



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 06:53 PM GMT

PDB ID : 1D1B  
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)  
COMPLEXED WITH O,P-DINITROPHENYL AMINOPROPYLDIPHOS  
PHATE BERYLLIUM 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 X-ray Structure 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/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

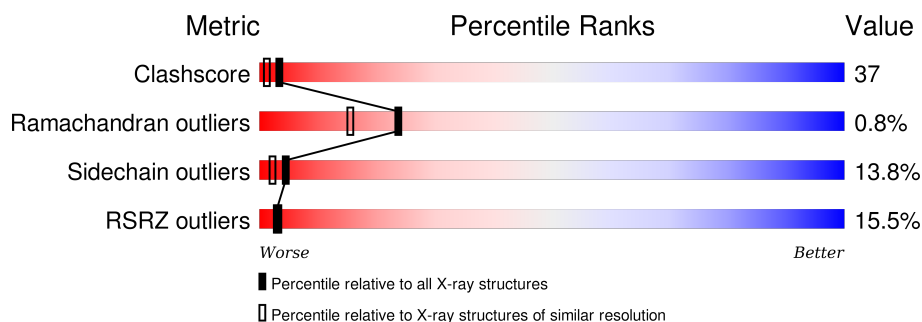
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	761	

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6374 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 MYOSIN.

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

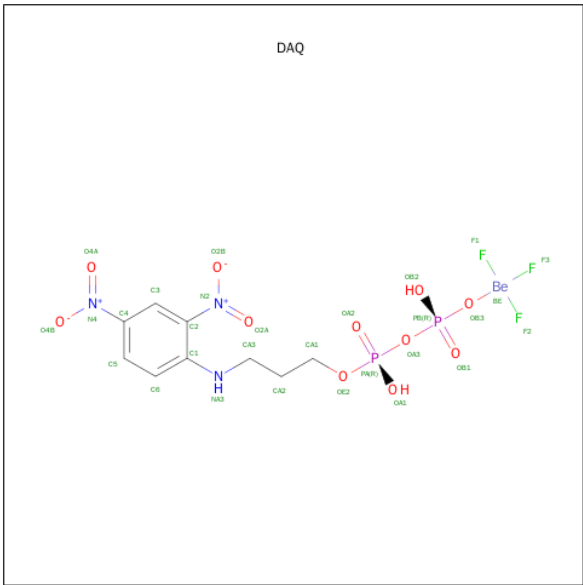
There are 3 discrepancies between the modelled and reference sequences:

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 AMINOPROPYLDIPHOSPHATE BERYLLIUM 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, $\alpha$ , $\beta$ , $\gamma$	103.88 Å   180.46 Å   54.07 Å 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 2.00 Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, $R_{free}$	0.204 , (Not available) 0.205 , (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> )	0.28 , 119.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 67444 reflections	Xtriage
$F_o, F_c$ correlation	0.94	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.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: 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 Too-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 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	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

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 37.

All (422) 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: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	Interatomic distance (Å)	Clash overlap (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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.67	0.77
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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%)	24 15

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%)	4 2

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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 [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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

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	23,29,29	1.30	2 (8%)	27,43,43	1.79	5 (18%)

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	-	0/22/29/29	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	DAQ	C1-NA3	2.33	1.44	1.37
3	A	999	DAQ	PA-OA1	3.21	1.56	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	DAQ	OA1-PA-OA2	-4.68	104.75	118.70
3	A	999	DAQ	C3-C2-C1	-3.13	118.94	121.62
3	A	999	DAQ	OA3-PA-OE2	2.02	109.14	101.36
3	A	999	DAQ	OA3-PA-OA2	2.24	114.16	108.79
3	A	999	DAQ	C3-C4-N4	4.39	122.65	118.80

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	DAQ	5	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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%)	0.74	114 (15%) 3 3	11, 36, 88, 100	0

All (114) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	10.3
1	A	53	VAL	9.8
1	A	27	LEU	8.6
1	A	65	VAL	8.4
1	A	24	LEU	8.2
1	A	494	TYR	7.2
1	A	67	GLY	6.7
1	A	56	THR	6.7
1	A	493	GLU	6.3
1	A	732	ILE	5.8
1	A	759	GLU	5.6
1	A	66	ASP	5.6
1	A	697	ILE	5.6
1	A	444	GLU	5.5
1	A	728	LYS	5.4
1	A	742	THR	5.4
1	A	68	GLN	5.3
1	A	725	ALA	5.3
1	A	25	PHE	5.2
1	A	706	TYR	5.0
1	A	713	PRO	4.7
1	A	700	ASP	4.7
1	A	731	ASN	4.6
1	A	59	SER	4.5
1	A	23	ASP	4.5
1	A	722	ALA	4.4
1	A	30	SER	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	202	ARG	4.2
1	A	2	ASN	4.1
1	A	711	ASN	4.1
1	A	733	ASP	4.1
1	A	698	TYR	3.9
1	A	714	ARG	3.9
1	A	751	LEU	3.9
1	A	744	ILE	3.9
1	A	29	VAL	3.9
1	A	692	PHE	3.8
1	A	758	ARG	3.8
1	A	5	HIS	3.8
1	A	716	ALA	3.8
1	A	26	LYS	3.8
1	A	536	PRO	3.7
1	A	707	LEU	3.7
1	A	362	GLY	3.7
1	A	74	LYS	3.6
1	A	39	PRO	3.6
1	A	718	ASP	3.6
1	A	756	GLU	3.6
1	A	723	THR	3.6
1	A	42	LYS	3.6
1	A	57	SER	3.6
1	A	729	HIS	3.6
1	A	730	LEU	3.5
1	A	506	PHE	3.5
1	A	696	ILE	3.4
1	A	757	ALA	3.4
1	A	492	GLU	3.3
1	A	290	ALA	3.3
1	A	274	THR	3.3
1	A	361	LYS	3.3
1	A	537	ASN	3.3
1	A	294	LYS	3.2
1	A	724	ASP	3.2
1	A	745	PHE	3.1
1	A	351	ILE	3.0
1	A	365	GLU	3.0
1	A	712	VAL	3.0
1	A	72	VAL	3.0
1	A	399	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	749	GLY	2.9
1	A	70	ARG	2.9
1	A	719	SER	2.8
1	A	366	GLY	2.8
1	A	743	LYS	2.8
1	A	348	ILE	2.8
1	A	702	VAL	2.8
1	A	687	ILE	2.7
1	A	741	ILE	2.7
1	A	22	SER	2.7
1	A	734	PRO	2.7
1	A	289	THR	2.6
1	A	701	PHE	2.6
1	A	40	ASP	2.6
1	A	31	ASP	2.6
1	A	347	ILE	2.6
1	A	405	VAL	2.6
1	A	699	ALA	2.5
1	A	429	LEU	2.5
1	A	504	ILE	2.5
1	A	443	GLN	2.5
1	A	753	ARG	2.5
1	A	693	PRO	2.4
1	A	76	ASP	2.4
1	A	32	LYS	2.4
1	A	689	ARG	2.4
1	A	489	LEU	2.4
1	A	54	SER	2.4
1	A	715	ASP	2.4
1	A	695	ARG	2.3
1	A	61	THR	2.3
1	A	721	LYS	2.3
1	A	60	PHE	2.3
1	A	752	ALA	2.2
1	A	209	GLY	2.2
1	A	69	ASP	2.2
1	A	158	ILE	2.2
1	A	364	GLY	2.1
1	A	203	ASN	2.1
1	A	4	ILE	2.1
1	A	352	LEU	2.1
1	A	367	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	34	TYR	2.0
1	A	422	VAL	2.0
1	A	691	GLY	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	DAQ	A	999	29/29	0.97	0.12	0.88	3,23,100,100	12
2	MG	A	998	1/1	0.99	0.07	-1.78	18,18,18,18	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.