



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:18 PM UTC

PDB ID : 1GLD / pdb_00001gld
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 : 2.93 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

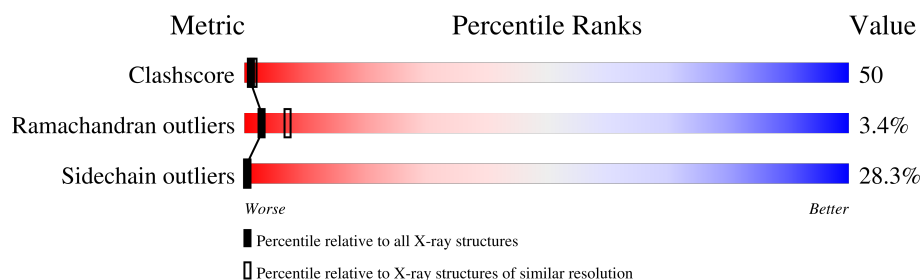
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.93 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	1184 (2.96-2.92)
Ramachandran outliers	187476	1131 (2.96-2.92)
Sidechain outliers	187428	1131 (2.96-2.92)

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	27% 32% 27% 11% .
2	G	501	30% 38% 24% 6% .

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
4	G3H	G	503	X	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 4957 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 IIIGlc.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	F	161	Total	C	N	O	S	0	0	0
			1150	738	181	229	2			

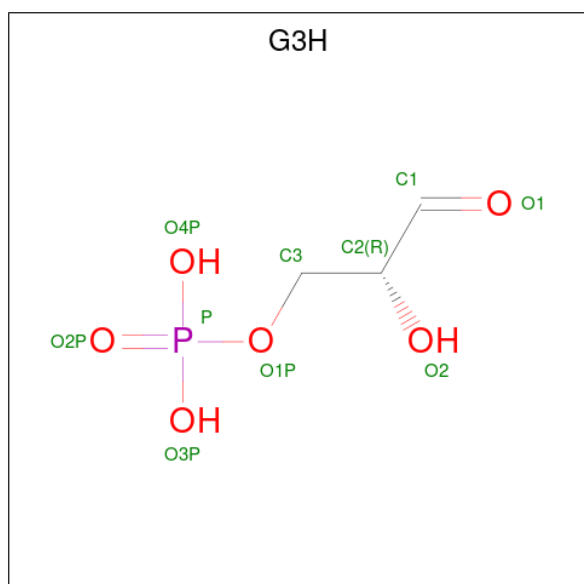
- Molecule 2 is a protein called GLYCEROL KINASE.

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 MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

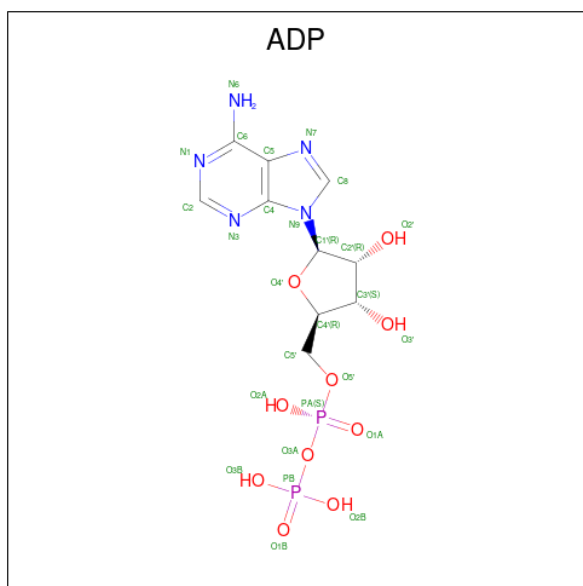
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Mn	0	0
			1	1		

- Molecule 4 is GLYCERALDEHYDE-3-PHOSPHATE (CCD ID: G3H) (formula: C₃H₇O₆P).



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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

- Molecule 6 is water.

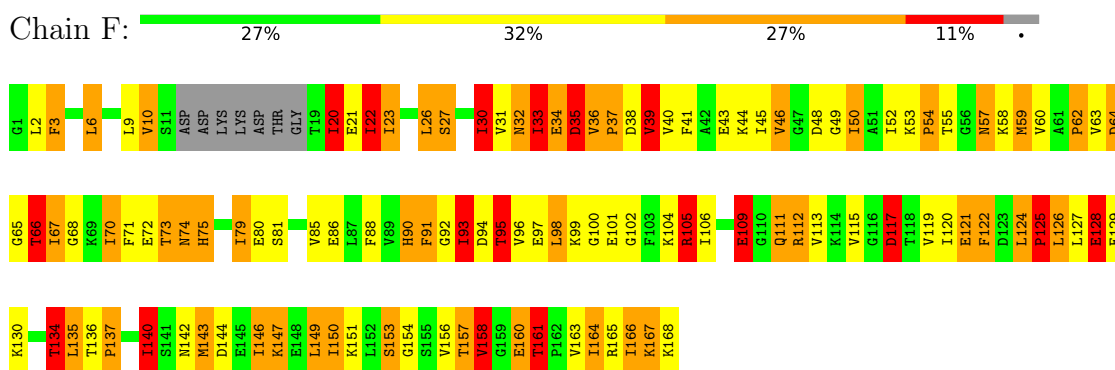
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	2	Total O 2 2	0	0
6	G	15	Total O 15 15	0	0

3 Residue-property plots

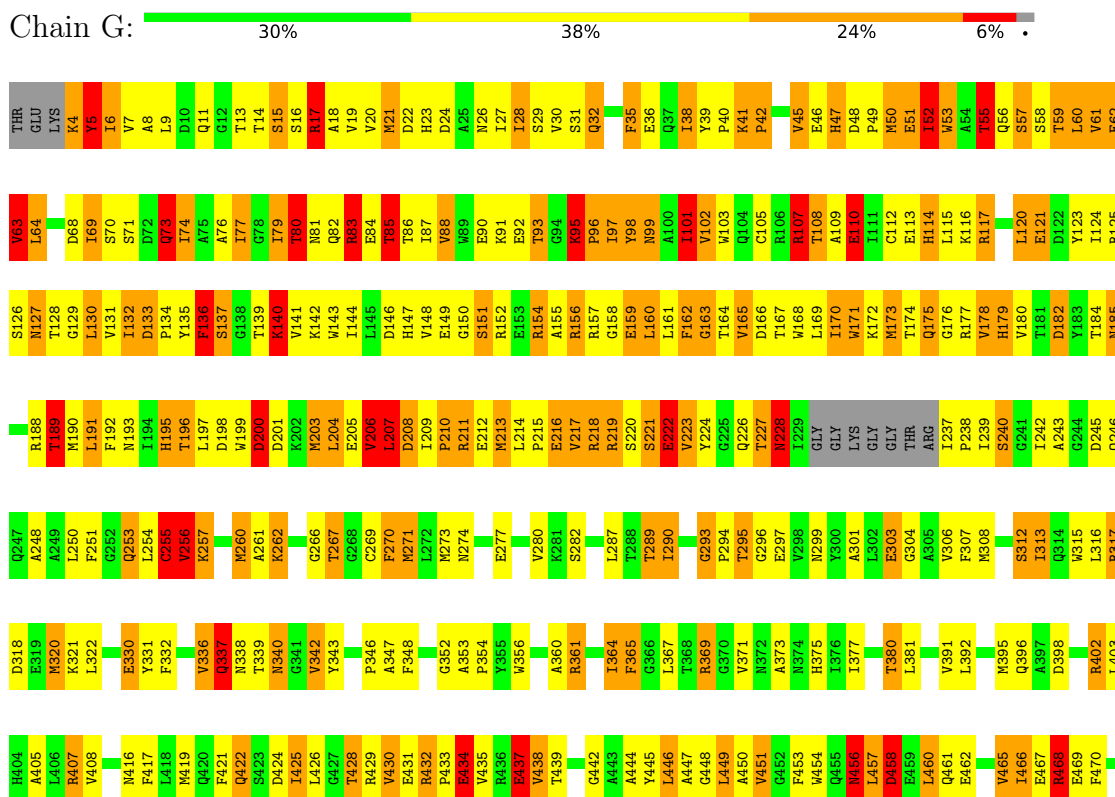
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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



G473	I474	E475	T476	T477	E478	R479		R482	Y483	A484	G485	W486	K487	K488	A489	V490		M494		E498	H499	ASP	GLU
------	------	------	------	------	------	------	--	------	------	------	------	------	------	------	------	------	--	------	--	------	------	-----	-----

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, α , β , γ	122.98Å 125.87Å 134.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	14.60 – 2.93	Depositor
% Data completeness (in resolution range)	(Not available) (14.60-2.93)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.134 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4957	wwPDB-VP
Average B, all atoms (Å ²)	33.0	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: ADP, G3H, MN

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	1.66	13/1165 (1.1%)	2.32	75/1583 (4.7%)
2	G	1.63	28/3831 (0.7%)	2.10	156/5211 (3.0%)
All	All	1.64	41/4996 (0.8%)	2.15	231/6794 (3.4%)

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	4	0
2	G	5	1
All	All	9	1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	408	VAL	CA-C	-7.87	1.44	1.52
2	G	377	ILE	CA-CB	-7.77	1.45	1.54
2	G	371	VAL	CA-CB	-6.70	1.45	1.54
1	F	91	PHE	CA-C	-6.67	1.44	1.52
2	G	336	VAL	C-N	-6.59	1.24	1.33
1	F	88	PHE	N-CA	-6.11	1.38	1.46
2	G	364	ILE	CA-CB	-6.03	1.47	1.54
2	G	110	GLU	CD-OE1	6.02	1.36	1.25
1	F	90	HIS	CA-C	-6.01	1.45	1.52
2	G	405	ALA	CA-C	-5.89	1.45	1.52
2	G	377	ILE	N-CA	-5.88	1.39	1.46
1	F	137	PRO	CA-C	-5.88	1.45	1.52
2	G	437	GLU	CD-OE2	5.78	1.36	1.25
1	F	72	GLU	CD-OE2	5.68	1.36	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	22	ILE	N-CA	-5.67	1.39	1.46
1	F	167	LYS	C-O	5.63	1.30	1.24
2	G	114	HIS	CA-C	-5.52	1.46	1.52
1	F	144	ASP	CG-OD2	5.48	1.35	1.25
2	G	62	GLU	CD-OE1	5.48	1.35	1.25
1	F	30	ILE	CA-CB	-5.48	1.48	1.54
2	G	295	THR	CA-C	-5.41	1.46	1.53
2	G	434	GLU	CD-OE1	5.39	1.35	1.25
2	G	38	ILE	CA-C	-5.36	1.46	1.52
1	F	46	VAL	CA-CB	-5.36	1.46	1.54
2	G	224	TYR	C-N	5.30	1.38	1.33
2	G	107	ARG	C-O	-5.26	1.18	1.24
2	G	216	GLU	CD-OE2	5.26	1.35	1.25
2	G	36	GLU	CD-OE1	5.25	1.35	1.25
1	F	121	GLU	CD-OE1	5.24	1.35	1.25
2	G	458	ASP	CG-OD1	5.21	1.35	1.25
2	G	206	VAL	CA-CB	-5.19	1.47	1.54
1	F	128	GLU	CD-OE2	5.15	1.35	1.25
2	G	424	ASP	C-N	-5.12	1.28	1.34
2	G	312	SER	C-N	-5.10	1.27	1.33
2	G	102	VAL	CA-C	-5.09	1.47	1.53
2	G	133	ASP	CG-OD2	5.07	1.34	1.25
2	G	371	VAL	N-CA	-5.07	1.40	1.46
2	G	24	ASP	CG-OD1	5.05	1.34	1.25
2	G	96	PRO	N-CA	-5.03	1.41	1.47
1	F	39	VAL	CA-CB	-5.02	1.47	1.54
2	G	498	GLU	CD-OE1	5.00	1.34	1.25

All (231) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	35	ASP	CA-CB-CG	13.69	126.29	112.60
2	G	42	PRO	N-CA-CB	11.42	115.24	103.25
1	F	111	GLN	N-CA-C	11.35	125.78	110.35
2	G	336	VAL	N-CA-C	11.14	124.72	113.47
2	G	332	PHE	CA-CB-CG	-9.71	104.09	113.80
2	G	85	THR	CA-C-N	9.61	135.16	121.42
2	G	85	THR	C-N-CA	9.61	135.16	121.42
2	G	185	ASN	CA-CB-CG	-9.56	103.04	112.60
2	G	107	ARG	N-CA-C	9.13	120.84	111.07
2	G	228	ASN	N-CA-C	8.91	121.10	108.54
1	F	35	ASP	N-CA-CB	8.78	124.97	110.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	95	LYS	CA-C-O	8.75	128.26	119.86
1	F	126	LEU	N-CA-C	-8.54	101.92	111.14
1	F	20	ILE	N-CA-C	8.50	120.07	108.17
2	G	92	GLU	CA-C-N	8.36	131.31	120.44
2	G	92	GLU	C-N-CA	8.36	131.31	120.44
2	G	200	ASP	CA-CB-CG	-8.33	104.27	112.60
2	G	114	HIS	CA-CB-CG	-8.30	105.50	113.80
1	F	93	ILE	N-CA-CB	8.11	121.68	111.46
2	G	317	ARG	N-CA-C	8.07	119.98	111.03
1	F	93	ILE	N-CA-C	7.99	119.39	107.80
2	G	52	ILE	O-C-N	7.88	130.06	121.94
1	F	137	PRO	CB-CA-C	-7.84	101.19	111.23
2	G	157	ARG	N-CA-C	-7.64	103.06	112.38
2	G	41	LYS	CA-C-N	7.53	129.25	119.84
2	G	41	LYS	C-N-CA	7.53	129.25	119.84
2	G	407	ARG	CA-C-N	-7.52	112.81	123.03
2	G	407	ARG	C-N-CA	-7.52	112.81	123.03
2	G	35	PHE	CA-CB-CG	-7.42	106.38	113.80
2	G	159	GLU	CA-C-N	7.42	133.43	123.05
2	G	159	GLU	C-N-CA	7.42	133.43	123.05
2	G	331	TYR	N-CA-C	7.41	119.36	111.28
1	F	55	THR	CB-CA-C	7.34	121.67	109.56
2	G	256	VAL	N-CA-C	7.33	124.58	109.34
1	F	102	GLY	N-CA-C	-7.24	105.08	114.85
2	G	63	VAL	N-CA-CB	7.16	119.73	110.57
2	G	114	HIS	O-C-N	7.13	129.73	122.03
2	G	178	VAL	N-CA-C	7.08	118.32	107.99
2	G	102	VAL	N-CA-C	7.07	117.76	110.05
2	G	218	ARG	N-CA-C	7.04	119.78	109.07
1	F	58	LYS	N-CA-C	7.04	119.89	108.76
2	G	52	ILE	N-CA-C	-7.04	103.47	110.30
2	G	136	PHE	CA-C-N	7.03	134.97	121.54
2	G	136	PHE	C-N-CA	7.03	134.97	121.54
2	G	136	PHE	O-C-N	7.01	130.79	122.94
2	G	93	THR	N-CA-C	6.94	118.50	111.07
2	G	369	ARG	N-CA-CB	6.92	121.07	110.14
2	G	417	PHE	CA-CB-CG	-6.91	106.89	113.80
2	G	47	HIS	CA-CB-CG	6.75	120.55	113.80
2	G	336	VAL	N-CA-CB	6.68	120.28	112.33
2	G	144	ILE	N-CA-C	6.66	117.36	110.36
2	G	42	PRO	CA-C-N	-6.66	108.37	121.41
2	G	42	PRO	C-N-CA	-6.66	108.37	121.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	430	VAL	CA-C-N	-6.64	113.83	123.00
2	G	430	VAL	C-N-CA	-6.64	113.83	123.00
2	G	330	GLU	N-CA-C	-6.63	103.97	111.07
1	F	124	LEU	CA-C-N	-6.59	111.60	119.84
1	F	124	LEU	C-N-CA	-6.59	111.60	119.84
2	G	74	ILE	N-CA-CB	6.59	118.51	111.00
1	F	122	PHE	N-CA-C	6.58	118.76	108.96
2	G	289	THR	N-CA-C	6.58	116.74	108.45
1	F	75	HIS	N-CA-C	-6.58	103.90	114.09
1	F	150	ILE	N-CA-CB	6.56	118.86	110.99
2	G	27	ILE	CB-CA-C	6.55	118.49	111.35
2	G	296	GLY	CA-C-N	-6.54	110.89	122.07
2	G	296	GLY	C-N-CA	-6.54	110.89	122.07
1	F	128	GLU	CA-C-N	-6.52	111.89	122.26
1	F	128	GLU	C-N-CA	-6.52	111.89	122.26
1	F	41	PHE	O-C-N	6.51	129.81	122.32
2	G	88	VAL	CA-C-N	-6.51	111.54	122.29
2	G	88	VAL	C-N-CA	-6.51	111.54	122.29
2	G	140	LYS	N-CA-CB	6.51	119.71	109.82
1	F	57	ASN	N-CA-C	6.48	124.60	110.80
2	G	36	GLU	N-CA-C	6.48	119.68	109.96
2	G	108	THR	CB-CA-C	-6.47	103.19	111.22
2	G	307	PHE	N-CA-C	6.47	118.34	111.28
2	G	424	ASP	CA-CB-CG	6.44	119.04	112.60
2	G	290	ILE	N-CA-C	6.39	117.79	108.53
2	G	179	HIS	CA-CB-CG	6.36	120.16	113.80
2	G	460	LEU	N-CA-C	6.35	121.81	113.30
2	G	160	LEU	N-CA-C	6.32	118.82	108.52
2	G	85	THR	O-C-N	6.29	130.96	122.59
1	F	112	ARG	N-CA-CB	6.29	120.41	110.23
2	G	196	THR	OG1-CB-CG2	6.24	121.78	109.30
2	G	456	ASN	CA-CB-CG	-6.21	106.39	112.60
1	F	153	SER	N-CA-C	6.19	117.58	108.86
1	F	32	ASN	O-C-N	6.18	130.53	122.93
1	F	54	PRO	N-CA-C	6.17	121.99	111.68
2	G	189	THR	N-CA-CB	-6.16	100.35	110.40
1	F	86	GLU	CA-C-N	-6.14	113.17	122.81
1	F	86	GLU	C-N-CA	-6.14	113.17	122.81
1	F	111	GLN	N-CA-CB	6.14	119.06	110.04
2	G	86	THR	N-CA-C	6.12	119.88	110.20
2	G	364	ILE	CA-CB-CG2	-6.12	100.10	110.50
2	G	42	PRO	CB-CA-C	6.12	121.65	111.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	432	ARG	CA-C-N	6.09	126.05	119.78
2	G	432	ARG	C-N-CA	6.09	126.05	119.78
2	G	15	SER	N-CA-C	6.08	118.02	108.96
1	F	134	THR	CB-CA-C	6.03	119.67	109.55
1	F	36	VAL	N-CA-C	6.00	114.83	108.95
1	F	36	VAL	N-CA-CB	6.00	115.66	110.08
2	G	195	HIS	CA-CB-CG	-6.00	107.81	113.80
2	G	27	ILE	N-CA-CB	5.97	117.85	111.46
1	F	38	ASP	CA-CB-CG	5.97	118.57	112.60
2	G	5	TYR	CB-CA-C	-5.96	99.54	110.62
1	F	41	PHE	CA-C-N	5.96	128.85	120.28
1	F	41	PHE	C-N-CA	5.96	128.85	120.28
2	G	196	THR	CA-CB-CG2	5.95	120.62	110.50
2	G	468	ARG	N-CA-C	5.95	118.19	108.55
2	G	365	PHE	N-CA-C	5.92	118.70	109.52
2	G	293	GLY	N-CA-C	-5.88	100.36	112.34
1	F	59	MET	CG-SD-CE	-5.84	88.05	100.90
1	F	27	SER	N-CA-C	5.84	118.74	109.81
1	F	124	LEU	C-N-CD	-5.83	101.12	125.00
2	G	38	ILE	CA-C-N	-5.82	115.60	123.46
2	G	38	ILE	C-N-CA	-5.82	115.60	123.46
1	F	41	PHE	CA-CB-CG	-5.81	107.99	113.80
2	G	318	ASP	CA-CB-CG	5.78	118.38	112.60
2	G	92	GLU	O-C-N	5.77	128.26	122.08
2	G	270	PHE	CA-CB-CG	-5.77	108.03	113.80
2	G	320	MET	N-CA-C	-5.75	105.15	111.82
2	G	61	VAL	O-C-N	5.74	128.16	121.96
2	G	76	ALA	N-CA-C	5.74	115.69	108.45
2	G	162	PHE	CA-CB-CG	-5.73	108.07	113.80
2	G	97	ILE	CA-CB-CG2	-5.73	100.77	110.50
2	G	253	GLN	CA-C-O	5.71	126.19	119.28
1	F	161	THR	N-CA-CB	-5.71	101.02	109.98
1	F	2	LEU	N-CA-CB	5.70	121.34	111.13
2	G	175	GLN	CB-CA-C	5.69	121.75	110.42
2	G	346	PRO	N-CA-CB	5.66	106.21	102.25
2	G	133	ASP	CA-C-O	5.65	124.78	119.13
2	G	380	THR	N-CA-C	-5.65	105.02	111.07
1	F	115	VAL	CA-C-N	-5.60	114.52	123.31
1	F	115	VAL	C-N-CA	-5.60	114.52	123.31
1	F	168	LYS	N-CA-C	5.59	126.65	111.00
1	F	20	ILE	N-CA-CB	5.58	118.84	111.25
1	F	137	PRO	N-CA-CB	5.57	108.20	103.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	125	PRO	N-CA-CB	5.57	109.10	103.25
2	G	303	GLU	CG-CD-OE1	-5.55	105.62	118.40
1	F	147	LYS	N-CA-C	5.55	118.17	111.40
1	F	39	VAL	N-CA-C	5.52	118.78	111.17
2	G	369	ARG	N-CA-C	5.52	118.81	111.75
2	G	61	VAL	CB-CA-C	-5.51	104.64	111.70
2	G	191	LEU	N-CA-CB	-5.50	102.30	110.61
2	G	337	GLN	N-CA-CB	5.50	119.79	110.49
2	G	121	GLU	N-CA-CB	5.50	118.17	109.82
1	F	140	ILE	N-CA-C	-5.49	100.50	108.36
1	F	62	PRO	N-CA-CB	5.49	109.01	103.25
2	G	456	ASN	N-CA-C	5.49	118.14	108.75
1	F	158	VAL	O-C-N	5.49	128.11	122.79
2	G	64	LEU	O-C-N	5.48	127.79	122.09
2	G	207	LEU	CB-CA-C	-5.48	101.90	110.94
2	G	449	LEU	CB-CA-C	-5.48	101.54	110.85
1	F	3	PHE	CB-CA-C	5.46	120.20	109.72
2	G	101	ILE	N-CA-CB	5.43	116.45	110.53
2	G	223	VAL	N-CA-CB	5.43	116.85	110.82
2	G	221	SER	N-CA-CB	5.42	119.60	110.77
2	G	165	VAL	N-CA-C	5.40	118.62	111.17
2	G	45	VAL	CA-C-O	-5.39	114.83	120.76
2	G	83	ARG	N-CA-C	5.39	117.48	110.53
1	F	75	HIS	CA-C-O	5.38	124.88	118.79
1	F	93	ILE	CB-CA-C	5.38	118.82	110.96
1	F	88	PHE	CB-CA-C	5.38	119.43	109.70
2	G	490	VAL	CB-CA-C	-5.36	105.01	111.88
2	G	137	SER	N-CA-C	5.36	122.22	110.80
2	G	371	VAL	CB-CA-C	-5.36	103.73	111.34
1	F	93	ILE	CA-C-O	5.35	126.26	120.53
1	F	168	LYS	N-CA-CB	5.35	119.60	110.50
1	F	64	ASP	N-CA-CB	5.35	118.13	110.06
2	G	17	ARG	CB-CA-C	5.34	120.88	110.30
2	G	63	VAL	CB-CA-C	-5.33	105.03	112.02
2	G	55	THR	N-CA-CB	-5.33	102.06	110.06
2	G	126	SER	CA-C-N	-5.33	113.19	122.36
2	G	126	SER	C-N-CA	-5.33	113.19	122.36
2	G	438	VAL	N-CA-C	5.33	116.69	110.62
2	G	306	VAL	CB-CA-C	-5.32	104.07	110.99
2	G	73	GLN	N-CA-C	5.32	119.62	113.18
2	G	485	GLY	N-CA-C	-5.32	105.96	112.77
1	F	64	ASP	CA-CB-CG	5.31	117.91	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	369	ARG	NE-CZ-NH2	5.31	123.98	119.20
2	G	80	THR	N-CA-CB	5.28	120.02	110.83
1	F	64	ASP	N-CA-C	-5.28	101.86	110.20
2	G	196	THR	CA-CB-OG1	5.28	117.51	109.60
2	G	165	VAL	CB-CA-C	5.27	119.75	112.05
1	F	164	ILE	CB-CA-C	-5.26	101.71	111.18
2	G	110	GLU	CB-CG-CD	5.23	121.50	112.60
2	G	342	VAL	N-CA-C	5.23	116.32	109.21
2	G	457	LEU	CA-C-N	-5.22	112.00	120.72
2	G	457	LEU	C-N-CA	-5.22	112.00	120.72
2	G	80	THR	CA-CB-OG1	5.21	117.42	109.60
2	G	316	LEU	CA-C-N	-5.21	113.54	120.63
2	G	316	LEU	C-N-CA	-5.21	113.54	120.63
2	G	499	HIS	CA-CB-CG	-5.21	108.59	113.80
1	F	160	GLU	N-CA-CB	5.20	119.28	110.49
2	G	86	THR	CA-C-N	5.19	130.26	122.58
2	G	86	THR	C-N-CA	5.19	130.26	122.58
2	G	257	LYS	CB-CA-C	5.17	119.25	109.37
1	F	70	ILE	N-CA-CB	5.16	119.75	111.23
2	G	168	TRP	O-C-N	-5.15	116.28	122.15
1	F	91	PHE	CA-CB-CG	-5.14	108.66	113.80
1	F	37	PRO	N-CA-CB	5.13	106.18	102.79
2	G	301	ALA	N-CA-C	5.12	116.30	108.42
2	G	27	ILE	CA-C-N	5.10	128.03	120.74
2	G	27	ILE	C-N-CA	5.10	128.03	120.74
2	G	280	VAL	CB-CA-C	-5.09	103.74	111.33
1	F	109	GLU	CA-C-N	-5.09	111.44	121.41
1	F	109	GLU	C-N-CA	-5.09	111.44	121.41
2	G	17	ARG	N-CA-C	5.08	117.14	109.41
1	F	66	THR	CA-C-N	-5.08	113.85	120.91
1	F	66	THR	C-N-CA	-5.08	113.85	120.91
2	G	212	GLU	O-C-N	5.07	127.50	122.12
2	G	337	GLN	CB-CA-C	-5.07	100.32	110.42
1	F	30	ILE	CB-CA-C	-5.07	103.56	111.26
2	G	79	ILE	N-CA-C	5.06	115.26	107.77
1	F	105	ARG	CA-C-N	-5.05	112.87	121.97
1	F	105	ARG	C-N-CA	-5.05	112.87	121.97
2	G	373	ALA	CA-C-N	5.05	127.05	120.28
2	G	373	ALA	C-N-CA	5.05	127.05	120.28
2	G	346	PRO	CA-N-CD	-5.04	104.94	112.00
2	G	255	CYS	N-CA-C	-5.04	100.06	110.80
1	F	57	ASN	CA-C-N	-5.03	111.97	121.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	57	ASN	C-N-CA	-5.03	111.97	121.63
1	F	117	ASP	CB-CA-C	5.03	117.80	109.70
2	G	340	ASN	CA-CB-CG	-5.02	107.58	112.60
2	G	147	HIS	CA-CB-CG	-5.02	108.78	113.80
2	G	102	VAL	CA-CB-CG2	-5.01	101.87	110.40
2	G	163	GLY	CA-C-N	5.00	130.32	122.21
2	G	163	GLY	C-N-CA	5.00	130.32	122.21
1	F	33	ILE	N-CA-CB	5.00	116.72	110.47
2	G	222	GLU	CA-C-N	-5.00	113.68	121.18
2	G	222	GLU	C-N-CA	-5.00	113.68	121.18

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	35	ASP	CA
1	F	93	ILE	CA
1	F	111	GLN	CA
1	F	168	LYS	CA
2	G	42	PRO	CA
2	G	70	SER	CA
2	G	175	GLN	CA
2	G	196	THR	CB
2	G	255	CYS	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	200	ASP	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	F	1150	0	1127	135	0
2	G	3752	0	3605	355	0
3	G	1	0	0	0	0
4	G	10	0	5	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	27	0	12	1	0
6	F	2	0	0	0	0
6	G	15	0	0	0	0
All	All	4957	0	4749	489	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 (489) 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:G:137:SER:HB2	2:G:189:THR:HA	1.34	1.04
2:G:271:MET:HE1	2:G:392:LEU:HA	1.45	0.98
1:F:91:PHE:HA	1:F:136:THR:HG23	1.45	0.98
1:F:43:GLU:HB2	1:F:45:ILE:HD11	1.46	0.98
2:G:189:THR:HG23	2:G:191:LEU:H	1.29	0.97
2:G:152:ARG:HH21	2:G:208:ASP:HB3	1.27	0.97
2:G:419:MET:HE2	2:G:419:MET:HA	1.48	0.96
1:F:54:PRO:HD2	1:F:134:THR:HG23	1.48	0.94
2:G:16:SER:HB2	2:G:55:THR:HG23	1.49	0.93
2:G:6:ILE:HD11	2:G:453:PHE:CE2	2.06	0.90
2:G:180:VAL:HG21	2:G:218:ARG:HG3	1.54	0.89
1:F:157:THR:CG2	1:F:160:GLU:HB2	2.02	0.89
2:G:308:MET:HE2	2:G:348:PHE:HB2	1.52	0.89
2:G:482:ARG:HG3	2:G:482:ARG:HH11	1.37	0.89
1:F:157:THR:HG23	1:F:160:GLU:HB2	1.56	0.88
2:G:274:ASN:HD21	2:G:299:ASN:HD22	1.22	0.88
2:G:117:ARG:HG3	2:G:117:ARG:HH11	1.38	0.87
2:G:396:GLN:NE2	2:G:403:LEU:H	1.73	0.86
2:G:35:PHE:HE2	2:G:47:HIS:HD2	1.22	0.85
2:G:204:LEU:HD21	2:G:214:LEU:HD11	1.55	0.85
2:G:38:ILE:HG22	2:G:40:PRO:HD3	1.56	0.85
2:G:141:VAL:HG11	2:G:209:ILE:HD13	1.59	0.85
2:G:431:GLU:HB2	2:G:466:ILE:HD13	1.59	0.83
1:F:106:ILE:HD11	1:F:121:GLU:HB2	1.61	0.83
2:G:45:VAL:H	2:G:105:CYS:HB2	1.41	0.83
2:G:189:THR:CG2	2:G:191:LEU:H	1.92	0.82
1:F:67:ILE:HD12	1:F:68:GLY:N	1.96	0.81
2:G:64:LEU:HD22	2:G:69:ILE:HG22	1.62	0.81
2:G:51:GLU:O	2:G:55:THR:HB	1.81	0.79
2:G:29:SER:OG	2:G:63:VAL:HG12	1.82	0.79

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:152:ARG:NH2	2:G:208:ASP:HB3	1.95	0.79
2:G:434:GLU:HA	2:G:467:GLU:HB2	1.64	0.79
1:F:3:PHE:HD1	1:F:6:LEU:HD11	1.46	0.79
2:G:83:ARG:HD3	4:G:503:G3H:O2	1.83	0.79
1:F:156:VAL:HG12	1:F:161:THR:HB	1.65	0.79
1:F:156:VAL:HG12	1:F:161:THR:CG2	2.12	0.78
2:G:35:PHE:HE2	2:G:47:HIS:CD2	2.01	0.78
2:G:6:ILE:HD12	2:G:6:ILE:H	1.47	0.78
2:G:154:ARG:HH11	2:G:154:ARG:HB3	1.48	0.78
2:G:255:CYS:HB3	2:G:260:MET:CB	2.14	0.77
2:G:5:TYR:HB3	2:G:21:MET:O	1.85	0.77
2:G:210:PRO:O	2:G:213:MET:HG2	1.84	0.77
2:G:396:GLN:HE21	2:G:403:LEU:H	1.33	0.76
2:G:60:LEU:O	2:G:63:VAL:HG23	1.85	0.76
2:G:255:CYS:HB3	2:G:260:MET:HB2	1.66	0.76
2:G:204:LEU:HD21	2:G:214:LEU:CD1	2.15	0.76
2:G:136:PHE:HB3	2:G:188:ARG:O	1.86	0.76
1:F:43:GLU:HB2	1:F:45:ILE:CD1	2.16	0.75
2:G:112:CYS:HB3	2:G:132:ILE:HG22	1.68	0.75
1:F:165:ARG:HG3	1:F:165:ARG:HH11	1.52	0.75
1:F:67:ILE:HD11	1:F:70:ILE:HG13	1.69	0.74
2:G:246:GLN:OE1	2:G:270:PHE:HB2	1.88	0.74
2:G:407:ARG:HD3	2:G:431:GLU:HG3	1.69	0.74
2:G:154:ARG:HH12	2:G:159:GLU:HB2	1.51	0.73
2:G:340:ASN:HB2	2:G:375:HIS:CD2	2.23	0.73
2:G:15:SER:HA	2:G:35:PHE:CE1	2.22	0.73
2:G:468:ARG:HG3	2:G:469:GLU:N	2.01	0.72
2:G:257:LYS:O	2:G:260:MET:HG3	1.89	0.72
2:G:180:VAL:CG2	2:G:218:ARG:HG3	2.18	0.72
2:G:98:TYR:HD1	2:G:99:ASN:N	1.88	0.72
1:F:48:ASP:CB	1:F:143:MET:HE2	2.20	0.71
2:G:308:MET:HE2	2:G:348:PHE:CB	2.19	0.71
2:G:262:LYS:C	2:G:262:LYS:HD2	2.16	0.71
2:G:419:MET:HA	2:G:419:MET:CE	2.20	0.71
2:G:35:PHE:CE2	2:G:47:HIS:HD2	2.07	0.71
2:G:120:LEU:O	2:G:124:ILE:HG13	1.91	0.71
1:F:163:VAL:HG23	1:F:164:ILE:HG13	1.71	0.71
2:G:197:LEU:HD12	2:G:197:LEU:N	2.05	0.71
2:G:271:MET:HE2	2:G:391:VAL:HG13	1.71	0.71
2:G:473:GLY:O	2:G:476:THR:HG22	1.90	0.71
2:G:154:ARG:HH11	2:G:154:ARG:CB	2.03	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:85:THR:HB	2:G:102:VAL:HA	1.72	0.70
2:G:11:GLN:OE1	2:G:165:VAL:HG11	1.92	0.70
1:F:73:THR:HG21	1:F:96:VAL:HG23	1.73	0.69
2:G:141:VAL:CG1	2:G:209:ILE:HD13	2.21	0.69
2:G:4:LYS:HA	2:G:73:GLN:O	1.91	0.69
2:G:6:ILE:HD11	2:G:453:PHE:CD2	2.26	0.69
1:F:119:VAL:HG12	1:F:120:ILE:HG13	1.74	0.69
2:G:101:ILE:HD13	2:G:107:ARG:HD3	1.75	0.69
2:G:64:LEU:HD22	2:G:69:ILE:CG2	2.22	0.69
2:G:152:ARG:HH21	2:G:208:ASP:CB	2.01	0.69
2:G:174:THR:O	2:G:176:GLY:N	2.25	0.69
2:G:179:HIS:CD2	2:G:215:PRO:HA	2.28	0.69
2:G:205:GLU:O	2:G:208:ASP:N	2.26	0.69
2:G:120:LEU:HD23	2:G:120:LEU:N	2.08	0.68
1:F:48:ASP:HB3	1:F:143:MET:HE2	1.73	0.68
2:G:6:ILE:HD12	2:G:6:ILE:N	2.08	0.68
2:G:221:SER:HB2	2:G:450:ALA:HB2	1.76	0.68
2:G:261:ALA:HB2	2:G:273:MET:HB2	1.76	0.67
1:F:74:ASN:HD22	1:F:105:ARG:HH11	1.42	0.67
2:G:74:ILE:HD11	2:G:237:ILE:N	2.10	0.67
2:G:52:ILE:O	2:G:55:THR:HG22	1.95	0.67
2:G:154:ARG:HH11	2:G:154:ARG:CG	2.07	0.66
2:G:154:ARG:HB3	2:G:154:ARG:NH1	2.10	0.66
2:G:330:GLU:OE2	2:G:416:ASN:N	2.29	0.66
2:G:304:GLY:HA3	2:G:391:VAL:CG2	2.25	0.66
2:G:154:ARG:O	2:G:159:GLU:HG3	1.94	0.66
2:G:200:ASP:HB3	2:G:203:MET:HB2	1.78	0.66
1:F:32:ASN:O	1:F:35:ASP:N	2.26	0.65
1:F:36:VAL:HG13	1:F:37:PRO:HD2	1.77	0.65
1:F:156:VAL:HA	1:F:161:THR:HG21	1.77	0.65
2:G:156:ARG:HG3	2:G:156:ARG:HH11	1.61	0.65
2:G:134:PRO:O	2:G:140:LYS:NZ	2.29	0.65
2:G:150:GLY:O	2:G:154:ARG:HD3	1.96	0.65
2:G:83:ARG:O	2:G:85:THR:N	2.26	0.65
1:F:3:PHE:CD1	1:F:6:LEU:HD11	2.29	0.65
2:G:105:CYS:SG	2:G:107:ARG:HD2	2.36	0.65
2:G:274:ASN:HD21	2:G:299:ASN:ND2	1.94	0.65
2:G:169:LEU:O	2:G:173:MET:HG2	1.97	0.64
1:F:70:ILE:HG13	1:F:109:GLU:HG2	1.80	0.64
2:G:85:THR:HG22	2:G:103:TRP:N	2.11	0.64
2:G:304:GLY:HA3	2:G:391:VAL:HG21	1.78	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:317:ARG:O	2:G:317:ARG:HG2	1.97	0.64
2:G:451:VAL:HG12	2:G:453:PHE:HB2	1.80	0.64
2:G:20:VAL:O	2:G:28:ILE:HB	1.97	0.64
2:G:217:VAL:C	2:G:218:ARG:HG2	2.23	0.64
2:G:18:ALA:HB2	2:G:59:THR:HG23	1.79	0.64
2:G:70:SER:OG	2:G:71:SER:N	2.27	0.64
2:G:434:GLU:HG2	2:G:465:VAL:HG13	1.79	0.64
2:G:336:VAL:O	2:G:338:ASN:N	2.32	0.63
2:G:206:VAL:HG12	2:G:207:LEU:HD23	1.80	0.63
2:G:130:LEU:HD13	2:G:136:PHE:CE1	2.34	0.63
1:F:27:SER:OG	1:F:158:VAL:HG12	1.99	0.63
2:G:422:GLN:HE21	2:G:422:GLN:C	2.06	0.63
1:F:45:ILE:N	1:F:45:ILE:HD12	2.13	0.63
2:G:458:ASP:OD1	2:G:458:ASP:N	2.30	0.63
2:G:468:ARG:HG2	2:G:470:PHE:CE1	2.34	0.63
1:F:66:THR:HG23	1:F:112:ARG:HA	1.80	0.63
2:G:432:ARG:HD2	2:G:467:GLU:OE1	1.99	0.63
1:F:156:VAL:HG12	1:F:161:THR:CB	2.29	0.62
2:G:56:GLN:HG2	2:G:169:LEU:HD11	1.80	0.62
1:F:74:ASN:ND2	1:F:105:ARG:HB2	2.14	0.62
2:G:160:LEU:C	2:G:161:LEU:HD23	2.25	0.62
2:G:50:MET:HE1	2:G:96:PRO:HD2	1.82	0.62
2:G:271:MET:SD	2:G:395:MET:HE2	2.40	0.62
1:F:43:GLU:CD	2:G:402:ARG:HH22	2.08	0.62
2:G:57:SER:O	2:G:60:LEU:HB3	1.99	0.61
2:G:101:ILE:CD1	2:G:107:ARG:HD3	2.29	0.61
2:G:428:THR:HG22	2:G:429:ARG:O	2.00	0.61
2:G:47:HIS:ND1	2:G:102:VAL:HG21	2.15	0.61
2:G:45:VAL:N	2:G:105:CYS:HB2	2.15	0.61
2:G:85:THR:HG22	2:G:103:TRP:H	1.64	0.61
2:G:121:GLU:HA	2:G:132:ILE:HD11	1.82	0.61
2:G:170:ILE:HD11	2:G:239:ILE:HG21	1.81	0.61
1:F:20:ILE:O	1:F:165:ARG:HA	2.00	0.61
2:G:152:ARG:HE	2:G:208:ASP:HB3	1.65	0.61
1:F:43:GLU:C	1:F:45:ILE:HD12	2.25	0.61
1:F:23:ILE:O	1:F:62:PRO:HB3	2.01	0.61
2:G:102:VAL:O	2:G:140:LYS:HE3	2.01	0.61
1:F:45:ILE:HD12	1:F:45:ILE:H	1.66	0.60
2:G:16:SER:CB	2:G:55:THR:HG23	2.28	0.60
2:G:77:ILE:HG22	2:G:239:ILE:HG23	1.82	0.60
1:F:39:VAL:O	1:F:45:ILE:HD13	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:189:THR:CG2	2:G:191:LEU:HB2	2.31	0.60
2:G:110:GLU:CD	2:G:110:GLU:H	2.09	0.60
2:G:155:ALA:HB2	2:G:160:LEU:HB2	1.84	0.59
2:G:361:ARG:HG2	2:G:361:ARG:HH11	1.67	0.59
2:G:475:GLU:OE1	2:G:475:GLU:N	2.29	0.59
1:F:165:ARG:HG3	1:F:165:ARG:NH1	2.17	0.59
2:G:110:GLU:O	2:G:113:GLU:HB2	2.02	0.59
2:G:226:GLN:HA	2:G:237:ILE:O	2.02	0.59
2:G:81:ASN:ND2	2:G:166:ASP:HB3	2.17	0.59
2:G:80:THR:HG21	2:G:248:ALA:CB	2.32	0.59
2:G:308:MET:HE2	2:G:348:PHE:CG	2.37	0.59
1:F:20:ILE:HG22	1:F:21:GLU:N	2.18	0.59
1:F:74:ASN:HD22	1:F:105:ARG:HB2	1.67	0.59
2:G:422:GLN:HE22	2:G:426:LEU:HG	1.67	0.59
2:G:434:GLU:CA	2:G:467:GLU:HB2	2.33	0.59
1:F:106:ILE:CD1	1:F:121:GLU:HB2	2.32	0.58
1:F:149:LEU:CD2	1:F:166:ILE:HG22	2.33	0.58
2:G:70:SER:O	2:G:73:GLN:HG3	2.03	0.58
2:G:124:ILE:CD1	2:G:203:MET:HE1	2.33	0.58
1:F:140:ILE:HD13	1:F:149:LEU:HD21	1.85	0.58
2:G:161:LEU:HD23	2:G:161:LEU:N	2.14	0.58
2:G:255:CYS:HB3	2:G:260:MET:HB3	1.85	0.58
2:G:85:THR:HG21	2:G:102:VAL:HG13	1.85	0.58
1:F:59:MET:HG3	1:F:122:PHE:CE2	2.39	0.58
1:F:104:LYS:O	1:F:106:ILE:HD12	2.03	0.58
2:G:156:ARG:HG3	2:G:156:ARG:NH1	2.18	0.58
2:G:182:ASP:HB3	2:G:242:ILE:CG2	2.33	0.58
1:F:149:LEU:HD22	1:F:166:ILE:HG22	1.86	0.57
2:G:53:TRP:HE3	2:G:53:TRP:HA	1.69	0.57
2:G:124:ILE:HD11	2:G:203:MET:HE1	1.85	0.57
2:G:343:TYR:HE2	2:G:485:GLY:HA3	1.69	0.57
2:G:445:TYR:HA	2:G:454:TRP:CZ3	2.38	0.57
1:F:26:LEU:C	1:F:26:LEU:HD23	2.29	0.57
2:G:431:GLU:HB2	2:G:466:ILE:CD1	2.32	0.57
1:F:39:VAL:HG12	1:F:43:GLU:HG3	1.85	0.57
2:G:102:VAL:HG12	2:G:103:TRP:N	2.19	0.57
2:G:196:THR:HG22	2:G:198:ASP:H	1.69	0.57
2:G:23:HIS:HA	2:G:453:PHE:CE2	2.40	0.57
2:G:114:HIS:O	2:G:117:ARG:N	2.37	0.57
2:G:130:LEU:HD13	2:G:136:PHE:CD1	2.40	0.57
1:F:117:ASP:OD1	1:F:117:ASP:N	2.35	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:90:GLU:HB2	2:G:93:THR:OG1	2.03	0.57
2:G:164:THR:H	2:G:167:THR:HB	1.70	0.57
2:G:442:GLY:O	2:G:445:TYR:HB2	2.05	0.57
2:G:85:THR:CG2	2:G:103:TRP:HD1	2.17	0.57
2:G:155:ALA:CB	2:G:160:LEU:HB2	2.34	0.56
1:F:22:ILE:CD1	1:F:166:ILE:HD13	2.36	0.56
1:F:40:VAL:HA	1:F:45:ILE:HD13	1.87	0.56
1:F:157:THR:HG22	1:F:161:THR:OG1	2.05	0.56
2:G:53:TRP:CD1	2:G:172:LYS:HE2	2.40	0.56
1:F:31:VAL:HG12	1:F:32:ASN:N	2.18	0.56
2:G:11:GLN:HG2	2:G:16:SER:OG	2.06	0.56
2:G:151:SER:O	2:G:160:LEU:HD12	2.06	0.56
2:G:170:ILE:HG22	2:G:171:TRP:N	2.20	0.56
2:G:108:THR:HB	2:G:139:THR:HB	1.86	0.56
1:F:74:ASN:ND2	1:F:105:ARG:HH11	2.04	0.56
2:G:53:TRP:HA	2:G:53:TRP:CE3	2.41	0.56
2:G:430:VAL:HB	2:G:470:PHE:HB2	1.88	0.55
1:F:70:ILE:HG21	1:F:105:ARG:HD2	1.88	0.55
2:G:274:ASN:ND2	2:G:299:ASN:HD22	1.99	0.55
2:G:7:VAL:HG22	2:G:20:VAL:HG22	1.89	0.55
2:G:184:THR:HG22	2:G:290:ILE:O	2.06	0.55
1:F:140:ILE:CD1	1:F:149:LEU:HD21	2.36	0.55
1:F:150:ILE:O	1:F:164:ILE:HG23	2.07	0.55
2:G:189:THR:HG23	2:G:191:LEU:N	2.11	0.55
2:G:101:ILE:HD13	2:G:107:ARG:CD	2.36	0.55
2:G:115:LEU:HD22	2:G:120:LEU:HD12	1.89	0.55
1:F:48:ASP:HB2	1:F:143:MET:HE2	1.87	0.55
2:G:59:THR:O	2:G:63:VAL:HG22	2.06	0.55
2:G:56:GLN:O	2:G:59:THR:HG22	2.08	0.54
1:F:67:ILE:HD11	1:F:70:ILE:CG1	2.38	0.54
1:F:27:SER:O	1:F:54:PRO:HA	2.08	0.54
2:G:102:VAL:HG12	2:G:103:TRP:H	1.73	0.54
2:G:90:GLU:OE1	2:G:93:THR:HG21	2.08	0.54
1:F:164:ILE:HG22	1:F:165:ARG:N	2.23	0.53
1:F:153:SER:OG	1:F:154:GLY:N	2.42	0.53
1:F:157:THR:N	1:F:161:THR:OG1	2.29	0.53
2:G:162:PHE:CG	2:G:163:GLY:N	2.76	0.53
2:G:74:ILE:HD12	2:G:74:ILE:O	2.09	0.53
2:G:171:TRP:HZ3	2:G:172:LYS:HD2	1.72	0.53
2:G:108:THR:HG21	2:G:139:THR:C	2.34	0.53
1:F:32:ASN:HB2	1:F:35:ASP:OD1	2.08	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:256:VAL:HG12	2:G:257:LYS:N	2.23	0.53
1:F:66:THR:HA	1:F:111:GLN:O	2.08	0.53
2:G:245:ASP:OD1	4:G:503:G3H:O2	2.26	0.53
2:G:11:GLN:HB2	2:G:56:GLN:HE21	1.74	0.53
2:G:61:VAL:HG12	2:G:62:GLU:N	2.19	0.53
2:G:117:ARG:HG3	2:G:117:ARG:NH1	2.10	0.53
1:F:101:GLU:HG2	1:F:126:LEU:HD21	1.89	0.52
2:G:98:TYR:CD1	2:G:99:ASN:N	2.75	0.52
2:G:155:ALA:O	2:G:158:GLY:HA2	2.09	0.52
1:F:143:MET:HE1	1:F:149:LEU:HG	1.91	0.52
1:F:70:ILE:HG21	1:F:105:ARG:CD	2.40	0.52
2:G:271:MET:CE	2:G:391:VAL:HG13	2.38	0.52
2:G:313:ILE:N	2:G:313:ILE:HD13	2.25	0.52
2:G:83:ARG:HB2	4:G:503:G3H:C1	2.40	0.52
2:G:87:ILE:HG22	2:G:88:VAL:N	2.24	0.52
2:G:152:ARG:HE	2:G:208:ASP:CG	2.18	0.52
2:G:254:LEU:O	2:G:255:CYS:O	2.28	0.52
1:F:32:ASN:HB3	1:F:34:GLU:HG2	1.91	0.52
1:F:67:ILE:HD12	1:F:67:ILE:C	2.34	0.52
2:G:48:ASP:HB3	2:G:51:GLU:HB2	1.92	0.51
2:G:165:VAL:O	2:G:169:LEU:HB2	2.09	0.51
2:G:189:THR:HG23	2:G:191:LEU:HB2	1.90	0.51
2:G:130:LEU:N	2:G:130:LEU:HD23	2.25	0.51
2:G:364:ILE:HG22	2:G:365:PHE:N	2.25	0.51
2:G:152:ARG:NE	2:G:208:ASP:HB3	2.24	0.51
2:G:80:THR:HG22	2:G:243:ALA:O	2.11	0.51
2:G:154:ARG:HH12	2:G:159:GLU:CB	2.22	0.51
2:G:19:VAL:HG12	2:G:21:MET:HE2	1.91	0.51
2:G:392:LEU:O	2:G:395:MET:HB3	2.11	0.51
2:G:98:TYR:CE2	2:G:143:TRP:HZ3	2.28	0.51
2:G:422:GLN:NE2	2:G:422:GLN:CA	2.73	0.51
2:G:180:VAL:HG23	2:G:216:GLU:O	2.11	0.51
1:F:98:LEU:O	1:F:99:LYS:HB2	2.10	0.51
2:G:6:ILE:HG22	2:G:7:VAL:H	1.76	0.51
2:G:47:HIS:ND1	2:G:102:VAL:CG2	2.74	0.51
2:G:193:ASN:HB3	2:G:196:THR:HG22	1.92	0.50
2:G:293:GLY:N	2:G:297:GLU:O	2.42	0.50
2:G:154:ARG:NH1	2:G:159:GLU:HB2	2.24	0.50
2:G:15:SER:CA	2:G:35:PHE:HE1	2.25	0.50
2:G:343:TYR:CE2	2:G:485:GLY:HA3	2.45	0.50
2:G:18:ALA:CB	2:G:63:VAL:HG21	2.41	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:22:ASP:OD2	2:G:26:ASN:HB2	2.12	0.50
2:G:154:ARG:HH11	2:G:154:ARG:HG2	1.76	0.49
2:G:155:ALA:C	2:G:158:GLY:H	2.20	0.49
2:G:223:VAL:HA	2:G:240:SER:HA	1.93	0.49
2:G:482:ARG:HG3	2:G:482:ARG:NH1	2.09	0.49
2:G:152:ARG:CZ	2:G:208:ASP:HB3	2.42	0.49
2:G:435:VAL:O	2:G:435:VAL:HG13	2.10	0.49
2:G:456:ASN:HD22	2:G:457:LEU:H	1.59	0.49
1:F:124:LEU:O	1:F:128:GLU:HB2	2.13	0.49
2:G:256:VAL:O	2:G:256:VAL:HG13	2.06	0.49
2:G:251:PHE:HE2	2:G:445:TYR:HB3	1.78	0.49
2:G:451:VAL:CG1	2:G:453:PHE:HB2	2.42	0.49
1:F:10:VAL:HG12	1:F:10:VAL:O	2.12	0.49
2:G:180:VAL:HA	2:G:216:GLU:O	2.13	0.49
1:F:33:ILE:HB	1:F:49:GLY:O	2.12	0.49
1:F:54:PRO:HD2	1:F:134:THR:CG2	2.32	0.49
2:G:226:GLN:CG	2:G:238:PRO:HA	2.42	0.49
2:G:133:ASP:C	2:G:135:TYR:H	2.21	0.49
2:G:162:PHE:O	2:G:179:HIS:HE1	1.96	0.49
2:G:18:ALA:HB1	2:G:63:VAL:HG21	1.94	0.49
1:F:85:VAL:HG21	1:F:166:ILE:HD11	1.94	0.48
2:G:97:ILE:O	2:G:98:TYR:HB2	2.12	0.48
2:G:166:ASP:OD1	2:G:166:ASP:N	2.41	0.48
2:G:17:ARG:HB2	2:G:31:SER:O	2.13	0.48
2:G:456:ASN:HD22	2:G:457:LEU:N	2.10	0.48
2:G:53:TRP:CE3	2:G:53:TRP:CA	2.96	0.48
2:G:131:VAL:O	2:G:136:PHE:HE2	1.96	0.48
1:F:30:ILE:HG22	1:F:31:VAL:N	2.29	0.48
1:F:79:ILE:HG12	1:F:80:GLU:N	2.27	0.48
2:G:155:ALA:HB2	2:G:160:LEU:HD12	1.96	0.48
1:F:20:ILE:O	1:F:166:ILE:N	2.44	0.48
1:F:73:THR:OG1	1:F:100:GLY:N	2.47	0.48
2:G:148:VAL:O	2:G:151:SER:HB2	2.14	0.48
2:G:227:THR:HG23	2:G:228:ASN:N	2.29	0.48
2:G:15:SER:HA	2:G:35:PHE:HE1	1.73	0.48
2:G:60:LEU:C	2:G:60:LEU:HD12	2.39	0.48
1:F:67:ILE:HD12	1:F:68:GLY:C	2.39	0.48
1:F:124:LEU:N	1:F:125:PRO:CD	2.76	0.48
2:G:80:THR:HG21	2:G:248:ALA:HB3	1.96	0.48
2:G:160:LEU:O	2:G:161:LEU:HD23	2.14	0.48
2:G:206:VAL:HG12	2:G:207:LEU:N	2.26	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:32:ASN:O	1:F:35:ASP:HA	2.13	0.47
2:G:189:THR:HG21	2:G:191:LEU:HB2	1.95	0.47
2:G:451:VAL:HG12	2:G:453:PHE:CB	2.44	0.47
1:F:156:VAL:HG12	1:F:161:THR:HG21	1.91	0.47
2:G:14:THR:HG1	2:G:267:THR:HG1	1.58	0.47
2:G:179:HIS:CD2	2:G:215:PRO:CA	2.96	0.47
2:G:193:ASN:HB3	2:G:196:THR:CG2	2.45	0.47
2:G:271:MET:HE1	2:G:392:LEU:CA	2.32	0.47
1:F:59:MET:HG3	1:F:122:PHE:HE2	1.78	0.47
1:F:75:HIS:HD2	1:F:95:THR:HB	1.79	0.47
2:G:23:HIS:HA	2:G:453:PHE:HE2	1.79	0.47
2:G:77:ILE:HG22	2:G:77:ILE:O	2.14	0.47
1:F:124:LEU:O	1:F:124:LEU:HG	2.13	0.47
1:F:50:ILE:HD11	1:F:163:VAL:HG21	1.96	0.47
2:G:5:TYR:CD1	2:G:5:TYR:N	2.82	0.47
2:G:152:ARG:HE	2:G:208:ASP:CB	2.25	0.47
2:G:426:LEU:HD23	2:G:426:LEU:HA	1.34	0.47
2:G:483:TYR:O	2:G:486:TRP:HB3	2.15	0.47
2:G:133:ASP:CG	2:G:134:PRO:HD2	2.39	0.47
2:G:46:GLU:OE2	2:G:107:ARG:NH2	2.34	0.46
2:G:11:GLN:CD	2:G:52:ILE:HG23	2.41	0.46
2:G:297:GLU:OE1	2:G:297:GLU:N	2.47	0.46
1:F:30:ILE:C	1:F:31:VAL:HG23	2.41	0.46
1:F:150:ILE:HB	1:F:165:ARG:HB2	1.98	0.46
2:G:428:THR:CG2	2:G:429:ARG:N	2.77	0.46
2:G:449:LEU:HD23	2:G:454:TRP:HB2	1.98	0.46
1:F:97:GLU:CG	1:F:98:LEU:HD13	2.45	0.46
2:G:431:GLU:O	2:G:433:PRO:HD3	2.15	0.46
2:G:460:LEU:C	2:G:462:GLU:H	2.24	0.46
1:F:164:ILE:CG2	1:F:165:ARG:N	2.78	0.46
2:G:221:SER:HB2	2:G:446:LEU:O	2.16	0.46
2:G:315:TRP:CH2	2:G:320:MET:HG3	2.50	0.46
1:F:20:ILE:HG22	1:F:21:GLU:H	1.79	0.46
2:G:132:ILE:H	2:G:132:ILE:HG12	1.51	0.46
1:F:31:VAL:CG1	1:F:32:ASN:N	2.79	0.45
2:G:115:LEU:HD11	2:G:207:LEU:HD21	1.99	0.45
2:G:95:LYS:HA	2:G:96:PRO:HD3	1.73	0.45
2:G:320:MET:HB3	2:G:320:MET:HE3	1.66	0.45
1:F:120:ILE:CG2	1:F:121:GLU:N	2.80	0.45
2:G:102:VAL:CG1	2:G:103:TRP:N	2.79	0.45
1:F:45:ILE:CD1	1:F:45:ILE:H	2.29	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:81:SER:HG	1:F:85:VAL:H	1.65	0.45
2:G:352:GLY:O	2:G:356:TRP:N	2.32	0.45
1:F:33:ILE:CG2	1:F:34:GLU:N	2.80	0.45
2:G:255:CYS:O	2:G:257:LYS:N	2.48	0.45
2:G:123:TYR:OH	2:G:200:ASP:OD1	2.33	0.45
2:G:211:ARG:HG3	2:G:214:LEU:HD12	1.99	0.45
1:F:26:LEU:HD21	1:F:52:ILE:CG2	2.47	0.45
1:F:106:ILE:HD12	1:F:106:ILE:N	2.32	0.45
2:G:8:ALA:O	2:G:9:LEU:HD12	2.17	0.45
2:G:127:ASN:HB3	2:G:193:ASN:ND2	2.31	0.45
2:G:282:SER:OG	2:G:398:ASP:OD2	2.29	0.45
2:G:381:LEU:HA	2:G:381:LEU:HD23	1.73	0.45
1:F:67:ILE:CD1	1:F:70:ILE:CG1	2.95	0.44
2:G:88:VAL:HA	2:G:161:LEU:O	2.17	0.44
1:F:62:PRO:C	1:F:63:VAL:HG13	2.42	0.44
2:G:98:TYR:CE2	2:G:143:TRP:CZ3	3.05	0.44
2:G:196:THR:HG22	2:G:198:ASP:N	2.31	0.44
1:F:165:ARG:NH1	1:F:165:ARG:CG	2.80	0.44
2:G:174:THR:C	2:G:176:GLY:H	2.26	0.44
2:G:432:ARG:HA	2:G:433:PRO:HD2	1.65	0.44
1:F:98:LEU:HD13	1:F:98:LEU:N	2.32	0.44
2:G:448:GLY:CA	2:G:453:PHE:HB3	2.48	0.44
1:F:143:MET:SD	1:F:146:ILE:HD13	2.57	0.44
2:G:303:GLU:CG	2:G:304:GLY:N	2.80	0.44
1:F:98:LEU:HD12	1:F:98:LEU:HA	1.32	0.44
1:F:166:ILE:O	1:F:166:ILE:HG12	2.17	0.44
2:G:312:SER:HB3	2:G:380:THR:CG2	2.48	0.44
2:G:195:HIS:CD2	2:G:195:HIS:H	2.36	0.44
1:F:36:VAL:CG1	1:F:37:PRO:HD2	2.44	0.44
2:G:85:THR:CG2	2:G:103:TRP:CD1	3.00	0.44
2:G:253:GLN:HG2	2:G:438:VAL:HG11	1.99	0.44
2:G:476:THR:O	2:G:479:ARG:HD3	2.17	0.44
2:G:35:PHE:CE2	2:G:47:HIS:CD2	2.90	0.43
2:G:53:TRP:NE1	2:G:172:LYS:HE2	2.33	0.43
2:G:133:ASP:C	2:G:135:TYR:N	2.76	0.43
2:G:197:LEU:N	2:G:197:LEU:CD1	2.79	0.43
2:G:250:LEU:HD11	2:G:255:CYS:HB2	2.00	0.43
1:F:59:MET:HB2	1:F:59:MET:HE2	1.54	0.43
1:F:81:SER:OG	1:F:85:VAL:HB	2.18	0.43
2:G:128:THR:OG1	2:G:130:LEU:HB2	2.18	0.43
2:G:199:TRP:CZ2	2:G:214:LEU:HB3	2.54	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:30:VAL:HG12	2:G:31:SER:N	2.33	0.43
2:G:80:THR:CG2	2:G:248:ALA:HB2	2.49	0.43
2:G:240:SER:OG	2:G:447:ALA:HB1	2.17	0.43
2:G:110:GLU:O	2:G:113:GLU:N	2.52	0.43
2:G:178:VAL:HG12	2:G:180:VAL:HG12	1.99	0.43
2:G:422:GLN:NE2	2:G:426:LEU:HG	2.32	0.43
1:F:91:PHE:HA	1:F:136:THR:CG2	2.33	0.43
2:G:13:THR:OG1	2:G:103:TRP:NE1	2.35	0.43
2:G:124:ILE:O	2:G:128:THR:OG1	2.31	0.43
2:G:322:LEU:HA	2:G:322:LEU:HD23	1.71	0.43
2:G:102:VAL:CG1	2:G:103:TRP:H	2.29	0.43
2:G:152:ARG:O	2:G:155:ALA:N	2.50	0.43
2:G:169:LEU:HD23	2:G:169:LEU:HA	1.71	0.43
2:G:347:ALA:O	2:G:361:ARG:HA	2.19	0.43
2:G:155:ALA:HB2	2:G:160:LEU:CB	2.48	0.43
2:G:179:HIS:CD2	2:G:215:PRO:HB3	2.54	0.43
2:G:360:ALA:O	2:G:361:ARG:HG2	2.19	0.43
1:F:45:ILE:CD1	1:F:45:ILE:N	2.81	0.43
2:G:173:MET:HB2	2:G:227:THR:OG1	2.19	0.43
2:G:336:VAL:O	2:G:337:GLN:HB2	2.19	0.43
2:G:342:VAL:HG12	2:G:343:TYR:N	2.32	0.43
1:F:91:PHE:CD1	1:F:91:PHE:C	2.96	0.43
2:G:83:ARG:HH11	4:G:503:G3H:C1	2.32	0.42
2:G:15:SER:HA	2:G:35:PHE:CD1	2.54	0.42
2:G:361:ARG:HG2	2:G:361:ARG:NH1	2.32	0.42
2:G:271:MET:CE	2:G:392:LEU:HA	2.33	0.42
2:G:313:ILE:HD12	2:G:313:ILE:HA	1.80	0.42
2:G:360:ALA:HB2	2:G:494:MET:HA	2.00	0.42
2:G:458:ASP:C	2:G:460:LEU:N	2.77	0.42
1:F:75:HIS:CD2	1:F:95:THR:HB	2.54	0.42
1:F:93:ILE:O	1:F:94:ASP:HB2	2.19	0.42
2:G:192:PHE:CD1	2:G:192:PHE:C	2.98	0.42
1:F:64:ASP:HA	1:F:113:VAL:O	2.20	0.42
1:F:98:LEU:N	1:F:98:LEU:CD1	2.79	0.42
2:G:182:ASP:HB3	2:G:242:ILE:HG22	2.01	0.42
1:F:50:ILE:HD11	1:F:163:VAL:CG2	2.49	0.42
1:F:149:LEU:CD2	1:F:166:ILE:CG2	2.98	0.42
2:G:70:SER:O	2:G:73:GLN:N	2.47	0.42
2:G:142:LYS:HE2	2:G:146:ASP:OD2	2.20	0.41
2:G:197:LEU:HD12	2:G:197:LEU:H	1.82	0.41
2:G:251:PHE:HE2	2:G:445:TYR:CB	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:266:GLY:HA2	5:G:504:ADP:O5'	2.20	0.41
2:G:451:VAL:O	2:G:451:VAL:HG13	2.20	0.41
1:F:52:ILE:HD13	1:F:52:ILE:HG21	1.82	0.41
2:G:4:LYS:C	2:G:5:TYR:CG	2.98	0.41
2:G:434:GLU:CB	2:G:467:GLU:HB2	2.50	0.41
2:G:196:THR:CG2	2:G:198:ASP:N	2.83	0.41
1:F:92:GLY:HA2	1:F:135:LEU:O	2.20	0.41
1:F:150:ILE:HG22	1:F:151:LYS:N	2.36	0.41
1:F:156:VAL:CG1	1:F:161:THR:HB	2.41	0.41
2:G:114:HIS:C	2:G:116:LYS:N	2.79	0.41
2:G:246:GLN:CD	2:G:270:PHE:HB2	2.44	0.41
2:G:353:ALA:HA	2:G:354:PRO:HA	1.75	0.41
1:F:39:VAL:H	1:F:39:VAL:HG23	1.13	0.41
1:F:65:GLY:O	1:F:113:VAL:N	2.41	0.41
1:F:146:ILE:O	1:F:146:ILE:HG12	2.20	0.41
1:F:163:VAL:C	1:F:164:ILE:HG13	2.46	0.41
2:G:85:THR:HB	2:G:101:ILE:O	2.20	0.41
2:G:260:MET:HB3	2:G:260:MET:HE2	1.78	0.41
2:G:32:GLN:HE21	2:G:32:GLN:HB2	1.64	0.41
2:G:68:ASP:O	2:G:69:ILE:HD12	2.21	0.41
2:G:174:THR:O	2:G:177:ARG:N	2.40	0.41
2:G:189:THR:HG23	2:G:191:LEU:CB	2.50	0.41
2:G:456:ASN:HD22	2:G:456:ASN:HA	1.51	0.41
2:G:457:LEU:HD23	2:G:457:LEU:HA	1.58	0.41
1:F:26:LEU:CD2	1:F:52:ILE:HD12	2.51	0.41
1:F:147:LYS:N	1:F:167:LYS:O	2.50	0.41
2:G:226:GLN:CG	2:G:238:PRO:CA	2.99	0.41
2:G:444:ALA:O	2:G:447:ALA:N	2.54	0.41
1:F:127:LEU:HD23	1:F:127:LEU:HA	1.76	0.40
2:G:156:ARG:C	2:G:158:GLY:N	2.76	0.40
2:G:221:SER:CB	2:G:450:ALA:HB2	2.49	0.40
2:G:468:ARG:HH11	2:G:468:ARG:HD2	1.69	0.40
1:F:136:THR:HA	1:F:137:PRO:HD2	1.88	0.40
2:G:109:ALA:O	2:G:113:GLU:HG2	2.21	0.40
2:G:174:THR:HB	2:G:178:VAL:HG23	2.03	0.40
1:F:54:PRO:CD	1:F:134:THR:HG23	2.35	0.40
2:G:47:HIS:O	2:G:49:PRO:HD3	2.20	0.40
2:G:115:LEU:HA	2:G:115:LEU:HD23	1.71	0.40
1:F:90:HIS:ND1	1:F:92:GLY:O	2.55	0.40
2:G:270:PHE:CD2	2:G:270:PHE:N	2.87	0.40
2:G:421:PHE:CZ	2:G:425:ILE:HD13	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:451:VAL:HG12	2:G:453:PHE:H	1.85	0.40
2:G:457:LEU:HD23	2:G:460:LEU:HD12	2.04	0.40
1:F:27:SER:HG	1:F:158:VAL:HG12	1.84	0.40
1:F:30:ILE:CG2	1:F:31:VAL:N	2.83	0.40
1:F:71:PHE:O	1:F:74:ASN:N	2.51	0.40
1:F:120:ILE:HG22	1:F:121:GLU:N	2.36	0.40
2:G:124:ILE:CD1	2:G:203:MET:CE	2.99	0.40
2:G:125:ARG:O	2:G:129:GLY:N	2.52	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%)	137 (87%)	15 (10%)	5 (3%)	3	8
2	G	485/501 (97%)	422 (87%)	46 (10%)	17 (4%)	3	7
All	All	642/669 (96%)	559 (87%)	61 (10%)	22 (3%)	3	7

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	57	ASN
2	G	42	PRO
2	G	175	GLN
2	G	206	VAL
2	G	255	CYS
2	G	256	VAL
2	G	211	ARG
2	G	222	GLU
1	F	74	ASN
1	F	95	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	109	GLU
2	G	98	TYR
2	G	149	GLU
2	G	437	GLU
2	G	461	GLN
2	G	479	ARG
1	F	125	PRO
2	G	84	GLU
2	G	99	ASN
2	G	210	PRO
2	G	219	ARG
2	G	294	PRO

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	121/145 (83%)	81 (67%)	40 (33%)	0	0
2	G	378/412 (92%)	277 (73%)	101 (27%)	0	0
All	All	499/557 (90%)	358 (72%)	141 (28%)	0	0

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	6	LEU
1	F	9	LEU
1	F	10	VAL
1	F	20	ILE
1	F	22	ILE
1	F	23	ILE
1	F	26	LEU
1	F	30	ILE
1	F	33	ILE
1	F	34	GLU
1	F	35	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	39	VAL
1	F	44	LYS
1	F	46	VAL
1	F	50	ILE
1	F	53	LYS
1	F	60	VAL
1	F	66	THR
1	F	67	ILE
1	F	73	THR
1	F	79	ILE
1	F	93	ILE
1	F	95	THR
1	F	98	LEU
1	F	105	ARG
1	F	117	ASP
1	F	128	GLU
1	F	129	GLU
1	F	130	LYS
1	F	134	THR
1	F	135	LEU
1	F	140	ILE
1	F	142	ASN
1	F	143	MET
1	F	146	ILE
1	F	149	LEU
1	F	157	THR
1	F	158	VAL
1	F	161	THR
1	F	166	ILE
2	G	4	LYS
2	G	5	TYR
2	G	6	ILE
2	G	17	ARG
2	G	21	MET
2	G	28	ILE
2	G	32	GLN
2	G	39	TYR
2	G	41	LYS
2	G	50	MET
2	G	51	GLU
2	G	52	ILE
2	G	53	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	55	THR
2	G	57	SER
2	G	58	SER
2	G	59	THR
2	G	60	LEU
2	G	63	VAL
2	G	69	ILE
2	G	73	GLN
2	G	77	ILE
2	G	79	ILE
2	G	80	THR
2	G	82	GLN
2	G	83	ARG
2	G	85	THR
2	G	91	LYS
2	G	95	LYS
2	G	101	ILE
2	G	107	ARG
2	G	110	GLU
2	G	117	ARG
2	G	120	LEU
2	G	127	ASN
2	G	130	LEU
2	G	132	ILE
2	G	136	PHE
2	G	140	LYS
2	G	151	SER
2	G	154	ARG
2	G	156	ARG
2	G	170	ILE
2	G	171	TRP
2	G	173	MET
2	G	182	ASP
2	G	185	ASN
2	G	189	THR
2	G	190	MET
2	G	201	ASP
2	G	203	MET
2	G	204	LEU
2	G	207	LEU
2	G	208	ASP
2	G	213	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	217	VAL
2	G	219	ARG
2	G	220	SER
2	G	222	GLU
2	G	227	THR
2	G	228	ASN
2	G	240	SER
2	G	255	CYS
2	G	256	VAL
2	G	260	MET
2	G	262	LYS
2	G	267	THR
2	G	269	CYS
2	G	271	MET
2	G	277	GLU
2	G	287	LEU
2	G	289	THR
2	G	295	THR
2	G	313	ILE
2	G	321	LYS
2	G	337	GLN
2	G	339	THR
2	G	361	ARG
2	G	367	LEU
2	G	369	ARG
2	G	402	ARG
2	G	422	GLN
2	G	425	ILE
2	G	428	THR
2	G	434	GLU
2	G	437	GLU
2	G	439	THR
2	G	446	LEU
2	G	451	VAL
2	G	456	ASN
2	G	458	ASP
2	G	465	VAL
2	G	466	ILE
2	G	468	ARG
2	G	474	ILE
2	G	477	THR
2	G	482	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	G	487	LYS
2	G	488	LYS
2	G	494	MET
2	G	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	74	ASN
1	F	142	ASN
2	G	47	HIS
2	G	81	ASN
2	G	104	GLN
2	G	299	ASN
2	G	374	ASN
2	G	387	GLN
2	G	396	GLN
2	G	422	GLN
2	G	456	ASN

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 3 ligands modelled in this entry, 1 is 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
4	G3H	G	503	3	8,9,9	2.39	2 (25%)	7,12,12	0.81	0
5	ADP	G	504	3	28,29,29	1.20	1 (3%)	43,45,45	3.30	6 (13%)

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	G3H	G	503	3	1/1/2/3	2/7/8/8	-
5	ADP	G	504	3	-	7/16/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	503	G3H	O1-C1	5.17	1.39	1.20
5	G	504	ADP	PA-O3A	4.67	1.64	1.59
4	G	503	G3H	C3-C2	3.64	1.56	1.51

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	504	ADP	O2A-PA-O3A	13.39	143.46	107.27
5	G	504	ADP	O3A-PA-O1A	-9.61	81.79	110.70
5	G	504	ADP	C4-N9-C1'	-8.39	107.01	126.63
5	G	504	ADP	C1'-N9-C8	8.35	145.63	127.09
5	G	504	ADP	O2'-C2'-C1'	5.05	127.48	110.10
5	G	504	ADP	O2B-PB-O3A	2.64	113.50	104.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	503	G3H	C2

All (9) torsion outliers are listed below:

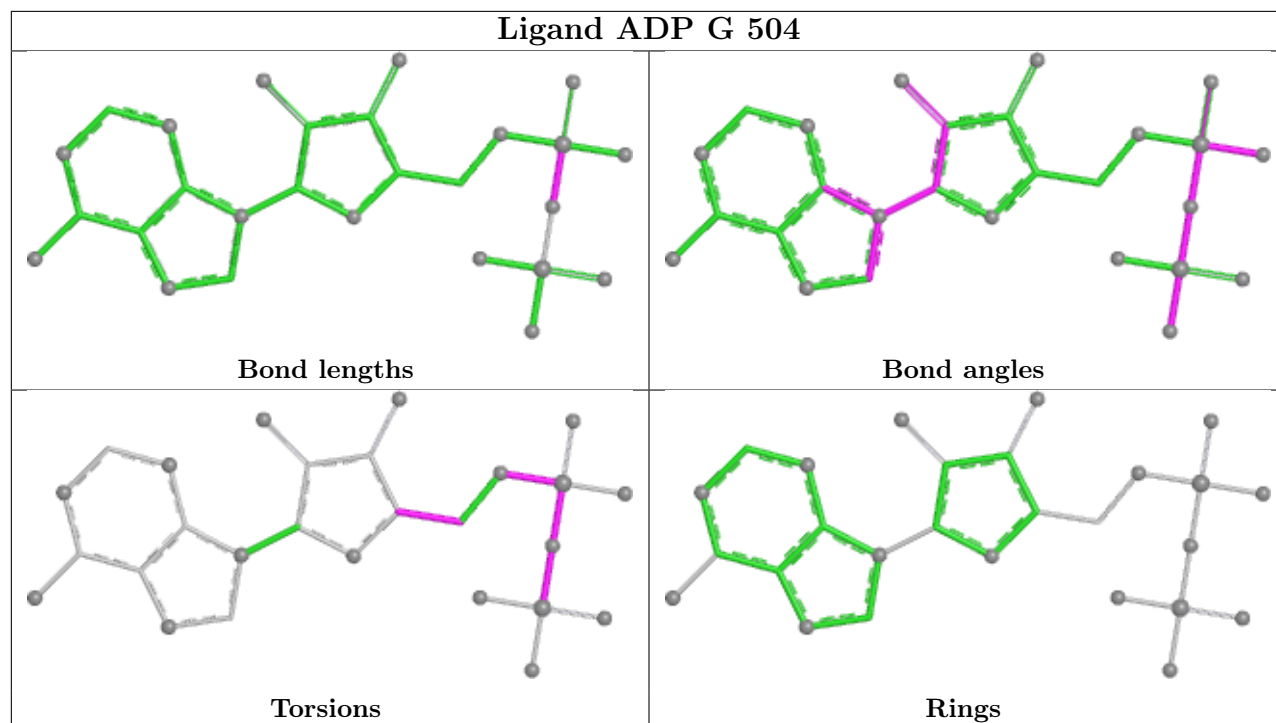
Mol	Chain	Res	Type	Atoms
4	G	503	G3H	C1-C2-C3-O1P
4	G	503	G3H	O2-C2-C3-O1P
5	G	504	ADP	PA-O3A-PB-O2B
5	G	504	ADP	PA-O3A-PB-O3B
5	G	504	ADP	C5'-O5'-PA-O1A
5	G	504	ADP	C3'-C4'-C5'-O5'
5	G	504	ADP	O4'-C4'-C5'-O5'
5	G	504	ADP	C5'-O5'-PA-O2A
5	G	504	ADP	PB-O3A-PA-O2A

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	503	G3H	4	0
5	G	504	ADP	1	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.