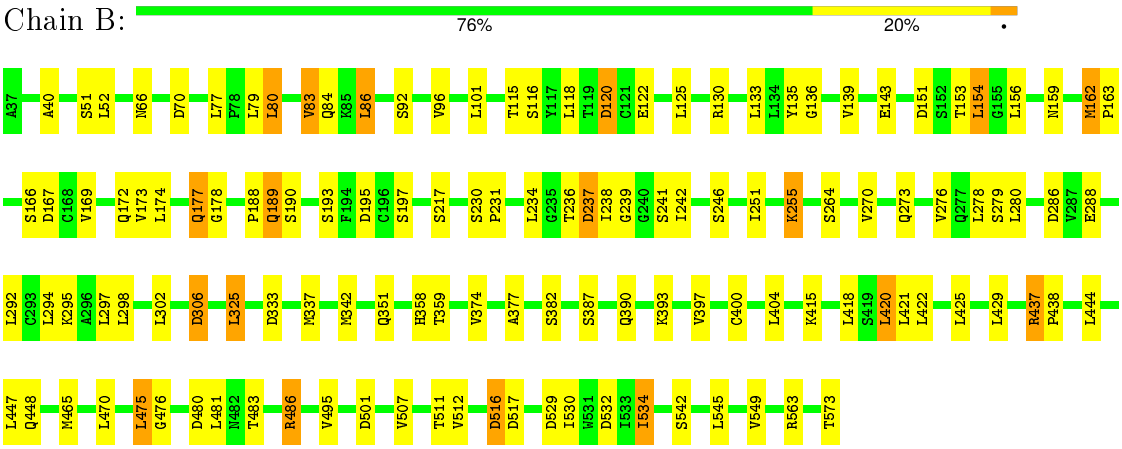
• Molecule 1: Fatty-acid amide hydrolase

Chain A:



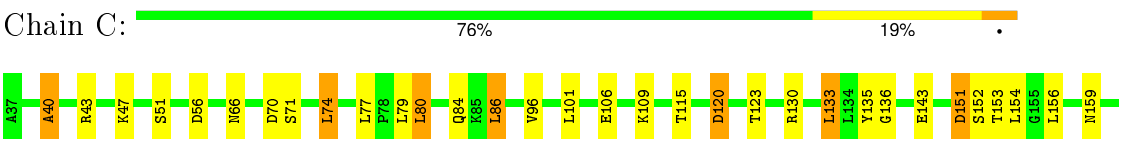
• Molecule 1: Fatty-acid amide hydrolase

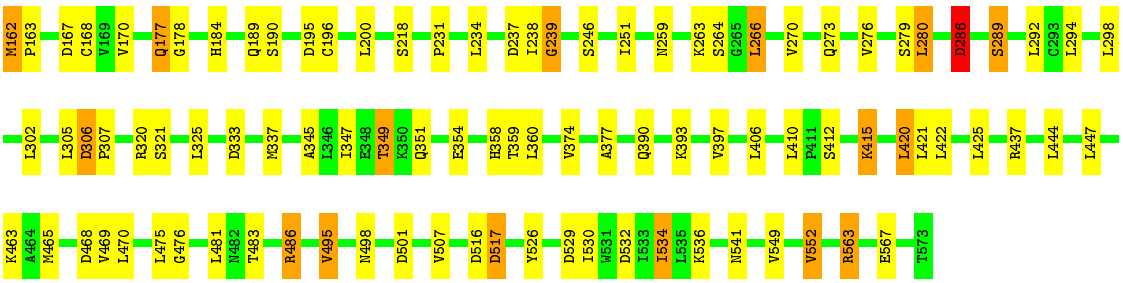
Chain B:



• Molecule 1: Fatty-acid amide hydrolase

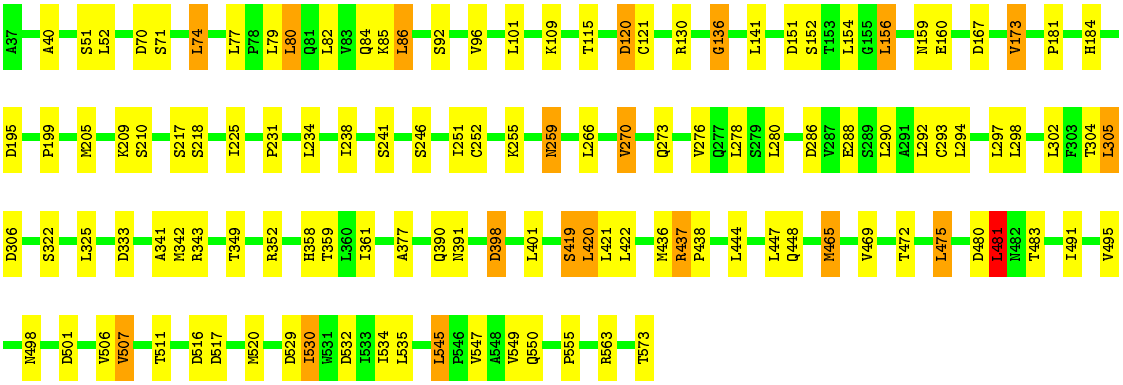
Chain C:





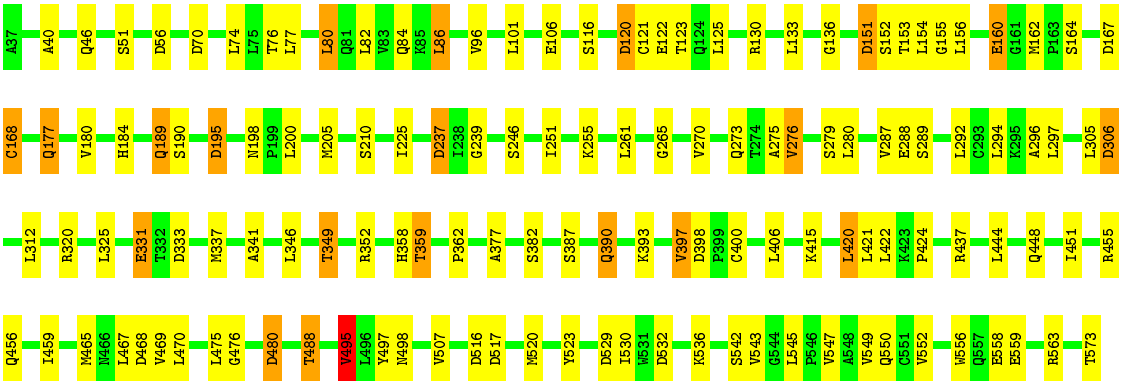
• Molecule 1: Fatty-acid amide hydrolase

Chain D:



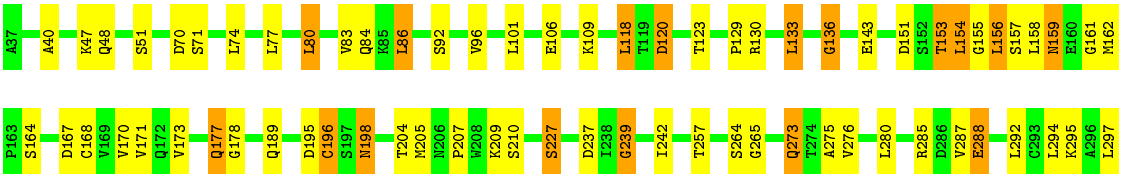
• Molecule 1: Fatty-acid amide hydrolase

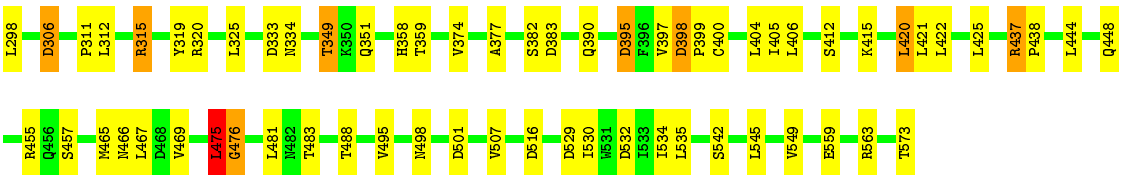
Chain E:



• Molecule 1: Fatty-acid amide hydrolase

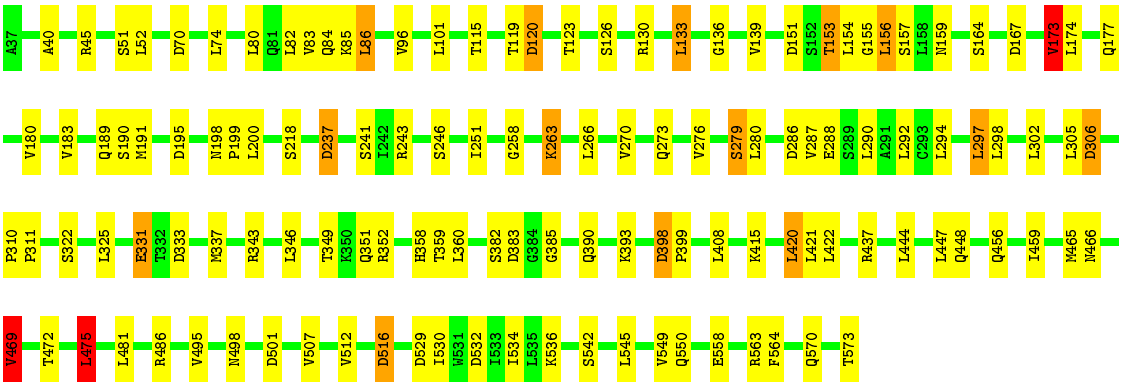
Chain F:





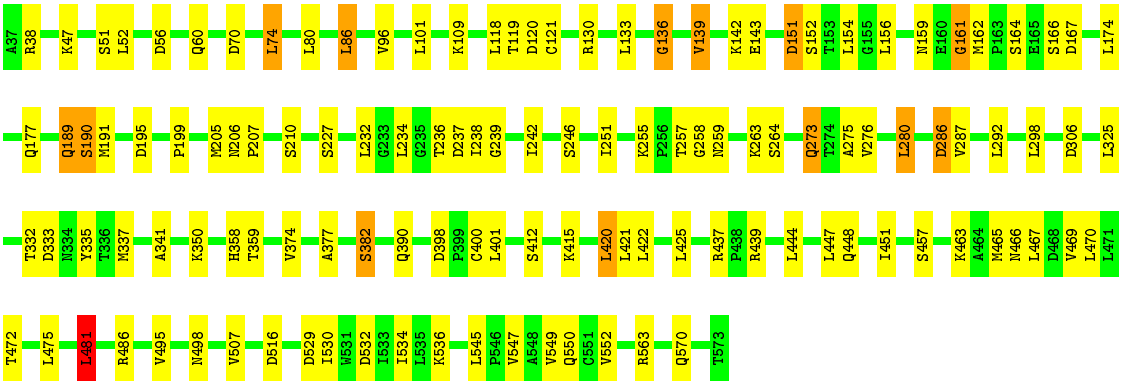
• Molecule 1: Fatty-acid amide hydrolase

Chain G:



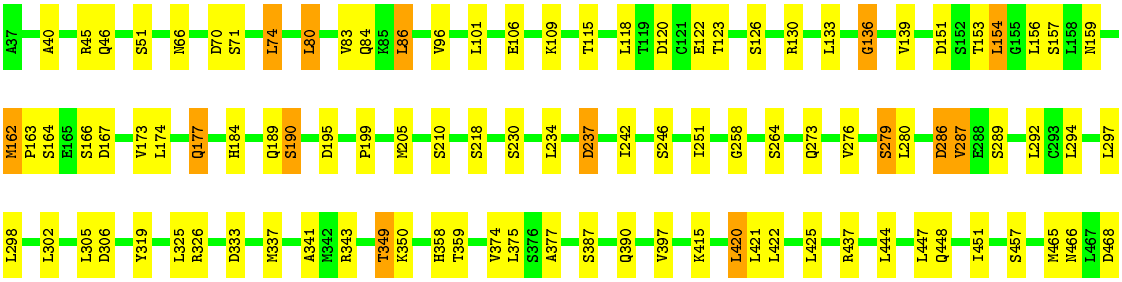
• Molecule 1: Fatty-acid amide hydrolase

Chain H:



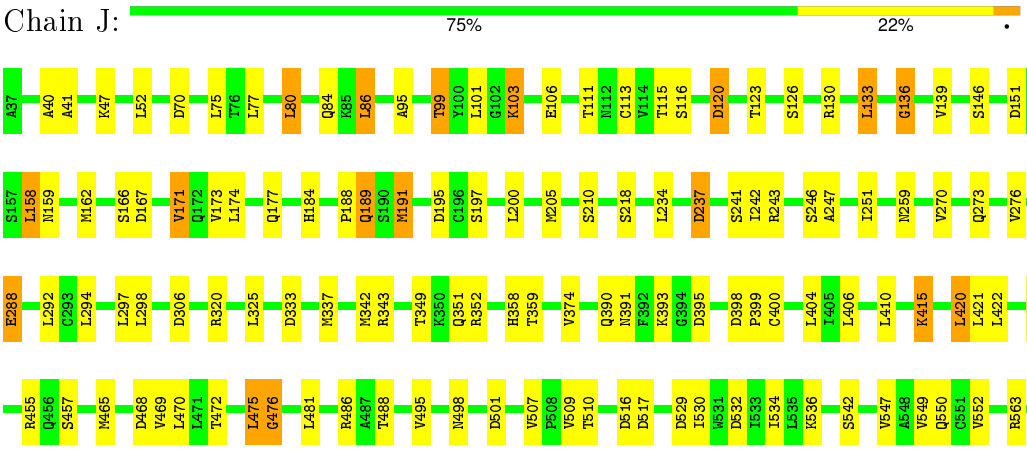
• Molecule 1: Fatty-acid amide hydrolase

Chain I:



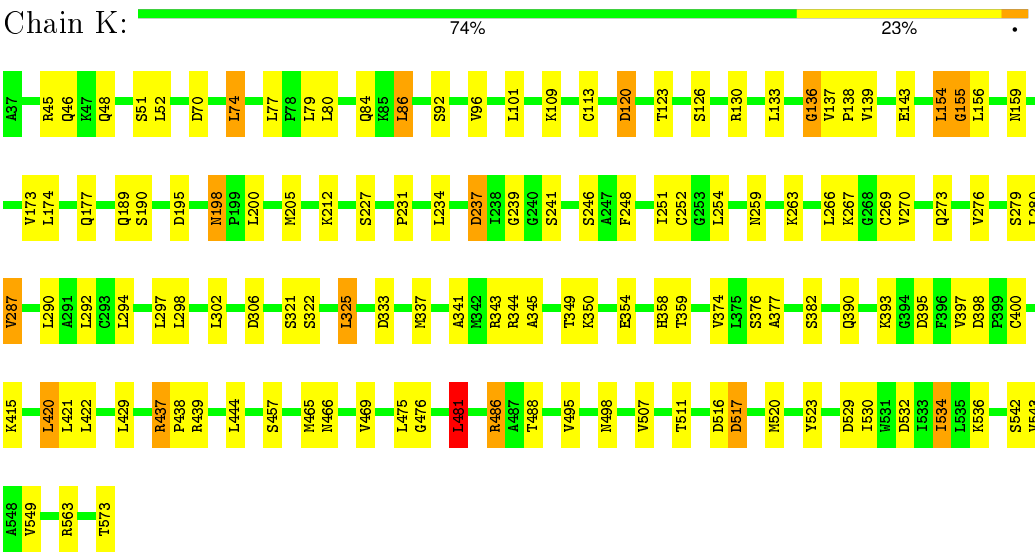
• Molecule 1: Fatty-acid amide hydrolase

Chain J:



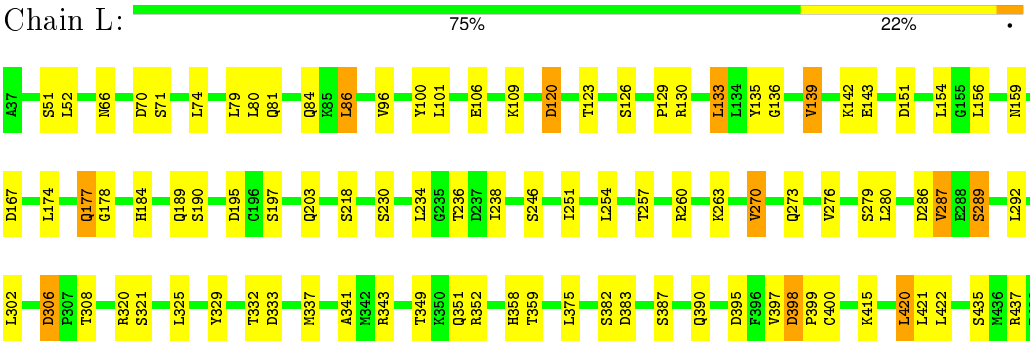
• Molecule 1: Fatty-acid amide hydrolase

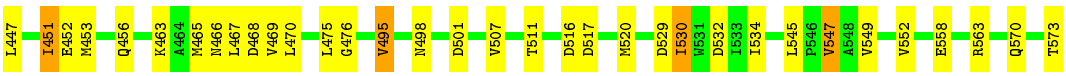
Chain K:



• Molecule 1: Fatty-acid amide hydrolase

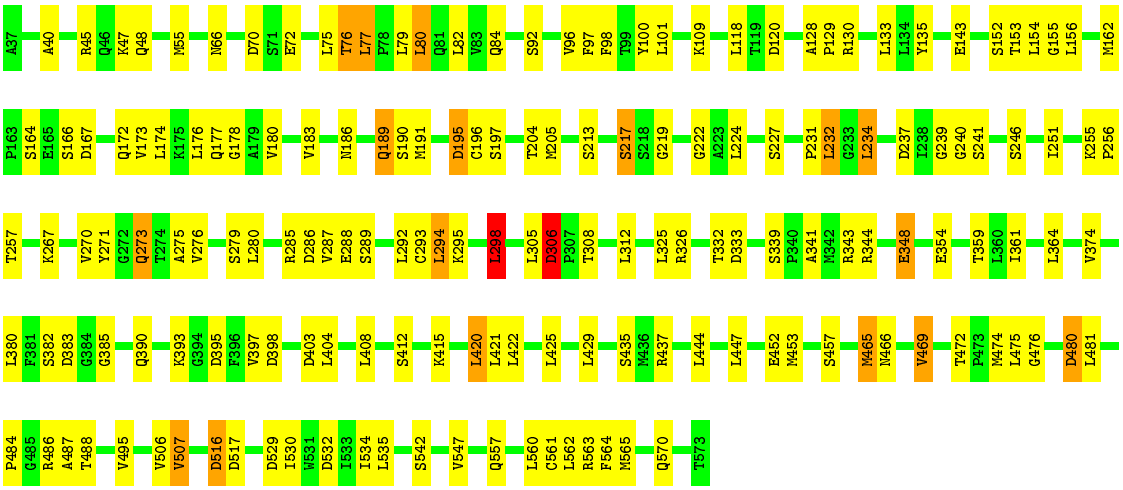
Chain L:





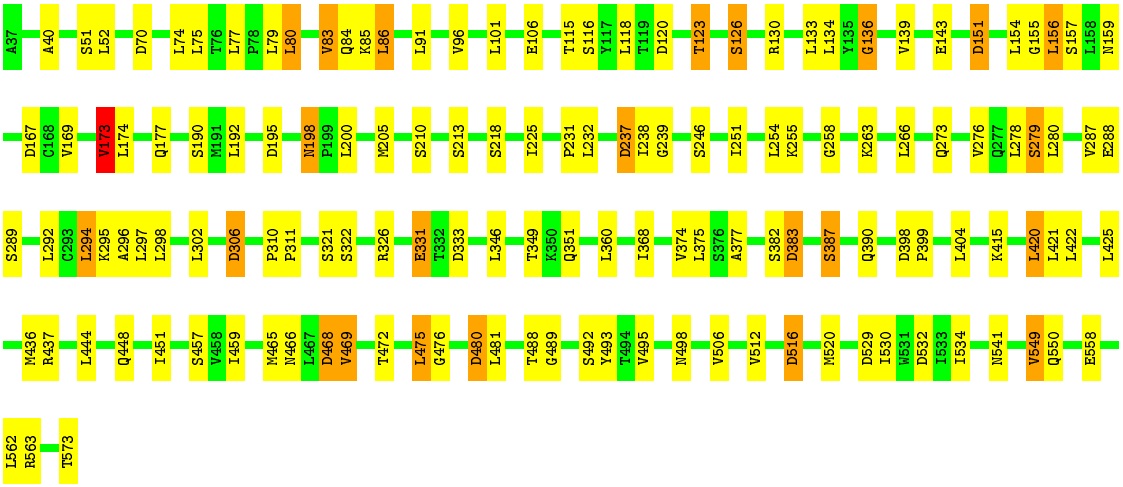
• Molecule 1: Fatty-acid amide hydrolase

Chain M:



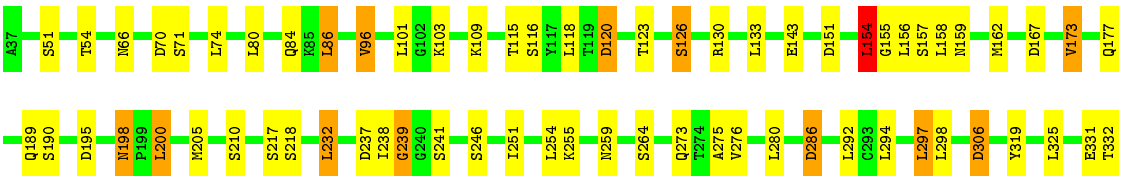
• Molecule 1: Fatty-acid amide hydrolase

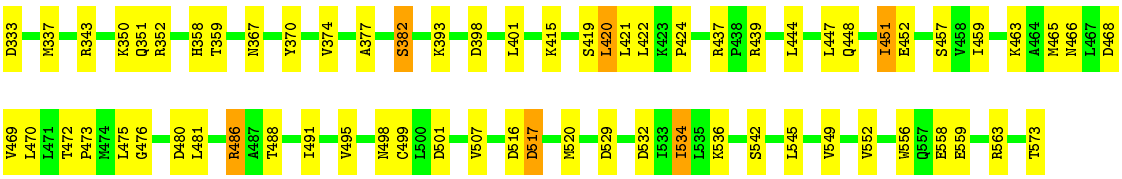
Chain N:



• Molecule 1: Fatty-acid amide hydrolase

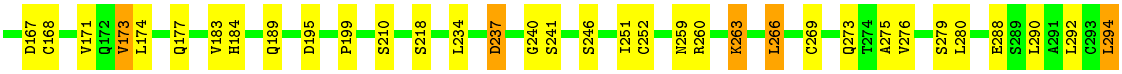
Chain O:

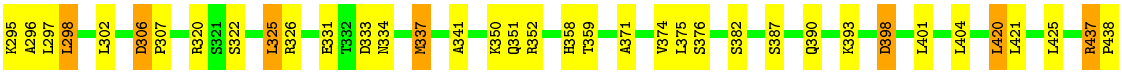




- Molecule 1: Fatty-acid amide hydrolase

Chain P:





4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	147.11Å 272.02Å 147.22Å 90.00° 115.21° 90.00°	Depositor
Resolution (Å)	141.42 – 2.80	Depositor
% Data completeness (in resolution range)	71.4 (141.42-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
Refinement program	REFMAC 5.1.19	Depositor
R, R_{free}	0.218 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	64524	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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	0.95	2/4102 (0.0%)	0.88	16/5589 (0.3%)
1	B	0.97	2/4100 (0.0%)	0.89	14/5586 (0.3%)
1	C	0.95	2/4100 (0.0%)	0.88	16/5586 (0.3%)
1	D	0.93	2/4100 (0.0%)	0.87	17/5586 (0.3%)
1	E	1.01	3/4100 (0.1%)	0.88	16/5586 (0.3%)
1	F	0.97	3/4100 (0.1%)	0.89	16/5586 (0.3%)
1	G	0.97	2/4102 (0.0%)	0.88	16/5589 (0.3%)
1	H	0.93	0/4100	0.88	14/5586 (0.3%)
1	I	0.96	2/4102 (0.0%)	0.86	14/5589 (0.3%)
1	J	0.97	2/4100 (0.0%)	0.87	15/5586 (0.3%)
1	K	0.98	3/4100 (0.1%)	0.89	16/5586 (0.3%)
1	L	1.02	2/4102 (0.0%)	0.88	16/5589 (0.3%)
1	M	1.13	2/4102 (0.0%)	0.93	15/5589 (0.3%)
1	N	1.09	2/4100 (0.0%)	0.89	14/5586 (0.3%)
1	O	0.96	1/4102 (0.0%)	0.88	17/5589 (0.3%)
1	P	1.00	3/4100 (0.1%)	0.88	16/5586 (0.3%)
All	All	0.99	33/65612 (0.1%)	0.88	248/89394 (0.3%)

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	2
1	B	0	3
1	C	0	2
1	D	0	4
1	E	0	4
1	F	0	6
1	G	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	6
1	I	0	5
1	J	0	4
1	K	0	3
1	L	0	1
1	M	0	4
1	N	0	4
1	O	0	4
1	P	0	2
All	All	0	57

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	469	VAL	CB-CG1	-6.53	1.39	1.52
1	A	549	VAL	CA-CB	6.08	1.67	1.54
1	A	287	VAL	CA-CB	5.88	1.67	1.54
1	D	507	VAL	CA-CB	5.77	1.66	1.54
1	F	83	VAL	CA-CB	5.72	1.66	1.54
1	C	552	VAL	CA-CB	5.70	1.66	1.54
1	M	469	VAL	CB-CG1	-5.55	1.41	1.52
1	G	173	VAL	CA-CB	5.53	1.66	1.54
1	N	173	VAL	CB-CG1	-5.50	1.41	1.52
1	L	287	VAL	CA-CB	5.49	1.66	1.54
1	I	349	THR	CA-CB	5.49	1.67	1.53
1	F	171	VAL	CB-CG2	-5.43	1.41	1.52
1	B	83	VAL	CA-CB	5.42	1.66	1.54
1	F	349	THR	CA-CB	5.42	1.67	1.53
1	J	171	VAL	CB-CG2	-5.39	1.41	1.52
1	E	349	THR	CA-CB	5.38	1.67	1.53
1	O	558	GLU	CD-OE1	-5.34	1.19	1.25
1	P	173	VAL	CA-CB	5.34	1.66	1.54
1	K	287	VAL	CB-CG1	-5.32	1.41	1.52
1	L	270	VAL	CA-CB	5.32	1.66	1.54
1	I	287	VAL	CA-CB	5.26	1.65	1.54
1	E	497	TYR	CE2-CZ	5.23	1.45	1.38
1	N	83	VAL	CA-CB	5.22	1.65	1.54
1	E	495	VAL	CA-CB	5.13	1.65	1.54
1	P	526	TYR	CD1-CE1	5.10	1.47	1.39
1	K	287	VAL	CA-CB	5.09	1.65	1.54
1	C	526	TYR	CD2-CE2	5.06	1.47	1.39
1	P	83	VAL	CA-CB	5.04	1.65	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	247	ALA	CA-CB	-5.03	1.41	1.52
1	M	507	VAL	CA-CB	5.03	1.65	1.54
1	D	270	VAL	CA-CB	5.03	1.65	1.54
1	B	270	VAL	CA-CB	5.01	1.65	1.54
1	K	248	PHE	CB-CG	5.01	1.59	1.51

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	237	ASP	CB-CG-OD2	8.76	126.18	118.30
1	H	333	ASP	CB-CG-OD2	8.51	125.96	118.30
1	A	529	ASP	CB-CG-OD2	8.42	125.88	118.30
1	D	333	ASP	CB-CG-OD2	8.38	125.84	118.30
1	B	529	ASP	CB-CG-OD2	8.37	125.83	118.30
1	C	420	LEU	CA-CB-CG	8.10	133.93	115.30
1	J	70	ASP	CB-CG-OD2	8.08	125.58	118.30
1	K	529	ASP	CB-CG-OD2	8.08	125.58	118.30
1	F	333	ASP	CB-CG-OD2	8.08	125.57	118.30
1	P	237	ASP	CB-CG-OD2	8.05	125.54	118.30
1	G	151	ASP	CB-CG-OD2	8.03	125.52	118.30
1	E	167	ASP	CB-CG-OD2	8.02	125.51	118.30
1	G	70	ASP	CB-CG-OD2	7.97	125.47	118.30
1	J	333	ASP	CB-CG-OD2	7.95	125.45	118.30
1	H	529	ASP	CB-CG-OD2	7.95	125.45	118.30
1	H	70	ASP	CB-CG-OD2	7.89	125.40	118.30
1	C	195	ASP	CB-CG-OD2	7.82	125.34	118.30
1	K	195	ASP	CB-CG-OD2	7.80	125.32	118.30
1	I	333	ASP	CB-CG-OD2	7.79	125.31	118.30
1	F	195	ASP	CB-CG-OD2	7.79	125.31	118.30
1	P	333	ASP	CB-CG-OD2	7.77	125.30	118.30
1	G	333	ASP	CB-CG-OD2	7.74	125.26	118.30
1	M	529	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	167	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	195	ASP	CB-CG-OD2	7.68	125.21	118.30
1	B	333	ASP	CB-CG-OD2	7.63	125.16	118.30
1	B	532	ASP	CB-CG-OD2	7.58	125.12	118.30
1	E	529	ASP	CB-CG-OD2	7.57	125.11	118.30
1	H	195	ASP	CB-CG-OD2	7.54	125.09	118.30
1	L	70	ASP	CB-CG-OD2	7.53	125.08	118.30
1	D	529	ASP	CB-CG-OD2	7.52	125.07	118.30
1	P	529	ASP	CB-CG-OD2	7.46	125.01	118.30
1	B	70	ASP	CB-CG-OD2	7.43	124.99	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	529	ASP	CB-CG-OD2	7.42	124.98	118.30
1	C	529	ASP	CB-CG-OD2	7.39	124.95	118.30
1	M	195	ASP	CB-CG-OD2	7.35	124.91	118.30
1	C	167	ASP	CB-CG-OD2	7.34	124.91	118.30
1	K	333	ASP	CB-CG-OD2	7.34	124.91	118.30
1	C	70	ASP	CB-CG-OD2	7.32	124.89	118.30
1	L	532	ASP	CB-CG-OD2	7.32	124.89	118.30
1	J	529	ASP	CB-CG-OD2	7.31	124.88	118.30
1	D	516	ASP	CB-CG-OD2	7.31	124.88	118.30
1	E	333	ASP	CB-CG-OD2	7.31	124.88	118.30
1	N	167	ASP	CB-CG-OD2	7.28	124.85	118.30
1	B	151	ASP	CB-CG-OD2	7.26	124.84	118.30
1	C	333	ASP	CB-CG-OD2	7.25	124.82	118.30
1	D	195	ASP	CB-CG-OD2	7.23	124.80	118.30
1	N	70	ASP	CB-CG-OD2	7.23	124.80	118.30
1	L	195	ASP	CB-CG-OD2	7.20	124.78	118.30
1	M	532	ASP	CB-CG-OD2	7.20	124.78	118.30
1	G	529	ASP	CB-CG-OD2	7.19	124.77	118.30
1	K	70	ASP	CB-CG-OD2	7.18	124.76	118.30
1	K	167	ASP	CB-CG-OD2	7.16	124.74	118.30
1	J	306	ASP	CB-CG-OD2	7.14	124.72	118.30
1	K	532	ASP	CB-CG-OD2	7.13	124.71	118.30
1	F	151	ASP	CB-CG-OD2	7.12	124.71	118.30
1	G	501	ASP	CB-CG-OD2	7.12	124.71	118.30
1	A	151	ASP	CB-CG-OD2	7.08	124.67	118.30
1	O	151	ASP	CB-CG-OD2	7.05	124.65	118.30
1	M	70	ASP	CB-CG-OD2	7.05	124.65	118.30
1	L	333	ASP	CB-CG-OD2	7.04	124.64	118.30
1	M	420	LEU	CA-CB-CG	7.03	131.46	115.30
1	L	167	ASP	CB-CG-OD2	7.02	124.62	118.30
1	O	333	ASP	CB-CG-OD2	7.01	124.61	118.30
1	E	420	LEU	CA-CB-CG	7.00	131.39	115.30
1	L	151	ASP	CB-CG-OD2	6.99	124.59	118.30
1	C	532	ASP	CB-CG-OD2	6.96	124.56	118.30
1	I	195	ASP	CB-CG-OD2	6.96	124.56	118.30
1	M	237	ASP	CB-CG-OD2	6.95	124.55	118.30
1	O	516	ASP	CB-CG-OD2	6.95	124.55	118.30
1	P	516	ASP	CB-CG-OD2	6.94	124.55	118.30
1	E	195	ASP	CB-CG-OD2	6.93	124.54	118.30
1	A	70	ASP	CB-CG-OD2	6.84	124.45	118.30
1	F	529	ASP	CB-CG-OD2	6.83	124.44	118.30
1	N	529	ASP	CB-CG-OD2	6.82	124.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	286	ASP	CB-CG-OD2	6.81	124.43	118.30
1	M	333	ASP	CB-CG-OD2	6.78	124.41	118.30
1	J	167	ASP	CB-CG-OD2	6.77	124.39	118.30
1	J	532	ASP	CB-CG-OD2	6.77	124.39	118.30
1	I	529	ASP	CB-CG-OD2	6.75	124.38	118.30
1	P	167	ASP	CB-CG-OD2	6.75	124.38	118.30
1	D	70	ASP	CB-CG-OD2	6.75	124.37	118.30
1	E	306	ASP	CB-CG-OD2	6.75	124.37	118.30
1	I	151	ASP	CB-CG-OD2	6.75	124.37	118.30
1	I	70	ASP	CB-CG-OD2	6.71	124.33	118.30
1	H	237	ASP	CB-CG-OD2	6.66	124.30	118.30
1	A	420	LEU	CA-CB-CG	6.65	130.59	115.30
1	E	151	ASP	CB-CG-OD2	6.65	124.28	118.30
1	A	501	ASP	CB-CG-OD2	6.61	124.25	118.30
1	N	151	ASP	CB-CG-OD2	6.60	124.24	118.30
1	G	167	ASP	CB-CG-OD2	6.60	124.24	118.30
1	O	237	ASP	CB-CG-OD2	6.60	124.24	118.30
1	F	532	ASP	CB-CG-OD2	6.60	124.24	118.30
1	P	195	ASP	CB-CG-OD2	6.57	124.21	118.30
1	F	237	ASP	CB-CG-OD2	6.56	124.20	118.30
1	G	532	ASP	CB-CG-OD2	6.55	124.20	118.30
1	M	398	ASP	CB-CG-OD2	6.54	124.19	118.30
1	E	516	ASP	CB-CG-OD2	6.54	124.19	118.30
1	B	420	LEU	CA-CB-CG	6.54	130.33	115.30
1	I	167	ASP	CB-CG-OD2	6.54	124.18	118.30
1	C	501	ASP	CB-CG-OD2	6.53	124.17	118.30
1	G	516	ASP	CB-CG-OD2	6.53	124.17	118.30
1	K	516	ASP	CB-CG-OD2	6.52	124.17	118.30
1	F	167	ASP	CB-CG-OD2	6.52	124.17	118.30
1	I	420	LEU	CA-CB-CG	6.50	130.26	115.30
1	O	195	ASP	CB-CG-OD2	6.49	124.14	118.30
1	N	333	ASP	CB-CG-OD2	6.49	124.14	118.30
1	I	516	ASP	CB-CG-OD2	6.46	124.11	118.30
1	B	167	ASP	CB-CG-OD2	6.43	124.09	118.30
1	K	237	ASP	CB-CG-OD2	6.42	124.08	118.30
1	J	501	ASP	CB-CG-OD2	6.42	124.08	118.30
1	G	420	LEU	CA-CB-CG	6.42	130.05	115.30
1	L	516	ASP	CB-CG-OD2	6.41	124.07	118.30
1	O	167	ASP	CB-CG-OD2	6.40	124.06	118.30
1	N	516	ASP	CB-CG-OD2	6.40	124.06	118.30
1	B	237	ASP	CB-CG-OD2	6.39	124.05	118.30
1	P	532	ASP	CB-CG-OD2	6.39	124.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	70	ASP	CB-CG-OD2	6.38	124.05	118.30
1	H	167	ASP	CB-CG-OD2	6.38	124.05	118.30
1	M	516	ASP	CB-CG-OD2	6.37	124.03	118.30
1	O	529	ASP	CB-CG-OD2	6.36	124.03	118.30
1	E	480	ASP	CB-CG-OD2	6.35	124.02	118.30
1	D	151	ASP	CB-CG-OD2	6.32	123.99	118.30
1	N	195	ASP	CB-CG-OD2	6.32	123.99	118.30
1	B	516	ASP	CB-CG-OD2	6.31	123.98	118.30
1	E	70	ASP	CB-CG-OD2	6.30	123.97	118.30
1	D	167	ASP	CB-CG-OD2	6.30	123.97	118.30
1	H	516	ASP	CB-CG-OD2	6.30	123.97	118.30
1	F	516	ASP	CB-CG-OD2	6.27	123.94	118.30
1	J	516	ASP	CB-CG-OD2	6.23	123.91	118.30
1	J	237	ASP	CB-CG-OD2	6.15	123.83	118.30
1	N	237	ASP	CB-CG-OD2	6.15	123.83	118.30
1	K	286	ASP	CB-CG-OD2	6.14	123.83	118.30
1	O	70	ASP	CB-CG-OD2	6.12	123.80	118.30
1	K	420	LEU	CA-CB-CG	6.10	129.33	115.30
1	O	532	ASP	CB-CG-OD2	6.10	123.79	118.30
1	E	532	ASP	CB-CG-OD2	6.05	123.74	118.30
1	C	516	ASP	CB-CG-OD2	6.04	123.73	118.30
1	D	420	LEU	CA-CB-CG	6.04	129.19	115.30
1	D	532	ASP	CB-CG-OD2	5.98	123.68	118.30
1	O	232	LEU	CA-CB-CG	5.92	128.93	115.30
1	A	333	ASP	CB-CG-OD2	5.92	123.62	118.30
1	A	516	ASP	CB-CG-OD2	5.91	123.62	118.30
1	J	195	ASP	CB-CG-OD2	5.91	123.62	118.30
1	O	306	ASP	CB-CG-OD2	5.90	123.61	118.30
1	I	532	ASP	CB-CG-OD2	5.89	123.60	118.30
1	C	151	ASP	CB-CG-OD2	5.88	123.59	118.30
1	N	420	LEU	CA-CB-CG	5.88	128.82	115.30
1	F	420	LEU	CA-CB-CG	5.88	128.82	115.30
1	J	420	LEU	CA-CB-CG	5.88	128.81	115.30
1	F	398	ASP	CB-CG-OD2	5.87	123.58	118.30
1	N	532	ASP	CB-CG-OD2	5.86	123.57	118.30
1	B	195	ASP	CB-CG-OD2	5.85	123.57	118.30
1	F	306	ASP	CB-CG-OD2	5.84	123.56	118.30
1	H	151	ASP	CB-CG-OD2	5.84	123.56	118.30
1	A	237	ASP	CB-CG-OD2	5.84	123.56	118.30
1	M	167	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	532	ASP	CB-CG-OD2	5.79	123.51	118.30
1	L	420	LEU	CA-CB-CG	5.76	128.55	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	468	ASP	CB-CG-OD2	5.76	123.48	118.30
1	K	120	ASP	CB-CG-OD2	5.76	123.48	118.30
1	P	70	ASP	CB-CG-OD2	5.75	123.47	118.30
1	K	74	LEU	CA-CB-CG	5.74	128.50	115.30
1	D	74	LEU	CA-CB-CG	5.72	128.46	115.30
1	G	195	ASP	CB-CG-OD2	5.72	123.45	118.30
1	L	517	ASP	CB-CG-OD2	5.71	123.44	118.30
1	B	517	ASP	CB-CG-OD2	5.69	123.42	118.30
1	N	306	ASP	CB-CG-OD2	5.68	123.41	118.30
1	L	286	ASP	CB-CG-OD2	5.67	123.40	118.30
1	J	468	ASP	CB-CG-OD2	5.64	123.37	118.30
1	J	151	ASP	CB-CG-OD2	5.64	123.37	118.30
1	C	468	ASP	CB-CG-OD2	5.63	123.37	118.30
1	E	398	ASP	CB-CG-OD2	5.63	123.37	118.30
1	O	420	LEU	CA-CB-CG	5.63	128.25	115.30
1	H	398	ASP	CB-CG-OD2	5.62	123.36	118.30
1	C	56	ASP	CB-CG-OD2	5.60	123.34	118.30
1	I	306	ASP	CB-CG-OD2	5.60	123.34	118.30
1	H	420	LEU	CA-CB-CG	5.58	128.14	115.30
1	I	468	ASP	CB-CG-OD2	5.57	123.31	118.30
1	M	286	ASP	CB-CG-OD2	5.57	123.31	118.30
1	K	306	ASP	CB-CG-OD2	5.57	123.31	118.30
1	D	120	ASP	CB-CG-OD2	5.51	123.26	118.30
1	E	468	ASP	CB-CG-OD2	5.51	123.26	118.30
1	F	501	ASP	CB-CG-OD2	5.50	123.25	118.30
1	A	403	ASP	CB-CG-OD2	5.49	123.24	118.30
1	B	306	ASP	CB-CG-OD2	5.48	123.24	118.30
1	P	566	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	H	532	ASP	CB-CG-OD2	5.48	123.23	118.30
1	D	398	ASP	CB-CG-OD2	5.46	123.22	118.30
1	E	120	ASP	CB-CG-OD2	5.45	123.20	118.30
1	O	120	ASP	CB-CG-OD2	5.44	123.20	118.30
1	D	306	ASP	CB-CG-OD2	5.43	123.19	118.30
1	F	156	LEU	CA-CB-CG	5.43	127.78	115.30
1	K	403	ASP	CB-CG-OD2	5.42	123.18	118.30
1	O	517	ASP	CB-CG-OD2	5.42	123.17	118.30
1	O	398	ASP	CB-CG-OD2	5.41	123.17	118.30
1	F	120	ASP	CB-CG-OD2	5.40	123.16	118.30
1	G	306	ASP	CB-CG-OD2	5.39	123.15	118.30
1	C	286	ASP	CB-CG-OD2	5.37	123.14	118.30
1	G	237	ASP	CB-CG-OD2	5.36	123.13	118.30
1	D	501	ASP	CB-CG-OD2	5.36	123.12	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	306	ASP	CB-CG-OD2	5.36	123.12	118.30
1	P	420	LEU	CA-CB-CG	5.35	127.59	115.30
1	O	501	ASP	CB-CG-OD2	5.33	123.10	118.30
1	I	480	ASP	CB-CG-OD2	5.33	123.09	118.30
1	K	517	ASP	CB-CG-OD2	5.33	123.09	118.30
1	P	306	ASP	CB-CG-OD2	5.32	123.09	118.30
1	G	120	ASP	CB-CG-OD2	5.31	123.08	118.30
1	I	286	ASP	CB-CG-OD2	5.30	123.07	118.30
1	O	286	ASP	CB-CG-OD2	5.30	123.07	118.30
1	H	56	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	120	ASP	CB-CG-OD2	5.29	123.06	118.30
1	C	120	ASP	CB-CG-OD2	5.29	123.06	118.30
1	N	120	ASP	CB-CG-OD2	5.27	123.04	118.30
1	N	156	LEU	CA-CB-CG	5.26	127.40	115.30
1	P	517	ASP	CB-CG-OD2	5.23	123.01	118.30
1	L	501	ASP	CB-CG-OD2	5.22	123.00	118.30
1	P	398	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	156	LEU	CA-CB-CG	5.20	127.26	115.30
1	P	501	ASP	CB-CG-OD2	5.19	122.97	118.30
1	H	232	LEU	CA-CB-CG	5.17	127.19	115.30
1	M	77	LEU	CA-CB-CG	5.17	127.18	115.30
1	G	398	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	501	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	306	ASP	CB-CG-OD2	5.15	122.93	118.30
1	A	120	ASP	CB-CG-OD2	5.14	122.93	118.30
1	J	120	ASP	CB-CG-OD2	5.13	122.92	118.30
1	F	395	ASP	CB-CG-OD2	5.12	122.90	118.30
1	H	286	ASP	CB-CG-OD2	5.11	122.90	118.30
1	P	468	ASP	CB-CG-OD2	5.09	122.88	118.30
1	A	468	ASP	CB-CG-OD2	5.09	122.88	118.30
1	J	395	ASP	CB-CG-OD2	5.09	122.88	118.30
1	D	286	ASP	CB-CG-OD2	5.08	122.88	118.30
1	G	156	LEU	CA-CB-CG	5.07	126.96	115.30
1	D	305	LEU	CA-CB-CG	5.06	126.95	115.30
1	D	517	ASP	CB-CG-OD2	5.06	122.86	118.30
1	E	56	ASP	CB-CG-OD2	5.06	122.86	118.30
1	M	480	ASP	CB-CG-OD2	5.06	122.85	118.30
1	L	120	ASP	CB-CG-OD2	5.03	122.83	118.30
1	L	398	ASP	CB-CG-OD2	5.03	122.83	118.30
1	C	517	ASP	CB-CG-OD2	5.02	122.82	118.30
1	N	480	ASP	CB-CG-OD2	5.02	122.81	118.30
1	P	151	ASP	CB-CG-OD2	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	403	ASP	CB-CG-OD2	5.01	122.81	118.30
1	I	237	ASP	CB-CG-OD2	5.01	122.81	118.30
1	E	237	ASP	CB-CG-OD2	5.01	122.81	118.30
1	L	306	ASP	CB-CG-OD2	5.01	122.81	118.30
1	K	398	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	120	ASP	Peptide
1	A	197	SER	Peptide
1	B	120	ASP	Peptide
1	B	40	ALA	Peptide
1	B	475	LEU	Peptide
1	C	120	ASP	Peptide
1	C	40	ALA	Peptide
1	D	120	ASP	Peptide
1	D	136	GLY	Peptide
1	D	40	ALA	Peptide
1	D	475	LEU	Peptide
1	E	120	ASP	Peptide
1	E	276	VAL	Peptide
1	E	359	THR	Peptide
1	E	40	ALA	Peptide
1	F	118	LEU	Peptide
1	F	120	ASP	Peptide
1	F	136	GLY	Peptide
1	F	161	GLY	Peptide
1	F	40	ALA	Peptide
1	F	475	LEU	Peptide
1	G	120	ASP	Peptide
1	G	40	ALA	Peptide
1	G	475	LEU	Peptide
1	H	118	LEU	Peptide
1	H	120	ASP	Peptide
1	H	136	GLY	Peptide
1	H	161	GLY	Peptide
1	H	190	SER	Peptide
1	H	38	ARG	Peptide
1	I	118	LEU	Peptide
1	I	120	ASP	Peptide

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Mol	Chain	Res	Type	Group
1	I	136	GLY	Peptide
1	I	190	SER	Peptide
1	I	40	ALA	Peptide
1	J	120	ASP	Peptide
1	J	136	GLY	Peptide
1	J	40	ALA	Peptide
1	J	475	LEU	Peptide
1	K	120	ASP	Peptide
1	K	136	GLY	Peptide
1	K	155	GLY	Peptide
1	L	120	ASP	Peptide
1	M	120	ASP	Peptide
1	M	155	GLY	Peptide
1	M	40	ALA	Peptide
1	M	476	GLY	Peptide
1	N	136	GLY	Peptide
1	N	40	ALA	Peptide
1	N	468	ASP	Peptide
1	N	475	LEU	Peptide
1	O	118	LEU	Peptide
1	O	120	ASP	Peptide
1	O	154	LEU	Peptide
1	O	468	ASP	Peptide
1	P	120	ASP	Peptide
1	P	136	GLY	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4010	0	3953	29	0
1	B	4008	0	3953	28	0
1	C	4008	0	3953	27	0
1	D	4008	0	3953	30	0
1	E	4008	0	3953	29	0
1	F	4008	0	3953	29	0
1	G	4010	0	3953	29	0
1	H	4008	0	3953	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	I	4010	0	3953	21	0
1	J	4008	0	3953	27	0
1	K	4008	0	3953	29	0
1	L	4010	0	3953	24	0
1	M	4010	0	3953	30	0
1	N	4008	0	3953	37	0
1	O	4010	0	3953	26	0
1	P	4008	0	3953	29	0
2	A	24	0	36	5	0
2	B	24	0	36	3	0
2	C	24	0	36	3	0
2	D	24	0	36	4	0
2	E	24	0	36	3	0
2	F	24	0	36	4	0
2	G	24	0	36	1	0
2	H	24	0	36	4	0
2	I	24	0	36	2	0
2	J	24	0	36	2	0
2	K	24	0	36	3	0
2	L	24	0	36	1	0
2	M	24	0	36	2	0
2	N	24	0	36	4	0
2	O	24	0	36	3	0
2	P	24	0	36	2	0
All	All	64524	0	63824	447	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 3.

All (447) 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:L:453:MET:CE	1:L:453:MET:SD	2.02	1.48
1:D:325:LEU:H	1:D:358:HIS:HD2	1.18	0.90
1:A:155:GLY:HA3	1:A:198:ASN:HD21	1.38	0.87
1:C:325:LEU:H	1:C:358:HIS:HD2	1.27	0.81
1:D:86:LEU:HG	1:D:136:GLY:HA3	1.64	0.80
1:K:397:VAL:HG11	1:K:405:ILE:HG21	1.64	0.80
1:A:155:GLY:CA	1:A:198:ASN:HD21	1.98	0.77
1:J:95:ALA:O	1:J:99:THR:OG1	2.05	0.74
1:I:86:LEU:HG	1:I:136:GLY:HA3	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:155:GLY:HA2	1:E:198:ASN:HD22	1.55	0.71
1:P:325:LEU:H	1:P:358:HIS:HD2	1.36	0.71
1:E:86:LEU:HG	1:E:136:GLY:HA3	1.72	0.71
1:K:325:LEU:H	1:K:358:HIS:HD2	1.37	0.70
1:O:325:LEU:H	1:O:358:HIS:HD2	1.40	0.69
1:J:325:LEU:H	1:J:358:HIS:HD2	1.40	0.69
1:A:325:LEU:H	1:A:358:HIS:HD2	1.39	0.69
1:K:86:LEU:HG	1:K:136:GLY:HA3	1.75	0.69
1:B:86:LEU:HG	1:B:136:GLY:HA3	1.73	0.69
1:G:325:LEU:H	1:G:358:HIS:HD2	1.41	0.68
1:C:495:VAL:HA	1:C:498:ASN:HD22	1.61	0.66
1:G:155:GLY:HA2	1:G:198:ASN:HD22	1.60	0.66
1:P:86:LEU:HD21	1:P:96:VAL:HG21	1.78	0.65
1:H:325:LEU:H	1:H:358:HIS:HD2	1.43	0.64
1:L:495:VAL:HG11	2:L:600:MAY:H15	1.79	0.64
1:A:86:LEU:HD21	1:A:96:VAL:HG21	1.79	0.64
1:L:142:LYS:NZ	1:L:236:THR:OG1	2.27	0.64
1:B:325:LEU:H	1:B:358:HIS:HD2	1.45	0.64
1:N:375:LEU:HD22	1:N:451:ILE:HG13	1.79	0.64
1:M:80:LEU:HD11	1:M:288:GLU:HB3	1.79	0.64
1:D:495:VAL:HG11	2:D:600:MAY:H15	1.79	0.64
1:G:246:SER:HA	1:G:251:ILE:HG13	1.79	0.63
1:C:495:VAL:HG11	2:C:600:MAY:H15	1.81	0.63
1:N:80:LEU:HD11	1:N:288:GLU:HB3	1.80	0.62
1:M:495:VAL:HG11	2:M:600:MAY:H15	1.82	0.62
1:E:495:VAL:HA	1:E:498:ASN:HD22	1.64	0.62
1:B:80:LEU:HD11	1:B:288:GLU:HB3	1.81	0.62
1:A:86:LEU:HG	1:A:136:GLY:HA3	1.82	0.62
1:N:331:GLU:HG3	1:N:346:LEU:HD12	1.81	0.62
1:E:495:VAL:HG11	2:E:600:MAY:H15	1.81	0.62
1:F:325:LEU:H	1:F:358:HIS:HD2	1.48	0.62
1:A:246:SER:HA	1:A:251:ILE:HG13	1.80	0.62
1:L:375:LEU:HD13	1:L:451:ILE:HG12	1.82	0.61
1:C:246:SER:HA	1:C:251:ILE:HG13	1.82	0.61
1:J:80:LEU:HD11	1:J:288:GLU:HB3	1.83	0.61
1:H:495:VAL:HA	1:H:498:ASN:HD22	1.65	0.61
1:A:495:VAL:HG11	2:A:600:MAY:H15	1.83	0.60
1:G:495:VAL:HA	1:G:498:ASN:HD22	1.67	0.60
1:B:154:LEU:O	1:B:189:GLN:O	2.20	0.60
1:G:243:ARG:HH22	1:G:498:ASN:HD21	1.50	0.59
1:F:86:LEU:HD21	1:F:96:VAL:HG21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:86:LEU:HG	1:H:136:GLY:HA3	1.83	0.59
1:A:486:ARG:HB2	1:A:534:ILE:HG21	1.85	0.59
1:O:495:VAL:HG11	2:O:600:MAY:H15	1.85	0.59
1:N:155:GLY:HA3	1:N:198:ASN:ND2	2.17	0.58
1:H:246:SER:HA	1:H:251:ILE:HG13	1.86	0.58
1:K:495:VAL:HA	1:K:498:ASN:HD22	1.68	0.58
1:J:246:SER:HA	1:J:251:ILE:HG13	1.86	0.58
1:A:162:MET:N	1:A:162:MET:SD	2.76	0.57
1:K:495:VAL:HG11	2:K:600:MAY:H15	1.85	0.57
1:D:173:VAL:HG22	1:D:297:LEU:HD23	1.86	0.57
1:K:154:LEU:HD21	1:K:267:LYS:HG2	1.86	0.57
1:I:495:VAL:HA	1:I:498:ASN:HD22	1.69	0.57
1:H:275:ALA:HB1	1:H:451:ILE:HD12	1.87	0.57
1:B:153:THR:HA	1:B:159:ASN:HB2	1.85	0.57
1:M:562:LEU:HA	1:M:565:MET:HB2	1.87	0.56
1:B:86:LEU:HD21	1:B:96:VAL:HG21	1.87	0.56
1:N:173:VAL:HG11	1:N:302:LEU:HD12	1.88	0.56
1:P:472:THR:HG21	1:P:550:GLN:HE21	1.71	0.56
1:G:258:GLY:HA2	1:G:279:SER:HB3	1.88	0.56
1:P:495:VAL:HG11	2:P:600:MAY:H15	1.87	0.56
1:L:189:GLN:HE22	1:L:397:VAL:HA	1.71	0.56
1:N:495:VAL:HA	1:N:498:ASN:HD22	1.71	0.56
1:I:237:ASP:HB2	1:I:242:ILE:HD12	1.88	0.56
1:F:495:VAL:HG11	2:F:600:MAY:H15	1.87	0.55
1:N:74:LEU:HD11	1:N:96:VAL:HG12	1.89	0.55
1:G:243:ARG:NH2	1:G:498:ASN:HD21	2.04	0.55
1:C:133:LEU:H	1:C:177:GLN:HG3	1.71	0.55
1:O:495:VAL:HA	1:O:498:ASN:HD22	1.71	0.55
1:C:189:GLN:HE22	1:C:397:VAL:HA	1.72	0.55
1:C:486:ARG:HB2	1:C:534:ILE:HG21	1.89	0.55
1:F:153:THR:HA	1:F:159:ASN:HB2	1.88	0.55
1:J:325:LEU:H	1:J:358:HIS:CD2	2.24	0.55
1:N:86:LEU:HG	1:N:136:GLY:HA3	1.87	0.55
1:G:139:VAL:HG21	1:G:174:LEU:HD13	1.88	0.55
1:A:155:GLY:HA3	1:A:198:ASN:ND2	2.16	0.55
1:O:155:GLY:HA2	1:O:198:ASN:HD22	1.72	0.55
1:P:294:LEU:HD22	1:P:298:LEU:HD22	1.87	0.55
1:K:325:LEU:H	1:K:358:HIS:CD2	2.23	0.55
1:P:371:ALA:HA	1:P:375:LEU:HD12	1.89	0.55
1:J:133:LEU:HB2	1:J:177:GLN:HE21	1.70	0.55
1:E:377:ALA:HA	2:E:600:MAY:H12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:238:ILE:HG22	2:H:600:MAY:HMB	1.88	0.54
1:G:153:THR:HA	1:G:159:ASN:HB2	1.89	0.54
1:J:86:LEU:HG	1:J:136:GLY:HA3	1.89	0.54
1:F:189:GLN:NE2	1:F:398:ASP:H	2.05	0.54
1:D:199:PRO:HD3	1:D:398:ASP:HB2	1.88	0.54
1:B:495:VAL:HG11	2:B:600:MAY:H15	1.90	0.54
1:B:189:GLN:HE22	1:B:397:VAL:HA	1.72	0.54
1:E:86:LEU:HD21	1:E:96:VAL:HG21	1.89	0.54
1:H:133:LEU:HB2	1:H:177:GLN:HE21	1.73	0.54
1:M:488:THR:HG23	2:M:600:MAY:H7A	1.90	0.54
1:N:86:LEU:HD21	1:N:96:VAL:HG21	1.89	0.54
1:A:263:LYS:HG2	1:A:266:LEU:HD22	1.90	0.53
1:G:243:ARG:HH22	1:G:498:ASN:ND2	2.05	0.53
1:G:80:LEU:HD21	1:G:288:GLU:HB3	1.89	0.53
1:E:325:LEU:H	1:E:358:HIS:HD2	1.56	0.53
1:J:111:THR:HG1	1:J:113:CYS:HG	1.57	0.53
1:I:495:VAL:HG11	2:I:600:MAY:H15	1.90	0.53
1:G:472:THR:HB	1:G:550:GLN:HB3	1.89	0.53
1:G:86:LEU:HD21	1:G:96:VAL:HG21	1.89	0.53
1:A:177:GLN:HG2	1:A:296:ALA:HB1	1.90	0.53
1:P:252:CYS:HB3	1:P:290:LEU:HD11	1.90	0.53
1:D:495:VAL:HA	1:D:498:ASN:HD22	1.74	0.53
1:F:86:LEU:HG	1:F:136:GLY:HA3	1.89	0.53
1:C:86:LEU:HG	1:C:136:GLY:HA3	1.91	0.53
1:N:472:THR:HG21	1:N:550:GLN:HE21	1.72	0.53
1:M:246:SER:HA	1:M:251:ILE:HG13	1.91	0.53
1:N:139:VAL:HG21	1:N:174:LEU:HD13	1.90	0.53
1:N:512:VAL:HG13	1:N:516:ASP:HB2	1.91	0.52
1:B:188:PRO:HA	1:B:197:SER:O	2.10	0.52
1:L:162:MET:N	1:L:162:MET:SD	2.79	0.52
1:E:470:LEU:HB3	1:E:552:VAL:HB	1.89	0.52
1:D:341:ALA:HB1	1:D:547:VAL:HG21	1.90	0.52
1:A:237:ASP:HB3	1:A:255:LYS:HG3	1.90	0.52
1:J:509:VAL:HG23	1:J:510:THR:HG22	1.92	0.52
1:K:377:ALA:HA	2:K:600:MAY:H12	1.92	0.52
1:G:263:LYS:HB3	1:G:266:LEU:HD22	1.92	0.52
1:K:341:ALA:HB1	1:K:547:VAL:HG21	1.92	0.52
1:H:273:GLN:OE1	1:H:275:ALA:O	2.28	0.52
1:B:133:LEU:H	1:B:177:GLN:HG3	1.75	0.52
1:O:367:ASN:HB3	1:O:370:TYR:HB3	1.92	0.52
1:K:246:SER:HA	1:K:251:ILE:HG13	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:475:LEU:HD22	1:F:476:GLY:H	1.74	0.51
1:L:246:SER:HA	1:L:251:ILE:HG13	1.93	0.51
1:O:198:ASN:HD21	1:O:200:LEU:HB2	1.74	0.51
1:N:258:GLY:HA2	1:N:279:SER:HB3	1.92	0.51
1:K:86:LEU:HD21	1:K:96:VAL:HG21	1.91	0.51
1:F:488:THR:HG23	2:F:600:MAY:H7A	1.92	0.51
1:L:86:LEU:HD21	1:L:96:VAL:HG21	1.92	0.51
1:H:139:VAL:HG21	1:H:174:LEU:HD13	1.92	0.51
1:O:470:LEU:HB3	1:O:552:VAL:HB	1.93	0.51
1:K:239:GLY:HA2	1:K:495:VAL:HG23	1.93	0.51
1:N:198:ASN:HD21	1:N:200:LEU:HB2	1.76	0.51
1:H:470:LEU:HB3	1:H:552:VAL:HB	1.92	0.51
1:F:495:VAL:HA	1:F:498:ASN:HD22	1.76	0.51
1:L:79:LEU:HD23	1:L:289:SER:HB3	1.93	0.51
1:P:260:ARG:NH2	1:P:558:GLU:OE1	2.44	0.50
1:H:495:VAL:HG11	2:H:600:MAY:H15	1.93	0.50
1:A:488:THR:HG23	2:A:600:MAY:H7A	1.93	0.50
1:J:472:THR:HG21	1:J:550:GLN:HE21	1.77	0.50
1:P:325:LEU:H	1:P:358:HIS:CD2	2.24	0.50
1:L:133:LEU:H	1:L:177:GLN:HG3	1.77	0.50
1:O:275:ALA:HB1	1:O:451:ILE:HD12	1.93	0.50
1:B:169:VAL:HA	1:B:172:GLN:HE21	1.77	0.50
1:J:139:VAL:HG21	1:J:174:LEU:HD13	1.94	0.50
1:I:325:LEU:H	1:I:358:HIS:HD2	1.59	0.50
1:I:319:TYR:O	1:I:566:ARG:NH1	2.45	0.49
1:I:154:LEU:O	1:I:189:GLN:O	2.30	0.49
1:I:246:SER:HA	1:I:251:ILE:HG13	1.93	0.49
1:M:232:LEU:HD11	1:M:293:CYS:HB2	1.95	0.49
1:O:486:ARG:HB2	1:O:534:ILE:HG21	1.94	0.49
1:F:325:LEU:H	1:F:358:HIS:CD2	2.28	0.49
1:N:169:VAL:O	1:N:173:VAL:HG12	2.12	0.49
1:O:86:LEU:HD21	1:O:96:VAL:HG21	1.94	0.49
1:J:495:VAL:HA	1:J:498:ASN:HD22	1.77	0.49
1:P:486:ARG:HB2	1:P:534:ILE:HG21	1.94	0.49
1:I:375:LEU:HD22	1:I:451:ILE:HG13	1.95	0.49
1:D:246:SER:HA	1:D:251:ILE:HG13	1.94	0.49
1:L:470:LEU:HB3	1:L:552:VAL:HB	1.94	0.49
1:M:239:GLY:HA2	1:M:495:VAL:HG23	1.94	0.49
1:C:162:MET:N	1:C:162:MET:SD	2.85	0.49
1:C:286:ASP:OD2	1:C:289:SER:OG	2.31	0.49
1:B:162:MET:N	1:B:162:MET:SD	2.85	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:469:VAL:HG11	1:M:564:PHE:CG	2.47	0.49
1:M:135:TYR:HA	1:M:178:GLY:HA3	1.95	0.49
1:J:470:LEU:HB3	1:J:552:VAL:HB	1.95	0.49
1:G:331:GLU:HG3	1:G:346:LEU:HD12	1.94	0.49
1:D:325:LEU:H	1:D:358:HIS:CD2	2.11	0.48
1:D:377:ALA:HA	2:D:600:MAY:H12	1.94	0.48
1:P:294:LEU:O	1:P:298:LEU:HB2	2.13	0.48
1:B:486:ARG:HG3	1:B:534:ILE:HG12	1.94	0.48
1:P:488:THR:HG23	2:P:600:MAY:H7A	1.94	0.48
1:A:495:VAL:HA	1:A:498:ASN:HD22	1.79	0.48
1:B:377:ALA:HA	2:B:600:MAY:H12	1.95	0.48
1:C:74:LEU:HD11	1:C:96:VAL:HG12	1.95	0.48
1:H:382:SER:HA	1:H:439:ARG:HH11	1.78	0.48
1:E:80:LEU:HD11	1:E:288:GLU:HB3	1.95	0.48
1:P:80:LEU:HD11	1:P:288:GLU:HB3	1.95	0.48
1:A:154:LEU:HD23	1:A:269:CYS:HB3	1.95	0.48
1:E:122:GLU:HA	1:E:125:LEU:HB2	1.94	0.48
1:A:472:THR:HB	1:A:550:GLN:HB3	1.95	0.48
1:C:86:LEU:HD21	1:C:96:VAL:HG21	1.96	0.48
1:A:243:ARG:HH22	1:A:498:ASN:HD21	1.61	0.48
1:N:239:GLY:HA2	1:N:495:VAL:HG23	1.96	0.48
1:J:495:VAL:HG11	2:J:600:MAY:H15	1.94	0.48
1:P:495:VAL:HA	1:P:498:ASN:HD22	1.79	0.47
1:J:488:THR:HG23	2:J:600:MAY:H7A	1.96	0.47
1:G:199:PRO:HD3	1:G:398:ASP:HB2	1.96	0.47
1:P:199:PRO:HD3	1:P:398:ASP:HB2	1.96	0.47
1:E:239:GLY:HA2	1:E:495:VAL:HG23	1.95	0.47
1:C:307:PRO:HB2	1:D:555:PRO:HD2	1.96	0.47
1:K:139:VAL:HG21	1:K:174:LEU:HD13	1.96	0.47
1:A:325:LEU:N	1:A:358:HIS:HD2	2.09	0.47
1:G:80:LEU:HD22	1:G:80:LEU:H	1.79	0.47
1:O:259:ASN:HB3	1:O:556:TRP:HH2	1.80	0.47
1:E:488:THR:HG23	2:E:600:MAY:H7A	1.97	0.47
1:A:238:ILE:HG22	2:A:600:MAY:HMB	1.95	0.47
1:G:86:LEU:HG	1:G:136:GLY:HA3	1.95	0.47
1:N:237:ASP:HB3	1:N:255:LYS:HG3	1.97	0.47
1:P:51:SER:HB3	1:P:117:TYR:H	1.79	0.47
1:D:86:LEU:HD21	1:D:96:VAL:HG21	1.96	0.47
1:E:168:CYS:HB2	1:E:265:GLY:HA3	1.96	0.47
1:E:80:LEU:H	1:E:80:LEU:HD22	1.80	0.47
1:P:133:LEU:H	1:P:177:GLN:HG3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:488:THR:HG23	2:O:600:MAY:H7A	1.97	0.46
1:G:189:GLN:NE2	1:G:398:ASP:H	2.12	0.46
1:H:341:ALA:HB1	1:H:547:VAL:HG21	1.98	0.46
1:F:397:VAL:HG11	1:F:405:ILE:HG21	1.97	0.46
1:P:275:ALA:HB1	1:P:451:ILE:HD12	1.97	0.46
1:I:258:GLY:HA2	1:I:279:SER:HB3	1.96	0.46
1:P:171:VAL:HA	1:P:174:LEU:HD12	1.97	0.46
1:C:80:LEU:H	1:C:80:LEU:HD22	1.81	0.46
1:E:523:TYR:HB3	1:E:536:LYS:HG3	1.98	0.46
1:E:312:LEU:HD11	1:F:311:PRO:HD2	1.96	0.46
1:D:238:ILE:HD12	1:D:278:LEU:HB2	1.98	0.46
1:I:377:ALA:HA	2:I:600:MAY:H12	1.97	0.46
1:P:177:GLN:HG2	1:P:296:ALA:HB1	1.98	0.46
1:C:79:LEU:HD13	1:C:231:PRO:HB2	1.97	0.46
1:A:153:THR:HA	1:A:159:ASN:HB2	1.97	0.46
1:B:512:VAL:HG13	1:B:516:ASP:HB2	1.97	0.46
1:F:319:TYR:HB2	1:F:559:GLU:HB2	1.96	0.46
1:M:273:GLN:NE2	1:M:275:ALA:O	2.49	0.46
1:J:75:LEU:HD13	1:J:103:LYS:HE3	1.97	0.46
1:M:195:ASP:HB2	1:M:484:PRO:HG2	1.98	0.46
1:H:236:THR:HG22	1:H:280:LEU:HB3	1.98	0.46
1:F:168:CYS:HB2	1:F:265:GLY:HA3	1.98	0.46
1:A:275:ALA:HB1	1:A:451:ILE:HD12	1.97	0.46
1:E:331:GLU:HG3	1:E:346:LEU:HD12	1.98	0.46
1:D:141:LEU:HD11	1:D:181:PRO:HB3	1.96	0.46
1:D:252:CYS:HB3	1:D:290:LEU:HD11	1.98	0.46
1:L:139:VAL:HG21	1:L:174:LEU:HD13	1.98	0.45
1:I:86:LEU:HD21	1:I:96:VAL:HG21	1.97	0.45
1:J:243:ARG:HH22	1:J:498:ASN:HD21	1.63	0.45
1:O:123:THR:HA	1:O:126:SER:HB2	1.98	0.45
1:D:217:SER:H	1:D:241:SER:CB	2.29	0.45
1:P:326:ARG:HE	1:P:326:ARG:HB3	1.53	0.45
1:H:74:LEU:HD13	1:H:96:VAL:HG12	1.99	0.45
1:F:196:CYS:HB3	1:F:204:THR:HB	1.98	0.45
1:N:79:LEU:O	1:N:83:VAL:HG12	2.17	0.45
1:C:239:GLY:HA2	1:C:495:VAL:HG23	1.99	0.45
1:N:495:VAL:HG11	2:N:600:MAY:H15	1.99	0.45
1:K:79:LEU:HD13	1:K:231:PRO:HB2	1.97	0.45
1:D:437:ARG:HA	1:D:438:PRO:HD3	1.83	0.45
1:B:255:LYS:HB3	1:B:255:LYS:HE3	1.64	0.45
1:D:491:ILE:HD11	2:D:600:MAY:C14	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:139:VAL:HG21	1:I:174:LEU:HD13	1.97	0.45
1:G:133:LEU:H	1:G:177:GLN:HG3	1.82	0.45
1:P:263:LYS:HA	1:P:266:LEU:HD13	1.98	0.45
1:C:377:ALA:HA	2:C:600:MAY:H12	1.99	0.44
1:B:162:MET:HA	1:B:163:PRO:HD2	1.89	0.44
1:L:306:ASP:OD2	1:L:308:THR:OG1	2.28	0.44
1:I:472:THR:HB	1:I:550:GLN:HB3	1.98	0.44
1:H:206:ASN:HA	1:H:207:PRO:HD2	1.85	0.44
1:L:435:SER:HA	1:L:439:ARG:HH22	1.82	0.44
1:D:472:THR:HG21	1:D:550:GLN:HE21	1.82	0.44
1:A:371:ALA:HA	1:A:375:LEU:HD12	2.00	0.44
1:F:80:LEU:HD11	1:F:288:GLU:HB3	1.99	0.44
1:L:495:VAL:HA	1:L:498:ASN:HD22	1.83	0.44
1:N:133:LEU:H	1:N:177:GLN:HG3	1.82	0.44
1:M:72:GLU:O	1:M:76:THR:OG1	2.34	0.44
1:D:481:LEU:HA	1:D:481:LEU:HD13	1.91	0.44
1:D:156:LEU:HG	1:D:391:ASN:HB3	1.98	0.44
1:M:361:ILE:HG21	1:M:465:MET:HG2	1.99	0.44
1:N:198:ASN:ND2	1:N:200:LEU:H	2.15	0.44
1:L:189:GLN:NE2	1:L:398:ASP:H	2.14	0.44
1:C:345:ALA:O	1:C:349:THR:HG23	2.17	0.44
1:M:385:GLY:HA3	1:M:408:LEU:HD22	1.99	0.44
1:I:74:LEU:HD11	1:I:96:VAL:HG12	2.00	0.44
1:O:377:ALA:HA	2:O:600:MAY:H12	1.99	0.44
1:O:246:SER:HA	1:O:251:ILE:HG13	1.98	0.44
1:E:225:ILE:HG22	1:E:251:ILE:HG21	1.98	0.44
1:N:123:THR:HA	1:N:126:SER:HB2	2.00	0.44
1:D:209:LYS:HD2	1:D:545:LEU:HD21	1.99	0.44
1:C:470:LEU:HB3	1:C:552:VAL:HB	2.00	0.44
1:M:128:ALA:HA	1:M:129:PRO:HD3	1.84	0.44
1:N:85:LYS:HB3	1:N:91:LEU:HD12	1.99	0.44
1:G:325:LEU:H	1:G:358:HIS:CD2	2.27	0.44
1:A:243:ARG:HH22	1:A:498:ASN:ND2	2.16	0.44
1:D:246:SER:HB2	1:D:506:VAL:HG11	1.98	0.44
1:B:139:VAL:HG21	1:B:174:LEU:HD13	2.00	0.44
1:C:170:VAL:HG11	1:C:280:LEU:HD11	2.00	0.44
1:N:294:LEU:HD12	1:N:562:LEU:HD11	1.99	0.44
1:D:259:ASN:HD22	1:D:259:ASN:HA	1.68	0.44
1:M:217:SER:H	1:M:241:SER:CB	2.30	0.44
1:I:133:LEU:H	1:I:177:GLN:HG3	1.83	0.44
1:B:246:SER:HA	1:B:251:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:151:ASP:HB3	1:E:153:THR:HG23	2.00	0.44
1:H:377:ALA:HA	2:H:600:MAY:H12	2.00	0.43
1:F:239:GLY:HA2	1:F:495:VAL:HG23	1.99	0.43
1:M:474:MET:HG2	1:M:506:VAL:HG21	2.00	0.43
1:K:523:TYR:HB3	1:K:536:LYS:HG3	2.00	0.43
1:C:40:ALA:HB1	1:C:43:ARG:HB2	2.00	0.43
1:C:563:ARG:HH12	1:C:567:GLU:HB2	1.83	0.43
1:K:162:MET:HA	1:K:163:PRO:HD2	1.95	0.43
1:I:80:LEU:HD22	1:I:80:LEU:H	1.83	0.43
1:F:377:ALA:HA	2:F:600:MAY:H12	2.00	0.43
1:F:189:GLN:HE21	1:F:398:ASP:H	1.65	0.43
1:E:246:SER:HA	1:E:251:ILE:HG13	1.99	0.43
1:J:188:PRO:HA	1:J:197:SER:O	2.19	0.43
1:C:263:LYS:HA	1:C:266:LEU:HD13	2.00	0.43
1:L:129:PRO:HD2	1:L:178:GLY:HA2	2.01	0.43
1:M:469:VAL:HG11	1:M:564:PHE:CD2	2.53	0.43
1:M:306:ASP:OD2	1:M:308:THR:OG1	2.25	0.43
1:O:80:LEU:HD22	1:O:80:LEU:H	1.83	0.43
1:E:275:ALA:HB2	1:E:448:GLN:HG3	2.01	0.43
1:C:238:ILE:HG22	2:C:600:MAY:HMB	1.99	0.43
1:D:238:ILE:HG22	2:D:600:MAY:HMB	2.01	0.43
1:G:495:VAL:HG11	2:G:600:MAY:H15	2.01	0.43
1:O:239:GLY:HA2	1:O:495:VAL:HG23	1.99	0.43
1:O:472:THR:HG22	1:O:473:PRO:O	2.19	0.43
1:C:410:LEU:HB2	1:C:415:LYS:HD2	1.99	0.43
1:K:198:ASN:HD21	1:K:200:LEU:HB2	1.84	0.43
1:E:237:ASP:HB3	1:E:255:LYS:HG3	2.01	0.43
1:N:79:LEU:HD13	1:N:231:PRO:HB2	2.00	0.43
1:K:437:ARG:HD3	1:K:439:ARG:HG3	2.00	0.43
1:M:294:LEU:HD22	1:M:298:LEU:HD22	2.00	0.43
1:J:398:ASP:HA	1:J:399:PRO:HD2	1.88	0.43
1:N:310:PRO:HA	1:N:311:PRO:HD3	1.82	0.43
1:H:335:TYR:OH	2:H:600:MAY:H19A	2.19	0.42
1:N:192:LEU:HG	2:N:600:MAY:H8	2.01	0.42
1:H:142:LYS:NZ	1:H:236:THR:OG1	2.49	0.42
1:O:217:SER:H	1:O:241:SER:CB	2.31	0.42
1:K:345:ALA:O	1:K:349:THR:HG23	2.19	0.42
1:E:189:GLN:HE22	1:E:397:VAL:HA	1.84	0.42
1:L:86:LEU:HG	1:L:136:GLY:HA3	2.00	0.42
1:O:74:LEU:HD11	1:O:96:VAL:HA	2.01	0.42
1:N:225:ILE:HB	1:N:251:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:79:LEU:HD13	1:D:231:PRO:HB2	2.01	0.42
1:N:349:THR:HG21	1:N:549:VAL:HG21	2.01	0.42
1:K:237:ASP:HA	1:K:241:SER:HB2	2.01	0.42
1:N:383:ASP:OD2	1:N:387:SER:OG	2.34	0.42
1:G:398:ASP:HA	1:G:399:PRO:HD2	1.88	0.42
1:E:556:TRP:HA	1:E:558:GLU:OE1	2.19	0.42
1:P:341:ALA:HB1	1:P:547:VAL:HG21	2.01	0.42
1:J:41:ALA:HB1	1:J:200:LEU:HA	2.01	0.42
1:J:189:GLN:HE21	1:J:398:ASP:H	1.66	0.42
1:G:512:VAL:HG13	1:G:516:ASP:HB2	2.01	0.42
1:O:325:LEU:H	1:O:358:HIS:CD2	2.28	0.42
1:L:135:TYR:HA	1:L:178:GLY:HA3	2.00	0.42
1:N:246:SER:HA	1:N:251:ILE:HG13	2.02	0.42
1:G:237:ASP:HA	1:G:241:SER:HB2	2.01	0.42
1:F:398:ASP:HA	1:F:399:PRO:HD2	1.76	0.42
1:C:162:MET:HA	1:C:163:PRO:HD2	1.93	0.42
1:B:237:ASP:HB3	1:B:255:LYS:HG3	2.01	0.42
1:M:196:CYS:SG	1:M:219:GLY:HA3	2.60	0.42
1:P:470:LEU:HB3	1:P:552:VAL:HB	2.02	0.42
1:F:207:PRO:HB3	1:F:227:SER:HB3	2.01	0.42
1:P:246:SER:HA	1:P:251:ILE:HG13	2.00	0.42
1:M:183:VAL:HG21	1:M:224:LEU:HD21	2.02	0.42
1:G:385:GLY:HA3	1:G:408:LEU:HD22	2.02	0.42
1:K:486:ARG:HB2	1:K:534:ILE:HD13	2.01	0.42
1:P:237:ASP:HA	1:P:241:SER:HB2	2.01	0.42
1:P:337:MET:HB3	1:P:523:TYR:CE2	2.54	0.42
1:B:238:ILE:HG22	2:B:600:MAY:HMB	2.02	0.42
1:M:341:ALA:HB2	1:M:516:ASP:HB3	2.02	0.42
1:A:310:PRO:HA	1:A:311:PRO:HD2	1.92	0.42
1:B:236:THR:HB	1:B:278:LEU:HD11	2.02	0.42
1:A:217:SER:H	1:A:241:SER:CB	2.33	0.42
1:K:137:VAL:HA	1:K:138:PRO:HD3	1.90	0.42
1:N:489:GLY:HA2	2:N:600:MAY:H18	2.01	0.41
1:J:237:ASP:HB2	1:J:242:ILE:HD12	2.02	0.41
1:H:189:GLN:HB2	1:H:199:PRO:HD3	2.02	0.41
1:J:237:ASP:HA	1:J:241:SER:HB2	2.02	0.41
1:B:135:TYR:HA	1:B:178:GLY:HA3	2.02	0.41
1:L:453:MET:CE	1:L:453:MET:CG	2.96	0.41
1:K:252:CYS:HB3	1:K:290:LEU:HD11	2.01	0.41
1:I:341:ALA:HB1	1:I:547:VAL:HG21	2.01	0.41
1:N:238:ILE:HD12	1:N:278:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:341:ALA:HB1	1:E:547:VAL:HG21	2.01	0.41
1:K:155:GLY:HA2	1:K:198:ASN:ND2	2.34	0.41
1:K:212:LYS:HG3	1:K:545:LEU:HD11	2.03	0.41
1:G:469:VAL:HG11	1:G:564:PHE:CG	2.56	0.41
1:A:135:TYR:HA	1:A:178:GLY:HA3	2.02	0.41
1:B:238:ILE:HD12	1:B:278:LEU:HB2	2.03	0.41
1:K:481:LEU:HA	1:K:481:LEU:HD13	1.96	0.41
1:O:154:LEU:HA	1:O:154:LEU:HD12	1.91	0.41
1:F:437:ARG:HA	1:F:438:PRO:HD3	1.94	0.41
1:L:398:ASP:HA	1:L:399:PRO:HD2	1.78	0.41
1:E:160:GLU:HG2	1:E:200:LEU:HD21	2.02	0.41
1:C:135:TYR:HA	1:C:178:GLY:HA3	2.03	0.41
1:M:174:LEU:HD11	1:M:234:LEU:HD22	2.02	0.41
2:A:600:MAY:H4	2:A:600:MAY:H7	1.94	0.41
1:N:177:GLN:HG2	1:N:296:ALA:HB1	2.03	0.41
1:L:341:ALA:HB1	1:L:547:VAL:HG21	2.02	0.41
1:L:325:LEU:H	1:L:358:HIS:CD2	2.38	0.41
1:M:255:LYS:HA	1:M:256:PRO:HD2	1.95	0.41
1:N:263:LYS:HA	1:N:266:LEU:HD13	2.01	0.41
1:I:162:MET:HA	1:I:163:PRO:HD2	1.90	0.41
1:M:557:GLN:HB3	1:M:560:LEU:HB3	2.03	0.41
1:O:173:VAL:HG22	1:O:297:LEU:HD12	2.03	0.41
1:P:437:ARG:HA	1:P:438:PRO:HD3	1.90	0.41
1:B:217:SER:H	1:B:241:SER:CB	2.34	0.41
1:A:367:ASN:HB3	1:A:370:TYR:HB3	2.02	0.41
1:J:410:LEU:HB2	1:J:415:LYS:HD2	2.02	0.41
1:H:472:THR:HB	1:H:550:GLN:HB3	2.02	0.41
1:H:472:THR:HG21	1:H:550:GLN:HE21	1.85	0.41
1:H:481:LEU:HA	1:H:481:LEU:HD13	2.00	0.41
1:I:473:PRO:HG2	1:I:493:TYR:CE1	2.56	0.41
1:B:122:GLU:HA	1:B:125:LEU:HB2	2.03	0.41
1:J:158:LEU:HD22	1:J:391:ASN:HD22	1.85	0.41
1:B:437:ARG:HA	1:B:438:PRO:HD3	1.87	0.41
1:O:382:SER:HA	1:O:439:ARG:HH11	1.85	0.41
1:F:155:GLY:CA	1:F:198:ASN:ND2	2.84	0.41
1:D:80:LEU:HD11	1:D:288:GLU:HB3	2.03	0.41
1:F:74:LEU:HD11	1:F:96:VAL:HG12	2.02	0.41
1:F:133:LEU:H	1:F:177:GLN:HG3	1.86	0.41
1:O:459:ILE:HD13	1:P:307:PRO:HD2	2.03	0.41
1:M:186:ASN:ND2	1:M:204:THR:OG1	2.54	0.41
1:O:319:TYR:HB2	1:O:559:GLU:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:171:VAL:HA	1:J:174:LEU:HD12	2.03	0.40
1:K:437:ARG:HA	1:K:438:PRO:HD3	1.96	0.40
1:M:79:LEU:HD13	1:M:231:PRO:HB2	2.03	0.40
1:E:177:GLN:HG2	1:E:296:ALA:HB1	2.03	0.40
1:D:361:ILE:HG21	1:D:465:MET:HG2	2.03	0.40
1:K:488:THR:HG23	2:K:600:MAY:H7A	2.02	0.40
1:H:207:PRO:HB3	1:H:227:SER:HB3	2.02	0.40
1:D:79:LEU:HD12	1:D:82:LEU:HD23	2.03	0.40
1:H:239:GLY:HA2	1:H:495:VAL:HG23	2.03	0.40
1:N:377:ALA:HA	2:N:600:MAY:H12	2.02	0.40
1:M:222:GLY:HA2	1:M:251:ILE:HD11	2.02	0.40
1:I:162:MET:N	1:I:162:MET:SD	2.94	0.40
1:F:129:PRO:HD2	1:F:178:GLY:HA2	2.04	0.40
1:L:260:ARG:NH2	1:L:558:GLU:OE2	2.48	0.40
1:A:192:LEU:HG	2:A:600:MAY:H8	2.03	0.40
1:M:344:ARG:O	1:M:348:GLU:HB2	2.21	0.40
1:F:273:GLN:OE1	1:F:275:ALA:O	2.39	0.40
1:G:173:VAL:HG22	1:G:297:LEU:HD12	2.03	0.40
1:F:312:LEU:HD22	1:F:315:ARG:HH12	1.86	0.40
1:G:310:PRO:HA	1:G:311:PRO:HD3	1.90	0.40
1:B:79:LEU:HD13	1:B:231:PRO:HB2	2.04	0.40
2:F:600:MAY:H7	2:F:600:MAY:H4	1.88	0.40
1:F:154:LEU:O	1:F:189:GLN:O	2.38	0.40
1:D:530:ILE:HG21	1:E:424:PRO:O	2.21	0.40
1:E:390:GLN:HE21	1:E:390:GLN:HB2	1.72	0.40
1:K:190:SER:HG	1:K:269:CYS:HG	1.67	0.40
1:N:398:ASP:HA	1:N:399:PRO:HD2	1.86	0.40
1:J:342:MET:HG3	1:J:476:GLY:HA2	2.03	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	535/537 (100%)	498 (93%)	31 (6%)	6 (1%)	17	50
1	B	535/537 (100%)	503 (94%)	24 (4%)	8 (2%)	13	40
1	C	535/537 (100%)	507 (95%)	23 (4%)	5 (1%)	21	55
1	D	535/537 (100%)	499 (93%)	31 (6%)	5 (1%)	21	55
1	E	535/537 (100%)	491 (92%)	36 (7%)	8 (2%)	13	40
1	F	535/537 (100%)	502 (94%)	27 (5%)	6 (1%)	17	50
1	G	535/537 (100%)	506 (95%)	26 (5%)	3 (1%)	30	65
1	H	535/537 (100%)	498 (93%)	31 (6%)	6 (1%)	17	50
1	I	535/537 (100%)	496 (93%)	37 (7%)	2 (0%)	39	74
1	J	535/537 (100%)	506 (95%)	26 (5%)	3 (1%)	30	65
1	K	535/537 (100%)	497 (93%)	32 (6%)	6 (1%)	17	50
1	L	535/537 (100%)	494 (92%)	36 (7%)	5 (1%)	21	55
1	M	535/537 (100%)	466 (87%)	57 (11%)	12 (2%)	8	28
1	N	535/537 (100%)	494 (92%)	33 (6%)	8 (2%)	13	40
1	O	535/537 (100%)	499 (93%)	30 (6%)	6 (1%)	17	50
1	P	535/537 (100%)	497 (93%)	34 (6%)	4 (1%)	26	62
All	All	8560/8592 (100%)	7953 (93%)	514 (6%)	93 (1%)	17	50

All (93) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	306	ASP
1	A	480	ASP
1	E	189	GLN
1	E	480	ASP
1	E	488	THR
1	F	306	ASP
1	L	530	ILE
1	M	189	GLN
1	M	480	ASP
1	N	306	ASP
1	N	480	ASP
1	N	488	THR
1	A	40	ALA
1	B	189	GLN
1	B	476	GLY
1	E	276	VAL

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Mol	Chain	Res	Type
1	G	475	LEU
1	H	258	GLY
1	I	276	VAL
1	J	476	GLY
1	K	481	LEU
1	M	98	PHE
1	M	197	SER
1	M	298	LEU
1	M	487	ALA
1	N	476	GLY
1	N	493	TYR
1	O	476	GLY
1	O	480	ASP
1	B	480	ASP
1	C	476	GLY
1	D	480	ASP
1	E	306	ASP
1	H	191	MET
1	J	191	MET
1	K	189	GLN
1	M	227	SER
1	N	276	VAL
1	A	197	SER
1	B	143	GLU
1	B	483	THR
1	C	276	VAL
1	C	306	ASP
1	D	276	VAL
1	D	481	LEU
1	F	227	SER
1	H	276	VAL
1	H	481	LEU
1	I	476	GLY
1	J	276	VAL
1	K	227	SER
1	L	197	SER
1	L	276	VAL
1	M	97	PHE
1	M	276	VAL
1	O	239	GLY
1	O	276	VAL
1	O	306	ASP

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Mol	Chain	Res	Type
1	P	276	VAL
1	A	276	VAL
1	B	276	VAL
1	B	306	ASP
1	F	276	VAL
1	F	483	THR
1	K	376	SER
1	L	321	SER
1	M	191	MET
1	N	492	SER
1	P	306	ASP
1	P	480	ASP
1	D	419	SER
1	E	455	ARG
1	F	476	GLY
1	G	191	MET
1	G	276	VAL
1	H	306	ASP
1	K	276	VAL
1	K	476	GLY
1	M	240	GLY
1	A	476	GLY
1	C	239	GLY
1	H	161	GLY
1	E	476	GLY
1	M	306	ASP
1	B	239	GLY
1	F	239	GLY
1	L	476	GLY
1	O	424	PRO
1	D	483	THR
1	N	469	VAL
1	P	240	GLY
1	C	483	THR
1	E	362	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	426/455 (94%)	354 (83%)	72 (17%)	2	7
1	B	425/455 (93%)	351 (83%)	74 (17%)	2	7
1	C	425/455 (93%)	341 (80%)	84 (20%)	1	5
1	D	425/455 (93%)	354 (83%)	71 (17%)	3	8
1	E	425/455 (93%)	345 (81%)	80 (19%)	2	6
1	F	425/455 (93%)	339 (80%)	86 (20%)	1	4
1	G	426/455 (94%)	345 (81%)	81 (19%)	2	5
1	H	425/455 (93%)	350 (82%)	75 (18%)	2	7
1	I	426/455 (94%)	344 (81%)	82 (19%)	2	5
1	J	425/455 (93%)	344 (81%)	81 (19%)	2	5
1	K	425/455 (93%)	341 (80%)	84 (20%)	1	5
1	L	426/455 (94%)	338 (79%)	88 (21%)	1	4
1	M	426/455 (94%)	323 (76%)	103 (24%)	1	2
1	N	425/455 (93%)	345 (81%)	80 (19%)	2	6
1	O	426/455 (94%)	340 (80%)	86 (20%)	1	4
1	P	425/455 (93%)	339 (80%)	86 (20%)	1	4
All	All	6806/7280 (94%)	5493 (81%)	1313 (19%)	2	5

All (1313) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LYS
1	A	74	LEU
1	A	77	LEU
1	A	82	LEU
1	A	84	GLN
1	A	86	LEU
1	A	101	LEU
1	A	106	GLU
1	A	115	THR
1	A	130	ARG
1	A	133	LEU
1	A	139	VAL
1	A	152	SER
1	A	154	LEU
1	A	156	LEU

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Mol	Chain	Res	Type
1	A	159	ASN
1	A	162	MET
1	A	164	SER
1	A	190	SER
1	A	200	LEU
1	A	205	MET
1	A	218	SER
1	A	259	ASN
1	A	270	VAL
1	A	273	GLN
1	A	279	SER
1	A	280	LEU
1	A	287	VAL
1	A	292	LEU
1	A	297	LEU
1	A	298	LEU
1	A	302	LEU
1	A	320	ARG
1	A	322	SER
1	A	343	ARG
1	A	344	ARG
1	A	347	ILE
1	A	349	THR
1	A	351	GLN
1	A	352	ARG
1	A	359	THR
1	A	360	LEU
1	A	374	VAL
1	A	383	ASP
1	A	390	GLN
1	A	393	LYS
1	A	395	ASP
1	A	400	CYS
1	A	406	LEU
1	A	415	LYS
1	A	420	LEU
1	A	421	LEU
1	A	422	LEU
1	A	425	LEU
1	A	437	ARG
1	A	444	LEU
1	A	447	LEU

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Mol	Chain	Res	Type
1	A	453	MET
1	A	465	MET
1	A	466	ASN
1	A	469	VAL
1	A	470	LEU
1	A	475	LEU
1	A	481	LEU
1	A	483	THR
1	A	511	THR
1	A	530	ILE
1	A	542	SER
1	A	545	LEU
1	A	549	VAL
1	A	563	ARG
1	A	573	THR
1	B	51	SER
1	B	52	LEU
1	B	66	ASN
1	B	77	LEU
1	B	80	LEU
1	B	83	VAL
1	B	84	GLN
1	B	86	LEU
1	B	92	SER
1	B	101	LEU
1	B	115	THR
1	B	116	SER
1	B	118	LEU
1	B	130	ARG
1	B	154	LEU
1	B	156	LEU
1	B	162	MET
1	B	166	SER
1	B	173	VAL
1	B	177	GLN
1	B	190	SER
1	B	193	SER
1	B	230	SER
1	B	234	LEU
1	B	242	ILE
1	B	255	LYS
1	B	264	SER

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Mol	Chain	Res	Type
1	B	273	GLN
1	B	279	SER
1	B	280	LEU
1	B	286	ASP
1	B	292	LEU
1	B	294	LEU
1	B	295	LYS
1	B	297	LEU
1	B	298	LEU
1	B	302	LEU
1	B	325	LEU
1	B	337	MET
1	B	342	MET
1	B	351	GLN
1	B	359	THR
1	B	374	VAL
1	B	382	SER
1	B	387	SER
1	B	390	GLN
1	B	393	LYS
1	B	400	CYS
1	B	404	LEU
1	B	415	LYS
1	B	418	LEU
1	B	420	LEU
1	B	421	LEU
1	B	422	LEU
1	B	425	LEU
1	B	429	LEU
1	B	437	ARG
1	B	444	LEU
1	B	447	LEU
1	B	448	GLN
1	B	465	MET
1	B	470	LEU
1	B	475	LEU
1	B	481	LEU
1	B	486	ARG
1	B	507	VAL
1	B	511	THR
1	B	530	ILE
1	B	534	ILE

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Mol	Chain	Res	Type
1	B	542	SER
1	B	545	LEU
1	B	549	VAL
1	B	563	ARG
1	B	573	THR
1	C	47	LYS
1	C	51	SER
1	C	66	ASN
1	C	71	SER
1	C	74	LEU
1	C	77	LEU
1	C	80	LEU
1	C	84	GLN
1	C	86	LEU
1	C	101	LEU
1	C	106	GLU
1	C	109	LYS
1	C	115	THR
1	C	123	THR
1	C	130	ARG
1	C	133	LEU
1	C	143	GLU
1	C	151	ASP
1	C	152	SER
1	C	153	THR
1	C	154	LEU
1	C	156	LEU
1	C	159	ASN
1	C	162	MET
1	C	168	CYS
1	C	177	GLN
1	C	184	HIS
1	C	190	SER
1	C	196	CYS
1	C	200	LEU
1	C	218	SER
1	C	234	LEU
1	C	259	ASN
1	C	264	SER
1	C	266	LEU
1	C	270	VAL
1	C	273	GLN

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Mol	Chain	Res	Type
1	C	279	SER
1	C	280	LEU
1	C	286	ASP
1	C	289	SER
1	C	292	LEU
1	C	294	LEU
1	C	298	LEU
1	C	302	LEU
1	C	305	LEU
1	C	306	ASP
1	C	320	ARG
1	C	321	SER
1	C	337	MET
1	C	347	ILE
1	C	349	THR
1	C	351	GLN
1	C	354	GLU
1	C	359	THR
1	C	360	LEU
1	C	374	VAL
1	C	390	GLN
1	C	393	LYS
1	C	406	LEU
1	C	412	SER
1	C	415	LYS
1	C	420	LEU
1	C	421	LEU
1	C	422	LEU
1	C	425	LEU
1	C	437	ARG
1	C	444	LEU
1	C	447	LEU
1	C	463	LYS
1	C	465	MET
1	C	469	VAL
1	C	475	LEU
1	C	481	LEU
1	C	486	ARG
1	C	495	VAL
1	C	507	VAL
1	C	517	ASP
1	C	530	ILE

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Mol	Chain	Res	Type
1	C	534	ILE
1	C	536	LYS
1	C	541	ASN
1	C	549	VAL
1	C	563	ARG
1	D	51	SER
1	D	52	LEU
1	D	71	SER
1	D	74	LEU
1	D	77	LEU
1	D	80	LEU
1	D	84	GLN
1	D	85	LYS
1	D	86	LEU
1	D	92	SER
1	D	101	LEU
1	D	109	LYS
1	D	115	THR
1	D	121	CYS
1	D	130	ARG
1	D	152	SER
1	D	154	LEU
1	D	156	LEU
1	D	159	ASN
1	D	160	GLU
1	D	173	VAL
1	D	184	HIS
1	D	205	MET
1	D	210	SER
1	D	218	SER
1	D	225	ILE
1	D	234	LEU
1	D	255	LYS
1	D	259	ASN
1	D	266	LEU
1	D	270	VAL
1	D	273	GLN
1	D	280	LEU
1	D	292	LEU
1	D	293	CYS
1	D	294	LEU
1	D	298	LEU

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Mol	Chain	Res	Type
1	D	302	LEU
1	D	304	THR
1	D	305	LEU
1	D	322	SER
1	D	342	MET
1	D	343	ARG
1	D	349	THR
1	D	352	ARG
1	D	359	THR
1	D	390	GLN
1	D	401	LEU
1	D	419	SER
1	D	420	LEU
1	D	421	LEU
1	D	422	LEU
1	D	436	MET
1	D	437	ARG
1	D	444	LEU
1	D	447	LEU
1	D	448	GLN
1	D	465	MET
1	D	469	VAL
1	D	475	LEU
1	D	481	LEU
1	D	507	VAL
1	D	511	THR
1	D	520	MET
1	D	530	ILE
1	D	534	ILE
1	D	535	LEU
1	D	545	LEU
1	D	549	VAL
1	D	563	ARG
1	D	573	THR
1	E	46	GLN
1	E	51	SER
1	E	74	LEU
1	E	76	THR
1	E	77	LEU
1	E	80	LEU
1	E	82	LEU
1	E	84	GLN

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Mol	Chain	Res	Type
1	E	86	LEU
1	E	101	LEU
1	E	106	GLU
1	E	116	SER
1	E	121	CYS
1	E	123	THR
1	E	130	ARG
1	E	133	LEU
1	E	152	SER
1	E	154	LEU
1	E	156	LEU
1	E	160	GLU
1	E	162	MET
1	E	164	SER
1	E	168	CYS
1	E	177	GLN
1	E	180	VAL
1	E	184	HIS
1	E	190	SER
1	E	195	ASP
1	E	205	MET
1	E	210	SER
1	E	261	LEU
1	E	270	VAL
1	E	273	GLN
1	E	279	SER
1	E	280	LEU
1	E	287	VAL
1	E	289	SER
1	E	292	LEU
1	E	294	LEU
1	E	297	LEU
1	E	305	LEU
1	E	320	ARG
1	E	331	GLU
1	E	337	MET
1	E	349	THR
1	E	352	ARG
1	E	359	THR
1	E	382	SER
1	E	387	SER
1	E	390	GLN

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Mol	Chain	Res	Type
1	E	393	LYS
1	E	397	VAL
1	E	400	CYS
1	E	406	LEU
1	E	415	LYS
1	E	420	LEU
1	E	421	LEU
1	E	422	LEU
1	E	437	ARG
1	E	444	LEU
1	E	451	ILE
1	E	456	GLN
1	E	459	ILE
1	E	465	MET
1	E	467	LEU
1	E	469	VAL
1	E	475	LEU
1	E	495	VAL
1	E	507	VAL
1	E	517	ASP
1	E	520	MET
1	E	530	ILE
1	E	542	SER
1	E	543	VAL
1	E	545	LEU
1	E	549	VAL
1	E	550	GLN
1	E	559	GLU
1	E	563	ARG
1	E	573	THR
1	F	47	LYS
1	F	48	GLN
1	F	51	SER
1	F	71	SER
1	F	77	LEU
1	F	80	LEU
1	F	84	GLN
1	F	86	LEU
1	F	92	SER
1	F	101	LEU
1	F	106	GLU
1	F	109	LYS

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Mol	Chain	Res	Type
1	F	118	LEU
1	F	123	THR
1	F	130	ARG
1	F	133	LEU
1	F	143	GLU
1	F	153	THR
1	F	154	LEU
1	F	156	LEU
1	F	157	SER
1	F	158	LEU
1	F	159	ASN
1	F	162	MET
1	F	164	SER
1	F	170	VAL
1	F	173	VAL
1	F	177	GLN
1	F	196	CYS
1	F	198	ASN
1	F	205	MET
1	F	209	LYS
1	F	210	SER
1	F	242	ILE
1	F	257	THR
1	F	264	SER
1	F	273	GLN
1	F	280	LEU
1	F	285	ARG
1	F	287	VAL
1	F	288	GLU
1	F	292	LEU
1	F	294	LEU
1	F	295	LYS
1	F	297	LEU
1	F	298	LEU
1	F	315	ARG
1	F	320	ARG
1	F	334	ASN
1	F	349	THR
1	F	351	GLN
1	F	359	THR
1	F	374	VAL
1	F	382	SER

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Mol	Chain	Res	Type
1	F	383	ASP
1	F	390	GLN
1	F	395	ASP
1	F	400	CYS
1	F	404	LEU
1	F	406	LEU
1	F	412	SER
1	F	415	LYS
1	F	420	LEU
1	F	421	LEU
1	F	422	LEU
1	F	425	LEU
1	F	437	ARG
1	F	444	LEU
1	F	448	GLN
1	F	455	ARG
1	F	457	SER
1	F	465	MET
1	F	466	ASN
1	F	467	LEU
1	F	469	VAL
1	F	475	LEU
1	F	481	LEU
1	F	507	VAL
1	F	530	ILE
1	F	534	ILE
1	F	535	LEU
1	F	542	SER
1	F	545	LEU
1	F	549	VAL
1	F	563	ARG
1	F	573	THR
1	G	45	ARG
1	G	51	SER
1	G	52	LEU
1	G	74	LEU
1	G	82	LEU
1	G	83	VAL
1	G	84	GLN
1	G	85	LYS
1	G	86	LEU
1	G	101	LEU

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Mol	Chain	Res	Type
1	G	115	THR
1	G	119	THR
1	G	123	THR
1	G	126	SER
1	G	130	ARG
1	G	133	LEU
1	G	153	THR
1	G	154	LEU
1	G	156	LEU
1	G	157	SER
1	G	164	SER
1	G	173	VAL
1	G	180	VAL
1	G	183	VAL
1	G	190	SER
1	G	200	LEU
1	G	218	SER
1	G	263	LYS
1	G	270	VAL
1	G	273	GLN
1	G	279	SER
1	G	280	LEU
1	G	287	VAL
1	G	290	LEU
1	G	292	LEU
1	G	294	LEU
1	G	297	LEU
1	G	298	LEU
1	G	302	LEU
1	G	305	LEU
1	G	306	ASP
1	G	322	SER
1	G	331	GLU
1	G	337	MET
1	G	343	ARG
1	G	349	THR
1	G	351	GLN
1	G	352	ARG
1	G	359	THR
1	G	360	LEU
1	G	382	SER
1	G	383	ASP

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Mol	Chain	Res	Type
1	G	390	GLN
1	G	393	LYS
1	G	415	LYS
1	G	420	LEU
1	G	421	LEU
1	G	422	LEU
1	G	437	ARG
1	G	444	LEU
1	G	447	LEU
1	G	448	GLN
1	G	456	GLN
1	G	459	ILE
1	G	465	MET
1	G	466	ASN
1	G	469	VAL
1	G	475	LEU
1	G	481	LEU
1	G	486	ARG
1	G	507	VAL
1	G	530	ILE
1	G	534	ILE
1	G	536	LYS
1	G	542	SER
1	G	545	LEU
1	G	549	VAL
1	G	558	GLU
1	G	563	ARG
1	G	570	GLN
1	G	573	THR
1	H	47	LYS
1	H	51	SER
1	H	52	LEU
1	H	60	GLN
1	H	74	LEU
1	H	80	LEU
1	H	86	LEU
1	H	101	LEU
1	H	109	LYS
1	H	119	THR
1	H	121	CYS
1	H	130	ARG
1	H	139	VAL

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Mol	Chain	Res	Type
1	H	143	GLU
1	H	151	ASP
1	H	152	SER
1	H	154	LEU
1	H	156	LEU
1	H	159	ASN
1	H	162	MET
1	H	164	SER
1	H	166	SER
1	H	189	GLN
1	H	190	SER
1	H	205	MET
1	H	210	SER
1	H	234	LEU
1	H	242	ILE
1	H	255	LYS
1	H	257	THR
1	H	259	ASN
1	H	263	LYS
1	H	264	SER
1	H	273	GLN
1	H	280	LEU
1	H	286	ASP
1	H	287	VAL
1	H	292	LEU
1	H	298	LEU
1	H	332	THR
1	H	337	MET
1	H	350	LYS
1	H	359	THR
1	H	374	VAL
1	H	382	SER
1	H	390	GLN
1	H	400	CYS
1	H	401	LEU
1	H	412	SER
1	H	415	LYS
1	H	420	LEU
1	H	421	LEU
1	H	422	LEU
1	H	425	LEU
1	H	437	ARG

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Mol	Chain	Res	Type
1	H	444	LEU
1	H	447	LEU
1	H	448	GLN
1	H	457	SER
1	H	463	LYS
1	H	465	MET
1	H	466	ASN
1	H	467	LEU
1	H	469	VAL
1	H	475	LEU
1	H	481	LEU
1	H	486	ARG
1	H	507	VAL
1	H	530	ILE
1	H	534	ILE
1	H	536	LYS
1	H	545	LEU
1	H	549	VAL
1	H	563	ARG
1	H	570	GLN
1	I	45	ARG
1	I	46	GLN
1	I	51	SER
1	I	66	ASN
1	I	71	SER
1	I	74	LEU
1	I	80	LEU
1	I	83	VAL
1	I	84	GLN
1	I	86	LEU
1	I	101	LEU
1	I	106	GLU
1	I	109	LYS
1	I	115	THR
1	I	122	GLU
1	I	123	THR
1	I	126	SER
1	I	130	ARG
1	I	153	THR
1	I	154	LEU
1	I	156	LEU
1	I	157	SER

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Mol	Chain	Res	Type
1	I	159	ASN
1	I	162	MET
1	I	164	SER
1	I	166	SER
1	I	173	VAL
1	I	177	GLN
1	I	184	HIS
1	I	190	SER
1	I	199	PRO
1	I	205	MET
1	I	210	SER
1	I	218	SER
1	I	230	SER
1	I	234	LEU
1	I	264	SER
1	I	273	GLN
1	I	279	SER
1	I	280	LEU
1	I	286	ASP
1	I	287	VAL
1	I	289	SER
1	I	292	LEU
1	I	294	LEU
1	I	297	LEU
1	I	298	LEU
1	I	302	LEU
1	I	305	LEU
1	I	326	ARG
1	I	337	MET
1	I	343	ARG
1	I	349	THR
1	I	350	LYS
1	I	359	THR
1	I	374	VAL
1	I	387	SER
1	I	390	GLN
1	I	397	VAL
1	I	415	LYS
1	I	420	LEU
1	I	421	LEU
1	I	422	LEU
1	I	425	LEU

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Mol	Chain	Res	Type
1	I	437	ARG
1	I	444	LEU
1	I	447	LEU
1	I	448	GLN
1	I	457	SER
1	I	465	MET
1	I	466	ASN
1	I	469	VAL
1	I	475	LEU
1	I	481	LEU
1	I	488	THR
1	I	507	VAL
1	I	530	ILE
1	I	534	ILE
1	I	545	LEU
1	I	549	VAL
1	I	563	ARG
1	I	573	THR
1	J	47	LYS
1	J	52	LEU
1	J	77	LEU
1	J	80	LEU
1	J	84	GLN
1	J	86	LEU
1	J	99	THR
1	J	101	LEU
1	J	103	LYS
1	J	106	GLU
1	J	115	THR
1	J	116	SER
1	J	123	THR
1	J	126	SER
1	J	130	ARG
1	J	133	LEU
1	J	146	SER
1	J	153	THR
1	J	154	LEU
1	J	156	LEU
1	J	158	LEU
1	J	159	ASN
1	J	162	MET
1	J	166	SER

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Mol	Chain	Res	Type
1	J	173	VAL
1	J	184	HIS
1	J	189	GLN
1	J	191	MET
1	J	205	MET
1	J	210	SER
1	J	218	SER
1	J	234	LEU
1	J	259	ASN
1	J	270	VAL
1	J	273	GLN
1	J	279	SER
1	J	280	LEU
1	J	287	VAL
1	J	288	GLU
1	J	292	LEU
1	J	294	LEU
1	J	297	LEU
1	J	298	LEU
1	J	320	ARG
1	J	337	MET
1	J	343	ARG
1	J	349	THR
1	J	351	GLN
1	J	352	ARG
1	J	359	THR
1	J	374	VAL
1	J	390	GLN
1	J	393	LYS
1	J	400	CYS
1	J	404	LEU
1	J	406	LEU
1	J	415	LYS
1	J	420	LEU
1	J	421	LEU
1	J	422	LEU
1	J	425	LEU
1	J	437	ARG
1	J	444	LEU
1	J	455	ARG
1	J	457	SER
1	J	465	MET

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Mol	Chain	Res	Type
1	J	469	VAL
1	J	475	LEU
1	J	481	LEU
1	J	486	ARG
1	J	507	VAL
1	J	517	ASP
1	J	530	ILE
1	J	534	ILE
1	J	536	LYS
1	J	542	SER
1	J	547	VAL
1	J	549	VAL
1	J	563	ARG
1	J	570	GLN
1	J	573	THR
1	K	45	ARG
1	K	46	GLN
1	K	48	GLN
1	K	51	SER
1	K	52	LEU
1	K	74	LEU
1	K	77	LEU
1	K	80	LEU
1	K	84	GLN
1	K	86	LEU
1	K	92	SER
1	K	101	LEU
1	K	109	LYS
1	K	113	CYS
1	K	123	THR
1	K	126	SER
1	K	130	ARG
1	K	133	LEU
1	K	143	GLU
1	K	154	LEU
1	K	156	LEU
1	K	159	ASN
1	K	162	MET
1	K	173	VAL
1	K	177	GLN
1	K	198	ASN
1	K	205	MET

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Mol	Chain	Res	Type
1	K	234	LEU
1	K	254	LEU
1	K	259	ASN
1	K	263	LYS
1	K	266	LEU
1	K	270	VAL
1	K	273	GLN
1	K	279	SER
1	K	280	LEU
1	K	283	MET
1	K	287	VAL
1	K	292	LEU
1	K	294	LEU
1	K	297	LEU
1	K	298	LEU
1	K	302	LEU
1	K	321	SER
1	K	322	SER
1	K	325	LEU
1	K	337	MET
1	K	343	ARG
1	K	344	ARG
1	K	350	LYS
1	K	354	GLU
1	K	359	THR
1	K	374	VAL
1	K	382	SER
1	K	390	GLN
1	K	393	LYS
1	K	395	ASP
1	K	400	CYS
1	K	415	LYS
1	K	420	LEU
1	K	421	LEU
1	K	422	LEU
1	K	429	LEU
1	K	437	ARG
1	K	444	LEU
1	K	457	SER
1	K	465	MET
1	K	466	ASN
1	K	469	VAL

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Mol	Chain	Res	Type
1	K	475	LEU
1	K	481	LEU
1	K	486	ARG
1	K	507	VAL
1	K	511	THR
1	K	517	ASP
1	K	520	MET
1	K	530	ILE
1	K	534	ILE
1	K	542	SER
1	K	543	VAL
1	K	545	LEU
1	K	549	VAL
1	K	563	ARG
1	K	573	THR
1	L	51	SER
1	L	52	LEU
1	L	66	ASN
1	L	71	SER
1	L	74	LEU
1	L	80	LEU
1	L	81	GLN
1	L	84	GLN
1	L	86	LEU
1	L	100	TYR
1	L	101	LEU
1	L	106	GLU
1	L	109	LYS
1	L	123	THR
1	L	126	SER
1	L	130	ARG
1	L	133	LEU
1	L	139	VAL
1	L	143	GLU
1	L	154	LEU
1	L	156	LEU
1	L	159	ASN
1	L	162	MET
1	L	164	SER
1	L	177	GLN
1	L	184	HIS
1	L	190	SER

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Mol	Chain	Res	Type
1	L	203	GLN
1	L	218	SER
1	L	230	SER
1	L	234	LEU
1	L	238	ILE
1	L	254	LEU
1	L	257	THR
1	L	263	LYS
1	L	270	VAL
1	L	273	GLN
1	L	279	SER
1	L	280	LEU
1	L	287	VAL
1	L	289	SER
1	L	292	LEU
1	L	295	LYS
1	L	298	LEU
1	L	302	LEU
1	L	320	ARG
1	L	329	TYR
1	L	332	THR
1	L	337	MET
1	L	343	ARG
1	L	349	THR
1	L	351	GLN
1	L	352	ARG
1	L	359	THR
1	L	382	SER
1	L	383	ASP
1	L	387	SER
1	L	390	GLN
1	L	395	ASP
1	L	400	CYS
1	L	415	LYS
1	L	420	LEU
1	L	421	LEU
1	L	422	LEU
1	L	437	ARG
1	L	444	LEU
1	L	447	LEU
1	L	451	ILE
1	L	452	GLU

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Mol	Chain	Res	Type
1	L	456	GLN
1	L	463	LYS
1	L	465	MET
1	L	466	ASN
1	L	467	LEU
1	L	469	VAL
1	L	475	LEU
1	L	495	VAL
1	L	507	VAL
1	L	511	THR
1	L	520	MET
1	L	530	ILE
1	L	534	ILE
1	L	545	LEU
1	L	547	VAL
1	L	549	VAL
1	L	563	ARG
1	L	570	GLN
1	L	573	THR
1	M	45	ARG
1	M	47	LYS
1	M	48	GLN
1	M	55	MET
1	M	66	ASN
1	M	75	LEU
1	M	76	THR
1	M	77	LEU
1	M	80	LEU
1	M	82	LEU
1	M	84	GLN
1	M	92	SER
1	M	96	VAL
1	M	100	TYR
1	M	101	LEU
1	M	109	LYS
1	M	118	LEU
1	M	130	ARG
1	M	133	LEU
1	M	143	GLU
1	M	152	SER
1	M	153	THR
1	M	154	LEU

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Mol	Chain	Res	Type
1	M	156	LEU
1	M	162	MET
1	M	164	SER
1	M	166	SER
1	M	172	GLN
1	M	173	VAL
1	M	176	LEU
1	M	177	GLN
1	M	180	VAL
1	M	189	GLN
1	M	190	SER
1	M	205	MET
1	M	213	SER
1	M	217	SER
1	M	232	LEU
1	M	234	LEU
1	M	257	THR
1	M	267	LYS
1	M	270	VAL
1	M	271	TYR
1	M	273	GLN
1	M	279	SER
1	M	280	LEU
1	M	285	ARG
1	M	287	VAL
1	M	289	SER
1	M	292	LEU
1	M	294	LEU
1	M	295	LYS
1	M	298	LEU
1	M	305	LEU
1	M	312	LEU
1	M	325	LEU
1	M	326	ARG
1	M	332	THR
1	M	339	SER
1	M	343	ARG
1	M	348	GLU
1	M	354	GLU
1	M	359	THR
1	M	364	LEU
1	M	374	VAL

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Mol	Chain	Res	Type
1	M	380	LEU
1	M	382	SER
1	M	383	ASP
1	M	390	GLN
1	M	393	LYS
1	M	395	ASP
1	M	397	VAL
1	M	404	LEU
1	M	412	SER
1	M	415	LYS
1	M	420	LEU
1	M	421	LEU
1	M	422	LEU
1	M	425	LEU
1	M	429	LEU
1	M	435	SER
1	M	437	ARG
1	M	444	LEU
1	M	447	LEU
1	M	452	GLU
1	M	453	MET
1	M	457	SER
1	M	465	MET
1	M	466	ASN
1	M	472	THR
1	M	475	LEU
1	M	481	LEU
1	M	486	ARG
1	M	507	VAL
1	M	517	ASP
1	M	530	ILE
1	M	534	ILE
1	M	535	LEU
1	M	542	SER
1	M	547	VAL
1	M	561	CYS
1	M	563	ARG
1	M	570	GLN
1	N	51	SER
1	N	52	LEU
1	N	75	LEU
1	N	77	LEU

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Mol	Chain	Res	Type
1	N	80	LEU
1	N	84	GLN
1	N	86	LEU
1	N	101	LEU
1	N	106	GLU
1	N	115	THR
1	N	116	SER
1	N	118	LEU
1	N	123	THR
1	N	126	SER
1	N	130	ARG
1	N	134	LEU
1	N	143	GLU
1	N	151	ASP
1	N	154	LEU
1	N	156	LEU
1	N	157	SER
1	N	159	ASN
1	N	173	VAL
1	N	190	SER
1	N	198	ASN
1	N	205	MET
1	N	210	SER
1	N	213	SER
1	N	218	SER
1	N	232	LEU
1	N	254	LEU
1	N	273	GLN
1	N	279	SER
1	N	280	LEU
1	N	287	VAL
1	N	289	SER
1	N	292	LEU
1	N	294	LEU
1	N	295	LYS
1	N	297	LEU
1	N	298	LEU
1	N	321	SER
1	N	322	SER
1	N	326	ARG
1	N	331	GLU
1	N	351	GLN

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Mol	Chain	Res	Type
1	N	360	LEU
1	N	368	ILE
1	N	374	VAL
1	N	382	SER
1	N	383	ASP
1	N	387	SER
1	N	390	GLN
1	N	404	LEU
1	N	415	LYS
1	N	420	LEU
1	N	421	LEU
1	N	422	LEU
1	N	425	LEU
1	N	436	MET
1	N	437	ARG
1	N	444	LEU
1	N	448	GLN
1	N	457	SER
1	N	459	ILE
1	N	465	MET
1	N	466	ASN
1	N	468	ASP
1	N	469	VAL
1	N	475	LEU
1	N	481	LEU
1	N	506	VAL
1	N	520	MET
1	N	530	ILE
1	N	534	ILE
1	N	541	ASN
1	N	549	VAL
1	N	558	GLU
1	N	563	ARG
1	N	573	THR
1	O	51	SER
1	O	54	THR
1	O	66	ASN
1	O	71	SER
1	O	84	GLN
1	O	86	LEU
1	O	96	VAL
1	O	101	LEU

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Mol	Chain	Res	Type
1	O	103	LYS
1	O	109	LYS
1	O	115	THR
1	O	116	SER
1	O	126	SER
1	O	130	ARG
1	O	133	LEU
1	O	143	GLU
1	O	154	LEU
1	O	156	LEU
1	O	157	SER
1	O	158	LEU
1	O	159	ASN
1	O	162	MET
1	O	173	VAL
1	O	177	GLN
1	O	189	GLN
1	O	190	SER
1	O	198	ASN
1	O	200	LEU
1	O	205	MET
1	O	210	SER
1	O	218	SER
1	O	232	LEU
1	O	238	ILE
1	O	254	LEU
1	O	255	LYS
1	O	264	SER
1	O	273	GLN
1	O	280	LEU
1	O	286	ASP
1	O	292	LEU
1	O	294	LEU
1	O	297	LEU
1	O	298	LEU
1	O	331	GLU
1	O	332	THR
1	O	337	MET
1	O	343	ARG
1	O	350	LYS
1	O	351	GLN
1	O	352	ARG

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Mol	Chain	Res	Type
1	O	359	THR
1	O	374	VAL
1	O	382	SER
1	O	393	LYS
1	O	401	LEU
1	O	415	LYS
1	O	419	SER
1	O	420	LEU
1	O	421	LEU
1	O	422	LEU
1	O	437	ARG
1	O	444	LEU
1	O	447	LEU
1	O	448	GLN
1	O	451	ILE
1	O	452	GLU
1	O	457	SER
1	O	463	LYS
1	O	465	MET
1	O	466	ASN
1	O	469	VAL
1	O	475	LEU
1	O	481	LEU
1	O	486	ARG
1	O	491	ILE
1	O	499	CYS
1	O	507	VAL
1	O	517	ASP
1	O	520	MET
1	O	534	ILE
1	O	536	LYS
1	O	542	SER
1	O	545	LEU
1	O	549	VAL
1	O	563	ARG
1	O	573	THR
1	P	52	LEU
1	P	54	THR
1	P	66	ASN
1	P	74	LEU
1	P	77	LEU
1	P	80	LEU

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Mol	Chain	Res	Type
1	P	83	VAL
1	P	84	GLN
1	P	86	LEU
1	P	90	GLU
1	P	92	SER
1	P	101	LEU
1	P	109	LYS
1	P	115	THR
1	P	119	THR
1	P	126	SER
1	P	130	ARG
1	P	143	GLU
1	P	152	SER
1	P	153	THR
1	P	156	LEU
1	P	159	ASN
1	P	162	MET
1	P	164	SER
1	P	168	CYS
1	P	173	VAL
1	P	183	VAL
1	P	184	HIS
1	P	189	GLN
1	P	210	SER
1	P	218	SER
1	P	234	LEU
1	P	259	ASN
1	P	263	LYS
1	P	266	LEU
1	P	269	CYS
1	P	273	GLN
1	P	279	SER
1	P	280	LEU
1	P	292	LEU
1	P	294	LEU
1	P	295	LYS
1	P	297	LEU
1	P	298	LEU
1	P	302	LEU
1	P	320	ARG
1	P	322	SER
1	P	325	LEU

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Mol	Chain	Res	Type
1	P	331	GLU
1	P	334	ASN
1	P	337	MET
1	P	350	LYS
1	P	351	GLN
1	P	352	ARG
1	P	359	THR
1	P	374	VAL
1	P	376	SER
1	P	382	SER
1	P	387	SER
1	P	390	GLN
1	P	393	LYS
1	P	401	LEU
1	P	404	LEU
1	P	420	LEU
1	P	421	LEU
1	P	425	LEU
1	P	437	ARG
1	P	444	LEU
1	P	463	LYS
1	P	465	MET
1	P	466	ASN
1	P	467	LEU
1	P	469	VAL
1	P	474	MET
1	P	475	LEU
1	P	481	LEU
1	P	507	VAL
1	P	511	THR
1	P	530	ILE
1	P	534	ILE
1	P	535	LEU
1	P	542	SER
1	P	545	LEU
1	P	549	VAL
1	P	559	GLU
1	P	563	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	87	GLN
1	A	159	ASN
1	A	189	GLN
1	A	198	ASN
1	A	259	ASN
1	A	358	HIS
1	A	498	ASN
1	B	48	GLN
1	B	172	GLN
1	B	189	GLN
1	B	198	ASN
1	B	259	ASN
1	B	273	GLN
1	B	358	HIS
1	B	498	ASN
1	C	48	GLN
1	C	189	GLN
1	C	198	ASN
1	C	259	ASN
1	C	273	GLN
1	C	358	HIS
1	C	391	ASN
1	C	498	ASN
1	D	48	GLN
1	D	87	GLN
1	D	189	GLN
1	D	198	ASN
1	D	259	ASN
1	D	273	GLN
1	D	351	GLN
1	D	358	HIS
1	D	498	ASN
1	E	189	GLN
1	E	259	ASN
1	E	358	HIS
1	E	498	ASN
1	F	48	GLN
1	F	189	GLN
1	F	198	ASN
1	F	259	ASN
1	F	273	GLN
1	F	358	HIS

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Mol	Chain	Res	Type
1	F	367	ASN
1	F	498	ASN
1	G	48	GLN
1	G	177	GLN
1	G	189	GLN
1	G	198	ASN
1	G	259	ASN
1	G	273	GLN
1	G	358	HIS
1	G	498	ASN
1	H	48	GLN
1	H	177	GLN
1	H	189	GLN
1	H	259	ASN
1	H	273	GLN
1	H	358	HIS
1	H	367	ASN
1	H	456	GLN
1	H	498	ASN
1	I	48	GLN
1	I	189	GLN
1	I	259	ASN
1	I	358	HIS
1	I	391	ASN
1	I	434	ASN
1	I	498	ASN
1	J	48	GLN
1	J	177	GLN
1	J	189	GLN
1	J	203	GLN
1	J	259	ASN
1	J	358	HIS
1	J	391	ASN
1	J	434	ASN
1	J	498	ASN
1	K	189	GLN
1	K	198	ASN
1	K	259	ASN
1	K	358	HIS
1	K	498	ASN
1	L	48	GLN
1	L	66	ASN

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Mol	Chain	Res	Type
1	L	189	GLN
1	L	198	ASN
1	L	273	GLN
1	L	358	HIS
1	L	390	GLN
1	L	498	ASN
1	M	48	GLN
1	M	172	GLN
1	M	198	ASN
1	M	273	GLN
1	M	334	ASN
1	M	351	GLN
1	M	498	ASN
1	N	48	GLN
1	N	189	GLN
1	N	198	ASN
1	N	259	ASN
1	N	358	HIS
1	N	448	GLN
1	N	498	ASN
1	O	48	GLN
1	O	177	GLN
1	O	189	GLN
1	O	198	ASN
1	O	259	ASN
1	O	273	GLN
1	O	358	HIS
1	O	498	ASN
1	P	48	GLN
1	P	66	ASN
1	P	189	GLN
1	P	259	ASN
1	P	273	GLN
1	P	358	HIS
1	P	390	GLN
1	P	434	ASN
1	P	498	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	MAY	A	600	1	20,23,24	0.39	0	19,23,26	0.81	1 (5%)
2	MAY	B	600	1	20,23,24	0.50	0	19,23,26	0.74	1 (5%)
2	MAY	C	600	1	20,23,24	0.35	0	19,23,26	0.79	1 (5%)
2	MAY	D	600	1	20,23,24	0.38	0	19,23,26	0.85	1 (5%)
2	MAY	E	600	1	20,23,24	0.51	0	19,23,26	0.81	1 (5%)
2	MAY	F	600	1	20,23,24	0.54	0	19,23,26	0.64	0
2	MAY	G	600	1	20,23,24	0.36	0	19,23,26	0.86	1 (5%)
2	MAY	H	600	1	20,23,24	0.53	0	19,23,26	0.82	1 (5%)
2	MAY	I	600	1	20,23,24	0.38	0	19,23,26	0.79	1 (5%)
2	MAY	J	600	1	20,23,24	0.44	0	19,23,26	0.76	1 (5%)
2	MAY	K	600	1	20,23,24	0.52	0	19,23,26	0.75	0
2	MAY	L	600	1	20,23,24	0.49	0	19,23,26	0.86	1 (5%)
2	MAY	M	600	1	20,23,24	0.36	0	19,23,26	0.81	1 (5%)
2	MAY	N	600	1	20,23,24	0.48	0	19,23,26	0.74	0
2	MAY	O	600	1	20,23,24	0.47	0	19,23,26	0.70	0
2	MAY	P	600	1	20,23,24	0.42	0	19,23,26	0.70	0

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
2	MAY	A	600	1	-	0/18/22/24	0/0/0/0
2	MAY	B	600	1	-	0/18/22/24	0/0/0/0
2	MAY	C	600	1	-	0/18/22/24	0/0/0/0
2	MAY	D	600	1	-	0/18/22/24	0/0/0/0
2	MAY	E	600	1	-	0/18/22/24	0/0/0/0
2	MAY	F	600	1	-	0/18/22/24	0/0/0/0
2	MAY	G	600	1	-	0/18/22/24	0/0/0/0
2	MAY	H	600	1	-	0/18/22/24	0/0/0/0
2	MAY	I	600	1	-	0/18/22/24	0/0/0/0
2	MAY	J	600	1	-	0/18/22/24	0/0/0/0
2	MAY	K	600	1	-	0/18/22/24	0/0/0/0
2	MAY	L	600	1	-	0/18/22/24	0/0/0/0
2	MAY	M	600	1	-	0/18/22/24	0/0/0/0
2	MAY	N	600	1	-	0/18/22/24	0/0/0/0
2	MAY	O	600	1	-	0/18/22/24	0/0/0/0
2	MAY	P	600	1	-	0/18/22/24	0/0/0/0

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	600	MAY	C3-C2-C1	-2.50	107.04	114.13
2	D	600	MAY	C3-C2-C1	-2.43	107.22	114.13
2	E	600	MAY	C3-C2-C1	-2.37	107.41	114.13
2	L	600	MAY	C3-C2-C1	-2.35	107.47	114.13
2	G	600	MAY	C3-C2-C1	-2.30	107.59	114.13
2	C	600	MAY	C3-C2-C1	-2.25	107.74	114.13
2	H	600	MAY	C3-C2-C1	-2.22	107.82	114.13
2	J	600	MAY	C3-C2-C1	-2.21	107.85	114.13
2	M	600	MAY	C3-C2-C1	-2.20	107.87	114.13
2	I	600	MAY	C3-C2-C1	-2.18	107.93	114.13
2	B	600	MAY	C3-C2-C1	-2.13	108.07	114.13

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 46 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	MAY	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	600	MAY	3	0
2	C	600	MAY	3	0
2	D	600	MAY	4	0
2	E	600	MAY	3	0
2	F	600	MAY	4	0
2	G	600	MAY	1	0
2	H	600	MAY	4	0
2	I	600	MAY	2	0
2	J	600	MAY	2	0
2	K	600	MAY	3	0
2	L	600	MAY	1	0
2	M	600	MAY	2	0
2	N	600	MAY	4	0
2	O	600	MAY	3	0
2	P	600	MAY	2	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates

EDS was not executed - this section will therefore be empty.

6.4 Ligands

EDS was not executed - this section will therefore be empty.

6.5 Other polymers

EDS was not executed - this section will therefore be empty.