



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 04:57 AM UTC

PDB ID : 1GLC / pdb_00001glc
Title : CATION PROMOTED ASSOCIATION (CPA) OF A REGULATORY AND
TARGET PROTEIN IS CONTROLLED BY PHOSPHORYLATION
Authors : Feese, M.D.; Meadow, N.D.; Roseman, S.; Pettigrew, D.W.; Remington, S.J.
Deposited on : 1994-03-07
Resolution : 2.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

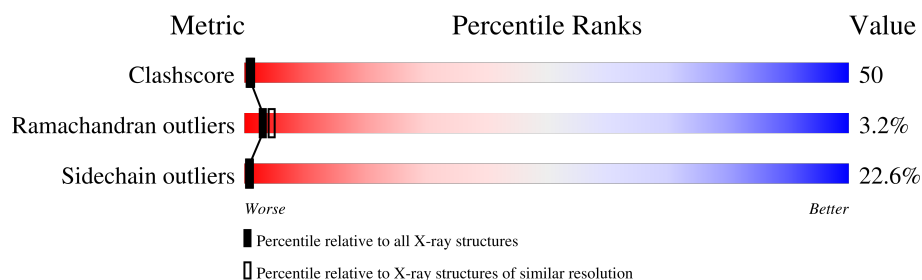
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))	
Clashscore	190562	1141	(2.66-2.66)
Ramachandran outliers	187476	1126	(2.66-2.66)
Sidechain outliers	187428	1126	(2.66-2.66)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	F	168	
2	G	501	

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
5	G3H	G	503	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 4990 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 GLUCOSE-SPECIFIC PROTEIN III_{Glc}.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace			
1	F	161	Total	C	N	O	S	0	0
			1157	741	181	233	2		

- Molecule 2 is a protein called GLYCEROL KINASE.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace				
2	G	489	Total	C	N	O	S	0	0	0
			3752	2379	644	710	19			

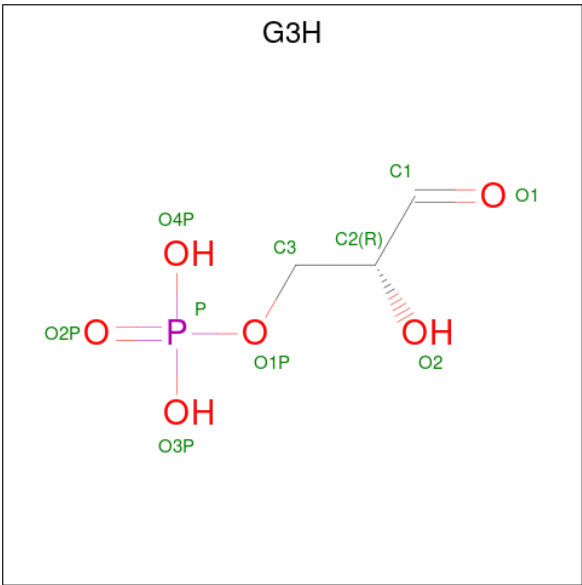
- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

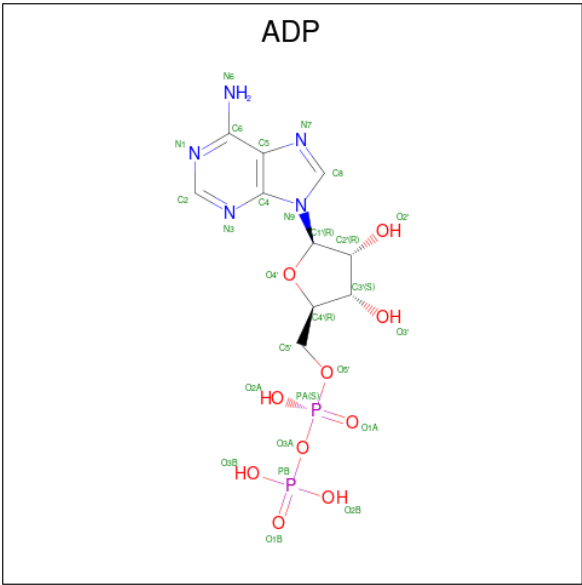
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	
4	G	1	Total 1	Mg 1	0	0

- Molecule 5 is GLYCERALDEHYDE-3-PHOSPHATE (CCD ID: G3H) (formula: C₃H₇O₆P).



Mol	Chain	Residues	Atoms	ZeroOcc			AltConf		
5	G	1	Total	C	O	P	0		0
			10	3	6	1			

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms	ZeroOcc				AltConf		
6	G	1	Total	C	N	O	P	0		0
			27	10	5	10	2			

- Molecule 7 is water.

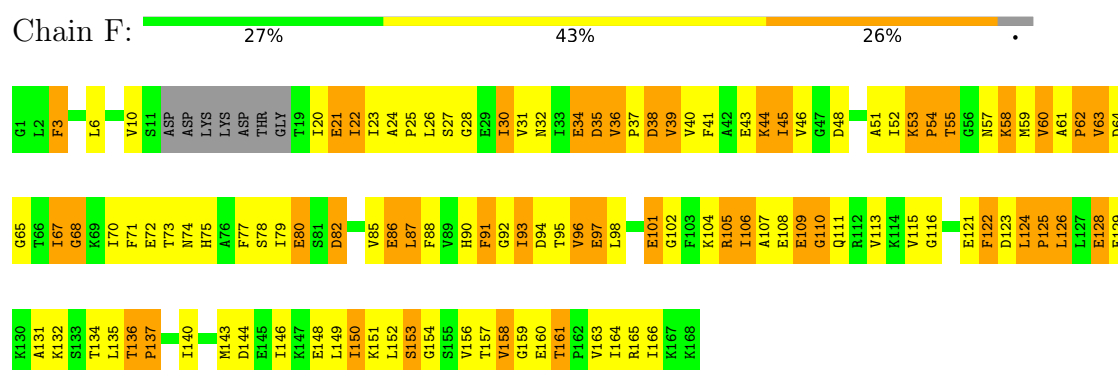
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	F	5	Total 5	O 5	0
7	G	37	Total 37	O 37	0

3 Residue-property plots

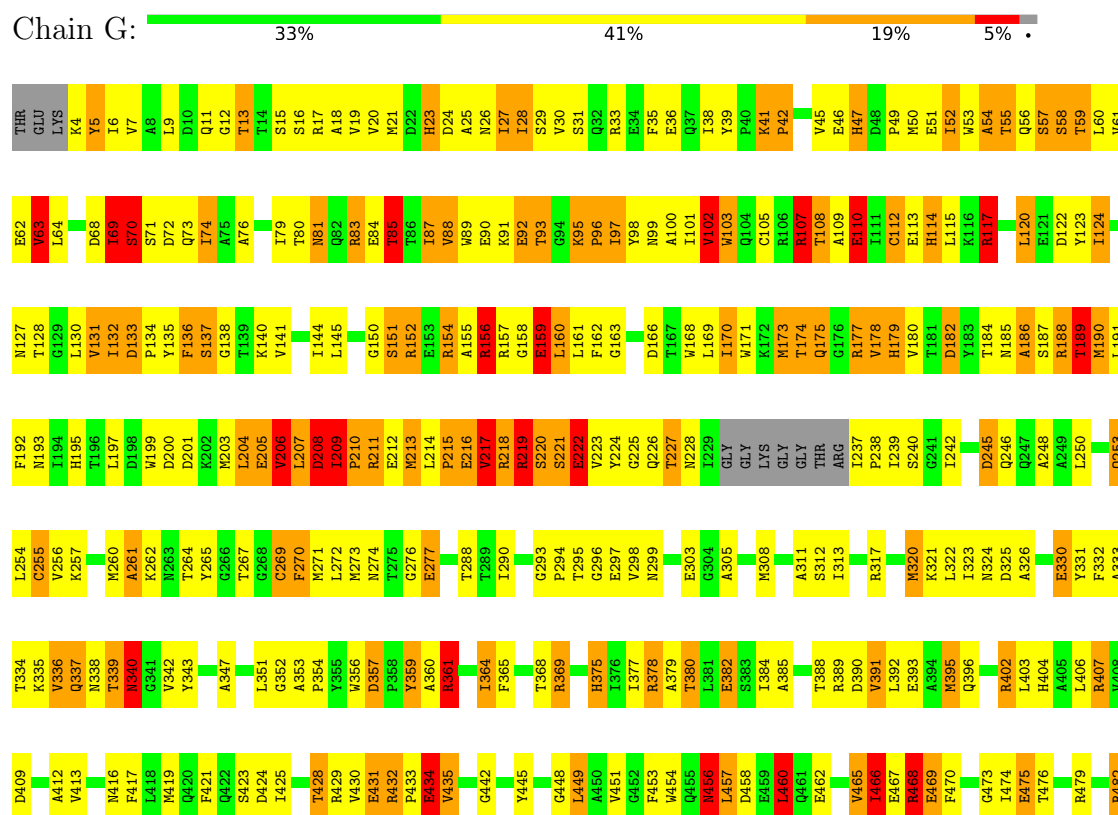
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

• Molecule 1: GLUCOSE-SPECIFIC PROTEIN IIIGlc



• Molecule 2: GLYCEROL KINASE



Y483	A484	G485	W486	K487	K488	A489	A493	E497	E498	H499	ASP	GLU
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4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	123.83Å 125.16Å 133.54Å	Depositor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.50 – 2.65	Depositor
% Data completeness (in resolution range)	(Not available) (14.50-2.65)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.166 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4990	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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: MG, G3H, ZN, ADP

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	F	1.77	22/1172 (1.9%)	2.16	51/1592 (3.2%)
2	G	1.69	37/3831 (1.0%)	2.12	162/5211 (3.1%)
All	All	1.71	59/5003 (1.2%)	2.13	213/6803 (3.1%)

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	F	1	0
2	G	2	1
All	All	3	1

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	87	LEU	CA-C	-7.33	1.43	1.52
2	G	110	GLU	CD-OE2	7.18	1.39	1.25
2	G	364	ILE	CA-CB	-7.03	1.45	1.54
1	F	91	PHE	N-CA	-6.68	1.38	1.46
1	F	63	VAL	CA-CB	-6.65	1.50	1.55
2	G	88	VAL	CA-CB	-6.56	1.46	1.54
1	F	144	ASP	CG-OD1	6.33	1.37	1.25
2	G	96	PRO	N-CA	-6.10	1.40	1.46
1	F	137	PRO	CA-C	-6.08	1.44	1.52
2	G	336	VAL	C-N	-6.04	1.25	1.33
2	G	377	ILE	CA-CB	-5.98	1.48	1.54
2	G	320	MET	C-N	-5.97	1.25	1.33
2	G	380	THR	N-CA	-5.95	1.39	1.46
2	G	406	LEU	N-CA	-5.95	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	114	HIS	CA-C	-5.90	1.45	1.52
2	G	39	TYR	N-CA	-5.87	1.40	1.46
1	F	22	ILE	N-CA	-5.81	1.39	1.46
2	G	206	VAL	CA-CB	-5.76	1.46	1.54
2	G	102	VAL	CA-C	-5.71	1.46	1.52
2	G	298	VAL	C-O	-5.70	1.17	1.24
2	G	62	GLU	CD-OE1	5.69	1.36	1.25
1	F	88	PHE	N-CA	-5.65	1.39	1.46
2	G	245	ASP	CG-OD2	5.62	1.36	1.25
2	G	239	ILE	CA-CB	-5.61	1.47	1.54
2	G	216	GLU	CD-OE2	5.59	1.35	1.25
1	F	90	HIS	CA-C	-5.59	1.46	1.52
2	G	359	TYR	C-O	-5.57	1.17	1.24
2	G	24	ASP	CG-OD1	5.57	1.35	1.25
2	G	331	TYR	CA-CB	-5.56	1.44	1.53
2	G	133	ASP	C-N	-5.54	1.28	1.34
2	G	205	GLU	CD-OE2	5.54	1.35	1.25
2	G	12	GLY	C-N	5.53	1.41	1.33
2	G	144	ILE	CA-CB	-5.52	1.48	1.54
1	F	30	ILE	CA-CB	-5.49	1.48	1.54
1	F	128	GLU	CD-OE2	5.45	1.35	1.25
2	G	357	ASP	CA-C	-5.43	1.46	1.52
2	G	385	ALA	CA-C	-5.39	1.45	1.52
1	F	148	GLU	CD-OE2	5.37	1.35	1.25
1	F	72	GLU	CD-OE2	5.37	1.35	1.25
2	G	337	GLN	CA-C	-5.34	1.45	1.52
2	G	87	ILE	CA-CB	-5.33	1.47	1.54
1	F	39	VAL	CA-CB	-5.21	1.47	1.54
2	G	277	GLU	CD-OE2	5.18	1.35	1.25
1	F	80	GLU	N-CA	-5.18	1.39	1.46
1	F	97	GLU	CD-OE1	5.17	1.35	1.25
1	F	106	ILE	CA-CB	-5.17	1.47	1.54
2	G	424	ASP	CG-OD2	5.15	1.35	1.25
1	F	82	ASP	CG-OD1	5.12	1.35	1.25
1	F	136	THR	C-O	-5.12	1.20	1.24
2	G	361	ARG	C-N	-5.10	1.28	1.33
2	G	298	VAL	CA-C	-5.10	1.46	1.52
1	F	44	LYS	CA-C	-5.09	1.46	1.53
2	G	38	ILE	CA-C	-5.08	1.46	1.52
2	G	208	ASP	CG-OD1	5.07	1.34	1.25
2	G	404	HIS	CA-C	-5.07	1.46	1.52
2	G	117	ARG	NE-CZ	5.06	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	158	VAL	CA-CB	-5.02	1.49	1.54
1	F	136	THR	CA-C	-5.00	1.47	1.52
1	F	101	GLU	CD-OE2	5.00	1.34	1.25

All (213) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	35	ASP	CA-CB-CG	10.76	123.36	112.60
2	G	245	ASP	CA-CB-CG	10.65	123.25	112.60
2	G	114	HIS	CA-CB-CG	-10.16	103.64	113.80
2	G	404	HIS	CA-CB-CG	-9.43	104.37	113.80
2	G	137	SER	N-CA-C	9.03	121.94	111.11
2	G	270	PHE	CA-CB-CG	-8.87	104.93	113.80
1	F	38	ASP	CA-CB-CG	8.80	121.40	112.60
2	G	456	ASN	CA-CB-CG	-8.64	103.96	112.60
2	G	336	VAL	N-CA-C	8.50	127.03	109.34
2	G	465	VAL	CB-CA-C	-8.22	99.67	111.34
2	G	144	ILE	N-CA-C	8.20	118.29	110.42
1	F	150	ILE	N-CA-CB	8.19	122.39	111.25
2	G	85	THR	CA-C-N	8.15	133.08	121.42
2	G	85	THR	C-N-CA	8.15	133.08	121.42
2	G	179	HIS	CA-CB-CG	8.09	121.89	113.80
2	G	47	HIS	CA-CB-CG	7.97	121.77	113.80
2	G	407	ARG	CA-C-N	-7.96	112.20	123.03
2	G	407	ARG	C-N-CA	-7.96	112.20	123.03
1	F	60	VAL	N-CA-CB	-7.94	97.08	111.92
2	G	245	ASP	N-CA-C	7.90	120.59	111.11
2	G	136	PHE	CA-CB-CG	-7.89	105.91	113.80
2	G	209	ILE	C-N-CD	-7.76	93.17	125.00
2	G	256	VAL	N-CA-C	7.65	125.26	109.34
2	G	92	GLU	CA-C-N	7.57	131.32	120.79
2	G	92	GLU	C-N-CA	7.57	131.32	120.79
1	F	93	ILE	CB-CA-C	7.52	121.45	110.77
1	F	126	LEU	N-CA-C	-7.49	102.81	110.97
2	G	27	ILE	N-CA-CB	7.47	119.45	111.46
2	G	335	LYS	N-CA-C	-7.43	104.30	113.15
2	G	189	THR	N-CA-CB	-7.33	99.02	110.30
2	G	70	SER	N-CA-CB	7.26	122.98	111.43
2	G	63	VAL	CB-CA-C	-7.15	102.68	112.04
2	G	460	LEU	N-CA-C	7.11	122.06	112.88
2	G	178	VAL	CB-CA-C	-7.11	102.76	111.08
2	G	157	ARG	N-CA-C	-7.11	104.60	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	67	ILE	N-CA-CB	7.00	118.79	110.95
2	G	432	ARG	O-C-N	6.97	127.74	121.19
2	G	63	VAL	CA-C-N	6.92	129.55	120.28
2	G	63	VAL	C-N-CA	6.92	129.55	120.28
2	G	174	THR	N-CA-C	-6.90	105.65	112.97
2	G	222	GLU	CA-C-N	-6.90	113.74	122.43
2	G	222	GLU	C-N-CA	-6.90	113.74	122.43
2	G	332	PHE	CA-CB-CG	-6.89	106.91	113.80
2	G	430	VAL	CA-C-N	-6.83	113.49	123.05
2	G	430	VAL	C-N-CA	-6.83	113.49	123.05
1	F	54	PRO	CA-C-N	6.83	134.58	121.54
1	F	54	PRO	C-N-CA	6.83	134.58	121.54
1	F	86	GLU	CA-C-N	-6.80	111.38	122.81
1	F	86	GLU	C-N-CA	-6.80	111.38	122.81
2	G	218	ARG	N-CA-C	6.78	119.73	109.23
2	G	493	ALA	CA-C-O	6.74	127.15	119.27
2	G	81	ASN	N-CA-CB	-6.69	101.15	111.46
2	G	52	ILE	O-C-N	6.66	128.82	121.90
2	G	71	SER	CA-C-N	6.61	129.14	120.28
2	G	71	SER	C-N-CA	6.61	129.14	120.28
2	G	253	GLN	CA-C-O	6.61	127.56	119.11
1	F	36	VAL	N-CA-CB	6.60	116.22	110.08
1	F	58	LYS	N-CA-C	6.60	118.23	108.60
1	F	150	ILE	N-CA-C	6.55	117.34	108.17
1	F	63	VAL	CB-CA-C	-6.52	105.61	111.74
2	G	69	ILE	N-CA-CB	-6.50	98.67	112.00
1	F	150	ILE	O-C-N	6.48	129.98	123.18
2	G	186	ALA	N-CA-C	6.48	119.16	111.71
2	G	41	LYS	CA-C-N	6.40	127.84	119.84
2	G	41	LYS	C-N-CA	6.40	127.84	119.84
1	F	53	LYS	CA-C-N	-6.40	111.84	119.84
1	F	53	LYS	C-N-CA	-6.40	111.84	119.84
1	F	144	ASP	CA-CB-CG	6.40	119.00	112.60
2	G	41	LYS	C-N-CD	-6.36	98.92	125.00
2	G	296	GLY	CA-C-N	-6.31	111.75	122.67
2	G	296	GLY	C-N-CA	-6.31	111.75	122.67
2	G	432	ARG	CA-C-N	6.26	126.17	119.85
2	G	432	ARG	C-N-CA	6.26	126.17	119.85
2	G	136	PHE	CA-C-N	6.23	128.95	120.54
2	G	136	PHE	C-N-CA	6.23	128.95	120.54
1	F	122	PHE	N-CA-C	6.22	118.23	108.96
1	F	54	PRO	N-CA-C	6.20	125.24	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	26	LEU	O-C-N		-6.19	115.98
2	G	293	GLY	CA-C-N		6.19	127.58
2	G	293	GLY	C-N-CA		6.19	127.58
1	F	34	GLU	CA-C-N		-6.17	112.98
1	F	34	GLU	C-N-CA		-6.17	112.98
2	G	320	MET	N-CA-C		-6.13	104.50
2	G	330	GLU	N-CA-C		-6.12	104.52
2	G	159	GLU	CA-C-N		6.10	131.59
2	G	159	GLU	C-N-CA		6.10	131.59
2	G	499	HIS	CA-CB-CG		-6.08	107.72
2	G	23	HIS	CA-CB-CG		-6.08	107.72
2	G	209	ILE	CA-C-N		6.06	127.41
2	G	209	ILE	C-N-CA		6.06	127.41
2	G	357	ASP	O-C-N		6.04	126.46
2	G	331	TYR	N-CA-C		6.03	117.53
2	G	368	THR	CA-CB-OG1		-6.03	100.56
2	G	74	ILE	N-CA-CB		6.02	118.52
1	F	93	ILE	N-CA-CB		6.01	119.45
2	G	88	VAL	CA-C-N		-6.01	110.58
2	G	88	VAL	C-N-CA		-6.01	110.58
2	G	93	THR	N-CA-C		5.98	118.32
2	G	61	VAL	CB-CA-C		-5.94	104.10
2	G	15	SER	N-CA-C		5.93	117.61
1	F	36	VAL	N-CA-C		-5.92	103.15
2	G	354	PRO	CB-CA-C		-5.92	97.21
2	G	390	ASP	CA-CB-CG		5.92	118.52
2	G	114	HIS	O-C-N		5.91	128.41
2	G	388	THR	CB-CA-C		-5.90	101.61
2	G	63	VAL	O-C-N		5.90	129.56
2	G	369	ARG	N-CA-C		5.89	119.72
1	F	153	SER	N-CA-C		5.87	117.88
2	G	468	ARG	CA-C-N		-5.86	114.44
2	G	468	ARG	C-N-CA		-5.86	114.44
2	G	215	PRO	N-CA-CB		5.86	109.40
2	G	38	ILE	CA-C-N		-5.84	114.89
2	G	38	ILE	C-N-CA		-5.84	114.89
2	G	177	ARG	CA-C-N		5.84	129.97
2	G	177	ARG	C-N-CA		5.84	129.97
2	G	185	ASN	CA-CB-CG		-5.82	106.78
2	G	76	ALA	N-CA-C		5.81	116.22
2	G	261	ALA	N-CA-C		5.80	118.92
1	F	92	GLY	CA-C-N		-5.78	115.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	92	GLY	C-N-CA		-5.78	115.41
2	G	107	ARG	N-CA-C		5.78	118.04
2	G	107	ARG	N-CA-CB		5.78	118.55
1	F	57	ASN	N-CA-C		5.77	123.09
2	G	63	VAL	N-CA-CB		5.77	118.83
2	G	72	ASP	N-CA-C		5.76	117.55
2	G	81	ASN	N-CA-C		5.75	116.99
1	F	161	THR	N-CA-CB		-5.73	100.96
2	G	112	CYS	N-CA-CB		5.72	119.03
1	F	35	ASP	N-CA-CB		5.67	119.51
2	G	188	ARG	CA-C-N		5.66	130.30
2	G	188	ARG	C-N-CA		5.66	130.30
2	G	245	ASP	CB-CG-OD2		-5.65	105.40
1	F	21	GLU	CA-C-N		-5.63	116.21
1	F	21	GLU	C-N-CA		-5.63	116.21
2	G	296	GLY	N-CA-C		-5.60	105.89
2	G	36	GLU	N-CA-C		5.59	118.34
2	G	466	ILE	N-CA-CB		5.58	118.17
1	F	71	PHE	N-CA-CB		5.56	118.20
1	F	64	ASP	N-CA-C		-5.54	101.44
2	G	434	GLU	N-CA-C		5.52	117.30
2	G	217	VAL	N-CA-C		5.51	116.67
2	G	305	ALA	CA-C-N		5.51	130.80
2	G	305	ALA	C-N-CA		5.51	130.80
2	G	375	HIS	CA-CB-CG		-5.49	108.31
2	G	382	GLU	CG-CD-OE2		-5.48	105.79
2	G	33	ARG	N-CA-CB		5.48	118.38
2	G	197	LEU	N-CA-C		5.48	119.13
2	G	160	LEU	N-CA-C		5.45	117.39
2	G	421	PHE	CA-CB-CG		-5.43	108.37
2	G	382	GLU	N-CA-C		5.41	117.93
2	G	110	GLU	N-CA-CB		5.41	117.91
2	G	108	THR	CA-CB-OG1		-5.41	101.49
2	G	288	THR	O-C-N		-5.40	117.07
2	G	209	ILE	O-C-N		5.38	127.24
1	F	39	VAL	N-CA-CB		-5.37	102.37
2	G	144	ILE	CB-CA-C		-5.36	105.11
1	F	62	PRO	N-CA-CB		5.35	108.87
2	G	5	TYR	N-CA-C		5.35	116.97
2	G	79	ILE	N-CA-C		5.34	115.55
2	G	431	GLU	CA-C-O		5.34	126.20
2	G	17	ARG	N-CA-C		5.34	117.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	217	VAL	CB-CA-C	5.33	117.42	110.96
1	F	62	PRO	O-C-N	5.33	129.84	122.64
2	G	178	VAL	N-CA-C	5.33	116.43	108.54
1	F	131	ALA	N-CA-C	5.33	117.59	110.35
2	G	330	GLU	CB-CA-C	-5.32	102.52	110.88
2	G	339	THR	N-CA-C	-5.32	106.64	113.02
1	F	132	LYS	N-CA-C	-5.29	105.59	111.36
1	F	3	PHE	N-CA-C	-5.29	107.00	112.93
2	G	188	ARG	N-CA-C	5.29	119.00	112.54
2	G	395	MET	CA-C-N	-5.28	113.21	120.28
2	G	395	MET	C-N-CA	-5.28	113.21	120.28
2	G	385	ALA	CB-CA-C	-5.26	102.05	110.79
2	G	428	THR	CA-CB-OG1	5.25	117.48	109.60
2	G	417	PHE	CA-CB-CG	-5.25	108.55	113.80
2	G	59	THR	CA-CB-OG1	-5.24	101.73	109.60
2	G	223	VAL	N-CA-CB	5.23	117.74	111.31
2	G	54	ALA	N-CA-CB	-5.21	102.17	109.94
2	G	114	HIS	N-CA-CB	5.21	117.53	109.98
2	G	340	ASN	CA-C-N	-5.20	115.27	122.86
2	G	340	ASN	C-N-CA	-5.20	115.27	122.86
1	F	129	GLU	CB-CA-C	5.19	118.74	109.29
2	G	290	ILE	N-CA-C	5.19	116.06	108.53
2	G	456	ASN	N-CA-C	5.19	117.91	109.24
2	G	325	ASP	CB-CA-C	-5.18	99.61	109.66
1	F	105	ARG	CA-C-N	-5.17	112.27	120.55
1	F	105	ARG	C-N-CA	-5.17	112.27	120.55
2	G	336	VAL	N-CA-CB	5.17	119.77	111.23
2	G	337	GLN	N-CA-CB	5.17	119.23	110.49
2	G	208	ASP	N-CA-C	5.17	118.52	111.39
2	G	28	ILE	N-CA-C	5.16	115.83	110.82
2	G	70	SER	N-CA-C	5.15	117.24	109.41
2	G	384	ILE	CA-CB-CG2	-5.15	101.75	110.50
2	G	379	ALA	O-C-N	5.14	128.59	122.27
1	F	57	ASN	CA-C-N	-5.13	113.02	121.80
1	F	57	ASN	C-N-CA	-5.13	113.02	121.80
2	G	156	ARG	CB-CA-C	-5.13	102.13	110.85
2	G	13	THR	N-CA-CB	5.12	117.43	110.01
2	G	388	THR	CA-CB-CG2	-5.12	101.80	110.50
2	G	120	LEU	N-CA-C	5.11	119.00	112.87
1	F	60	VAL	CB-CA-C	-5.10	101.58	110.71
1	F	158	VAL	N-CA-C	5.09	116.78	109.51
2	G	449	LEU	CB-CA-C	-5.09	102.03	110.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	80	GLU	N-CA-CB		-5.08	102.57
2	G	103	TRP	CA-C-N		5.07	127.08
2	G	103	TRP	C-N-CA		5.07	127.08
2	G	88	VAL	CA-CB-CG1		-5.07	101.78
2	G	330	GLU	CB-CG-CD		5.07	121.21
2	G	240	SER	CA-C-N		-5.05	117.72
2	G	240	SER	C-N-CA		-5.05	117.72
2	G	87	ILE	N-CA-C		5.04	115.91
1	F	45	ILE	N-CA-CB		-5.01	104.16
2	G	30	VAL	CB-CA-C		-5.00	102.69

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	55	THR	CA
2	G	42	PRO	CA
2	G	255	CYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	340	ASN	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	1157	0	1133	144	0
2	G	3752	0	3605	342	0
3	F	1	0	0	0	0
4	G	1	0	0	0	0
5	G	10	0	5	3	0
6	G	27	0	12	0	0
7	F	5	0	0	2	0
7	G	37	0	0	2	0
All	All	4990	0	4755	485	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 50.

All (485) 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:F:74:ASN:HD22	1:F:105:ARG:NH1	1.47	1.11
2:G:7:VAL:HG22	2:G:20:VAL:HG22	1.27	1.06
2:G:431:GLU:HB2	2:G:466:ILE:HD13	1.39	1.05
2:G:396:GLN:NE2	2:G:403:LEU:H	1.54	1.05
2:G:35:PHE:HE1	2:G:47:HIS:HD2	1.09	1.00
1:F:23:ILE:HD13	1:F:115:VAL:HG11	1.44	0.98
2:G:396:GLN:HE21	2:G:403:LEU:H	1.08	0.96
2:G:85:THR:HG22	2:G:103:TRP:H	1.31	0.95
1:F:74:ASN:HD22	1:F:105:ARG:HH11	1.08	0.94
2:G:9:LEU:HD11	2:G:60:LEU:HD13	1.49	0.94
1:F:30:ILE:HD11	1:F:163:VAL:HG12	1.49	0.91
2:G:456:ASN:HD22	2:G:457:LEU:H	1.18	0.91
2:G:189:THR:HG22	2:G:191:LEU:H	1.36	0.90
2:G:45:VAL:H	2:G:105:CYS:HB2	1.35	0.90
1:F:75:HIS:HE1	1:F:96:VAL:HB	1.37	0.89
1:F:156:VAL:HG12	1:F:161:THR:CG2	2.03	0.89
2:G:85:THR:HG22	2:G:103:TRP:N	1.88	0.87
2:G:35:PHE:CE1	2:G:47:HIS:HD2	1.94	0.86
2:G:117:ARG:HG3	2:G:117:ARG:HH11	1.39	0.86
2:G:189:THR:CG2	2:G:191:LEU:H	1.90	0.85
2:G:274:ASN:HD21	2:G:299:ASN:HD22	1.23	0.85
2:G:35:PHE:HE1	2:G:47:HIS:CD2	1.96	0.84
1:F:70:ILE:HG13	1:F:109:GLU:HG2	1.60	0.84
2:G:112:CYS:HB3	2:G:132:ILE:HG22	1.57	0.83
2:G:11:GLN:HB2	2:G:56:GLN:HE21	1.43	0.83
1:F:157:THR:CG2	1:F:160:GLU:HB2	2.08	0.83
2:G:152:ARG:NH2	2:G:208:ASP:HB3	1.93	0.83
1:F:74:ASN:ND2	1:F:105:ARG:NH1	2.28	0.82
1:F:157:THR:HG22	1:F:160:GLU:HB2	1.62	0.82
2:G:182:ASP:HB3	2:G:242:ILE:CG2	2.11	0.81
2:G:105:CYS:SG	2:G:107:ARG:HD2	2.20	0.81
2:G:473:GLY:O	2:G:476:THR:HG22	1.79	0.81
1:F:143:MET:HE1	1:F:149:LEU:HD13	1.62	0.80
2:G:152:ARG:HG3	2:G:152:ARG:HH11	1.45	0.80
2:G:445:TYR:HA	2:G:454:TRP:CZ3	2.15	0.80
2:G:60:LEU:O	2:G:63:VAL:HG23	1.82	0.80
1:F:38:ASP:OD1	1:F:40:VAL:HG22	1.81	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:VAL:HG12	1:F:161:THR:HB	1.65	0.79
1:F:67:ILE:HD11	1:F:70:ILE:HG12	1.64	0.79
2:G:152:ARG:HH21	2:G:208:ASP:HB3	1.48	0.79
2:G:154:ARG:HH11	2:G:154:ARG:HB3	1.47	0.79
1:F:124:LEU:HB3	1:F:125:PRO:HD3	1.65	0.78
2:G:155:ALA:HB2	2:G:160:LEU:HB2	1.65	0.78
2:G:29:SER:OG	2:G:63:VAL:HG12	1.83	0.78
2:G:456:ASN:HD22	2:G:457:LEU:N	1.81	0.78
2:G:246:GLN:OE1	2:G:270:PHE:HB2	1.84	0.77
1:F:54:PRO:HD2	1:F:134:THR:HG23	1.66	0.77
2:G:101:ILE:HD13	2:G:107:ARG:HD3	1.65	0.76
1:F:65:GLY:HA2	1:F:82:ASP:OD1	1.84	0.76
2:G:41:LYS:HG3	2:G:42:PRO:N	1.98	0.76
2:G:83:ARG:HD3	5:G:503:G3H:O2	1.85	0.76
2:G:190:MET:O	2:G:203:MET:HG3	1.84	0.75
2:G:468:ARG:HG3	2:G:469:GLU:N	2.01	0.75
1:F:165:ARG:HG3	1:F:165:ARG:HH11	1.52	0.75
1:F:106:ILE:HD11	1:F:121:GLU:HB2	1.67	0.74
2:G:396:GLN:NE2	2:G:403:LEU:N	2.33	0.74
2:G:23:HIS:HA	2:G:453:PHE:CE1	2.23	0.74
2:G:56:GLN:O	2:G:59:THR:HG22	1.88	0.74
2:G:5:TYR:HB3	2:G:21:MET:O	1.89	0.73
2:G:85:THR:HG21	2:G:102:VAL:HG13	1.70	0.73
1:F:67:ILE:HD11	1:F:70:ILE:CG1	2.19	0.73
2:G:250:LEU:HD11	2:G:255:CYS:HB2	1.70	0.72
2:G:51:GLU:O	2:G:55:THR:HB	1.90	0.72
2:G:74:ILE:HD11	2:G:237:ILE:N	2.05	0.71
1:F:156:VAL:HG12	1:F:161:THR:CB	2.19	0.71
1:F:40:VAL:HA	1:F:45:ILE:HD12	1.73	0.71
1:F:143:MET:SD	1:F:146:ILE:HD11	2.30	0.71
2:G:64:LEU:HD22	2:G:69:ILE:CG2	2.21	0.70
2:G:23:HIS:HA	2:G:453:PHE:HE1	1.56	0.70
2:G:206:VAL:HG12	2:G:207:LEU:HD23	1.73	0.70
2:G:20:VAL:O	2:G:28:ILE:HB	1.91	0.70
2:G:47:HIS:ND1	2:G:102:VAL:HG21	2.07	0.70
2:G:137:SER:HB2	2:G:189:THR:HA	1.73	0.69
1:F:30:ILE:CD1	1:F:163:VAL:HG12	2.21	0.69
2:G:431:GLU:O	2:G:433:PRO:HD3	1.93	0.69
2:G:255:CYS:HB3	2:G:260:MET:CB	2.23	0.69
2:G:255:CYS:HB3	2:G:260:MET:HB3	1.74	0.69
1:F:106:ILE:CD1	1:F:121:GLU:HG3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:90:GLU:HB2	2:G:93:THR:OG1	1.93	0.69
1:F:140:ILE:HD13	1:F:149:LEU:CD1	2.23	0.68
1:F:165:ARG:HG3	1:F:165:ARG:NH1	2.04	0.68
1:F:31:VAL:HG12	1:F:32:ASN:N	2.08	0.68
2:G:339:THR:HG22	2:G:378:ARG:HG2	1.75	0.67
2:G:136:PHE:HB3	2:G:188:ARG:O	1.94	0.67
2:G:154:ARG:HH11	2:G:154:ARG:CB	2.07	0.67
2:G:174:THR:HB	2:G:178:VAL:HG23	1.75	0.67
2:G:50:MET:HE1	2:G:96:PRO:CD	2.24	0.67
1:F:73:THR:HG21	1:F:96:VAL:HG23	1.76	0.67
2:G:407:ARG:HD3	2:G:431:GLU:HG3	1.75	0.66
1:F:156:VAL:CG1	1:F:161:THR:HB	2.25	0.66
2:G:123:TYR:O	2:G:127:ASN:ND2	2.28	0.66
2:G:226:GLN:HA	2:G:238:PRO:HA	1.77	0.66
2:G:468:ARG:HG2	2:G:470:PHE:CE1	2.31	0.66
2:G:154:ARG:O	2:G:159:GLU:HG3	1.96	0.66
2:G:50:MET:HE1	2:G:96:PRO:HD2	1.77	0.66
2:G:156:ARG:HG3	2:G:156:ARG:HH11	1.61	0.66
2:G:201:ASP:OD1	2:G:211:ARG:NH1	2.27	0.66
2:G:347:ALA:HB2	2:G:351:LEU:HD21	1.78	0.66
1:F:27:SER:OG	1:F:158:VAL:HG12	1.96	0.65
1:F:75:HIS:CE1	1:F:96:VAL:HB	2.28	0.65
2:G:7:VAL:CG2	2:G:20:VAL:HG22	2.18	0.65
1:F:156:VAL:HG12	1:F:161:THR:HG21	1.78	0.65
2:G:205:GLU:HG2	2:G:206:VAL:N	2.12	0.65
2:G:13:THR:OG1	2:G:103:TRP:NE1	2.28	0.65
2:G:160:LEU:C	2:G:161:LEU:HD23	2.22	0.64
2:G:257:LYS:O	2:G:260:MET:HG3	1.96	0.64
1:F:32:ASN:HB2	1:F:35:ASP:OD1	1.98	0.64
2:G:154:ARG:HH11	2:G:154:ARG:CG	2.10	0.64
2:G:250:LEU:CD1	2:G:255:CYS:HB2	2.27	0.64
2:G:11:GLN:CB	2:G:56:GLN:HE21	2.11	0.64
2:G:27:ILE:HD13	2:G:27:ILE:N	2.12	0.64
2:G:330:GLU:OE2	2:G:416:ASN:N	2.31	0.64
2:G:340:ASN:HB2	2:G:375:HIS:CD2	2.32	0.64
2:G:155:ALA:CB	2:G:160:LEU:HB2	2.27	0.64
1:F:124:LEU:CB	1:F:125:PRO:HD3	2.24	0.63
2:G:85:THR:CG2	2:G:102:VAL:HA	2.28	0.63
2:G:90:GLU:OE2	2:G:154:ARG:NH2	2.31	0.63
2:G:128:THR:HB	7:G:539:HOH:O	1.99	0.63
1:F:23:ILE:HD13	1:F:115:VAL:CG1	2.26	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:ILE:HD11	1:F:121:GLU:CB	2.28	0.63
2:G:46:GLU:OE2	2:G:107:ARG:NH2	2.27	0.63
2:G:52:ILE:O	2:G:55:THR:HG22	1.99	0.63
2:G:161:LEU:HD23	2:G:161:LEU:N	2.13	0.63
2:G:145:LEU:HB2	2:G:152:ARG:HH12	1.64	0.63
2:G:201:ASP:CG	2:G:211:ARG:HH12	2.06	0.62
2:G:271:MET:SD	2:G:395:MET:HE2	2.39	0.62
2:G:120:LEU:HD23	2:G:120:LEU:N	2.12	0.62
1:F:20:ILE:O	1:F:165:ARG:HA	1.99	0.62
1:F:36:VAL:HG13	1:F:37:PRO:HD2	1.81	0.62
2:G:361:ARG:HG2	2:G:361:ARG:HH11	1.63	0.62
2:G:432:ARG:HD2	2:G:467:GLU:OE1	1.99	0.62
2:G:456:ASN:ND2	2:G:457:LEU:H	1.94	0.62
2:G:31:SER:HB2	2:G:59:THR:OG1	2.00	0.62
2:G:265:TYR:HB3	2:G:412:ALA:HB3	1.81	0.62
2:G:85:THR:CG2	2:G:103:TRP:H	2.09	0.62
2:G:186:ALA:O	2:G:189:THR:HB	2.00	0.62
2:G:110:GLU:O	2:G:113:GLU:HB2	2.00	0.61
2:G:127:ASN:ND2	2:G:127:ASN:N	2.47	0.61
2:G:45:VAL:H	2:G:105:CYS:CB	2.12	0.61
2:G:47:HIS:CE1	2:G:102:VAL:HG21	2.36	0.61
1:F:106:ILE:HD11	1:F:121:GLU:HG3	1.81	0.61
2:G:482:ARG:HG3	2:G:482:ARG:HH11	1.65	0.61
2:G:431:GLU:HB2	2:G:466:ILE:CD1	2.25	0.61
2:G:182:ASP:HB3	2:G:242:ILE:HG21	1.81	0.61
2:G:91:LYS:NZ	2:G:158:GLY:O	2.29	0.60
2:G:189:THR:CG2	2:G:191:LEU:HB2	2.31	0.60
2:G:90:GLU:OE1	2:G:93:THR:HG21	2.01	0.60
2:G:152:ARG:O	2:G:155:ALA:N	2.34	0.60
1:F:140:ILE:HD13	1:F:149:LEU:HD11	1.83	0.60
2:G:428:THR:HG22	2:G:429:ARG:O	2.01	0.60
2:G:271:MET:HG2	2:G:395:MET:HE1	1.83	0.60
2:G:174:THR:OG1	2:G:178:VAL:HB	2.01	0.60
1:F:96:VAL:HG12	7:F:170:HOH:O	2.01	0.60
2:G:18:ALA:HB1	2:G:63:VAL:HG21	1.84	0.60
2:G:150:GLY:O	2:G:154:ARG:HD3	2.02	0.59
2:G:145:LEU:HB2	2:G:152:ARG:NH1	2.17	0.59
2:G:174:THR:HG21	2:G:178:VAL:HG21	1.85	0.59
1:F:67:ILE:CD1	1:F:70:ILE:HG12	2.31	0.59
2:G:154:ARG:HH12	2:G:159:GLU:HB2	1.66	0.59
1:F:38:ASP:O	1:F:41:PHE:HB2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:150:ILE:O	1:F:164:ILE:HA	2.03	0.59
1:F:31:VAL:HG12	1:F:32:ASN:H	1.67	0.58
2:G:19:VAL:HG13	2:G:27:ILE:HG23	1.84	0.58
1:F:106:ILE:HD11	1:F:121:GLU:CG	2.34	0.58
1:F:140:ILE:CD1	1:F:149:LEU:HD11	2.33	0.58
2:G:11:GLN:HB2	2:G:56:GLN:NE2	2.15	0.58
2:G:85:THR:CG2	2:G:103:TRP:HD1	2.16	0.58
2:G:347:ALA:HB2	2:G:351:LEU:CD2	2.33	0.58
2:G:308:MET:CE	2:G:311:ALA:HB3	2.33	0.58
1:F:74:ASN:ND2	1:F:105:ARG:HH11	1.92	0.58
2:G:155:ALA:HB2	2:G:160:LEU:CB	2.33	0.58
1:F:124:LEU:O	1:F:128:GLU:HB2	2.04	0.58
2:G:16:SER:OG	2:G:55:THR:HG23	2.03	0.58
1:F:85:VAL:HG12	1:F:86:GLU:N	2.19	0.57
2:G:343:TYR:CE2	2:G:485:GLY:HA3	2.39	0.57
2:G:152:ARG:HG3	2:G:152:ARG:NH1	2.18	0.57
2:G:187:SER:HB2	7:G:519:HOH:O	2.04	0.57
2:G:59:THR:O	2:G:63:VAL:HG22	2.04	0.57
1:F:40:VAL:O	1:F:46:VAL:HG23	2.04	0.57
2:G:218:ARG:NH2	2:G:222:GLU:OE1	2.35	0.57
2:G:169:LEU:O	2:G:173:MET:HG2	2.05	0.57
1:F:146:ILE:HG12	1:F:146:ILE:O	2.03	0.56
2:G:392:LEU:C	2:G:392:LEU:HD23	2.30	0.56
2:G:21:MET:CG	2:G:27:ILE:HD12	2.35	0.56
2:G:88:VAL:O	2:G:97:ILE:HG23	2.04	0.56
1:F:140:ILE:HD13	1:F:149:LEU:HD12	1.86	0.56
2:G:170:ILE:HG22	2:G:171:TRP:N	2.19	0.56
2:G:333:ALA:HB1	2:G:378:ARG:HB2	1.88	0.56
2:G:272:LEU:N	2:G:272:LEU:HD12	2.20	0.56
1:F:25:PRO:HB3	1:F:62:PRO:HG3	1.87	0.56
2:G:261:ALA:HB2	2:G:273:MET:HB2	1.88	0.56
2:G:98:TYR:CD1	2:G:99:ASN:N	2.73	0.56
2:G:173:MET:C	2:G:175:GLN:H	2.12	0.56
2:G:162:PHE:O	2:G:179:HIS:HE1	1.88	0.56
2:G:336:VAL:O	2:G:338:ASN:N	2.39	0.56
1:F:61:ALA:HB2	1:F:113:VAL:HG21	1.88	0.55
2:G:88:VAL:HG12	2:G:89:TRP:N	2.21	0.55
1:F:93:ILE:C	1:F:93:ILE:HD12	2.30	0.55
2:G:336:VAL:HG23	2:G:338:ASN:O	2.06	0.55
2:G:204:LEU:HD21	2:G:214:LEU:CD1	2.36	0.55
2:G:458:ASP:OD1	2:G:458:ASP:N	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:102:GLY:O	1:F:122:PHE:HA	2.06	0.55
1:F:22:ILE:HD11	1:F:166:ILE:HD13	1.88	0.54
2:G:26:ASN:O	2:G:28:ILE:HD13	2.06	0.54
2:G:53:TRP:HA	2:G:53:TRP:CE3	2.42	0.54
2:G:162:PHE:CG	2:G:163:GLY:N	2.75	0.54
1:F:30:ILE:HG22	1:F:31:VAL:N	2.23	0.54
1:F:48:ASP:CB	1:F:143:MET:HE2	2.37	0.54
1:F:106:ILE:HD12	1:F:106:ILE:N	2.22	0.54
2:G:11:GLN:CD	2:G:52:ILE:HG23	2.32	0.54
2:G:130:LEU:HD13	2:G:136:PHE:CD1	2.42	0.54
1:F:153:SER:OG	1:F:154:GLY:N	2.39	0.54
2:G:205:GLU:O	2:G:208:ASP:N	2.27	0.54
2:G:364:ILE:HG22	2:G:365:PHE:N	2.22	0.54
1:F:104:LYS:O	1:F:106:ILE:HD12	2.08	0.54
1:F:150:ILE:HG22	1:F:151:LYS:N	2.23	0.54
2:G:117:ARG:HG3	2:G:117:ARG:NH1	2.15	0.54
1:F:94:ASP:O	1:F:97:GLU:HG2	2.09	0.53
2:G:180:VAL:HG23	2:G:216:GLU:O	2.08	0.53
2:G:416:ASN:OD1	2:G:432:ARG:NH2	2.32	0.53
2:G:18:ALA:CB	2:G:63:VAL:HG21	2.38	0.53
2:G:179:HIS:CD2	2:G:215:PRO:HA	2.44	0.53
2:G:475:GLU:H	2:G:475:GLU:CD	2.14	0.53
2:G:483:TYR:O	2:G:486:TRP:HB3	2.08	0.53
2:G:21:MET:HG2	2:G:27:ILE:HD12	1.90	0.53
2:G:80:THR:CG2	2:G:245:ASP:HA	2.39	0.53
2:G:45:VAL:N	2:G:105:CYS:HB2	2.16	0.53
2:G:195:HIS:N	2:G:195:HIS:CD2	2.76	0.53
2:G:246:GLN:CD	2:G:270:PHE:HB2	2.32	0.53
2:G:274:ASN:OD1	2:G:276:GLY:N	2.29	0.52
2:G:47:HIS:HE1	2:G:102:VAL:HG11	1.74	0.52
2:G:74:ILE:HD12	2:G:74:ILE:O	2.10	0.52
2:G:154:ARG:HB3	2:G:154:ARG:NH1	2.20	0.52
2:G:475:GLU:OE1	2:G:475:GLU:N	2.28	0.52
2:G:152:ARG:CZ	2:G:208:ASP:HB3	2.40	0.52
2:G:155:ALA:C	2:G:158:GLY:H	2.18	0.52
2:G:391:VAL:HG12	2:G:392:LEU:N	2.24	0.52
2:G:210:PRO:O	2:G:212:GLU:N	2.43	0.52
2:G:445:TYR:HA	2:G:454:TRP:HZ3	1.72	0.52
2:G:50:MET:HE1	2:G:96:PRO:HD3	1.92	0.52
2:G:343:TYR:CZ	2:G:485:GLY:HA3	2.45	0.52
1:F:91:PHE:O	1:F:95:THR:HG21	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:155:ALA:O	2:G:158:GLY:HA2	2.08	0.52
2:G:254:LEU:O	2:G:255:CYS:O	2.28	0.52
2:G:6:ILE:HD13	2:G:454:TRP:CH2	2.45	0.52
2:G:389:ARG:HG3	2:G:389:ARG:O	2.09	0.52
2:G:255:CYS:HB3	2:G:260:MET:HB2	1.92	0.52
1:F:10:VAL:HG12	1:F:10:VAL:O	2.10	0.51
1:F:43:GLU:OE1	2:G:402:ARG:NH2	2.43	0.51
2:G:80:THR:HG22	2:G:245:ASP:HA	1.91	0.51
2:G:123:TYR:OH	2:G:200:ASP:OD1	2.26	0.51
2:G:219:ARG:HD3	2:G:221:SER:O	2.11	0.51
2:G:134:PRO:O	2:G:140:LYS:NZ	2.33	0.51
2:G:297:GLU:N	2:G:297:GLU:OE1	2.44	0.51
1:F:67:ILE:HD12	1:F:68:GLY:N	2.26	0.50
2:G:220:SER:HB3	2:G:242:ILE:O	2.11	0.50
1:F:22:ILE:CD1	1:F:166:ILE:HD13	2.41	0.50
2:G:47:HIS:ND1	2:G:102:VAL:CG2	2.74	0.50
2:G:87:ILE:HG22	2:G:88:VAL:N	2.26	0.50
2:G:5:TYR:O	2:G:74:ILE:HA	2.11	0.50
2:G:204:LEU:HD11	2:G:214:LEU:HD11	1.93	0.50
2:G:435:VAL:O	2:G:435:VAL:HG13	2.11	0.50
1:F:36:VAL:CG1	1:F:37:PRO:HD2	2.42	0.50
1:F:62:PRO:C	1:F:63:VAL:HG13	2.37	0.50
2:G:4:LYS:HG3	2:G:73:GLN:O	2.11	0.50
1:F:31:VAL:CG1	1:F:32:ASN:N	2.75	0.50
1:F:3:PHE:HB3	1:F:6:LEU:HD12	1.92	0.49
1:F:101:GLU:O	1:F:126:LEU:HD21	2.12	0.49
2:G:431:GLU:CB	2:G:466:ILE:HD13	2.27	0.49
1:F:48:ASP:HB3	1:F:143:MET:HE2	1.93	0.49
1:F:106:ILE:HD12	1:F:106:ILE:H	1.77	0.49
1:F:108:GLU:O	1:F:110:GLY:N	2.44	0.49
1:F:123:ASP:O	1:F:125:PRO:N	2.45	0.49
2:G:312:SER:HB3	2:G:380:THR:CG2	2.42	0.49
1:F:67:ILE:HA	1:F:79:ILE:HB	1.93	0.49
1:F:27:SER:HG	1:F:158:VAL:H	1.60	0.49
2:G:35:PHE:CE1	2:G:47:HIS:CD2	2.83	0.49
2:G:52:ILE:C	2:G:55:THR:HG22	2.35	0.49
2:G:52:ILE:HA	2:G:55:THR:HG22	1.94	0.49
2:G:174:THR:HG21	2:G:178:VAL:CG2	2.42	0.49
2:G:182:ASP:HB3	2:G:242:ILE:HG22	1.91	0.49
2:G:271:MET:C	2:G:272:LEU:HD12	2.37	0.49
1:F:77:PHE:HE2	1:F:79:ILE:CG2	2.25	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:131:VAL:O	2:G:136:PHE:HE2	1.95	0.49
2:G:170:ILE:O	2:G:173:MET:N	2.41	0.49
2:G:184:THR:O	2:G:187:SER:OG	2.30	0.49
2:G:152:ARG:HH21	2:G:208:ASP:CB	2.23	0.49
1:F:40:VAL:HA	1:F:45:ILE:CD1	2.42	0.49
1:F:86:GLU:O	1:F:140:ILE:HA	2.13	0.49
2:G:85:THR:HG23	2:G:103:TRP:HD1	1.77	0.49
2:G:115:LEU:HD22	2:G:120:LEU:HD12	1.95	0.48
2:G:210:PRO:O	2:G:213:MET:HG2	2.13	0.48
2:G:18:ALA:HB2	2:G:59:THR:HG23	1.96	0.48
2:G:16:SER:CB	2:G:55:THR:HG23	2.43	0.48
1:F:106:ILE:HD13	1:F:121:GLU:HG3	1.95	0.48
2:G:434:GLU:HA	2:G:467:GLU:HB2	1.96	0.48
2:G:360:ALA:O	2:G:361:ARG:HG2	2.14	0.47
1:F:124:LEU:O	1:F:124:LEU:HD12	2.14	0.47
2:G:189:THR:HG23	2:G:191:LEU:HG	1.96	0.47
2:G:154:ARG:HH11	2:G:154:ARG:HG2	1.79	0.47
1:F:115:VAL:HG12	1:F:116:GLY:N	2.30	0.47
2:G:49:PRO:HD3	2:G:100:ALA:H	1.78	0.47
2:G:434:GLU:HB3	2:G:465:VAL:HB	1.95	0.47
1:F:20:ILE:HB	1:F:166:ILE:HG12	1.97	0.47
1:F:93:ILE:O	1:F:94:ASP:HB2	2.14	0.47
2:G:85:THR:HG22	2:G:102:VAL:HA	1.96	0.47
1:F:27:SER:OG	1:F:158:VAL:N	2.41	0.47
1:F:77:PHE:CE2	1:F:79:ILE:HG22	2.50	0.47
1:F:94:ASP:HA	7:F:170:HOH:O	2.15	0.47
2:G:52:ILE:CA	2:G:55:THR:HG22	2.45	0.47
2:G:80:THR:HG21	2:G:248:ALA:CB	2.45	0.47
1:F:124:LEU:N	1:F:125:PRO:CD	2.77	0.47
2:G:456:ASN:ND2	2:G:457:LEU:N	2.56	0.47
1:F:52:ILE:HG22	1:F:53:LYS:O	2.15	0.47
1:F:164:ILE:CG2	1:F:165:ARG:N	2.78	0.47
2:G:174:THR:HB	2:G:178:VAL:CG2	2.44	0.47
2:G:253:GLN:NE2	2:G:409:ASP:OD2	2.42	0.47
1:F:150:ILE:CG2	1:F:151:LYS:N	2.79	0.46
2:G:428:THR:CG2	2:G:429:ARG:N	2.78	0.46
2:G:151:SER:O	2:G:160:LEU:HD12	2.15	0.46
2:G:160:LEU:O	2:G:213:MET:HB3	2.16	0.46
2:G:308:MET:HE1	2:G:311:ALA:CB	2.45	0.46
1:F:59:MET:HB2	1:F:59:MET:HE2	1.59	0.46
2:G:83:ARG:HH22	2:G:303:GLU:CD	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:28:ILE:HD12	2:G:28:ILE:HA	1.71	0.46
2:G:342:VAL:HA	2:G:365:PHE:O	2.15	0.46
1:F:32:ASN:HB3	1:F:34:GLU:HG2	1.97	0.46
1:F:78:SER:C	1:F:79:ILE:HG22	2.40	0.46
2:G:199:TRP:HZ2	2:G:215:PRO:HD2	1.81	0.46
2:G:262:LYS:CE	2:G:272:LEU:HD13	2.45	0.46
1:F:158:VAL:C	1:F:160:GLU:H	2.23	0.46
2:G:124:ILE:HD11	2:G:203:MET:HE1	1.98	0.46
2:G:141:VAL:CG2	2:G:162:PHE:CD1	2.98	0.46
2:G:206:VAL:HG12	2:G:207:LEU:N	2.26	0.46
2:G:246:GLN:HG3	2:G:270:PHE:CG	2.51	0.46
2:G:6:ILE:CD1	2:G:454:TRP:CH2	2.99	0.46
2:G:41:LYS:CG	2:G:42:PRO:N	2.76	0.46
2:G:204:LEU:HA	2:G:204:LEU:HD12	1.71	0.46
2:G:317:ARG:HA	2:G:323:ILE:HG13	1.98	0.46
2:G:248:ALA:O	2:G:442:GLY:HA3	2.15	0.46
2:G:174:THR:O	2:G:177:ARG:N	2.37	0.45
2:G:193:ASN:OD1	2:G:195:HIS:N	2.34	0.45
1:F:96:VAL:O	1:F:96:VAL:HG22	2.15	0.45
2:G:352:GLY:O	2:G:356:TRP:N	2.33	0.45
2:G:499:HIS:N	2:G:499:HIS:CD2	2.82	0.45
1:F:79:ILE:CG1	1:F:80:GLU:N	2.78	0.45
2:G:189:THR:HG23	2:G:191:LEU:HB2	1.98	0.45
2:G:317:ARG:HD2	2:G:324:ASN:O	2.16	0.45
2:G:428:THR:HG22	2:G:429:ARG:N	2.31	0.45
2:G:476:THR:O	2:G:479:ARG:HD3	2.16	0.45
1:F:51:ALA:O	1:F:52:ILE:HG13	2.16	0.45
1:F:85:VAL:CG1	1:F:86:GLU:N	2.79	0.45
2:G:190:MET:HB3	2:G:190:MET:HE3	1.42	0.45
1:F:143:MET:CE	1:F:149:LEU:HD13	2.40	0.45
1:F:157:THR:HG23	1:F:160:GLU:HB2	1.93	0.45
2:G:21:MET:HG3	2:G:27:ILE:HD12	1.98	0.45
2:G:53:TRP:HA	2:G:53:TRP:HE3	1.77	0.45
1:F:28:GLY:HA2	1:F:55:THR:HG23	1.98	0.45
1:F:67:ILE:O	1:F:67:ILE:HG13	2.16	0.45
2:G:114:HIS:O	2:G:117:ARG:N	2.47	0.45
2:G:182:ASP:HA	2:G:218:ARG:O	2.17	0.45
1:F:105:ARG:HG3	1:F:107:ALA:O	2.17	0.45
2:G:156:ARG:C	2:G:158:GLY:H	2.25	0.45
1:F:48:ASP:HB2	1:F:143:MET:HE2	1.99	0.45
1:F:52:ILE:O	1:F:54:PRO:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:50:MET:O	2:G:54:ALA:HB2	2.17	0.45
2:G:458:ASP:C	2:G:460:LEU:N	2.75	0.45
1:F:70:ILE:HD13	1:F:70:ILE:HG21	1.63	0.44
2:G:21:MET:HG2	2:G:27:ILE:CD1	2.46	0.44
2:G:189:THR:HG23	2:G:191:LEU:CB	2.46	0.44
1:F:40:VAL:HB	1:F:46:VAL:HG22	1.99	0.44
2:G:7:VAL:HG22	2:G:20:VAL:CG2	2.21	0.44
2:G:130:LEU:N	2:G:130:LEU:HD23	2.30	0.44
2:G:210:PRO:C	2:G:212:GLU:H	2.25	0.44
2:G:308:MET:HE3	2:G:311:ALA:HB3	1.99	0.44
2:G:445:TYR:N	2:G:445:TYR:CD1	2.85	0.44
2:G:486:TRP:O	2:G:489:ALA:HB3	2.17	0.44
1:F:31:VAL:CG1	1:F:32:ASN:H	2.29	0.44
2:G:109:ALA:HA	2:G:134:PRO:HG3	2.00	0.44
2:G:189:THR:HG21	2:G:191:LEU:HB2	1.99	0.44
2:G:313:ILE:HG21	2:G:326:ALA:HB1	2.00	0.44
2:G:210:PRO:C	2:G:212:GLU:N	2.76	0.44
2:G:423:SER:OG	2:G:428:THR:O	2.30	0.44
1:F:30:ILE:CG2	1:F:31:VAL:N	2.79	0.44
1:F:158:VAL:CG2	1:F:159:GLY:N	2.77	0.43
2:G:27:ILE:N	2:G:27:ILE:CD1	2.80	0.43
2:G:11:GLN:CB	2:G:56:GLN:NE2	2.80	0.43
2:G:128:THR:C	2:G:130:LEU:H	2.26	0.43
2:G:189:THR:HG23	2:G:191:LEU:H	1.77	0.43
1:F:79:ILE:HG12	1:F:80:GLU:N	2.27	0.43
1:F:143:MET:HA	1:F:146:ILE:HD13	2.00	0.43
2:G:123:TYR:CD1	2:G:123:TYR:C	2.96	0.43
1:F:67:ILE:HD11	1:F:70:ILE:HG13	1.98	0.43
2:G:225:GLY:O	2:G:238:PRO:HA	2.18	0.43
2:G:246:GLN:HG3	2:G:270:PHE:CB	2.49	0.43
2:G:270:PHE:CD2	2:G:270:PHE:N	2.87	0.43
1:F:136:THR:HA	1:F:137:PRO:HD2	1.93	0.43
2:G:74:ILE:CD1	2:G:237:ILE:N	2.80	0.43
2:G:95:LYS:HA	2:G:96:PRO:HD3	1.63	0.43
2:G:211:ARG:HA	2:G:214:LEU:HD12	2.00	0.43
2:G:219:ARG:O	2:G:224:TYR:OH	2.29	0.43
2:G:21:MET:HA	2:G:26:ASN:O	2.19	0.43
2:G:360:ALA:C	2:G:361:ARG:HG2	2.43	0.43
1:F:30:ILE:C	1:F:31:VAL:HG23	2.43	0.43
1:F:165:ARG:HH11	1:F:165:ARG:CG	2.23	0.43
2:G:108:THR:H	2:G:108:THR:HG23	1.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:141:VAL:HG21	2:G:162:PHE:CD1	2.53	0.43
2:G:107:ARG:C	2:G:109:ALA:H	2.27	0.43
2:G:13:THR:HB	2:G:267:THR:HG21	2.00	0.42
2:G:64:LEU:HD22	2:G:69:ILE:HG21	2.01	0.42
2:G:133:ASP:C	2:G:135:TYR:H	2.27	0.42
2:G:192:PHE:CE2	2:G:217:VAL:HG21	2.54	0.42
2:G:264:THR:O	2:G:269:CYS:HA	2.19	0.42
1:F:63:VAL:HG23	1:F:79:ILE:HD11	2.01	0.42
2:G:57:SER:HB2	2:G:58:SER:H	1.37	0.42
2:G:199:TRP:CZ2	2:G:215:PRO:HD2	2.54	0.42
2:G:80:THR:HG21	2:G:248:ALA:HB3	2.00	0.42
2:G:107:ARG:HG2	2:G:108:THR:HG23	2.01	0.42
1:F:135:LEU:HD23	1:F:135:LEU:HA	1.78	0.42
2:G:141:VAL:CG1	2:G:209:ILE:HD13	2.48	0.42
2:G:272:LEU:HG	2:G:303:GLU:HB2	2.01	0.42
2:G:313:ILE:N	2:G:313:ILE:HD13	2.34	0.42
2:G:334:THR:C	2:G:336:VAL:H	2.28	0.42
1:F:61:ALA:CB	1:F:113:VAL:HG21	2.50	0.42
2:G:53:TRP:HB2	2:G:168:TRP:HE1	1.84	0.42
2:G:70:SER:H	2:G:73:GLN:HG3	1.84	0.42
2:G:226:GLN:CG	2:G:238:PRO:HB3	2.50	0.42
1:F:23:ILE:CD1	1:F:115:VAL:HG21	2.50	0.42
1:F:77:PHE:CE2	1:F:79:ILE:CG2	3.03	0.42
2:G:85:THR:CG2	2:G:103:TRP:CD1	2.99	0.42
2:G:88:VAL:CG1	2:G:89:TRP:N	2.81	0.42
2:G:113:GLU:O	2:G:117:ARG:HB2	2.20	0.42
1:F:98:LEU:N	1:F:98:LEU:CD1	2.80	0.42
1:F:152:LEU:HD21	1:F:165:ARG:HH12	1.85	0.42
2:G:101:ILE:CD1	2:G:107:ARG:HD3	2.43	0.42
1:F:44:LYS:HE2	1:F:48:ASP:OD1	2.20	0.42
2:G:18:ALA:HB3	2:G:63:VAL:CG2	2.50	0.42
2:G:83:ARG:C	2:G:85:THR:H	2.28	0.42
2:G:85:THR:HB	2:G:102:VAL:HA	2.00	0.42
2:G:265:TYR:CD2	2:G:413:VAL:HG12	2.55	0.42
2:G:320:MET:HE3	2:G:320:MET:HB3	1.73	0.42
1:F:158:VAL:C	1:F:160:GLU:N	2.78	0.41
1:F:39:VAL:H	1:F:39:VAL:HG23	1.17	0.41
1:F:158:VAL:HG23	1:F:159:GLY:N	2.35	0.41
2:G:135:TYR:OH	5:G:503:G3H:O1	2.26	0.41
2:G:457:LEU:HD23	2:G:457:LEU:HA	1.70	0.41
1:F:36:VAL:HA	1:F:37:PRO:HD3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:204:LEU:HD21	2:G:214:LEU:HD12	2.02	0.41
2:G:497:GLU:HG3	2:G:498:GLU:H	1.85	0.41
1:F:23:ILE:CG2	1:F:24:ALA:N	2.82	0.41
2:G:353:ALA:HB2	2:G:356:TRP:CZ2	2.56	0.41
2:G:448:GLY:CA	2:G:453:PHE:HB3	2.51	0.41
2:G:174:THR:CB	2:G:178:VAL:CG2	2.99	0.41
2:G:482:ARG:HG3	2:G:482:ARG:NH1	2.32	0.41
1:F:21:GLU:HG3	1:F:165:ARG:HD3	2.03	0.41
1:F:164:ILE:HG22	1:F:165:ARG:N	2.34	0.41
2:G:173:MET:O	2:G:227:THR:OG1	2.36	0.41
2:G:206:VAL:CG1	2:G:207:LEU:HD23	2.48	0.41
2:G:378:ARG:O	2:G:382:GLU:HG3	2.20	0.41
1:F:74:ASN:HB3	1:F:105:ARG:HH11	1.85	0.41
2:G:322:LEU:HA	2:G:322:LEU:HD23	1.90	0.41
1:F:91:PHE:CD1	1:F:91:PHE:C	2.98	0.41
1:F:111:GLN:H	1:F:111:GLN:HG2	1.41	0.41
2:G:89:TRP:HA	2:G:97:ILE:CG2	2.51	0.41
2:G:154:ARG:CG	2:G:154:ARG:NH1	2.77	0.41
2:G:189:THR:HG23	2:G:191:LEU:CG	2.50	0.41
2:G:101:ILE:HD13	2:G:107:ARG:CD	2.44	0.41
2:G:84:GLU:HG2	2:G:136:PHE:HA	2.03	0.40
2:G:419:MET:HE2	2:G:419:MET:HA	2.03	0.40
2:G:84:GLU:HB2	2:G:103:TRP:HB3	2.02	0.40
2:G:141:VAL:HG12	2:G:209:ILE:HD13	2.02	0.40
2:G:156:ARG:HG3	2:G:156:ARG:NH1	2.31	0.40
2:G:458:ASP:C	2:G:460:LEU:H	2.28	0.40
1:F:86:GLU:C	1:F:87:LEU:HG	2.47	0.40
1:F:152:LEU:HD23	1:F:152:LEU:HA	1.88	0.40
2:G:23:HIS:C	2:G:25:ALA:H	2.29	0.40
2:G:357:ASP:OD1	2:G:359:TYR:HB2	2.20	0.40
2:G:389:ARG:O	2:G:393:GLU:HG3	2.21	0.40
2:G:460:LEU:C	2:G:462:GLU:N	2.80	0.40
2:G:81:ASN:ND2	2:G:166:ASP:HB3	2.37	0.40
2:G:189:THR:HG22	2:G:190:MET:N	2.36	0.40
1:F:67:ILE:HD12	1:F:67:ILE:C	2.46	0.40
2:G:41:LYS:HA	2:G:42:PRO:HD2	1.93	0.40
2:G:83:ARG:HH11	5:G:503:G3H:C2	2.34	0.40
2:G:343:TYR:OH	2:G:485:GLY:HA3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	F	113/168 (67%)	97 (86%)	10 (9%)	6 (5%)	1	2
2	G	485/501 (97%)	423 (87%)	49 (10%)	13 (3%)	4	6
All	All	598/669 (89%)	520 (87%)	59 (10%)	19 (3%)	3	4

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	109	GLU
2	G	42	PRO
2	G	219	ARG
2	G	255	CYS
1	F	124	LEU
2	G	57	SER
2	G	175	GLN
2	G	206	VAL
2	G	211	ARG
2	G	138	GLY
1	F	125	PRO
2	G	58	SER
2	G	68	ASP
2	G	210	PRO
2	G	294	PRO
2	G	92	GLU
1	F	68	GLY
1	F	110	GLY
1	F	96	VAL

5.3.2 Protein sidechains

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	F	5/145 (3%)	2 (40%)	3 (60%)	0	0
2	G	292/412 (71%)	228 (78%)	64 (22%)	1	1
All	All	297/557 (53%)	230 (77%)	67 (23%)	1	1

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	55	THR
1	F	58	LYS
1	F	60	VAL
2	G	55	THR
2	G	63	VAL
2	G	69	ILE
2	G	70	SER
2	G	83	ARG
2	G	85	THR
2	G	95	LYS
2	G	97	ILE
2	G	102	VAL
2	G	107	ARG
2	G	110	GLU
2	G	117	ARG
2	G	122	ASP
2	G	124	ILE
2	G	131	VAL
2	G	132	ILE
2	G	151	SER
2	G	152	ARG
2	G	154	ARG
2	G	156	ARG
2	G	159	GLU
2	G	170	ILE
2	G	173	MET
2	G	182	ASP
2	G	189	THR
2	G	190	MET
2	G	204	LEU
2	G	206	VAL
2	G	207	LEU
2	G	208	ASP

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Mol	Chain	Res	Type
2	G	209	ILE
2	G	213	MET
2	G	217	VAL
2	G	219	ARG
2	G	220	SER
2	G	221	SER
2	G	222	GLU
2	G	227	THR
2	G	228	ASN
2	G	269	CYS
2	G	277	GLU
2	G	295	THR
2	G	321	LYS
2	G	337	GLN
2	G	361	ARG
2	G	369	ARG
2	G	378	ARG
2	G	391	VAL
2	G	402	ARG
2	G	425	ILE
2	G	434	GLU
2	G	435	VAL
2	G	449	LEU
2	G	451	VAL
2	G	456	ASN
2	G	457	LEU
2	G	460	LEU
2	G	466	ILE
2	G	468	ARG
2	G	469	GLU
2	G	474	ILE
2	G	475	GLU
2	G	482	ARG
2	G	487	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	G	56	GLN
2	G	179	HIS
2	G	185	ASN
2	G	299	ASN

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Mol	Chain	Res	Type
2	G	387	GLN
2	G	396	GLN
2	G	456	ASN
2	G	499	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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
6	ADP	G	504	4	28,29,29	1.28	1 (3%)	43,45,45	2.42	5 (11%)
5	G3H	G	503	4	8,9,9	2.56	4 (50%)	7,12,12	1.20	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
6	ADP	G	504	4	-	1/16/32/32	0/3/3/3
5	G3H	G	503	4	1/1/2/3	1/7/8/8	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	503	G3H	O1-C1	5.54	1.41	1.20
6	G	504	ADP	PA-O3A	5.35	1.65	1.59
5	G	503	G3H	C3-C2	3.38	1.56	1.51
5	G	503	G3H	P-O1P	2.21	1.67	1.60
5	G	503	G3H	O2-C2	-2.17	1.40	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	504	ADP	C1'-N9-C8	8.67	146.34	127.09
6	G	504	ADP	C4-N9-C1'	-8.05	107.81	126.63
6	G	504	ADP	O2'-C2'-C1'	7.07	134.45	110.10
6	G	504	ADP	O3A-PA-O1A	4.49	124.22	110.70
6	G	504	ADP	O2B-PB-O3A	2.87	114.25	104.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	503	G3H	C2

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	G	503	G3H	O1-C1-C2-C3
6	G	504	ADP	C3'-C4'-C5'-O5'

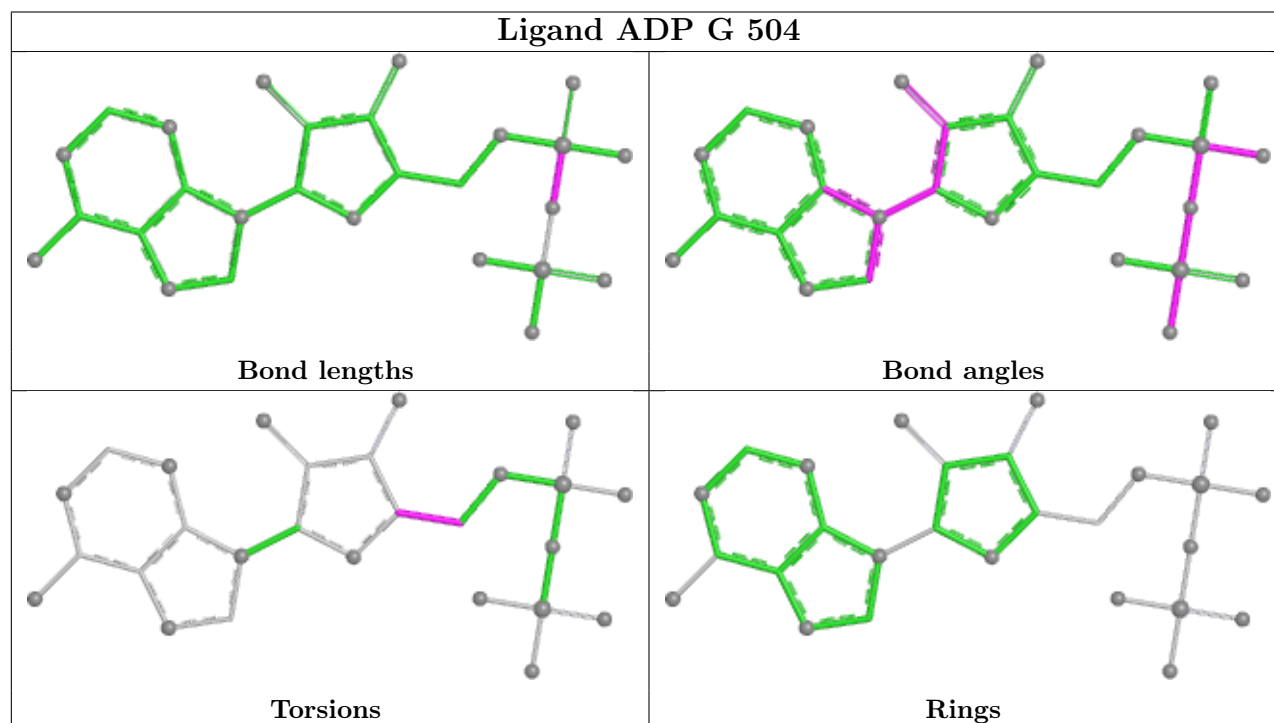
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	G	503	G3H	3	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 than 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.



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 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.