



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:12 am BST

PDB ID : 1GLC  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
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

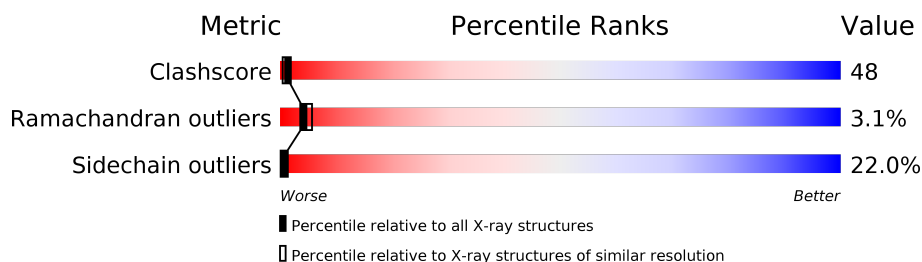
# 1 Overall quality at a glance

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	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	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	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			

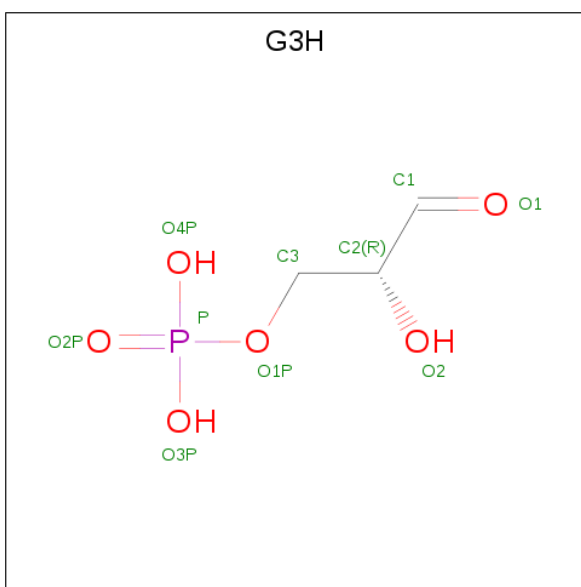
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 5 is GLYCERALDEHYDE-3-PHOSPHATE (three-letter code: G3H) (formula: C<sub>3</sub>H<sub>7</sub>O<sub>6</sub>P).



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 (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



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.

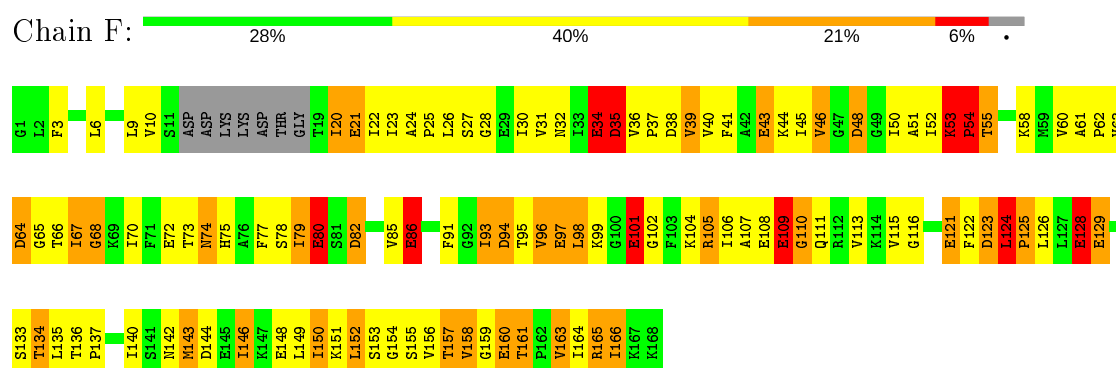
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	F	5	Total 5	O 5	0	0
7	G	37	Total 37	O 37	0	0

### 3 Residue-property plots

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

Note EDS was not executed.

#### • Molecule 1: GLUCOSE-SPECIFIC PROTEIN IIIGlc



## 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 a, b, c, $\alpha$ , $\beta$ , $\gamma$	123.83Å 125.16Å 133.54Å 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 <sup>2</sup> )	37.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: G3H, ZN, MG, 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	1.43	15/1172 (1.3%)	1.74	22/1592 (1.4%)
2	G	1.33	27/3831 (0.7%)	1.75	83/5211 (1.6%)
All	All	1.36	42/5003 (0.8%)	1.75	105/6803 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	1	0
2	G	2	1
All	All	3	1

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	110	GLU	CD-OE2	12.13	1.39	1.25
2	G	62	GLU	CD-OE1	9.56	1.36	1.25
2	G	216	GLU	CD-OE2	9.39	1.35	1.25
2	G	205	GLU	CD-OE2	9.30	1.35	1.25
1	F	128	GLU	CD-OE2	9.13	1.35	1.25
1	F	148	GLU	CD-OE2	9.00	1.35	1.25
1	F	72	GLU	CD-OE2	9.00	1.35	1.25
2	G	277	GLU	CD-OE2	8.67	1.35	1.25
1	F	97	GLU	CD-OE1	8.66	1.35	1.25
1	F	101	GLU	CD-OE2	8.37	1.34	1.25
2	G	498	GLU	CD-OE1	8.20	1.34	1.25
2	G	475	GLU	CD-OE2	8.18	1.34	1.25
2	G	159	GLU	CD-OE1	8.07	1.34	1.25
1	F	129	GLU	CD-OE1	8.07	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	43	GLU	CD-OE2	8.05	1.34	1.25
1	F	80	GLU	CD-OE2	7.96	1.34	1.25
2	G	437	GLU	CD-OE2	7.82	1.34	1.25
2	G	36	GLU	CD-OE1	7.68	1.34	1.25
1	F	86	GLU	CD-OE1	7.64	1.34	1.25
2	G	51	GLU	CD-OE1	7.62	1.34	1.25
2	G	212	GLU	CD-OE2	7.41	1.33	1.25
2	G	393	GLU	CD-OE1	7.39	1.33	1.25
1	F	121	GLU	CD-OE1	7.27	1.33	1.25
2	G	34	GLU	CD-OE1	7.27	1.33	1.25
1	F	21	GLU	CD-OE2	7.17	1.33	1.25
2	G	90	GLU	CD-OE2	7.12	1.33	1.25
2	G	434	GLU	CD-OE1	6.88	1.33	1.25
2	G	382	GLU	CD-OE2	6.70	1.33	1.25
2	G	297	GLU	CD-OE2	6.64	1.32	1.25
2	G	478	GLU	CD-OE1	6.61	1.32	1.25
2	G	283	GLU	CD-OE2	6.48	1.32	1.25
2	G	469	GLU	CD-OE1	6.46	1.32	1.25
2	G	431	GLU	CD-OE2	6.08	1.32	1.25
2	G	319	GLU	CD-OE1	6.05	1.32	1.25
1	F	34	GLU	CD-OE2	5.98	1.32	1.25
2	G	467	GLU	CD-OE2	5.81	1.32	1.25
1	F	160	GLU	CD-OE2	5.78	1.32	1.25
2	G	382	GLU	CD-OE1	5.49	1.31	1.25
2	G	258	GLU	CD-OE1	5.46	1.31	1.25
1	F	144	ASP	CG-OD1	5.22	1.37	1.25
1	F	109	GLU	CD-OE2	5.16	1.31	1.25
2	G	113	GLU	CD-OE2	5.15	1.31	1.25

All (105) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	245	ASP	CB-CG-OD2	-14.33	105.40	118.30
2	G	209	ILE	C-N-CD	-12.47	93.17	120.60
2	G	328	ASP	CB-CG-OD1	-12.30	107.23	118.30
2	G	41	LYS	C-N-CD	-9.85	98.92	120.60
2	G	328	ASP	CB-CG-OD2	9.09	126.48	118.30
2	G	378	ARG	NE-CZ-NH2	-8.61	116.00	120.30
2	G	482	ARG	NE-CZ-NH1	8.45	124.53	120.30
2	G	70	SER	N-CA-CB	8.32	122.98	110.50
1	F	94	ASP	CB-CG-OD2	-8.26	110.87	118.30
2	G	201	ASP	CB-CG-OD1	-8.21	110.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	200	ASP	CB-CG-OD2	-8.10	111.01	118.30
2	G	482	ARG	NE-CZ-NH2	-8.05	116.28	120.30
1	F	35	ASP	CB-CG-OD1	7.97	125.47	118.30
2	G	156	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	G	318	ASP	CB-CG-OD1	7.85	125.37	118.30
1	F	48	ASP	CB-CG-OD2	-7.83	111.25	118.30
2	G	325	ASP	CB-CG-OD2	-7.79	111.29	118.30
2	G	117	ARG	NE-CZ-NH1	7.74	124.17	120.30
2	G	133	ASP	CB-CG-OD2	-7.72	111.35	118.30
2	G	388	THR	CA-CB-CG2	-7.57	101.80	112.40
2	G	166	ASP	CB-CG-OD2	7.55	125.10	118.30
2	G	201	ASP	CB-CG-OD2	7.55	125.09	118.30
2	G	106	ARG	NE-CZ-NH2	-7.48	116.56	120.30
2	G	468	ARG	NE-CZ-NH2	-7.47	116.56	120.30
2	G	198	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	F	124	LEU	C-N-CD	-7.14	104.90	120.60
1	F	94	ASP	CB-CG-OD1	6.98	124.58	118.30
2	G	361	ARG	NE-CZ-NH1	6.94	123.77	120.30
1	F	82	ASP	CB-CG-OD2	6.94	124.54	118.30
2	G	402	ARG	NE-CZ-NH1	6.93	123.77	120.30
2	G	146	ASP	CB-CG-OD2	-6.89	112.09	118.30
1	F	35	ASP	CB-CG-OD2	-6.87	112.11	118.30
2	G	182	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	F	53	LYS	C-N-CD	-6.70	105.85	120.60
2	G	275	THR	CA-CB-CG2	-6.58	103.19	112.40
1	F	60	VAL	N-CA-CB	-6.55	97.08	111.50
1	F	48	ASP	CB-CG-OD1	6.50	124.15	118.30
2	G	107	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	G	331	TYR	CB-CG-CD1	-6.40	117.16	121.00
2	G	318	ASP	CB-CG-OD2	-6.38	112.56	118.30
2	G	122	ASP	CB-CG-OD2	-6.28	112.65	118.30
2	G	182	ASP	CB-CG-OD1	6.28	123.95	118.30
2	G	382	GLU	CG-CD-OE2	-6.26	105.79	118.30
2	G	190	MET	CG-SD-CE	-6.25	90.20	100.20
2	G	458	ASP	CB-CG-OD1	-6.24	112.69	118.30
2	G	83	ARG	NE-CZ-NH2	-6.23	117.18	120.30
2	G	198	ASP	CB-CG-OD1	6.20	123.88	118.30
2	G	465	VAL	CB-CA-C	-6.17	99.67	111.40
2	G	48	ASP	CB-CG-OD1	-6.17	112.74	118.30
2	G	88	VAL	CA-CB-CG1	-6.08	101.78	110.90
2	G	389	ARG	NE-CZ-NH1	6.07	123.34	120.30
2	G	188	ARG	NE-CZ-NH2	6.07	123.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	407	ARG	NE-CZ-NH1	6.03	123.31	120.30
2	G	133	ASP	CB-CG-OD1	5.95	123.66	118.30
2	G	189	THR	N-CA-CB	-5.94	99.02	110.30
2	G	336	VAL	N-CA-C	5.94	127.03	111.00
2	G	219	ARG	NE-CZ-NH1	5.93	123.27	120.30
2	G	354	PRO	CB-CA-C	-5.92	97.21	112.00
2	G	218	ARG	NE-CZ-NH1	5.89	123.25	120.30
1	F	64	ASP	CB-CG-OD2	-5.86	113.03	118.30
2	G	114	HIS	CA-CB-CG	-5.86	103.64	113.60
1	F	82	ASP	CB-CG-OD1	-5.86	113.03	118.30
2	G	166	ASP	CB-CG-OD1	-5.85	113.03	118.30
2	G	361	ARG	NE-CZ-NH2	-5.84	117.38	120.30
2	G	288	THR	CA-CB-CG2	-5.83	104.25	112.40
1	F	64	ASP	CB-CG-OD1	5.82	123.53	118.30
2	G	188	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	F	144	ASP	CB-CG-OD1	-5.71	113.16	118.30
2	G	54	ALA	N-CA-CB	-5.66	102.17	110.10
2	G	106	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	G	357	ASP	CB-CG-OD2	-5.64	113.22	118.30
2	G	390	ASP	CB-CG-OD1	-5.60	113.26	118.30
2	G	409	ASP	CB-CG-OD1	5.58	123.32	118.30
2	G	102	VAL	CA-CB-CG2	-5.57	102.55	110.90
2	G	404	HIS	CA-CB-CG	-5.43	104.37	113.60
2	G	200	ASP	CB-CG-OD1	5.41	123.17	118.30
2	G	325	ASP	CB-CA-C	-5.40	99.61	110.40
2	G	458	ASP	CB-CG-OD2	5.38	123.14	118.30
2	G	385	ALA	CB-CA-C	-5.37	102.05	110.10
1	F	123	ASP	CB-CG-OD1	-5.36	113.47	118.30
2	G	390	ASP	CB-CG-OD2	5.35	123.12	118.30
2	G	357	ASP	CB-CG-OD1	5.32	123.09	118.30
2	G	402	ARG	NE-CZ-NH2	-5.30	117.65	120.30
2	G	208	ASP	CB-CG-OD1	-5.28	113.55	118.30
2	G	256	VAL	N-CA-C	5.28	125.26	111.00
2	G	69	ILE	N-CA-CB	-5.27	98.67	110.80
2	G	123	TYR	CB-CG-CD2	-5.26	117.84	121.00
2	G	81	ASN	N-CA-CB	-5.25	101.15	110.60
2	G	477	THR	CA-CB-CG2	-5.22	105.09	112.40
2	G	108	THR	CA-CB-CG2	-5.22	105.09	112.40
2	G	389	ARG	NE-CZ-NH2	-5.20	117.70	120.30
2	G	407	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	F	60	VAL	CB-CA-C	-5.17	101.58	111.40
2	G	22	ASP	CB-CG-OD1	-5.16	113.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	54	PRO	C-N-CA	5.15	134.58	121.70
1	F	152	LEU	CA-CB-CG	-5.12	103.51	115.30
1	F	144	ASP	CB-CG-OD2	5.10	122.89	118.30
2	G	22	ASP	CB-CG-OD2	5.09	122.89	118.30
2	G	215	PRO	N-CA-CB	5.08	109.40	103.30
1	F	54	PRO	N-CA-C	5.05	125.24	112.10
1	F	150	ILE	N-CA-CB	5.04	122.39	110.80
2	G	317	ARG	NE-CZ-NH2	-5.03	117.78	120.30
2	G	24	ASP	CB-CG-OD1	-5.02	113.78	118.30
2	G	382	GLU	CG-CD-OE1	5.02	128.34	118.30
1	F	150	ILE	CA-C-N	-5.02	106.16	117.20

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	137	0
2	G	3752	0	3605	327	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	3	0
All	All	4990	0	4755	463	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 48.

All (463) 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
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
1:F:156:VAL:HG12	1:F:161:THR:HB	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:13:THR:HG1	2:G:103:TRP:HE1	1.33	0.75
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:HH11	1:F:165:ARG:HG3	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:206:VAL:HG12	2:G:207:LEU:HD23	1.73	0.70
2:G:23:HIS:HA	2:G:453:PHE:HE1	1.56	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:308:MET:HE3	2:G:311:ALA:HB3	1.73	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:ILE:CD1	1:F:121:GLU:HG3	2.22	0.69
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:NH1	1:F:165:ARG:HG3	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
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: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: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:N	2:G:27:ILE:HD13	2.12	0.64
2:G:340:ASN:HB2	2:G:375:HIS:CD2	2.32	0.64
2:G:330:GLU:OE2	2:G:416:ASN:N	2.31	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:128:THR:HB	7:G:539:HOH:O	1.99	0.63
2:G:90:GLU:OE2	2:G:154:ARG:NH2	2.31	0.63
2:G:85:THR:CG2	2:G:102:VAL:HA	2.28	0.63
1:F:106:ILE:HD11	1:F:121:GLU:CB	2.28	0.63
1:F:23:ILE:HD13	1:F:115:VAL:CG1	2.26	0.63
2:G:46:GLU:OE2	2:G:107:ARG:NH2	2.27	0.63
2:G:161:LEU:N	2:G:161:LEU:HD23	2.13	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:52:ILE:O	2:G:55:THR:HG22	1.99	0.63
2:G:145:LEU:HB2	2:G:152:ARG:HH12	1.64	0.63
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:HH11	2:G:361:ARG:HG2	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:458:ASP:OD1	2:G:458:ASP:N	2.33	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:189:THR:CG2	2:G:191:LEU:HB2	2.31	0.60
2:G:152:ARG:O	2:G:155:ALA:N	2.34	0.60
2:G:90:GLU:OE1	2:G:93:THR:HG21	2.01	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: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:160:LEU:C	2:G:161:LEU:HD23	2.22	0.59
2:G:150:GLY:O	2:G:154:ARG:HD3	2.02	0.59
2:G:271:MET:HG2	2:G:395:MET:HE1	1.84	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:140:ILE:CD1	1:F:149:LEU:HD11	2.33	0.58
2:G:85:THR:CG2	2:G:103:TRP:HD1	2.16	0.58
2:G:11:GLN:HB2	2:G:56:GLN:NE2	2.15	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:91:LYS:NZ	2:G:158:GLY:O	2.29	0.58
2:G:155:ALA:HB2	2:G:160:LEU:CB	2.33	0.58
2:G:201:ASP:CG	2:G:211:ARG:HH12	2.06	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: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: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:143:MET:HE1	1:F:149:LEU:HD13	1.88	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
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
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:162:PHE:CG	2:G:163:GLY:N	2.75	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:106:ILE:HD12	1:F:106:ILE:N	2.22	0.54
1:F:30:ILE:HG22	1:F:31:VAL:N	2.23	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: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: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:391:VAL:HG12	2:G:392:LEU:N	2.24	0.52
1:F:143:MET:CE	1:F:149:LEU:HD13	2.40	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:343:TYR:CZ	2:G:485:GLY:HA3	2.45	0.52
2:G:392:LEU:HD23	2:G:392:LEU:C	2.30	0.52
1:F:91:PHE:O	1:F:95:THR:HG21	2.10	0.52
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:389:ARG:O	2:G:389:ARG:HG3	2.09	0.52
2:G:6:ILE:HD13	2:G:454:TRP:CH2	2.45	0.52
2:G:255:CYS:HB3	2:G:260:MET:HB2	1.92	0.52
2:G:173:MET:C	2:G:175:GLN:H	2.12	0.51
1:F:10:VAL:O	1:F:10:VAL:HG12	2.10	0.51
1:F:43:GLU:OE1	2:G:402:ARG:NH2	2.43	0.51
1:F:93:ILE:C	1:F:93:ILE:HD12	2.30	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:297:GLU:OE1	2:G:297:GLU:N	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:335:LYS:NZ	7:G:527:HOH:O	2.41	0.50
2:G:87:ILE:HG22	2:G:88:VAL:N	2.26	0.50
2:G:134:PRO:O	2:G:140:LYS:NZ	2.33	0.50
2:G:204:LEU:HD11	2:G:214:LEU:HD11	1.93	0.50
2:G:435:VAL:HG13	2:G:435:VAL:O	2.11	0.50
2:G:5:TYR:O	2:G:74:ILE:HA	2.11	0.50
1:F:36:VAL:CG1	1:F:37:PRO:HD2	2.42	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:101:GLU:O	1:F:126:LEU:HD21	2.12	0.49
1:F:3:PHE:HB3	1:F:6:LEU:HD12	1.92	0.49
2:G:431:GLU:CB	2:G:466:ILE:HD13	2.27	0.49
2:G:11:GLN:CD	2:G:52:ILE:HG23	2.32	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
2:G:35:PHE:CE1	2:G:47:HIS:CD2	2.83	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
1:F:77:PHE:HE2	1:F:79:ILE:CG2	2.25	0.49
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: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:475:GLU:CD	2:G:475:GLU:H	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:190:MET:HB3	2:G:190:MET:HE3	1.57	0.48
2:G:360:ALA:O	2:G:361:ARG:HG2	2.14	0.47
1:F:124:LEU:HD12	1:F:124:LEU:O	2.14	0.47
2:G:155:ALA:C	2:G:158:GLY:H	2.18	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:27:SER:HG	1:F:158:VAL:H	1.62	0.47
1:F:115:VAL:HG12	1:F:116:GLY:N	2.30	0.47
2:G:434:GLU:HB3	2:G:465:VAL:HB	1.95	0.47
2:G:49:PRO:HD3	2:G:100:ALA:H	1.78	0.47
1:F:93:ILE:O	1:F:94:ASP:HB2	2.14	0.47
1:F:20:ILE:HB	1:F:166:ILE:HG12	1.97	0.47
2:G:85:THR:HG22	2:G:102:VAL:HA	1.96	0.47
2:G:246:GLN:CD	2:G:270:PHE:HB2	2.32	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:80:THR:HG21	2:G:248:ALA:CB	2.45	0.47
2:G:52:ILE:CA	2:G:55:THR:HG22	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:164:ILE:CG2	1:F:165:ARG:N	2.78	0.47
1:F:52:ILE:HG22	1:F:53:LYS:O	2.15	0.47
2:G:174:THR:HB	2:G:178:VAL:CG2	2.44	0.47
2:G:184:THR:O	2:G:187:SER:OG	2.30	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: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
2:G:21:MET:HE1	2:G:444:ALA:HB2	1.97	0.46
1:F:32:ASN:HB3	1:F:34:GLU:HG2	1.97	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:48:ASP:HB3	1:F:143:MET:HE1	1.96	0.46
2:G:124:ILE:HD11	2:G:203:MET:HE1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:204:LEU:HD12	2:G:204:LEU:HA	1.71	0.46
2:G:317:ARG:HA	2:G:323:ILE:HG13	1.98	0.46
2:G:41:LYS:CG	2:G:42:PRO:N	2.76	0.46
2:G:6:ILE:CD1	2:G:454:TRP:CH2	2.99	0.46
2:G:52:ILE:C	2:G:55:THR:HG22	2.35	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:HG22	1:F:96:VAL:O	2.15	0.45
2:G:352:GLY:O	2:G:356:TRP:N	2.33	0.45
2:G:499:HIS:CD2	2:G:499:HIS:N	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
1:F:157:THR:HG23	1:F:160:GLU:HB2	1.93	0.45
2:G:13:THR:OG1	2:G:103:TRP:NE1	2.28	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:62:PRO:C	1:F:63:VAL:HG13	2.37	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:271:MET:CG	2:G:395:MET:HE1	2.47	0.45
1:F:52:ILE:O	1:F:54:PRO:HD3	2.16	0.45
2:G:50:MET:O	2:G:54:ALA:HB2	2.17	0.45
1:F:70:ILE:HD13	1:F:70:ILE:HG21	1.63	0.44
2:G:189:THR:HG23	2:G:191:LEU:CB	2.46	0.44
2:G:21:MET:HG2	2:G:27:ILE:CD1	2.46	0.44
1:F:40:VAL:HB	1:F:46:VAL:HG22	1.99	0.44
1:F:79:ILE:HG12	1:F:80:GLU:N	2.27	0.44
2:G:271:MET:C	2:G:272:LEU:HD12	2.37	0.44
2:G:130:LEU:N	2:G:130:LEU:HD23	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:7:VAL:HG22	2:G:20:VAL:CG2	2.21	0.44
2:G:445:TYR:CD1	2:G:445:TYR:N	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:190:MET:HB2	2:G:190:MET:HE2	1.76	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:189:THR:HG23	2:G:191:LEU:H	1.77	0.43
1:F:143:MET:HA	1:F:146:ILE:HD13	2.00	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:N	2:G:270:PHE:CD2	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:211:ARG:HA	2:G:214:LEU:HD12	2.00	0.43
2:G:95:LYS:HA	2:G:96:PRO:HD3	1.63	0.43
2:G:21:MET:HA	2:G:26:ASN:O	2.19	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
2:G:141:VAL:HG21	2:G:162:PHE:CD1	2.53	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: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:199:TRP:CZ2	2:G:215:PRO:HD2	2.54	0.42
2:G:57:SER:HB2	2:G:58:SER:H	1.37	0.42
2:G:107:ARG:HG2	2:G:108:THR:HG23	2.01	0.42
2:G:80:THR:HG21	2:G:248:ALA:HB3	2.00	0.42
1:F:135:LEU:HA	1:F:135:LEU:HD23	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
1:F:61:ALA:CB	1:F:113:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:53:TRP:HB2	2:G:168:TRP:HE1	1.84	0.42
2:G:226:GLN:CG	2:G:238:PRO:HB3	2.50	0.42
2:G:70:SER:H	2:G:73:GLN:HG3	1.84	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:113:GLU:O	2:G:117:ARG:HB2	2.20	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
1:F:152:LEU:HD21	1:F:165:ARG:HH12	1.85	0.42
1:F:98:LEU:CD1	1:F:98:LEU:N	2.80	0.42
2:G:101:ILE:CD1	2:G:107:ARG:HD3	2.43	0.42
2:G:90:GLU:HB2	2:G:93:THR:HG1	1.84	0.42
1:F:44:LYS:HE2	1:F:48:ASP:OD1	2.20	0.42
2:G:85:THR:HB	2:G:102:VAL:HA	2.00	0.42
2:G:18:ALA:HB3	2:G:63:VAL:CG2	2.50	0.42
2:G:265:TYR:CD2	2:G:413:VAL:HG12	2.55	0.42
1:F:158:VAL:HG23	1:F:159:GLY:N	2.35	0.41
1:F:39:VAL:HG23	1:F:39:VAL:H	1.17	0.41
2:G:457:LEU:HA	2:G:457:LEU:HD23	1.70	0.41
2:G:135:TYR:OH	5:G:503:G3H:O1	2.26	0.41
1:F:36:VAL:HA	1:F:37:PRO:HD3	1.80	0.41
1:F:78:SER:C	1:F:79:ILE:HG22	2.40	0.41
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
2:G:83:ARG:HH22	2:G:303:GLU:CD	2.24	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
1:F:158:VAL:C	1:F:160:GLU:H	2.23	0.41
2:G:482:ARG:HG3	2:G:482:ARG:NH1	2.32	0.41
1:F:164:ILE:HG22	1:F:165:ARG:N	2.34	0.41
1:F:21:GLU:HG3	1:F:165:ARG:HD3	2.03	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:HD23	2:G:322:LEU:HA	1.90	0.41
1:F:111:GLN:HG2	1:F:111:GLN:H	1.41	0.41
2:G:189:THR:HG23	2:G:191:LEU:CG	2.50	0.41
2:G:89:TRP:HA	2:G:97:ILE:CG2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:154:ARG:NH1	2:G:154:ARG:CG	2.77	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
1:F:27:SER:HG	1:F:158:VAL:HG12	1.86	0.40
2:G:156:ARG:HG3	2:G:156:ARG:NH1	2.31	0.40
2:G:141:VAL:HG12	2:G:209:ILE:HD13	2.02	0.40
2:G:84:GLU:HB2	2:G:103:TRP:HB3	2.02	0.40
1:F:152:LEU:HD23	1:F:152:LEU:HA	1.88	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:271:MET:SD	2:G:395:MET:HE1	2.62	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
2:G:343:TYR:OH	2:G:485:GLY:HA3	2.22	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

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	157/168 (94%)	134 (85%)	16 (10%)	7 (4%)	2	2
2	G	485/501 (97%)	423 (87%)	49 (10%)	13 (3%)	5	6
All	All	642/669 (96%)	557 (87%)	65 (10%)	20 (3%)	4	5

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	109	GLU
2	G	42	PRO

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Mol	Chain	Res	Type
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	54	PRO
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	123/145 (85%)	86 (70%)	37 (30%)	0	0
2	G	378/412 (92%)	305 (81%)	73 (19%)	1	1
All	All	501/557 (90%)	391 (78%)	110 (22%)	1	0

All (110) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	9	LEU
1	F	20	ILE
1	F	26	LEU
1	F	34	GLU
1	F	35	ASP

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Mol	Chain	Res	Type
1	F	39	VAL
1	F	46	VAL
1	F	50	ILE
1	F	53	LYS
1	F	55	THR
1	F	58	LYS
1	F	64	ASP
1	F	66	THR
1	F	67	ILE
1	F	74	ASN
1	F	79	ILE
1	F	80	GLU
1	F	86	GLU
1	F	93	ILE
1	F	98	LEU
1	F	99	LYS
1	F	101	GLU
1	F	105	ARG
1	F	128	GLU
1	F	129	GLU
1	F	133	SER
1	F	134	THR
1	F	142	ASN
1	F	143	MET
1	F	146	ILE
1	F	155	SER
1	F	157	THR
1	F	158	VAL
1	F	161	THR
1	F	163	VAL
1	F	165	ARG
1	F	166	ILE
2	G	4	LYS
2	G	5	TYR
2	G	6	ILE
2	G	11	GLN
2	G	17	ARG
2	G	21	MET
2	G	24	ASP
2	G	27	ILE
2	G	28	ILE
2	G	29	SER

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Mol	Chain	Res	Type
2	G	32	GLN
2	G	39	TYR
2	G	47	HIS
2	G	51	GLU
2	G	55	THR
2	G	63	VAL
2	G	69	ILE
2	G	70	SER
2	G	73	GLN
2	G	80	THR
2	G	83	ARG
2	G	85	THR
2	G	95	LYS
2	G	97	ILE
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	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
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	227	THR
2	G	228	ASN

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Mol	Chain	Res	Type
2	G	255	CYS
2	G	262	LYS
2	G	269	CYS
2	G	277	GLU
2	G	295	THR
2	G	314	GLN
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	456	ASN
2	G	457	LEU
2	G	460	LEU
2	G	468	ARG
2	G	474	ILE
2	G	482	ARG
2	G	487	LYS

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

Mol	Chain	Res	Type
1	F	74	ASN
1	F	142	ASN
2	G	47	HIS
2	G	56	GLN
2	G	81	ASN
2	G	179	HIS
2	G	185	ASN
2	G	284	ASN
2	G	299	ASN
2	G	396	GLN
2	G	456	ASN
2	G	499	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	$\# Z  > 2$
5	G3H	G	503	4	8,9,9	2.47	4 (50%)	10,12,12	1.20	0
6	ADP	G	504	4	24,29,29	0.98	1 (4%)	29,45,45	2.67	6 (20%)

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
5	G3H	G	503	4	1/1/2/3	1/7/8/8	-
6	ADP	G	504	4	-	1/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	503	G3H	O1-C1	5.29	1.41	1.19
5	G	503	G3H	C3-C2	3.38	1.56	1.51
6	G	504	ADP	C8-N7	-2.32	1.30	1.34
5	G	503	G3H	P-O1P	2.20	1.67	1.60
5	G	503	G3H	O2-C2	-2.04	1.40	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	504	ADP	C1'-N9-C4	-10.72	107.81	126.64
6	G	504	ADP	O2'-C2'-C1'	6.39	134.45	110.85
6	G	504	ADP	PA-O3A-PB	-3.53	120.70	132.83
6	G	504	ADP	O2B-PB-O3A	2.87	114.25	104.64
6	G	504	ADP	C4-C5-N7	2.24	111.73	109.40
6	G	504	ADP	C3'-C2'-C1'	2.21	104.31	100.98

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	G	503	G3H	C2

All (2) torsion outliers are listed below:

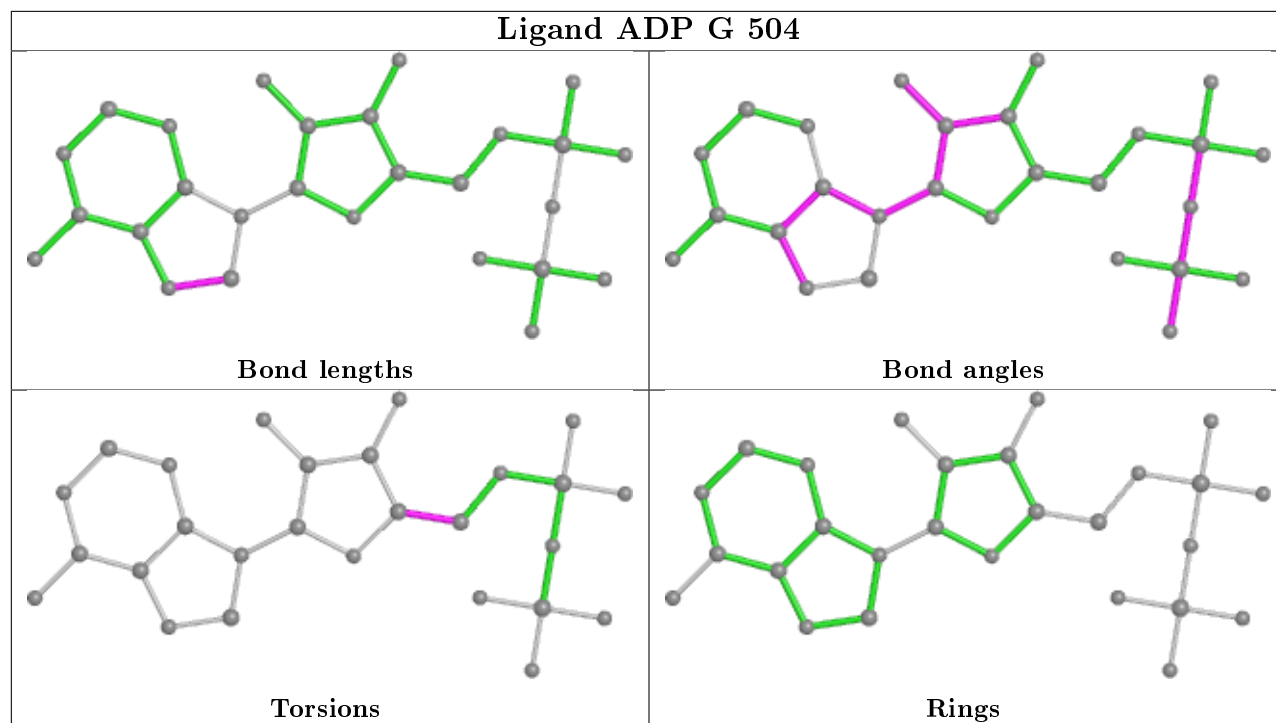
Mol	Chain	Res	Type	Atoms
5	G	503	G3H	O1-C1-C2-C3
6	G	504	ADP	C3'-C4'-C5'-O5'

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.