



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 12:42 PM GMT

PDB ID : 1D1B  
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)  
COMPLEXED WITH O,P-DINITROPHENYL AMINOPROPYLDIPHOS  
PHATEBERYLLIUM TRIFLUORIDE.  
Authors : Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Pate, E.; Yount, R.G.; Rayment, I.  
Deposited on : 1999-09-15  
Resolution : 2.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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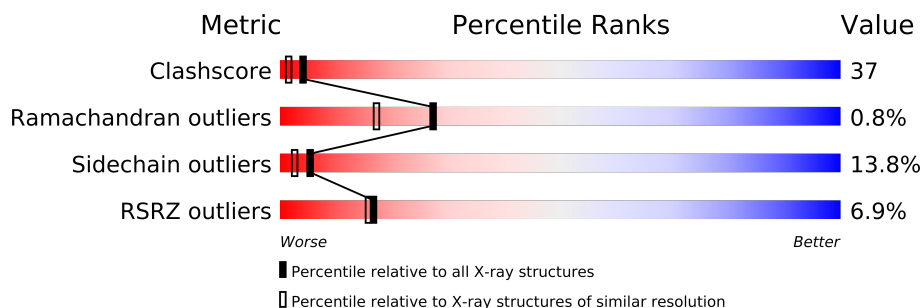
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance


The reported resolution of this entry is 2.00 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	79885	6188 (2.00-2.00)
Ramachandran outliers	78287	6102 (2.00-2.00)
Sidechain outliers	78261	6100 (2.00-2.00)
RSRZ outliers	66119	4890 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	761	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6374 atoms, of which 0 are hydrogen and 0 are deuterium.

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 MYOSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	736	Total	C	N	O	S	0	0	0
			5803	3689	997	1101	16			

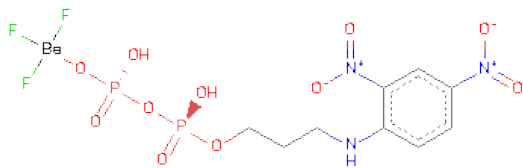
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	CYS	TYR	SEE REMARK 999	UNP P08799
A	760	PRO	GLN	ENGINEERED	UNP P08799
A	761	ASN	ARG	ENGINEERED	UNP P08799

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is O,P-DINITROPHENYL AMINOPROPYLDIPHOSPHATEBERYLLIUM TRIFLUORIDE (three-letter code: DAQ) (formula: C<sub>9</sub>H<sub>12</sub>BeF<sub>3</sub>N<sub>3</sub>O<sub>11</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Be	C	F	N	O	P		
3	A	1	29	1	9	3	3	11	2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	541	Total	O	0	0
			541	541		



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.88Å 180.46Å 54.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 28.84 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (25.00-2.00) 97.1 (28.84-2.00)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.32 (at 2.00Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.204 , (Not available) 0.207 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 111.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67444 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	6374	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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: MG, DAQ

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	1.84	43/5914 (0.7%)	1.70	97/7992 (1.2%)

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

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ASP	CG-OD2	80.26	3.10	1.25
1	A	40	ASP	CB-CG	53.89	2.65	1.51
1	A	40	ASP	CG-OD1	50.48	2.41	1.25
1	A	657	ILE	CG1-CD1	21.70	3.00	1.50
1	A	99	GLU	CD-OE2	8.03	1.34	1.25
1	A	459	GLU	CD-OE2	7.70	1.34	1.25
1	A	567	GLU	CD-OE2	7.33	1.33	1.25
1	A	187	GLU	CD-OE2	7.31	1.33	1.25
1	A	273	GLU	CD-OE2	7.28	1.33	1.25
1	A	55	GLU	CD-OE2	6.87	1.33	1.25
1	A	93	GLU	CD-OE2	6.78	1.33	1.25
1	A	89	GLU	CD-OE2	6.75	1.33	1.25
1	A	636	GLU	CD-OE2	6.56	1.32	1.25
1	A	180	GLU	CD-OE2	6.52	1.32	1.25
1	A	646	GLU	CD-OE2	6.49	1.32	1.25
1	A	755	GLU	CD-OE2	6.41	1.32	1.25
1	A	492	GLU	CD-OE2	6.40	1.32	1.25
1	A	444	GLU	CD-OE2	6.33	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	GLU	CD-OE2	6.29	1.32	1.25
1	A	683	GLU	CD-OE2	6.18	1.32	1.25
1	A	412	GLU	CD-OE2	6.15	1.32	1.25
1	A	559	GLU	CD-OE2	6.09	1.32	1.25
1	A	531	GLU	CD-OE2	6.05	1.32	1.25
1	A	390	GLU	CD-OE2	5.98	1.32	1.25
1	A	365	GLU	CD-OE2	5.96	1.32	1.25
1	A	668	GLU	CD-OE2	5.89	1.32	1.25
1	A	490	GLU	CD-OE2	5.87	1.32	1.25
1	A	302	GLU	CD-OE2	5.82	1.32	1.25
1	A	476	GLU	CD-OE2	5.80	1.32	1.25
1	A	212	GLU	CD-OE2	5.78	1.32	1.25
1	A	360	GLU	CD-OE2	5.74	1.31	1.25
1	A	756	GLU	CD-OE2	5.70	1.31	1.25
1	A	48	GLU	CD-OE2	5.67	1.31	1.25
1	A	339	GLU	CD-OE2	5.66	1.31	1.25
1	A	150	GLU	CD-OE2	5.61	1.31	1.25
1	A	322	GLU	CD-OE2	5.51	1.31	1.25
1	A	89	GLU	CD-OE1	-5.46	1.19	1.25
1	A	51	GLU	CD-OE2	5.38	1.31	1.25
1	A	340	GLU	CD-OE2	5.34	1.31	1.25
1	A	138	GLU	CD-OE2	5.27	1.31	1.25
1	A	597	GLU	CD-OE2	5.13	1.31	1.25
1	A	560	GLU	CD-OE2	5.10	1.31	1.25
1	A	244	GLU	CD-OE2	5.09	1.31	1.25

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	40	ASP	CB-CG-OD1	-51.79	71.69	118.30
1	A	40	ASP	CB-CG-OD2	-21.04	99.37	118.30
1	A	657	ILE	CB-CG1-CD1	-19.29	59.90	113.90
1	A	238	ARG	NE-CZ-NH1	14.89	127.74	120.30
1	A	238	ARG	NE-CZ-NH2	-14.51	113.05	120.30
1	A	202	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	A	45	ASP	CB-CG-OD2	-10.20	109.12	118.30
1	A	713	PRO	N-CA-CB	10.02	115.32	103.30
1	A	562	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	40	ASP	CA-CB-CG	8.85	132.87	113.40
1	A	70	ARG	NE-CZ-NH1	8.81	124.71	120.30
1	A	45	ASP	CB-CG-OD1	8.68	126.12	118.30
1	A	530	ASP	CB-CG-OD1	8.44	125.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	428	ARG	NE-CZ-NH2	-8.27	116.16	120.30
1	A	689	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	605	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	A	620	ARG	NE-CZ-NH1	8.05	124.33	120.30
1	A	605	ASP	CB-CG-OD1	7.78	125.30	118.30
1	A	686	ARG	NE-CZ-NH1	7.75	124.18	120.30
1	A	75	ASP	CB-CG-OD2	-7.70	111.37	118.30
1	A	595	ASP	CB-CG-OD1	7.64	125.18	118.30
1	A	160	ASP	CB-CG-OD2	-7.58	111.48	118.30
1	A	147	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	A	590	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	454	ASP	CB-CG-OD1	7.39	124.95	118.30
1	A	44	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	A	669	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	A	147	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	A	332	ASP	CB-CG-OD2	-7.05	111.96	118.30
1	A	583	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	A	590	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	371	ASP	CB-CG-OD1	6.97	124.58	118.30
1	A	583	ASP	CB-CG-OD1	6.97	124.57	118.30
1	A	704	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	520	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	A	419	ASP	CB-CG-OD2	-6.70	112.27	118.30
1	A	571	THR	CA-CB-CG2	-6.66	103.08	112.40
1	A	614	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	A	669	ASP	CB-CG-OD1	6.56	124.20	118.30
1	A	202	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	419	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	530	ASP	CB-CG-OD2	-6.45	112.49	118.30
1	A	148	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	A	677	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	602	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	72	VAL	CB-CA-C	-6.29	99.44	111.40
1	A	86	ASP	CB-CG-OD1	6.26	123.94	118.30
1	A	686	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	A	314	ASP	CB-CG-OD2	-6.26	112.67	118.30
1	A	160	ASP	CB-CG-OD1	6.24	123.91	118.30
1	A	562	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	31	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	538	ALA	N-CA-CB	6.17	118.73	110.10
1	A	175	LEU	CB-CG-CD1	-6.09	100.65	111.00
1	A	21	ASP	CB-CG-OD2	-6.08	112.83	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	168	ASP	CB-CG-OD1	6.07	123.76	118.30
1	A	674	ASP	CB-CG-OD2	-6.07	112.84	118.30
1	A	168	ASP	CB-CG-OD2	-6.05	112.86	118.30
1	A	505	ASP	CB-CG-OD1	6.05	123.74	118.30
1	A	733	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	A	518	ASP	CB-CG-OD1	6.00	123.70	118.30
1	A	447	ALA	N-CA-CB	5.97	118.45	110.10
1	A	23	ASP	CB-CG-OD2	-5.96	112.94	118.30
1	A	371	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	A	33	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	A	700	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	595	ASP	CB-CG-OD2	-5.83	113.06	118.30
1	A	320	ASP	CB-CG-OD1	5.77	123.49	118.30
1	A	602	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	31	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	535	PHE	CA-CB-CG	-5.66	100.32	113.90
1	A	151	VAL	CA-CB-CG1	5.65	119.37	110.90
1	A	494	TYR	N-CA-CB	5.65	120.77	110.60
1	A	169	ASP	CB-CG-OD1	5.63	123.37	118.30
1	A	238	ARG	CD-NE-CZ	5.58	131.42	123.60
1	A	109	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	A	542	THR	N-CA-CB	-5.51	99.83	110.30
1	A	505	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	6	ASP	CB-CG-OD1	5.48	123.23	118.30
1	A	724	ASP	CB-CG-OD1	5.47	123.22	118.30
1	A	141	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	76	ASP	CB-CG-OD1	5.42	123.18	118.30
1	A	129	PHE	N-CA-CB	5.42	120.35	110.60
1	A	332	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	66	ASP	CB-CG-OD2	-5.36	113.47	118.30
1	A	700	ASP	CB-CG-OD1	5.29	123.06	118.30
1	A	715	ASP	CB-CG-OD1	5.28	123.05	118.30
1	A	141	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	518	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	515	ASP	CB-CG-OD1	5.22	122.99	118.30
1	A	320	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	440	VAL	CA-CB-CG2	-5.12	103.21	110.90
1	A	113	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	21	ASP	CB-CG-OD1	5.06	122.86	118.30
1	A	620	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	75	ASP	CB-CA-C	5.01	120.42	110.40
1	A	70	ARG	NE-CZ-NH2	-5.01	117.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	ASP	Sidechain

## 5.2 Close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5803	0	5638	421	0
2	A	1	0	0	0	0
3	A	29	0	10	5	0
4	A	541	0	0	30	0
All	All	6374	0	5648	422	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 37.

All (422) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:289:THR:HB	1:A:292:GLU:OE2	1.38	1.19
1:A:532:GLN:OE1	1:A:542:THR:HG22	1.38	1.19
1:A:289:THR:HG22	1:A:291:GLU:H	1.05	1.14
1:A:62:PHE:HE2	1:A:72:VAL:CG2	1.61	1.12
1:A:686:ARG:HB2	1:A:686:ARG:HH11	0.95	1.10
1:A:63:LYS:HE2	1:A:67:GLY:HA2	1.32	1.09
1:A:7:ARG:HH11	1:A:7:ARG:HG3	1.08	1.08
1:A:398:ILE:HD12	1:A:407:GLN:HG3	1.34	1.05
1:A:296:LEU:HB3	1:A:298:LEU:CD1	1.89	1.03
1:A:686:ARG:CB	1:A:686:ARG:HH11	1.72	1.02
1:A:62:PHE:HE2	1:A:72:VAL:HG23	1.23	1.01
1:A:734:PRO:HA	1:A:737:TYR:CZ	1.94	1.01
1:A:35:ILE:HD11	1:A:77:ALA:HB1	1.44	0.99
1:A:750:GLN:HE21	1:A:754:ILE:HD12	1.28	0.99
1:A:686:ARG:NH1	1:A:686:ARG:HB2	1.77	0.98
1:A:409:LEU:HD22	1:A:413:LYS:HE3	1.46	0.96

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:GLU:O	1:A:274:THR:OG1	1.85	0.94
1:A:62:PHE:CE2	1:A:72:VAL:HG23	2.02	0.94
1:A:62:PHE:CE2	1:A:72:VAL:CG2	2.52	0.93
1:A:706:TYR:CD1	1:A:713:PRO:HA	2.03	0.93
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.04	0.93
1:A:80:ARG:NH2	1:A:83:ILE:HD11	1.83	0.92
1:A:753:ARG:HA	1:A:756:GLU:HB2	1.51	0.91
1:A:289:THR:HG22	1:A:291:GLU:N	1.84	0.91
1:A:697:ILE:HB	1:A:700:ASP:HB2	1.54	0.90
1:A:80:ARG:CZ	1:A:83:ILE:HD11	2.01	0.90
1:A:55:GLU:HG2	1:A:56:THR:O	1.73	0.89
1:A:737:TYR:HB3	1:A:746:PHE:CE1	2.09	0.88
1:A:487:PHE:CE2	1:A:505:ASP:HB2	2.10	0.87
1:A:432:TRP:CZ2	1:A:436:LYS:HD2	2.08	0.87
1:A:296:LEU:HB3	1:A:298:LEU:HD13	1.57	0.86
1:A:296:LEU:HB3	1:A:298:LEU:HD11	1.55	0.86
1:A:60:PHE:CE1	1:A:74:LYS:HA	2.10	0.85
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.79	0.85
1:A:35:ILE:HD11	1:A:77:ALA:CB	2.07	0.85
1:A:736:GLN:HB3	1:A:750:GLN:HG2	1.57	0.83
1:A:219:ASN:HB3	1:A:220:PRO:HD3	1.59	0.83
1:A:487:PHE:CD2	1:A:505:ASP:HB2	2.12	0.83
1:A:695:ARG:HA	1:A:744:ILE:O	1.79	0.82
1:A:191:LYS:HA	1:A:191:LYS:HE2	1.60	0.82
1:A:342:MET:HE1	1:A:342:MET:HA	1.61	0.82
1:A:43:GLU:OE1	1:A:43:GLU:HA	1.74	0.81
1:A:99:GLU:HG2	1:A:686:ARG:HH21	1.46	0.81
1:A:40:ASP:OD1	1:A:42:LYS:HG2	1.80	0.81
1:A:289:THR:O	1:A:293:LYS:HD2	1.79	0.81
1:A:99:GLU:HG2	1:A:686:ARG:NH2	1.97	0.80
1:A:399:LEU:HD23	1:A:403:ASP:O	1.80	0.80
1:A:97:LEU:HB2	1:A:689:ARG:HD3	1.63	0.80
1:A:342:MET:HA	1:A:342:MET:CE	2.12	0.80
1:A:398:ILE:HD12	1:A:407:GLN:CG	2.12	0.79
1:A:34:TYR:CD1	1:A:51:GLU:HA	2.18	0.78
1:A:84:LYS:C	1:A:84:LYS:HD2	2.04	0.78
1:A:7:ARG:HG3	1:A:7:ARG:NH1	1.85	0.78
1:A:289:THR:CB	1:A:292:GLU:OE2	2.27	0.78
1:A:319:SER:OG	1:A:322:GLU:HG2	1.83	0.78
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.66	0.77
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.14	0.77
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.67	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:371:ASP:OD2	1:A:373:THR:N	2.15	0.77
1:A:398:ILE:CD1	1:A:407:GLN:HG3	2.14	0.76
1:A:706:TYR:HD1	1:A:713:PRO:HA	1.49	0.76
1:A:482:PHE:CE1	1:A:486:MET:HE2	2.20	0.76
1:A:687:ILE:HG22	1:A:688:THR:N	1.97	0.76
1:A:87:GLY:H	1:A:105:ASN:ND2	1.82	0.76
1:A:695:ARG:HD3	1:A:745:PHE:CE2	2.20	0.75
1:A:219:ASN:HA	4:A:1403:HOH:O	1.87	0.75
1:A:337:SER:O	1:A:341:GLN:HG3	1.87	0.74
1:A:735:GLU:HA	1:A:738:ARG:HH21	1.53	0.74
1:A:668:GLU:OE1	4:A:1203:HOH:O	2.06	0.74
1:A:391:LYS:NZ	1:A:391:LYS:HB3	2.03	0.73
1:A:327:THR:HG22	1:A:331:MET:HE2	1.70	0.73
1:A:296:LEU:CB	1:A:298:LEU:HD13	2.18	0.73
1:A:750:GLN:HE21	1:A:754:ILE:CD1	2.01	0.72
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.19	0.72
3:A:999:DAQ:HA22	4:A:1509:HOH:O	1.90	0.72
1:A:513:THR:O	1:A:517:ILE:HD12	1.88	0.71
1:A:504:ILE:HG13	1:A:504:ILE:O	1.89	0.71
1:A:63:LYS:HE2	1:A:67:GLY:CA	2.17	0.71
1:A:698:TYR:CZ	1:A:720:GLN:HG2	2.25	0.71
1:A:692:PHE:HB3	1:A:745:PHE:HB3	1.71	0.71
1:A:682:LEU:HB3	1:A:686:ARG:HH22	1.55	0.70
1:A:354:LEU:O	1:A:418:ARG:HD3	1.90	0.70
1:A:540:ASP:OD2	4:A:1264:HOH:O	2.09	0.70
1:A:321:SER:O	1:A:325:LYS:HE2	1.92	0.70
1:A:382:PHE:O	1:A:603:SER:OG	2.09	0.70
1:A:63:LYS:CE	1:A:67:GLY:HA2	2.18	0.70
1:A:391:LYS:HZ2	1:A:395:GLU:HB2	1.58	0.69
1:A:273:GLU:O	4:A:1523:HOH:O	2.11	0.69
1:A:399:LEU:HD22	1:A:401:GLY:H	1.58	0.68
1:A:137:GLN:O	1:A:137:GLN:HG3	1.94	0.67
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.59	0.67
1:A:734:PRO:HA	1:A:737:TYR:CE1	2.29	0.67
1:A:368:VAL:HG12	1:A:369:LEU:H	1.60	0.67
1:A:737:TYR:HB3	1:A:746:PHE:HE1	1.58	0.67
1:A:336:PHE:O	1:A:341:GLN:NE2	2.26	0.67
1:A:127:ASN:HD21	3:A:999:DAQ:HA21	1.59	0.66
1:A:298:LEU:N	1:A:298:LEU:HD12	2.09	0.66
1:A:97:LEU:HD13	1:A:685:ILE:HG23	1.77	0.66
1:A:219:ASN:HB3	1:A:220:PRO:CD	2.24	0.66
1:A:367:ALA:HB3	1:A:394:MET:HG2	1.78	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.28	0.66
1:A:752:ALA:O	1:A:756:GLU:N	2.29	0.66
1:A:34:TYR:HE1	1:A:51:GLU:HB2	1.61	0.66
1:A:532:GLN:OE1	1:A:542:THR:CG2	2.31	0.66
1:A:736:GLN:NE2	1:A:753:ARG:HH22	1.93	0.66
1:A:40:ASP:CB	1:A:40:ASP:CG	2.64	0.66
1:A:396:PRO:HD2	1:A:407:GLN:O	1.96	0.65
1:A:367:ALA:O	1:A:408:HIS:NE2	2.27	0.65
1:A:736:GLN:HG3	1:A:750:GLN:OE1	1.97	0.65
1:A:56:THR:CG2	1:A:57:SER:N	2.59	0.65
1:A:60:PHE:HE1	1:A:74:LYS:HA	1.60	0.65
1:A:682:LEU:O	1:A:686:ARG:NH1	2.30	0.64
1:A:35:ILE:CD1	1:A:77:ALA:HB1	2.23	0.64
1:A:62:PHE:HE2	1:A:72:VAL:HG21	1.60	0.64
1:A:60:PHE:O	1:A:72:VAL:N	2.30	0.64
1:A:322:GLU:O	1:A:325:LYS:HB2	1.96	0.64
1:A:694:ASN:C	1:A:695:ARG:HG2	2.18	0.64
1:A:489:LEU:N	1:A:489:LEU:HD23	2.06	0.64
1:A:682:LEU:HD22	1:A:686:ARG:NH2	2.12	0.63
1:A:56:THR:HG23	1:A:57:SER:H	1.63	0.63
1:A:692:PHE:O	1:A:695:ARG:NE	2.31	0.63
1:A:409:LEU:HD22	1:A:413:LYS:CE	2.25	0.63
1:A:695:ARG:HA	1:A:745:PHE:HA	1.81	0.63
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.34	0.63
1:A:371:ASP:OD2	1:A:372:LYS:N	2.32	0.63
1:A:399:LEU:CD2	1:A:400:ALA:N	2.62	0.62
1:A:687:ILE:O	1:A:690:LYS:HG3	1.99	0.62
1:A:681:VAL:O	1:A:685:ILE:HG13	1.99	0.62
1:A:696:ILE:O	1:A:743:LYS:HB3	2.00	0.62
1:A:727:LEU:O	1:A:731:ASN:HA	2.00	0.62
1:A:300:GLY:O	1:A:303:SER:HB2	2.00	0.62
1:A:72:VAL:HG12	1:A:73:LYS:N	2.14	0.61
1:A:60:PHE:N	1:A:72:VAL:O	2.31	0.61
1:A:372:LYS:O	1:A:376:ASN:ND2	2.33	0.61
1:A:621:ALA:HB3	1:A:627:PHE:HA	1.82	0.61
1:A:409:LEU:CD2	1:A:413:LYS:HE3	2.27	0.61
1:A:378:ALA:O	1:A:381:VAL:HG22	2.01	0.60
1:A:64:THR:HG23	1:A:68:GLN:O	2.00	0.60
1:A:176:LEU:HD12	1:A:176:LEU:N	2.17	0.60
1:A:724:ASP:O	1:A:728:LYS:N	2.34	0.60
1:A:391:LYS:HZ1	1:A:391:LYS:HB3	1.65	0.60
1:A:331:MET:HE3	1:A:345:PHE:HZ	1.67	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:621:ALA:HB2	1:A:628:ILE:HG23	1.84	0.60
1:A:535:PHE:N	1:A:535:PHE:CD2	2.69	0.60
1:A:302:GLU:H	1:A:302:GLU:CD	2.05	0.59
1:A:742:THR:OG1	1:A:743:LYS:HG3	2.02	0.59
1:A:56:THR:HG22	1:A:58:ASP:H	1.68	0.59
1:A:87:GLY:H	1:A:105:ASN:HD21	1.48	0.59
1:A:62:PHE:CE2	1:A:72:VAL:HG21	2.35	0.59
1:A:56:THR:CG2	1:A:57:SER:H	2.15	0.59
1:A:741:ILE:C	1:A:742:THR:HG23	2.23	0.59
1:A:40:ASP:OD1	1:A:40:ASP:CG	2.41	0.58
1:A:30:SER:HA	4:A:1282:HOH:O	2.03	0.58
1:A:298:LEU:CD1	1:A:298:LEU:N	2.66	0.58
1:A:415:SER:O	1:A:418:ARG:HB3	2.03	0.58
1:A:695:ARG:HB3	1:A:745:PHE:CD1	2.38	0.58
1:A:218:ALA:O	1:A:221:ILE:HB	2.04	0.58
1:A:544:ILE:HG13	1:A:544:ILE:O	2.03	0.58
1:A:706:TYR:HB2	1:A:712:VAL:O	2.03	0.58
1:A:217:GLN:O	1:A:220:PRO:HD2	2.03	0.58
1:A:357:ILE:O	1:A:357:ILE:HG22	2.03	0.57
1:A:735:GLU:CB	1:A:738:ARG:HH21	2.17	0.57
1:A:219:ASN:CB	1:A:220:PRO:CD	2.80	0.57
1:A:590:ASP:N	1:A:591:PRO:HD3	2.20	0.57
1:A:687:ILE:CG2	1:A:688:THR:N	2.66	0.57
1:A:704:ARG:NH2	1:A:755:GLU:OE1	2.33	0.57
1:A:399:LEU:HD22	1:A:400:ALA:N	2.20	0.57
1:A:83:ILE:HG13	1:A:86:ASP:OD1	2.05	0.56
1:A:2:ASN:ND2	1:A:5:HIS:CE1	2.73	0.56
1:A:722:ALA:O	1:A:726:VAL:HG23	2.05	0.56
1:A:290:ALA:HA	1:A:293:LYS:HD2	1.87	0.56
1:A:753:ARG:O	1:A:756:GLU:O	2.24	0.56
1:A:213:GLN:O	1:A:217:GLN:HG2	2.05	0.56
1:A:331:MET:HE3	1:A:345:PHE:CZ	2.40	0.56
1:A:410:ASN:OD1	1:A:413:LYS:HB2	2.06	0.56
1:A:399:LEU:HD21	1:A:401:GLY:O	2.04	0.56
1:A:736:GLN:CB	1:A:750:GLN:HG2	2.34	0.56
1:A:290:ALA:HA	1:A:293:LYS:CD	2.35	0.56
1:A:585:LEU:O	1:A:589:LYS:HD3	2.05	0.56
1:A:686:ARG:CG	1:A:686:ARG:HH11	2.18	0.55
1:A:397:ARG:HB3	1:A:404:LEU:HD22	1.87	0.55
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.41	0.55
1:A:311:GLY:N	4:A:1083:HOH:O	2.15	0.55
1:A:718:ASP:O	1:A:721:LYS:N	2.40	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:698:TYR:HB3	1:A:719:SER:HB3	1.87	0.55
1:A:308:ASN:OD1	1:A:309:GLN:NE2	2.40	0.55
1:A:133:PRO:HB2	4:A:1225:HOH:O	2.06	0.55
1:A:706:TYR:HB2	1:A:712:VAL:HG12	1.90	0.54
1:A:323:GLU:HA	1:A:326:ILE:HG13	1.88	0.54
1:A:662:GLN:NE2	4:A:1397:HOH:O	2.39	0.54
1:A:61:THR:HA	1:A:70:ARG:O	2.07	0.54
1:A:749:GLY:O	1:A:753:ARG:HG3	2.07	0.54
1:A:750:GLN:NE2	1:A:754:ILE:HD12	2.10	0.54
1:A:505:ASP:O	1:A:508:LEU:HD23	2.07	0.54
1:A:238:ARG:CD	1:A:264:GLU:OE2	2.56	0.54
1:A:259:GLN:OE1	4:A:1413:HOH:O	2.17	0.54
1:A:190:LYS:O	4:A:1242:HOH:O	2.18	0.54
1:A:219:ASN:OD1	1:A:220:PRO:N	2.42	0.53
1:A:654:ARG:NH2	1:A:679:ASN:O	2.38	0.53
1:A:331:MET:CE	1:A:345:PHE:HZ	2.21	0.53
1:A:442:CYS:SG	1:A:443:GLN:N	2.82	0.53
1:A:697:ILE:CB	1:A:700:ASP:HB2	2.33	0.53
1:A:323:GLU:HA	1:A:323:GLU:OE1	2.08	0.53
1:A:389:LEU:HG	1:A:393:LEU:HD12	1.90	0.53
1:A:695:ARG:HB3	1:A:745:PHE:CG	2.44	0.53
1:A:219:ASN:N	1:A:220:PRO:HD2	2.22	0.53
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.91	0.53
1:A:745:PHE:CD1	1:A:745:PHE:N	2.76	0.53
1:A:399:LEU:HD22	1:A:401:GLY:N	2.23	0.53
1:A:399:LEU:HD23	1:A:400:ALA:H	1.73	0.53
1:A:628:ILE:HD11	1:A:633:GLN:HB2	1.91	0.53
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.48	0.53
1:A:506:PHE:O	1:A:509:ASP:HB2	2.08	0.53
1:A:695:ARG:CD	1:A:745:PHE:CE2	2.91	0.52
1:A:741:ILE:HG22	1:A:742:THR:HG23	1.89	0.52
1:A:102:VAL:HG21	1:A:685:ILE:HD12	1.92	0.52
1:A:701:PHE:CD1	1:A:705:TYR:CD2	2.97	0.52
1:A:391:LYS:NZ	1:A:395:GLU:HB2	2.23	0.52
1:A:2:ASN:HD22	1:A:5:HIS:CE1	2.27	0.52
1:A:666:LYS:HE3	4:A:1208:HOH:O	2.10	0.52
1:A:694:ASN:O	1:A:745:PHE:HA	2.10	0.52
1:A:399:LEU:HD23	1:A:400:ALA:N	2.25	0.52
1:A:323:GLU:O	1:A:326:ILE:HB	2.09	0.52
1:A:147:ARG:HB2	1:A:149:ASN:ND2	2.25	0.51
1:A:695:ARG:NE	1:A:745:PHE:CD2	2.79	0.51
1:A:732:ILE:HG22	1:A:733:ASP:N	2.25	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:504:ILE:HG12	1:A:506:PHE:CE1	2.46	0.51
1:A:619:SER:HB3	1:A:627:PHE:CE2	2.46	0.51
1:A:745:PHE:HD1	1:A:745:PHE:N	2.09	0.51
1:A:722:ALA:O	1:A:725:ALA:HB3	2.11	0.51
1:A:2:ASN:O	1:A:5:HIS:N	2.34	0.51
1:A:172:ASN:HB2	4:A:1439:HOH:O	2.10	0.51
1:A:646:GLU:OE1	4:A:1195:HOH:O	2.19	0.51
1:A:59:SER:HB2	1:A:72:VAL:O	2.12	0.50
1:A:72:VAL:CG1	1:A:73:LYS:N	2.73	0.50
1:A:695:ARG:O	1:A:743:LYS:HD3	2.11	0.50
1:A:695:ARG:CA	1:A:744:ILE:O	2.56	0.50
1:A:409:LEU:CD2	1:A:413:LYS:CE	2.89	0.50
1:A:701:PHE:CE1	1:A:705:TYR:CD2	2.99	0.50
1:A:292:GLU:O	1:A:296:LEU:HB2	2.12	0.50
1:A:84:LYS:O	1:A:84:LYS:HD2	2.12	0.50
1:A:482:PHE:CE1	1:A:486:MET:CE	2.94	0.50
1:A:217:GLN:C	1:A:220:PRO:HD2	2.33	0.49
1:A:391:LYS:NZ	1:A:395:GLU:CB	2.75	0.49
1:A:702:VAL:HG21	1:A:722:ALA:HB3	1.94	0.49
1:A:735:GLU:CA	1:A:738:ARG:HH21	2.24	0.49
1:A:389:LEU:HG	1:A:393:LEU:CD1	2.42	0.49
1:A:59:SER:CB	1:A:72:VAL:O	2.60	0.49
1:A:679:ASN:HB2	4:A:1117:HOH:O	2.12	0.49
1:A:567:GLU:HA	1:A:579:TYR:O	2.12	0.49
1:A:734:PRO:CA	1:A:737:TYR:CZ	2.84	0.49
1:A:147:ARG:CG	1:A:147:ARG:HH11	2.25	0.49
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.95	0.49
1:A:315:ILE:HD13	4:A:1416:HOH:O	2.13	0.49
1:A:682:LEU:HD22	1:A:686:ARG:HH21	1.76	0.48
1:A:238:ARG:HD3	1:A:264:GLU:OE2	2.13	0.48
1:A:389:LEU:HD11	1:A:393:LEU:HD11	1.95	0.48
1:A:397:ARG:HA	1:A:406:ALA:HA	1.94	0.48
1:A:97:LEU:H	1:A:689:ARG:NE	2.12	0.48
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.45	0.48
1:A:683:GLU:CG	1:A:687:ILE:HD12	2.42	0.48
1:A:702:VAL:HG13	1:A:712:VAL:HG11	1.96	0.48
1:A:331:MET:CE	1:A:345:PHE:CZ	2.96	0.48
1:A:698:TYR:CE1	1:A:720:GLN:HG2	2.48	0.48
1:A:736:GLN:HB3	1:A:750:GLN:CG	2.38	0.48
1:A:654:ARG:NH1	4:A:1200:HOH:O	2.05	0.48
1:A:697:ILE:HD13	1:A:743:LYS:HG2	1.96	0.48
1:A:127:ASN:OD1	3:A:999:DAQ:O2A	2.31	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:56:THR:HG22	1:A:57:SER:N	2.28	0.48
1:A:147:ARG:CB	1:A:149:ASN:ND2	2.76	0.48
1:A:590:ASP:N	1:A:591:PRO:CD	2.76	0.47
1:A:191:LYS:CA	1:A:191:LYS:HE2	2.37	0.47
1:A:594:GLN:HG3	1:A:594:GLN:O	2.14	0.47
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.49	0.47
1:A:375:LEU:HD12	1:A:389:LEU:HD23	1.96	0.47
1:A:313:VAL:HG23	1:A:313:VAL:O	2.13	0.47
1:A:686:ARG:NH1	1:A:686:ARG:CB	2.57	0.47
1:A:482:PHE:HE1	1:A:486:MET:CE	2.28	0.47
1:A:98:ASN:OD1	1:A:100:PRO:HD2	2.15	0.47
1:A:191:LYS:CE	1:A:191:LYS:HA	2.38	0.47
1:A:698:TYR:CE2	1:A:720:GLN:HG2	2.49	0.47
1:A:504:ILE:HG23	1:A:504:ILE:O	2.15	0.47
1:A:621:ALA:HB2	1:A:628:ILE:H	1.79	0.47
1:A:40:ASP:OD1	1:A:42:LYS:CG	2.59	0.47
1:A:345:PHE:HD1	1:A:345:PHE:HA	1.57	0.47
1:A:308:ASN:C	1:A:308:ASN:OD1	2.54	0.46
1:A:172:ASN:ND2	4:A:1439:HOH:O	2.27	0.46
1:A:289:THR:CG2	1:A:290:ALA:N	2.78	0.46
1:A:80:ARG:NE	1:A:83:ILE:HD11	2.30	0.46
1:A:406:ALA:C	1:A:407:GLN:HG2	2.36	0.46
1:A:697:ILE:HG22	1:A:700:ASP:H	1.80	0.46
1:A:683:GLU:HG3	1:A:687:ILE:HD12	1.97	0.46
1:A:380:THR:HG22	1:A:381:VAL:N	2.29	0.46
1:A:285:LEU:HD11	1:A:304:PHE:CE1	2.51	0.46
1:A:749:GLY:C	1:A:753:ARG:NH1	2.69	0.46
1:A:219:ASN:CB	1:A:220:PRO:HD3	2.36	0.46
1:A:147:ARG:NH1	1:A:147:ARG:CG	2.78	0.46
1:A:609:THR:OG1	4:A:1267:HOH:O	2.20	0.46
1:A:520:ARG:HD3	4:A:1146:HOH:O	2.16	0.46
1:A:368:VAL:HG12	1:A:369:LEU:N	2.28	0.46
1:A:238:ARG:HH11	1:A:264:GLU:CD	2.18	0.46
1:A:72:VAL:HG12	1:A:73:LYS:O	2.15	0.46
1:A:601:LYS:O	1:A:613:ASN:OD1	2.34	0.46
1:A:59:SER:HB2	1:A:73:LYS:HA	1.98	0.46
1:A:692:PHE:CE1	1:A:747:ARG:HG2	2.50	0.46
1:A:109:ARG:HB3	1:A:114:LEU:HB2	1.97	0.46
1:A:273:GLU:C	1:A:274:THR:HG1	2.09	0.46
1:A:223:GLU:O	1:A:227:ASN:HB2	2.15	0.46
1:A:107:ARG:NH2	4:A:1031:HOH:O	2.37	0.46
1:A:372:LYS:HB3	1:A:376:ASN:HD21	1.81	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:296:LEU:HA	1:A:296:LEU:HD12	1.65	0.45
1:A:692:PHE:CE1	1:A:747:ARG:CG	2.99	0.45
1:A:324:PHE:HD2	1:A:325:LYS:HZ3	1.65	0.45
1:A:727:LEU:O	1:A:731:ASN:CA	2.65	0.45
1:A:395:GLU:HA	1:A:407:GLN:O	2.16	0.45
1:A:706:TYR:CD1	1:A:713:PRO:CA	2.90	0.45
1:A:321:SER:O	1:A:325:LYS:CE	2.63	0.45
1:A:692:PHE:CD1	1:A:747:ARG:HG2	2.52	0.45
1:A:685:ILE:HG22	1:A:686:ARG:HD3	1.99	0.45
1:A:34:TYR:CD1	1:A:51:GLU:CA	2.96	0.45
1:A:38:ASN:OD1	1:A:38:ASN:N	2.50	0.45
1:A:52:ILE:C	1:A:52:ILE:HD12	2.36	0.45
1:A:695:ARG:HB3	1:A:745:PHE:CE1	2.52	0.45
1:A:750:GLN:OE1	1:A:753:ARG:NH2	2.50	0.45
1:A:701:PHE:O	1:A:705:TYR:HD2	1.99	0.45
1:A:730:LEU:HD23	1:A:730:LEU:HA	1.59	0.45
1:A:292:GLU:O	1:A:293:LYS:C	2.54	0.45
1:A:339:GLU:HB3	1:A:340:GLU:H	1.63	0.45
1:A:490:GLU:HA	1:A:490:GLU:OE1	2.17	0.45
1:A:698:TYR:CE1	1:A:720:GLN:CG	3.00	0.44
1:A:698:TYR:O	1:A:702:VAL:HG23	2.17	0.44
1:A:372:LYS:HB3	1:A:372:LYS:HE2	1.50	0.44
1:A:297:HIS:C	1:A:298:LEU:HD12	2.38	0.44
1:A:147:ARG:HB2	1:A:150:GLU:HB2	1.99	0.44
1:A:595:ASP:HB3	4:A:1461:HOH:O	2.17	0.44
1:A:262:LEU:HB3	4:A:1411:HOH:O	2.17	0.44
1:A:694:ASN:HB2	1:A:746:PHE:HB2	2.00	0.44
1:A:375:LEU:CD1	1:A:389:LEU:HD23	2.48	0.44
1:A:193:ILE:HG21	1:A:193:ILE:HD13	1.75	0.44
1:A:325:LYS:O	1:A:329:GLN:HB2	2.18	0.44
1:A:473:TYR:OH	1:A:518:ASP:OD2	2.30	0.44
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.44	0.44
1:A:40:ASP:HA	1:A:41:PRO:HD3	1.78	0.44
1:A:686:ARG:NH1	1:A:686:ARG:CG	2.81	0.44
1:A:754:ILE:HG22	1:A:755:GLU:N	2.32	0.44
1:A:191:LYS:CE	1:A:191:LYS:CA	2.95	0.43
1:A:341:GLN:O	1:A:345:PHE:CD2	2.71	0.43
1:A:182:GLY:HA2	3:A:999:DAQ:HA11	2.00	0.43
1:A:309:GLN:NE2	4:A:1456:HOH:O	2.49	0.43
1:A:85:PHE:HE2	4:A:1285:HOH:O	2.00	0.43
1:A:325:LYS:HA	1:A:325:LYS:HD3	1.49	0.43
1:A:129:PHE:CE1	1:A:662:GLN:HA	2.53	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:337:SER:OG	1:A:339:GLU:HB3	2.19	0.43
1:A:190:LYS:HE3	1:A:223:GLU:OE2	2.18	0.43
1:A:64:THR:OG1	1:A:68:GLN:N	2.52	0.43
1:A:692:PHE:O	1:A:695:ARG:CZ	2.67	0.43
1:A:738:ARG:HD3	1:A:738:ARG:HA	1.48	0.42
1:A:362:GLY:HA3	1:A:368:VAL:CG2	2.49	0.42
1:A:175:LEU:N	1:A:175:LEU:HD12	2.34	0.42
1:A:289:THR:C	1:A:291:GLU:N	2.71	0.42
1:A:737:TYR:C	1:A:737:TYR:CD1	2.92	0.42
1:A:508:LEU:CD2	1:A:508:LEU:N	2.81	0.42
1:A:735:GLU:CB	1:A:738:ARG:NH2	2.81	0.42
1:A:149:ASN:ND2	1:A:150:GLU:OE1	2.52	0.42
1:A:64:THR:CG2	1:A:68:GLN:O	2.67	0.42
1:A:485:HIS:ND1	4:A:1136:HOH:O	2.14	0.42
1:A:719:SER:O	1:A:723:THR:N	2.52	0.42
1:A:38:ASN:C	1:A:40:ASP:H	2.22	0.42
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.84	0.42
1:A:410:ASN:OD1	1:A:410:ASN:C	2.57	0.42
1:A:289:THR:HG22	1:A:290:ALA:N	2.33	0.42
1:A:704:ARG:HG3	1:A:704:ARG:O	2.18	0.42
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.19	0.42
1:A:415:SER:OG	1:A:418:ARG:NH2	2.48	0.42
1:A:342:MET:O	1:A:346:LYS:N	2.48	0.42
1:A:19:GLN:N	4:A:1258:HOH:O	2.39	0.42
1:A:379:SER:O	1:A:383:GLY:N	2.48	0.42
1:A:289:THR:C	1:A:291:GLU:H	2.20	0.42
1:A:293:LYS:O	1:A:297:HIS:N	2.53	0.42
1:A:350:GLY:HA2	1:A:381:VAL:HG21	2.02	0.42
1:A:412:GLU:HG2	1:A:413:LYS:N	2.34	0.41
1:A:462:LYS:HE3	1:A:462:LYS:HB2	1.71	0.41
1:A:424:ALA:O	1:A:428:ARG:HB2	2.20	0.41
1:A:614:ASP:O	1:A:616:ASN:N	2.53	0.41
1:A:158:ILE:HG23	1:A:158:ILE:HD13	1.71	0.41
1:A:164:ARG:HA	1:A:164:ARG:HD3	1.81	0.41
1:A:45:ASP:OD1	1:A:677:ARG:NH1	2.49	0.41
1:A:682:LEU:CB	1:A:686:ARG:HH22	2.28	0.41
1:A:696:ILE:C	1:A:743:LYS:HB3	2.40	0.41
1:A:342:MET:O	1:A:346:LYS:HG3	2.21	0.41
1:A:706:TYR:CB	1:A:712:VAL:HG12	2.49	0.41
1:A:706:TYR:CD1	1:A:714:ARG:N	2.88	0.41
1:A:399:LEU:HA	1:A:403:ASP:O	2.21	0.41
1:A:724:ASP:HA	1:A:739:PHE:HZ	1.84	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:280:ILE:HG13	1:A:280:ILE:O	2.20	0.41
1:A:449:PHE:CD2	1:A:449:PHE:C	2.94	0.41
1:A:508:LEU:HD13	4:A:1376:HOH:O	2.21	0.41
1:A:669:ASP:HB3	4:A:1271:HOH:O	2.20	0.41
1:A:391:LYS:HZ3	1:A:395:GLU:HB3	1.84	0.41
1:A:51:GLU:O	1:A:53:VAL:HG23	2.20	0.41
1:A:127:ASN:ND2	3:A:999:DAQ:HA21	2.32	0.41
1:A:370:LYS:HE2	1:A:370:LYS:HB3	1.84	0.41
1:A:597:GLU:OE1	1:A:612:PHE:CD2	2.74	0.41
1:A:290:ALA:HA	1:A:293:LYS:HD3	2.02	0.41
1:A:288:ALA:O	1:A:293:LYS:HE3	2.20	0.41
1:A:34:TYR:CE1	1:A:51:GLU:CB	2.89	0.41
1:A:51:GLU:OE1	1:A:53:VAL:HG22	2.21	0.41
1:A:367:ALA:CB	1:A:394:MET:HG2	2.49	0.41
1:A:620:ARG:O	4:A:1316:HOH:O	2.22	0.41
1:A:734:PRO:O	1:A:737:TYR:O	2.39	0.41
1:A:287:GLY:O	1:A:325:LYS:NZ	2.54	0.41
1:A:238:ARG:HD2	1:A:264:GLU:OE2	2.20	0.41
1:A:391:LYS:HZ2	1:A:395:GLU:CB	2.30	0.40
1:A:219:ASN:N	1:A:220:PRO:CD	2.84	0.40
1:A:219:ASN:C	1:A:221:ILE:N	2.74	0.40
1:A:222:LEU:HD23	1:A:222:LEU:HA	1.80	0.40
1:A:697:ILE:CG2	1:A:698:TYR:N	2.84	0.40
1:A:610:LYS:HA	1:A:610:LYS:HD2	1.64	0.40
1:A:399:LEU:C	1:A:399:LEU:CD2	2.89	0.40
1:A:399:LEU:CD2	1:A:401:GLY:N	2.84	0.40
1:A:102:VAL:HG21	1:A:685:ILE:CD1	2.51	0.40
1:A:732:ILE:HG21	1:A:750:GLN:CD	2.42	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	726/761 (95%)	679 (94%)	41 (6%)	6 (1%)	27	17

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	714	ARG
1	A	719	SER
1	A	7	ARG
1	A	362	GLY
1	A	32	LYS
1	A	713	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	615/665 (92%)	530 (86%)	85 (14%)	<b>5</b> <b>2</b>

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	13	LYS
1	A	23	ASP
1	A	28	THR
1	A	31	ASP
1	A	32	LYS
1	A	38	ASN
1	A	42	LYS
1	A	46	SER
1	A	52	ILE
1	A	54	SER
1	A	56	THR
1	A	57	SER
1	A	59	SER
1	A	60	PHE
1	A	63	LYS
1	A	66	ASP
1	A	84	LYS
1	A	95	SER
1	A	149	ASN
1	A	150	GLU

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Mol	Chain	Res	Type
1	A	151	VAL
1	A	158	ILE
1	A	159	SER
1	A	164	ARG
1	A	170	ARG
1	A	211	LEU
1	A	241	LYS
1	A	257	SER
1	A	258	ILE
1	A	259	GLN
1	A	273	GLU
1	A	296	LEU
1	A	313	VAL
1	A	321	SER
1	A	325	LYS
1	A	326	ILE
1	A	329	GLN
1	A	342	MET
1	A	368	VAL
1	A	370	LYS
1	A	372	LYS
1	A	376	ASN
1	A	379	SER
1	A	387	SER
1	A	399	LEU
1	A	404	LEU
1	A	436	LYS
1	A	439	ASN
1	A	446	LYS
1	A	462	LYS
1	A	486	MET
1	A	492	GLU
1	A	504	ILE
1	A	510	SER
1	A	520	ARG
1	A	542	THR
1	A	589	LYS
1	A	594	GLN
1	A	609	THR
1	A	640	SER
1	A	654	ARG
1	A	657	ILE

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Mol	Chain	Res	Type
1	A	661	LYS
1	A	666	LYS
1	A	674	ASP
1	A	686	ARG
1	A	687	ILE
1	A	689	ARG
1	A	690	LYS
1	A	695	ARG
1	A	704	ARG
1	A	711	ASN
1	A	715	ASP
1	A	720	GLN
1	A	721	LYS
1	A	733	ASP
1	A	736	GLN
1	A	738	ARG
1	A	742	THR
1	A	743	LYS
1	A	744	ILE
1	A	745	PHE
1	A	750	GLN
1	A	754	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	105	ASN
1	A	149	ASN
1	A	234	ASN
1	A	235	ASN
1	A	283	GLN
1	A	309	GLN
1	A	329	GLN
1	A	338	GLN
1	A	376	ASN
1	A	479	GLN
1	A	491	GLN
1	A	594	GLN
1	A	613	ASN
1	A	736	GLN



### 5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z  > 2$
3	DAQ	A	999	2	28,29,29	1.88	5 (17%)	36,43,43	1.71	6 (16%)

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
3	DAQ	A	999	2	-	0/23/29/29	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	DAQ	PB-OB3	6.06	1.64	1.51
3	A	999	DAQ	C2-N2	4.78	1.53	1.46
3	A	999	DAQ	F3-BE	-2.90	1.49	1.55
3	A	999	DAQ	F2-BE	-2.21	1.50	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	DAQ	C1-NA3	2.17	1.44	1.38

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	DAQ	C3-C4-N4	4.98	122.65	118.71
3	A	999	DAQ	C3-C2-N2	4.64	120.48	115.82
3	A	999	DAQ	C3-C2-C1	-3.01	118.94	121.69
3	A	999	DAQ	O2B-N2-O2A	-3.00	115.28	121.35
3	A	999	DAQ	O2B-N2-C2	2.13	123.81	117.25
3	A	999	DAQ	O4B-N4-C4	2.13	118.51	114.42

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	736/761 (96%)	0.10	51 (6%) 17 16	11, 36, 88, 100	0

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	8.5
1	A	24	LEU	7.0
1	A	53	VAL	5.6
1	A	65	VAL	5.5
1	A	27	LEU	5.0
1	A	493	GLU	4.7
1	A	494	TYR	4.5
1	A	742	THR	4.1
1	A	725	ALA	4.1
1	A	67	GLY	4.0
1	A	722	ALA	3.9
1	A	759	GLU	3.9
1	A	25	PHE	3.7
1	A	56	THR	3.7
1	A	59	SER	3.7
1	A	728	LYS	3.6
1	A	68	GLN	3.5
1	A	444	GLU	3.3
1	A	723	THR	3.3
1	A	713	PRO	3.2
1	A	733	ASP	2.8
1	A	697	ILE	2.8
1	A	23	ASP	2.8
1	A	66	ASP	2.8
1	A	732	ILE	2.8
1	A	274	THR	2.7
1	A	756	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	724	ASP	2.7
1	A	70	ARG	2.7
1	A	2	ASN	2.6
1	A	699	ALA	2.6
1	A	29	VAL	2.6
1	A	536	PRO	2.6
1	A	731	ASN	2.6
1	A	757	ALA	2.5
1	A	706	TYR	2.5
1	A	751	LEU	2.5
1	A	202	ARG	2.5
1	A	729	HIS	2.5
1	A	744	ILE	2.4
1	A	700	ASP	2.4
1	A	711	ASN	2.4
1	A	721	LYS	2.3
1	A	57	SER	2.3
1	A	712	VAL	2.3
1	A	74	LYS	2.3
1	A	698	TYR	2.2
1	A	506	PHE	2.2
1	A	702	VAL	2.2
1	A	714	ARG	2.1
1	A	351	ILE	2.1

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DAQ	A	999	29/29	0.11	1.39	3,23,100,100	12
2	MG	A	998	1/1	0.07	-0.51	18,18,18,18	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.