Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 07:59 PM EDT

PDB ID	:	1K3T
Title	:	Structure of Glycosomal Glyceraldehyde-3-Phosphate Dehydrogenase from Trypanosoma cruzi Complexed with Chalepin, a Coumarin Derivative Inhibitor
Authors	:	Pavao, F.
Deposited on	:	2001-10-04
Resolution	:	1.95 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:

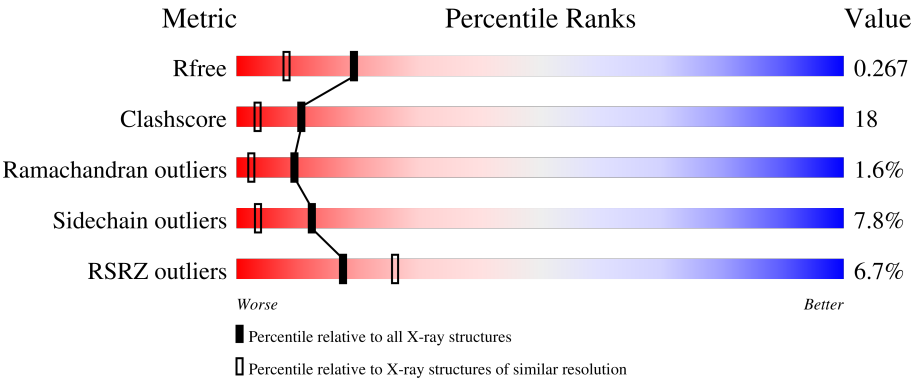
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 1.95 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))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	359	2% 69% 25% 6%
1	B	359	5% 64% 28% 7%
1	C	359	18% 51% 39% 9%
1	D	359	2% 66% 24% 8%

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
2	BRZ	C	960	-	-	X	-

2 Entry composition

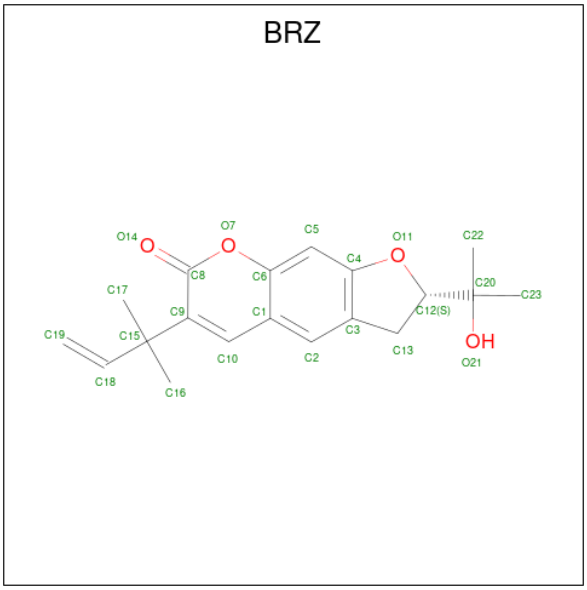
There are 3 unique types of molecules in this entry. The entry contains 11942 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glyceraldehyde-3-phosphate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	0	0
			2744	1725	486	519	14			
1	B	359	Total	C	N	O	S	0	0	0
			2744	1725	486	519	14			
1	C	359	Total	C	N	O	S	0	1	0
			2750	1728	487	520	15			
1	D	359	Total	C	N	O	S	0	0	0
			2744	1725	486	519	14			

- Molecule 2 is 6-(1,1-DIMETHYLALLYL)-2-(1-HYDROXY-1-METHYLETHYL)-2,3-DIHYDRO-7H-FURO[3,2-G]CHROMEN-7-ONE (three-letter code: BRZ) (formula: $C_{19}H_{22}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	O		0	0
			23	19	4			

- Molecule 3 is water.

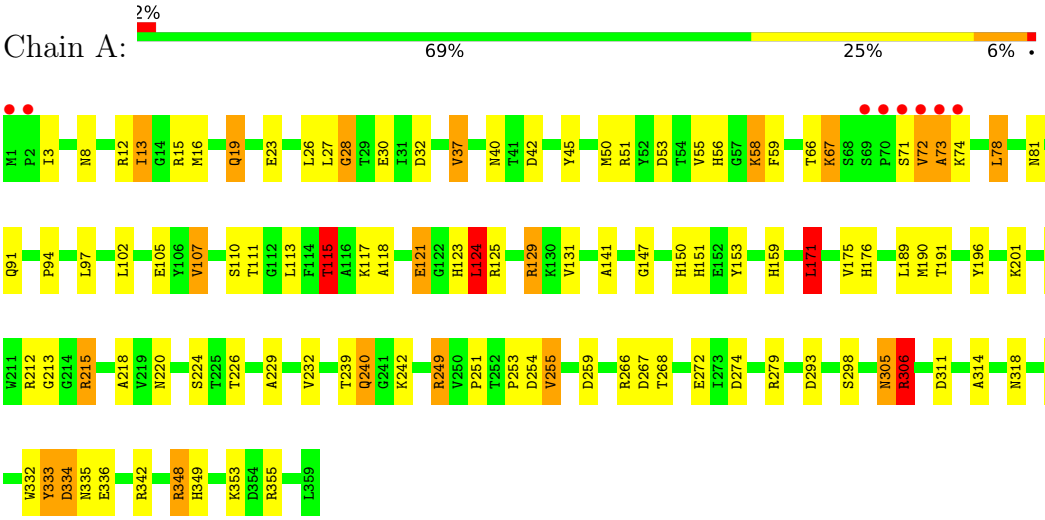
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	271	Total O 271 271	0	0
3	B	223	Total O 223 223	0	0
3	C	161	Total O 161 161	0	0
3	D	282	Total O 282 282	0	0

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

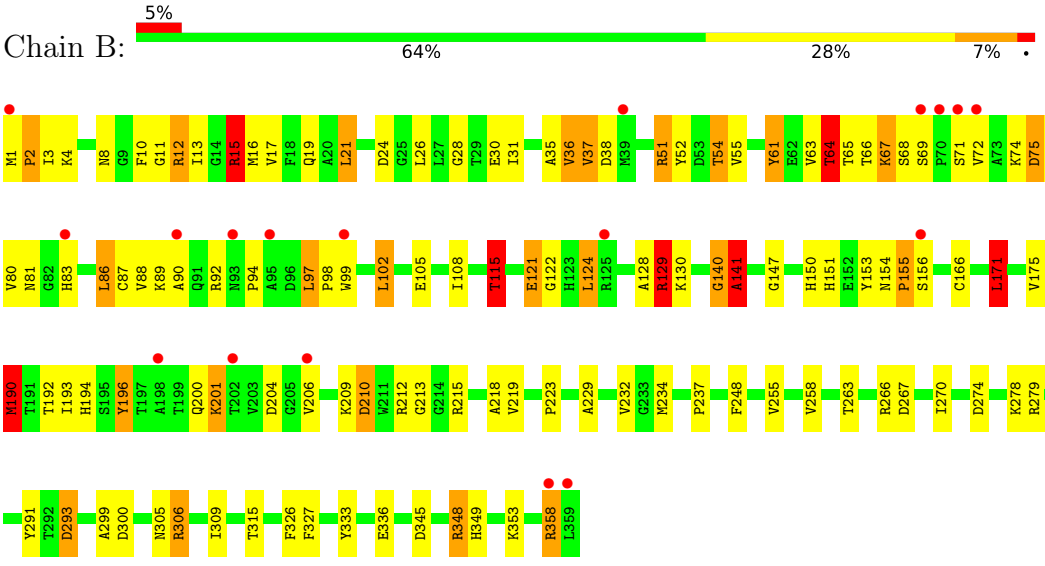
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain A:



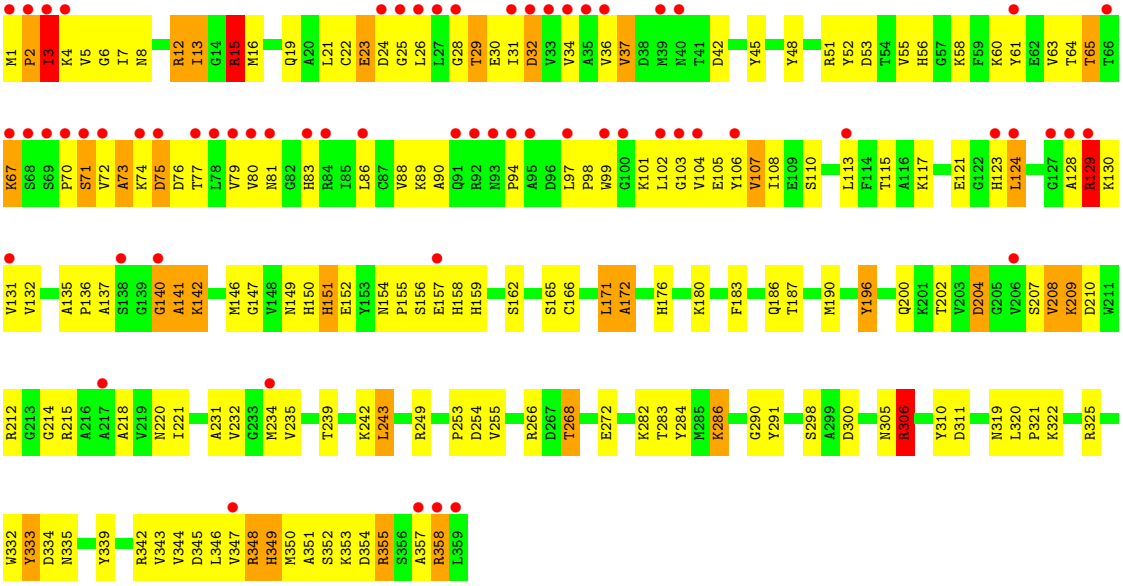
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain B:



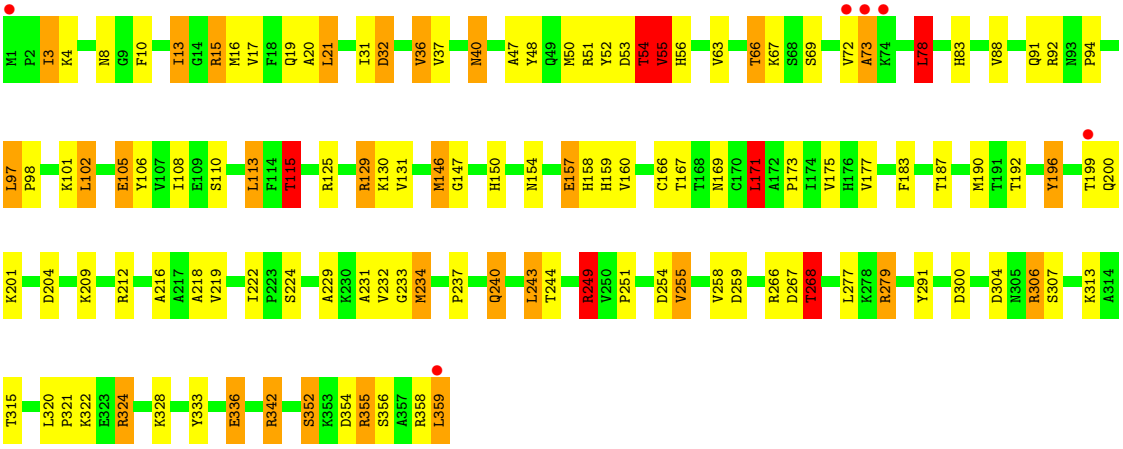
• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain C:



• Molecule 1: Glyceraldehyde-3-phosphate dehydrogenase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.08Å 84.97Å 105.24Å 90.00° 96.32° 90.00°	Depositor
Resolution (Å)	15.00 – 1.95 44.54 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (15.00-1.95) 77.9 (44.54-1.95)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 1.95Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.201 , 0.280 0.197 , 0.267	Depositor DCC
R_{free} test set	2483 reflections (3.04%)	wwPDB-VP
Wilson B-factor (Å^2)	22.5	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 69.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11942	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BRZ

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	A	0.78	0/2797	1.76	64/3792 (1.7%)
1	B	0.74	0/2797	1.72	62/3792 (1.6%)
1	C	0.66	0/2803	1.63	40/3800 (1.1%)
1	D	0.79	0/2797	1.95	70/3792 (1.8%)
All	All	0.74	0/11194	1.77	236/15176 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

All (236) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	125	ARG	CD-NE-CZ	31.38	167.52	123.60
1	D	249	ARG	CD-NE-CZ	20.97	152.95	123.60
1	D	279	ARG	CD-NE-CZ	19.71	151.19	123.60
1	D	266	ARG	CD-NE-CZ	18.29	149.21	123.60
1	C	129	ARG	CD-NE-CZ	17.83	148.56	123.60
1	C	15	ARG	NE-CZ-NH1	17.26	128.93	120.30
1	D	204	ASP	CB-CG-OD1	16.38	133.04	118.30
1	A	215	ARG	NE-CZ-NH2	14.61	127.61	120.30
1	A	212	ARG	NE-CZ-NH2	-14.25	113.18	120.30
1	D	249	ARG	NE-CZ-NH1	14.15	127.37	120.30
1	D	129	ARG	NE-CZ-NH1	-14.11	113.24	120.30
1	A	125	ARG	CD-NE-CZ	11.96	140.35	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	279	ARG	NE-CZ-NH1	11.72	126.16	120.30
1	D	342	ARG	NE-CZ-NH1	11.63	126.12	120.30
1	C	15	ARG	CD-NE-CZ	11.04	139.06	123.60
1	C	325	ARG	NE-CZ-NH1	10.61	125.61	120.30
1	A	15	ARG	CD-NE-CZ	10.47	138.25	123.60
1	C	15	ARG	NH1-CZ-NH2	-10.30	108.07	119.40
1	D	355	ARG	NE-CZ-NH1	9.97	125.29	120.30
1	D	355	ARG	CD-NE-CZ	9.92	137.48	123.60
1	D	243	LEU	CA-CB-CG	9.89	138.05	115.30
1	B	279	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	D	51	ARG	NE-CZ-NH1	-9.68	115.46	120.30
1	D	359	LEU	CA-CB-CG	9.62	137.43	115.30
1	A	212	ARG	NE-CZ-NH1	9.44	125.02	120.30
1	B	210	ASP	CB-CG-OD2	-9.44	109.80	118.30
1	B	141	ALA	N-CA-CB	9.31	123.13	110.10
1	D	21	LEU	CA-CB-CG	9.23	136.53	115.30
1	C	311	ASP	CB-CG-OD2	-9.21	110.02	118.30
1	A	12	ARG	CD-NE-CZ	9.00	136.21	123.60
1	C	355	ARG	NE-CZ-NH2	8.91	124.75	120.30
1	A	215	ARG	NE-CZ-NH1	-8.88	115.86	120.30
1	B	345	ASP	CB-CG-OD1	8.78	126.20	118.30
1	B	155	PRO	CA-C-N	8.67	136.27	117.20
1	D	306	ARG	NE-CZ-NH2	-8.62	115.99	120.30
1	A	348	ARG	NE-CZ-NH2	8.61	124.61	120.30
1	A	311	ASP	CB-CG-OD2	8.59	126.03	118.30
1	B	15	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	C	306	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	B	92	ARG	CD-NE-CZ	8.46	135.44	123.60
1	A	45	TYR	CB-CG-CD2	-8.45	115.93	121.00
1	A	78	LEU	CA-CB-CG	8.40	134.62	115.30
1	B	267	ASP	CB-CG-OD2	-8.33	110.81	118.30
1	B	24	ASP	CB-CG-OD1	8.25	125.72	118.30
1	D	52	TYR	CB-CG-CD1	-8.24	116.06	121.00
1	A	334	ASP	CB-CG-OD2	8.21	125.69	118.30
1	A	153	TYR	CB-CG-CD2	-8.15	116.11	121.00
1	B	266	ARG	CG-CD-NE	8.06	128.72	111.80
1	A	259	ASP	CB-CG-OD2	8.04	125.53	118.30
1	C	234	MET	CA-CB-CG	8.04	126.96	113.30
1	C	212	ARG	NE-CZ-NH2	-7.96	116.32	120.30
1	C	196	TYR	CB-CG-CD2	-7.88	116.27	121.00
1	B	293	ASP	N-CA-CB	7.87	124.77	110.60
1	D	342	ARG	CD-NE-CZ	7.82	134.54	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	12	ARG	NE-CZ-NH2	-7.81	116.39	120.30
1	B	15	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	B	285	MET	CG-SD-CE	7.68	112.49	100.20
1	A	45	TYR	CB-CG-CD1	7.61	125.56	121.00
1	B	306	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	B	51	ARG	NE-CZ-NH1	7.54	124.07	120.30
1	D	125	ARG	NE-CZ-NH2	7.43	124.01	120.30
1	D	266	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	C	196	TYR	CB-CG-CD1	7.40	125.44	121.00
1	D	51	ARG	CD-NE-CZ	7.37	133.92	123.60
1	B	12	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	A	115	THR	N-CA-CB	-7.33	96.38	110.30
1	C	48	TYR	CB-CG-CD1	7.30	125.38	121.00
1	B	333	TYR	CB-CG-CD2	7.28	125.37	121.00
1	A	159	HIS	CA-CB-CG	-7.26	101.25	113.60
1	A	314	ALA	N-CA-CB	7.24	120.24	110.10
1	B	190	MET	CA-CB-CG	7.22	125.58	113.30
1	A	267	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	D	342	ARG	NH1-CZ-NH2	-7.01	111.69	119.40
1	C	300	ASP	CB-CG-OD2	6.99	124.59	118.30
1	B	358	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	D	15	ARG	NE-CZ-NH2	6.97	123.78	120.30
1	A	125	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	C	172	ALA	CB-CA-C	6.87	120.40	110.10
1	D	267	ASP	CB-CG-OD1	6.85	124.46	118.30
1	A	30	GLU	OE1-CD-OE2	-6.82	115.11	123.30
1	B	61	TYR	CB-CG-CD2	6.82	125.09	121.00
1	A	323	GLU	OE1-CD-OE2	-6.81	115.13	123.30
1	A	121	GLU	OE1-CD-OE2	-6.80	115.14	123.30
1	B	333	TYR	CB-CG-CD1	-6.80	116.92	121.00
1	D	15	ARG	NE-CZ-NH1	-6.79	116.91	120.30
1	D	48	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	D	66	THR	N-CA-CB	6.68	123.00	110.30
1	C	306	ARG	NH1-CZ-NH2	6.68	126.74	119.40
1	D	204	ASP	OD1-CG-OD2	-6.67	110.63	123.30
1	A	124	LEU	CA-CB-CG	6.67	130.64	115.30
1	D	249	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	A	53	ASP	CB-CG-OD2	6.64	124.28	118.30
1	C	48	TYR	CB-CG-CD2	-6.54	117.08	121.00
1	D	115	THR	N-CA-CB	-6.53	97.89	110.30
1	C	129	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	C	204	ASP	CB-CG-OD1	6.52	124.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	C	266	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	266	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	B	193	ILE	C-N-CA	6.41	137.73	121.70
1	C	12	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	37	VAL	CA-CB-CG1	6.40	120.50	110.90
1	D	234	MET	CA-CB-CG	6.39	124.17	113.30
1	B	24	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	C	306	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	D	101	LYS	CB-CG-CD	6.29	127.95	111.60
1	B	204	ASP	CA-CB-CG	6.29	127.23	113.40
1	D	51	ARG	CG-CD-NE	-6.28	98.62	111.80
1	A	51	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	B	348	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	D	51	ARG	CB-CA-C	-6.26	97.89	110.40
1	A	336	GLU	OE1-CD-OE2	-6.20	115.86	123.30
1	D	53	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	B	309	ILE	CA-CB-CG1	6.19	122.75	111.00
1	D	113	LEU	CA-CB-CG	6.17	129.50	115.30
1	A	32	ASP	CB-CG-OD1	6.15	123.84	118.30
1	D	129	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	311	ASP	OD1-CG-OD2	-6.13	111.64	123.30
1	B	237	PRO	O-C-N	-6.13	112.89	122.70
1	D	16	MET	CB-CA-C	6.12	122.63	110.40
1	A	293	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	A	125	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	B	38	ASP	CB-CG-OD2	6.05	123.74	118.30
1	D	324	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	B	36	VAL	CA-CB-CG2	-6.01	101.88	110.90
1	B	192	THR	CA-CB-CG2	6.01	120.82	112.40
1	D	55	VAL	CG1-CB-CG2	-6.01	101.28	110.90
1	B	38	ASP	CB-CG-OD1	-5.99	112.91	118.30
1	B	54	THR	CA-CB-OG1	5.99	121.57	109.00
1	B	348	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	A	279	ARG	NH1-CZ-NH2	-5.95	112.86	119.40
1	B	92	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	D	266	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	204	ASP	CB-CG-OD1	5.90	123.61	118.30
1	D	78	LEU	CA-CB-CG	5.86	128.77	115.30
1	B	171	LEU	CB-CG-CD2	5.85	120.94	111.00
1	C	231	ALA	N-CA-CB	5.84	118.28	110.10
1	B	156	SER	N-CA-CB	5.83	119.25	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	15	ARG	CB-CG-CD	5.80	126.69	111.60
1	A	306	ARG	CD-NE-CZ	5.78	131.69	123.60
1	C	348	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	A	129	ARG	CD-NE-CZ	5.76	131.67	123.60
1	A	141	ALA	N-CA-CB	5.74	118.13	110.10
1	B	279	ARG	NE-CZ-NH2	-5.73	117.43	120.30
1	A	153	TYR	CB-CG-CD1	5.73	124.44	121.00
1	D	324	ARG	NE-CZ-NH2	-5.69	117.46	120.30
1	A	12	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	B	140	GLY	N-CA-C	-5.67	98.93	113.10
1	C	291	TYR	CB-CG-CD1	-5.67	117.60	121.00
1	A	267	ASP	CB-CG-OD1	5.65	123.38	118.30
1	A	23	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	B	155	PRO	CA-C-O	-5.64	106.66	120.20
1	D	92	ARG	CD-NE-CZ	5.64	131.50	123.60
1	D	16	MET	CA-CB-CG	5.62	122.84	113.30
1	D	216	ALA	CB-CA-C	5.61	118.52	110.10
1	D	125	ARG	NE-CZ-NH1	-5.61	117.49	120.30
1	B	293	ASP	CA-CB-CG	5.58	125.69	113.40
1	C	12	ARG	CD-NE-CZ	5.58	131.42	123.60
1	A	81	ASN	C-N-CA	5.58	134.02	122.30
1	A	249	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	D	54	THR	N-CA-CB	5.56	120.86	110.30
1	D	167	THR	CA-CB-CG2	-5.56	104.62	112.40
1	B	129	ARG	CD-NE-CZ	5.56	131.38	123.60
1	D	324	ARG	CD-NE-CZ	5.55	131.38	123.60
1	A	333	TYR	CB-CG-CD1	5.54	124.33	121.00
1	A	342	ARG	CD-NE-CZ	5.53	131.34	123.60
1	A	27	LEU	N-CA-CB	5.52	121.43	110.40
1	D	36	VAL	N-CA-CB	5.52	123.64	111.50
1	B	129	ARG	CG-CD-NE	5.51	123.37	111.80
1	B	35	ALA	CB-CA-C	-5.51	101.84	110.10
1	C	3	ILE	N-CA-CB	5.48	123.41	110.80
1	A	171	LEU	CB-CG-CD2	5.47	120.30	111.00
1	B	234	MET	CB-CA-C	-5.45	99.50	110.40
1	D	16	MET	N-CA-CB	-5.45	100.79	110.60
1	A	333	TYR	O-C-N	5.44	131.41	122.70
1	B	86	LEU	CA-CB-CG	-5.43	102.81	115.30
1	D	171	LEU	CB-CG-CD1	5.43	120.23	111.00
1	D	300	ASP	CB-CG-OD1	-5.43	113.42	118.30
1	C	355	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	B	267	ASP	CB-CG-OD1	5.42	123.18	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	15	ARG	NE-CZ-NH2	5.40	123.00	120.30
1	D	336	GLU	OE1-CD-OE2	-5.39	116.83	123.30
1	B	54	THR	N-CA-CB	5.38	120.53	110.30
1	B	61	TYR	CB-CG-CD1	-5.36	117.79	121.00
1	C	334	ASP	N-CA-C	-5.36	96.54	111.00
1	C	334	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	121	GLU	O-C-N	-5.35	114.11	123.20
1	D	306	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	C	310	TYR	CB-CG-CD1	-5.34	117.80	121.00
1	D	171	LEU	CB-CA-C	-5.33	100.07	110.20
1	D	291	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	B	75	ASP	CB-CG-OD2	5.30	123.07	118.30
1	C	333	TYR	N-CA-CB	5.30	120.14	110.60
1	D	267	ASP	CB-CG-OD2	-5.29	113.53	118.30
1	D	304	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	B	64	THR	N-CA-CB	-5.29	100.25	110.30
1	B	274	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	249	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	333	TYR	CB-CG-CD2	-5.27	117.84	121.00
1	D	32	ASP	CB-CG-OD2	5.27	123.05	118.30
1	B	248	PHE	N-CA-CB	5.27	120.08	110.60
1	A	84	ARG	NE-CZ-NH1	-5.25	117.67	120.30
1	B	306	ARG	CG-CD-NE	-5.25	100.77	111.80
1	C	196	TYR	N-CA-CB	5.25	120.05	110.60
1	C	358	ARG	CD-NE-CZ	-5.25	116.25	123.60
1	A	210	ASP	N-CA-CB	-5.23	101.18	110.60
1	D	229	ALA	CB-CA-C	5.22	117.93	110.10
1	D	66	THR	CA-CB-OG1	5.22	119.96	109.00
1	D	146	MET	CA-C-O	5.20	131.02	120.10
1	A	13	ILE	N-CA-CB	5.20	122.75	110.80
1	C	210	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	D	129	ARG	CD-NE-CZ	5.17	130.84	123.60
1	D	352	SER	N-CA-CB	5.16	118.24	110.50
1	D	40	ASN	CA-CB-CG	5.15	124.73	113.40
1	D	268	THR	CB-CA-C	-5.14	97.71	111.60
1	B	300	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	C	311	ASP	CB-CG-OD1	5.11	122.90	118.30
1	D	158	HIS	CA-CB-CG	5.10	122.28	113.60
1	C	286	LYS	CA-CB-CG	5.10	124.62	113.40
1	B	115	THR	N-CA-CB	-5.09	100.63	110.30
1	A	323	GLU	CB-CG-CD	5.08	127.92	114.20
1	D	212	ARG	CD-NE-CZ	5.08	130.71	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	ASP	CB-CG-OD2	-5.06	113.74	118.30
1	B	52	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	A	334	ASP	CB-CG-OD1	-5.04	113.77	118.30
1	A	333	TYR	N-CA-CB	5.03	119.66	110.60
1	D	20	ALA	CB-CA-C	5.03	117.65	110.10
1	A	129	ARG	CG-CD-NE	5.03	122.36	111.80
1	B	327	PHE	CB-CG-CD1	-5.03	117.28	120.80
1	C	290	GLY	N-CA-C	-5.03	100.53	113.10
1	A	212	ARG	CG-CD-NE	5.02	122.34	111.80
1	C	140	GLY	N-CA-C	-5.01	100.56	113.10
1	B	215	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	A	229	ALA	CB-CA-C	5.01	117.62	110.10
1	A	28	GLY	CA-C-O	-5.00	111.59	120.60
1	A	240	GLN	CB-CG-CD	5.00	124.60	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	28	GLY	Mainchain

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	A	2744	0	2749	83	0
1	B	2744	0	2749	85	0
1	C	2750	0	2752	168	0
1	D	2744	0	2749	82	0
2	C	23	0	22	17	0
3	A	271	0	0	15	0
3	B	223	0	0	12	0
3	C	161	0	0	17	0
3	D	282	0	0	11	0
All	All	11942	0	11021	405	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 18.

All (405) 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:C:166[A]:CYS:SG	2:C:960:BRZ:HC18	1.96	1.05
1:C:166[A]:CYS:H	2:C:960:BRZ:HC73	1.27	0.97
1:A:94:PRO:HA	1:A:97:LEU:HD23	1.46	0.97
1:C:166[B]:CYS:H	2:C:960:BRZ:HC73	1.28	0.96
1:A:40:ASN:HD21	1:A:42:ASP:HB3	1.31	0.95
1:A:220:ASN:HD21	1:D:54:THR:HG21	1.33	0.93
1:C:107:VAL:HG13	1:C:131:VAL:HG22	1.53	0.90
1:B:64:THR:HG22	1:B:79:VAL:HB	1.53	0.90
1:C:121:GLU:HA	1:C:124:LEU:HD22	1.56	0.87
1:C:176:HIS:CE1	1:C:180:LYS:HD2	2.09	0.85
1:B:66:THR:HG22	1:B:67:LYS:H	1.41	0.84
1:C:166[A]:CYS:SG	2:C:960:BRZ:C18	2.66	0.83
1:C:358:ARG:HD2	3:C:1025:HOH:O	1.77	0.83
1:A:8:ASN:ND2	1:A:37:VAL:HG22	1.94	0.82
1:A:117:LYS:O	1:A:121:GLU:HG3	1.78	0.82
1:D:47:ALA:HA	1:D:50:MET:HE3	1.60	0.82
1:D:190:MET:CE	1:D:192:THR:HB	2.11	0.81
1:C:70:PRO:O	1:C:71:SER:HB2	1.80	0.80
1:A:305:ASN:HB3	3:A:527:HOH:O	1.81	0.79
1:A:196:TYR:HB3	3:A:538:HOH:O	1.80	0.79
1:D:50:MET:HG2	3:D:530:HOH:O	1.82	0.79
1:C:154:ASN:HD22	1:C:157:GLU:H	1.30	0.78
1:C:8:ASN:HD22	1:C:37:VAL:HG13	1.49	0.77
1:B:37:VAL:HB	1:B:88:VAL:HG22	1.66	0.76
1:B:190:MET:HE1	1:B:258:VAL:HG22	1.66	0.75
1:C:115:THR:HG23	1:C:137:ALA:HA	1.68	0.75
1:C:239:THR:HB	1:C:243:LEU:HD22	1.68	0.74
1:A:55:VAL:HG23	1:A:56:HIS:CD2	2.23	0.74
1:D:3:ILE:HG22	1:D:355:ARG:NH2	2.02	0.74
1:A:8:ASN:HD22	1:A:37:VAL:HG22	1.51	0.73
1:B:68:SER:HB3	1:B:86:LEU:HD21	1.69	0.73
1:C:8:ASN:HA	1:C:37:VAL:HG13	1.72	0.72
1:B:190:MET:HG2	1:B:229:ALA:HB2	1.71	0.72
1:C:1:MET:HB3	1:C:2:PRO:CD	2.19	0.72
1:D:190:MET:HE3	1:D:258:VAL:HG22	1.72	0.71
1:A:13:ILE:HG23	1:A:110:SER:HB2	1.72	0.71
1:C:61:TYR:HD2	1:C:81:ASN:HB2	1.55	0.71
1:A:115:THR:HB	3:A:376:HOH:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:183:PHE:CD1	1:C:268:THR:HG21	2.26	0.71
1:B:54:THR:HG21	1:C:220:ASN:HD21	1.53	0.70
1:B:115:THR:HG22	3:B:498:HOH:O	1.91	0.70
1:B:10:PHE:CG	1:B:36:VAL:HG21	2.25	0.70
1:A:105:GLU:HG3	1:A:129:ARG:HD2	1.73	0.70
1:B:196:TYR:HB3	3:B:485:HOH:O	1.91	0.70
1:C:154:ASN:HD22	1:C:157:GLU:N	1.89	0.70
1:D:166:CYS:HB3	3:D:533:HOH:O	1.90	0.70
1:B:166:CYS:HB3	3:B:525:HOH:O	1.91	0.69
1:C:106:TYR:OH	1:C:351:ALA:HA	1.91	0.69
1:C:146:MET:HE3	1:C:346:LEU:HB2	1.74	0.69
1:A:40:ASN:ND2	1:A:42:ASP:H	1.90	0.69
1:A:3:ILE:HG23	1:A:355:ARG:NH2	2.08	0.69
1:A:218:ALA:HA	1:A:251:PRO:HB3	1.75	0.68
1:A:324:ARG:HG3	3:A:610:HOH:O	1.93	0.68
1:A:40:ASN:HD21	1:A:42:ASP:CB	2.07	0.67
1:A:305:ASN:C	1:A:305:ASN:HD22	1.97	0.67
1:B:129:ARG:HH21	1:B:358:ARG:HH21	1.43	0.67
1:C:354:ASP:O	1:C:358:ARG:HG3	1.96	0.66
1:D:8:ASN:ND2	1:D:37:VAL:HG22	2.10	0.66
1:C:147:GLY:H	1:C:150:HIS:CD2	2.13	0.66
1:A:115:THR:HG21	3:A:467:HOH:O	1.94	0.66
1:A:215:ARG:HH21	1:D:54:THR:HG22	1.60	0.66
1:C:349:HIS:CE1	1:C:353:LYS:HZ2	2.13	0.66
1:D:3:ILE:HD12	1:D:106:TYR:CD1	2.31	0.66
1:D:115:THR:HB	3:D:522:HOH:O	1.96	0.66
1:D:336:GLU:HA	3:D:516:HOH:O	1.96	0.66
1:C:355:ARG:HG2	3:C:1058:HOH:O	1.96	0.65
1:D:130:LYS:NZ	1:D:159:HIS:HD2	1.94	0.65
1:C:34:VAL:HG12	1:C:102:LEU:HD23	1.78	0.65
1:C:28:GLY:HA2	1:C:32:ASP:OD2	1.97	0.65
1:D:201:LYS:HE2	3:D:527:HOH:O	1.97	0.64
1:C:1:MET:HB3	1:C:2:PRO:HD2	1.78	0.64
1:D:3:ILE:HG22	1:D:355:ARG:HH22	1.61	0.64
1:B:10:PHE:CD1	1:B:36:VAL:HG21	2.32	0.64
1:C:208:VAL:HG13	1:C:209:LYS:HG2	1.80	0.63
1:B:8:ASN:HD22	1:B:37:VAL:HG22	1.63	0.63
1:C:305:ASN:HB3	3:C:1055:HOH:O	1.98	0.63
1:A:3:ILE:HG23	1:A:355:ARG:HH21	1.63	0.63
1:B:54:THR:HG23	1:C:204:ASP:OD1	1.99	0.63
1:B:190:MET:HE3	1:B:258:VAL:HG13	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166[A]:CYS:HB2	2:C:960:BRZ:O14	1.98	0.62
1:B:171:LEU:HD13	1:B:232:VAL:HG21	1.82	0.62
3:C:1018:HOH:O	1:D:187:THR:HG22	2.00	0.62
1:C:7:ILE:HB	1:C:36:VAL:HG12	1.82	0.62
1:D:4:LYS:NZ	1:D:32:ASP:OD1	2.34	0.61
1:D:13:ILE:HG22	1:D:110:SER:HB2	1.82	0.61
1:C:31:ILE:HD11	1:C:348:ARG:HD3	1.81	0.61
1:C:221:ILE:HD12	3:D:439:HOH:O	2.00	0.61
1:C:51:ARG:HG2	1:C:52:TYR:CE2	2.36	0.60
1:C:176:HIS:NE2	1:C:180:LYS:HD2	2.15	0.60
1:C:335:ASN:HB2	2:C:960:BRZ:HC92	1.82	0.60
1:A:37:VAL:HG23	1:A:90:ALA:HA	1.83	0.60
1:A:204:ASP:OD1	1:D:54:THR:HG23	2.01	0.60
1:B:129:ARG:HD2	3:B:535:HOH:O	2.01	0.60
1:A:318:ASN:HB3	3:A:585:HOH:O	2.02	0.59
1:C:51:ARG:HG3	3:C:1014:HOH:O	2.02	0.59
1:B:51:ARG:HD3	3:B:444:HOH:O	2.01	0.59
1:A:213:GLY:HA2	1:A:249:ARG:HH12	1.68	0.59
1:C:129:ARG:HD2	1:C:358:ARG:NH1	2.17	0.59
1:A:37:VAL:HG21	1:A:97:LEU:HD11	1.85	0.59
1:B:219:VAL:HG11	1:C:253:PRO:HG3	1.84	0.59
1:A:220:ASN:ND2	1:D:54:THR:HG21	2.11	0.59
1:A:147:GLY:H	1:A:150:HIS:HD2	1.48	0.59
1:C:15:ARG:O	1:C:19:GLN:HG3	2.03	0.59
1:C:26:LEU:HD13	1:C:348:ARG:HD3	1.84	0.59
1:C:154:ASN:ND2	1:C:157:GLU:H	1.99	0.59
1:C:166[A]:CYS:SG	2:C:960:BRZ:C17	2.91	0.59
1:D:50:MET:HE1	1:D:63:VAL:HG11	1.83	0.59
1:D:222:ILE:O	1:D:249:ARG:HD3	2.03	0.59
1:B:190:MET:O	1:B:190:MET:HG3	2.03	0.59
1:A:107:VAL:HG13	1:A:131:VAL:HG22	1.83	0.58
1:C:147:GLY:H	1:C:150:HIS:HD2	1.50	0.58
1:C:339:TYR:O	1:C:343:VAL:HG23	2.03	0.58
1:D:47:ALA:HA	1:D:50:MET:CE	2.32	0.58
1:B:200:GLN:O	1:B:201:LYS:HE3	2.04	0.58
1:B:11:GLY:O	1:B:15:ARG:HB2	2.03	0.58
1:D:259:ASP:OD1	1:D:328:LYS:NZ	2.35	0.58
1:A:67:LYS:HB2	1:A:72:VAL:HB	1.84	0.57
1:C:166[A]:CYS:H	2:C:960:BRZ:C17	2.11	0.57
1:C:129:ARG:HD2	1:C:358:ARG:HH12	1.68	0.57
1:C:348:ARG:O	1:C:351:ALA:N	2.36	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:GLY:O	1:B:141:ALA:CB	2.50	0.57
1:D:130:LYS:HZ3	1:D:159:HIS:HD2	1.51	0.57
1:A:19:GLN:OE1	1:A:50:MET:HG2	2.05	0.57
1:A:147:GLY:H	1:A:150:HIS:CD2	2.22	0.57
1:C:320:LEU:HG	1:D:244:THR:HG22	1.85	0.57
1:C:55:VAL:HG13	1:C:56:HIS:CD2	2.40	0.57
1:B:28:GLY:HA3	1:B:83:HIS:CE1	2.39	0.57
1:D:17:VAL:HG11	1:D:108:ILE:HD13	1.87	0.57
1:A:215:ARG:NH2	1:D:54:THR:HG22	2.20	0.57
1:B:98:PRO:HG2	1:B:102:LEU:HD22	1.86	0.57
1:C:166[A]:CYS:SG	1:C:335:ASN:O	2.62	0.56
1:A:224:SER:HB2	1:A:249:ARG:HH21	1.70	0.56
1:B:54:THR:HG22	1:C:215:ARG:HH21	1.70	0.56
1:C:110:SER:HA	3:C:983:HOH:O	2.06	0.56
1:C:72:VAL:O	1:C:73:ALA:HB2	2.06	0.56
1:B:176:HIS:HE1	3:B:471:HOH:O	1.88	0.56
1:D:171:LEU:HD22	1:D:175:VAL:HG23	1.87	0.56
1:C:3:ILE:HD11	1:C:355:ARG:HH21	1.70	0.56
1:C:6:GLY:HA3	1:C:99:TRP:CZ3	2.41	0.56
1:C:142:LYS:NZ	1:C:152:GLU:OE1	2.38	0.56
1:C:183:PHE:CE1	1:C:268:THR:HG21	2.41	0.56
1:B:8:ASN:ND2	1:B:37:VAL:HG22	2.21	0.55
1:C:186:GLN:HG2	1:C:187:THR:HG23	1.89	0.55
1:A:111:THR:HB	1:A:113:LEU:HD13	1.88	0.55
1:C:183:PHE:HD1	1:C:268:THR:HG21	1.70	0.55
1:C:298:SER:HB3	1:C:332:TRP:CZ3	2.42	0.55
1:B:129:ARG:HH21	1:B:358:ARG:NH2	2.05	0.55
1:D:131:VAL:HB	1:D:160:VAL:HG22	1.89	0.55
1:B:78:LEU:HD23	1:B:87:CYS:SG	2.47	0.55
1:C:98:PRO:HB2	1:C:101:LYS:HB2	1.89	0.55
1:D:224:SER:HB2	1:D:249:ARG:NH1	2.21	0.55
1:A:107:VAL:HG11	1:A:123:HIS:HB3	1.89	0.54
1:A:118:ALA:HA	1:A:121:GLU:CD	2.27	0.54
1:A:349:HIS:NE2	1:A:353:LYS:HE2	2.21	0.54
1:B:129:ARG:O	1:B:130:LYS:HD3	2.07	0.54
1:B:105:GLU:HB3	1:B:129:ARG:HD3	1.89	0.54
1:A:71:SER:O	1:A:73:ALA:N	2.40	0.54
1:C:3:ILE:CG1	1:C:355:ARG:HH21	2.20	0.54
1:C:166[A]:CYS:HG	2:C:960:BRZ:HC18	1.72	0.54
1:A:176:HIS:HD2	3:A:487:HOH:O	1.89	0.54
1:A:150:HIS:HE1	3:A:536:HOH:O	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:ARG:O	1:C:16:MET:HG3	2.08	0.54
1:C:108:ILE:HD11	1:C:347:VAL:HG21	1.90	0.54
1:C:166[B]:CYS:SG	2:C:960:BRZ:C18	2.95	0.54
1:A:115:THR:HG22	3:A:462:HOH:O	2.08	0.54
1:B:218:ALA:HB3	3:B:400:HOH:O	2.07	0.54
1:C:5:VAL:HG22	1:C:106:TYR:HB2	1.90	0.54
1:A:220:ASN:HD21	1:D:54:THR:CG2	2.15	0.53
1:B:3:ILE:HB	1:B:31:ILE:HD13	1.90	0.53
1:C:358:ARG:HB2	3:C:1103:HOH:O	2.07	0.53
1:B:21:LEU:HD13	1:B:26:LEU:HB2	1.89	0.53
1:B:130:LYS:NZ	1:B:155:PRO:O	2.41	0.53
2:C:960:BRZ:C18	2:C:960:BRZ:O14	2.56	0.53
1:C:121:GLU:O	1:C:124:LEU:HB2	2.09	0.53
2:C:960:BRZ:C19	2:C:960:BRZ:C8	2.85	0.53
1:D:190:MET:CE	1:D:258:VAL:HG22	2.38	0.53
1:C:155:PRO:HB3	1:C:354:ASP:CB	2.39	0.53
1:C:348:ARG:O	1:C:349:HIS:C	2.47	0.53
1:B:99:TRP:HA	1:B:99:TRP:CE3	2.43	0.53
1:C:207:SER:HB3	1:C:214:GLY:CA	2.39	0.53
1:B:54:THR:HG22	1:C:215:ARG:NH2	2.24	0.53
1:B:147:GLY:H	1:B:150:HIS:CD2	2.27	0.53
1:B:153:TYR:HD2	1:B:353:LYS:HD3	1.74	0.53
1:C:130:LYS:CD	1:C:159:HIS:HA	2.39	0.53
1:C:117:LYS:HB2	1:C:140:GLY:O	2.10	0.52
1:C:154:ASN:HB3	1:C:157:GLU:HB2	1.92	0.52
1:A:13:ILE:CG2	1:A:110:SER:HB2	2.38	0.52
1:D:8:ASN:HD22	1:D:37:VAL:HG22	1.73	0.52
1:A:226:THR:HB	3:A:557:HOH:O	2.09	0.52
1:C:132:VAL:HG22	1:C:350:MET:HE1	1.91	0.52
1:C:344:VAL:O	1:C:348:ARG:HG3	2.10	0.52
1:A:19:GLN:HG3	1:A:59:PHE:CE1	2.45	0.51
1:A:26:LEU:HD13	1:A:348:ARG:HD2	1.92	0.51
1:C:104:VAL:O	1:C:128:ALA:HA	2.09	0.51
1:A:13:ILE:HD12	1:A:13:ILE:O	2.10	0.51
1:A:171:LEU:HD13	1:A:232:VAL:HG21	1.93	0.51
1:B:151:HIS:HB2	3:B:414:HOH:O	2.10	0.51
1:C:22:CYS:O	1:C:23:GLU:C	2.49	0.51
1:D:105:GLU:OE1	1:D:129:ARG:NH2	2.43	0.51
1:C:61:TYR:CD2	1:C:81:ASN:HB2	2.42	0.51
1:D:21:LEU:HD11	1:D:31:ILE:HD13	1.93	0.51
1:A:26:LEU:HD21	1:A:348:ARG:NH2	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:GLU:CB	1:B:129:ARG:HD3	2.41	0.51
1:D:94:PRO:HA	1:D:97:LEU:HD22	1.92	0.51
1:A:239:THR:HA	1:A:242:LYS:HD2	1.93	0.51
1:C:166[A]:CYS:SG	1:C:339:TYR:HB2	2.52	0.50
1:A:3:ILE:HG12	3:A:617:HOH:O	2.10	0.50
1:A:305:ASN:HD22	1:A:306:ARG:N	2.09	0.50
1:D:50:MET:CE	1:D:63:VAL:HG11	2.41	0.50
1:C:321:PRO:O	1:C:322:LYS:HB2	2.10	0.50
1:C:89:LYS:HG2	1:C:90:ALA:H	1.77	0.50
1:A:176:HIS:HE1	3:A:430:HOH:O	1.95	0.50
1:C:28:GLY:N	1:C:31:ILE:O	2.44	0.50
1:C:239:THR:HA	1:C:242:LYS:HD2	1.93	0.50
1:D:354:ASP:O	1:D:358:ARG:HG3	2.12	0.50
1:C:166[A]:CYS:SG	1:C:339:TYR:CB	3.00	0.50
1:D:183:PHE:CD1	1:D:268:THR:HG21	2.47	0.50
1:A:91:GLN:HB2	1:A:97:LEU:HD22	1.94	0.49
1:C:21:LEU:HD11	1:C:31:ILE:HG21	1.94	0.49
1:B:13:ILE:HD11	3:B:443:HOH:O	2.10	0.49
1:C:146:MET:CE	1:C:346:LEU:HA	2.42	0.49
1:D:37:VAL:HB	1:D:88:VAL:HG22	1.94	0.49
1:B:349:HIS:NE2	1:B:353:LYS:HD2	2.27	0.49
1:D:50:MET:HE1	1:D:78:LEU:HG	1.94	0.49
1:D:268:THR:O	1:D:324:ARG:HA	2.12	0.49
1:B:124:LEU:HA	1:B:128:ALA:O	2.13	0.49
1:C:172:ALA:HB2	1:C:232:VAL:HG22	1.94	0.49
1:C:283:THR:OG1	1:C:284:TYR:N	2.38	0.49
1:C:342:ARG:HA	1:C:345:ASP:HB2	1.94	0.49
1:C:3:ILE:CD1	1:C:355:ARG:HH21	2.25	0.49
1:C:4:LYS:HD3	1:C:103:GLY:O	2.13	0.48
1:C:306:ARG:HD2	3:C:1086:HOH:O	2.13	0.48
1:A:196:TYR:CD2	1:A:251:PRO:HA	2.48	0.48
1:A:326:PHE:CE1	1:B:263:THR:HG23	2.48	0.48
1:B:1:MET:HB3	1:B:4:LYS:NZ	2.28	0.48
1:B:66:THR:HG22	1:B:67:LYS:N	2.20	0.48
1:C:154:ASN:ND2	1:C:157:GLU:HG3	2.28	0.48
1:D:91:GLN:HB2	1:D:97:LEU:HD13	1.95	0.48
1:A:253:PRO:HG3	3:A:481:HOH:O	2.12	0.48
1:B:12:ARG:HG2	1:B:16:MET:CE	2.44	0.48
1:D:146:MET:HB2	1:D:342:ARG:HD3	1.94	0.48
1:A:305:ASN:C	1:A:305:ASN:ND2	2.66	0.48
1:B:65:THR:HG22	1:B:78:LEU:HD13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:206:VAL:HG13	1:C:45:TYR:HE2	1.77	0.48
1:C:166[B]:CYS:H	2:C:960:BRZ:C17	2.14	0.47
1:C:355:ARG:HA	3:C:1058:HOH:O	2.14	0.47
1:D:218:ALA:HA	1:D:251:PRO:HB3	1.96	0.47
1:D:231:ALA:O	1:D:234:MET:HG2	2.14	0.47
1:D:355:ARG:NH1	3:D:482:HOH:O	2.45	0.47
1:B:89:LYS:NZ	1:B:90:ALA:O	2.34	0.47
1:D:233:GLY:O	1:D:240:GLN:HG3	2.14	0.47
1:B:176:HIS:HD2	3:B:402:HOH:O	1.97	0.47
1:B:210:ASP:OD2	1:B:213:GLY:HA3	2.15	0.47
1:B:278:LYS:HE2	1:B:291:TYR:CE2	2.49	0.47
1:C:146:MET:HE3	1:C:346:LEU:CB	2.44	0.47
1:C:346:LEU:O	1:C:349:HIS:HB3	2.14	0.47
1:A:254:ASP:OD2	1:A:334:ASP:OD1	2.32	0.46
1:B:154:ASN:HD22	1:B:154:ASN:HA	1.63	0.46
1:C:42:ASP:HA	3:C:1026:HOH:O	2.14	0.46
1:D:10:PHE:CE1	1:D:36:VAL:HG11	2.50	0.46
1:A:72:VAL:O	1:A:73:ALA:C	2.54	0.46
1:C:149:ASN:ND2	1:C:235:VAL:HG22	2.30	0.46
1:C:351:ALA:O	1:C:355:ARG:HG3	2.16	0.46
1:A:190:MET:HG2	1:A:191:THR:N	2.29	0.46
1:B:61:TYR:CD1	1:B:81:ASN:HB2	2.51	0.46
1:B:69:SER:O	1:B:72:VAL:HG23	2.15	0.46
1:D:173:PRO:O	1:D:177:VAL:HG23	2.15	0.46
3:A:481:HOH:O	1:D:219:VAL:HG11	2.16	0.46
1:D:358:ARG:O	1:D:359:LEU:HD23	2.15	0.46
1:B:270:ILE:HD11	1:B:315:THR:CG2	2.46	0.46
1:D:15:ARG:O	1:D:19:GLN:HG3	2.15	0.46
1:D:21:LEU:HD11	1:D:31:ILE:CD1	2.45	0.46
1:B:270:ILE:HD11	1:B:315:THR:HG22	1.98	0.46
1:B:129:ARG:HE	1:B:358:ARG:NH2	2.14	0.46
1:C:136:PRO:HG3	1:C:165:SER:HB3	1.97	0.46
1:D:196:TYR:CD2	1:D:251:PRO:HA	2.52	0.45
1:D:224:SER:HB2	1:D:249:ARG:CZ	2.46	0.45
1:A:254:ASP:O	1:A:255:VAL:HB	2.16	0.45
1:C:70:PRO:O	1:C:71:SER:CB	2.57	0.45
1:A:118:ALA:HA	1:A:121:GLU:OE1	2.17	0.45
1:C:140:GLY:O	1:C:141:ALA:HB2	2.17	0.45
1:A:268:THR:OG1	1:A:272:GLU:HG3	2.15	0.45
1:C:89:LYS:HG2	1:C:90:ALA:N	2.31	0.45
1:C:154:ASN:ND2	1:C:157:GLU:N	2.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:196:TYR:HA	1:D:200:GLN:NE2	2.32	0.45
1:A:151:HIS:HD2	3:A:452:HOH:O	1.98	0.45
1:C:53:ASP:HB2	3:C:986:HOH:O	2.17	0.45
1:C:166[A]:CYS:SG	2:C:960:BRZ:HC71	2.56	0.45
1:C:218:ALA:HB3	3:C:1027:HOH:O	2.17	0.45
1:B:180:LYS:HD3	1:B:284:TYR:CE2	2.52	0.44
1:D:32:ASP:OD2	1:D:83:HIS:HE1	2.01	0.44
1:D:67:LYS:HE3	1:D:73:ALA:O	2.18	0.44
1:B:121:GLU:O	1:B:122:GLY:C	2.55	0.44
1:B:12:ARG:HD3	3:B:539:HOH:O	2.16	0.44
1:B:212:ARG:NH1	1:B:223:PRO:HG2	2.32	0.44
1:D:356:SER:HB2	3:D:627:HOH:O	2.16	0.44
1:C:8:ASN:HD22	1:C:37:VAL:CG1	2.25	0.44
1:C:137:ALA:HB2	1:C:162:SER:HB2	1.98	0.44
1:C:37:VAL:HG21	1:C:97:LEU:HD11	2.00	0.44
1:D:98:PRO:O	1:D:102:LEU:HD22	2.18	0.44
1:A:58:LYS:HE3	3:C:977:HOH:O	2.18	0.44
1:D:147:GLY:H	1:D:150:HIS:CD2	2.36	0.44
1:B:67:LYS:NZ	1:B:67:LYS:HB3	2.33	0.44
1:C:298:SER:HB3	1:C:332:TRP:HZ3	1.83	0.44
2:C:960:BRZ:HC32	2:C:960:BRZ:HC11	1.70	0.44
1:A:298:SER:HB3	1:A:332:TRP:HZ3	1.83	0.43
1:C:1:MET:HE1	1:C:30:GLU:HG3	2.00	0.43
1:C:129:ARG:HD2	1:C:358:ARG:NH2	2.33	0.43
1:D:190:MET:HG3	1:D:258:VAL:HG13	1.99	0.43
1:C:155:PRO:HB3	1:C:354:ASP:HB2	1.99	0.43
1:A:19:GLN:HE22	1:A:50:MET:HA	1.83	0.43
1:A:305:ASN:ND2	1:A:306:ARG:HD3	2.33	0.43
1:B:76:ASP:HA	3:B:521:HOH:O	2.17	0.43
1:A:224:SER:CB	1:A:249:ARG:HE	2.32	0.43
1:D:55:VAL:HG13	1:D:56:HIS:CD2	2.54	0.43
1:D:169:ASN:O	1:D:307:SER:HB3	2.19	0.43
1:D:177:VAL:HG11	1:D:277:LEU:HD23	2.00	0.43
1:B:69:SER:OG	1:B:71:SER:HB3	2.19	0.43
1:C:8:ASN:ND2	1:C:37:VAL:HG13	2.27	0.43
1:C:55:VAL:HG21	1:C:254:ASP:CB	2.49	0.43
1:C:86:LEU:CD2	1:C:88:VAL:HG12	2.48	0.43
1:C:135:ALA:HB1	1:C:136:PRO:CD	2.49	0.43
1:C:166[A]:CYS:SG	2:C:960:BRZ:C15	3.06	0.43
1:A:224:SER:HB2	1:A:249:ARG:HE	1.82	0.43
1:B:99:TRP:HA	1:B:99:TRP:HE3	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:171:LEU:HD13	1:C:232:VAL:HG21	2.01	0.43
1:D:56:HIS:NE2	1:D:336:GLU:OE1	2.51	0.43
1:C:130:LYS:HD3	1:C:159:HIS:HA	2.00	0.43
1:A:171:LEU:HD22	1:A:175:VAL:HG23	2.01	0.43
1:C:99:TRP:HE3	1:C:104:VAL:HB	1.84	0.43
1:C:98:PRO:HG2	1:C:102:LEU:HD13	2.01	0.42
1:C:129:ARG:HD2	1:C:358:ARG:CZ	2.49	0.42
1:B:299:ALA:CB	1:D:54:THR:HB	2.49	0.42
1:D:254:ASP:O	1:D:255:VAL:HB	2.19	0.42
1:A:218:ALA:CA	1:A:251:PRO:HB3	2.48	0.42
1:B:17:VAL:HG11	1:B:108:ILE:HD13	2.02	0.42
1:C:29:THR:OG1	1:C:30:GLU:N	2.47	0.42
1:C:63:VAL:HG22	1:C:80:VAL:HG22	2.01	0.42
1:C:207:SER:HB3	1:C:214:GLY:HA3	2.01	0.42
1:D:171:LEU:HD13	1:D:232:VAL:HG21	2.02	0.42
1:C:151:HIS:HD2	1:C:353:LYS:NZ	2.17	0.42
1:C:282:LYS:O	1:C:286:LYS:HD3	2.19	0.42
1:A:91:GLN:HB2	1:A:97:LEU:CD2	2.49	0.42
1:B:54:THR:CG2	1:C:215:ARG:HH21	2.31	0.42
1:C:3:ILE:HG13	1:C:355:ARG:HH21	1.84	0.42
1:C:107:VAL:HG11	1:C:123:HIS:HB3	2.02	0.42
1:A:201:LYS:HA	1:A:201:LYS:HD3	1.92	0.42
1:C:28:GLY:HA3	1:C:83:HIS:CE1	2.54	0.42
1:C:142:LYS:HG3	1:C:158:HIS:NE2	2.34	0.42
1:C:319:ASN:HB3	3:C:1096:HOH:O	2.18	0.42
1:D:183:PHE:HD1	1:D:268:THR:HG21	1.84	0.42
1:C:268:THR:HG22	1:C:272:GLU:OE1	2.20	0.42
1:D:320:LEU:HA	1:D:321:PRO:HD3	1.84	0.42
1:B:4:LYS:HA	1:B:4:LYS:HD2	1.94	0.42
1:A:189:LEU:HG	1:B:326:PHE:HE2	1.85	0.42
1:B:1:MET:HA	1:B:2:PRO:HD2	1.91	0.42
1:D:313:LYS:HD2	3:D:638:HOH:O	2.18	0.42
1:B:105:GLU:OE1	1:B:129:ARG:CZ	2.68	0.41
1:C:67:LYS:HG2	3:C:1120:HOH:O	2.19	0.41
1:C:196:TYR:HA	1:C:200:GLN:NE2	2.34	0.41
1:C:146:MET:HB2	1:C:342:ARG:HD3	2.01	0.41
1:C:105:GLU:OE1	1:C:129:ARG:NH2	2.54	0.41
1:C:166[A]:CYS:SG	1:C:339:TYR:CG	3.13	0.41
1:B:12:ARG:NE	1:B:336:GLU:OE2	2.50	0.41
1:B:171:LEU:HD22	1:B:175:VAL:HG23	2.02	0.41
1:C:6:GLY:HA3	1:C:99:TRP:HZ3	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:15:ARG:HG3	1:D:15:ARG:HH11	1.86	0.41
1:D:130:LYS:HZ2	1:D:159:HIS:HD2	1.68	0.41
1:D:199:THR:HA	3:D:518:HOH:O	2.19	0.41
1:A:196:TYR:HD2	1:A:251:PRO:HA	1.85	0.41
1:C:209:LYS:HG2	1:C:209:LYS:H	1.57	0.41
1:D:209:LYS:HE2	1:D:209:LYS:HB3	1.89	0.41
1:B:129:ARG:NH2	1:B:358:ARG:HH21	2.15	0.41
1:C:58:LYS:HB2	1:C:60:LYS:NZ	2.36	0.41
1:C:107:VAL:HG21	1:C:123:HIS:ND1	2.36	0.41
1:A:213:GLY:HA2	1:A:249:ARG:NH1	2.34	0.41
1:C:107:VAL:CG1	1:C:131:VAL:HG22	2.37	0.41
1:D:222:ILE:HB	1:D:249:ARG:HB2	2.02	0.41
1:A:121:GLU:O	1:A:124:LEU:HB2	2.20	0.41
1:A:40:ASN:HD21	1:A:42:ASP:H	1.65	0.41
1:B:15:ARG:O	1:B:19:GLN:HG3	2.20	0.41
1:B:30:GLU:OE2	1:B:348:ARG:NH1	2.53	0.41
1:B:94:PRO:HA	1:B:97:LEU:CD2	2.51	0.41
1:C:1:MET:HB2	1:C:29:THR:O	2.21	0.41
1:C:25:GLY:HA2	3:C:1110:HOH:O	2.21	0.41
1:D:154:ASN:ND2	1:D:157:GLU:OE1	2.54	0.41
1:C:13:ILE:HA	1:C:13:ILE:HD13	1.78	0.41
1:C:99:TRP:O	1:C:103:GLY:N	2.53	0.41
1:C:105:GLU:HG3	1:C:106:TYR:H	1.87	0.41
1:C:286:LYS:HE2	1:C:286:LYS:HB3	1.78	0.41
2:C:960:BRZ:O14	2:C:960:BRZ:C19	2.69	0.41
1:C:60:LYS:HD3	1:C:60:LYS:HA	1.96	0.40
1:C:75:ASP:OD1	1:C:75:ASP:N	2.54	0.40
1:C:115:THR:HB	3:C:1075:HOH:O	2.21	0.40
1:D:315:THR:HG23	1:D:328:LYS:O	2.21	0.40
1:A:209:LYS:HD2	1:A:209:LYS:O	2.21	0.40
1:A:298:SER:HB3	1:A:332:TRP:CZ3	2.57	0.40
1:B:63:VAL:HG13	1:B:80:VAL:HG22	2.03	0.40
1:C:94:PRO:O	1:C:97:LEU:HD23	2.21	0.40
1:C:135:ALA:HB1	1:C:136:PRO:HD2	2.03	0.40
1:D:150:HIS:HE1	3:D:587:HOH:O	2.04	0.40
1:B:1:MET:HB3	1:B:4:LYS:HZ3	1.87	0.40
1:C:65:THR:HA	1:C:77:THR:O	2.21	0.40
1:C:86:LEU:HD23	1:C:88:VAL:HG12	2.04	0.40
1:C:64:THR:OG1	1:C:79:VAL:HB	2.22	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	A	357/359 (99%)	346 (97%)	8 (2%)	3 (1%)	19 9
1	B	357/359 (99%)	336 (94%)	18 (5%)	3 (1%)	19 9
1	C	358/359 (100%)	320 (89%)	24 (7%)	14 (4%)	3 0
1	D	357/359 (99%)	340 (95%)	14 (4%)	3 (1%)	19 9
All	All	1429/1436 (100%)	1342 (94%)	64 (4%)	23 (2%)	9 2

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	72	VAL
1	C	3	ILE
1	C	73	ALA
1	C	141	ALA
1	A	255	VAL
1	B	141	ALA
1	B	255	VAL
1	C	29	THR
1	C	74	LYS
1	C	208	VAL
1	C	255	VAL
1	C	357	ALA
1	D	73	ALA
1	D	255	VAL
1	B	2	PRO
1	C	71	SER
1	C	151	HIS
1	C	349	HIS
1	A	73	ALA
1	C	23	GLU
1	C	76	ASP
1	C	2	PRO
1	D	72	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	A	296/296 (100%)	277 (94%)	19 (6%)	17	6
1	B	296/296 (100%)	273 (92%)	23 (8%)	12	3
1	C	297/296 (100%)	273 (92%)	24 (8%)	11	3
1	D	296/296 (100%)	270 (91%)	26 (9%)	10	2
All	All	1185/1184 (100%)	1093 (92%)	92 (8%)	12	3

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	MET
1	A	19	GLN
1	A	58	LYS
1	A	66	THR
1	A	67	LYS
1	A	74	LYS
1	A	78	LEU
1	A	84	ARG
1	A	102	LEU
1	A	107	VAL
1	A	115	THR
1	A	124	LEU
1	A	171	LEU
1	A	240	GLN
1	A	266	ARG
1	A	305	ASN
1	A	306	ARG
1	A	333	TYR
1	A	335	ASN
1	B	15	ARG
1	B	21	LEU
1	B	37	VAL
1	B	55	VAL
1	B	64	THR

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Mol	Chain	Res	Type
1	B	67	LYS
1	B	74	LYS
1	B	75	ASP
1	B	97	LEU
1	B	102	LEU
1	B	115	THR
1	B	124	LEU
1	B	129	ARG
1	B	171	LEU
1	B	190	MET
1	B	194	HIS
1	B	196	TYR
1	B	201	LYS
1	B	209	LYS
1	B	286	LYS
1	B	293	ASP
1	B	305	ASN
1	B	306	ARG
1	C	13	ILE
1	C	15	ARG
1	C	24	ASP
1	C	32	ASP
1	C	37	VAL
1	C	65	THR
1	C	67	LYS
1	C	75	ASP
1	C	107	VAL
1	C	113	LEU
1	C	124	LEU
1	C	129	ARG
1	C	142	LYS
1	C	156	SER
1	C	171	LEU
1	C	190	MET
1	C	202	THR
1	C	209	LYS
1	C	243	LEU
1	C	249	ARG
1	C	268	THR
1	C	306	ARG
1	C	333	TYR
1	C	352	SER

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Mol	Chain	Res	Type
1	D	3	ILE
1	D	13	ILE
1	D	40	ASN
1	D	54	THR
1	D	55	VAL
1	D	66	THR
1	D	69	SER
1	D	78	LEU
1	D	97	LEU
1	D	102	LEU
1	D	105	GLU
1	D	113	LEU
1	D	115	THR
1	D	157	GLU
1	D	171	LEU
1	D	196	TYR
1	D	237	PRO
1	D	240	GLN
1	D	243	LEU
1	D	249	ARG
1	D	268	THR
1	D	279	ARG
1	D	306	ARG
1	D	322	LYS
1	D	333	TYR
1	D	352	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
1	A	40	ASN
1	A	49	GLN
1	A	150	HIS
1	A	151	HIS
1	A	159	HIS
1	A	176	HIS
1	A	200	GLN
1	A	305	ASN
1	B	8	ASN
1	B	49	GLN
1	B	83	HIS

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Mol	Chain	Res	Type
1	B	150	HIS
1	B	154	ASN
1	B	176	HIS
1	B	200	GLN
1	B	305	ASN
1	C	8	ASN
1	C	83	HIS
1	C	91	GLN
1	C	150	HIS
1	C	151	HIS
1	C	154	ASN
1	C	200	GLN
1	C	349	HIS
1	D	8	ASN
1	D	150	HIS
1	D	159	HIS
1	D	176	HIS
1	D	200	GLN
1	D	341	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)

1 ligand is modelled in this entry.

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	$\#\|Z\| > 2$
2	BRZ	C	960	1	22,25,25	2.04	6 (27%)	33,40,40	3.87	21 (63%)

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
2	BRZ	C	960	1	-	8/15/23/23	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	960	BRZ	C9-C8	4.74	1.55	1.40
2	C	960	BRZ	C10-C1	4.17	1.51	1.42
2	C	960	BRZ	O7-C6	3.60	1.42	1.36
2	C	960	BRZ	C13-C12	2.50	1.56	1.54
2	C	960	BRZ	C5-C4	2.33	1.40	1.36
2	C	960	BRZ	C10-C9	-2.21	1.34	1.37

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	960	BRZ	O11-C12-C20	11.30	120.08	108.38
2	C	960	BRZ	C5-C6-C1	-6.92	115.63	123.10
2	C	960	BRZ	O21-C20-C12	6.40	123.30	107.89
2	C	960	BRZ	C10-C9-C15	-5.49	115.53	121.75
2	C	960	BRZ	C23-C20-C12	-5.46	100.77	110.61
2	C	960	BRZ	C3-C2-C1	-5.01	112.39	121.28
2	C	960	BRZ	C9-C15-C18	-4.95	99.62	110.48
2	C	960	BRZ	C17-C15-C18	4.49	129.36	107.99
2	C	960	BRZ	O11-C12-C13	4.22	108.67	106.25
2	C	960	BRZ	C10-C9-C8	4.09	130.40	117.27
2	C	960	BRZ	C15-C9-C8	-3.90	114.04	121.91
2	C	960	BRZ	C15-C18-C19	3.83	139.47	126.70
2	C	960	BRZ	O7-C6-C5	3.71	120.43	116.03
2	C	960	BRZ	C10-C1-C2	-2.95	116.36	122.16
2	C	960	BRZ	C4-C5-C6	-2.82	116.74	120.06
2	C	960	BRZ	O7-C6-C1	2.79	123.94	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	960	BRZ	C23-C20-C22	-2.79	106.56	110.56
2	C	960	BRZ	C13-C12-C20	2.49	119.47	115.94
2	C	960	BRZ	C17-C15-C9	-2.26	104.14	111.48
2	C	960	BRZ	C9-C10-C1	-2.19	118.05	121.92
2	C	960	BRZ	C13-C3-C4	2.04	110.26	108.05

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	960	BRZ	O11-C12-C20-O21
2	C	960	BRZ	O11-C12-C20-C22
2	C	960	BRZ	O11-C12-C20-C23
2	C	960	BRZ	C13-C12-C20-O21
2	C	960	BRZ	C13-C12-C20-C22
2	C	960	BRZ	C13-C12-C20-C23
2	C	960	BRZ	C17-C15-C9-C8
2	C	960	BRZ	C17-C15-C18-C19

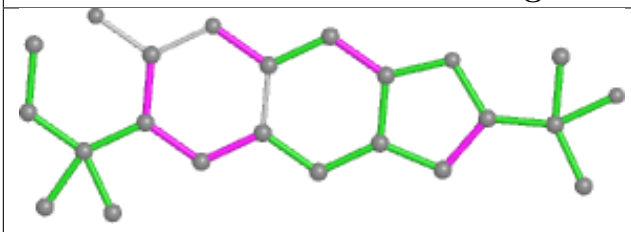
There are no ring outliers.

1 monomer is involved in 17 short contacts:

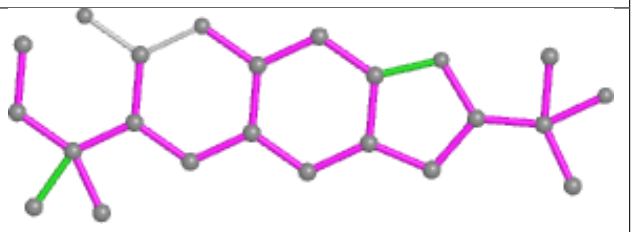
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	960	BRZ	17	0

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.

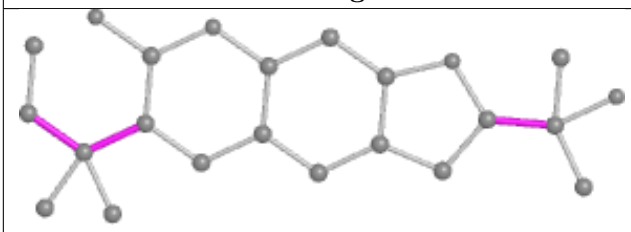
Ligand BRZ C 960



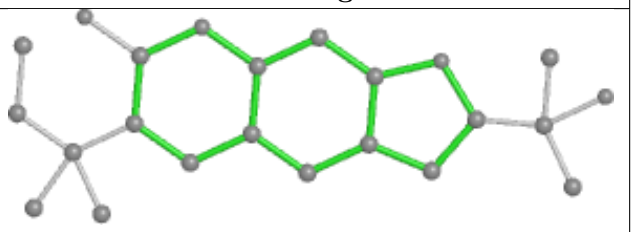
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	359/359 (100%)	-0.14	8 (2%) 62 70	13, 23, 41, 65	0
1	B	359/359 (100%)	0.22	18 (5%) 28 39	12, 28, 51, 64	0
1	C	359/359 (100%)	1.01	64 (17%) 1 1	16, 38, 81, 104	0
1	D	359/359 (100%)	-0.06	6 (1%) 70 77	14, 24, 41, 55	0
All	All	1436/1436 (100%)	0.26	96 (6%) 17 26	12, 27, 63, 104	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	12.4
1	C	358	ARG	10.9
1	C	357	ALA	9.0
1	C	359	LEU	8.2
1	C	72	VAL	8.0
1	C	102	LEU	7.8
1	C	71	SER	7.3
1	C	70	PRO	6.8
1	C	123	HIS	6.6
1	C	3	ILE	6.4
1	C	95	ALA	6.4
1	A	72	VAL	6.3
1	C	124	LEU	6.2
1	D	359	LEU	5.8
1	A	71	SER	5.8
1	C	2	PRO	5.8
1	C	68	SER	5.5
1	A	1	MET	5.5
1	C	129	ARG	5.1
1	C	39	MET	4.9
1	C	128	ALA	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	83	HIS	4.5
1	C	80	VAL	4.5
1	C	93	ASN	4.3
1	B	90	ALA	4.3
1	C	99	TRP	4.1
1	B	1	MET	4.1
1	C	69	SER	4.1
1	D	1	MET	4.0
1	B	206	VAL	4.0
1	C	92	ARG	3.9
1	C	100	GLY	3.9
1	B	72	VAL	3.9
1	B	71	SER	3.8
1	C	94	PRO	3.8
1	C	78	LEU	3.7
1	C	131	VAL	3.7
1	C	113	LEU	3.6
1	C	66	THR	3.6
1	A	73	ALA	3.6
1	B	69	SER	3.5
1	C	33	VAL	3.5
1	D	73	ALA	3.5
1	A	70	PRO	3.5
1	B	70	PRO	3.4
1	C	91	GLN	3.3
1	B	359	LEU	3.2
1	C	74	LYS	3.1
1	C	97	LEU	3.1
1	C	103	GLY	3.1
1	B	156	SER	3.1
1	B	93	ASN	3.1
1	C	127	GLY	3.1
1	B	125	ARG	2.9
1	C	138	SER	2.9
1	C	81	ASN	2.9
1	B	202	THR	2.8
1	C	35	ALA	2.8
1	C	157	GLU	2.8
1	B	358	ARG	2.7
1	B	83	HIS	2.7
1	D	72	VAL	2.6
1	B	39	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	27	LEU	2.5
1	D	199	THR	2.5
1	C	61	TYR	2.4
1	C	206	VAL	2.4
1	B	95	ALA	2.3
1	C	25	GLY	2.3
1	A	2	PRO	2.3
1	C	67	LYS	2.3
1	C	234	MET	2.2
1	B	198	ALA	2.2
1	C	24	ASP	2.2
1	C	106	TYR	2.2
1	C	31	ILE	2.2
1	C	77	THR	2.2
1	C	140	GLY	2.2
1	C	34	VAL	2.2
1	A	69	SER	2.2
1	C	217	ALA	2.2
1	B	99	TRP	2.1
1	C	36	VAL	2.1
1	C	28	GLY	2.1
1	C	79	VAL	2.1
1	C	104	VAL	2.1
1	C	84	ARG	2.1
1	C	347	VAL	2.1
1	C	86	LEU	2.1
1	C	75	ASP	2.1
1	C	4	LYS	2.1
1	D	74	LYS	2.1
1	C	40	ASN	2.0
1	C	32	ASP	2.0
1	C	26	LEU	2.0
1	A	74	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands

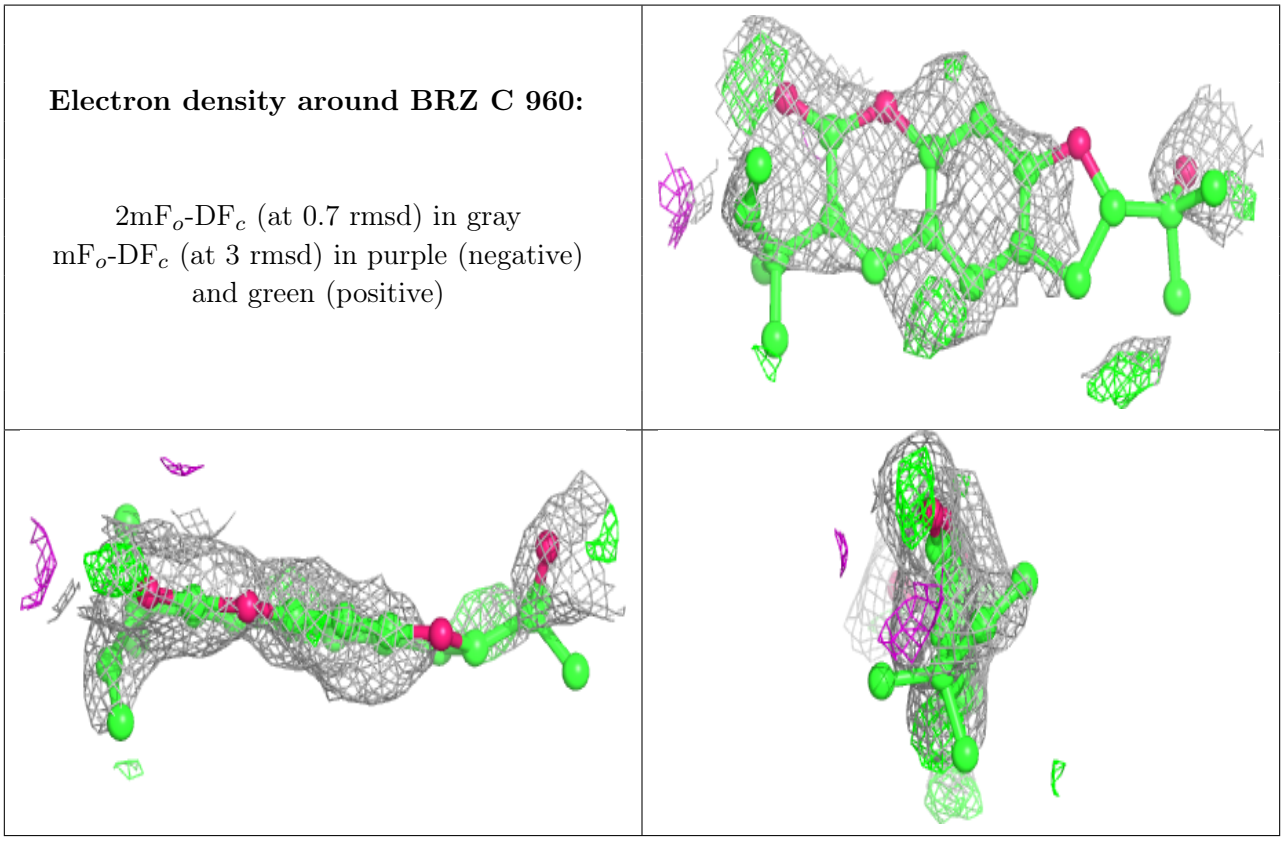
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	BRZ	C	960	23/23	0.62	0.35	68,70,71,71	23

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around BRZ C 960:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



6.5 Other polymers

There are no such residues in this entry.