



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:54 PM GMT

PDB ID : 1MMG
Title : X-RAY STRUCTURES OF THE MGADP, MGATPGAMMAS, AND
MGAMPPNP COMPLEXES OF THE DICTYOSTELIUM DISCOIDEUM
MYOSIN MOTOR DOMAIN
Authors : Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Rayment, I.
Deposited on : 1997-07-18
Resolution : 2.10 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

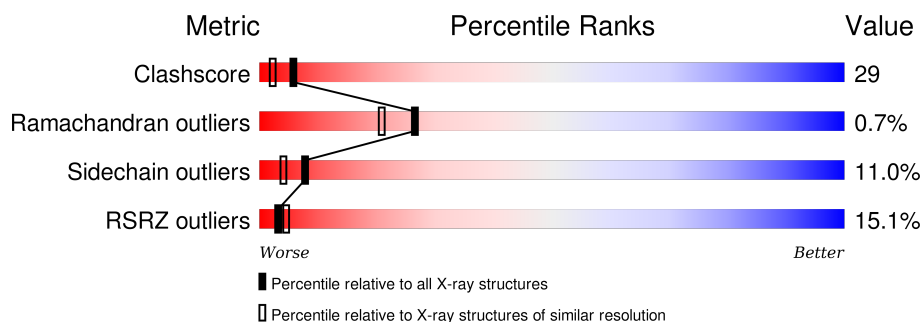
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 2.10 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	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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 ≥ 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	762	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6234 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	741	Total	C	N	O	S	0	0	0
			5865	3724	1011	1114	16			

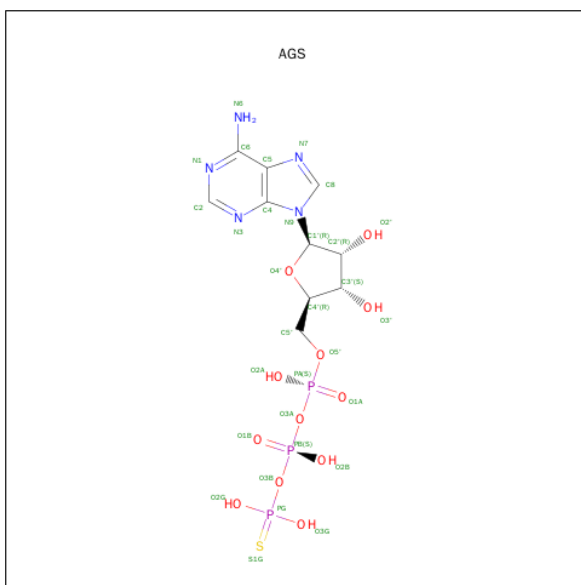
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	65	SER	VAL	CONFLICT	UNP P08799
A	273	THR	GLU	CONFLICT	UNP P08799
A	312	CYS	TYR	CONFLICT	UNP P08799
A	321	GLU	SER	CONFLICT	UNP P08799
A	322	ASP	GLU	CONFLICT	UNP P08799
A	443	SER	GLN	CONFLICT	UNP P08799
A	489	VAL	LEU	CONFLICT	UNP P08799
A	628	LEU	ILE	CONFLICT	UNP P08799
A	684	ALA	GLY	CONFLICT	UNP P08799
A	707	ASP	LEU	CONFLICT	UNP P08799
A	737	PHE	TYR	CONFLICT	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 PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	337	Total O 337 337	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.80 Å 179.90 Å 54.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 29.97 – 1.91	Depositor EDS
% Data completeness (in resolution range)	92.0 (30.00-2.10) 95.0 (29.97-1.91)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.94 (at 1.91 Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.198 , (Not available) 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.499	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 115.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 75608 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6234	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.97% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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, AGS

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	1.18	41/5975 (0.7%)	1.57	94/8071 (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	1	0

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	212	GLU	CD-OE2	8.83	1.35	1.25
1	A	187	GLU	CD-OE1	8.34	1.34	1.25
1	A	339	GLU	CD-OE1	8.30	1.34	1.25
1	A	683	GLU	CD-OE1	8.30	1.34	1.25
1	A	89	GLU	CD-OE1	7.92	1.34	1.25
1	A	636	GLU	CD-OE1	7.87	1.34	1.25
1	A	444	GLU	CD-OE2	7.54	1.33	1.25
1	A	531	GLU	CD-OE1	7.38	1.33	1.25
1	A	497	GLU	CD-OE1	7.16	1.33	1.25
1	A	735	GLU	CD-OE1	7.02	1.33	1.25
1	A	340	GLU	CD-OE1	7.01	1.33	1.25
1	A	492	GLU	CD-OE1	6.96	1.33	1.25
1	A	51	GLU	CD-OE1	6.96	1.33	1.25
1	A	668	GLU	CD-OE2	6.93	1.33	1.25
1	A	580	GLU	CD-OE2	6.92	1.33	1.25
1	A	360	GLU	CD-OE2	6.82	1.33	1.25
1	A	55	GLU	CD-OE1	6.76	1.33	1.25
1	A	490	GLU	CD-OE1	6.69	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	302	GLU	CD-OE2	6.49	1.32	1.25
1	A	395	GLU	CD-OE2	6.42	1.32	1.25
1	A	567	GLU	CD-OE2	6.39	1.32	1.25
1	A	646	GLU	CD-OE1	6.32	1.32	1.25
1	A	291	GLU	CD-OE2	6.19	1.32	1.25
1	A	321	GLU	CD-OE2	6.15	1.32	1.25
1	A	390	GLU	CD-OE1	6.15	1.32	1.25
1	A	292	GLU	CD-OE1	6.11	1.32	1.25
1	A	586	GLU	CD-OE2	5.79	1.32	1.25
1	A	323	GLU	CD-OE2	5.72	1.31	1.25
1	A	99	GLU	CD-OE2	5.67	1.31	1.25
1	A	180	GLU	CD-OE1	5.66	1.31	1.25
1	A	43	GLU	CD-OE1	5.58	1.31	1.25
1	A	717	GLU	CD-OE2	5.42	1.31	1.25
1	A	150	GLU	CD-OE1	5.42	1.31	1.25
1	A	412	GLU	CD-OE1	5.41	1.31	1.25
1	A	755	GLU	CD-OE1	5.40	1.31	1.25
1	A	476	GLU	CD-OE1	5.33	1.31	1.25
1	A	756	GLU	CD-OE1	5.32	1.31	1.25
1	A	540	ASP	CG-OD1	5.25	1.37	1.25
1	A	457	GLY	CA-C	5.22	1.60	1.51
1	A	560	GLU	CD-OE2	5.21	1.31	1.25
1	A	264	GLU	CD-OE2	-5.20	1.20	1.25

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	605	ASP	CB-CG-OD1	-11.88	107.61	118.30
1	A	148	ARG	NE-CZ-NH2	-11.53	114.54	120.30
1	A	238	ARG	NE-CZ-NH1	10.96	125.78	120.30
1	A	419	ASP	CB-CG-OD2	-9.97	109.32	118.30
1	A	605	ASP	CB-CG-OD2	9.64	126.97	118.30
1	A	428	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	23	ASP	CB-CG-OD2	-9.11	110.10	118.30
1	A	6	ASP	CB-CG-OD2	-8.98	110.22	118.30
1	A	168	ASP	CB-CG-OD1	8.83	126.25	118.30
1	A	674	ASP	CB-CG-OD1	-8.83	110.35	118.30
1	A	238	ARG	NE-CZ-NH2	-8.73	115.94	120.30
1	A	160	ASP	CB-CG-OD1	-8.36	110.77	118.30
1	A	147	ARG	NE-CZ-NH1	8.29	124.45	120.30
1	A	168	ASP	CB-CG-OD2	-8.29	110.84	118.30
1	A	76	ASP	CB-CG-OD2	-8.23	110.89	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	590	ASP	CB-CG-OD1	-7.88	111.21	118.30
1	A	614	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	614	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	A	419	ASP	CB-CG-OD1	7.67	125.20	118.30
1	A	403	ASP	CB-CG-OD1	-7.63	111.43	118.30
1	A	669	ASP	CB-CG-OD1	-7.60	111.46	118.30
1	A	44	ARG	NE-CZ-NH1	7.55	124.07	120.30
1	A	509	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	202	ARG	CB-CA-C	7.23	124.86	110.40
1	A	562	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	7	ARG	NE-CZ-NH2	-7.10	116.75	120.30
1	A	689	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	A	729	HIS	CA-CB-CG	-7.09	101.55	113.60
1	A	583	ASP	CB-CG-OD1	-6.97	112.02	118.30
1	A	267	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	700	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	A	509	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	707	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	A	518	ASP	CB-CG-OD2	-6.88	112.11	118.30
1	A	332	ASP	CB-CG-OD1	-6.86	112.13	118.30
1	A	686	ARG	NE-CZ-NH2	-6.77	116.92	120.30
1	A	428	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	6	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	23	ASP	CB-CG-OD1	6.59	124.23	118.30
1	A	44	ARG	CD-NE-CZ	6.53	132.74	123.60
1	A	535	PHE	CB-CG-CD1	-6.52	116.24	120.80
1	A	66	ASP	CB-CG-OD1	-6.50	112.45	118.30
1	A	276	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	358	LYS	N-CA-CB	6.42	122.16	110.60
1	A	322	ASP	CB-CG-OD1	6.40	124.06	118.30
1	A	738	ARG	NE-CZ-NH1	6.21	123.40	120.30
1	A	718	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	A	131	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	141	ASP	CB-CG-OD1	-6.04	112.87	118.30
1	A	170	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	A	147	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	57	SER	N-CA-CB	-6.00	101.50	110.50
1	A	58	ASP	CB-CG-OD2	6.00	123.70	118.30
1	A	371	ASP	CB-CG-OD2	5.97	123.67	118.30
1	A	249	ASN	CA-CB-CG	-5.97	100.28	113.40
1	A	530	ASP	CB-CG-OD2	5.96	123.67	118.30
1	A	735	GLU	N-CA-CB	5.94	121.30	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	443	SER	N-CA-CB	5.91	119.36	110.50
1	A	489	VAL	CB-CA-C	5.90	122.61	111.40
1	A	530	ASP	CB-CG-OD1	-5.86	113.02	118.30
1	A	700	ASP	CB-CG-OD2	5.79	123.52	118.30
1	A	707	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	535	PHE	CA-CB-CG	-5.67	100.28	113.90
1	A	518	ASP	CB-CG-OD1	5.66	123.39	118.30
1	A	58	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	A	58	ASP	CB-CA-C	-5.62	99.15	110.40
1	A	595	ASP	CB-CG-OD1	-5.61	113.25	118.30
1	A	583	ASP	CB-CG-OD2	5.57	123.31	118.30
1	A	320	ASP	CB-CG-OD1	-5.56	113.29	118.30
1	A	86	ASP	CB-CG-OD2	5.56	123.30	118.30
1	A	345	PHE	CB-CG-CD1	-5.52	116.94	120.80
1	A	620	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	164	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	A	403	ASP	CB-CG-OD2	5.39	123.15	118.30
1	A	35	ILE	CA-CB-CG2	5.39	121.67	110.90
1	A	298	LEU	CA-CB-CG	-5.36	102.97	115.30
1	A	602	ASP	CB-CG-OD2	-5.30	113.53	118.30
1	A	31	ASP	CB-CG-OD1	-5.29	113.54	118.30
1	A	86	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	A	484	HIS	CA-CB-CG	-5.25	104.68	113.60
1	A	538	ALA	N-CA-CB	5.25	117.44	110.10
1	A	40	ASP	CB-CG-OD1	-5.24	113.58	118.30
1	A	631	ALA	CB-CA-C	-5.24	102.24	110.10
1	A	31	ASP	CB-CG-OD2	5.23	123.01	118.30
1	A	669	ASP	CB-CG-OD2	5.22	123.00	118.30
1	A	7	ARG	NE-CZ-NH1	5.17	122.89	120.30
1	A	686	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	713	PRO	N-CA-CB	5.10	109.42	103.30
1	A	595	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	724	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	A	687	ILE	CB-CA-C	-5.04	101.52	111.60
1	A	76	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	47	TYR	CB-CA-C	-5.03	100.34	110.40

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	489	VAL	CA

There are no planarity outliers.

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	5865	0	5757	337	0
2	A	1	0	0	0	0
3	A	31	0	12	3	0
4	A	337	0	0	5	0
All	All	6234	0	5769	337	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 29.

All (337) 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:61:THR:HG23	1:A:71:GLN:HG2	1.17	1.10
1:A:290:ALA:HA	1:A:293:LYS:HD2	1.35	1.07
1:A:735:GLU:HA	1:A:738:ARG:HH21	1.19	1.02
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.42	1.01
1:A:735:GLU:HA	1:A:738:ARG:NH2	1.76	1.01
1:A:532:GLN:HE22	1:A:542:THR:CG2	1.75	0.98
1:A:219:ASN:N	1:A:220:PRO:HD2	1.82	0.93
1:A:62:PHE:HE1	1:A:72:VAL:HG12	1.34	0.92
1:A:286:ALA:HB1	1:A:321:GLU:HG3	1.48	0.91
1:A:742:THR:HG22	1:A:743:LYS:HD2	1.51	0.91
1:A:654:ARG:NH1	4:A:8067:HOH:O	2.02	0.91
1:A:735:GLU:CA	1:A:738:ARG:HH21	1.83	0.90
1:A:139:MET:HA	1:A:142:ILE:HD12	1.54	0.90
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.07	0.89
1:A:412:GLU:HG3	1:A:413:LYS:N	1.88	0.89
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.11	0.85
1:A:202:ARG:HH11	1:A:252:PHE:HB3	1.41	0.84
1:A:202:ARG:HH11	1:A:252:PHE:CB	1.91	0.82
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.15	0.82
1:A:61:THR:CG2	1:A:71:GLN:HG2	2.06	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:286:ALA:HB1	1:A:321:GLU:CG	2.11	0.81
1:A:286:ALA:CB	1:A:321:GLU:HG3	2.10	0.81
1:A:532:GLN:NE2	1:A:542:THR:CG2	2.42	0.81
1:A:61:THR:HG23	1:A:71:GLN:CG	2.08	0.81
1:A:730:LEU:HB2	1:A:732:ILE:HD12	1.62	0.81
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.11	0.81
1:A:538:ALA:HB1	1:A:542:THR:HG21	1.62	0.80
1:A:40:ASP:OD1	1:A:42:LYS:HB2	1.82	0.80
1:A:692:PHE:CE1	1:A:747:ARG:HG3	2.15	0.80
1:A:509:ASP:OD2	1:A:557:LYS:NZ	2.13	0.80
1:A:289:THR:OG1	1:A:292:GLU:HG3	1.82	0.79
1:A:87:GLY:H	1:A:105:ASN:ND2	1.79	0.79
1:A:580:GLU:HG3	1:A:582:GLN:OE1	1.82	0.79
1:A:395:GLU:HA	1:A:407:GLN:O	1.82	0.79
1:A:59:SER:CA	1:A:74:LYS:HG3	2.14	0.78
1:A:296:LEU:HB2	1:A:298:LEU:CD1	2.14	0.78
1:A:146:ARG:HD3	1:A:151:VAL:HG13	1.66	0.78
1:A:497:GLU:OE2	1:A:742:THR:HB	1.84	0.78
1:A:296:LEU:HB2	1:A:298:LEU:HD11	1.65	0.77
1:A:62:PHE:CE1	1:A:72:VAL:HG12	2.18	0.77
1:A:358:LYS:HG2	1:A:359:PHE:N	1.98	0.75
1:A:735:GLU:CA	1:A:738:ARG:NH2	2.45	0.75
1:A:397:ARG:HA	1:A:406:ALA:HA	1.68	0.75
1:A:210:VAL:O	1:A:214:GLN:HG3	1.88	0.74
1:A:385:ASN:OD1	1:A:386:PRO:HD2	1.85	0.74
1:A:288:ALA:O	1:A:293:LYS:HE2	1.87	0.74
1:A:290:ALA:CA	1:A:293:LYS:HD2	2.15	0.74
1:A:396:PRO:O	1:A:398:ILE:HD12	1.88	0.74
1:A:399:LEU:HD11	1:A:401:GLY:O	1.86	0.74
1:A:698:TYR:CZ	1:A:720:GLN:HG2	2.23	0.73
1:A:742:THR:CG2	1:A:743:LYS:HD2	2.17	0.73
1:A:732:ILE:HG22	1:A:737:PHE:CE2	2.24	0.73
1:A:412:GLU:HG3	1:A:413:LYS:H	1.54	0.73
1:A:35:ILE:HD12	1:A:35:ILE:O	1.88	0.73
1:A:692:PHE:CD1	1:A:747:ARG:HG2	2.25	0.72
1:A:289:THR:HB	1:A:291:GLU:CD	2.10	0.72
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.91	0.72
1:A:296:LEU:CB	1:A:298:LEU:HD11	2.19	0.71
1:A:300:GLY:HA3	1:A:302:GLU:OE2	1.90	0.71
1:A:27:LEU:O	4:A:8229:HOH:O	2.09	0.71
1:A:732:ILE:HG22	1:A:737:PHE:HE2	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:683:GLU:HG3	1:A:686:ARG:NH1	2.05	0.70
1:A:289:THR:HB	1:A:291:GLU:OE2	1.91	0.70
1:A:273:THR:O	1:A:274:THR:OG1	2.09	0.69
1:A:44:ARG:HG3	1:A:44:ARG:HH11	1.58	0.69
1:A:290:ALA:HA	1:A:293:LYS:CD	2.20	0.69
1:A:532:GLN:HE22	1:A:542:THR:HG21	1.57	0.69
1:A:40:ASP:HB3	1:A:43:GLU:HG2	1.73	0.68
1:A:319:SER:OG	1:A:322:ASP:HB2	1.94	0.68
1:A:249:ASN:H	1:A:249:ASN:ND2	1.74	0.67
1:A:532:GLN:NE2	1:A:542:THR:HG22	2.10	0.67
1:A:60:PHE:CD2	1:A:74:LYS:HA	2.29	0.67
1:A:399:LEU:HD12	1:A:401:GLY:H	1.59	0.66
1:A:692:PHE:CD1	1:A:747:ARG:CG	2.78	0.66
1:A:703:LYS:HD3	1:A:704:ARG:N	2.11	0.66
1:A:692:PHE:CZ	1:A:738:ARG:HG2	2.31	0.66
1:A:686:ARG:HA	1:A:689:ARG:NH1	2.11	0.65
1:A:491:GLN:O	1:A:495:LEU:HD22	1.96	0.65
1:A:532:GLN:HE22	1:A:538:ALA:HB1	1.62	0.65
1:A:51:GLU:O	1:A:62:PHE:HB2	1.98	0.64
1:A:72:VAL:HG22	1:A:73:LYS:O	1.97	0.64
1:A:329:GLN:O	1:A:332:ASP:HB2	1.96	0.64
1:A:87:GLY:H	1:A:105:ASN:HD21	1.45	0.64
1:A:710:PRO:HG2	1:A:729:HIS:CE1	2.33	0.63
1:A:710:PRO:HD2	1:A:729:HIS:CE1	2.33	0.63
1:A:336:PHE:O	1:A:341:GLN:NE2	2.30	0.62
1:A:98:ASN:O	1:A:102:VAL:HG23	1.98	0.62
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.79	0.62
1:A:614:ASP:OD1	1:A:615:PRO:HD2	1.99	0.62
1:A:181:SER:OG	3:A:999:AGS:O2G	2.14	0.62
1:A:64:THR:HG23	1:A:68:GLN:O	1.99	0.62
1:A:698:TYR:CE1	1:A:720:GLN:HG2	2.36	0.61
1:A:124:VAL:HG13	1:A:656:ILE:HD12	1.81	0.61
1:A:498:LYS:HG2	1:A:498:LYS:O	1.99	0.60
1:A:59:SER:N	1:A:74:LYS:HG3	2.16	0.60
1:A:59:SER:HA	1:A:74:LYS:HG3	1.84	0.60
1:A:706:TYR:HB2	1:A:712:VAL:HG12	1.84	0.60
1:A:742:THR:HG22	1:A:743:LYS:CD	2.27	0.60
1:A:137:GLN:O	1:A:137:GLN:HG3	2.02	0.59
1:A:484:HIS:O	1:A:487:PHE:HB3	2.02	0.59
1:A:34:TYR:CD1	1:A:51:GLU:HA	2.38	0.59
1:A:567:GLU:HB3	1:A:578:MET:CE	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:SER:O	1:A:341:GLN:HG3	2.02	0.59
1:A:593:GLN:HB2	1:A:596:LEU:HD12	1.84	0.59
1:A:45:ASP:CG	1:A:677:ARG:NH2	2.56	0.58
1:A:359:PHE:HB3	1:A:411:VAL:HG22	1.84	0.58
1:A:62:PHE:HE1	1:A:72:VAL:CG1	2.13	0.58
1:A:397:ARG:HD2	1:A:404:LEU:CD2	2.33	0.58
1:A:37:TYR:O	1:A:47:TYR:HA	2.03	0.58
1:A:753:ARG:O	1:A:756:GLU:HB2	2.03	0.58
1:A:491:GLN:O	1:A:495:LEU:HD13	2.02	0.58
1:A:709:ALA:HB2	1:A:726:VAL:HA	1.85	0.58
1:A:202:ARG:NH1	1:A:252:PHE:CB	2.66	0.58
1:A:523:PRO:HD2	4:A:8295:HOH:O	2.03	0.58
1:A:696:ILE:O	1:A:743:LYS:HA	2.03	0.58
1:A:703:LYS:CD	1:A:704:ARG:N	2.67	0.58
1:A:372:LYS:HE3	1:A:390:GLU:OE2	2.04	0.57
1:A:398:ILE:HD13	1:A:407:GLN:CG	2.33	0.57
1:A:6:ASP:OD1	1:A:8:THR:OG1	2.18	0.57
1:A:726:VAL:O	1:A:730:LEU:HG	2.04	0.57
1:A:31:ASP:OD1	1:A:31:ASP:N	2.37	0.57
1:A:399:LEU:HD12	1:A:401:GLY:N	2.20	0.57
1:A:59:SER:HB2	1:A:72:VAL:O	2.05	0.57
1:A:2:ASN:ND2	1:A:5:HIS:CE1	2.73	0.57
1:A:213:GLN:O	1:A:217:GLN:HG2	2.06	0.56
1:A:724:ASP:O	1:A:728:LYS:HB2	2.05	0.56
1:A:296:LEU:O	1:A:297:HIS:HB2	2.04	0.56
1:A:146:ARG:HD3	1:A:151:VAL:CG1	2.34	0.56
1:A:2:ASN:HD22	1:A:5:HIS:CE1	2.24	0.56
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.35	0.55
1:A:289:THR:O	1:A:291:GLU:N	2.39	0.55
1:A:487:PHE:O	1:A:491:GLN:HB2	2.06	0.55
1:A:289:THR:C	1:A:291:GLU:N	2.60	0.55
1:A:383:GLY:HA3	1:A:604:SER:OG	2.07	0.55
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.89	0.55
1:A:223:GLU:O	1:A:227:ASN:HB2	2.07	0.54
1:A:542:THR:HG22	1:A:543:LEU:N	2.22	0.54
1:A:36:TRP:CZ3	1:A:49:CYS:HB2	2.42	0.54
1:A:692:PHE:CD1	1:A:747:ARG:HG3	2.43	0.54
1:A:697:ILE:HB	1:A:700:ASP:OD2	2.07	0.54
1:A:730:LEU:CB	1:A:732:ILE:HD12	2.35	0.54
1:A:243:ILE:O	1:A:451:GLY:HA2	2.07	0.54
1:A:735:GLU:C	1:A:738:ARG:HH21	2.10	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:MET:HA	1:A:142:ILE:CD1	2.34	0.54
1:A:567:GLU:HB3	1:A:578:MET:HE2	1.90	0.54
1:A:698:TYR:OH	1:A:739:PHE:HD1	1.91	0.54
1:A:642:MET:O	1:A:646:GLU:OE1	2.26	0.54
1:A:319:SER:CB	1:A:322:ASP:HB2	2.38	0.54
1:A:723:THR:HG22	1:A:739:PHE:CZ	2.43	0.53
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.27	0.53
1:A:725:ALA:O	1:A:729:HIS:N	2.34	0.53
1:A:698:TYR:HE1	1:A:739:PHE:CE1	2.26	0.53
1:A:176:LEU:HD12	1:A:176:LEU:N	2.24	0.53
1:A:532:GLN:NE2	1:A:538:ALA:HB1	2.23	0.53
1:A:533:SER:O	1:A:589:LYS:HE3	2.09	0.53
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.26	0.53
1:A:397:ARG:HD2	1:A:404:LEU:HD21	1.91	0.53
1:A:327:THR:HG22	1:A:331:MET:HE2	1.91	0.53
1:A:60:PHE:N	1:A:72:VAL:O	2.33	0.52
1:A:732:ILE:CG2	1:A:737:PHE:HE2	2.21	0.52
1:A:72:VAL:CG2	1:A:73:LYS:N	2.72	0.52
1:A:43:GLU:HG3	1:A:43:GLU:O	2.10	0.52
1:A:3:PRO:HA	1:A:6:ASP:HB3	1.92	0.52
1:A:59:SER:OG	1:A:71:GLN:OE1	2.27	0.52
1:A:184:GLY:HA2	3:A:999:AGS:O1A	2.10	0.52
1:A:217:GLN:O	1:A:220:PRO:HG2	2.09	0.52
1:A:289:THR:C	1:A:291:GLU:H	2.12	0.51
1:A:700:ASP:O	1:A:703:LYS:HD2	2.10	0.51
1:A:35:ILE:HD13	1:A:37:TYR:HB3	1.92	0.51
1:A:293:LYS:HA	1:A:298:LEU:HD12	1.93	0.51
1:A:730:LEU:CB	1:A:732:ILE:CD1	2.88	0.51
1:A:735:GLU:HB3	1:A:738:ARG:HH22	1.74	0.51
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.44	0.51
1:A:710:PRO:HD2	1:A:729:HIS:NE2	2.26	0.51
1:A:354:LEU:O	1:A:418:ARG:HD3	2.10	0.51
1:A:692:PHE:CE1	1:A:747:ARG:CG	2.88	0.51
1:A:730:LEU:CD1	1:A:732:ILE:HD11	2.41	0.51
1:A:26:LYS:HA	1:A:29:VAL:HG23	1.92	0.51
1:A:730:LEU:HB2	1:A:732:ILE:CD1	2.39	0.50
1:A:738:ARG:N	1:A:745:PHE:O	2.37	0.50
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.47	0.50
1:A:544:ILE:HG13	1:A:544:ILE:O	2.12	0.50
1:A:202:ARG:NH1	1:A:252:PHE:HB2	2.27	0.50
1:A:535:PHE:N	1:A:535:PHE:CD2	2.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:SER:HA	3:A:999:AGS:S1G	2.52	0.49
1:A:597:GLU:OE1	1:A:612:PHE:HD2	1.94	0.49
1:A:456:SER:OG	1:A:457:GLY:O	2.29	0.49
1:A:43:GLU:CG	1:A:43:GLU:O	2.60	0.49
1:A:6:ASP:C	1:A:8:THR:H	2.16	0.49
1:A:375:LEU:O	1:A:379:SER:OG	2.30	0.49
1:A:756:GLU:OE2	4:A:8220:HOH:O	2.20	0.49
1:A:698:TYR:O	1:A:702:VAL:HG23	2.12	0.49
1:A:538:ALA:CB	1:A:542:THR:HG21	2.38	0.49
1:A:737:PHE:HB3	1:A:746:PHE:CD1	2.48	0.49
1:A:59:SER:HA	1:A:74:LYS:H	1.78	0.49
1:A:538:ALA:HB1	1:A:542:THR:CG2	2.39	0.49
1:A:202:ARG:HH11	1:A:252:PHE:HB2	1.76	0.48
1:A:385:ASN:O	1:A:388:VAL:N	2.45	0.48
1:A:750:GLN:O	1:A:750:GLN:NE2	2.45	0.48
1:A:269:VAL:HG12	1:A:306:TYR:CZ	2.48	0.48
1:A:540:ASP:HB3	1:A:581:ILE:HG23	1.95	0.48
1:A:532:GLN:OE1	1:A:542:THR:HG23	2.13	0.48
1:A:37:TYR:OH	1:A:65:SER:N	2.41	0.48
1:A:202:ARG:NH1	1:A:253:ILE:O	2.46	0.48
1:A:90:ASP:HB3	1:A:93:GLU:HG3	1.94	0.48
1:A:97:LEU:HB2	1:A:689:ARG:HD3	1.96	0.48
1:A:656:ILE:HD13	1:A:676:LEU:HD21	1.95	0.48
1:A:36:TRP:NE1	1:A:80:ARG:HG3	2.29	0.48
1:A:726:VAL:O	1:A:729:HIS:HB3	2.14	0.48
1:A:146:ARG:CD	1:A:151:VAL:CG1	2.92	0.48
1:A:495:LEU:N	1:A:495:LEU:CD1	2.75	0.48
1:A:682:LEU:O	1:A:686:ARG:HG3	2.14	0.47
1:A:308:ASN:C	1:A:308:ASN:OD1	2.53	0.47
1:A:732:ILE:CG2	1:A:737:PHE:CE2	2.93	0.47
1:A:2:ASN:O	1:A:5:HIS:N	2.41	0.47
1:A:53:VAL:HG23	1:A:62:PHE:HA	1.96	0.47
1:A:60:PHE:O	1:A:71:GLN:HA	2.13	0.47
1:A:738:ARG:HD3	1:A:738:ARG:HA	1.54	0.47
1:A:35:ILE:CD1	1:A:37:TYR:HD2	2.28	0.47
1:A:149:ASN:ND2	1:A:149:ASN:H	2.10	0.47
1:A:696:ILE:N	1:A:696:ILE:HD12	2.30	0.47
1:A:289:THR:HG1	1:A:292:GLU:HG3	1.79	0.47
1:A:35:ILE:HD11	1:A:37:TYR:HD2	1.80	0.47
1:A:185:LYS:HE3	1:A:456:SER:HA	1.97	0.47
1:A:32:LYS:HB3	1:A:34:TYR:CE2	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:TYR:CD1	1:A:720:GLN:HA	2.50	0.46
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.50	0.46
1:A:385:ASN:HB3	1:A:388:VAL:HG21	1.97	0.46
1:A:410:ASN:O	1:A:414:SER:HB2	2.15	0.46
1:A:238:ARG:HD3	1:A:264:GLU:OE1	2.15	0.46
1:A:386:PRO:O	1:A:390:GLU:HB2	2.16	0.46
1:A:62:PHE:CE1	1:A:72:VAL:CG1	2.95	0.46
1:A:410:ASN:OD1	1:A:410:ASN:C	2.54	0.46
1:A:358:LYS:NZ	1:A:359:PHE:O	2.38	0.46
1:A:341:GLN:O	1:A:345:PHE:CD2	2.69	0.46
1:A:568:PHE:CA	1:A:578:MET:HE1	2.46	0.46
1:A:181:SER:O	1:A:657:ILE:HD12	2.16	0.46
1:A:139:MET:CA	1:A:142:ILE:HD12	2.36	0.45
1:A:686:ARG:O	1:A:689:ARG:HB3	2.17	0.45
1:A:397:ARG:HD2	1:A:404:LEU:HD23	1.97	0.45
1:A:546:LYS:O	1:A:550:HIS:HD2	1.98	0.45
1:A:532:GLN:HB3	1:A:532:GLN:HE21	1.29	0.45
1:A:535:PHE:HA	1:A:536:PRO:HD2	1.69	0.45
1:A:628:LEU:HD11	1:A:632:ALA:HB1	1.98	0.45
1:A:362:GLY:O	1:A:363:ALA:C	2.54	0.45
1:A:60:PHE:HD2	1:A:74:LYS:HA	1.79	0.45
1:A:497:GLU:CD	1:A:742:THR:HB	2.37	0.45
1:A:377:ALA:O	1:A:381:VAL:HG22	2.16	0.45
1:A:710:PRO:CG	1:A:729:HIS:CE1	3.00	0.45
1:A:710:PRO:CD	1:A:729:HIS:CE1	2.99	0.45
1:A:735:GLU:O	1:A:738:ARG:NH2	2.50	0.45
1:A:362:GLY:O	1:A:364:GLY:N	2.50	0.45
1:A:590:ASP:N	1:A:591:PRO:HD3	2.32	0.45
1:A:345:PHE:HD1	1:A:345:PHE:HA	1.56	0.45
1:A:324:PHE:O	1:A:328:ARG:HB2	2.17	0.45
1:A:694:ASN:HB2	1:A:746:PHE:HB2	1.98	0.44
1:A:696:ILE:HG22	1:A:697:ILE:O	2.16	0.44
1:A:37:TYR:O	1:A:47:TYR:CA	2.65	0.44
1:A:683:GLU:HG3	1:A:686:ARG:HH12	1.80	0.44
1:A:124:VAL:CG1	1:A:656:ILE:HD12	2.46	0.44
1:A:2:ASN:HA	1:A:3:PRO:HD2	1.79	0.44
1:A:719:SER:HA	1:A:722:ALA:HB3	2.00	0.44
1:A:597:GLU:O	1:A:601:LYS:HG3	2.17	0.44
1:A:293:LYS:O	1:A:297:HIS:N	2.51	0.44
1:A:698:TYR:CE2	1:A:720:GLN:CG	3.01	0.44
1:A:621:ALA:HB2	1:A:628:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:692:PHE:CE2	1:A:738:ARG:HG2	2.52	0.44
1:A:358:LYS:CG	1:A:359:PHE:N	2.74	0.44
1:A:585:LEU:O	1:A:589:LYS:HG3	2.17	0.44
1:A:602:ASP:O	1:A:603:SER:C	2.56	0.44
1:A:87:GLY:N	1:A:105:ASN:HD21	2.12	0.43
1:A:628:LEU:HA	1:A:628:LEU:HD12	1.43	0.43
1:A:34:TYR:HE1	1:A:51:GLU:HB2	1.73	0.43
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.58	0.43
1:A:737:PHE:HB3	1:A:746:PHE:CE1	2.53	0.43
1:A:202:ARG:HD3	1:A:252:PHE:CB	2.48	0.43
1:A:319:SER:HB3	1:A:322:ASP:HB2	2.00	0.43
1:A:701:PHE:CE1	1:A:705:TYR:CD2	3.06	0.43
1:A:690:LYS:HE2	1:A:690:LYS:HB3	1.45	0.43
1:A:6:ASP:O	1:A:8:THR:N	2.52	0.43
1:A:597:GLU:OE1	1:A:612:PHE:CD2	2.72	0.43
1:A:691:GLY:O	1:A:747:ARG:CD	2.67	0.43
1:A:710:PRO:HG2	1:A:729:HIS:HE1	1.79	0.43
1:A:698:TYR:CE1	1:A:739:PHE:CE1	3.07	0.43
1:A:350:GLY:CA	1:A:381:VAL:HG21	2.49	0.43
1:A:96:TYR:OH	1:A:753:ARG:CZ	2.67	0.43
1:A:698:TYR:CZ	1:A:720:GLN:CG	3.00	0.42
1:A:94:LEU:O	1:A:97:LEU:HD11	2.19	0.42
1:A:146:ARG:HD2	1:A:151:VAL:HG11	2.01	0.42
1:A:38:ASN:HA	1:A:46:SER:O	2.19	0.42
1:A:610:LYS:HB3	1:A:610:LYS:HE2	1.67	0.42
1:A:219:ASN:H	1:A:220:PRO:HD2	1.78	0.42
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.72	0.42
1:A:399:LEU:HD12	1:A:400:ALA:N	2.34	0.42
1:A:132:ILE:HG22	1:A:134:ILE:HG23	2.00	0.42
1:A:60:PHE:CD2	1:A:74:LYS:HG2	2.55	0.42
1:A:385:ASN:HB3	1:A:388:VAL:HG23	2.01	0.42
1:A:232:ARG:HG2	1:A:232:ARG:NH1	2.34	0.42
1:A:348:ILE:HA	1:A:348:ILE:HD13	1.86	0.42
1:A:712:VAL:HG21	1:A:725:ALA:HB3	2.00	0.42
1:A:395:GLU:HG2	1:A:408:HIS:HA	2.00	0.42
1:A:693:PRO:HD2	1:A:747:ARG:HA	2.02	0.42
1:A:394:MET:HG2	1:A:414:SER:OG	2.19	0.42
1:A:300:GLY:O	1:A:304:PHE:CD2	2.72	0.42
1:A:495:LEU:HD13	1:A:495:LEU:H	1.84	0.42
1:A:521:GLN:HA	1:A:522:PRO:C	2.41	0.42
1:A:296:LEU:HB2	1:A:298:LEU:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:SER:HB3	1:A:752:ALA:HB2	2.02	0.42
1:A:688:THR:HA	4:A:8198:HOH:O	2.20	0.42
1:A:369:LEU:O	1:A:372:LYS:NZ	2.34	0.41
1:A:35:ILE:HD12	1:A:35:ILE:C	2.40	0.41
1:A:491:GLN:HB3	1:A:491:GLN:HE21	1.55	0.41
1:A:750:GLN:NE2	1:A:750:GLN:HA	2.35	0.41
1:A:91:MET:CE	1:A:106:LEU:HD13	2.50	0.41
1:A:222:LEU:HA	1:A:222:LEU:HD23	1.79	0.41
1:A:217:GLN:C	1:A:220:PRO:HG2	2.41	0.41
1:A:495:LEU:HD13	1:A:495:LEU:N	2.35	0.41
1:A:158:ILE:HG22	1:A:175:LEU:HD21	2.03	0.41
1:A:59:SER:C	1:A:74:LYS:HG3	2.41	0.41
1:A:289:THR:O	1:A:292:GLU:N	2.54	0.41
1:A:385:ASN:HA	1:A:386:PRO:HD3	1.94	0.41
1:A:488:LYS:HE3	1:A:488:LYS:HB2	1.84	0.41
1:A:693:PRO:HD2	1:A:746:PHE:O	2.20	0.41
1:A:289:THR:HB	1:A:291:GLU:OE1	2.20	0.41
1:A:698:TYR:CE1	1:A:739:PHE:CD1	3.09	0.41
1:A:372:LYS:O	1:A:376:ASN:CG	2.59	0.41
1:A:229:LYS:NZ	1:A:274:THR:O	2.52	0.41
1:A:702:VAL:HG13	1:A:712:VAL:HG11	2.03	0.41
1:A:542:THR:CG2	1:A:543:LEU:N	2.84	0.40
1:A:567:GLU:HA	1:A:579:TYR:O	2.22	0.40
1:A:138:GLU:H	1:A:138:GLU:CD	2.25	0.40
1:A:175:LEU:HG	1:A:651:HIS:HB2	2.03	0.40
1:A:40:ASP:HB3	1:A:43:GLU:CG	2.48	0.40
1:A:60:PHE:CE2	1:A:74:LYS:HG2	2.56	0.40
1:A:704:ARG:HG2	1:A:705:TYR:CZ	2.57	0.40
1:A:292:GLU:O	1:A:296:LEU:N	2.55	0.40
1:A:442:CYS:SG	1:A:443:SER:N	2.95	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	733/762 (96%)	695 (95%)	33 (4%)	5 (1%)	26	21

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	ALA
1	A	711	ASN
1	A	7	ARG
1	A	290	ALA
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	629/666 (94%)	560 (89%)	69 (11%)	8	4

All (69) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	24	LEU
1	A	28	THR
1	A	31	ASP
1	A	32	LYS
1	A	44	ARG
1	A	46	SER
1	A	56	THR
1	A	57	SER
1	A	66	ASP
1	A	71	GLN
1	A	72	VAL
1	A	83	ILE
1	A	95	SER

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Mol	Chain	Res	Type
1	A	97	LEU
1	A	150	GLU
1	A	158	ILE
1	A	198	SER
1	A	202	ARG
1	A	219	ASN
1	A	238	ARG
1	A	249	ASN
1	A	266	SER
1	A	285	LEU
1	A	291	GLU
1	A	303	SER
1	A	316	LYS
1	A	328	ARG
1	A	342	MET
1	A	360	GLU
1	A	368	VAL
1	A	370	LYS
1	A	372	LYS
1	A	375	LEU
1	A	379	SER
1	A	399	LEU
1	A	408	HIS
1	A	412	GLU
1	A	414	SER
1	A	436	LYS
1	A	446	LYS
1	A	471	ILE
1	A	489	VAL
1	A	491	GLN
1	A	495	LEU
1	A	499	ILE
1	A	509	ASP
1	A	510	SER
1	A	542	THR
1	A	544	ILE
1	A	546	LYS
1	A	553	LYS
1	A	565	LYS
1	A	609	THR
1	A	610	LYS
1	A	619	SER

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Mol	Chain	Res	Type
1	A	640	SER
1	A	646	GLU
1	A	666	LYS
1	A	669	ASP
1	A	690	LYS
1	A	703	LYS
1	A	721	LYS
1	A	728	LYS
1	A	735	GLU
1	A	738	ARG
1	A	743	LYS
1	A	744	ILE
1	A	753	ARG

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

Mol	Chain	Res	Type
1	A	105	ASN
1	A	149	ASN
1	A	219	ASN
1	A	234	ASN
1	A	249	ASN
1	A	283	GLN
1	A	329	GLN
1	A	407	GLN
1	A	439	ASN
1	A	491	GLN
1	A	532	GLN
1	A	594	GLN
1	A	606	ASN
1	A	613	ASN
1	A	662	GLN
1	A	729	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no 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	AGS	A	999	2	24,33,33	1.74	3 (12%)	28,52,52	1.97	5 (17%)

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	AGS	A	999	2	-	0/15/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	AGS	O4'-C1'	-3.44	1.36	1.41
3	A	999	AGS	C6-N6	-3.13	1.25	1.34
3	A	999	AGS	PG-S1G	5.93	2.02	1.90

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	AGS	N3-C2-N1	-6.44	123.96	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	AGS	C1'-N9-C4	-4.16	120.67	126.94
3	A	999	AGS	C2'-C3'-C4'	-2.63	97.21	102.61
3	A	999	AGS	O3'-C3'-C2'	2.74	120.73	111.83
3	A	999	AGS	C2-N1-C6	3.68	125.35	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	AGS	3	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, 95th 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	741/762 (97%)	0.66	112 (15%) 3 4	12, 37, 84, 100	0

All (112) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	56	THR	6.5
1	A	710	PRO	6.3
1	A	53	VAL	6.2
1	A	444	GLU	5.9
1	A	494	TYR	5.6
1	A	715	ASP	5.5
1	A	25	PHE	5.4
1	A	737	PHE	5.3
1	A	500	ASN	5.2
1	A	67	GLY	5.2
1	A	498	LYS	5.1
1	A	706	TYR	5.0
1	A	443	SER	5.0
1	A	27	LEU	4.9
1	A	59	SER	4.9
1	A	68	GLN	4.8
1	A	495	LEU	4.6
1	A	707	ASP	4.5
1	A	716	ALA	4.5
1	A	66	ASP	4.5
1	A	362	GLY	4.4
1	A	65	SER	4.3
1	A	497	GLU	4.3
1	A	708	LEU	4.2
1	A	61	THR	4.1
1	A	348	ILE	4.0
1	A	405	VAL	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	499	ILE	3.8
1	A	72	VAL	3.8
1	A	537	ASN	3.7
1	A	5	HIS	3.6
1	A	725	ALA	3.4
1	A	742	THR	3.4
1	A	366	GLY	3.3
1	A	743	LYS	3.3
1	A	711	ASN	3.3
1	A	23	ASP	3.3
1	A	744	ILE	3.3
1	A	42	LYS	3.2
1	A	429	LEU	3.2
1	A	39	PRO	3.2
1	A	70	ARG	3.1
1	A	709	ALA	3.1
1	A	713	PRO	3.1
1	A	717	GLU	3.1
1	A	496	LYS	3.1
1	A	280	ILE	3.1
1	A	734	PRO	3.1
1	A	426	TYR	3.0
1	A	536	PRO	3.0
1	A	225	PHE	2.9
1	A	338	GLN	2.9
1	A	698	TYR	2.9
1	A	294	LYS	2.9
1	A	26	LYS	2.9
1	A	62	PHE	2.9
1	A	689	ARG	2.9
1	A	58	ASP	2.8
1	A	404	LEU	2.8
1	A	77	ALA	2.8
1	A	40	ASP	2.8
1	A	2	ASN	2.8
1	A	723	THR	2.8
1	A	735	GLU	2.8
1	A	347	ILE	2.8
1	A	158	ILE	2.7
1	A	30	SER	2.7
1	A	365	GLU	2.7
1	A	728	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	24	LEU	2.7
1	A	508	LEU	2.6
1	A	402	ARG	2.6
1	A	367	ALA	2.6
1	A	401	GLY	2.5
1	A	712	VAL	2.5
1	A	399	LEU	2.5
1	A	316	LYS	2.5
1	A	57	SER	2.5
1	A	718	ASP	2.5
1	A	29	VAL	2.5
1	A	4	ILE	2.5
1	A	222	LEU	2.4
1	A	124	VAL	2.4
1	A	288	ALA	2.4
1	A	74	LYS	2.4
1	A	705	TYR	2.4
1	A	364	GLY	2.4
1	A	31	ASP	2.3
1	A	703	LYS	2.3
1	A	724	ASP	2.3
1	A	351	ILE	2.3
1	A	60	PHE	2.3
1	A	726	VAL	2.3
1	A	202	ARG	2.2
1	A	730	LEU	2.2
1	A	406	ALA	2.2
1	A	76	ASP	2.2
1	A	177	ILE	2.2
1	A	740	GLY	2.2
1	A	509	ASP	2.2
1	A	28	THR	2.1
1	A	106	LEU	2.1
1	A	615	PRO	2.1
1	A	44	ARG	2.1
1	A	714	ARG	2.1
1	A	422	VAL	2.1
1	A	727	LEU	2.1
1	A	653	VAL	2.1
1	A	319	SER	2.1
1	A	155	ILE	2.0
1	A	370	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	692	PHE	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, 95th 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(\AA^2)	Q<0.9
3	AGS	A	999	31/31	0.94	0.14	0.76	11,38,100,100	0
2	MG	A	998	1/1	0.99	0.05	-2.89	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.