Full wwPDB X-ray Structure Validation Report (i)

Jan 28, 2024 – 01:28 AM EST

PDB ID	:	1GLE
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 (i) 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 (1)) were used in the production of this report:

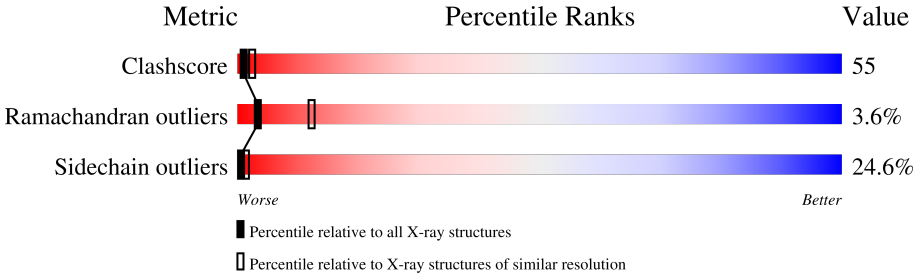
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.94 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	141614	3218 (2.98-2.90)
Ramachandran outliers	138981	3122 (2.98-2.90)
Sidechain outliers	138945	3124 (2.98-2.90)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	F	168	24% 48% 19% 5% •
2	G	501	29% 43% 20% 5% •

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 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 IIIGlc.

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

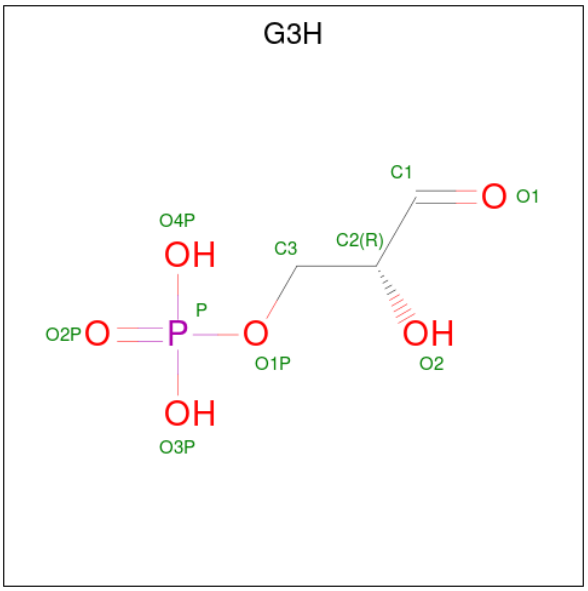
- Molecule 2 is a protein called GLYCEROL KINASE.

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

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

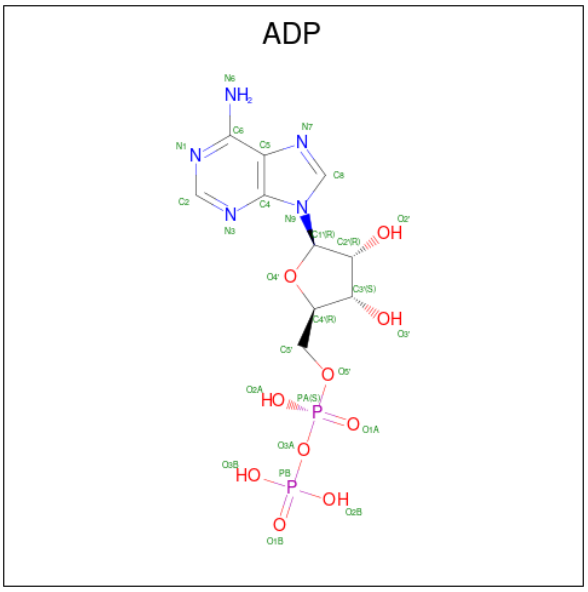
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
3	F	1	1	1	0	0
			Total	Zn		
3	G	1	1	1	0	0

- Molecule 4 is GLYCERALDEHYDE-3-PHOSPHATE (three-letter code: G3H) (formula: $C_3H_7O_6P$).



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

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



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

- Molecule 6 is water.

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

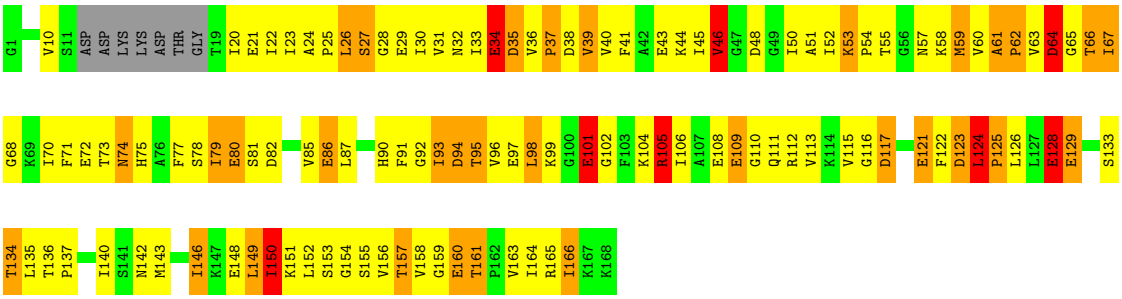
3 Residue-property plots (i)

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.

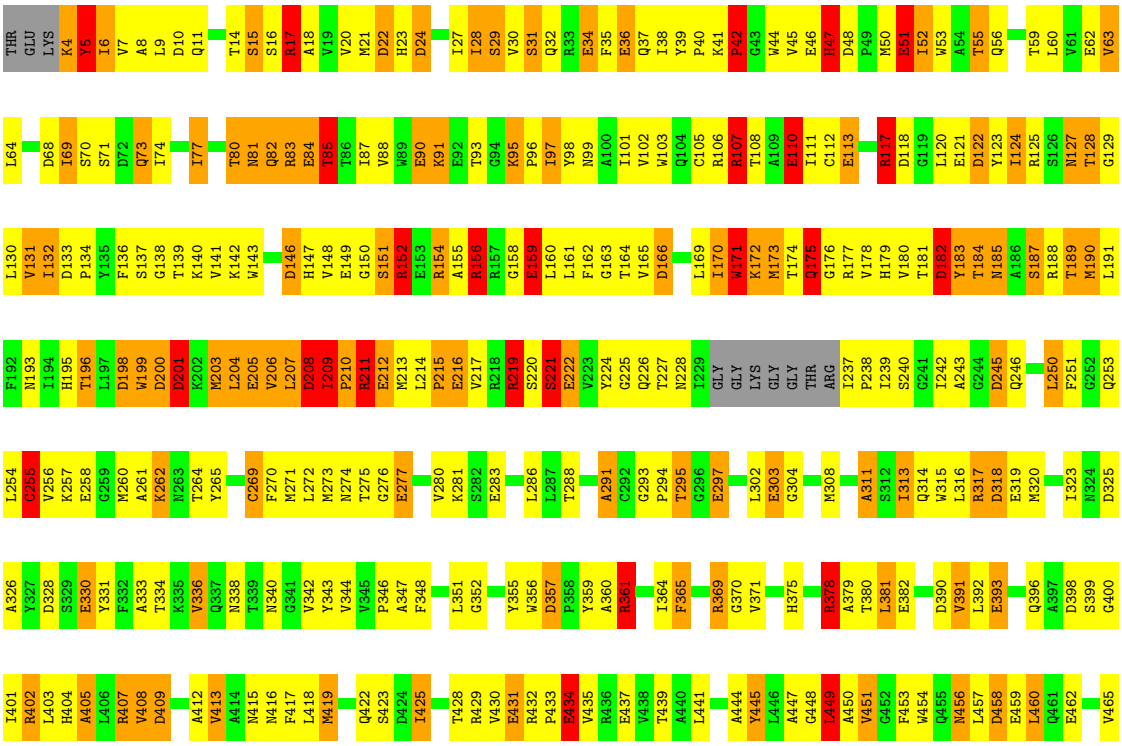
• Molecule 1: GLUCOSE-SPECIFIC PROTEIN IIIGlc

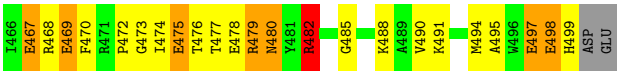
Chain F: 24% 48% 19% 5% •



• Molecule 2: GLYCEROL KINASE

Chain G: 29% 43% 20% 5% •




I466
E467
R468
E469
F470
R471
P472
G473
I474
E475
T476
T477
E478
R479
N480
Y481
R482
G485
K488
A489
V490
K491
M494
A495
W496
E497
E498
H499
ASP
GLU

4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.45	15/1172 (1.3%)	1.81	24/1592 (1.5%)
2	G	1.31	31/3831 (0.8%)	1.77	93/5211 (1.8%)
All	All	1.34	46/5003 (0.9%)	1.78	117/6803 (1.7%)

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 (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	110	GLU	CD-OE2	11.00	1.37	1.25
2	G	393	GLU	CD-OE1	9.82	1.36	1.25
2	G	62	GLU	CD-OE2	9.63	1.36	1.25
1	F	101	GLU	CD-OE2	9.56	1.36	1.25
2	G	216	GLU	CD-OE2	9.46	1.36	1.25
2	G	51	GLU	CD-OE1	9.31	1.35	1.25
1	F	80	GLU	CD-OE1	9.04	1.35	1.25
1	F	148	GLU	CD-OE2	8.92	1.35	1.25
1	F	72	GLU	CD-OE2	8.92	1.35	1.25
2	G	437	GLU	CD-OE2	8.91	1.35	1.25
1	F	97	GLU	CD-OE1	8.90	1.35	1.25
2	G	159	GLU	CD-OE1	8.75	1.35	1.25
1	F	129	GLU	CD-OE1	8.37	1.34	1.25
1	F	128	GLU	CD-OE2	8.36	1.34	1.25
2	G	205	GLU	CD-OE2	8.20	1.34	1.25
1	F	121	GLU	CD-OE1	8.18	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	498	GLU	CD-OE1	8.09	1.34	1.25
1	F	43	GLU	CD-OE2	8.01	1.34	1.25
2	G	431	GLU	CD-OE2	7.93	1.34	1.25
1	F	86	GLU	CD-OE1	7.82	1.34	1.25
2	G	277	GLU	CD-OE2	7.57	1.33	1.25
2	G	34	GLU	CD-OE1	7.54	1.33	1.25
2	G	382	GLU	CD-OE2	7.45	1.33	1.25
1	F	109	GLU	CD-OE2	7.34	1.33	1.25
2	G	434	GLU	CD-OE1	7.31	1.33	1.25
2	G	475	GLU	CD-OE2	7.26	1.33	1.25
2	G	469	GLU	CD-OE1	7.12	1.33	1.25
2	G	90	GLU	CD-OE2	7.03	1.33	1.25
1	F	21	GLU	CD-OE2	6.98	1.33	1.25
2	G	258	GLU	CD-OE1	6.94	1.33	1.25
2	G	297	GLU	CD-OE2	6.94	1.33	1.25
2	G	212	GLU	CD-OE2	6.64	1.32	1.25
1	F	34	GLU	CD-OE2	6.62	1.32	1.25
2	G	283	GLU	CD-OE2	6.45	1.32	1.25
1	F	29	GLU	CD-OE1	6.45	1.32	1.25
2	G	36	GLU	CD-OE2	6.43	1.32	1.25
2	G	330	GLU	CD-OE1	6.16	1.32	1.25
2	G	467	GLU	CD-OE2	5.63	1.31	1.25
2	G	319	GLU	CD-OE1	5.58	1.31	1.25
2	G	478	GLU	CD-OE1	5.56	1.31	1.25
1	F	160	GLU	CD-OE2	5.28	1.31	1.25
2	G	222	GLU	CD-OE1	5.25	1.31	1.25
2	G	117	ARG	NE-CZ	5.22	1.39	1.33
2	G	303	GLU	CD-OE1	5.12	1.31	1.25
2	G	331	TYR	CB-CG	-5.07	1.44	1.51
2	G	113	GLU	CD-OE2	5.01	1.31	1.25

All (117) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	209	ILE	C-N-CD	-12.36	93.41	120.60
2	G	369	ARG	NE-CZ-NH1	11.41	126.00	120.30
1	F	124	LEU	C-N-CD	-10.71	97.05	120.60
2	G	361	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	F	94	ASP	CB-CG-OD2	-10.02	109.29	118.30
1	F	48	ASP	CB-CG-OD2	-9.81	109.47	118.30
2	G	245	ASP	CB-CG-OD2	-9.71	109.56	118.30
2	G	133	ASP	CB-CG-OD2	-9.41	109.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	328	ASP	CB-CG-OD1	-9.36	109.88	118.30
2	G	200	ASP	CB-CG-OD2	-8.99	110.21	118.30
2	G	219	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	F	104	LYS	N-CA-CB	-8.70	94.94	110.60
2	G	479	ARG	NE-CZ-NH1	8.51	124.56	120.30
2	G	402	ARG	NE-CZ-NH1	8.15	124.38	120.30
2	G	245	ASP	CB-CG-OD1	8.00	125.50	118.30
2	G	117	ARG	NE-CZ-NH1	7.88	124.24	120.30
2	G	152	ARG	NE-CZ-NH1	7.74	124.17	120.30
1	F	82	ASP	CB-CG-OD2	7.57	125.11	118.30
1	F	48	ASP	CB-CG-OD1	7.47	125.03	118.30
2	G	133	ASP	CB-CG-OD1	7.41	124.97	118.30
2	G	328	ASP	CB-CG-OD2	7.38	124.94	118.30
1	F	64	ASP	CB-CG-OD1	7.32	124.89	118.30
1	F	64	ASP	CB-CG-OD2	-7.29	111.74	118.30
2	G	479	ARG	NE-CZ-NH2	-7.29	116.66	120.30
2	G	458	ASP	CB-CG-OD1	-7.17	111.85	118.30
2	G	390	ASP	CB-CG-OD1	-7.16	111.85	118.30
2	G	325	ASP	CB-CG-OD2	-7.16	111.86	118.30
2	G	275	THR	CA-CB-CG2	-7.06	102.51	112.40
2	G	482	ARG	NE-CZ-NH2	-6.95	116.83	120.30
2	G	334	THR	CA-CB-CG2	-6.92	102.71	112.40
2	G	288	THR	CA-CB-CG2	-6.91	102.72	112.40
2	G	221	SER	N-CA-CB	6.85	120.77	110.50
1	F	35	ASP	CB-CG-OD1	6.79	124.41	118.30
2	G	42	PRO	N-CA-CB	6.75	111.40	103.30
1	F	59	MET	CG-SD-CE	-6.73	89.43	100.20
2	G	156	ARG	NE-CZ-NH2	-6.64	116.98	120.30
2	G	317	ARG	NE-CZ-NH2	-6.59	117.01	120.30
2	G	325	ASP	CB-CA-C	-6.56	97.29	110.40
1	F	94	ASP	CB-CG-OD1	6.51	124.16	118.30
2	G	182	ASP	CB-CG-OD1	6.48	124.13	118.30
2	G	70	SER	N-CA-CB	6.43	120.15	110.50
1	F	35	ASP	CB-CG-OD2	-6.43	112.51	118.30
2	G	198	ASP	CB-CG-OD2	-6.42	112.52	118.30
2	G	106	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	G	182	ASP	CB-CG-OD2	-6.38	112.55	118.30
2	G	419	MET	CA-CB-CG	-6.37	102.47	113.30
2	G	409	ASP	CB-CG-OD2	-6.33	112.60	118.30
2	G	361	ARG	NE-CZ-NH2	-6.31	117.14	120.30
2	G	156	ARG	NE-CZ-NH1	6.30	123.45	120.30
2	G	146	ASP	CB-CG-OD2	-6.29	112.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	465	VAL	CB-CA-C	-6.27	99.49	111.40
1	F	71	PHE	N-CA-CB	6.25	121.85	110.60
1	F	95	THR	CA-CB-CG2	-6.24	103.67	112.40
2	G	171	TRP	CA-CB-CG	6.22	125.52	113.70
2	G	48	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	F	150	ILE	CA-C-N	-6.20	103.57	117.20
2	G	10	ASP	CB-CG-OD2	6.14	123.83	118.30
2	G	318	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	G	183	TYR	CB-CG-CD2	6.11	124.66	121.00
2	G	128	THR	CA-CB-CG2	-6.05	103.93	112.40
2	G	409	ASP	CB-CG-OD1	6.04	123.74	118.30
2	G	336	VAL	N-CA-C	6.03	127.29	111.00
2	G	47	HIS	N-CA-CB	6.00	121.40	110.60
1	F	60	VAL	N-CA-CB	-5.98	98.35	111.50
2	G	185	ASN	CA-CB-CG	-5.94	100.33	113.40
2	G	482	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	G	404	HIS	CA-CB-CG	-5.89	103.59	113.60
1	F	82	ASP	CB-CG-OD1	-5.88	113.01	118.30
2	G	311	ALA	CB-CA-C	-5.88	101.28	110.10
2	G	407	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	F	123	ASP	CB-CG-OD1	-5.75	113.13	118.30
1	F	55	THR	N-CA-CB	5.74	121.21	110.30
2	G	47	HIS	CA-CB-CG	5.73	123.35	113.60
2	G	198	ASP	CB-CG-OD1	5.64	123.38	118.30
2	G	184	THR	CA-CB-CG2	-5.63	104.52	112.40
2	G	166	ASP	CB-CG-OD2	5.62	123.35	118.30
2	G	17	ARG	CB-CA-C	5.61	121.62	110.40
1	F	61	ALA	C-N-CD	-5.58	108.32	120.60
2	G	5	TYR	CB-CA-C	-5.55	99.29	110.40
2	G	380	THR	CA-CB-OG1	-5.54	97.38	109.00
2	G	15	SER	CB-CA-C	-5.52	99.61	110.10
2	G	369	ARG	N-CA-CB	5.50	120.50	110.60
2	G	107	ARG	NE-CZ-NH1	5.49	123.05	120.30
2	G	291	ALA	CB-CA-C	-5.49	101.86	110.10
2	G	201	ASP	CB-CG-OD2	-5.47	113.37	118.30
2	G	10	ASP	CB-CG-OD1	-5.47	113.38	118.30
1	F	46	VAL	CA-CB-CG1	-5.46	102.71	110.90
2	G	407	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	F	105	ARG	NE-CZ-NH1	5.44	123.02	120.30
2	G	449	LEU	CB-CA-C	-5.42	99.91	110.20
2	G	408	VAL	CB-CA-C	-5.38	101.18	111.40
2	G	378	ARG	NE-CZ-NH2	-5.37	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	219	ARG	NE-CZ-NH2	-5.37	117.62	120.30
2	G	215	PRO	N-CA-CB	5.35	109.72	103.30
2	G	208	ASP	CB-CG-OD1	-5.34	113.49	118.30
2	G	390	ASP	CB-CG-OD2	5.32	123.09	118.30
2	G	118	ASP	CB-CG-OD1	5.29	123.06	118.30
2	G	405	ALA	N-CA-CB	5.26	117.46	110.10
2	G	5	TYR	CB-CG-CD2	-5.23	117.86	121.00
2	G	122	ASP	CB-CG-OD2	-5.22	113.60	118.30
2	G	318	ASP	CB-CG-OD1	5.22	123.00	118.30
2	G	381	LEU	CB-CG-CD2	-5.20	102.16	111.00
2	G	106	ARG	NE-CZ-NH1	5.19	122.90	120.30
2	G	22	ASP	CB-CG-OD2	5.18	122.97	118.30
2	G	480	ASN	N-CA-CB	5.18	119.92	110.60
2	G	190	MET	CG-SD-CE	-5.15	91.97	100.20
1	F	150	ILE	O-C-N	5.14	130.93	122.70
2	G	22	ASP	CB-CG-OD1	-5.12	113.69	118.30
2	G	445	TYR	CB-CG-CD2	-5.11	117.93	121.00
2	G	175	GLN	CB-CA-C	5.09	120.57	110.40
2	G	357	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	F	57	ASN	N-CA-C	5.06	124.66	111.00
2	G	172	LYS	N-CA-CB	5.05	119.69	110.60
2	G	408	VAL	CA-CB-CG2	-5.04	103.33	110.90
2	G	497	GLU	CG-CD-OE2	-5.04	108.21	118.30
2	G	365	PHE	CB-CG-CD1	5.03	124.32	120.80
2	G	297	GLU	OE1-CD-OE2	5.02	129.33	123.30

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	138	0
2	G	3752	0	3605	392	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	G	10	0	5	5	0
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	530	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 55.

All (530) 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
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: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:419:MET:CE	2:G:419:MET:HA	2.05	0.85
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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: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: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: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
1:F:40:VAL:O	1:F:46:VAL:HG23	1.90	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:271:MET:C	2:G:272:LEU:HD12	2.08	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
1:F:31:VAL:HG12	1:F:32:ASN:N	2.06	0.70
2:G:201:ASP:CG	2:G:211:ARG:HH12	1.94	0.70
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
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:124:ILE:HD11	2:G:203:MET:HE1	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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:308:MET:HE2	2:G:348:PHE:HB2	1.80	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:261:ALA:HB2	2:G:273:MET:HB2	1.83	0.60
2:G:308:MET:HE3	2:G:348:PHE:CD1	2.36	0.60
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:448:GLY:HA3	2:G:454:TRP:CE3	2.37	0.59
1:F:93:ILE:HD12	1:F:93:ILE:C	2.22	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:38:ILE:HG22	2:G:40:PRO:HD3	1.87	0.57
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: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: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:HG21	2:G:102:VAL:HG13	1.90	0.54
2:G:85:THR:N	6:G:541:HOH:O	2.40	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:396:GLN:NE2	2:G:403:LEU:H	2.06	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
2:G:459:GLU:C	2:G:460:LEU:HD23	2.29	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:124:ILE:O	2:G:128:THR:OG1	2.20	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: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
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
2:G:392:LEU:C	2:G:392:LEU:HD23	2.32	0.51
1:F:124:LEU:O	1:F:128:GLU:HB2	2.11	0.50
2:G:124:ILE:HD11	2:G:203:MET:CE	2.39	0.50
2:G:435:VAL:O	2:G:435:VAL:HG13	2.11	0.50
1:F:28:GLY:HA3	1:F:53:LYS:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:419:MET:HA	2:G:419:MET:HE1	1.90	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
2:G:342:VAL:HG12	2:G:343:TYR: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:52:ILE:O	1:F:52:ILE:HG22	2.11	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: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: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:364:ILE:HG22	2:G:365:PHE:N	2.28	0.49
1:F:59:MET:HB3	1:F:59:MET:HE3	1.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:GLU:C	1:F:87:LEU:HG	2.33	0.48
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:428:THR:CG2	2:G:429:ARG:N	2.75	0.48
2:G:468:ARG:CG	2:G:469:GLU:N	2.76	0.48
1:F:66:THR:HG23	1:F:112:ARG:HA	1.95	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:419:MET:HA	2:G:419:MET:HE2	1.91	0.47
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:342:VAL:CG1	2:G:343:TYR:N	2.77	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: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:200:ASP:HB3	2:G:203:MET:HB2	1.97	0.47
1:F:27:SER:HG	1:F:158:VAL:HG12	1.80	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
2:G:490:VAL:HG12	2:G:491:LYS:N	2.29	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: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:11:GLN:CD	2:G:52:ILE:HG23	2.36	0.46
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: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
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
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
1:F:164:ILE:HG22	1:F:165:ARG:N	2.30	0.46
2:G:53:TRP:CE3	2:G:53:TRP:CA	2.96	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
2:G:128:THR:C	2:G:130:LEU:H	2.19	0.46
2:G:173:MET:C	2:G:175:GLN:H	2.19	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
2:G:428:THR:HG22	2:G:429:ARG:N	2.29	0.45
2:G:448:GLY:HA3	2:G:454:TRP:CZ3	2.51	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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
2:G:308:MET:CE	2:G:348:PHE:HB2	2.47	0.44
1:F:150:ILE:HD12	1:F:150:ILE:H	1.83	0.44
2:G:42:PRO:C	2:G:44:TRP:H	2.21	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
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:155:ALA:HB2	2:G:160:LEU:HD12	1.99	0.44
2:G:85:THR:CB	2:G:102:VAL:HA	2.45	0.43
1:F:108:GLU:C	1:F:110:GLY:H	2.21	0.43
1:F:39:VAL:O	1:F:45:ILE:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:14:THR:HA	6:G:506:HOH:O	2.17	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:152:ARG:HE	2:G:208:ASP:CG	2.22	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
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
2:G:209:ILE:HA	2:G:210:PRO:HD2	1.36	0.43
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:475:GLU:H	2:G:475:GLU:CD	2.17	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:160:LEU:C	2:G:161:LEU:HD23	2.40	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
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:371:VAL:HG13	2:G:375:HIS:HB2	2.01	0.42
2:G:155:ALA:C	2:G:158:GLY:H	2.23	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:357:ASP:C	2:G:359:TYR:H	2.24	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: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
2:G:304:GLY:HA3	2:G:391:VAL:HG21	2.02	0.41
1:F:36:VAL:C	1:F:38:ASP:H	2.23	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:91:PHE:CD1	1:F:91:PHE:C	2.94	0.41
2:G:102:VAL:H	2:G:102:VAL:HG23	1.69	0.41
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:245:ASP:OD1	4:G:503:G3H:O2	2.30	0.41
2:G:246:GLN:CD	2:G:270:PHE:HB2	2.41	0.41
2:G:408:VAL:O	2:G:433:PRO:HG2	2.21	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:407:ARG:CD	2:G:431:GLU:HG3	2.38	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%)	133 (85%)	18 (12%)	6 (4%)	3 11
2	G	485/501 (97%)	410 (84%)	58 (12%)	17 (4%)	3 13
All	All	642/669 (96%)	543 (85%)	76 (12%)	23 (4%)	3 12

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

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Mol	Chain	Res	Type
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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	F	123/145 (85%)	88 (72%)	35 (28%)	0 1
2	G	378/412 (92%)	290 (77%)	88 (23%)	1 2
All	All	501/557 (90%)	378 (75%)	123 (25%)	0 1

All (123) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	20	ILE
1	F	26	LEU
1	F	27	SER
1	F	34	GLU
1	F	35	ASP
1	F	39	VAL

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Mol	Chain	Res	Type
1	F	44	LYS
1	F	46	VAL
1	F	50	ILE
1	F	53	LYS
1	F	58	LYS
1	F	64	ASP
1	F	66	THR
1	F	67	ILE
1	F	74	ASN
1	F	79	ILE
1	F	93	ILE
1	F	95	THR
1	F	98	LEU
1	F	99	LYS
1	F	101	GLU
1	F	105	ARG
1	F	111	GLN
1	F	117	ASP
1	F	128	GLU
1	F	129	GLU
1	F	134	THR
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	161	THR
1	F	166	ILE
2	G	4	LYS
2	G	5	TYR
2	G	6	ILE
2	G	17	ARG
2	G	24	ASP
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	37	GLN
2	G	41	LYS

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Mol	Chain	Res	Type
2	G	47	HIS
2	G	50	MET
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
2	G	82	GLN
2	G	83	ARG
2	G	85	THR
2	G	91	LYS
2	G	95	LYS
2	G	97	ILE
2	G	107	ARG
2	G	110	GLU
2	G	117	ARG
2	G	122	ASP
2	G	124	ILE
2	G	127	ASN
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	201	ASP
2	G	203	MET
2	G	204	LEU
2	G	207	LEU
2	G	208	ASP
2	G	209	ILE

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Mol	Chain	Res	Type
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	250	LEU
2	G	255	CYS
2	G	262	LYS
2	G	269	CYS
2	G	277	GLU
2	G	295	THR
2	G	313	ILE
2	G	361	ARG
2	G	369	ARG
2	G	378	ARG
2	G	391	VAL
2	G	398	ASP
2	G	402	ARG
2	G	413	VAL
2	G	425	ILE
2	G	434	GLU
2	G	449	LEU
2	G	451	VAL
2	G	456	ASN
2	G	460	LEU
2	G	474	ILE
2	G	477	THR
2	G	480	ASN
2	G	482	ARG
2	G	488	LYS

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

Mol	Chain	Res	Type
1	F	74	ASN
1	F	142	ASN
2	G	32	GLN
2	G	47	HIS
2	G	56	GLN

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Mol	Chain	Res	Type
2	G	81	ASN
2	G	185	ASN
2	G	228	ASN
2	G	396	GLN
2	G	404	HIS
2	G	456	ASN
2	G	499	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	G3H	G	503	-	8,9,9	2.25	1 (12%)	10,12,12	0.95	0
5	ADP	G	504	-	24,29,29	0.79	0	29,45,45	2.38	8 (27%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	503	G3H	O1-C1	6.03	1.44	1.19

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	G	504	ADP	C1'-N9-C4	-8.24	112.16	126.64
5	G	504	ADP	O2'-C2'-C1'	5.86	132.51	110.85
5	G	504	ADP	PA-O3A-PB	-3.89	119.48	132.83
5	G	504	ADP	C5-C6-N6	3.21	125.23	120.35
5	G	504	ADP	O2'-C2'-C3'	-3.16	101.59	111.82
5	G	504	ADP	O2B-PB-O3A	2.51	113.07	104.64
5	G	504	ADP	C3'-C2'-C1'	2.06	104.08	100.98
5	G	504	ADP	O4'-C4'-C3'	2.02	109.10	105.11

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

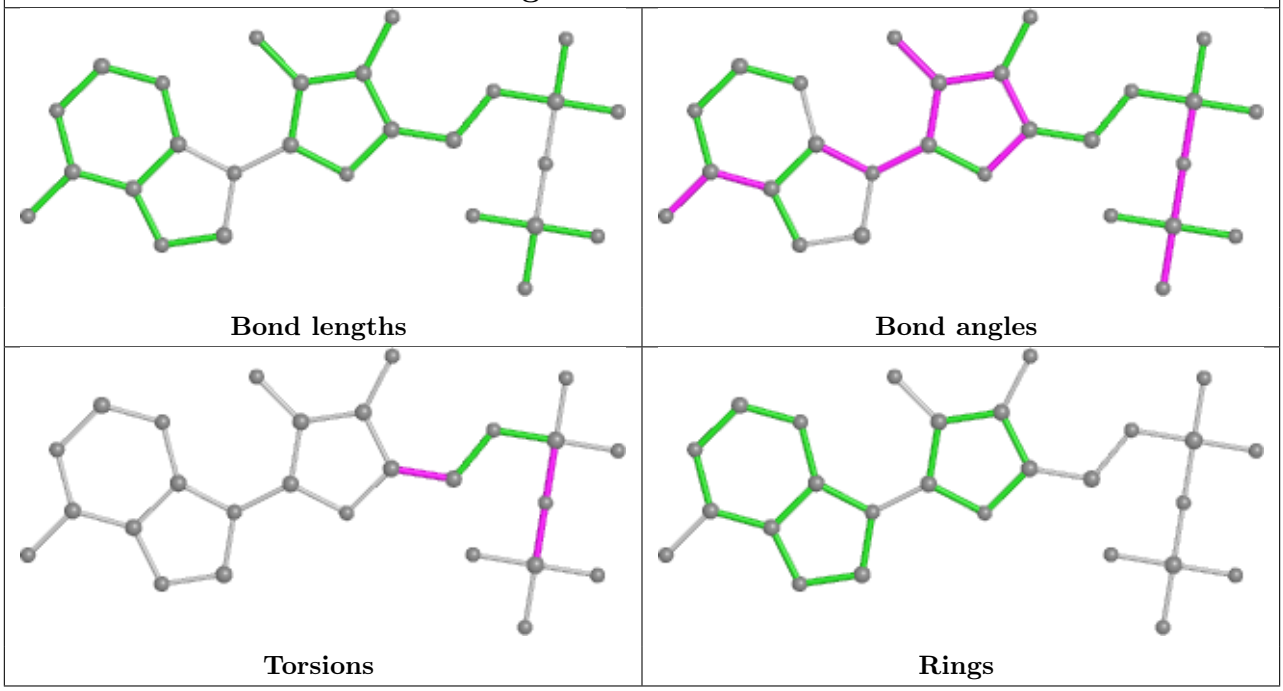
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	503	G3H	5	0

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

Ligand ADP G 504



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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.