Full wwPDB X-ray Structure Validation Report ⓘ

Jun 3, 2020 – 03:15 am BST

PDB ID	:	4FAB
Title	:	THREE-DIMENSIONAL STRUCTURE OF A FLUORESCEIN-FAB COMPLEX CRYSTALLIZED IN 2-METHYL-2,4-PENTANEDIOL
Authors	:	Herron, J.N.; He, X.; Mason, M.L.; Vossjunior, E.W.; Edmundson, A.B.
Deposited on	:	1989-04-10
Resolution	:	2.70 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

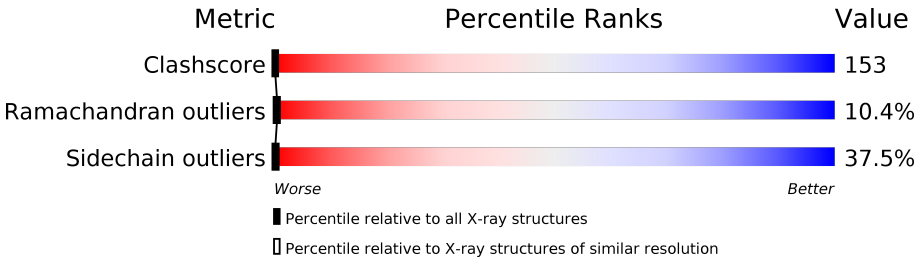
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	L	219	11% 45% 29% 15%
2	H	216	6% 38% 37% 19%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLU	H	218	-	-	X	-
4	MPD	H	219	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3395 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 IGG2A-KAPPA 4-4-20 FAB (LIGHT CHAIN).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	219	Total	C	N	O	S	0	0	0
			1700	1060	291	342	7			

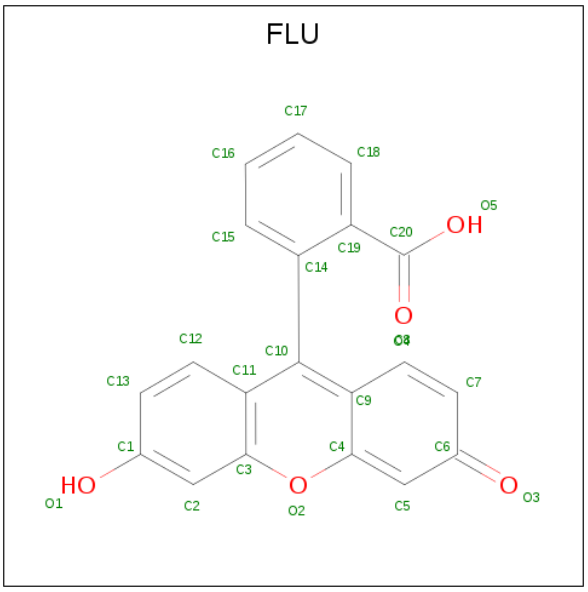
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	2	VAL	ILE	CONFLICT	GB 1589925
L	7	THR	SER	CONFLICT	GB 1589925
L	29	LEU	VAL	CONFLICT	GB 1589925
L	33	GLN	ASN	CONFLICT	GB 1589925
L	39	ARG	GLU	CONFLICT	GB 1589925
L	41	TYR	PHE	CONFLICT	GB 1589925
L	51	VAL	LEU	CONFLICT	GB 1589925
L	92	PHE	TYR	CONFLICT	GB 1589925
L	94	SER	PHE	CONFLICT	GB 1589925
L	96	SER	ALA	CONFLICT	GB 1589925
L	97	THR	SER	CONFLICT	GB 1589925
L	217	ASN	GLY	CONFLICT	GB 1589925

- Molecule 2 is a protein called IGG2A-KAPPA 4-4-20 FAB (HEAVY CHAIN).

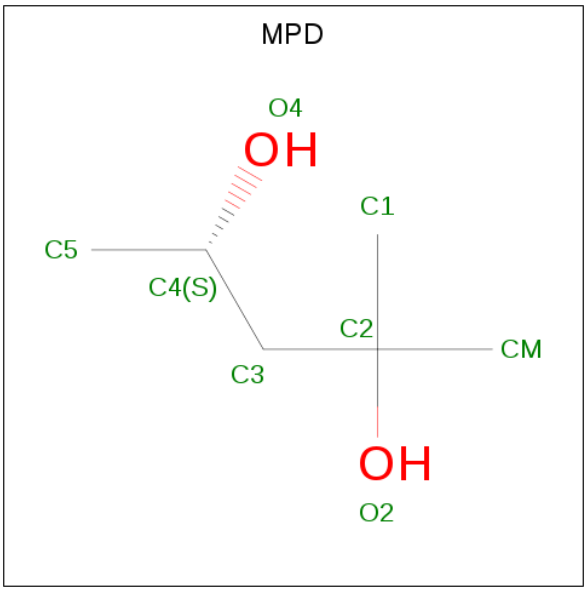
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	216	Total	C	N	O	S	0	0	0
			1662	1050	269	333	10			

- Molecule 3 is 2-(6-HYDROXY-3-OXO-3H-XANTHEN-9-YL)-BENZOIC ACID (three-letter code: FLU) (formula: $C_{20}H_{12}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	H	1	Total	C	O	0	0
			25	20	5		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	H	1	Total	C	O	0	0
			8	6	2		

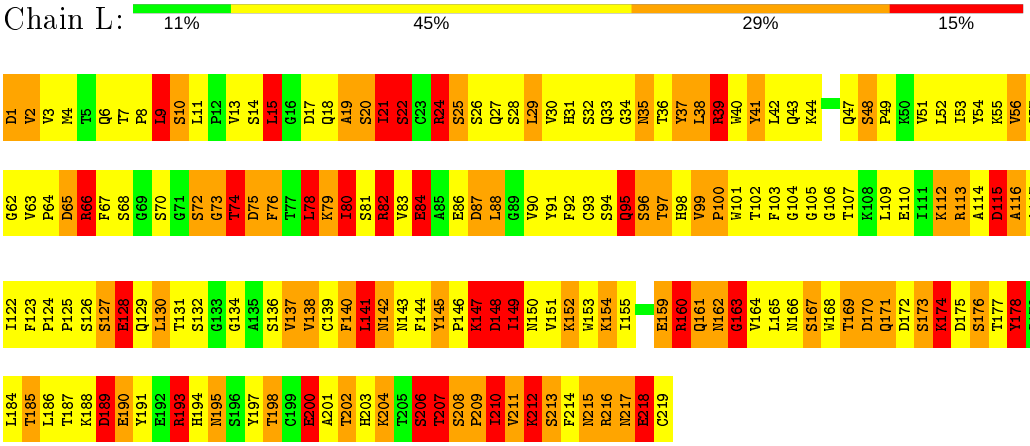
3 Residue-property plots (i)

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

Note EDS was not executed.

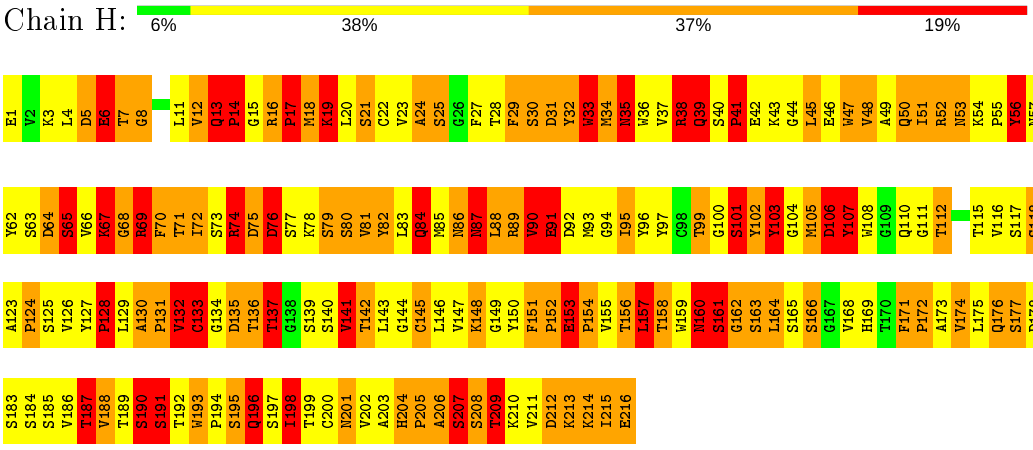
- Molecule 1: IGG2A-KAPPA 4-4-20 FAB (LIGHT CHAIN)

Chain L:



- Molecule 2: IGG2A-KAPPA 4-4-20 FAB (HEAVY CHAIN)

Chain H:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	58.30Å 43.90Å 42.50Å 82.10° 87.30° 84.60°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.70)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.215 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3395	wwPDB-VP
Average B, all atoms (Å^2)	13.0	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: MPD, FLU

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	L	1.26	3/1739 (0.2%)	2.40	108/2359 (4.6%)
2	H	1.34	6/1706 (0.4%)	2.56	125/2326 (5.4%)
All	All	1.30	9/3445 (0.3%)	2.48	233/4685 (5.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	8	GLY	N-CA	-7.37	1.34	1.46
2	H	161	SER	CB-OG	6.24	1.50	1.42
2	H	190	SER	CA-CB	5.96	1.61	1.52
2	H	196	GLN	CA-CB	-5.82	1.41	1.53
2	H	80	SER	CB-OG	-5.53	1.35	1.42
1	L	34	GLY	N-CA	5.26	1.53	1.46
1	L	74	THR	CB-OG1	5.18	1.53	1.43
1	L	116	ALA	CA-CB	5.12	1.63	1.52
2	H	162	GLY	N-CA	5.06	1.53	1.46

All (233) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	193	ARG	NE-CZ-NH2	-21.80	109.40	120.30
2	H	16	ARG	NE-CZ-NH1	20.66	130.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	196	GLN	CA-CB-CG	17.09	151.00	113.40
2	H	204	HIS	CA-CB-CG	16.39	141.47	113.60
2	H	74	ARG	NE-CZ-NH2	-16.28	112.16	120.30
2	H	16	ARG	CA-CB-CG	13.59	143.30	113.40
1	L	66	ARG	CD-NE-CZ	13.01	141.81	123.60
2	H	80	SER	CA-CB-OG	12.78	145.71	111.20
1	L	84	GLU	CA-CB-CG	12.22	140.28	113.40
2	H	16	ARG	NE-CZ-NH2	-11.81	114.39	120.30
2	H	110	GLN	CA-CB-CG	11.76	139.28	113.40
2	H	106	ASP	CB-CG-OD2	-11.75	107.72	118.30
1	L	113	ARG	NE-CZ-NH2	11.46	126.03	120.30
2	H	15	GLY	N-CA-C	11.18	141.06	113.10
1	L	207	THR	N-CA-CB	11.11	131.41	110.30
2	H	142	THR	N-CA-CB	10.99	131.18	110.30
2	H	33	TRP	CA-CB-CG	10.72	134.07	113.70
1	L	75	ASP	CB-CG-OD2	-10.60	108.76	118.30
2	H	16	ARG	CD-NE-CZ	10.57	138.39	123.60
2	H	38	ARG	CD-NE-CZ	10.36	138.10	123.60
1	L	115	ASP	CB-CG-OD1	10.31	127.58	118.30
1	L	113	ARG	CD-NE-CZ	10.20	137.88	123.60
1	L	65	ASP	CB-CG-OD2	-10.17	109.15	118.30
1	L	142	ASN	CA-CB-CG	10.13	135.69	113.40
2	H	74	ARG	NE-CZ-NH1	9.94	125.27	120.30
2	H	91	GLU	OE1-CD-OE2	-9.43	111.99	123.30
2	H	38	ARG	NE-CZ-NH1	9.13	124.86	120.30
2	H	8	GLY	N-CA-C	9.08	135.80	113.10
1	L	116	ALA	N-CA-CB	-8.89	97.66	110.10
2	H	89	ARG	NE-CZ-NH2	8.73	124.67	120.30
1	L	148	ASP	CB-CG-OD1	8.69	126.12	118.30
2	H	213	LYS	CB-CA-C	8.61	127.63	110.40
2	H	153	GLU	CG-CD-OE1	8.47	135.24	118.30
2	H	91	GLU	CB-CG-CD	8.37	136.80	114.20
2	H	103	TYR	CB-CG-CD1	-8.29	116.03	121.00
1	L	190	GLU	CA-CB-CG	8.27	131.60	113.40
2	H	89	ARG	NE-CZ-NH1	-8.27	116.17	120.30
1	L	160	ARG	CD-NE-CZ	8.26	135.16	123.60
1	L	116	ALA	N-CA-C	8.24	133.26	111.00
2	H	110	GLN	N-CA-CB	8.24	125.43	110.60
1	L	84	GLU	OE1-CD-OE2	8.22	133.17	123.30
1	L	160	ARG	NE-CZ-NH2	-8.15	116.22	120.30
2	H	35	ASN	CA-CB-CG	8.14	131.30	113.40
1	L	162	ASN	CB-CA-C	8.01	126.41	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	113	ARG	CA-CB-CG	8.00	131.01	113.40
2	H	76	ASP	CB-CG-OD2	7.89	125.40	118.30
2	H	91	GLU	CG-CD-OE1	7.86	134.03	118.30
1	L	200	GLU	CA-CB-CG	7.82	130.61	113.40
2	H	106	ASP	CA-CB-CG	-7.82	96.20	113.40
1	L	41	TYR	CB-CG-CD1	7.71	125.62	121.00
2	H	13	GLN	CA-CB-CG	7.70	130.33	113.40
1	L	21	ILE	CB-CA-C	7.51	126.62	111.60
1	L	193	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	L	115	ASP	CA-CB-CG	7.45	129.80	113.40
2	H	160	ASN	CA-CB-CG	-7.44	97.03	113.40
1	L	35	ASN	CA-CB-CG	-7.38	97.17	113.40
2	H	84	GLN	CB-CG-CD	7.35	130.72	111.60
1	L	115	ASP	CA-C-O	-7.35	104.67	120.10
1	L	84	GLU	N-CA-CB	7.28	123.71	110.60
1	L	9	LEU	CA-CB-CG	7.25	131.98	115.30
1	L	41	TYR	CB-CG-CD2	-7.23	116.66	121.00
2	H	38	ARG	CG-CD-NE	7.21	126.94	111.80
2	H	215	ILE	CB-CA-C	7.17	125.93	111.60
1	L	193	ARG	N-CA-CB	7.16	123.49	110.60
2	H	78	LYS	N-CA-C	-7.13	91.73	111.00
2	H	101	SER	CB-CA-C	7.13	123.64	110.10
1	L	72	SER	N-CA-CB	7.12	121.19	110.50
2	H	17	PRO	N-CA-C	7.11	130.59	112.10
2	H	196	GLN	N-CA-CB	7.10	123.39	110.60
2	H	153	GLU	CG-CD-OE2	-7.08	104.13	118.30
2	H	41	PRO	N-CA-CB	-7.01	94.89	103.30
1	L	78	LEU	CA-CB-CG	7.00	131.39	115.30
1	L	24	ARG	N-CA-CB	6.96	123.12	110.60
1	L	216	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	L	189	ASP	CB-CG-OD1	6.92	124.52	118.30
2	H	17	PRO	N-CA-CB	-6.89	95.03	102.60
2	H	7	THR	C-N-CA	6.85	136.69	122.30
2	H	67	LYS	CA-CB-CG	6.85	128.46	113.40
1	L	149	ILE	N-CA-CB	6.84	126.52	110.80
1	L	160	ARG	NE-CZ-NH1	6.79	123.70	120.30
1	L	171	GLN	N-CA-CB	6.79	122.82	110.60
2	H	181	THR	CB-CA-C	6.76	129.85	111.60
1	L	39	ARG	NE-CZ-NH1	-6.71	116.95	120.30
2	H	71	THR	CA-C-O	6.71	134.18	120.10
2	H	166	SER	CB-CA-C	6.70	122.83	110.10
1	L	193	ARG	CD-NE-CZ	-6.68	114.25	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	153	GLU	N-CA-C	6.66	128.99	111.00
1	L	65	ASP	CB-CG-OD1	6.64	124.28	118.30
2	H	69	ARG	NE-CZ-NH1	6.64	123.62	120.30
2	H	56	TYR	CA-CB-CG	-6.63	100.80	113.40
1	L	66	ARG	NE-CZ-NH2	6.62	123.61	120.30
2	H	19	LYS	CB-CA-C	-6.61	97.19	110.40
1	L	178	TYR	CB-CG-CD1	6.59	124.95	121.00
2	H	157	LEU	CB-CA-C	6.55	122.64	110.20
2	H	195	SER	O-C-N	6.53	133.15	122.70
1	L	193	ARG	CB-CA-C	-6.50	97.41	110.40
1	L	210	ILE	CB-CA-C	-6.49	98.63	111.60
1	L	207	THR	O-C-N	6.48	133.07	122.70
1	L	171	GLN	CB-CA-C	-6.47	97.46	110.40
2	H	103	TYR	CB-CG-CD2	6.46	124.88	121.00
1	L	58	ASN	CA-CB-CG	-6.45	99.20	113.40
1	L	127	SER	CB-CA-C	6.44	122.33	110.10
1	L	113	ARG	CB-CG-CD	6.38	128.19	111.60
2	H	21	SER	N-CA-CB	-6.37	100.94	110.50
2	H	53	ASN	CB-CA-C	6.34	123.08	110.40
2	H	61	TYR	N-CA-CB	6.33	122.00	110.60
2	H	133	CYS	CA-CB-SG	6.32	125.38	114.00
2	H	130	ALA	N-CA-CB	-6.32	101.26	110.10
1	L	174	LYS	N-CA-C	6.31	128.04	111.00
1	L	130	LEU	CB-CA-C	6.27	122.11	110.20
1	L	167	SER	N-CA-CB	6.21	119.81	110.50
1	L	78	LEU	CB-CA-C	6.18	121.94	110.20
2	H	19	LYS	N-CA-CB	6.17	121.70	110.60
2	H	14	PRO	CB-CA-C	6.15	127.37	112.00
1	L	140	PHE	N-CA-CB	6.15	121.67	110.60
2	H	212	ASP	CB-CG-OD2	6.14	123.83	118.30
1	L	176	SER	CB-CA-C	6.13	121.74	110.10
1	L	178	TYR	CA-CB-CG	6.12	125.02	113.40
1	L	113	ARG	NH1-CZ-NH2	-6.11	112.67	119.40
1	L	212	LYS	CA-CB-CG	6.10	126.83	113.40
1	L	74	THR	CA-CB-CG2	6.09	120.92	112.40
2	H	32	TYR	CB-CG-CD1	6.03	124.62	121.00
2	H	154	PRO	N-CA-C	6.02	127.76	112.10
1	L	171	GLN	O-C-N	6.02	132.33	122.70
2	H	84	GLN	CB-CA-C	6.01	122.41	110.40
1	L	95	GLN	N-CA-CB	6.00	121.41	110.60
1	L	216	ARG	CD-NE-CZ	6.00	132.00	123.60
2	H	13	GLN	O-C-N	5.99	132.47	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	76	ASP	OD1-CG-OD2	-5.97	111.95	123.30
1	L	58	ASN	OD1-CG-ND2	5.96	135.62	121.90
1	L	145	TYR	CA-CB-CG	-5.96	102.08	113.40
2	H	5	ASP	CB-CG-OD1	5.94	123.65	118.30
1	L	82	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	L	176	SER	N-CA-CB	-5.92	101.63	110.50
2	H	71	THR	N-CA-CB	5.88	121.47	110.30
2	H	191	SER	CB-CA-C	5.88	121.27	110.10
1	L	97	THR	N-CA-CB	5.87	121.46	110.30
1	L	174	LYS	CB-CA-C	-5.87	98.67	110.40
2	H	19	LYS	CB-CG-CD	5.86	126.84	111.60
2	H	118	SER	CA-CB-OG	5.84	126.98	111.20
2	H	52	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	H	5	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	L	34	GLY	N-CA-C	-5.83	98.53	113.10
1	L	128	GLU	OE1-CD-OE2	5.81	130.28	123.30
2	H	89	ARG	CD-NE-CZ	-5.79	115.49	123.60
2	H	152	PRO	C-N-CA	5.79	136.18	121.70
2	H	7	THR	CA-C-O	5.78	132.23	120.10
2	H	45	LEU	CB-CA-C	5.74	121.11	110.20
1	L	171	GLN	CB-CG-CD	5.74	126.52	111.60
2	H	135	ASP	CB-CA-C	5.73	121.87	110.40
2	H	16	ARG	CB-CG-CD	5.72	126.48	111.60
1	L	193	ARG	CG-CD-NE	-5.72	99.79	111.80
2	H	173	ALA	CB-CA-C	5.71	118.67	110.10
1	L	95	GLN	CB-CG-CD	5.70	126.43	111.60
2	H	88	LEU	CB-CA-C	5.70	121.03	110.20
2	H	190	SER	N-CA-C	5.70	126.39	111.00
1	L	95	GLN	CA-CB-CG	5.70	125.93	113.40
2	H	47	TRP	CA-CB-CG	5.68	124.50	113.70
1	L	75	ASP	OD1-CG-OD2	5.68	134.09	123.30
2	H	56	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	L	25	SER	N-CA-C	5.67	126.30	111.00
2	H	137	THR	N-CA-CB	-5.63	99.61	110.30
2	H	24	ALA	N-CA-CB	-5.62	102.24	110.10
1	L	95	GLN	CA-C-N	-5.61	104.86	117.20
1	L	25	SER	N-CA-CB	-5.61	102.09	110.50
2	H	39	GLN	CA-CB-CG	5.61	125.73	113.40
2	H	176	GLN	O-C-N	5.60	131.66	122.70
2	H	58	TYR	O-C-N	5.59	131.65	122.70
1	L	149	ILE	O-C-N	5.59	131.64	122.70
1	L	217	ASN	CA-CB-CG	-5.59	101.11	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	148	LYS	CA-CB-CG	5.59	125.69	113.40
1	L	20	SER	N-CA-C	-5.58	95.93	111.00
2	H	82	TYR	CB-CG-CD2	5.58	124.35	121.00
1	L	116	ALA	CB-CA-C	-5.57	101.74	110.10
2	H	71	THR	C-N-CA	5.56	135.60	121.70
2	H	177	SER	CB-CA-C	5.55	120.64	110.10
2	H	87	ASN	CA-CB-CG	5.51	125.52	113.40
1	L	163	GLY	N-CA-C	5.51	126.87	113.10
2	H	17	PRO	O-C-N	-5.46	113.97	122.70
1	L	19	ALA	CA-C-N	-5.45	105.22	117.20
1	L	65	ASP	CA-CB-CG	-5.44	101.43	113.40
2	H	195	SER	C-N-CA	-5.43	108.11	121.70
2	H	17	PRO	CA-C-O	5.43	133.24	120.20
1	L	170	ASP	CA-C-O	-5.42	108.72	120.10
2	H	90	VAL	CA-C-O	-5.41	108.74	120.10
2	H	80	SER	CB-CA-C	5.41	120.37	110.10
2	H	39	GLN	N-CA-CB	5.40	120.32	110.60
2	H	162	GLY	N-CA-C	-5.39	99.63	113.10
2	H	16	ARG	N-CA-CB	-5.38	100.91	110.60
2	H	1	GLU	CB-CG-CD	5.37	128.70	114.20
2	H	161	SER	CB-CA-C	5.37	120.29	110.10
1	L	37	TYR	CA-CB-CG	5.35	123.56	113.40
1	L	200	GLU	CG-CD-OE1	5.34	128.97	118.30
2	H	196	GLN	CB-CA-C	5.33	121.07	110.40
2	H	132	VAL	CB-CA-C	5.33	121.52	111.40
2	H	90	VAL	CA-C-N	5.31	128.89	117.20
2	H	141	VAL	CB-CA-C	5.31	121.49	111.40
1	L	24	ARG	CA-CB-CG	5.31	125.08	113.40
1	L	170	ASP	CB-CG-OD1	5.30	123.07	118.30
1	L	137	VAL	CA-CB-CG2	5.29	118.83	110.90
1	L	22	SER	O-C-N	5.29	131.16	122.70
1	L	186	LEU	CA-CB-CG	5.28	127.45	115.30
1	L	79	LYS	CA-CB-CG	5.27	125.00	113.40
2	H	110	GLN	N-CA-C	-5.27	96.76	111.00
1	L	147	LYS	CA-CB-CG	5.27	124.99	113.40
1	L	80	ILE	N-CA-C	-5.25	96.81	111.00
2	H	81	VAL	O-C-N	5.24	131.08	122.70
1	L	24	ARG	CB-CG-CD	5.24	125.21	111.60
1	L	59	ARG	NE-CZ-NH2	-5.23	117.69	120.30
2	H	209	THR	N-CA-CB	-5.22	100.37	110.30
2	H	160	ASN	N-CA-C	5.22	125.10	111.00
2	H	179	LEU	CA-CB-CG	5.21	127.29	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	31	ASP	CA-CB-CG	-5.21	101.94	113.40
1	L	193	ARG	O-C-N	5.21	131.03	122.70
2	H	87	ASN	CB-CG-OD1	5.20	132.00	121.60
2	H	195	SER	N-CA-CB	5.20	118.30	110.50
1	L	181	SER	N-CA-CB	5.16	118.25	110.50
2	H	6	GLU	N-CA-CB	5.15	119.87	110.60
2	H	136	THR	N-CA-CB	5.15	120.08	110.30
1	L	141	LEU	N-CA-CB	-5.14	100.12	110.40
1	L	115	ASP	CA-C-N	5.13	128.50	117.20
1	L	173	SER	CA-C-N	5.13	128.50	117.20
2	H	142	THR	CA-C-N	-5.13	105.91	117.20
2	H	78	LYS	CA-C-N	-5.12	105.94	117.20
2	H	187	THR	N-CA-C	-5.11	97.21	111.00
1	L	218	GLU	CA-C-O	5.09	130.80	120.10
2	H	5	ASP	CA-CB-CG	-5.08	102.23	113.40
1	L	160	ARG	CB-CG-CD	5.07	124.79	111.60
1	L	159	GLU	CB-CA-C	5.03	120.47	110.40
1	L	145	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	H	91	GLU	CA-CB-CG	5.03	124.46	113.40
2	H	42	GLU	CG-CD-OE2	-5.02	108.26	118.30
2	H	107	TYR	CB-CA-C	5.01	120.41	110.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	L	193	ARG	Sidechain
1	L	39	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	1700	0	1641	375	2
2	H	1662	0	1597	671	3
3	H	25	0	10	12	0
4	H	8	0	14	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	3395	0	3262	1019	4

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 153.

All (1019) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:31:ASP:HA	2:H:53:ASN:ND2	1.41	1.32
1:L:214:PHE:HB2	2:H:133:CYS:SG	1.75	1.27
1:L:190:GLU:HA	1:L:193:ARG:NH2	1.47	1.27
2:H:51:ILE:HD11	2:H:72:ILE:CD1	1.68	1.24
2:H:105:MET:HG3	2:H:106:ASP:N	1.45	1.20
2:H:38:ARG:NH1	2:H:96:TYR:OH	1.72	1.20
2:H:137:THR:O	2:H:141:VAL:HG22	1.41	1.18
2:H:62:TYR:CE1	2:H:71:THR:HA	1.79	1.18
1:L:193:ARG:CZ	1:L:193:ARG:HB2	1.67	1.18
2:H:153:GLU:OE2	2:H:180:TYR:CZ	1.99	1.15
2:H:19:LYS:O	2:H:19:LYS:HG3	1.46	1.15
2:H:124:PRO:HB3	2:H:150:TYR:HB3	1.27	1.14
2:H:131:PRO:HD3	2:H:143:LEU:HD23	1.19	1.14
2:H:20:LEU:HD13	2:H:85:MET:CE	1.78	1.14
2:H:69:ARG:HB3	2:H:87:ASN:ND2	1.63	1.13
1:L:174:LYS:HG3	1:L:175:ASP:H	0.98	1.11
2:H:157:LEU:HD12	2:H:158:THR:N	1.65	1.10
2:H:39:GLN:HB3	2:H:45:LEU:HD23	1.29	1.10
1:L:146:PRO:HG2	1:L:204:LYS:HG3	1.29	1.09
2:H:205:PRO:O	2:H:207:SER:N	1.86	1.08
2:H:131:PRO:HD3	2:H:143:LEU:CD2	1.82	1.08
1:L:144:PHE:CE1	1:L:149:ILE:HD11	1.88	1.08
2:H:51:ILE:CG1	2:H:72:ILE:HG13	1.83	1.07
2:H:161:SER:HB3	2:H:197:SER:OG	1.54	1.07
1:L:174:LYS:CG	1:L:175:ASP:H	1.64	1.07
1:L:149:ILE:HG22	1:L:150:ASN:H	1.13	1.07
2:H:160:ASN:HB3	2:H:199:THR:OG1	1.54	1.06
2:H:86:ASN:O	2:H:87:ASN:HB3	1.48	1.06
2:H:206:ALA:O	2:H:207:SER:HB3	1.52	1.05
2:H:106:ASP:HB2	4:H:219:MPD:HM3	1.37	1.05
2:H:51:ILE:HD11	2:H:72:ILE:HD12	1.38	1.05
1:L:155:ILE:H	1:L:159:GLU:HB2	1.17	1.05
1:L:122:ILE:HG22	1:L:212:LYS:HG3	1.37	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:157:LEU:CD1	2:H:158:THR:H	1.69	1.04
1:L:190:GLU:HA	1:L:193:ARG:HH21	1.02	1.04
2:H:158:THR:HG22	2:H:201:ASN:HB2	1.40	1.03
2:H:29:PHE:CG	2:H:79:SER:HB2	1.93	1.03
2:H:29:PHE:CD1	2:H:79:SER:HB2	1.94	1.03
2:H:105:MET:CG	2:H:106:ASP:H	1.71	1.03
1:L:194:HIS:O	1:L:216:ARG:HD3	1.58	1.03
2:H:143:LEU:HD22	2:H:215:ILE:HG21	1.36	1.02
1:L:2:VAL:HG22	1:L:26:SER:HB3	1.39	1.02
2:H:189:THR:O	2:H:194:PRO:HD3	1.58	1.02
1:L:32:SER:O	1:L:35:ASN:ND2	1.92	1.02
1:L:52:LEU:HA	1:L:63:VAL:HG21	1.35	1.02
2:H:197:SER:O	2:H:198:ILE:HB	1.53	1.02
2:H:87:ASN:O	2:H:89:ARG:NH1	1.93	1.02
2:H:161:SER:HB2	2:H:198:ILE:HA	1.42	1.02
2:H:69:ARG:CB	2:H:87:ASN:HD21	1.73	1.01
2:H:90:VAL:HA	2:H:116:VAL:HG11	1.43	1.01
2:H:40:SER:HB2	2:H:43:LYS:HG3	1.43	1.00
2:H:51:ILE:HD11	2:H:72:ILE:CG1	1.91	1.00
2:H:106:ASP:CB	4:H:219:MPD:HM3	1.92	0.99
2:H:164:LEU:HB2	2:H:193:TRP:CZ2	1.97	0.99
2:H:62:TYR:CZ	2:H:72:ILE:HG22	1.98	0.98
2:H:20:LEU:HD13	2:H:85:MET:HE3	1.39	0.98
1:L:120:VAL:HG11	1:L:212:LYS:HB2	1.46	0.98
2:H:64:ASP:HA	2:H:67:LYS:HD3	1.46	0.98
2:H:137:THR:HA	2:H:141:VAL:HG13	1.45	0.97
2:H:169:HIS:NE2	2:H:185:SER:OG	1.94	0.97
1:L:219:CYS:OXT	2:H:133:CYS:HB3	1.64	0.97
2:H:124:PRO:CB	2:H:150:TYR:HB3	1.94	0.97
2:H:162:GLY:HA2	2:H:197:SER:H	1.30	0.97
1:L:197:TYR:HB2	1:L:214:PHE:CE2	2.00	0.97
2:H:190:SER:C	2:H:194:PRO:HG2	1.84	0.96
2:H:158:THR:CG2	2:H:201:ASN:HB2	1.94	0.96
2:H:160:ASN:O	2:H:198:ILE:HA	1.64	0.96
2:H:157:LEU:HD12	2:H:158:THR:H	0.82	0.96
2:H:159:TRP:CE3	2:H:198:ILE:HD11	1.99	0.96
1:L:174:LYS:HD2	1:L:175:ASP:HB3	1.46	0.95
1:L:31:HIS:HB2	1:L:97:THR:HG23	1.47	0.95
2:H:64:ASP:CA	2:H:67:LYS:HD3	1.95	0.95
1:L:42:LEU:HD21	1:L:44:LYS:HZ3	1.29	0.95
2:H:45:LEU:HD13	2:H:108:TRP:CH2	2.02	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:51:ILE:HG23	2:H:60:THR:HG22	1.47	0.94
2:H:31:ASP:CA	2:H:53:ASN:ND2	2.29	0.94
1:L:215:ASN:O	1:L:218:GLU:N	2.01	0.94
2:H:61:TYR:OH	2:H:67:LYS:HE3	1.66	0.94
2:H:191:SER:HA	2:H:194:PRO:HB2	1.45	0.94
2:H:20:LEU:HD13	2:H:85:MET:SD	2.08	0.94
2:H:31:ASP:HA	2:H:53:ASN:HD22	1.32	0.93
2:H:164:LEU:HD12	2:H:165:SER:N	1.82	0.93
2:H:162:GLY:O	2:H:163:SER:HB2	1.68	0.93
2:H:40:SER:HB2	2:H:43:LYS:CG	1.99	0.93
2:H:23:VAL:HG22	2:H:80:SER:HB3	1.51	0.93
2:H:51:ILE:CD1	2:H:72:ILE:HG13	2.00	0.92
2:H:90:VAL:HG12	2:H:116:VAL:HG22	1.52	0.92
2:H:136:THR:OG1	2:H:140:SER:OG	1.85	0.92
2:H:41:PRO:HD2	2:H:94:GLY:HA2	1.51	0.92
2:H:62:TYR:HE1	2:H:71:THR:HA	1.29	0.92
1:L:215:ASN:H	1:L:219:CYS:HB3	1.32	0.92
2:H:54:LYS:HB2	2:H:55:PRO:HD3	1.52	0.92
1:L:174:LYS:HG3	1:L:175:ASP:N	1.80	0.91
2:H:214:LYS:NZ	2:H:214:LYS:HB3	1.83	0.91
2:H:17:PRO:O	2:H:85:MET:C	2.08	0.91
2:H:191:SER:C	2:H:194:PRO:HD2	1.91	0.91
1:L:198:THR:HB	1:L:213:SER:OG	1.71	0.91
1:L:195:ASN:HA	1:L:216:ARG:HB2	1.53	0.91
2:H:92:ASP:O	2:H:96:TYR:OH	1.89	0.90
2:H:16:ARG:N	2:H:17:PRO:HD3	1.86	0.90
2:H:19:LYS:O	2:H:19:LYS:CG	2.17	0.90
2:H:5:ASP:C	2:H:5:ASP:OD2	2.10	0.90
1:L:41:TYR:HE2	1:L:51:VAL:HG12	1.37	0.90
1:L:193:ARG:CB	1:L:193:ARG:CZ	2.50	0.90
2:H:12:VAL:O	2:H:116:VAL:HG23	1.72	0.90
2:H:171:PHE:N	2:H:171:PHE:CD1	2.34	0.90
2:H:40:SER:HA	2:H:94:GLY:HA3	1.54	0.90
1:L:124:PRO:HD2	2:H:132:VAL:HG11	1.54	0.90
1:L:174:LYS:CG	1:L:175:ASP:N	2.35	0.89
2:H:77:SER:O	2:H:79:SER:OG	1.91	0.89
2:H:85:MET:O	2:H:88:LEU:HG	1.73	0.89
2:H:130:ALA:O	2:H:132:VAL:HG12	1.73	0.89
2:H:40:SER:O	2:H:43:LYS:HB2	1.72	0.89
2:H:51:ILE:HD11	2:H:72:ILE:HG13	1.54	0.89
2:H:161:SER:HB2	2:H:198:ILE:CA	2.01	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:163:SER:O	2:H:193:TRP:CZ2	2.26	0.89
1:L:41:TYR:CE2	1:L:51:VAL:HG12	2.07	0.88
2:H:16:ARG:H	2:H:17:PRO:HD3	1.35	0.88
2:H:203:ALA:HA	2:H:210:LYS:HA	1.56	0.88
2:H:17:PRO:HA	2:H:86:ASN:HA	1.56	0.88
2:H:29:PHE:HB2	2:H:79:SER:OG	1.71	0.88
2:H:31:ASP:HA	2:H:53:ASN:HD21	1.14	0.88
2:H:40:SER:HA	2:H:94:GLY:CA	2.04	0.88
2:H:69:ARG:HB3	2:H:87:ASN:HD21	1.29	0.88
1:L:203:HIS:CE1	1:L:204:LYS:HG2	2.07	0.88
2:H:200:CYS:C	2:H:201:ASN:HD22	1.76	0.88
2:H:108:TRP:HE1	4:H:219:MPD:H31	1.39	0.87
1:L:214:PHE:CB	2:H:133:CYS:SG	2.62	0.87
1:L:149:ILE:HG22	1:L:150:ASN:N	1.89	0.87
1:L:215:ASN:CB	1:L:218:GLU:O	2.22	0.87
1:L:29:LEU:HD13	1:L:95:GLN:HB2	1.54	0.87
2:H:61:TYR:CZ	2:H:67:LYS:HE3	2.10	0.87
2:H:171:PHE:N	2:H:171:PHE:HD1	1.69	0.86
2:H:85:MET:HB2	2:H:88:LEU:HD21	1.56	0.86
1:L:6:GLN:HE21	1:L:21:ILE:HD11	1.40	0.86
2:H:198:ILE:HD13	2:H:199:THR:N	1.90	0.86
2:H:176:GLN:HG2	2:H:177:SER:OG	1.73	0.86
1:L:120:VAL:CG1	1:L:212:LYS:HB2	2.06	0.86
2:H:159:TRP:HE3	2:H:198:ILE:HD11	1.41	0.85
2:H:182:LEU:HG	2:H:183:SER:N	1.90	0.85
1:L:144:PHE:CE1	1:L:149:ILE:CD1	2.59	0.85
1:L:144:PHE:CD1	1:L:149:ILE:HD11	2.11	0.85
2:H:158:THR:HG22	2:H:201:ASN:CB	2.05	0.85
1:L:146:PRO:HG2	1:L:204:LYS:CG	2.07	0.85
2:H:69:ARG:CA	2:H:87:ASN:HD21	1.90	0.84
2:H:193:TRP:N	2:H:194:PRO:CD	2.41	0.84
2:H:199:THR:HG22	2:H:214:LYS:HG3	1.56	0.84
1:L:52:LEU:HA	1:L:63:VAL:CG2	2.08	0.84
2:H:62:TYR:OH	2:H:71:THR:HB	1.76	0.84
1:L:190:GLU:CA	1:L:193:ARG:NH2	2.39	0.84
2:H:39:GLN:HB2	2:H:44:GLY:C	1.96	0.83
2:H:64:ASP:N	2:H:67:LYS:HD3	1.93	0.83
1:L:29:LEU:HD13	1:L:95:GLN:CB	2.07	0.83
1:L:120:VAL:CG2	1:L:141:LEU:HD23	2.07	0.83
1:L:59:ARG:HG2	1:L:59:ARG:HH11	1.44	0.83
2:H:164:LEU:HB2	2:H:193:TRP:HZ2	1.39	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:81:SER:O	1:L:82:ARG:HB3	1.79	0.83
2:H:17:PRO:HG2	2:H:88:LEU:HD12	1.59	0.83
2:H:190:SER:OG	2:H:191:SER:N	2.02	0.83
2:H:38:ARG:HG2	2:H:96:TYR:CE2	2.14	0.83
1:L:146:PRO:CG	1:L:204:LYS:HG3	2.08	0.83
1:L:142:ASN:OD1	2:H:169:HIS:NE2	2.12	0.82
1:L:218:GLU:N	1:L:218:GLU:OE1	2.12	0.82
1:L:168:TRP:HE1	1:L:180:MET:HE3	1.44	0.82
2:H:164:LEU:HD12	2:H:165:SER:H	1.41	0.82
2:H:20:LEU:HD22	2:H:85:MET:HE1	1.59	0.82
2:H:191:SER:HA	2:H:194:PRO:CB	2.09	0.82
2:H:51:ILE:HG12	2:H:72:ILE:HG23	1.61	0.82
1:L:165:LEU:HD21	2:H:174:VAL:CG1	2.09	0.82
1:L:7:THR:O	1:L:22:SER:HB2	1.80	0.82
2:H:45:LEU:HD13	2:H:108:TRP:HH2	1.40	0.81
1:L:17:ASP:O	1:L:82:ARG:HA	1.78	0.81
2:H:127:TYR:HD2	2:H:146:LEU:CD2	1.94	0.81
2:H:29:PHE:CG	2:H:79:SER:CB	2.63	0.81
2:H:6:GLU:HB2	2:H:112:THR:HB	1.61	0.81
1:L:94:SER:HA	1:L:102:THR:O	1.81	0.81
2:H:70:PHE:CZ	2:H:85:MET:HB3	2.15	0.81
2:H:106:ASP:HB2	4:H:219:MPD:CM	2.11	0.81
2:H:22:CYS:HB2	2:H:36:TRP:CH2	2.16	0.81
2:H:90:VAL:HG12	2:H:116:VAL:CG2	2.10	0.80
1:L:206:SER:OG	1:L:208:SER:O	1.98	0.80
2:H:136:THR:HG23	2:H:140:SER:O	1.80	0.80
2:H:12:VAL:HG11	2:H:17:PRO:HG2	1.61	0.80
2:H:120:LYS:CD	2:H:120:LYS:H	1.94	0.80
2:H:191:SER:N	2:H:194:PRO:HG2	1.97	0.80
1:L:124:PRO:HB3	1:L:214:PHE:CE1	2.17	0.80
1:L:42:LEU:HD21	1:L:44:LYS:NZ	1.96	0.79
2:H:126:VAL:HG22	2:H:147:VAL:HB	1.65	0.79
2:H:189:THR:O	2:H:194:PRO:CD	2.30	0.79
2:H:171:PHE:H	2:H:171:PHE:HD1	1.28	0.79
2:H:162:GLY:C	2:H:196:GLN:HE21	1.86	0.79
2:H:62:TYR:CE1	2:H:71:THR:CA	2.64	0.79
2:H:124:PRO:HB3	2:H:150:TYR:CB	2.09	0.79
1:L:149:ILE:CG2	1:L:150:ASN:H	1.92	0.79
1:L:88:LEU:HD12	1:L:172:ASP:OD1	1.83	0.79
2:H:100:GLY:O	2:H:106:ASP:HB2	1.83	0.78
2:H:39:GLN:HB2	2:H:44:GLY:O	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:VAL:HG12	1:L:4:MET:HG2	1.65	0.78
2:H:99:THR:HB	4:H:219:MPD:CM	2.14	0.78
2:H:28:THR:O	2:H:29:PHE:C	2.21	0.78
2:H:14:PRO:HG3	2:H:90:VAL:CG1	2.13	0.78
1:L:18:GLN:HG3	1:L:80:ILE:O	1.83	0.78
2:H:5:ASP:OD2	2:H:6:GLU:N	2.16	0.78
2:H:61:TYR:CD1	2:H:62:TYR:N	2.51	0.78
1:L:155:ILE:N	1:L:159:GLU:HB2	1.97	0.78
2:H:86:ASN:O	2:H:87:ASN:CB	2.28	0.78
1:L:215:ASN:HB2	1:L:218:GLU:O	1.84	0.78
2:H:27:PHE:HZ	2:H:34:MET:CE	1.97	0.78
2:H:103:TYR:CD1	3:H:218:FLU:H18	2.19	0.78
1:L:1:ASP:CG	1:L:100:PRO:HG3	2.05	0.77
1:L:141:LEU:HD12	1:L:180:MET:HB3	1.65	0.77
2:H:120:LYS:CD	2:H:120:LYS:N	2.46	0.77
2:H:90:VAL:HA	2:H:116:VAL:CG1	2.15	0.77
2:H:120:LYS:O	2:H:120:LYS:HD3	1.85	0.77
2:H:205:PRO:C	2:H:207:SER:H	1.88	0.77
2:H:153:GLU:OE2	2:H:180:TYR:CE2	2.38	0.77
1:L:166:ASN:OD1	1:L:182:SER:HB2	1.84	0.77
1:L:120:VAL:HG23	1:L:141:LEU:HD23	1.66	0.76
1:L:161:GLN:CD	1:L:162:ASN:H	1.89	0.76
2:H:27:PHE:HZ	2:H:34:MET:HE1	1.49	0.76
2:H:211:VAL:HG23	2:H:212:ASP:N	2.00	0.76
2:H:106:ASP:CG	4:H:219:MPD:HM3	2.06	0.76
2:H:31:ASP:C	2:H:53:ASN:ND2	2.39	0.76
2:H:51:ILE:HG12	2:H:72:ILE:CG2	2.15	0.76
1:L:129:GLN:HG2	1:L:134:GLY:O	1.85	0.76
2:H:39:GLN:O	2:H:39:GLN:HG2	1.85	0.76
2:H:43:LYS:NZ	2:H:91:GLU:OE1	2.19	0.76
1:L:147:LYS:O	1:L:149:ILE:CD1	2.34	0.76
2:H:105:MET:CG	2:H:106:ASP:N	2.33	0.75
1:L:174:LYS:HD2	1:L:175:ASP:CB	2.16	0.75
2:H:188:VAL:HG22	2:H:193:TRP:HD1	1.51	0.75
2:H:62:TYR:O	2:H:67:LYS:HD2	1.86	0.75
1:L:130:LEU:HD22	1:L:188:LYS:HG3	1.69	0.75
1:L:149:ILE:N	1:L:149:ILE:HD12	1.99	0.75
1:L:6:GLN:NE2	1:L:21:ILE:HD11	2.02	0.75
1:L:217:ASN:HB3	1:L:218:GLU:OE1	1.86	0.75
2:H:193:TRP:N	2:H:194:PRO:HD2	2.02	0.75
2:H:17:PRO:CA	2:H:86:ASN:HA	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:190:SER:O	2:H:194:PRO:HG2	1.86	0.75
1:L:215:ASN:HB3	1:L:218:GLU:O	1.87	0.75
2:H:64:ASP:OD1	2:H:64:ASP:N	2.15	0.74
1:L:33:GLN:HA	1:L:35:ASN:HD21	1.53	0.74
2:H:49:ALA:HB1	2:H:72:ILE:HB	1.70	0.74
2:H:120:LYS:HD2	2:H:120:LYS:N	2.02	0.74
1:L:149:ILE:CD1	1:L:149:ILE:N	2.50	0.74
1:L:33:GLN:CA	1:L:35:ASN:HD21	2.01	0.74
1:L:96:SER:HB3	3:H:218:FLU:O3	1.88	0.74
1:L:96:SER:CB	3:H:218:FLU:O3	2.36	0.73
1:L:53:ILE:CG2	1:L:56:VAL:O	2.37	0.73
1:L:11:LEU:HD23	1:L:109:LEU:HD11	1.70	0.73
1:L:160:ARG:O	1:L:161:GLN:O	2.06	0.73
2:H:120:LYS:H	2:H:120:LYS:HD3	1.52	0.73
2:H:155:VAL:HG23	2:H:156:THR:N	2.01	0.73
2:H:203:ALA:HB2	2:H:210:LYS:HB2	1.69	0.73
2:H:54:LYS:HG2	2:H:58:TYR:OH	1.87	0.73
2:H:85:MET:CB	2:H:88:LEU:HD21	2.18	0.73
1:L:154:LYS:O	1:L:198:THR:HG23	1.88	0.73
2:H:17:PRO:O	2:H:85:MET:O	2.07	0.73
1:L:37:TYR:HB2	1:L:97:THR:OG1	1.88	0.73
2:H:127:TYR:HD2	2:H:146:LEU:HD22	1.52	0.73
2:H:150:TYR:CZ	2:H:155:VAL:CG1	2.71	0.73
2:H:90:VAL:HG12	2:H:116:VAL:HG13	1.71	0.73
2:H:14:PRO:HG3	2:H:90:VAL:HG11	1.69	0.72
2:H:86:ASN:ND2	2:H:86:ASN:O	2.22	0.72
1:L:161:GLN:OE1	1:L:162:ASN:N	2.20	0.72
4:H:219:MPD:O2	4:H:219:MPD:H52	1.90	0.72
2:H:27:PHE:CZ	2:H:34:MET:HE1	2.23	0.72
2:H:61:TYR:CE1	2:H:62:TYR:C	2.62	0.72
2:H:63:SER:O	2:H:67:LYS:N	2.21	0.72
1:L:124:PRO:CD	2:H:132:VAL:HG11	2.19	0.72
1:L:100:PRO:O	2:H:47:TRP:CE3	2.41	0.72
2:H:69:ARG:CB	2:H:87:ASN:ND2	2.37	0.72
1:L:148:ASP:C	1:L:149:ILE:HD12	2.09	0.72
2:H:163:SER:O	2:H:193:TRP:HZ2	1.71	0.72
2:H:69:ARG:C	2:H:87:ASN:HD21	1.91	0.72
1:L:51:VAL:HG21	2:H:105:MET:HE2	1.72	0.72
1:L:1:ASP:HA	1:L:100:PRO:CD	2.17	0.72
2:H:71:THR:O	2:H:84:GLN:NE2	2.23	0.72
2:H:64:ASP:O	2:H:66:VAL:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:142:THR:HA	2:H:186:VAL:O	1.90	0.71
1:L:193:ARG:NH1	1:L:193:ARG:HB2	2.03	0.71
2:H:207:SER:OG	2:H:208:SER:N	2.23	0.71
1:L:165:LEU:CD2	2:H:174:VAL:CG1	2.69	0.71
2:H:124:PRO:HA	2:H:148:LYS:O	1.90	0.71
1:L:38:LEU:C	1:L:38:LEU:HD12	2.11	0.71
1:L:55:LYS:HD3	2:H:104:GLY:HA3	1.72	0.71
2:H:207:SER:O	2:H:208:SER:C	2.29	0.71
2:H:36:TRP:CD1	2:H:72:ILE:HD13	2.24	0.71
1:L:65:ASP:OD2	1:L:65:ASP:O	2.08	0.71
1:L:4:MET:CE	1:L:95:GLN:HB3	2.21	0.71
2:H:93:MET:HE2	2:H:115:THR:CG2	2.19	0.70
2:H:153:GLU:CB	2:H:154:PRO:HD3	2.21	0.70
2:H:93:MET:HG3	2:H:115:THR:HA	1.71	0.70
2:H:40:SER:OG	2:H:93:MET:O	2.08	0.70
2:H:29:PHE:CB	2:H:79:SER:CB	2.69	0.70
1:L:19:ALA:O	1:L:79:LYS:HA	1.91	0.70
2:H:168:VAL:HA	2:H:185:SER:O	1.91	0.70
1:L:161:GLN:CG	1:L:162:ASN:N	2.53	0.70
1:L:120:VAL:CG1	1:L:212:LYS:HG2	2.21	0.70
2:H:24:ALA:HB1	2:H:27:PHE:CZ	2.27	0.70
1:L:161:GLN:HG3	1:L:162:ASN:N	2.06	0.70
2:H:51:ILE:HG23	2:H:60:THR:CG2	2.20	0.70
2:H:128:PRO:HG2	2:H:128:PRO:O	1.92	0.70
2:H:153:GLU:HB3	2:H:154:PRO:HD3	1.72	0.70
2:H:164:LEU:N	2:H:193:TRP:HE1	1.87	0.70
2:H:37:VAL:HG13	2:H:46:GLU:O	1.92	0.70
1:L:4:MET:HE1	1:L:95:GLN:HB3	1.72	0.69
1:L:29:LEU:CD1	1:L:95:GLN:HB3	2.22	0.69
2:H:103:TYR:H	3:H:218:FLU:C17	2.04	0.69
2:H:3:LYS:C	2:H:4:LEU:HD12	2.13	0.69
2:H:71:THR:C	2:H:83:LEU:HD12	2.12	0.69
1:L:84:GLU:O	1:L:87:ASP:HB2	1.92	0.69
1:L:29:LEU:CD1	1:L:95:GLN:CB	2.70	0.69
1:L:67:PHE:CZ	1:L:87:ASP:OD1	2.45	0.69
2:H:153:GLU:OE2	2:H:180:TYR:OH	2.11	0.69
1:L:129:GLN:O	1:L:132:SER:HB2	1.93	0.69
2:H:6:GLU:HG3	2:H:111:GLY:HA2	1.72	0.69
2:H:164:LEU:CD1	2:H:165:SER:H	2.04	0.69
2:H:169:HIS:O	2:H:171:PHE:HE1	1.76	0.69
2:H:35:ASN:ND2	2:H:99:THR:OG1	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:152:LYS:HZ3	1:L:154:LYS:HE2	1.58	0.69
2:H:106:ASP:OD1	4:H:219:MPD:HM3	1.93	0.69
2:H:11:LEU:O	2:H:12:VAL:HG23	1.92	0.69
2:H:23:VAL:HG22	2:H:80:SER:CB	2.22	0.69
2:H:3:LYS:O	2:H:24:ALA:HA	1.93	0.69
2:H:62:TYR:CZ	2:H:71:THR:HB	2.28	0.69
2:H:124:PRO:CA	2:H:150:TYR:HB3	2.22	0.68
2:H:12:VAL:HG11	2:H:17:PRO:CG	2.23	0.68
2:H:214:LYS:HB3	2:H:214:LYS:HZ3	1.56	0.68
1:L:193:ARG:O	1:L:193:ARG:CG	2.40	0.68
2:H:32:TYR:CD2	2:H:101:SER:O	2.46	0.68
2:H:178:ASP:O	2:H:178:ASP:OD1	2.11	0.68
1:L:51:VAL:HG21	2:H:105:MET:CE	2.23	0.68
2:H:191:SER:CA	2:H:194:PRO:HG2	2.24	0.68
1:L:59:ARG:HD3	1:L:63:VAL:CG1	2.22	0.68
2:H:162:GLY:CA	2:H:197:SER:H	2.04	0.68
2:H:51:ILE:HG12	2:H:72:ILE:HG13	1.75	0.68
1:L:115:ASP:OD2	1:L:175:ASP:O	2.11	0.68
1:L:120:VAL:HG12	1:L:212:LYS:HG2	1.74	0.68
2:H:163:SER:C	2:H:193:TRP:CZ2	2.67	0.68
2:H:205:PRO:C	2:H:207:SER:N	2.45	0.68
1:L:100:PRO:O	1:L:101:TRP:HB2	1.92	0.67
1:L:122:ILE:HG13	1:L:123:PHE:N	2.09	0.67
2:H:6:GLU:N	2:H:6:GLU:OE2	2.27	0.67
1:L:122:ILE:HG13	1:L:123:PHE:H	1.58	0.67
2:H:136:THR:C	2:H:140:SER:O	2.33	0.67
2:H:199:THR:HG22	2:H:214:LYS:CG	2.24	0.67
2:H:6:GLU:CG	2:H:111:GLY:HA2	2.23	0.67
2:H:77:SER:C	2:H:79:SER:N	2.45	0.67
2:H:105:MET:HG3	2:H:106:ASP:H	0.75	0.67
2:H:93:MET:HE2	2:H:115:THR:HA	1.75	0.67
2:H:17:PRO:CG	2:H:88:LEU:HD12	2.24	0.67
2:H:51:ILE:HG13	2:H:72:ILE:HG13	1.72	0.67
1:L:32:SER:C	1:L:35:ASN:ND2	2.48	0.67
1:L:52:LEU:CA	1:L:63:VAL:HG21	2.17	0.67
2:H:160:ASN:O	2:H:198:ILE:HG12	1.95	0.66
2:H:24:ALA:HB1	2:H:27:PHE:CE2	2.30	0.66
2:H:130:ALA:O	2:H:132:VAL:CG1	2.43	0.66
1:L:39:ARG:NH2	1:L:96:SER:OG	2.28	0.66
2:H:13:GLN:C	2:H:14:PRO:O	2.30	0.66
1:L:190:GLU:HA	1:L:193:ARG:HH22	1.58	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:191:TYR:CE1	1:L:216:ARG:HG3	2.31	0.66
1:L:60:PHE:CE1	1:L:61:SER:HB3	2.30	0.66
2:H:20:LEU:CD1	2:H:85:MET:SD	2.83	0.66
2:H:93:MET:HE2	2:H:115:THR:HG23	1.76	0.66
2:H:90:VAL:HG12	2:H:116:VAL:CG1	2.25	0.66
2:H:93:MET:CE	2:H:116:VAL:H	2.08	0.66
1:L:193:ARG:NH2	1:L:193:ARG:HB2	2.09	0.66
2:H:11:LEU:HD21	2:H:151:PHE:HZ	1.60	0.66
1:L:11:LEU:HD21	1:L:19:ALA:HB2	1.78	0.66
2:H:40:SER:N	2:H:43:LYS:HB2	2.10	0.66
2:H:169:HIS:CD2	2:H:185:SER:OG	2.49	0.65
1:L:165:LEU:HD21	2:H:174:VAL:HG12	1.77	0.65
2:H:191:SER:CA	2:H:194:PRO:CG	2.74	0.65
2:H:3:LYS:O	2:H:4:LEU:HD12	1.95	0.65
2:H:61:TYR:CE1	2:H:63:SER:HA	2.31	0.65
2:H:62:TYR:CE1	2:H:72:ILE:N	2.62	0.65
2:H:135:ASP:O	2:H:136:THR:C	2.35	0.65
1:L:113:ARG:NH1	1:L:175:ASP:HA	2.12	0.65
2:H:212:ASP:O	2:H:213:LYS:HG2	1.96	0.65
2:H:93:MET:HE3	2:H:116:VAL:H	1.61	0.65
1:L:38:LEU:HD12	1:L:39:ARG:N	2.11	0.65
2:H:151:PHE:CE2	2:H:152:PRO:HB3	2.32	0.65
2:H:27:PHE:CZ	2:H:34:MET:CE	2.79	0.65
2:H:39:GLN:HB3	2:H:45:LEU:CD2	2.18	0.65
2:H:40:SER:HA	2:H:94:GLY:HA2	1.78	0.65
2:H:146:LEU:HD21	2:H:148:LYS:HE3	1.77	0.65
2:H:147:VAL:O	2:H:147:VAL:HG22	1.96	0.65
2:H:164:LEU:N	2:H:193:TRP:NE1	2.45	0.65
2:H:191:SER:HA	2:H:194:PRO:CG	2.27	0.65
2:H:209:THR:HG23	2:H:210:LYS:N	2.11	0.65
2:H:62:TYR:HE1	2:H:71:THR:CA	2.04	0.65
2:H:162:GLY:C	2:H:196:GLN:NE2	2.50	0.65
2:H:36:TRP:O	2:H:48:VAL:HB	1.97	0.64
2:H:40:SER:C	2:H:43:LYS:HB2	2.16	0.64
2:H:70:PHE:O	2:H:71:THR:CG2	2.45	0.64
2:H:62:TYR:OH	2:H:72:ILE:N	2.30	0.64
2:H:40:SER:CB	2:H:93:MET:O	2.46	0.64
1:L:24:ARG:HE	1:L:24:ARG:C	2.01	0.64
2:H:20:LEU:CD1	2:H:85:MET:CE	2.67	0.64
1:L:65:ASP:C	1:L:67:PHE:H	2.00	0.64
2:H:136:THR:CG2	2:H:137:THR:N	2.59	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:158:THR:CG2	2:H:201:ASN:CB	2.69	0.64
2:H:203:ALA:HB2	2:H:210:LYS:HE3	1.80	0.64
1:L:103:PHE:N	1:L:103:PHE:CD1	2.65	0.64
1:L:155:ILE:HG23	1:L:197:TYR:CE1	2.32	0.64
1:L:33:GLN:C	1:L:35:ASN:H	2.01	0.64
2:H:203:ALA:CB	2:H:210:LYS:HB2	2.26	0.64
2:H:22:CYS:HB2	2:H:36:TRP:CZ2	2.33	0.64
2:H:122:THR:HG22	2:H:123:ALA:H	1.62	0.64
2:H:161:SER:HB3	2:H:197:SER:HG	1.62	0.64
2:H:169:HIS:O	2:H:171:PHE:CE1	2.51	0.64
2:H:214:LYS:NZ	2:H:214:LYS:CB	2.61	0.64
1:L:8:PRO:HG2	1:L:10:SER:O	1.97	0.64
2:H:211:VAL:CG2	2:H:212:ASP:N	2.60	0.63
1:L:161:GLN:CG	1:L:162:ASN:H	2.12	0.63
2:H:28:THR:O	2:H:30:SER:N	2.32	0.63
1:L:124:PRO:CD	2:H:132:VAL:CG1	2.77	0.63
1:L:155:ILE:HB	1:L:159:GLU:HG3	1.79	0.63
2:H:70:PHE:CE2	2:H:85:MET:HG2	2.33	0.63
1:L:141:LEU:CD1	1:L:180:MET:HB3	2.29	0.63
1:L:204:LYS:N	1:L:204:LYS:HD2	2.12	0.63
2:H:164:LEU:CD1	2:H:165:SER:N	2.60	0.63
1:L:120:VAL:HG12	1:L:212:LYS:CG	2.29	0.63
1:L:44:LYS:NZ	1:L:86:GLU:O	2.32	0.63
2:H:137:THR:CA	2:H:141:VAL:HG13	2.25	0.63
2:H:5:ASP:O	2:H:22:CYS:HA	1.98	0.63
2:H:52:ARG:O	2:H:74:ARG:NH2	2.32	0.63
2:H:103:TYR:H	3:H:218:FLU:C18	2.12	0.62
2:H:150:TYR:CE2	2:H:155:VAL:CG1	2.81	0.62
2:H:24:ALA:HB3	2:H:29:PHE:CE1	2.33	0.62
1:L:59:ARG:NH2	1:L:67:PHE:O	2.28	0.62
2:H:103:TYR:O	3:H:218:FLU:O4	2.18	0.62
2:H:35:ASN:HB2	2:H:49:ALA:O	1.99	0.62
2:H:48:VAL:HG12	2:H:49:ALA:N	2.14	0.62
2:H:162:GLY:N	2:H:197:SER:C	2.53	0.62
2:H:17:PRO:HD2	2:H:88:LEU:HD12	1.82	0.62
2:H:157:LEU:HD22	2:H:202:VAL:HG22	1.81	0.62
2:H:77:SER:O	2:H:79:SER:N	2.31	0.62
1:L:174:LYS:HZ1	1:L:175:ASP:CG	2.02	0.62
2:H:101:SER:O	2:H:102:TYR:HB2	1.99	0.62
2:H:164:LEU:CG	2:H:165:SER:H	2.13	0.62
1:L:10:SER:OG	1:L:11:LEU:N	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:136:SER:HA	1:L:184:LEU:O	2.00	0.62
1:L:53:ILE:HG21	1:L:56:VAL:O	2.00	0.62
2:H:147:VAL:O	2:H:147:VAL:CG2	2.46	0.62
2:H:155:VAL:CG2	2:H:156:THR:N	2.63	0.62
2:H:99:THR:HB	4:H:219:MPD:HM1	1.81	0.62
1:L:59:ARG:HD3	1:L:63:VAL:HG12	1.81	0.62
2:H:38:ARG:HG2	2:H:96:TYR:CD2	2.35	0.62
2:H:193:TRP:CE3	2:H:196:GLN:OE1	2.53	0.62
2:H:64:ASP:O	2:H:65:SER:C	2.38	0.62
2:H:13:GLN:O	2:H:14:PRO:O	2.17	0.61
1:L:113:ARG:HG3	1:L:176:SER:HB2	1.82	0.61
1:L:4:MET:HG3	1:L:102:THR:HB	1.82	0.61
2:H:22:CYS:CB	2:H:36:TRP:CZ2	2.83	0.61
2:H:40:SER:CA	2:H:43:LYS:HB2	2.29	0.61
2:H:93:MET:CE	2:H:115:THR:HG23	2.30	0.61
1:L:21:ILE:CG1	1:L:107:THR:HG21	2.31	0.61
1:L:21:ILE:HD13	1:L:22:SER:N	2.15	0.61
1:L:32:SER:C	1:L:35:ASN:HD21	2.01	0.61
2:H:201:ASN:HD22	2:H:201:ASN:N	1.97	0.61
1:L:215:ASN:N	1:L:219:CYS:HB3	2.09	0.61
1:L:52:LEU:HB2	1:L:53:ILE:HD12	1.82	0.61
2:H:117:SER:HB2	2:H:178:ASP:OD1	2.00	0.61
2:H:57:ASN:O	2:H:58:TYR:HB2	2.00	0.61
2:H:82:TYR:HB3	2:H:84:GLN:OE1	1.99	0.61
1:L:11:LEU:HD23	1:L:109:LEU:CD1	2.31	0.61
1:L:81:SER:O	1:L:82:ARG:CB	2.48	0.61
1:L:82:ARG:HG3	1:L:82:ARG:O	2.00	0.61
1:L:15:LEU:HD13	1:L:15:LEU:N	2.15	0.61
1:L:203:HIS:CG	1:L:204:LYS:N	2.67	0.61
2:H:21:SER:HA	2:H:82:TYR:CD1	2.35	0.61
2:H:61:TYR:OH	2:H:67:LYS:CE	2.45	0.61
2:H:64:ASP:N	2:H:67:LYS:CD	2.64	0.61
2:H:62:TYR:HE1	2:H:72:ILE:H	1.45	0.61
1:L:210:ILE:O	1:L:210:ILE:HG22	2.00	0.61
2:H:99:THR:CB	4:H:219:MPD:O2	2.49	0.61
2:H:61:TYR:HE1	2:H:63:SER:HA	1.66	0.61
2:H:75:ASP:O	2:H:79:SER:HA	2.01	0.61
2:H:204:HIS:CD2	2:H:206:ALA:HB3	2.35	0.61
1:L:3:VAL:N	1:L:26:SER:HB2	2.16	0.61
1:L:98:HIS:O	1:L:99:VAL:C	2.39	0.60
2:H:56:TYR:O	2:H:59:GLU:OE2	2.19	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:69:ARG:CA	2:H:87:ASN:ND2	2.62	0.60
1:L:91:TYR:CE2	1:L:109:LEU:HD23	2.36	0.60
1:L:164:VAL:HA	1:L:183:THR:O	2.01	0.60
1:L:161:GLN:HG3	1:L:163:GLY:N	2.17	0.60
2:H:206:ALA:O	2:H:207:SER:CB	2.35	0.60
1:L:38:LEU:HD23	1:L:76:PHE:CZ	2.36	0.60
2:H:152:PRO:HD2	2:H:206:ALA:HB1	1.84	0.60
2:H:62:TYR:HE1	2:H:72:ILE:N	2.00	0.60
2:H:160:ASN:O	2:H:198:ILE:CG1	2.49	0.60
2:H:93:MET:CE	2:H:115:THR:CG2	2.79	0.60
1:L:1:ASP:HA	1:L:100:PRO:HD3	1.84	0.60
1:L:95:GLN:O	1:L:101:TRP:HA	2.01	0.60
1:L:56:VAL:CG2	1:L:57:SER:N	2.65	0.60
1:L:122:ILE:CG2	1:L:212:LYS:HG3	2.23	0.60
1:L:78:LEU:HD22	1:L:79:LYS:N	2.17	0.60
2:H:17:PRO:CD	2:H:88:LEU:HD12	2.32	0.59
1:L:39:ARG:NH1	4:H:219:MPD:H32	2.16	0.59
1:L:6:GLN:OE1	1:L:92:PHE:HA	2.02	0.59
1:L:120:VAL:CG1	1:L:212:LYS:CB	2.78	0.59
2:H:31:ASP:CA	2:H:53:ASN:HD21	2.00	0.59
2:H:150:TYR:CE1	2:H:155:VAL:HG11	2.37	0.59
2:H:81:VAL:HG22	2:H:82:TYR:N	2.16	0.59
2:H:99:THR:HB	4:H:219:MPD:HM2	1.83	0.59
1:L:128:GLU:O	1:L:132:SER:OG	2.14	0.59
1:L:165:LEU:CD2	2:H:174:VAL:HG11	2.32	0.59
2:H:11:LEU:HD21	2:H:151:PHE:CZ	2.37	0.59
2:H:51:ILE:CG2	2:H:60:THR:HG22	2.28	0.59
1:L:21:ILE:HD13	1:L:21:ILE:C	2.23	0.59
2:H:90:VAL:CG1	2:H:116:VAL:HG22	2.28	0.59
2:H:143:LEU:HD22	2:H:215:ILE:CG2	2.24	0.59
2:H:66:VAL:O	2:H:67:LYS:O	2.21	0.59
1:L:161:GLN:HG3	1:L:163:GLY:H	1.67	0.59
1:L:168:TRP:HE1	1:L:180:MET:CE	2.15	0.59
1:L:200:GLU:HB2	1:L:211:VAL:HG12	1.83	0.59
1:L:15:LEU:HD22	1:L:15:LEU:H	1.68	0.59
1:L:116:ALA:HB1	1:L:143:ASN:O	2.03	0.59
2:H:87:ASN:O	2:H:89:ARG:CZ	2.50	0.58
1:L:120:VAL:CG1	1:L:212:LYS:CG	2.80	0.58
1:L:124:PRO:HD3	2:H:132:VAL:HG13	1.84	0.58
1:L:90:VAL:HG12	1:L:92:PHE:CE1	2.38	0.58
2:H:90:VAL:CG1	2:H:116:VAL:HG13	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:127:TYR:CD2	2:H:146:LEU:CD2	2.83	0.58
1:L:155:ILE:HG23	1:L:197:TYR:CD1	2.39	0.58
1:L:52:LEU:CB	1:L:53:ILE:HD12	2.33	0.58
2:H:161:SER:HB2	2:H:198:ILE:N	2.18	0.58
2:H:164:LEU:HB2	2:H:193:TRP:CE2	2.38	0.58
2:H:62:TYR:OH	2:H:72:ILE:O	2.20	0.58
2:H:40:SER:HB3	2:H:93:MET:O	2.04	0.58
2:H:31:ASP:CA	2:H:53:ASN:HD22	2.04	0.58
2:H:93:MET:HE2	2:H:115:THR:CA	2.34	0.58
2:H:5:ASP:OD2	2:H:6:GLU:C	2.42	0.58
2:H:162:GLY:HA2	2:H:197:SER:N	2.10	0.58
1:L:18:GLN:OE1	1:L:81:SER:HA	2.03	0.58
2:H:134:GLY:O	2:H:137:THR:CB	2.52	0.58
2:H:150:TYR:CZ	2:H:155:VAL:HG13	2.39	0.58
2:H:39:GLN:O	2:H:39:GLN:CG	2.50	0.58
1:L:193:ARG:O	1:L:193:ARG:HG3	2.04	0.58
1:L:59:ARG:CD	1:L:63:VAL:HG12	2.33	0.58
1:L:66:ARG:HD2	1:L:80:ILE:CG2	2.33	0.58
2:H:13:GLN:O	2:H:14:PRO:C	2.41	0.57
2:H:151:PHE:CD2	2:H:151:PHE:C	2.77	0.57
4:H:219:MPD:O2	4:H:219:MPD:C5	2.51	0.57
1:L:129:GLN:CG	1:L:134:GLY:O	2.52	0.57
1:L:29:LEU:HD11	1:L:95:GLN:HB3	1.86	0.57
2:H:191:SER:O	2:H:192:THR:C	2.40	0.57
2:H:70:PHE:CE1	2:H:85:MET:HB3	2.39	0.57
2:H:90:VAL:O	2:H:92:ASP:N	2.37	0.57
2:H:91:GLU:HG3	2:H:91:GLU:O	2.04	0.57
1:L:35:ASN:ND2	1:L:35:ASN:N	2.44	0.57
2:H:198:ILE:C	2:H:198:ILE:HD13	2.23	0.57
2:H:33:TRP:CE2	2:H:52:ARG:HD3	2.40	0.57
2:H:40:SER:OG	2:H:43:LYS:HE2	2.05	0.57
1:L:124:PRO:HD3	2:H:132:VAL:CG1	2.33	0.57
2:H:73:SER:O	2:H:81:VAL:HG23	2.04	0.57
1:L:189:ASP:C	1:L:193:ARG:HH22	2.08	0.57
2:H:136:THR:O	2:H:137:THR:C	2.44	0.57
2:H:108:TRP:CD1	4:H:219:MPD:HM1	2.40	0.57
2:H:6:GLU:CG	2:H:111:GLY:CA	2.83	0.57
2:H:17:PRO:O	2:H:86:ASN:N	2.37	0.57
2:H:99:THR:CB	4:H:219:MPD:HO2	2.17	0.57
2:H:45:LEU:HD21	2:H:97:TYR:HE1	1.70	0.57
1:L:203:HIS:CG	1:L:204:LYS:H	2.22	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:2:VAL:HG13	1:L:26:SER:HB2	1.86	0.57
2:H:106:ASP:CB	4:H:219:MPD:H11	2.34	0.57
2:H:64:ASP:CG	2:H:67:LYS:NZ	2.58	0.57
2:H:209:THR:CG2	2:H:210:LYS:N	2.67	0.56
2:H:29:PHE:HB2	2:H:79:SER:CB	2.34	0.56
2:H:33:TRP:CZ2	2:H:52:ARG:HD3	2.40	0.56
2:H:36:TRP:CD1	2:H:72:ILE:CD1	2.87	0.56
2:H:136:THR:CG2	2:H:137:THR:H	2.17	0.56
2:H:158:THR:HG22	2:H:201:ASN:O	2.04	0.56
2:H:197:SER:O	2:H:198:ILE:CB	2.40	0.56
2:H:33:TRP:CD1	2:H:50:GLN:OE1	2.59	0.56
1:L:161:GLN:HG2	1:L:184:LEU:HD11	1.87	0.56
1:L:59:ARG:NH1	1:L:59:ARG:HG2	2.18	0.56
2:H:90:VAL:CB	2:H:116:VAL:HG13	2.35	0.56
2:H:162:GLY:O	2:H:163:SER:CB	2.48	0.56
2:H:24:ALA:HB3	2:H:29:PHE:CD1	2.40	0.56
2:H:38:ARG:O	2:H:45:LEU:HA	2.05	0.56
1:L:31:HIS:CB	1:L:97:THR:HG23	2.29	0.56
1:L:136:SER:OG	2:H:148:LYS:NZ	2.38	0.56
1:L:147:LYS:HB3	1:L:178:TYR:CE2	2.40	0.56
1:L:154:LYS:HB3	1:L:198:THR:HG23	1.87	0.56
2:H:162:GLY:CA	2:H:197:SER:O	2.53	0.56
2:H:151:PHE:CD2	2:H:152:PRO:N	2.74	0.56
2:H:39:GLN:O	2:H:40:SER:C	2.44	0.56
1:L:21:ILE:HG12	1:L:107:THR:HG21	1.88	0.56
1:L:117:ALA:HB1	1:L:118:PRO:HD2	1.88	0.56
1:L:184:LEU:HD12	1:L:185:THR:H	1.69	0.56
2:H:189:THR:OG1	2:H:193:TRP:HB2	2.05	0.55
2:H:66:VAL:HB	2:H:70:PHE:HB2	1.88	0.55
2:H:121:THR:HG22	2:H:151:PHE:HE2	1.70	0.55
2:H:29:PHE:CB	2:H:79:SER:OG	2.48	0.55
1:L:49:PRO:HG2	2:H:45:LEU:HD11	1.87	0.55
2:H:136:THR:HG23	2:H:137:THR:N	2.21	0.55
2:H:83:LEU:HD23	2:H:85:MET:HE2	1.88	0.55
1:L:110:GLU:OE1	1:L:178:TYR:OH	2.11	0.55
1:L:11:LEU:HG	1:L:13:VAL:HG13	1.88	0.55
1:L:120:VAL:HG22	1:L:141:LEU:HD23	1.88	0.55
1:L:202:THR:HG23	1:L:209:PRO:HD3	1.87	0.55
1:L:30:VAL:HG22	1:L:36:THR:OG1	2.06	0.55
2:H:169:HIS:CE1	2:H:185:SER:OG	2.58	0.55
1:L:130:LEU:C	1:L:132:SER:H	2.08	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:28:SER:C	1:L:30:VAL:H	2.10	0.55
1:L:91:TYR:CD2	1:L:109:LEU:HD23	2.41	0.55
2:H:20:LEU:CD1	2:H:85:MET:HE3	2.25	0.55
1:L:168:TRP:NE1	1:L:180:MET:CE	2.70	0.55
1:L:3:VAL:HG12	1:L:24:ARG:NH2	2.22	0.55
2:H:161:SER:HB3	2:H:197:SER:CB	2.36	0.55
2:H:179:LEU:N	2:H:179:LEU:HD23	2.21	0.55
2:H:158:THR:HG23	2:H:201:ASN:HB2	1.86	0.55
2:H:40:SER:HG	2:H:93:MET:C	2.10	0.55
1:L:21:ILE:HD12	1:L:40:TRP:CZ3	2.41	0.55
2:H:100:GLY:O	4:H:219:MPD:H12	2.06	0.55
1:L:65:ASP:C	1:L:67:PHE:N	2.60	0.55
1:L:27:GLN:C	1:L:74:THR:HG23	2.27	0.55
2:H:159:TRP:CE3	2:H:198:ILE:CD1	2.83	0.54
2:H:188:VAL:HG22	2:H:193:TRP:CD1	2.39	0.54
1:L:168:TRP:NE1	1:L:180:MET:HE3	2.18	0.54
1:L:52:LEU:C	1:L:53:ILE:HD12	2.28	0.54
2:H:176:GLN:HG2	2:H:177:SER:HG	1.68	0.54
1:L:96:SER:O	3:H:218:FLU:H5	2.07	0.54
2:H:106:ASP:HB3	4:H:219:MPD:H11	1.88	0.54
2:H:162:GLY:N	2:H:197:SER:O	2.41	0.54
2:H:22:CYS:O	2:H:80:SER:HB2	2.07	0.54
1:L:94:SER:CA	1:L:102:THR:O	2.55	0.54
1:L:56:VAL:HG22	1:L:57:SER:H	1.72	0.54
2:H:144:GLY:HA2	2:H:184:SER:O	2.08	0.54
2:H:76:ASP:O	2:H:79:SER:HA	2.07	0.54
2:H:27:PHE:CE1	2:H:32:TYR:CD2	2.96	0.54
1:L:104:GLY:O	1:L:106:GLY:N	2.40	0.54
1:L:174:LYS:NZ	1:L:175:ASP:CG	2.60	0.54
1:L:67:PHE:CE2	1:L:80:ILE:HD13	2.43	0.54
2:H:193:TRP:H	2:H:194:PRO:CD	2.19	0.54
2:H:99:THR:CB	4:H:219:MPD:HM2	2.38	0.54
1:L:138:VAL:HG11	2:H:129:LEU:HD13	1.90	0.54
2:H:117:SER:HB2	2:H:178:ASP:CG	2.29	0.54
2:H:207:SER:O	2:H:208:SER:O	2.26	0.53
2:H:61:TYR:CE1	2:H:62:TYR:O	2.61	0.53
2:H:93:MET:HB2	2:H:116:VAL:HG12	1.90	0.53
1:L:42:LEU:CD2	1:L:44:LYS:HZ3	2.13	0.53
2:H:153:GLU:CA	2:H:153:GLU:OE2	2.55	0.53
2:H:126:VAL:HG12	2:H:213:LYS:HG3	1.90	0.53
2:H:81:VAL:HG22	2:H:82:TYR:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:161:GLN:OE1	1:L:162:ASN:HB2	2.08	0.53
1:L:130:LEU:CD2	1:L:188:LYS:HG3	2.38	0.53
1:L:138:VAL:O	1:L:138:VAL:HG12	2.08	0.53
1:L:118:PRO:HB3	1:L:144:PHE:CD2	2.44	0.53
2:H:54:LYS:HG2	2:H:58:TYR:CZ	2.43	0.53
1:L:29:LEU:HD21	1:L:95:GLN:HG2	1.90	0.53
2:H:153:GLU:CD	2:H:180:TYR:CZ	2.81	0.53
1:L:168:TRP:CD1	1:L:180:MET:HG3	2.44	0.53
2:H:142:THR:HG22	2:H:187:THR:N	2.24	0.53
2:H:161:SER:CB	2:H:198:ILE:N	2.71	0.53
2:H:45:LEU:HD21	2:H:97:TYR:CE1	2.44	0.53
1:L:123:PHE:CE2	1:L:140:PHE:CE1	2.97	0.53
1:L:152:LYS:NZ	1:L:154:LYS:HE2	2.24	0.53
2:H:45:LEU:CD1	2:H:108:TRP:CH2	2.86	0.53
2:H:16:ARG:HH21	2:H:86:ASN:HB2	1.74	0.53
2:H:38:ARG:NH1	2:H:96:TYR:CZ	2.61	0.53
2:H:90:VAL:C	2:H:92:ASP:H	2.11	0.52
1:L:123:PHE:CD2	1:L:138:VAL:HG12	2.44	0.52
2:H:124:PRO:N	2:H:150:TYR:HB3	2.23	0.52
2:H:69:ARG:C	2:H:87:ASN:ND2	2.61	0.52
2:H:120:LYS:H	2:H:120:LYS:HD2	1.65	0.52
2:H:191:SER:CA	2:H:194:PRO:HD2	2.38	0.52
2:H:49:ALA:HB1	2:H:72:ILE:CB	2.38	0.52
1:L:215:ASN:O	1:L:216:ARG:C	2.47	0.52
1:L:29:LEU:CD2	1:L:95:GLN:HG2	2.40	0.52
2:H:150:TYR:CE2	2:H:155:VAL:HG12	2.44	0.52
2:H:99:THR:CB	4:H:219:MPD:CM	2.87	0.52
2:H:134:GLY:C	2:H:137:THR:OG1	2.47	0.52
2:H:57:ASN:O	2:H:58:TYR:CB	2.58	0.52
2:H:69:ARG:HB3	2:H:87:ASN:CG	2.28	0.52
2:H:136:THR:HG22	2:H:137:THR:H	1.75	0.52
1:L:78:LEU:HD22	1:L:79:LYS:H	1.75	0.52
2:H:131:PRO:HD3	2:H:143:LEU:HD21	1.84	0.52
2:H:70:PHE:CZ	2:H:85:MET:CB	2.91	0.52
2:H:117:SER:HB2	2:H:178:ASP:OD2	2.09	0.52
2:H:64:ASP:OD1	2:H:67:LYS:NZ	2.42	0.52
2:H:108:TRP:NE1	4:H:219:MPD:H31	2.17	0.51
1:L:44:LYS:O	1:L:47:GLN:HB2	2.09	0.51
1:L:38:LEU:HD23	1:L:76:PHE:CE2	2.45	0.51
2:H:61:TYR:CE2	2:H:67:LYS:HE3	2.45	0.51
1:L:43:GLN:HE22	2:H:39:GLN:HE22	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:21:SER:HB2	2:H:82:TYR:HE1	1.74	0.51
2:H:169:HIS:N	2:H:169:HIS:ND1	2.58	0.51
1:L:184:LEU:HD12	1:L:185:THR:N	2.25	0.51
1:L:2:VAL:CG2	1:L:26:SER:HB3	2.27	0.51
1:L:35:ASN:O	1:L:37:TYR:CD2	2.63	0.51
2:H:38:ARG:NH1	2:H:96:TYR:CE2	2.78	0.51
2:H:70:PHE:O	2:H:71:THR:HG22	2.11	0.51
1:L:147:LYS:HB3	1:L:178:TYR:CZ	2.45	0.51
2:H:150:TYR:CZ	2:H:180:TYR:HB2	2.46	0.51
2:H:139:SER:O	2:H:190:SER:CA	2.59	0.50
2:H:203:ALA:CB	2:H:210:LYS:CB	2.88	0.50
2:H:49:ALA:CB	2:H:72:ILE:HB	2.41	0.50
2:H:72:ILE:HD12	2:H:81:VAL:CG2	2.41	0.50
2:H:6:GLU:HG2	2:H:111:GLY:C	2.31	0.50
2:H:164:LEU:CB	2:H:193:TRP:HE1	2.24	0.50
2:H:62:TYR:CE2	2:H:72:ILE:HG22	2.45	0.50
1:L:59:ARG:CG	1:L:59:ARG:HH11	2.15	0.50
2:H:80:SER:HG	2:H:82:TYR:HH	1.57	0.50
2:H:82:TYR:CB	2:H:84:GLN:OE1	2.59	0.50
2:H:12:VAL:CG1	2:H:17:PRO:CG	2.90	0.50
2:H:193:TRP:CE3	2:H:196:GLN:NE2	2.80	0.50
2:H:193:TRP:H	2:H:194:PRO:HD2	1.77	0.50
1:L:194:HIS:C	1:L:197:TYR:OH	2.49	0.50
2:H:203:ALA:HA	2:H:210:LYS:CA	2.35	0.50
2:H:63:SER:C	2:H:67:LYS:HD2	2.32	0.50
1:L:28:SER:O	1:L:30:VAL:N	2.43	0.50
2:H:121:THR:HA	2:H:151:PHE:HD2	1.77	0.50
2:H:66:VAL:O	2:H:67:LYS:C	2.49	0.50
2:H:121:THR:HA	2:H:151:PHE:CD2	2.47	0.50
2:H:35:ASN:CB	2:H:49:ALA:O	2.59	0.50
1:L:91:TYR:O	1:L:106:GLY:HA2	2.12	0.50
2:H:162:GLY:H	2:H:197:SER:C	2.14	0.49
2:H:40:SER:HB2	2:H:43:LYS:CD	2.41	0.49
2:H:92:ASP:O	2:H:96:TYR:CZ	2.64	0.49
1:L:124:PRO:HG3	1:L:214:PHE:CD1	2.46	0.49
2:H:204:HIS:O	2:H:207:SER:O	2.30	0.49
1:L:141:LEU:HD11	1:L:151:VAL:HG21	1.93	0.49
1:L:165:LEU:CD2	2:H:174:VAL:HG12	2.37	0.49
2:H:36:TRP:HD1	2:H:72:ILE:CD1	2.24	0.49
2:H:70:PHE:CE2	2:H:85:MET:CG	2.94	0.49
2:H:71:THR:O	2:H:83:LEU:HA	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:150:ASN:O	1:L:201:ALA:HA	2.12	0.49
2:H:28:THR:OG1	2:H:31:ASP:HB2	2.12	0.49
2:H:81:VAL:CG2	2:H:82:TYR:H	2.26	0.49
1:L:145:TYR:CE2	1:L:178:TYR:OH	2.65	0.49
1:L:66:ARG:HD3	1:L:82:ARG:O	2.12	0.49
2:H:17:PRO:HG2	2:H:88:LEU:CD1	2.37	0.49
2:H:198:ILE:CD1	2:H:198:ILE:C	2.81	0.49
1:L:165:LEU:HD21	2:H:174:VAL:CB	2.41	0.49
2:H:63:SER:C	2:H:67:LYS:CD	2.80	0.49
2:H:62:TYR:OH	2:H:72:ILE:HG22	2.11	0.49
2:H:123:ALA:HB1	2:H:124:PRO:HD2	1.93	0.49
2:H:75:ASP:O	2:H:76:ASP:O	2.30	0.49
1:L:60:PHE:CD1	1:L:61:SER:N	2.80	0.49
1:L:7:THR:OG1	1:L:22:SER:CB	2.60	0.49
1:L:87:ASP:O	1:L:91:TYR:OH	2.19	0.49
2:H:142:THR:HG22	2:H:187:THR:CA	2.43	0.49
2:H:215:ILE:O	2:H:216:GLU:CB	2.61	0.49
1:L:174:LYS:NZ	1:L:175:ASP:OD2	2.37	0.49
1:L:183:THR:HG22	1:L:183:THR:O	2.12	0.49
2:H:134:GLY:O	2:H:137:THR:OG1	2.31	0.49
1:L:125:PRO:HG3	1:L:191:TYR:CE2	2.47	0.49
1:L:3:VAL:H	1:L:26:SER:HB2	1.76	0.49
2:H:20:LEU:O	2:H:82:TYR:HA	2.13	0.48
1:L:15:LEU:HA	1:L:83:VAL:O	2.12	0.48
1:L:29:LEU:HD12	1:L:38:LEU:HB2	1.95	0.48
1:L:28:SER:HA	1:L:73:GLY:O	2.12	0.48
1:L:93:CYS:SG	1:L:93:CYS:O	2.70	0.48
2:H:22:CYS:HB3	2:H:36:TRP:CZ2	2.48	0.48
2:H:29:PHE:CZ	2:H:34:MET:SD	3.06	0.48
2:H:90:VAL:C	2:H:92:ASP:N	2.67	0.48
2:H:61:TYR:C	2:H:61:TYR:CD1	2.87	0.48
1:L:9:LEU:HD22	1:L:9:LEU:H	1.77	0.48
2:H:61:TYR:CG	2:H:62:TYR:N	2.81	0.48
1:L:31:HIS:HB2	1:L:37:TYR:HD2	1.78	0.48
1:L:40:TRP:CE2	1:L:78:LEU:HB3	2.49	0.48
1:L:56:VAL:HG22	1:L:57:SER:N	2.28	0.48
2:H:54:LYS:HB2	2:H:55:PRO:CD	2.32	0.48
2:H:35:ASN:ND2	2:H:99:THR:HG1	2.10	0.48
1:L:123:PHE:HD2	1:L:138:VAL:HG12	1.78	0.48
1:L:11:LEU:HD21	1:L:19:ALA:CB	2.44	0.48
1:L:2:VAL:HG13	1:L:26:SER:CB	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:69:ARG:O	2:H:87:ASN:ND2	2.46	0.48
1:L:15:LEU:HD12	1:L:83:VAL:HG12	1.96	0.48
1:L:54:TYR:CD1	2:H:105:MET:CE	2.97	0.48
2:H:151:PHE:CZ	2:H:152:PRO:HB3	2.49	0.48
2:H:39:GLN:C	2:H:40:SER:O	2.46	0.48
2:H:51:ILE:CD1	2:H:72:ILE:CD1	2.64	0.48
2:H:81:VAL:CG2	2:H:82:TYR:N	2.77	0.48
2:H:89:ARG:O	2:H:92:ASP:OD2	2.32	0.48
2:H:128:PRO:O	2:H:128:PRO:CG	2.56	0.48
2:H:16:ARG:N	2:H:17:PRO:CD	2.68	0.48
2:H:191:SER:N	2:H:194:PRO:CG	2.71	0.48
2:H:48:VAL:CG1	2:H:49:ALA:N	2.77	0.48
2:H:70:PHE:O	2:H:71:THR:HG23	2.12	0.48
1:L:118:PRO:HG2	1:L:118:PRO:O	2.14	0.48
1:L:165:LEU:HD21	2:H:174:VAL:HB	1.95	0.48
2:H:127:TYR:CD2	2:H:146:LEU:HD22	2.42	0.48
2:H:120:LYS:O	2:H:122:THR:OG1	2.25	0.48
2:H:145:CYS:O	2:H:183:SER:HA	2.13	0.47
2:H:163:SER:C	2:H:193:TRP:CE2	2.87	0.47
2:H:64:ASP:CG	2:H:67:LYS:HZ2	2.17	0.47
1:L:8:PRO:O	1:L:107:THR:OG1	2.22	0.47
2:H:162:GLY:H	2:H:197:SER:CA	2.27	0.47
2:H:85:MET:HB2	2:H:88:LEU:CD2	2.35	0.47
1:L:149:ILE:CG2	1:L:150:ASN:N	2.57	0.47
1:L:62:GLY:O	1:L:63:VAL:C	2.52	0.47
2:H:195:SER:C	2:H:196:GLN:O	2.52	0.47
1:L:155:ILE:HG13	1:L:159:GLU:CB	2.44	0.47
2:H:106:ASP:OD1	2:H:106:ASP:C	2.52	0.47
2:H:22:CYS:O	2:H:80:SER:HA	2.14	0.47
1:L:31:HIS:HB3	1:L:35:ASN:O	2.15	0.47
1:L:112:LYS:O	1:L:112:LYS:HG3	2.13	0.47
2:H:4:LEU:HD12	2:H:4:LEU:N	2.30	0.47
1:L:174:LYS:HG3	1:L:175:ASP:OD1	2.15	0.47
2:H:4:LEU:HD21	2:H:100:GLY:N	2.30	0.47
2:H:22:CYS:C	2:H:23:VAL:HG23	2.35	0.47
1:L:204:LYS:C	1:L:206:SER:H	2.18	0.47
1:L:136:SER:CA	1:L:184:LEU:O	2.62	0.46
1:L:147:LYS:O	1:L:149:ILE:HD13	2.11	0.46
1:L:95:GLN:O	1:L:95:GLN:NE2	2.48	0.46
2:H:20:LEU:CD2	2:H:85:MET:HE1	2.38	0.46
2:H:90:VAL:HB	2:H:116:VAL:HG13	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:145:TYR:CD1	1:L:146:PRO:HA	2.51	0.46
1:L:38:LEU:HD23	1:L:76:PHE:CE1	2.51	0.46
2:H:131:PRO:O	2:H:131:PRO:HG2	2.16	0.46
2:H:139:SER:O	2:H:190:SER:HA	2.14	0.46
2:H:21:SER:CB	2:H:82:TYR:HE1	2.28	0.46
1:L:30:VAL:O	1:L:30:VAL:HG12	2.15	0.46
1:L:38:LEU:C	1:L:38:LEU:CD1	2.83	0.46
1:L:94:SER:OG	1:L:95:GLN:N	2.48	0.46
2:H:190:SER:C	2:H:191:SER:OG	2.53	0.46
2:H:89:ARG:HH11	2:H:89:ARG:CG	2.26	0.46
1:L:166:ASN:OD1	1:L:182:SER:CB	2.61	0.46
2:H:103:TYR:HA	3:H:218:FLU:C18	2.45	0.46
2:H:176:GLN:O	2:H:177:SER:C	2.54	0.46
2:H:6:GLU:HG3	2:H:112:THR:N	2.31	0.46
2:H:69:ARG:NH2	2:H:87:ASN:OD1	2.46	0.46
2:H:157:LEU:HD12	2:H:158:THR:O	2.16	0.46
2:H:40:SER:HB2	2:H:43:LYS:CB	2.46	0.46
2:H:49:ALA:HB1	2:H:72:ILE:HG12	1.98	0.46
1:L:154:LYS:CB	1:L:198:THR:HG23	2.46	0.46
1:L:29:LEU:HD23	1:L:98:HIS:CD2	2.51	0.46
1:L:7:THR:OG1	1:L:22:SER:HB2	2.15	0.46
2:H:136:THR:CG2	2:H:140:SER:O	2.60	0.45
2:H:89:ARG:HG2	2:H:89:ARG:NH1	2.30	0.45
2:H:39:GLN:O	2:H:40:SER:O	2.33	0.45
2:H:17:PRO:N	2:H:87:ASN:H	2.14	0.45
1:L:6:GLN:HA	1:L:22:SER:O	2.16	0.45
2:H:38:ARG:NE	2:H:48:VAL:CG2	2.80	0.45
1:L:114:ALA:O	1:L:145:TYR:HB3	2.16	0.45
1:L:136:SER:HB3	1:L:185:THR:HG23	1.98	0.45
1:L:59:ARG:NH1	1:L:59:ARG:CG	2.74	0.45
1:L:154:LYS:NZ	1:L:200:GLU:CD	2.69	0.45
2:H:149:GLY:O	2:H:179:LEU:HD12	2.17	0.45
2:H:20:LEU:HD22	2:H:85:MET:CE	2.39	0.45
2:H:105:MET:O	2:H:106:ASP:HB3	2.16	0.45
2:H:161:SER:CB	2:H:197:SER:OG	2.45	0.45
2:H:36:TRP:HA	2:H:97:TYR:O	2.15	0.45
2:H:85:MET:CB	2:H:88:LEU:CD2	2.93	0.45
1:L:115:ASP:O	1:L:116:ALA:HB2	2.17	0.45
1:L:142:ASN:OD1	2:H:169:HIS:CD2	2.70	0.45
1:L:51:VAL:CG2	2:H:105:MET:CE	2.95	0.45
2:H:20:LEU:HB2	2:H:85:MET:HE3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:66:ARG:HD2	1:L:80:ILE:HG22	1.98	0.45
2:H:166:SER:CB	2:H:188:VAL:HG23	2.47	0.45
2:H:72:ILE:HA	2:H:82:TYR:O	2.16	0.45
1:L:152:LYS:HZ2	1:L:200:GLU:HG2	1.80	0.45
1:L:44:LYS:HE3	1:L:86:GLU:O	2.17	0.45
1:L:95:GLN:HE21	1:L:102:THR:N	2.14	0.45
2:H:100:GLY:O	2:H:106:ASP:CB	2.59	0.45
2:H:32:TYR:CE2	2:H:101:SER:O	2.70	0.45
1:L:169:THR:CG2	2:H:171:PHE:CD2	3.00	0.45
2:H:123:ALA:HB2	2:H:208:SER:HB3	1.98	0.45
2:H:62:TYR:HH	2:H:72:ILE:HG22	1.82	0.45
1:L:3:VAL:HG12	1:L:24:ARG:HH22	1.82	0.45
2:H:120:LYS:HD3	2:H:120:LYS:N	2.21	0.45
2:H:164:LEU:CA	2:H:193:TRP:HE1	2.29	0.45
3:H:218:FLU:H8	3:H:218:FLU:C15	2.45	0.45
1:L:123:PHE:CE2	1:L:140:PHE:HE1	2.35	0.45
2:H:49:ALA:CB	2:H:72:ILE:HG12	2.47	0.44
2:H:57:ASN:O	2:H:58:TYR:CD2	2.70	0.44
1:L:44:LYS:CE	1:L:86:GLU:O	2.66	0.44
1:L:53:ILE:HG23	1:L:56:VAL:O	2.14	0.44
2:H:180:TYR:C	2:H:181:THR:HG22	2.37	0.44
2:H:159:TRP:CD1	2:H:168:VAL:HG11	2.52	0.44
2:H:164:LEU:CB	2:H:193:TRP:NE1	2.80	0.44
2:H:40:SER:N	2:H:43:LYS:CB	2.79	0.44
1:L:200:GLU:HB2	1:L:211:VAL:CG1	2.46	0.44
2:H:150:TYR:CZ	2:H:155:VAL:HG11	2.47	0.44
2:H:27:PHE:HZ	2:H:34:MET:HE3	1.75	0.44
2:H:30:SER:HA	2:H:76:ASP:OD1	2.17	0.44
1:L:124:PRO:HD2	2:H:132:VAL:CG1	2.33	0.44
1:L:1:ASP:HA	1:L:100:PRO:HD2	1.95	0.44
2:H:116:VAL:O	2:H:116:VAL:HG13	2.18	0.44
2:H:153:GLU:HB3	2:H:154:PRO:CD	2.43	0.44
2:H:198:ILE:HD13	2:H:199:THR:H	1.79	0.44
3:H:218:FLU:C8	3:H:218:FLU:C15	2.94	0.44
2:H:27:PHE:CZ	2:H:34:MET:HE3	2.51	0.44
2:H:51:ILE:CD1	2:H:72:ILE:CG1	2.67	0.44
1:L:123:PHE:HA	1:L:124:PRO:HD3	1.77	0.44
1:L:13:VAL:O	1:L:112:LYS:HB3	2.18	0.44
1:L:204:LYS:H	1:L:204:LYS:HD2	1.80	0.44
2:H:153:GLU:CD	2:H:180:TYR:OH	2.56	0.44
2:H:192:THR:N	2:H:194:PRO:HD2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:82:ARG:CG	1:L:82:ARG:O	2.64	0.44
2:H:191:SER:CA	2:H:194:PRO:CD	2.95	0.44
2:H:70:PHE:CZ	2:H:85:MET:CG	3.01	0.44
1:L:141:LEU:HD13	1:L:180:MET:SD	2.58	0.44
1:L:24:ARG:HB2	1:L:74:THR:O	2.18	0.44
2:H:6:GLU:CG	2:H:112:THR:N	2.80	0.43
2:H:157:LEU:HD11	2:H:200:CYS:SG	2.58	0.43
2:H:61:TYR:CD1	2:H:62:TYR:C	2.91	0.43
2:H:51:ILE:CD1	2:H:72:ILE:HD12	2.27	0.43
1:L:55:LYS:CD	2:H:104:GLY:HA3	2.44	0.43
2:H:37:VAL:CG1	2:H:46:GLU:O	2.65	0.43
2:H:40:SER:O	2:H:43:LYS:CB	2.54	0.43
2:H:19:LYS:CE	2:H:82:TYR:CD1	3.01	0.43
1:L:96:SER:HB2	3:H:218:FLU:O3	2.18	0.43
2:H:57:ASN:O	2:H:58:TYR:HD2	2.01	0.43
2:H:124:PRO:O	2:H:124:PRO:HG2	2.19	0.43
2:H:189:THR:OG1	2:H:192:THR:OG1	2.25	0.43
2:H:212:ASP:C	2:H:213:LYS:HG2	2.38	0.43
2:H:189:THR:O	2:H:194:PRO:CG	2.66	0.43
2:H:3:LYS:HG2	2:H:25:SER:O	2.18	0.43
2:H:64:ASP:CG	2:H:67:LYS:HZ3	2.21	0.43
2:H:72:ILE:O	2:H:72:ILE:CG2	2.67	0.43
1:L:141:LEU:HD12	1:L:180:MET:O	2.18	0.43
1:L:197:TYR:CB	1:L:214:PHE:CE2	2.87	0.43
1:L:60:PHE:CZ	1:L:61:SER:HB3	2.54	0.43
2:H:6:GLU:HG2	2:H:111:GLY:CA	2.49	0.43
2:H:150:TYR:CE2	2:H:180:TYR:HB2	2.52	0.43
2:H:160:ASN:CB	2:H:199:THR:OG1	2.45	0.43
2:H:90:VAL:HG12	2:H:116:VAL:CB	2.49	0.43
2:H:35:ASN:HB3	2:H:50:GLN:HA	2.00	0.43
2:H:61:TYR:HE1	2:H:63:SER:CA	2.29	0.43
2:H:61:TYR:CE1	2:H:63:SER:N	2.86	0.43
1:L:160:ARG:O	1:L:161:GLN:C	2.57	0.43
2:H:19:LYS:HE2	2:H:82:TYR:CD1	2.54	0.43
2:H:70:PHE:CD2	2:H:83:LEU:HD21	2.54	0.43
1:L:48:SER:HA	1:L:49:PRO:HD3	1.83	0.43
1:L:59:ARG:HD3	1:L:63:VAL:HG11	1.99	0.43
2:H:12:VAL:O	2:H:116:VAL:HA	2.19	0.42
2:H:191:SER:C	2:H:194:PRO:CD	2.76	0.42
2:H:188:VAL:CG2	2:H:193:TRP:HD1	2.27	0.42
2:H:57:ASN:C	2:H:58:TYR:CD2	2.93	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:PHE:CZ	2:H:85:MET:SD	3.11	0.42
1:L:161:GLN:CG	1:L:184:LEU:HD11	2.49	0.42
1:L:24:ARG:NE	1:L:24:ARG:C	2.69	0.42
2:H:161:SER:O	2:H:162:GLY:C	2.57	0.42
2:H:166:SER:HB3	2:H:187:THR:O	2.19	0.42
1:L:65:ASP:O	1:L:67:PHE:N	2.52	0.42
1:L:68:SER:O	1:L:78:LEU:HA	2.19	0.42
1:L:129:GLN:O	1:L:132:SER:CB	2.64	0.42
2:H:72:ILE:N	2:H:83:LEU:HD12	2.34	0.42
1:L:153:TRP:NE1	1:L:182:SER:OG	2.53	0.42
1:L:218:GLU:N	1:L:218:GLU:CD	2.73	0.42
2:H:28:THR:C	2:H:30:SER:N	2.71	0.42
1:L:168:TRP:C	1:L:169:THR:HG22	2.38	0.42
2:H:143:LEU:CD1	2:H:198:ILE:HG21	2.50	0.42
2:H:103:TYR:CE1	3:H:218:FLU:H18	2.54	0.42
2:H:50:GLN:HG2	2:H:51:ILE:N	2.34	0.42
2:H:51:ILE:HA	2:H:59:GLU:O	2.20	0.42
1:L:174:LYS:CE	1:L:175:ASP:CG	2.88	0.42
1:L:190:GLU:N	1:L:193:ARG:HH22	2.17	0.42
2:H:137:THR:HA	2:H:141:VAL:CG1	2.33	0.42
1:L:21:ILE:HD12	1:L:40:TRP:CH2	2.55	0.42
1:L:54:TYR:HB3	2:H:105:MET:HE3	2.02	0.42
2:H:136:THR:O	2:H:140:SER:O	2.37	0.42
2:H:12:VAL:CG1	2:H:17:PRO:HG3	2.49	0.42
2:H:41:PRO:C	2:H:43:LYS:H	2.23	0.42
1:L:41:TYR:CE2	1:L:51:VAL:CG1	2.91	0.42
2:H:159:TRP:CD1	2:H:168:VAL:CG1	3.03	0.42
2:H:37:VAL:HG21	4:H:219:MPD:H53	2.02	0.42
2:H:95:ILE:HD12	2:H:95:ILE:N	2.35	0.42
1:L:204:LYS:C	1:L:206:SER:N	2.72	0.42
2:H:131:PRO:CD	2:H:143:LEU:HD23	2.14	0.41
2:H:157:LEU:CD1	2:H:158:THR:N	2.50	0.41
2:H:54:LYS:HE3	2:H:58:TYR:OH	2.20	0.41
1:L:149:ILE:HD13	1:L:149:ILE:N	2.34	0.41
1:L:63:VAL:HA	1:L:64:PRO:HD3	1.81	0.41
2:H:127:TYR:HA	2:H:128:PRO:HD3	1.90	0.41
1:L:152:LYS:NZ	1:L:152:LYS:CB	2.83	0.41
1:L:60:PHE:CE1	1:L:61:SER:CB	3.02	0.41
2:H:210:LYS:CG	2:H:210:LYS:O	2.68	0.41
2:H:70:PHE:CE2	2:H:85:MET:SD	3.13	0.41
1:L:152:LYS:HE2	1:L:152:LYS:HB3	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:155:ILE:HG13	1:L:159:GLU:HB2	2.01	0.41
2:H:174:VAL:CG1	2:H:175:LEU:N	2.83	0.41
2:H:24:ALA:CB	2:H:34:MET:HE1	2.50	0.41
1:L:215:ASN:HB3	1:L:218:GLU:OE1	2.20	0.41
1:L:39:ARG:HH11	1:L:39:ARG:HD2	1.56	0.41
1:L:147:LYS:HA	1:L:178:TYR:CD2	2.56	0.41
2:H:106:ASP:OD1	4:H:219:MPD:CM	2.65	0.41
1:L:88:LEU:CD1	1:L:172:ASP:OD1	2.62	0.41
1:L:191:TYR:CE1	1:L:216:ARG:CG	3.03	0.41
1:L:198:THR:CB	1:L:213:SER:OG	2.58	0.41
2:H:90:VAL:CA	2:H:116:VAL:CG1	2.93	0.41
2:H:171:PHE:HA	2:H:172:PRO:HD3	1.98	0.41
2:H:60:THR:HG1	2:H:62:TYR:HE2	1.66	0.41
1:L:144:PHE:HE1	1:L:147:LYS:O	2.03	0.41
1:L:194:HIS:O	1:L:197:TYR:OH	2.36	0.41
2:H:61:TYR:CE1	2:H:63:SER:CA	3.02	0.41
1:L:120:VAL:C	1:L:121:SER:OG	2.59	0.41
1:L:174:LYS:CD	1:L:175:ASP:H	2.27	0.41
1:L:154:LYS:NZ	1:L:200:GLU:OE2	2.50	0.41
2:H:124:PRO:HB3	2:H:150:TYR:CG	2.55	0.41
2:H:191:SER:N	2:H:194:PRO:HD2	2.35	0.41
2:H:29:PHE:O	2:H:30:SER:C	2.58	0.41
2:H:72:ILE:O	2:H:72:ILE:HG23	2.21	0.41
1:L:9:LEU:CD2	1:L:9:LEU:H	2.34	0.41
2:H:54:LYS:CB	2:H:55:PRO:CD	2.98	0.41
2:H:70:PHE:HD2	2:H:83:LEU:HD21	1.86	0.41
2:H:85:MET:O	2:H:87:ASN:N	2.53	0.41
1:L:175:ASP:OD2	1:L:177:THR:CG2	2.69	0.41
2:H:107:TYR:HA	2:H:107:TYR:HD2	1.39	0.40
2:H:145:CYS:HB3	2:H:157:LEU:HD21	2.03	0.40
2:H:147:VAL:HG13	2:H:182:LEU:HD23	2.03	0.40
2:H:165:SER:O	2:H:165:SER:OG	2.27	0.40
1:L:203:HIS:H	1:L:206:SER:HB2	1.86	0.40
2:H:58:TYR:C	2:H:59:GLU:O	2.60	0.40
1:L:95:GLN:NE2	1:L:101:TRP:HA	2.36	0.40
2:H:159:TRP:CZ3	2:H:198:ILE:CD1	3.05	0.40
2:H:122:THR:O	2:H:204:HIS:HE1	2.04	0.40
2:H:3:LYS:CG	2:H:25:SER:O	2.70	0.40
1:L:187:THR:OG1	1:L:190:GLU:N	2.42	0.40
2:H:40:SER:CB	2:H:43:LYS:CD	3.00	0.40
2:H:67:LYS:HB3	2:H:68:GLY:H	1.26	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:92:ASP:O	2:H:96:TYR:CE1	2.74	0.40
1:L:184:LEU:HD12	1:L:184:LEU:HA	1.79	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:57:SER:CB	1:L:216:ARG:NH2[1_645]	1.99	0.21
2:H:16:ARG:NH1	2:H:135:ASP:OD2[1_546]	2.07	0.13
1:L:70:SER:OG	2:H:209:THR:OG1[1_655]	2.14	0.06
2:H:16:ARG:CG	2:H:135:ASP:OD1[1_546]	2.14	0.06

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	L	217/219 (99%)	173 (80%)	29 (13%)	15 (7%)	1	1
2	H	214/216 (99%)	145 (68%)	39 (18%)	30 (14%)	0	0
All	All	431/435 (99%)	318 (74%)	68 (16%)	45 (10%)	0	0

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	73	GLY
1	L	82	ARG
1	L	105	GLY
1	L	161	GLN
1	L	174	LYS
1	L	206	SER
1	L	207	THR
2	H	17	PRO

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Mol	Chain	Res	Type
2	H	18	MET
2	H	41	PRO
2	H	65	SER
2	H	67	LYS
2	H	76	ASP
2	H	87	ASN
2	H	102	TYR
2	H	137	THR
2	H	153	GLU
2	H	163	SER
2	H	190	SER
2	H	198	ILE
2	H	206	ALA
2	H	207	SER
2	H	208	SER
1	L	15	LEU
1	L	29	LEU
1	L	160	ARG
1	L	163	GLY
2	H	8	GLY
2	H	30	SER
2	H	91	GLU
2	H	196	GLN
1	L	56	VAL
1	L	61	SER
1	L	66	ARG
2	H	68	GLY
2	H	161	SER
2	H	29	PHE
2	H	86	ASN
2	H	103	TYR
1	L	115	ASP
2	H	106	ASP
2	H	128	PRO
2	H	90	VAL
2	H	14	PRO
2	H	131	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	L	197/197 (100%)	125 (64%)	72 (36%)	0 0
2	H	190/190 (100%)	117 (62%)	73 (38%)	0 0
All	All	387/387 (100%)	242 (62%)	145 (38%)	0 0

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1	ASP
1	L	2	VAL
1	L	9	LEU
1	L	10	SER
1	L	14	SER
1	L	15	LEU
1	L	20	SER
1	L	21	ILE
1	L	22	SER
1	L	24	ARG
1	L	25	SER
1	L	38	LEU
1	L	48	SER
1	L	59	ARG
1	L	66	ARG
1	L	72	SER
1	L	74	THR
1	L	75	ASP
1	L	76	PHE
1	L	78	LEU
1	L	80	ILE
1	L	84	GLU
1	L	87	ASP
1	L	88	LEU
1	L	95	GLN
1	L	96	SER
1	L	99	VAL
1	L	100	PRO
1	L	112	LYS
1	L	115	ASP
1	L	118	PRO

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Mol	Chain	Res	Type
1	L	121	SER
1	L	126	SER
1	L	127	SER
1	L	128	GLU
1	L	131	THR
1	L	137	VAL
1	L	138	VAL
1	L	139	CYS
1	L	141	LEU
1	L	147	LYS
1	L	148	ASP
1	L	149	ILE
1	L	152	LYS
1	L	154	LYS
1	L	160	ARG
1	L	167	SER
1	L	169	THR
1	L	170	ASP
1	L	171	GLN
1	L	173	SER
1	L	174	LYS
1	L	178	TYR
1	L	182	SER
1	L	183	THR
1	L	185	THR
1	L	189	ASP
1	L	195	ASN
1	L	198	THR
1	L	200	GLU
1	L	202	THR
1	L	204	LYS
1	L	206	SER
1	L	207	THR
1	L	208	SER
1	L	209	PRO
1	L	210	ILE
1	L	211	VAL
1	L	212	LYS
1	L	213	SER
1	L	215	ASN
1	L	218	GLU
2	H	6	GLU

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Mol	Chain	Res	Type
2	H	7	THR
2	H	12	VAL
2	H	13	GLN
2	H	14	PRO
2	H	17	PRO
2	H	18	MET
2	H	19	LYS
2	H	25	SER
2	H	33	TRP
2	H	34	MET
2	H	35	ASN
2	H	38	ARG
2	H	39	GLN
2	H	41	PRO
2	H	48	VAL
2	H	50	GLN
2	H	51	ILE
2	H	56	TYR
2	H	60	THR
2	H	64	ASP
2	H	65	SER
2	H	67	LYS
2	H	69	ARG
2	H	70	PHE
2	H	72	ILE
2	H	74	ARG
2	H	75	ASP
2	H	76	ASP
2	H	79	SER
2	H	84	GLN
2	H	87	ASN
2	H	95	ILE
2	H	99	THR
2	H	101	SER
2	H	105	MET
2	H	107	TYR
2	H	112	THR
2	H	118	SER
2	H	120	LYS
2	H	124	PRO
2	H	125	SER
2	H	128	PRO

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Mol	Chain	Res	Type
2	H	132	VAL
2	H	133	CYS
2	H	141	VAL
2	H	145	CYS
2	H	151	PHE
2	H	153	GLU
2	H	156	THR
2	H	157	LEU
2	H	158	THR
2	H	160	ASN
2	H	164	LEU
2	H	171	PHE
2	H	172	PRO
2	H	174	VAL
2	H	179	LEU
2	H	181	THR
2	H	182	LEU
2	H	187	THR
2	H	188	VAL
2	H	190	SER
2	H	191	SER
2	H	193	TRP
2	H	196	GLN
2	H	198	ILE
2	H	201	ASN
2	H	205	PRO
2	H	207	SER
2	H	209	THR
2	H	214	LYS
2	H	216	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	27	GLN
1	L	35	ASN
1	L	43	GLN
1	L	98	HIS
2	H	13	GLN
2	H	35	ASN
2	H	50	GLN
2	H	53	ASN

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Mol	Chain	Res	Type
2	H	110	GLN
2	H	160	ASN
2	H	196	GLN
2	H	201	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	MPD	H	219	-	7,7,7	0.85	0	9,10,10	1.12	1 (11%)
3	FLU	H	218	-	24,28,28	3.96	10 (41%)	28,41,41	2.09	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	H	219	-	-	1/5/5/5	-
3	FLU	H	218	-	-	0/4/12/12	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	218	FLU	C19-C20	-12.64	1.35	1.47
3	H	218	FLU	C14-C10	-10.22	1.38	1.50
3	H	218	FLU	O3-C6	7.52	1.36	1.23
3	H	218	FLU	C12-C11	-3.16	1.35	1.42
3	H	218	FLU	C17-C16	2.80	1.45	1.38
3	H	218	FLU	C7-C6	2.69	1.43	1.37
3	H	218	FLU	C8-C9	-2.43	1.36	1.40
3	H	218	FLU	C13-C1	2.16	1.43	1.38
3	H	218	FLU	C18-C19	2.14	1.43	1.40
3	H	218	FLU	C15-C14	-2.09	1.36	1.40

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	218	FLU	C8-C9-C10	-6.39	118.61	122.70
3	H	218	FLU	C18-C19-C14	3.86	122.51	118.67
3	H	218	FLU	C12-C11-C3	3.18	120.18	116.50
3	H	218	FLU	C15-C14-C10	-2.64	113.98	119.41
4	H	219	MPD	CM-C2-C1	-2.40	105.57	110.57
3	H	218	FLU	C17-C16-C15	2.04	123.30	120.19

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	H	219	MPD	C2-C3-C4-C5

There are no ring outliers.

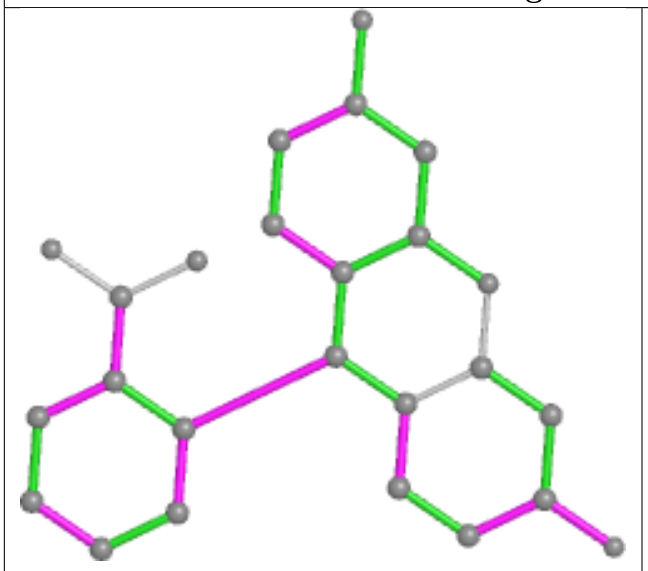
2 monomers are involved in 35 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	H	219	MPD	23	0
3	H	218	FLU	12	0

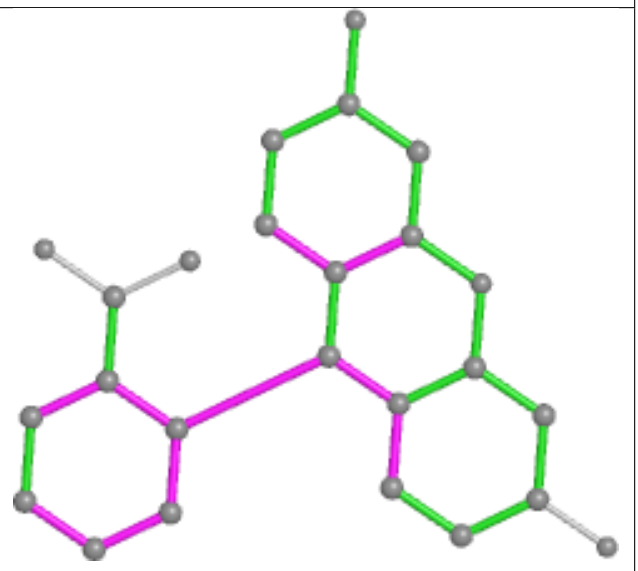
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

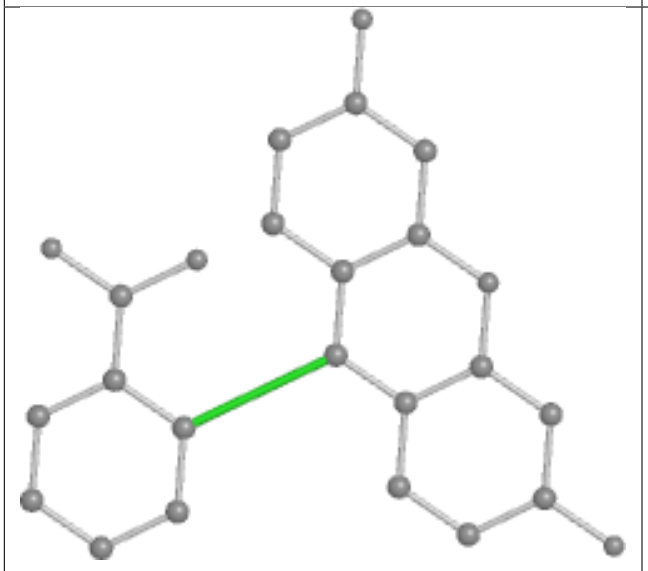
Ligand FLU H 218



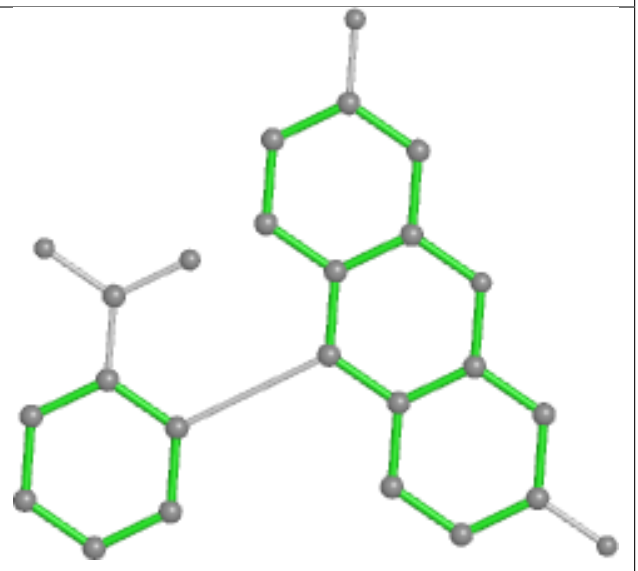
Bond lengths



Bond angles



Torsions



Rings

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.