



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 11:20 AM UTC

PDB ID : 1GLE / pdb_00001gle
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 : 2.94 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

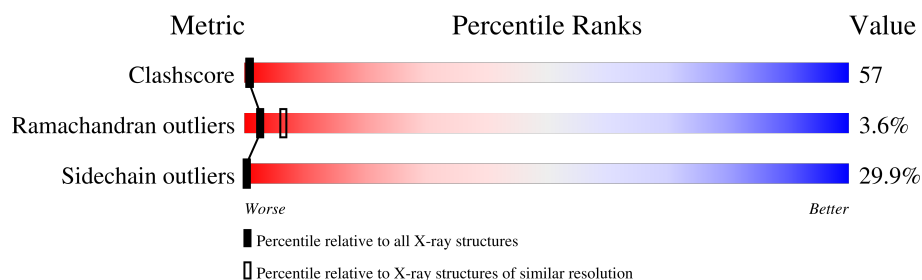
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 Å.

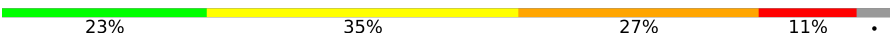
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	
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
4	G3H	G	503	X	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4996 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			

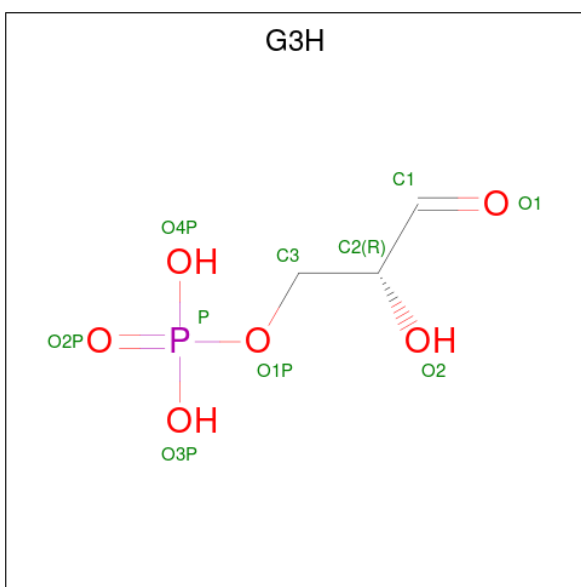
- Molecule 2 is a protein called GLYCEROL KINASE.

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 (CCD ID: ZN) (formula: Zn).

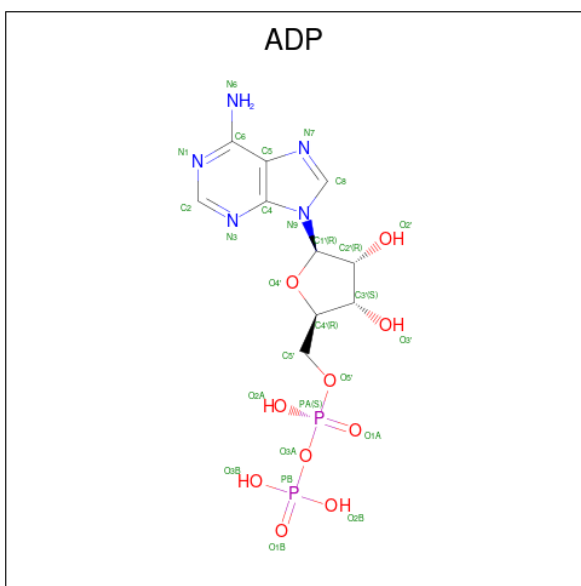
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	F	1	Total	Zn	0	0
			1	1		
3	G	1	Total	Zn	0	0
			1	1		

- 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	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	7	Total 7	O 7	0	0
6	G	41	Total 41	O 41	0	0

3 Residue-property plots

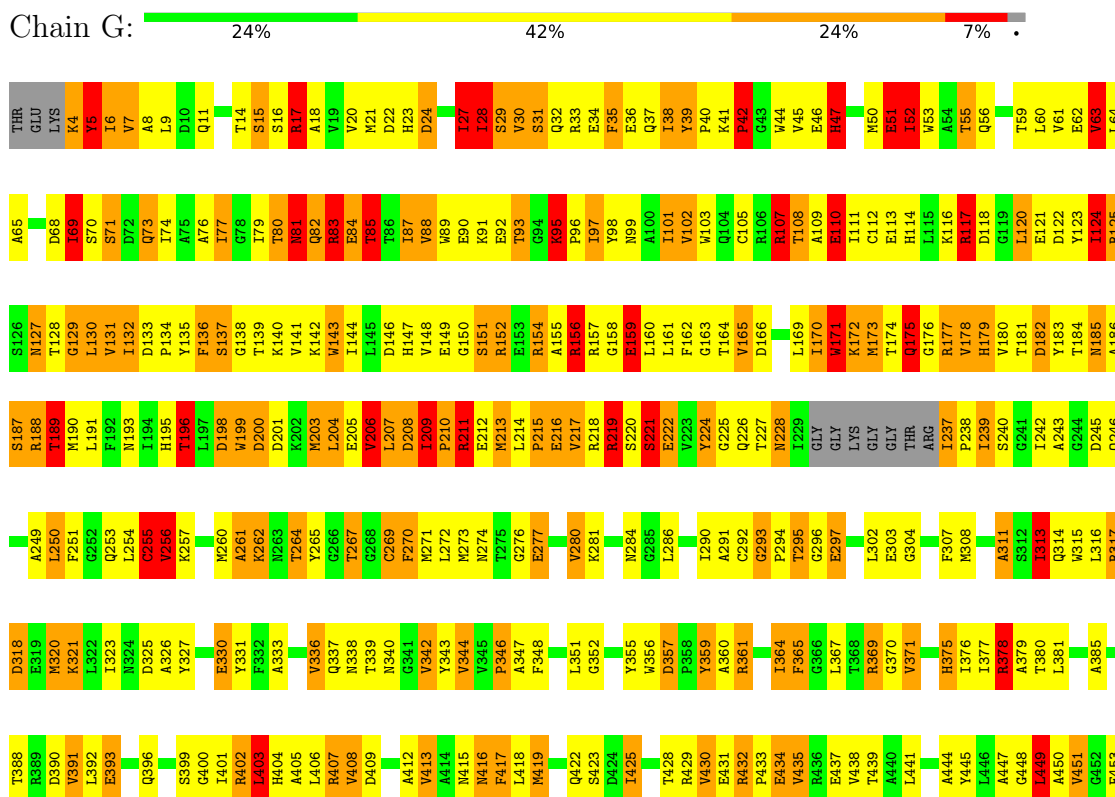
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



W454	Q455	M456	L457	D458	E459	L460	Q461	K463	A464	V465	L466	E467	R468	E469	F470	R471	P472	G473	I474	E475	T476	T477	E478	R479	M480	Y481	R482		G485	W486	K487	K488	A489	V490	K491	R492	A493	M494	A495	W496	E497	E498	H499	ASP	GLU
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4 Data and refinement statistics

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

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	124.03Å 125.11Å 133.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	21.80 – 2.94	Depositor
% Data completeness (in resolution range)	(Not available) (21.80-2.94)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.149 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4996	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, G3H, ZN

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	1.76	19/1172 (1.6%)	2.28	64/1592 (4.0%)
2	G	1.63	39/3831 (1.0%)	2.17	165/5211 (3.2%)
All	All	1.66	58/5003 (1.2%)	2.20	229/6803 (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
2	G	2	0

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	39	TYR	N-CA	-7.25	1.37	1.46
2	G	38	ILE	CA-C	-7.12	1.44	1.52
1	F	104	LYS	CA-C	6.96	1.62	1.52
1	F	91	PHE	CA-C	-6.76	1.44	1.52
2	G	101	ILE	CA-CB	-6.64	1.45	1.54
2	G	342	VAL	CA-CB	-6.63	1.46	1.54
1	F	137	PRO	CA-C	-6.61	1.44	1.52
2	G	377	ILE	CA-CB	-6.58	1.46	1.54
2	G	110	GLU	CD-OE2	6.53	1.37	1.25
1	F	39	VAL	CA-CB	-6.29	1.47	1.54
2	G	117	ARG	NE-CZ	6.17	1.39	1.33
1	F	144	ASP	CG-OD1	5.96	1.36	1.25
2	G	388	THR	CA-C	-5.90	1.45	1.52
2	G	393	GLU	CD-OE1	5.85	1.36	1.25
2	G	216	GLU	N-CA	-5.82	1.38	1.46
1	F	90	HIS	CA-C	-5.80	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	91	PHE	N-CA	-5.78	1.39	1.46
2	G	24	ASP	CG-OD1	5.75	1.36	1.25
2	G	62	GLU	CD-OE2	5.73	1.36	1.25
2	G	359	TYR	CA-C	-5.71	1.44	1.52
1	F	101	GLU	CD-OE2	5.69	1.36	1.25
1	F	87	LEU	N-CA	-5.68	1.39	1.46
2	G	216	GLU	CD-OE2	5.63	1.36	1.25
2	G	406	LEU	N-CA	-5.62	1.39	1.46
1	F	103	PHE	CA-C	-5.59	1.45	1.52
1	F	46	VAL	CA-CB	-5.56	1.47	1.54
2	G	336	VAL	C-N	-5.56	1.25	1.33
2	G	280	VAL	CA-CB	-5.55	1.48	1.54
2	G	51	GLU	CD-OE1	5.55	1.35	1.25
2	G	102	VAL	CA-C	-5.44	1.47	1.53
2	G	124	ILE	CA-CB	-5.40	1.48	1.54
1	F	80	GLU	CD-OE1	5.39	1.35	1.25
2	G	219	ARG	NE-CZ	5.36	1.39	1.33
2	G	124	ILE	N-CA	-5.34	1.40	1.46
2	G	331	TYR	CA-CB	-5.34	1.45	1.53
1	F	148	GLU	CD-OE2	5.32	1.35	1.25
1	F	72	GLU	CD-OE2	5.32	1.35	1.25
2	G	437	GLU	CD-OE2	5.32	1.35	1.25
1	F	97	GLU	CD-OE1	5.31	1.35	1.25
2	G	118	ASP	CG-OD2	5.30	1.35	1.25
2	G	408	VAL	CA-C	-5.25	1.47	1.52
2	G	39	TYR	CA-C	-5.23	1.45	1.52
2	G	159	GLU	CD-OE1	5.22	1.35	1.25
2	G	336	VAL	CA-C	-5.21	1.47	1.52
1	F	119	VAL	C-N	-5.19	1.27	1.33
2	G	313	ILE	N-CA	-5.16	1.40	1.46
2	G	320	MET	C-N	-5.14	1.26	1.33
1	F	46	VAL	CA-C	-5.13	1.45	1.52
2	G	388	THR	C-N	-5.13	1.27	1.34
2	G	37	GLN	C-N	-5.12	1.27	1.33
2	G	270	PHE	CA-C	-5.10	1.46	1.52
2	G	89	TRP	CA-C	-5.09	1.46	1.52
2	G	385	ALA	CA-CB	-5.07	1.45	1.53
2	G	224	TYR	C-N	5.06	1.38	1.33
1	F	136	THR	CA-C	-5.05	1.47	1.52
2	G	198	ASP	CG-OD2	5.04	1.34	1.25
2	G	378	ARG	C-N	-5.01	1.27	1.34
1	F	129	GLU	CD-OE1	5.00	1.34	1.25

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	336	VAL	N-CA-C	14.68	127.29	113.20
2	G	185	ASN	CA-CB-CG	-12.27	100.33	112.60
1	F	36	VAL	N-CA-CB	10.74	120.07	110.08
2	G	404	HIS	CA-CB-CG	-10.21	103.59	113.80
2	G	107	ARG	N-CA-C	9.56	121.30	111.07
2	G	47	HIS	CA-CB-CG	9.55	123.35	113.80
2	G	93	THR	N-CA-C	9.29	121.09	110.97
2	G	92	GLU	CA-C-N	9.25	132.86	120.65
2	G	92	GLU	C-N-CA	9.25	132.86	120.65
2	G	270	PHE	CA-CB-CG	-9.25	104.55	113.80
1	F	104	LYS	N-CA-CB	-9.20	94.94	110.49
2	G	85	THR	CA-C-N	9.20	133.93	120.87
2	G	85	THR	C-N-CA	9.20	133.93	120.87
2	G	95	LYS	CA-C-O	9.14	129.01	119.69
1	F	35	ASP	CA-CB-CG	8.83	121.43	112.60
1	F	158	VAL	N-CA-C	8.43	120.34	109.30
1	F	39	VAL	N-CA-C	8.38	120.17	110.62
1	F	86	GLU	CA-C-N	-8.32	110.86	122.93
1	F	86	GLU	C-N-CA	-8.32	110.86	122.93
2	G	380	THR	CA-CB-OG1	-8.15	97.38	109.60
2	G	114	HIS	CA-CB-CG	-8.10	105.70	113.80
2	G	432	ARG	CA-C-N	7.96	127.72	119.76
2	G	432	ARG	C-N-CA	7.96	127.72	119.76
1	F	40	VAL	O-C-N	7.95	129.90	121.87
1	F	71	PHE	N-CA-CB	7.95	121.85	109.69
1	F	41	PHE	CA-CB-CG	-7.79	106.01	113.80
2	G	42	PRO	N-CA-CB	7.76	111.40	103.25
2	G	465	VAL	CB-CA-C	-7.75	99.49	111.26
2	G	460	LEU	N-CA-C	7.74	123.86	112.94
2	G	209	ILE	C-N-CD	-7.71	93.41	125.00
1	F	67	ILE	N-CA-CB	7.68	119.32	110.49
2	G	179	HIS	CA-CB-CG	7.62	121.42	113.80
2	G	480	ASN	N-CA-C	7.59	120.44	111.71
2	G	27	ILE	N-CA-CB	7.58	119.58	111.46
1	F	135	LEU	CA-C-N	-7.58	112.59	122.98
1	F	135	LEU	C-N-CA	-7.58	112.59	122.98
2	G	83	ARG	N-CA-C	7.55	120.77	110.35
2	G	61	VAL	N-CA-CB	-7.51	102.74	110.62
2	G	466	ILE	N-CA-CB	7.47	119.96	110.99
2	G	261	ALA	N-CA-C	7.34	120.61	109.23
2	G	52	ILE	O-C-N	7.30	129.07	121.91
2	G	458	ASP	CA-CB-CG	-7.30	105.30	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	200	ASP	CA-CB-CG	-7.29	105.31	112.60
1	F	55	THR	N-CA-CB	7.27	121.21	110.53
1	F	111	GLN	N-CA-C	7.26	119.94	110.43
1	F	60	VAL	N-CA-CB	-7.25	98.35	111.92
1	F	126	LEU	N-CA-C	-7.18	103.39	111.07
1	F	150	ILE	O-C-N	7.17	130.93	123.18
1	F	64	ASP	CA-CB-CG	7.13	119.73	112.60
2	G	357	ASP	O-C-N	7.13	127.36	121.44
2	G	186	ALA	N-CA-C	7.12	119.03	111.28
2	G	28	ILE	N-CA-C	7.11	119.11	111.58
2	G	417	PHE	CA-CB-CG	-7.10	106.70	113.80
1	F	34	GLU	CA-C-N	-6.99	111.46	122.65
1	F	34	GLU	C-N-CA	-6.99	111.46	122.65
2	G	237	ILE	CA-C-N	-6.98	113.05	120.66
2	G	237	ILE	C-N-CA	-6.98	113.05	120.66
2	G	52	ILE	N-CA-C	-6.91	103.78	110.42
2	G	15	SER	N-CA-C	6.89	118.57	108.86
1	F	150	ILE	N-CA-C	6.87	118.37	108.48
2	G	69	ILE	N-CA-CB	-6.82	99.97	111.23
1	F	124	LEU	C-N-CD	-6.82	97.05	125.00
2	G	144	ILE	CB-CA-C	-6.77	103.30	111.97
2	G	5	TYR	N-CA-C	6.76	119.43	108.76
2	G	125	ARG	CA-C-N	6.63	129.83	120.28
2	G	125	ARG	C-N-CA	6.63	129.83	120.28
2	G	416	ASN	CA-CB-CG	-6.63	105.97	112.60
1	F	55	THR	N-CA-C	6.62	121.64	113.50
1	F	105	ARG	N-CA-C	6.60	119.58	108.23
2	G	157	ARG	N-CA-C	-6.58	104.36	112.38
2	G	129	GLY	N-CA-C	-6.58	106.72	115.40
2	G	221	SER	N-CA-CB	6.58	120.77	110.71
2	G	369	ARG	N-CA-CB	6.56	120.50	110.14
2	G	317	ARG	N-CA-C	6.53	118.48	111.36
2	G	449	LEU	CB-CA-C	-6.52	99.91	110.74
2	G	357	ASP	CA-C-N	6.52	127.48	120.83
2	G	357	ASP	C-N-CA	6.52	127.48	120.83
1	F	57	ASN	N-CA-C	6.51	124.66	110.80
1	F	58	LYS	N-CA-C	6.49	118.72	108.79
1	F	112	ARG	CA-C-N	-6.47	114.04	122.51
1	F	112	ARG	C-N-CA	-6.47	114.04	122.51
2	G	342	VAL	N-CA-C	6.43	117.88	109.58
2	G	52	ILE	CB-CA-C	-6.36	103.83	111.97
2	G	63	VAL	CA-C-N	6.35	128.70	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	63	VAL	C-N-CA	6.35	128.70	120.44
2	G	480	ASN	N-CA-CB	6.30	119.92	110.22
2	G	47	HIS	N-CA-CB	6.29	121.40	111.20
2	G	330	GLU	N-CA-C	-6.28	104.36	111.14
1	F	122	PHE	N-CA-C	6.27	118.31	108.96
2	G	171	TRP	CA-CB-CG	6.27	125.52	113.60
2	G	376	ILE	N-CA-C	6.26	116.43	110.42
2	G	107	ARG	N-CA-CB	6.23	119.04	110.01
2	G	108	THR	CB-CA-C	-6.22	103.51	111.22
1	F	150	ILE	N-CA-CB	6.21	122.19	111.39
2	G	198	ASP	CA-CB-CG	6.19	118.79	112.60
1	F	27	SER	N-CA-C	6.17	119.61	109.85
1	F	131	ALA	N-CA-C	6.17	119.20	110.50
2	G	215	PRO	N-CA-CB	6.16	109.72	103.25
2	G	290	ILE	N-CA-C	6.16	117.88	108.71
2	G	296	GLY	N-CA-C	-6.16	106.21	115.32
2	G	156	ARG	N-CA-CB	6.15	119.26	110.16
2	G	365	PHE	N-CA-C	6.15	118.52	109.24
2	G	432	ARG	O-C-N	6.14	128.17	121.36
1	F	117	ASP	CB-CA-C	6.13	119.47	109.90
2	G	42	PRO	N-CA-C	6.13	125.10	112.47
2	G	33	ARG	N-CA-CB	6.12	119.31	110.37
2	G	116	LYS	CA-C-N	6.12	128.49	120.28
2	G	116	LYS	C-N-CA	6.12	128.49	120.28
2	G	218	ARG	N-CA-C	6.10	118.44	109.24
1	F	93	ILE	CB-CA-C	6.07	119.19	110.33
2	G	344	VAL	CB-CA-C	-6.06	103.11	110.99
2	G	307	PHE	CA-C-N	-6.04	114.48	122.99
2	G	307	PHE	C-N-CA	-6.04	114.48	122.99
2	G	188	ARG	N-CA-C	6.03	119.89	112.54
2	G	371	VAL	CB-CA-C	-6.03	102.35	111.33
2	G	375	HIS	CA-CB-CG	-5.99	107.81	113.80
2	G	407	ARG	CA-C-N	-5.98	114.89	123.03
2	G	407	ARG	C-N-CA	-5.98	114.89	123.03
2	G	35	PHE	CA-CB-CG	-5.98	107.82	113.80
2	G	487	LYS	N-CA-CB	5.96	118.88	110.12
2	G	311	ALA	CB-CA-C	-5.95	101.28	110.81
2	G	408	VAL	CB-CA-C	-5.95	101.18	110.52
2	G	118	ASP	CB-CA-C	5.94	120.16	110.95
2	G	5	TYR	CB-CA-C	-5.94	99.29	110.16
2	G	165	VAL	N-CA-C	5.92	117.36	110.62
1	F	92	GLY	CA-C-N	-5.92	114.77	122.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	92	GLY	C-N-CA	-5.92	114.77	122.99
2	G	189	THR	N-CA-CB	-5.91	101.12	110.28
2	G	293	GLY	CA-C-N	5.89	127.20	119.84
2	G	293	GLY	C-N-CA	5.89	127.20	119.84
2	G	339	THR	N-CA-C	-5.86	106.11	113.20
2	G	178	VAL	CB-CA-C	-5.86	103.54	111.15
1	F	86	GLU	N-CA-C	5.85	118.05	108.52
2	G	144	ILE	N-CA-CB	5.84	117.38	110.55
2	G	419	MET	CA-CB-CG	-5.82	102.47	114.10
2	G	188	ARG	CA-C-N	5.81	129.14	120.31
2	G	188	ARG	C-N-CA	5.81	129.14	120.31
2	G	228	ASN	N-CA-C	5.80	119.06	107.62
2	G	159	GLU	CA-C-N	5.79	131.16	123.05
2	G	159	GLU	C-N-CA	5.79	131.16	123.05
2	G	38	ILE	CB-CA-C	-5.79	102.21	110.83
2	G	325	ASP	CB-CA-C	-5.79	97.29	109.38
1	F	128	GLU	CA-C-N	-5.75	113.21	122.23
1	F	128	GLU	C-N-CA	-5.75	113.21	122.23
2	G	280	VAL	CB-CA-C	-5.74	102.54	111.26
2	G	222	GLU	CA-C-N	-5.72	115.22	122.43
2	G	222	GLU	C-N-CA	-5.72	115.22	122.43
2	G	380	THR	N-CA-C	-5.72	104.96	111.14
2	G	17	ARG	CB-CA-C	5.72	121.62	110.30
1	F	32	ASN	O-C-N	5.71	129.96	122.93
1	F	33	ILE	N-CA-C	-5.71	104.11	110.62
1	F	35	ASP	N-CA-CB	5.69	118.87	110.56
2	G	346	PRO	N-CA-CB	5.68	106.80	102.36
2	G	256	VAL	N-CA-C	5.67	121.12	109.34
2	G	63	VAL	O-C-N	5.66	129.25	121.90
2	G	30	VAL	CB-CA-C	-5.65	101.96	110.55
2	G	71	SER	CA-C-N	5.63	127.82	120.28
2	G	71	SER	C-N-CA	5.63	127.82	120.28
2	G	378	ARG	CA-C-O	5.63	126.46	120.10
2	G	137	SER	N-CA-C	5.62	120.58	111.37
2	G	406	LEU	CA-C-N	-5.61	113.40	121.42
2	G	406	LEU	C-N-CA	-5.61	113.40	121.42
2	G	172	LYS	N-CA-CB	5.60	119.69	110.39
2	G	284	ASN	N-CA-C	5.60	118.05	110.88
1	F	156	VAL	O-C-N	5.58	129.33	123.02
2	G	390	ASP	CB-CA-C	-5.57	102.13	110.88
1	F	33	ILE	O-C-N	5.55	127.33	121.89
2	G	249	ALA	N-CA-C	-5.55	106.64	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	136	PHE	CA-CB-CG	-5.54	108.26	113.80
2	G	178	VAL	N-CA-C	5.51	116.17	108.89
2	G	37	GLN	N-CA-CB	5.51	119.42	110.77
1	F	64	ASP	N-CA-CB	5.51	118.75	109.94
2	G	63	VAL	CB-CA-C	-5.50	104.83	112.04
2	G	277	GLU	CA-C-N	-5.47	115.28	122.99
2	G	277	GLU	C-N-CA	-5.47	115.28	122.99
1	F	57	ASN	CA-C-N	-5.44	111.66	121.62
1	F	57	ASN	C-N-CA	-5.44	111.66	121.62
2	G	38	ILE	O-C-N	5.44	128.89	123.18
2	G	438	VAL	N-CA-C	5.43	116.21	110.72
1	F	39	VAL	CB-CA-C	-5.43	104.92	112.04
1	F	85	VAL	CA-C-N	-5.42	115.46	123.05
1	F	85	VAL	C-N-CA	-5.42	115.46	123.05
2	G	143	TRP	N-CA-C	-5.42	105.28	111.07
2	G	430	VAL	CA-C-N	-5.40	115.59	122.77
2	G	430	VAL	C-N-CA	-5.40	115.59	122.77
2	G	76	ALA	N-CA-C	5.39	115.66	108.38
1	F	146	ILE	N-CA-C	5.35	115.56	107.75
2	G	63	VAL	N-CA-CB	5.34	118.22	110.52
2	G	79	ILE	N-CA-C	5.32	115.56	108.11
1	F	60	VAL	N-CA-C	5.29	117.39	108.81
2	G	65	ALA	CA-C-N	5.28	127.61	120.38
2	G	65	ALA	C-N-CA	5.28	127.61	120.38
1	F	128	GLU	N-CA-C	5.27	117.77	111.71
2	G	70	SER	N-CA-CB	5.27	120.15	111.62
2	G	209	ILE	CA-C-N	5.23	126.38	119.84
2	G	209	ILE	C-N-CA	5.23	126.38	119.84
1	F	59	MET	CG-SD-CE	-5.21	89.43	100.90
2	G	297	GLU	CB-CG-CD	-5.17	103.81	112.60
2	G	307	PHE	N-CA-C	5.17	116.91	111.28
1	F	38	ASP	CA-CB-CG	5.16	117.76	112.60
2	G	267	THR	N-CA-C	-5.16	104.92	111.11
1	F	150	ILE	CB-CA-C	-5.15	102.95	110.62
1	F	94	ASP	N-CA-C	-5.14	106.30	112.58
2	G	359	TYR	CA-CB-CG	-5.14	104.64	113.90
2	G	81	ASN	N-CA-C	5.14	117.22	109.41
1	F	150	ILE	CA-C-N	5.11	129.49	122.84
1	F	150	ILE	C-N-CA	5.11	129.49	122.84
2	G	196	THR	N-CA-C	-5.11	106.87	113.01
2	G	385	ALA	CA-C-N	-5.10	113.50	120.44
2	G	385	ALA	C-N-CA	-5.10	113.50	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	175	GLN	CB-CA-C	5.10	120.57	110.42
2	G	177	ARG	CA-C-N	5.10	128.70	121.66
2	G	177	ARG	C-N-CA	5.10	128.70	121.66
2	G	318	ASP	CA-CB-CG	5.10	117.70	112.60
2	G	464	ALA	N-CA-C	5.09	119.14	111.81
1	F	87	LEU	N-CA-C	5.08	117.76	109.59
2	G	217	VAL	N-CA-CB	-5.08	105.27	111.21
2	G	292	CYS	N-CA-C	5.07	117.83	109.72
2	G	327	TYR	CA-C-N	5.07	127.78	120.38
2	G	327	TYR	C-N-CA	5.07	127.78	120.38
2	G	321	LYS	N-CA-C	5.06	119.41	113.23
2	G	375	HIS	O-C-N	5.05	127.27	122.07
2	G	403	LEU	O-C-N	5.04	128.81	122.86
1	F	62	PRO	N-CA-CB	5.04	108.54	103.25
1	F	125	PRO	N-CA-CB	5.02	108.52	103.25
2	G	15	SER	CB-CA-C	-5.01	99.61	111.65
1	F	103	PHE	O-C-N	5.01	128.69	123.03
2	G	88	VAL	CA-C-N	-5.01	113.12	121.64
2	G	88	VAL	C-N-CA	-5.01	113.12	121.64

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	G	255	CYS	CA
2	G	480	ASN	CA

There are no planarity outliers.

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	1157	0	1133	148	0
2	G	3752	0	3605	408	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	G	10	0	5	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	27	0	12	0	0
6	F	7	0	0	1	0
6	G	41	0	0	5	0
All	All	4996	0	4755	555	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 57.

All (555) 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:40:VAL:HA	1:F:45:ILE:HD12	1.18	1.10
2:G:7:VAL:HG22	2:G:20:VAL:HG22	1.32	1.09
2:G:419:MET:HE2	2:G:419:MET:HA	1.38	1.04
1:F:30:ILE:HD11	1:F:163:VAL:HG12	1.38	1.03
2:G:152:ARG:HH21	2:G:208:ASP:HB3	1.32	0.95
1:F:140:ILE:HD13	1:F:149:LEU:HD12	1.46	0.94
1:F:67:ILE:HA	1:F:79:ILE:HB	1.50	0.94
1:F:23:ILE:HD13	1:F:115:VAL:HG11	1.47	0.93
1:F:73:THR:HG21	1:F:96:VAL:HG23	1.50	0.92
1:F:36:VAL:HG13	1:F:37:PRO:HD2	1.51	0.91
1:F:106:ILE:HD11	1:F:121:GLU:HG3	1.51	0.91
2:G:308:MET:HE2	2:G:348:PHE:HB2	1.52	0.91
2:G:121:GLU:HA	2:G:132:ILE:HD11	1.53	0.88
1:F:157:THR:HG23	1:F:160:GLU:HB2	1.55	0.87
2:G:206:VAL:HG12	2:G:207:LEU:HD23	1.56	0.87
2:G:333:ALA:HB1	2:G:378:ARG:HB2	1.57	0.87
2:G:74:ILE:HD11	2:G:237:ILE:N	1.89	0.87
2:G:182:ASP:HB3	2:G:242:ILE:CG2	2.05	0.86
2:G:152:ARG:NH2	2:G:208:ASP:HB3	1.89	0.86
2:G:407:ARG:HD3	2:G:431:GLU:HG3	1.55	0.86
2:G:77:ILE:HG22	2:G:239:ILE:HG23	1.59	0.85
1:F:40:VAL:CA	1:F:45:ILE:HD12	2.05	0.82
2:G:16:SER:HB2	2:G:55:THR:HG23	1.61	0.82
1:F:40:VAL:HA	1:F:45:ILE:CD1	2.06	0.82
1:F:157:THR:CG2	1:F:160:GLU:HB2	2.09	0.81
2:G:189:THR:CG2	2:G:191:LEU:H	1.93	0.81
1:F:67:ILE:HD11	1:F:70:ILE:HG13	1.63	0.81
2:G:45:VAL:H	2:G:105:CYS:HB2	1.44	0.81
1:F:143:MET:SD	1:F:146:ILE:HD11	2.20	0.81
2:G:473:GLY:O	2:G:476:THR:HG22	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:85:THR:HG22	2:G:103:TRP:H	1.46	0.80
2:G:85:THR:HG22	2:G:103:TRP:N	1.96	0.80
2:G:271:MET:HE1	2:G:392:LEU:HB2	1.63	0.80
2:G:29:SER:OG	2:G:63:VAL:HG12	1.82	0.80
2:G:105:CYS:SG	2:G:107:ARG:HD2	2.22	0.80
2:G:445:TYR:HA	2:G:454:TRP:CZ3	2.17	0.80
1:F:106:ILE:CD1	1:F:121:GLU:HG3	2.12	0.79
2:G:419:MET:HA	2:G:419:MET:CE	2.05	0.79
2:G:51:GLU:O	2:G:55:THR:HB	1.82	0.79
2:G:60:LEU:O	2:G:63:VAL:HG23	1.82	0.78
2:G:101:ILE:HD13	2:G:107:ARG:HD3	1.65	0.78
2:G:156:ARG:HG3	2:G:156:ARG:HH11	1.49	0.78
1:F:143:MET:HA	1:F:146:ILE:HD13	1.65	0.78
2:G:98:TYR:HD1	2:G:99:ASN:H	1.32	0.77
2:G:271:MET:C	2:G:272:LEU:HD12	2.08	0.77
2:G:64:LEU:HD22	2:G:69:ILE:CG2	2.15	0.77
2:G:435:VAL:HG12	6:G:521:HOH:O	1.84	0.77
2:G:5:TYR:HB3	2:G:21:MET:O	1.85	0.76
2:G:52:ILE:O	2:G:55:THR:HG22	1.84	0.76
2:G:174:THR:HG21	2:G:178:VAL:HG21	1.66	0.76
2:G:83:ARG:HH11	4:G:503:G3H:H2	1.51	0.76
2:G:189:THR:HG22	2:G:191:LEU:H	1.52	0.75
2:G:246:GLN:OE1	2:G:270:PHE:HB2	1.85	0.75
2:G:15:SER:HA	2:G:35:PHE:CE1	2.21	0.75
1:F:30:ILE:CD1	1:F:163:VAL:HG12	2.17	0.75
1:F:79:ILE:HG12	1:F:80:GLU:N	2.01	0.75
2:G:201:ASP:CG	2:G:211:ARG:HH12	1.94	0.75
2:G:250:LEU:HD11	2:G:255:CYS:HB2	1.68	0.75
2:G:155:ALA:HB2	2:G:160:LEU:HB2	1.69	0.74
1:F:75:HIS:CE1	1:F:96:VAL:HB	2.22	0.74
2:G:35:PHE:CE2	2:G:47:HIS:HD2	2.05	0.74
2:G:182:ASP:HB3	2:G:242:ILE:HG22	1.69	0.74
2:G:35:PHE:HE2	2:G:47:HIS:CD2	2.05	0.74
2:G:403:LEU:HD23	2:G:405:ALA:O	1.88	0.74
2:G:35:PHE:HE2	2:G:47:HIS:HD2	1.33	0.74
1:F:156:VAL:CG1	1:F:161:THR:HB	2.17	0.73
2:G:11:GLN:HB2	2:G:56:GLN:HE21	1.53	0.73
1:F:156:VAL:HG12	1:F:161:THR:CG2	2.19	0.73
1:F:106:ILE:HD11	1:F:121:GLU:CG	2.18	0.73
2:G:255:CYS:HB3	2:G:260:MET:HB3	1.71	0.73
1:F:156:VAL:HG12	1:F:161:THR:HB	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:40:VAL:O	1:F:46:VAL:HG23	1.90	0.72
1:F:140:ILE:HD13	1:F:149:LEU:CD1	2.19	0.72
2:G:154:ARG:HG2	2:G:154:ARG:HH11	1.54	0.72
1:F:93:ILE:HD12	1:F:93:ILE:O	1.90	0.72
2:G:117:ARG:HG3	2:G:117:ARG:HH11	1.55	0.72
1:F:38:ASP:OD1	1:F:40:VAL:HG22	1.88	0.71
2:G:482:ARG:HG3	2:G:482:ARG:HH11	1.54	0.71
2:G:255:CYS:HB3	2:G:260:MET:CB	2.21	0.71
2:G:360:ALA:HB2	2:G:494:MET:HA	1.74	0.70
1:F:23:ILE:O	1:F:62:PRO:HB3	1.91	0.70
2:G:136:PHE:HB3	2:G:188:ARG:O	1.92	0.70
2:G:142:LYS:HE2	2:G:146:ASP:OD2	1.92	0.70
1:F:27:SER:OG	1:F:158:VAL:HG12	1.92	0.69
2:G:130:LEU:HD13	2:G:136:PHE:CD1	2.27	0.69
1:F:31:VAL:HG12	1:F:32:ASN:N	2.06	0.69
2:G:77:ILE:CG2	2:G:239:ILE:HG23	2.23	0.69
2:G:330:GLU:OE2	2:G:416:ASN:N	2.25	0.69
2:G:11:GLN:CB	2:G:56:GLN:HE21	2.06	0.69
2:G:141:VAL:CG1	2:G:209:ILE:HD13	2.23	0.69
2:G:68:ASP:O	2:G:69:ILE:HD12	1.94	0.68
2:G:152:ARG:HH21	2:G:208:ASP:CB	2.05	0.68
2:G:428:THR:HG22	2:G:429:ARG:O	1.93	0.68
1:F:150:ILE:HD12	1:F:165:ARG:O	1.94	0.68
2:G:112:CYS:SG	2:G:134:PRO:HD3	2.33	0.68
1:F:26:LEU:HD21	1:F:52:ILE:HG21	1.75	0.68
2:G:141:VAL:HG11	2:G:209:ILE:HD13	1.76	0.68
2:G:196:THR:HG22	2:G:198:ASP:H	1.59	0.68
2:G:23:HIS:HA	2:G:453:PHE:CE2	2.29	0.67
2:G:88:VAL:HA	2:G:161:LEU:O	1.94	0.67
2:G:155:ALA:CB	2:G:160:LEU:HB2	2.24	0.67
2:G:16:SER:CB	2:G:55:THR:HG23	2.25	0.67
2:G:174:THR:HB	2:G:178:VAL:HG23	1.77	0.66
2:G:154:ARG:HG2	2:G:154:ARG:NH1	2.10	0.66
2:G:313:ILE:HG21	2:G:326:ALA:HB1	1.77	0.66
2:G:46:GLU:OE2	2:G:107:ARG:NH2	2.26	0.66
1:F:117:ASP:N	1:F:117:ASP:OD1	2.29	0.65
2:G:7:VAL:CG2	2:G:20:VAL:HG22	2.18	0.65
2:G:90:GLU:OE1	2:G:93:THR:HG21	1.95	0.65
2:G:179:HIS:CD2	2:G:215:PRO:HA	2.31	0.65
2:G:127:ASN:N	2:G:127:ASN:ND2	2.42	0.65
2:G:189:THR:CG2	2:G:191:LEU:HB2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:201:ASP:OD2	2:G:211:ARG:NH1	2.29	0.65
2:G:83:ARG:HD3	4:G:503:G3H:O2	1.97	0.65
1:F:63:VAL:HG21	1:F:81:SER:HB3	1.79	0.65
2:G:308:MET:HE2	2:G:348:PHE:CB	2.26	0.65
2:G:151:SER:O	2:G:160:LEU:HD12	1.97	0.64
2:G:130:LEU:HD13	2:G:136:PHE:CE1	2.30	0.64
1:F:36:VAL:CG1	1:F:37:PRO:HD2	2.23	0.64
2:G:53:TRP:HA	2:G:53:TRP:CE3	2.30	0.64
2:G:190:MET:O	2:G:203:MET:HG3	1.96	0.64
2:G:56:GLN:O	2:G:59:THR:HG22	1.97	0.64
2:G:468:ARG:HG2	2:G:470:PHE:CE2	2.32	0.64
2:G:21:MET:SD	2:G:441:LEU:HD23	2.37	0.64
2:G:431:GLU:O	2:G:433:PRO:HD3	1.98	0.64
1:F:93:ILE:HD12	1:F:93:ILE:C	2.22	0.63
2:G:497:GLU:HG3	2:G:498:GLU:H	1.64	0.63
2:G:8:ALA:O	2:G:9:LEU:HD12	1.99	0.63
1:F:38:ASP:O	1:F:41:PHE:HB2	1.99	0.63
2:G:154:ARG:O	2:G:159:GLU:HG3	1.99	0.63
1:F:106:ILE:HD11	1:F:121:GLU:CB	2.28	0.63
2:G:53:TRP:HA	2:G:53:TRP:HE3	1.63	0.63
1:F:75:HIS:HE1	1:F:96:VAL:HB	1.60	0.62
2:G:154:ARG:HH11	2:G:154:ARG:CG	2.12	0.62
2:G:155:ALA:HB2	2:G:160:LEU:CB	2.29	0.62
2:G:336:VAL:O	2:G:338:ASN:N	2.32	0.62
1:F:54:PRO:HD2	1:F:134:THR:HG23	1.80	0.62
1:F:93:ILE:O	1:F:94:ASP:HB2	1.98	0.62
2:G:23:HIS:HA	2:G:453:PHE:HE2	1.64	0.62
2:G:317:ARG:O	2:G:317:ARG:HG2	1.99	0.62
1:F:150:ILE:HG22	1:F:151:LYS:N	2.15	0.62
2:G:291:ALA:HB1	6:G:505:HOH:O	1.98	0.62
2:G:22:ASP:OD1	2:G:24:ASP:N	2.32	0.62
2:G:108:THR:HB	2:G:139:THR:HB	1.82	0.62
2:G:9:LEU:HD11	2:G:60:LEU:HD13	1.80	0.61
2:G:120:LEU:O	2:G:124:ILE:HG13	2.01	0.61
1:F:150:ILE:O	1:F:164:ILE:HA	2.00	0.61
2:G:451:VAL:HG12	2:G:453:PHE:HB2	1.82	0.61
1:F:96:VAL:HG12	6:F:175:HOH:O	2.01	0.61
2:G:123:TYR:O	2:G:127:ASN:ND2	2.33	0.61
2:G:182:ASP:HB3	2:G:242:ILE:HG21	1.83	0.61
1:F:150:ILE:HG22	1:F:151:LYS:H	1.66	0.60
2:G:261:ALA:HB2	2:G:273:MET:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:156:VAL:HB	1:F:161:THR:HB	1.81	0.60
2:G:468:ARG:HG3	2:G:469:GLU:N	2.13	0.60
2:G:120:LEU:HD23	2:G:120:LEU:N	2.14	0.60
2:G:265:TYR:CD2	2:G:413:VAL:HG12	2.37	0.60
1:F:156:VAL:HG12	1:F:161:THR:CB	2.30	0.60
2:G:47:HIS:HE1	2:G:102:VAL:CG1	2.14	0.60
2:G:90:GLU:OE2	2:G:154:ARG:NH2	2.35	0.60
2:G:165:VAL:O	2:G:169:LEU:HB2	2.02	0.60
2:G:313:ILE:N	2:G:313:ILE:HD13	2.15	0.60
2:G:27:ILE:N	2:G:27:ILE:HD12	2.16	0.60
1:F:61:ALA:HB2	1:F:113:VAL:HG21	1.83	0.60
2:G:18:ALA:HB1	2:G:63:VAL:HG21	1.84	0.60
2:G:432:ARG:HD2	2:G:467:GLU:OE1	2.01	0.60
2:G:121:GLU:CA	2:G:132:ILE:HD11	2.28	0.60
2:G:183:TYR:CD2	2:G:219:ARG:HA	2.37	0.59
1:F:26:LEU:HD21	1:F:52:ILE:CG2	2.32	0.59
1:F:32:ASN:HB3	1:F:34:GLU:HG2	1.83	0.59
2:G:124:ILE:O	2:G:128:THR:OG1	2.20	0.59
2:G:448:GLY:HA3	2:G:454:TRP:CE3	2.37	0.59
2:G:456:ASN:HD22	2:G:457:LEU:H	1.50	0.59
2:G:174:THR:HG21	2:G:178:VAL:CG2	2.33	0.58
2:G:47:HIS:HE1	2:G:102:VAL:HG11	1.68	0.58
2:G:343:TYR:OH	2:G:485:GLY:HA3	2.04	0.58
1:F:156:VAL:CB	1:F:161:THR:HB	2.34	0.58
2:G:85:THR:HB	2:G:102:VAL:HA	1.83	0.58
2:G:18:ALA:CB	2:G:63:VAL:HG21	2.32	0.58
2:G:91:LYS:N	2:G:159:GLU:O	2.29	0.58
2:G:183:TYR:HD2	2:G:219:ARG:HA	1.68	0.58
2:G:87:ILE:HG22	2:G:88:VAL:N	2.18	0.58
2:G:333:ALA:CB	2:G:378:ARG:HB2	2.32	0.58
2:G:205:GLU:O	2:G:208:ASP:N	2.29	0.57
1:F:59:MET:HG3	1:F:122:PHE:CE1	2.39	0.57
2:G:459:GLU:C	2:G:460:LEU:HD23	2.29	0.57
2:G:59:THR:O	2:G:63:VAL:HG22	2.04	0.57
2:G:214:LEU:N	2:G:214:LEU:HD23	2.17	0.57
2:G:101:ILE:HG22	2:G:140:LYS:HD3	1.86	0.57
2:G:303:GLU:HG3	2:G:304:GLY:N	2.18	0.57
1:F:40:VAL:HB	1:F:46:VAL:HG22	1.87	0.57
2:G:85:THR:CG2	2:G:103:TRP:HD1	2.17	0.57
1:F:67:ILE:HG13	1:F:67:ILE:O	2.03	0.57
2:G:38:ILE:HG22	2:G:40:PRO:HD3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:110:GLU:O	2:G:113:GLU:HB2	2.05	0.57
2:G:147:HIS:O	2:G:148:VAL:HG23	2.05	0.57
2:G:370:GLY:HA3	6:G:544:HOH:O	2.04	0.57
2:G:204:LEU:HD21	2:G:214:LEU:CD1	2.34	0.56
2:G:343:TYR:CZ	2:G:485:GLY:HA3	2.40	0.56
2:G:357:ASP:OD1	2:G:359:TYR:HB2	2.04	0.56
2:G:162:PHE:CG	2:G:163:GLY:N	2.73	0.56
1:F:143:MET:HA	1:F:146:ILE:CD1	2.36	0.56
2:G:352:GLY:O	2:G:356:TRP:N	2.36	0.56
2:G:434:GLU:CB	2:G:467:GLU:HB2	2.36	0.56
2:G:31:SER:HB2	2:G:59:THR:OG1	2.06	0.55
2:G:476:THR:O	2:G:479:ARG:HD3	2.06	0.55
2:G:179:HIS:CD2	2:G:215:PRO:HB3	2.42	0.55
2:G:392:LEU:C	2:G:392:LEU:HD23	2.32	0.55
2:G:64:LEU:HD22	2:G:69:ILE:HG22	1.87	0.55
1:F:67:ILE:HD12	1:F:68:GLY:N	2.21	0.55
2:G:174:THR:O	2:G:176:GLY:N	2.40	0.55
2:G:46:GLU:HG3	2:G:107:ARG:HH12	1.72	0.55
1:F:23:ILE:HG21	1:F:159:GLY:HA2	1.88	0.55
2:G:30:VAL:HG12	2:G:31:SER:N	2.22	0.55
2:G:124:ILE:HD11	2:G:203:MET:HE1	1.88	0.55
2:G:210:PRO:O	2:G:212:GLU:N	2.40	0.55
2:G:330:GLU:OE2	2:G:416:ASN:HB2	2.07	0.55
2:G:189:THR:HG23	2:G:191:LEU:H	1.67	0.54
2:G:102:VAL:HG12	2:G:103:TRP:N	2.23	0.54
2:G:293:GLY:O	2:G:295:THR:N	2.40	0.54
1:F:140:ILE:HG21	1:F:146:ILE:HD12	1.90	0.54
2:G:448:GLY:CA	2:G:453:PHE:HB3	2.38	0.54
2:G:101:ILE:CG2	2:G:140:LYS:HD3	2.37	0.54
2:G:475:GLU:OE1	2:G:475:GLU:N	2.29	0.54
2:G:20:VAL:O	2:G:28:ILE:HB	2.08	0.54
2:G:85:THR:N	6:G:541:HOH:O	2.40	0.54
2:G:85:THR:HG21	2:G:102:VAL:HG13	1.90	0.54
2:G:174:THR:O	2:G:177:ARG:N	2.37	0.54
2:G:180:VAL:HA	2:G:216:GLU:O	2.08	0.54
2:G:458:ASP:OD1	2:G:458:ASP:N	2.37	0.53
2:G:342:VAL:HA	2:G:365:PHE:O	2.09	0.53
1:F:86:GLU:C	1:F:87:LEU:HG	2.33	0.53
1:F:93:ILE:HG13	1:F:133:SER:HB3	1.89	0.53
2:G:184:THR:O	2:G:187:SER:OG	2.25	0.53
2:G:246:GLN:HG3	2:G:270:PHE:CG	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:108:GLU:O	1:F:110:GLY:N	2.38	0.53
2:G:125:ARG:O	2:G:129:GLY:N	2.40	0.53
2:G:396:GLN:NE2	2:G:403:LEU:H	2.06	0.53
2:G:124:ILE:HD11	2:G:203:MET:CE	2.39	0.53
2:G:174:THR:CB	2:G:178:VAL:HG23	2.38	0.53
2:G:35:PHE:CE2	2:G:47:HIS:CD2	2.88	0.53
2:G:83:ARG:O	2:G:85:THR:N	2.35	0.53
2:G:84:GLU:HG2	2:G:136:PHE:HA	1.90	0.53
2:G:102:VAL:O	2:G:140:LYS:NZ	2.36	0.53
1:F:31:VAL:CG1	1:F:32:ASN:N	2.72	0.52
1:F:123:ASP:O	1:F:125:PRO:N	2.42	0.52
1:F:156:VAL:HG12	1:F:161:THR:HG21	1.89	0.52
2:G:85:THR:CG2	2:G:102:VAL:HA	2.39	0.52
2:G:444:ALA:O	2:G:447:ALA:HB3	2.10	0.52
2:G:102:VAL:HG12	2:G:103:TRP:H	1.75	0.52
1:F:31:VAL:HG12	1:F:32:ASN:H	1.74	0.52
2:G:11:GLN:OE1	2:G:165:VAL:HG11	2.10	0.52
2:G:127:ASN:N	2:G:127:ASN:HD22	2.08	0.52
2:G:360:ALA:CB	2:G:494:MET:HA	2.40	0.52
2:G:74:ILE:HD12	2:G:74:ILE:O	2.10	0.52
2:G:195:HIS:N	2:G:195:HIS:CD2	2.78	0.51
2:G:297:GLU:N	2:G:297:GLU:OE1	2.42	0.51
2:G:160:LEU:O	2:G:161:LEU:HD23	2.10	0.51
2:G:11:GLN:CD	2:G:52:ILE:HG23	2.36	0.51
2:G:56:GLN:HG2	2:G:169:LEU:HD11	1.92	0.51
2:G:17:ARG:HA	2:G:31:SER:O	2.11	0.51
2:G:189:THR:HG23	2:G:191:LEU:HB2	1.91	0.51
2:G:314:GLN:O	2:G:318:ASP:N	2.37	0.51
2:G:499:HIS:N	2:G:499:HIS:CD2	2.79	0.51
2:G:475:GLU:H	2:G:475:GLU:CD	2.17	0.51
1:F:150:ILE:HD12	1:F:150:ILE:N	2.25	0.51
2:G:254:LEU:O	2:G:255:CYS:O	2.28	0.51
2:G:85:THR:HB	2:G:101:ILE:O	2.11	0.51
2:G:180:VAL:HG23	2:G:216:GLU:O	2.10	0.51
2:G:425:ILE:HG13	2:G:425:ILE:O	2.11	0.51
1:F:65:GLY:HA3	1:F:81:SER:HA	1.93	0.51
2:G:434:GLU:HB2	2:G:467:GLU:HB2	1.92	0.51
1:F:74:ASN:HB3	1:F:105:ARG:HH11	1.75	0.51
2:G:255:CYS:HB3	2:G:260:MET:HB2	1.91	0.51
1:F:124:LEU:O	1:F:128:GLU:HB2	2.11	0.50
2:G:435:VAL:O	2:G:435:VAL:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:28:GLY:HA3	1:F:53:LYS:O	2.11	0.50
2:G:173:MET:C	2:G:175:GLN:H	2.19	0.50
2:G:15:SER:HA	2:G:35:PHE:CD1	2.46	0.50
2:G:82:GLN:OE1	2:G:85:THR:HG21	2.11	0.50
2:G:155:ALA:O	2:G:158:GLY:HA2	2.11	0.50
2:G:250:LEU:CD1	2:G:255:CYS:HB2	2.39	0.50
2:G:64:LEU:HD22	2:G:69:ILE:HG21	1.92	0.50
2:G:315:TRP:CH2	2:G:320:MET:HG3	2.47	0.50
2:G:317:ARG:HA	2:G:323:ILE:HG13	1.94	0.50
2:G:131:VAL:O	2:G:136:PHE:HE2	1.94	0.50
2:G:152:ARG:CZ	2:G:208:ASP:HB3	2.42	0.50
2:G:270:PHE:N	2:G:270:PHE:CD1	2.79	0.50
2:G:422:GLN:O	2:G:422:GLN:HG3	2.09	0.50
2:G:88:VAL:O	2:G:97:ILE:HG23	2.11	0.50
2:G:360:ALA:O	2:G:361:ARG:HG2	2.12	0.50
1:F:10:VAL:HG12	1:F:10:VAL:O	2.11	0.50
1:F:106:ILE:HD11	1:F:121:GLU:HB2	1.92	0.50
2:G:434:GLU:CA	2:G:467:GLU:HB2	2.42	0.50
2:G:316:LEU:HA	2:G:320:MET:HB2	1.92	0.49
2:G:81:ASN:HD22	2:G:81:ASN:H	1.59	0.49
1:F:23:ILE:HD12	1:F:115:VAL:HG21	1.93	0.49
2:G:170:ILE:HG22	2:G:171:TRP:N	2.26	0.49
1:F:150:ILE:HD13	1:F:165:ARG:HB2	1.94	0.49
2:G:47:HIS:ND1	2:G:102:VAL:HG22	2.27	0.49
2:G:162:PHE:O	2:G:179:HIS:HE1	1.95	0.49
1:F:150:ILE:CG2	1:F:151:LYS:H	2.25	0.49
2:G:189:THR:HG23	2:G:191:LEU:CB	2.42	0.49
1:F:52:ILE:O	1:F:52:ILE:HG22	2.11	0.49
1:F:73:THR:HG23	1:F:75:HIS:HD1	1.77	0.49
2:G:45:VAL:N	2:G:105:CYS:HB2	2.21	0.49
2:G:272:LEU:HG	2:G:303:GLU:HB2	1.94	0.49
1:F:26:LEU:CD2	1:F:52:ILE:HG21	2.42	0.49
1:F:64:ASP:HA	1:F:113:VAL:O	2.12	0.49
2:G:11:GLN:CG	2:G:56:GLN:HE21	2.25	0.49
2:G:42:PRO:C	2:G:44:TRP:H	2.21	0.49
2:G:47:HIS:ND1	2:G:102:VAL:CG2	2.76	0.49
2:G:204:LEU:HD21	2:G:214:LEU:HD11	1.95	0.49
1:F:25:PRO:HB3	1:F:62:PRO:HG3	1.95	0.49
1:F:51:ALA:O	1:F:52:ILE:HG13	2.11	0.49
2:G:189:THR:HG21	2:G:191:LEU:HB2	1.95	0.49
2:G:342:VAL:HG12	2:G:343:TYR:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:364:ILE:HG22	2:G:365:PHE:N	2.28	0.49
2:G:81:ASN:HD22	2:G:81:ASN:N	2.11	0.48
2:G:84:GLU:CG	2:G:136:PHE:HA	2.43	0.48
2:G:174:THR:OG1	2:G:178:VAL:HB	2.13	0.48
1:F:78:SER:HA	1:F:87:LEU:O	2.13	0.48
2:G:80:THR:HG22	2:G:245:ASP:HA	1.95	0.48
2:G:128:THR:C	2:G:130:LEU:H	2.19	0.48
2:G:428:THR:CG2	2:G:429:ARG:N	2.75	0.48
1:F:108:GLU:C	1:F:110:GLY:H	2.21	0.48
1:F:66:THR:HG23	1:F:112:ARG:HA	1.95	0.48
2:G:50:MET:HE1	2:G:96:PRO:HD2	1.96	0.48
2:G:352:GLY:O	2:G:355:TYR:N	2.47	0.48
1:F:85:VAL:HG12	1:F:86:GLU:N	2.27	0.48
1:F:40:VAL:HB	1:F:46:VAL:CG2	2.44	0.48
2:G:181:THR:HG23	2:G:182:ASP:O	2.14	0.48
2:G:456:ASN:HD22	2:G:457:LEU:N	2.12	0.48
1:F:146:ILE:HG12	1:F:146:ILE:O	2.13	0.48
2:G:169:LEU:HD23	2:G:169:LEU:HA	1.66	0.47
2:G:315:TRP:CE3	2:G:316:LEU:HD23	2.49	0.47
2:G:205:GLU:HG2	2:G:206:VAL:N	2.29	0.47
2:G:343:TYR:CE2	2:G:485:GLY:HA3	2.49	0.47
1:F:36:VAL:HG21	1:F:137:PRO:HG3	1.96	0.47
2:G:152:ARG:HE	2:G:208:ASP:CG	2.22	0.47
2:G:311:ALA:O	2:G:314:GLN:HB2	2.14	0.47
1:F:33:ILE:CG2	1:F:34:GLU:N	2.78	0.47
2:G:160:LEU:C	2:G:161:LEU:HD23	2.40	0.47
2:G:200:ASP:HB3	2:G:203:MET:HB2	1.97	0.47
1:F:91:PHE:HA	1:F:136:THR:HG23	1.96	0.47
2:G:80:THR:CG2	2:G:245:ASP:HA	2.45	0.47
2:G:313:ILE:HG21	2:G:326:ALA:CB	2.44	0.47
2:G:344:VAL:HG23	2:G:379:ALA:CB	2.45	0.47
2:G:448:GLY:HA2	2:G:453:PHE:HB3	1.96	0.47
1:F:30:ILE:CG2	1:F:31:VAL:N	2.78	0.47
2:G:141:VAL:CG2	2:G:162:PHE:CE1	2.98	0.47
2:G:155:ALA:C	2:G:158:GLY:H	2.23	0.47
2:G:221:SER:OG	2:G:450:ALA:HB2	2.14	0.47
2:G:272:LEU:HD12	2:G:272:LEU:N	2.30	0.47
2:G:351:LEU:HB3	2:G:355:TYR:HB2	1.97	0.47
2:G:98:TYR:CD1	2:G:99:ASN:HB2	2.51	0.46
2:G:441:LEU:HD23	2:G:441:LEU:HA	1.70	0.46
1:F:23:ILE:CG2	1:F:24:ALA:N	2.78	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:27:SER:HG	1:F:158:VAL:HG12	1.80	0.46
1:F:77:PHE:CE2	1:F:79:ILE:HG22	2.50	0.46
2:G:141:VAL:CG2	2:G:162:PHE:CD1	2.98	0.46
2:G:219:ARG:HH22	2:G:295:THR:HB	1.81	0.46
2:G:415:ASN:OD1	2:G:417:PHE:HB3	2.14	0.46
2:G:193:ASN:HB3	2:G:196:THR:HG22	1.98	0.46
2:G:179:HIS:CD2	2:G:215:PRO:CA	2.98	0.46
2:G:357:ASP:C	2:G:359:TYR:H	2.24	0.46
1:F:90:HIS:ND1	1:F:92:GLY:O	2.48	0.46
2:G:150:GLY:O	2:G:154:ARG:HD3	2.15	0.46
2:G:225:GLY:O	2:G:238:PRO:HA	2.15	0.46
2:G:408:VAL:O	2:G:408:VAL:HG23	2.12	0.46
1:F:115:VAL:HG12	1:F:116:GLY:N	2.31	0.46
2:G:182:ASP:CB	2:G:242:ILE:HG22	2.43	0.46
2:G:468:ARG:CG	2:G:469:GLU:N	2.76	0.46
1:F:23:ILE:CG2	1:F:159:GLY:HA2	2.45	0.46
1:F:106:ILE:CD1	1:F:121:GLU:N	2.78	0.46
2:G:53:TRP:CE3	2:G:53:TRP:CA	2.96	0.46
1:F:36:VAL:C	1:F:38:ASP:H	2.23	0.46
2:G:11:GLN:HB2	2:G:56:GLN:NE2	2.24	0.46
1:F:61:ALA:CB	1:F:113:VAL:HG21	2.46	0.46
1:F:65:GLY:HA3	1:F:80:GLU:O	2.16	0.46
1:F:91:PHE:CD1	1:F:91:PHE:C	2.94	0.46
2:G:226:GLN:HA	2:G:238:PRO:HA	1.98	0.46
1:F:164:ILE:CG2	1:F:165:ARG:N	2.78	0.46
2:G:408:VAL:HG22	2:G:431:GLU:O	2.15	0.46
1:F:98:LEU:N	1:F:98:LEU:CD1	2.79	0.45
1:F:164:ILE:HG22	1:F:165:ARG:N	2.30	0.45
2:G:246:GLN:CD	2:G:270:PHE:HB2	2.41	0.45
2:G:448:GLY:HA3	2:G:454:TRP:CZ3	2.51	0.45
2:G:342:VAL:CG1	2:G:343:TYR:N	2.77	0.45
2:G:52:ILE:O	2:G:56:GLN:N	2.34	0.45
1:F:22:ILE:HD11	1:F:166:ILE:HD13	1.98	0.45
1:F:23:ILE:CD1	1:F:115:VAL:HG21	2.47	0.45
1:F:32:ASN:HB3	1:F:34:GLU:CG	2.46	0.45
2:G:189:THR:HG23	2:G:191:LEU:N	2.32	0.45
2:G:246:GLN:HG3	2:G:270:PHE:CB	2.47	0.45
2:G:60:LEU:HD12	2:G:60:LEU:HA	1.65	0.45
2:G:199:TRP:CE2	2:G:214:LEU:HB3	2.52	0.45
1:F:30:ILE:HG22	1:F:31:VAL:N	2.32	0.45
2:G:27:ILE:N	2:G:27:ILE:CD1	2.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:46:GLU:CG	2:G:107:ARG:HH12	2.28	0.45
2:G:83:ARG:NH1	4:G:503:G3H:H2	2.25	0.45
2:G:260:MET:HB3	2:G:260:MET:HE2	1.70	0.45
2:G:381:LEU:HA	2:G:381:LEU:HD23	1.49	0.45
1:F:63:VAL:HG21	1:F:81:SER:CB	2.45	0.45
1:F:77:PHE:HE2	1:F:79:ILE:CG2	2.30	0.45
1:F:124:LEU:N	1:F:125:PRO:CD	2.79	0.45
2:G:178:VAL:CG1	2:G:180:VAL:HG12	2.47	0.45
2:G:204:LEU:HD12	2:G:204:LEU:HA	1.34	0.45
2:G:210:PRO:C	2:G:212:GLU:N	2.75	0.45
2:G:245:ASP:HB2	2:G:439:THR:HG21	1.98	0.45
2:G:494:MET:O	2:G:495:ALA:HB3	2.16	0.45
1:F:125:PRO:C	1:F:128:GLU:H	2.25	0.44
1:F:78:SER:C	1:F:79:ILE:HG22	2.43	0.44
2:G:130:LEU:HD13	2:G:136:PHE:CG	2.52	0.44
2:G:302:LEU:HD23	2:G:302:LEU:HA	1.66	0.44
2:G:428:THR:HG22	2:G:429:ARG:N	2.29	0.44
2:G:6:ILE:CD1	2:G:454:TRP:CH2	3.00	0.44
2:G:18:ALA:HB3	2:G:63:VAL:CG2	2.47	0.44
2:G:142:LYS:O	2:G:142:LYS:HG3	2.16	0.44
2:G:164:THR:OG1	2:G:166:ASP:OD1	2.29	0.44
2:G:206:VAL:HG12	2:G:207:LEU:N	2.30	0.44
1:F:150:ILE:HD12	1:F:150:ILE:H	1.83	0.44
1:F:153:SER:OG	1:F:154:GLY:N	2.49	0.44
2:G:15:SER:CA	2:G:35:PHE:CE1	2.98	0.44
2:G:55:THR:CG2	2:G:56:GLN:N	2.80	0.44
2:G:98:TYR:HD1	2:G:99:ASN:N	2.08	0.44
2:G:178:VAL:HG12	2:G:180:VAL:HG12	1.99	0.44
2:G:430:VAL:HB	2:G:470:PHE:HB2	2.00	0.44
1:F:101:GLU:O	1:F:126:LEU:HD21	2.17	0.44
2:G:83:ARG:HH11	4:G:503:G3H:C2	2.25	0.44
2:G:84:GLU:HB2	2:G:103:TRP:HB3	1.98	0.44
2:G:253:GLN:NE2	2:G:409:ASP:HB3	2.32	0.44
2:G:286:LEU:HD23	2:G:286:LEU:HA	1.84	0.44
1:F:85:VAL:CG1	1:F:86:GLU:N	2.80	0.44
1:F:124:LEU:O	1:F:124:LEU:HD12	2.18	0.44
1:F:125:PRO:HA	1:F:128:GLU:HB2	2.00	0.44
2:G:251:PHE:O	2:G:254:LEU:HD23	2.18	0.44
2:G:482:ARG:HG3	2:G:482:ARG:NH1	2.25	0.44
1:F:158:VAL:CG2	1:F:159:GLY:N	2.79	0.44
1:F:70:ILE:HD13	1:F:105:ARG:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:158:VAL:HG23	1:F:159:GLY:N	2.32	0.44
2:G:15:SER:HA	2:G:35:PHE:HE1	1.79	0.44
2:G:95:LYS:HG3	2:G:96:PRO:N	2.32	0.44
2:G:107:ARG:C	2:G:109:ALA:H	2.25	0.44
2:G:155:ALA:HB2	2:G:160:LEU:HD12	1.99	0.44
1:F:142:ASN:C	1:F:144:ASP:H	2.26	0.43
2:G:85:THR:CB	2:G:102:VAL:HA	2.45	0.43
2:G:458:ASP:C	2:G:460:LEU:N	2.76	0.43
1:F:39:VAL:O	1:F:45:ILE:HD12	2.18	0.43
2:G:14:THR:HA	6:G:506:HOH:O	2.17	0.43
2:G:210:PRO:C	2:G:212:GLU:H	2.26	0.43
2:G:255:CYS:O	2:G:257:LYS:N	2.49	0.43
1:F:157:THR:HG22	1:F:160:GLU:HB2	1.97	0.43
2:G:179:HIS:CG	2:G:215:PRO:HB3	2.53	0.43
2:G:346:PRO:HB3	2:G:348:PHE:HE1	1.83	0.43
2:G:396:GLN:HE21	2:G:403:LEU:H	1.66	0.43
1:F:24:ALA:HA	1:F:25:PRO:HD3	1.76	0.43
1:F:102:GLY:O	1:F:122:PHE:HA	2.18	0.43
2:G:11:GLN:HG2	2:G:16:SER:OG	2.18	0.43
2:G:130:LEU:CD1	2:G:136:PHE:CD1	3.00	0.43
2:G:196:THR:HG22	2:G:198:ASP:N	2.31	0.43
2:G:490:VAL:HG12	2:G:491:LYS:N	2.29	0.43
1:F:115:VAL:CG1	1:F:116:GLY:N	2.82	0.43
2:G:137:SER:HB2	2:G:189:THR:HA	2.00	0.43
2:G:280:VAL:HG12	2:G:281:LYS:N	2.32	0.43
1:F:30:ILE:C	1:F:31:VAL:HG23	2.44	0.43
2:G:124:ILE:CD1	2:G:203:MET:HE2	2.49	0.43
2:G:209:ILE:HA	2:G:210:PRO:HD2	1.36	0.43
1:F:40:VAL:C	1:F:46:VAL:HG23	2.44	0.42
2:G:340:ASN:HB2	2:G:375:HIS:CD2	2.53	0.42
2:G:419:MET:O	2:G:422:GLN:HB3	2.19	0.42
2:G:460:LEU:C	2:G:462:GLU:N	2.77	0.42
2:G:460:LEU:C	2:G:462:GLU:H	2.26	0.42
2:G:31:SER:OG	2:G:63:VAL:HG13	2.19	0.42
2:G:80:THR:HG23	2:G:243:ALA:O	2.19	0.42
2:G:222:GLU:O	2:G:240:SER:HA	2.19	0.42
2:G:451:VAL:O	2:G:451:VAL:HG13	2.19	0.42
1:F:157:THR:N	1:F:161:THR:OG1	2.36	0.42
2:G:315:TRP:CZ2	2:G:320:MET:CG	3.03	0.42
1:F:143:MET:CE	1:F:146:ILE:HD11	2.49	0.42
1:F:31:VAL:CG1	1:F:32:ASN:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:39:VAL:H	1:F:39:VAL:HG23	1.22	0.42
2:G:45:VAL:O	2:G:105:CYS:HB2	2.20	0.42
2:G:90:GLU:HB2	2:G:93:THR:OG1	2.20	0.42
2:G:170:ILE:HG21	2:G:178:VAL:HG11	2.01	0.42
2:G:221:SER:CB	2:G:450:ALA:HB2	2.49	0.42
2:G:271:MET:HE1	2:G:392:LEU:CB	2.43	0.42
2:G:371:VAL:HG13	2:G:375:HIS:HB2	2.01	0.42
1:F:67:ILE:HD12	1:F:67:ILE:C	2.45	0.42
2:G:185:ASN:HD22	2:G:185:ASN:HA	1.54	0.42
1:F:46:VAL:HG23	1:F:46:VAL:H	1.54	0.42
2:G:458:ASP:C	2:G:460:LEU:H	2.27	0.42
2:G:18:ALA:HB2	2:G:59:THR:HG23	2.01	0.42
2:G:105:CYS:SG	2:G:107:ARG:CD	3.02	0.42
2:G:162:PHE:CD2	2:G:163:GLY:N	2.87	0.42
2:G:347:ALA:HB2	2:G:351:LEU:HD21	2.00	0.42
1:F:135:LEU:HD23	1:F:135:LEU:HA	1.45	0.42
2:G:264:THR:O	2:G:269:CYS:HA	2.20	0.42
1:F:39:VAL:C	1:F:41:PHE:N	2.78	0.41
1:F:152:LEU:HD23	1:F:152:LEU:HA	1.83	0.41
2:G:111:ILE:H	2:G:111:ILE:HG13	1.68	0.41
2:G:11:GLN:CB	2:G:56:GLN:NE2	2.78	0.41
2:G:39:TYR:HA	2:G:40:PRO:HD2	1.88	0.41
2:G:224:TYR:HD1	2:G:239:ILE:O	2.03	0.41
2:G:399:SER:O	2:G:401:ILE:N	2.53	0.41
1:F:22:ILE:HG23	1:F:62:PRO:HB2	2.02	0.41
2:G:213:MET:HE3	2:G:213:MET:HB3	1.91	0.41
2:G:434:GLU:HA	2:G:467:GLU:HB2	2.00	0.41
2:G:392:LEU:HD23	2:G:393:GLU:N	2.36	0.41
2:G:423:SER:OG	2:G:472:PRO:HD3	2.20	0.41
1:F:59:MET:HE3	1:F:59:MET:HB3	1.75	0.41
2:G:304:GLY:HA3	2:G:391:VAL:HG21	2.02	0.41
1:F:43:GLU:CD	2:G:402:ARG:NH2	2.79	0.41
1:F:136:THR:HA	1:F:137:PRO:HD2	1.99	0.41
2:G:183:TYR:CE2	2:G:219:ARG:N	2.89	0.41
2:G:457:LEU:HD23	2:G:457:LEU:HA	1.95	0.41
2:G:108:THR:HG22	2:G:143:TRP:HB2	2.01	0.41
2:G:265:TYR:HB3	2:G:412:ALA:HB3	2.03	0.41
2:G:274:ASN:OD1	2:G:276:GLY:N	2.47	0.41
2:G:432:ARG:HA	2:G:433:PRO:HD2	1.77	0.41
1:F:58:LYS:C	1:F:122:PHE:HE1	2.28	0.41
2:G:102:VAL:H	2:G:102:VAL:HG23	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:189:THR:CG2	2:G:191:LEU:N	2.74	0.41
2:G:246:GLN:OE1	2:G:262:LYS:NZ	2.54	0.41
2:G:250:LEU:HD12	2:G:250:LEU:O	2.21	0.41
2:G:85:THR:CG2	2:G:103:TRP:H	2.26	0.41
2:G:95:LYS:HA	2:G:96:PRO:HD3	1.74	0.41
2:G:124:ILE:CD1	2:G:203:MET:CE	2.98	0.41
2:G:154:ARG:HH12	2:G:159:GLU:HB2	1.85	0.41
2:G:161:LEU:HD12	2:G:171:TRP:NE1	2.36	0.41
2:G:219:ARG:O	2:G:224:TYR:OH	2.26	0.41
2:G:408:VAL:O	2:G:433:PRO:HG2	2.21	0.41
1:F:59:MET:HB2	1:F:59:MET:HE2	1.57	0.41
2:G:85:THR:CG2	2:G:103:TRP:CD1	3.02	0.41
2:G:265:TYR:CD2	2:G:413:VAL:CG1	3.03	0.41
2:G:103:TRP:H	2:G:103:TRP:CD1	2.39	0.40
2:G:6:ILE:HD11	2:G:454:TRP:CH2	2.57	0.40
2:G:53:TRP:NE1	2:G:172:LYS:HE3	2.37	0.40
2:G:170:ILE:O	2:G:173:MET:N	2.39	0.40
2:G:497:GLU:HG3	2:G:498:GLU:N	2.33	0.40
1:F:67:ILE:HD11	1:F:70:ILE:CG1	2.40	0.40
2:G:4:LYS:HA	2:G:73:GLN:O	2.21	0.40
2:G:17:ARG:HE	2:G:17:ARG:HB3	1.69	0.40
2:G:108:THR:CB	2:G:111:ILE:HD12	2.51	0.40
2:G:174:THR:CB	2:G:178:VAL:CG2	3.00	0.40
2:G:418:LEU:HD12	2:G:418:LEU:O	2.21	0.40
2:G:445:TYR:N	2:G:445:TYR:CD1	2.89	0.40
2:G:449:LEU:HD23	2:G:454:TRP:HB2	2.02	0.40
2:G:490:VAL:C	2:G:492:ARG:N	2.79	0.40
1:F:149:LEU:HD23	1:F:149:LEU:O	2.21	0.40
2:G:351:LEU:HD23	2:G:351:LEU:HA	1.82	0.40
2:G:460:LEU:O	2:G:462:GLU:N	2.44	0.40
2:G:133:ASP:C	2:G:135:TYR:N	2.78	0.40
2:G:193:ASN:CG	2:G:196:THR:HB	2.46	0.40
2:G:407:ARG:CD	2:G:431:GLU:HG3	2.38	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	157/168 (94%)	133 (85%)	18 (12%)	6 (4%)	2	5
2	G	485/501 (97%)	410 (84%)	58 (12%)	17 (4%)	3	7
All	All	642/669 (96%)	543 (85%)	76 (12%)	23 (4%)	2	6

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	109	GLU
1	F	124	LEU
2	G	42	PRO
2	G	175	GLN
2	G	255	CYS
2	G	294	PRO
1	F	125	PRO
2	G	71	SER
2	G	138	GLY
2	G	211	ARG
2	G	84	GLU
2	G	85	THR
2	G	219	ARG
2	G	256	VAL
2	G	400	GLY
1	F	62	PRO
2	G	149	GLU
2	G	210	PRO
1	F	34	GLU
1	F	37	PRO
2	G	199	TRP
2	G	170	ILE
2	G	206	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%)	77 (63%)	46 (37%)	0	0
2	G	378/412 (92%)	274 (72%)	104 (28%)	0	0
All	All	501/557 (90%)	351 (70%)	150 (30%)	0	0

All (150) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	9	LEU
1	F	10	VAL
1	F	20	ILE
1	F	26	LEU
1	F	27	SER
1	F	30	ILE
1	F	34	GLU
1	F	35	ASP
1	F	39	VAL
1	F	44	LYS
1	F	46	VAL
1	F	50	ILE
1	F	52	ILE
1	F	53	LYS
1	F	58	LYS
1	F	60	VAL
1	F	63	VAL
1	F	64	ASP
1	F	66	THR
1	F	67	ILE
1	F	72	GLU
1	F	74	ASN
1	F	79	ILE
1	F	93	ILE
1	F	95	THR
1	F	98	LEU
1	F	99	LYS

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Mol	Chain	Res	Type
1	F	101	GLU
1	F	105	ARG
1	F	111	GLN
1	F	117	ASP
1	F	120	ILE
1	F	126	LEU
1	F	128	GLU
1	F	129	GLU
1	F	134	THR
1	F	140	ILE
1	F	142	ASN
1	F	146	ILE
1	F	149	LEU
1	F	150	ILE
1	F	155	SER
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	7	VAL
2	G	17	ARG
2	G	27	ILE
2	G	28	ILE
2	G	29	SER
2	G	31	SER
2	G	32	GLN
2	G	34	GLU
2	G	36	GLU
2	G	41	LYS
2	G	47	HIS
2	G	51	GLU
2	G	52	ILE
2	G	55	THR
2	G	63	VAL
2	G	69	ILE
2	G	73	GLN
2	G	77	ILE
2	G	80	THR
2	G	81	ASN

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Mol	Chain	Res	Type
2	G	82	GLN
2	G	83	ARG
2	G	85	THR
2	G	87	ILE
2	G	95	LYS
2	G	97	ILE
2	G	107	ARG
2	G	110	GLU
2	G	117	ARG
2	G	120	LEU
2	G	122	ASP
2	G	124	ILE
2	G	127	ASN
2	G	130	LEU
2	G	131	VAL
2	G	132	ILE
2	G	151	SER
2	G	152	ARG
2	G	154	ARG
2	G	156	ARG
2	G	159	GLU
2	G	171	TRP
2	G	173	MET
2	G	182	ASP
2	G	187	SER
2	G	189	THR
2	G	196	THR
2	G	203	MET
2	G	204	LEU
2	G	206	VAL
2	G	207	LEU
2	G	208	ASP
2	G	209	ILE
2	G	211	ARG
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
2	G	239	ILE

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Mol	Chain	Res	Type
2	G	250	LEU
2	G	255	CYS
2	G	256	VAL
2	G	262	LYS
2	G	264	THR
2	G	267	THR
2	G	269	CYS
2	G	277	GLU
2	G	295	THR
2	G	313	ILE
2	G	321	LYS
2	G	337	GLN
2	G	361	ARG
2	G	364	ILE
2	G	367	LEU
2	G	369	ARG
2	G	378	ARG
2	G	391	VAL
2	G	402	ARG
2	G	403	LEU
2	G	413	VAL
2	G	425	ILE
2	G	434	GLU
2	G	435	VAL
2	G	449	LEU
2	G	451	VAL
2	G	456	ASN
2	G	458	ASP
2	G	460	LEU
2	G	466	ILE
2	G	468	ARG
2	G	474	ILE
2	G	475	GLU
2	G	477	THR
2	G	480	ASN
2	G	482	ARG
2	G	487	LYS
2	G	488	LYS
2	G	498	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	F	32	ASN
1	F	74	ASN
1	F	111	GLN
1	F	142	ASN
2	G	32	GLN
2	G	47	HIS
2	G	56	GLN
2	G	81	ASN
2	G	185	ASN
2	G	228	ASN
2	G	284	ASN
2	G	314	GLN
2	G	387	GLN
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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	ADP	G	504	-	28,29,29	1.16	1 (3%)	43,45,45	2.83	7 (16%)
4	G3H	G	503	-	8,9,9	2.35	1 (12%)	7,12,12	1.06	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	ADP	G	504	-	-	6/16/32/32	0/3/3/3
4	G3H	G	503	-	1/1/2/3	2/7/8/8	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	503	G3H	O1-C1	6.32	1.44	1.20
5	G	504	ADP	PA-O3A	4.94	1.64	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	504	ADP	O2A-PA-O3A	11.21	137.56	107.27
5	G	504	ADP	O3A-PA-O1A	-7.69	87.58	110.70
5	G	504	ADP	O2'-C2'-C1'	6.51	132.51	110.10
5	G	504	ADP	C1'-N9-C8	6.25	140.97	127.09
5	G	504	ADP	C4-N9-C1'	-6.19	112.16	126.63
5	G	504	ADP	O2'-C2'-C3'	-3.19	101.59	111.82
5	G	504	ADP	O2B-PB-O3A	2.51	113.07	104.64

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	G	503	G3H	C2

All (8) 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	C3'-C4'-C5'-O5'

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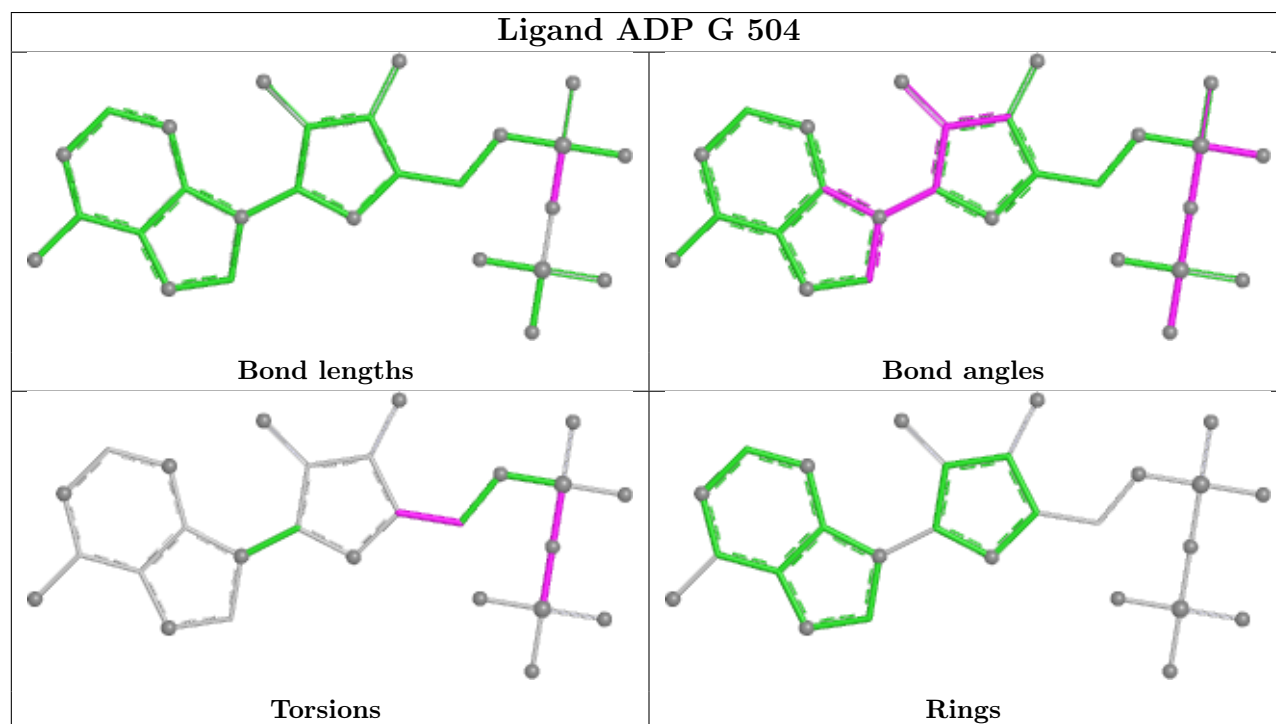
Mol	Chain	Res	Type	Atoms
5	G	504	ADP	O4'-C4'-C5'-O5'
5	G	504	ADP	PA-O3A-PB-O2B
5	G	504	ADP	PB-O3A-PA-O1A
5	G	504	ADP	PA-O3A-PB-O3B
5	G	504	ADP	PB-O3A-PA-O2A

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	503	G3H	4	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.