



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2014 – 12:57 AM GMT

PDB ID : 1D0Y
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH O-NITROPHENYL AMINOETHYLDIPHOSPHA
TEBERYLLIUM FLUORIDE.
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
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

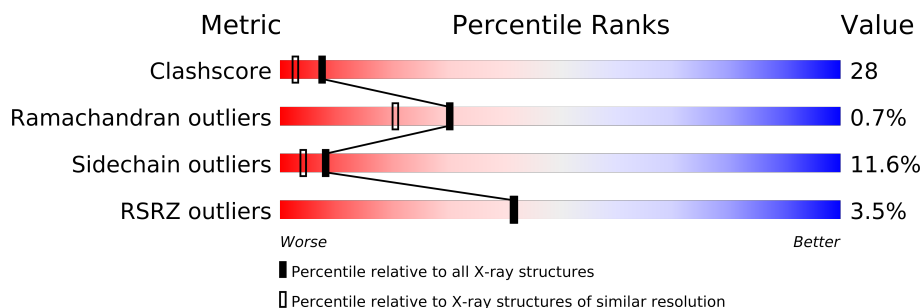
The following versions of software and data (see [references](#)) were used in the production of this report:

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 ≥ 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 6623 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 S1DC MOTOR DOMAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	741	Total	C	N	O	S	0	0	0
			5889	3745	1014	1114	16			

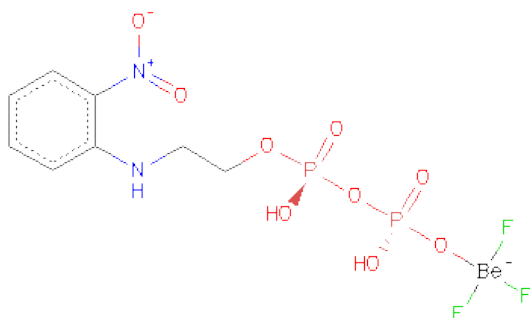
There are 3 discrepancies between the modelled and reference sequences:

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-NITROPHENYL AMINOETHYLDIPHOSPHATEBERYLLIUM TRIFLUORIDE (three-letter code: ONP) (formula: C₈H₁₁BeF₃N₂O₉P₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	Be	C	F	N	O	P	0	0
			25	1	8	3	2	9	2		

- Molecule 4 is water.

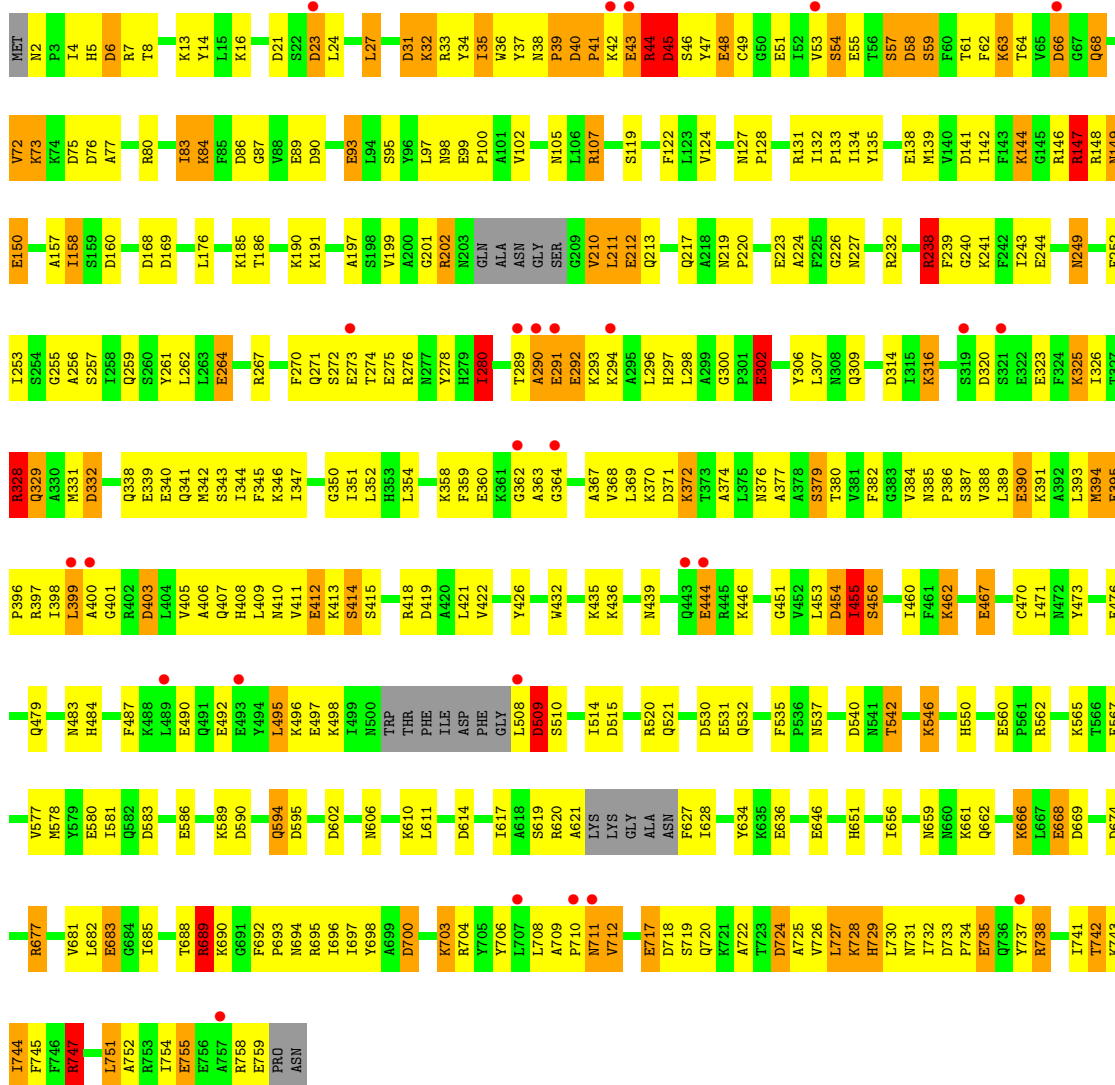
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	708	Total O 708 708	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: MYOSIN S1DC MOTOR DOMAIN

Chain A: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.80Å 180.30Å 54.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 19.95 – 2.01	Depositor EDS
% Data completeness (in resolution range)	86.6 (25.00-2.00) 84.6 (19.95-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.01Å)	Xtriage
Refinement program	TNT V. 5-E	Depositor
R, R_{free}	0.178 , (Not available) 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.45 , 126.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 58085 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6623	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 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

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

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	1.05	36/6001 (0.6%)	1.51	98/8102 (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 (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	668	GLU	CD-OE2	9.01	1.35	1.25
1	A	531	GLU	CD-OE2	8.92	1.35	1.25
1	A	89	GLU	CD-OE2	8.30	1.34	1.25
1	A	390	GLU	CD-OE2	7.47	1.33	1.25
1	A	51	GLU	CD-OE2	7.33	1.33	1.25
1	A	683	GLU	CD-OE2	7.19	1.33	1.25
1	A	412	GLU	CD-OE2	7.17	1.33	1.25
1	A	275	GLU	CD-OE2	7.12	1.33	1.25
1	A	735	GLU	CD-OE2	7.01	1.33	1.25
1	A	291	GLU	CD-OE2	7.00	1.33	1.25
1	A	55	GLU	CD-OE2	6.76	1.33	1.25
1	A	444	GLU	CD-OE2	6.76	1.33	1.25
1	A	567	GLU	CD-OE2	6.61	1.32	1.25
1	A	360	GLU	CD-OE2	6.51	1.32	1.25
1	A	717	GLU	CD-OE2	6.49	1.32	1.25
1	A	492	GLU	CD-OE2	6.48	1.32	1.25
1	A	302	GLU	CD-OE2	6.47	1.32	1.25
1	A	646	GLU	CD-OE2	6.23	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	395	GLU	CD-OE2	6.20	1.32	1.25
1	A	212	GLU	CD-OE2	6.11	1.32	1.25
1	A	244	GLU	CD-OE2	6.01	1.32	1.25
1	A	467	GLU	CD-OE2	5.94	1.32	1.25
1	A	586	GLU	CD-OE2	5.86	1.32	1.25
1	A	490	GLU	CD-OE2	5.77	1.32	1.25
1	A	476	GLU	CD-OE2	5.66	1.31	1.25
1	A	755	GLU	CD-OE2	5.64	1.31	1.25
1	A	636	GLU	CD-OE2	5.61	1.31	1.25
1	A	264	GLU	CD-OE1	-5.55	1.19	1.25
1	A	560	GLU	CD-OE2	5.49	1.31	1.25
1	A	580	GLU	CD-OE2	5.48	1.31	1.25
1	A	292	GLU	CD-OE2	5.43	1.31	1.25
1	A	339	GLU	CD-OE2	5.40	1.31	1.25
1	A	93	GLU	CD-OE2	5.24	1.31	1.25
1	A	497	GLU	CD-OE2	5.21	1.31	1.25
1	A	340	GLU	CD-OE2	5.19	1.31	1.25
1	A	48	GLU	CD-OE2	5.06	1.31	1.25

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	ARG	NE-CZ-NH1	11.26	125.93	120.30
1	A	238	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	A	276	ARG	NE-CZ-NH1	10.47	125.53	120.30
1	A	238	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	A	131	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	A	700	ASP	CB-CG-OD2	-8.77	110.41	118.30
1	A	66	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	A	314	ASP	CB-CG-OD2	-8.66	110.51	118.30
1	A	620	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	A	669	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	A	58	ASP	CB-CG-OD1	8.05	125.55	118.30
1	A	590	ASP	CB-CG-OD2	-7.95	111.14	118.30
1	A	148	ARG	NE-CZ-NH2	-7.90	116.35	120.30
1	A	419	ASP	CB-CG-OD1	7.88	125.40	118.30
1	A	419	ASP	CB-CG-OD2	-7.82	111.26	118.30
1	A	135	TYR	CB-CG-CD1	-7.72	116.37	121.00
1	A	169	ASP	CB-CG-OD1	7.66	125.20	118.30
1	A	328	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	A	168	ASP	CB-CG-OD2	-7.31	111.72	118.30
1	A	21	ASP	CB-CG-OD2	-7.25	111.78	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	6	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	A	23	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	620	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	332	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	157	ALA	N-CA-CB	7.06	119.99	110.10
1	A	168	ASP	CB-CG-OD1	7.06	124.65	118.30
1	A	724	ASP	CB-CG-OD2	-6.95	112.04	118.30
1	A	148	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	A	267	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	A	314	ASP	CB-CG-OD1	6.86	124.48	118.30
1	A	689	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	A	634	TYR	CB-CG-CD1	-6.82	116.91	121.00
1	A	520	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	A	76	ASP	CB-CG-OD2	-6.74	112.23	118.30
1	A	677	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	A	703	LYS	CB-CA-C	6.64	123.68	110.40
1	A	371	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	33	ARG	NE-CZ-NH1	6.49	123.54	120.30
1	A	724	ASP	CB-CG-OD1	6.32	123.99	118.30
1	A	44	ARG	NE-CZ-NH2	6.25	123.42	120.30
1	A	729	HIS	CA-CB-CG	-6.25	102.98	113.60
1	A	131	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	A	276	ARG	NE-CZ-NH2	-6.22	117.19	120.30
1	A	718	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	A	23	ASP	CB-CG-OD1	6.21	123.89	118.30
1	A	75	ASP	CB-CG-OD2	-6.20	112.72	118.30
1	A	58	ASP	CB-CG-OD2	-6.18	112.73	118.30
1	A	7	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	602	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	107	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	A	700	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	455	ILE	CA-CB-CG2	6.10	123.09	110.90
1	A	332	ASP	CB-CG-OD1	6.08	123.77	118.30
1	A	515	ASP	CB-CG-OD1	6.07	123.77	118.30
1	A	31	ASP	CB-CG-OD1	6.02	123.72	118.30
1	A	371	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	147	ARG	NE-CZ-NH2	-5.95	117.33	120.30
1	A	320	ASP	CB-CG-OD1	5.94	123.64	118.30
1	A	674	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	249	ASN	CA-CB-CG	-5.90	100.42	113.40
1	A	595	ASP	CB-CG-OD2	-5.88	113.01	118.30
1	A	562	ARG	NE-CZ-NH2	-5.81	117.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	747	ARG	NE-CZ-NH1	-5.75	117.42	120.30
1	A	160	ASP	CB-CG-OD1	5.75	123.47	118.30
1	A	320	ASP	CB-CG-OD2	-5.73	113.15	118.30
1	A	669	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	590	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	509	ASP	CB-CA-C	-5.71	98.97	110.40
1	A	583	ASP	CB-CG-OD1	5.70	123.43	118.30
1	A	45	ASP	CA-C-N	-5.67	104.72	117.20
1	A	43	GLU	O-C-N	-5.60	113.74	122.70
1	A	232	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	403	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	606	ASN	CB-CA-C	5.54	121.48	110.40
1	A	141	ASP	CB-CG-OD1	5.54	123.28	118.30
1	A	509	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	6	ASP	CB-CG-OD1	5.45	123.20	118.30
1	A	76	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	122	PHE	CB-CA-C	-5.43	99.55	110.40
1	A	614	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	328	ARG	NE-CZ-NH2	-5.37	117.61	120.30
1	A	66	ASP	CB-CG-OD1	5.32	123.09	118.30
1	A	530	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	717	GLU	N-CA-CB	5.25	120.05	110.60
1	A	454	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	583	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	614	ASP	CB-CG-OD2	-5.19	113.62	118.30
1	A	141	ASP	CB-CG-OD2	-5.18	113.63	118.30
1	A	435	LYS	CB-CA-C	5.17	120.73	110.40
1	A	75	ASP	CB-CG-OD1	5.14	122.93	118.30
1	A	119	SER	N-CA-CB	5.13	118.20	110.50
1	A	520	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	712	VAL	N-CA-C	5.12	124.82	111.00
1	A	57	SER	N-CA-CB	-5.10	102.85	110.50
1	A	602	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	280	ILE	CB-CA-C	-5.09	101.41	111.60
1	A	530	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	31	ASP	CB-CG-OD2	-5.03	113.78	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	ASP	Mainchain

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	5889	0	5792	323	0
2	A	1	0	0	0	0
3	A	25	0	9	1	0
4	A	708	0	0	40	0
All	All	6623	0	5801	324	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 28.

All (324) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.19	1.18
1:A:40:ASP:HB3	1:A:42:LYS:HB2	1.29	1.10
1:A:35:ILE:HD11	1:A:77:ALA:HB1	1.27	1.08
1:A:342:MET:HG3	1:A:346:LYS:HE3	1.44	0.99
1:A:40:ASP:C	1:A:42:LYS:H	1.67	0.96
1:A:2:ASN:HB3	1:A:5:HIS:HD2	1.32	0.94
1:A:53:VAL:HG11	1:A:63:LYS:HD2	1.48	0.93
1:A:62:PHE:HE2	1:A:72:VAL:HG22	1.31	0.92
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.72	0.91
1:A:290:ALA:HA	1:A:293:LYS:HD2	1.50	0.91
1:A:35:ILE:HD11	1:A:77:ALA:CB	2.00	0.91
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.00	0.90
1:A:40:ASP:CB	1:A:42:LYS:HB2	2.02	0.90
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.04	0.88
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.09	0.85
1:A:737:TYR:CE1	4:A:1460:HOH:O	2.30	0.85
1:A:395:GLU:HA	1:A:407:GLN:O	1.76	0.84
1:A:219:ASN:HB3	4:A:1642:HOH:O	1.76	0.84
1:A:2:ASN:HB3	1:A:5:HIS:CD2	2.13	0.83
1:A:397:ARG:HA	1:A:406:ALA:HA	1.57	0.83
1:A:594:GLN:HE21	1:A:594:GLN:HA	1.43	0.83
1:A:147:ARG:HG3	1:A:150:GLU:OE1	1.80	0.82
1:A:191:LYS:HA	1:A:191:LYS:HE2	1.62	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:147:ARG:HB2	1:A:149:ASN:ND2	1.96	0.80
1:A:202:ARG:NH1	1:A:252:PHE:HB3	1.96	0.80
1:A:144:LYS:HD3	4:A:1130:HOH:O	1.83	0.78
1:A:734:PRO:HA	1:A:737:TYR:CZ	2.19	0.78
1:A:249:ASN:ND2	4:A:1255:HOH:O	2.14	0.77
1:A:84:LYS:HE2	1:A:704:ARG:CZ	2.15	0.77
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.15	0.77
1:A:202:ARG:HH11	1:A:252:PHE:HB3	1.47	0.76
1:A:735:GLU:O	1:A:738:ARG:NH2	2.19	0.76
1:A:97:LEU:HB2	1:A:689:ARG:HD3	1.67	0.76
1:A:40:ASP:HB3	1:A:42:LYS:CB	2.15	0.75
1:A:147:ARG:HB2	1:A:149:ASN:HD21	1.51	0.74
1:A:410:ASN:OD1	1:A:413:LYS:HB2	1.89	0.73
1:A:722:ALA:O	1:A:725:ALA:HB3	1.87	0.73
1:A:289:THR:HG23	1:A:292:GLU:OE2	1.89	0.72
1:A:40:ASP:C	1:A:42:LYS:N	2.40	0.72
1:A:399:LEU:HD11	1:A:401:GLY:O	1.87	0.72
1:A:149:ASN:HD22	1:A:150:GLU:N	1.87	0.72
1:A:40:ASP:O	1:A:42:LYS:N	2.24	0.71
1:A:62:PHE:CE2	1:A:72:VAL:HG22	2.21	0.71
1:A:62:PHE:HE2	1:A:72:VAL:CG2	2.04	0.70
1:A:342:MET:HG3	1:A:346:LYS:CE	2.19	0.70
1:A:697:ILE:HB	1:A:700:ASP:OD1	1.91	0.70
1:A:546:LYS:NZ	4:A:1507:HOH:O	2.25	0.69
1:A:99:GLU:OE2	4:A:1390:HOH:O	2.10	0.69
1:A:302:GLU:H	1:A:302:GLU:CD	1.95	0.69
1:A:495:LEU:HD12	4:A:1223:HOH:O	1.92	0.69
1:A:202:ARG:HG3	4:A:1175:HOH:O	1.91	0.68
1:A:176:LEU:HD12	1:A:176:LEU:N	2.09	0.68
1:A:662:GLN:NE2	4:A:1139:HOH:O	2.26	0.68
1:A:343:SER:O	1:A:347:ILE:HG13	1.94	0.68
1:A:328:ARG:HD2	4:A:1459:HOH:O	1.93	0.67
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.76	0.67
1:A:249:ASN:H	1:A:249:ASN:ND2	1.91	0.67
1:A:342:MET:HE3	1:A:342:MET:HA	1.78	0.66
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.76	0.66
1:A:42:LYS:O	1:A:43:GLU:HG3	1.96	0.66
1:A:87:GLY:H	1:A:105:ASN:ND2	1.93	0.66
1:A:84:LYS:HE2	1:A:704:ARG:NE	2.11	0.66
1:A:362:GLY:O	1:A:364:GLY:N	2.29	0.65
1:A:496:LYS:NZ	1:A:496:LYS:HB3	2.10	0.65
1:A:64:THR:HG23	1:A:68:GLN:O	1.97	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:484:HIS:O	1:A:487:PHE:HB3	1.97	0.64
1:A:627:PHE:N	4:A:1426:HOH:O	2.30	0.64
1:A:185:LYS:HE3	1:A:456:SER:HA	1.79	0.64
1:A:241:LYS:H	1:A:455:ILE:HD12	1.63	0.64
1:A:202:ARG:HH11	1:A:202:ARG:HG3	1.62	0.63
1:A:38:ASN:C	1:A:40:ASP:H	2.01	0.63
1:A:344:ILE:HD11	1:A:432:TRP:HZ3	1.63	0.62
1:A:698:TYR:CZ	1:A:720:GLN:HG2	2.33	0.62
1:A:59:SER:HB2	1:A:72:VAL:O	1.99	0.62
1:A:202:ARG:NH1	1:A:252:PHE:CB	2.62	0.62
1:A:462:LYS:HG2	4:A:1572:HOH:O	1.99	0.62
1:A:35:ILE:CD1	1:A:77:ALA:HB1	2.17	0.62
1:A:138:GLU:O	1:A:142:ILE:HD12	1.99	0.61
1:A:331:MET:CE	1:A:345:PHE:HZ	2.14	0.61
1:A:453:LEU:CD1	1:A:455:ILE:HD13	2.30	0.61
1:A:47:TYR:CE1	1:A:100:PRO:HG3	2.35	0.61
1:A:58:ASP:HA	4:A:1238:HOH:O	2.00	0.61
1:A:238:ARG:HD3	1:A:264:GLU:OE2	2.01	0.61
1:A:724:ASP:OD2	1:A:728:LYS:HD2	2.01	0.61
1:A:138:GLU:HB3	4:A:1632:HOH:O	2.00	0.60
1:A:224:ALA:O	1:A:280:ILE:HG13	2.00	0.60
1:A:290:ALA:CA	1:A:293:LYS:HD2	2.29	0.60
1:A:594:GLN:HE21	1:A:594:GLN:CA	2.13	0.60
1:A:62:PHE:CE2	1:A:72:VAL:CG2	2.81	0.60
1:A:698:TYR:CE1	1:A:720:GLN:HG3	2.37	0.60
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.37	0.60
1:A:40:ASP:HB3	1:A:42:LYS:H	1.67	0.59
1:A:158:ILE:HD11	1:A:651:HIS:HB3	1.83	0.59
1:A:147:ARG:O	1:A:150:GLU:HB2	2.01	0.59
1:A:202:ARG:HG3	1:A:202:ARG:NH1	2.16	0.59
1:A:432:TRP:CZ2	1:A:436:LYS:HE2	2.37	0.58
1:A:191:LYS:HE2	1:A:191:LYS:CA	2.33	0.58
1:A:397:ARG:C	1:A:398:ILE:HD12	2.23	0.58
1:A:139:MET:HA	1:A:142:ILE:HD12	1.86	0.58
1:A:399:LEU:HD12	1:A:400:ALA:N	2.19	0.57
1:A:331:MET:CE	1:A:345:PHE:CZ	2.87	0.57
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.86	0.57
1:A:280:ILE:N	1:A:280:ILE:HD12	2.18	0.57
1:A:316:LYS:HB2	1:A:316:LYS:NZ	2.16	0.57
1:A:149:ASN:ND2	1:A:150:GLU:N	2.52	0.57
3:A:999:ONP:NA3	3:A:999:ONP:O2B	2.38	0.56
1:A:40:ASP:OD2	1:A:42:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.88	0.56
1:A:710:PRO:HG3	1:A:729:HIS:CE1	2.40	0.56
1:A:391:LYS:HE3	4:A:1613:HOH:O	2.06	0.56
1:A:379:SER:HB2	1:A:386:PRO:HG3	1.87	0.56
1:A:496:LYS:HG3	4:A:1353:HOH:O	2.06	0.56
1:A:32:LYS:HB3	1:A:34:TYR:CE2	2.40	0.56
1:A:124:VAL:HG13	1:A:656:ILE:CD1	2.36	0.56
1:A:621:ALA:HB2	1:A:628:ILE:HG12	1.88	0.56
1:A:550:HIS:HD2	4:A:1076:HOH:O	1.89	0.56
1:A:40:ASP:CG	1:A:42:LYS:HB2	2.27	0.56
1:A:399:LEU:HD12	1:A:399:LEU:C	2.25	0.56
1:A:398:ILE:HD13	1:A:407:GLN:CG	2.36	0.55
1:A:710:PRO:HD3	1:A:729:HIS:CG	2.40	0.55
1:A:758:ARG:HA	4:A:1236:HOH:O	2.05	0.55
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.87	0.55
1:A:362:GLY:HA3	4:A:1567:HOH:O	2.06	0.55
1:A:698:TYR:CD1	1:A:720:GLN:HG3	2.42	0.55
1:A:331:MET:HE3	1:A:345:PHE:CZ	2.42	0.55
1:A:2:ASN:CB	1:A:5:HIS:HD2	2.13	0.54
1:A:733:ASP:OD2	1:A:734:PRO:HD2	2.07	0.54
1:A:83:ILE:HD11	4:A:1421:HOH:O	2.08	0.54
1:A:532:GLN:OE1	1:A:542:THR:HB	2.06	0.54
1:A:692:PHE:CD1	1:A:747:ARG:HG2	2.42	0.54
1:A:399:LEU:HD13	1:A:403:ASP:O	2.08	0.54
1:A:201:GLY:HA2	1:A:212:GLU:OE2	2.06	0.54
1:A:385:ASN:HB3	1:A:388:VAL:HB	1.90	0.54
1:A:84:LYS:HG3	1:A:704:ARG:NH2	2.23	0.54
1:A:737:TYR:O	1:A:738:ARG:NE	2.36	0.53
1:A:202:ARG:N	1:A:212:GLU:OE2	2.37	0.53
1:A:202:ARG:HH11	1:A:202:ARG:CG	2.20	0.53
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.43	0.53
1:A:219:ASN:HD21	1:A:243:ILE:CD1	2.22	0.53
1:A:197:ALA:HA	1:A:253:ILE:HD11	1.91	0.53
1:A:372:LYS:O	1:A:376:ASN:ND2	2.42	0.53
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.43	0.53
1:A:385:ASN:HB3	1:A:388:VAL:CB	2.38	0.53
1:A:302:GLU:HG2	4:A:1651:HOH:O	2.09	0.53
1:A:217:GLN:NE2	4:A:1451:HOH:O	2.26	0.53
1:A:95:SER:HB3	1:A:752:ALA:HB2	1.90	0.53
1:A:694:ASN:C	1:A:695:ARG:HG3	2.29	0.53
1:A:149:ASN:HD22	1:A:150:GLU:H	1.55	0.53
1:A:331:MET:HE1	1:A:345:PHE:HZ	1.73	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:186:THR:HG22	1:A:190:LYS:HE3	1.91	0.53
1:A:399:LEU:HD11	1:A:401:GLY:C	2.30	0.52
1:A:367:ALA:O	1:A:408:HIS:HE1	1.91	0.52
1:A:6:ASP:OD1	1:A:8:THR:HG23	2.09	0.52
1:A:219:ASN:CB	4:A:1642:HOH:O	2.45	0.52
1:A:698:TYR:CZ	1:A:720:GLN:CG	2.91	0.52
1:A:540:ASP:HB3	1:A:581:ILE:HG23	1.90	0.52
1:A:359:PHE:HB3	1:A:411:VAL:HG22	1.91	0.52
1:A:730:LEU:HB2	1:A:732:ILE:HG12	1.91	0.52
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.50	0.52
1:A:219:ASN:HD21	1:A:243:ILE:HD13	1.75	0.52
1:A:436:LYS:O	1:A:439:ASN:HB2	2.10	0.51
1:A:132:ILE:HG22	1:A:134:ILE:HG23	1.91	0.51
1:A:410:ASN:O	1:A:414:SER:HB2	2.10	0.51
1:A:41:PRO:C	1:A:43:GLU:H	2.07	0.51
1:A:2:ASN:HD21	1:A:146:ARG:NH2	2.08	0.51
1:A:309:GLN:HB2	4:A:1174:HOH:O	2.09	0.51
1:A:226:GLY:HA3	1:A:239:PHE:CE2	2.47	0.50
1:A:210:VAL:CG2	1:A:211:LEU:N	2.74	0.50
1:A:2:ASN:ND2	1:A:5:HIS:NE2	2.60	0.50
1:A:710:PRO:O	1:A:711:ASN:ND2	2.44	0.50
1:A:384:VAL:O	1:A:386:PRO:HD3	2.11	0.50
1:A:296:LEU:O	1:A:297:HIS:HB2	2.12	0.50
1:A:342:MET:HA	1:A:342:MET:CE	2.42	0.49
1:A:62:PHE:HD1	1:A:63:LYS:O	1.95	0.49
1:A:709:ALA:HB2	1:A:726:VAL:HA	1.94	0.49
1:A:273:GLU:O	1:A:274:THR:OG1	2.15	0.49
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.47	0.49
1:A:2:ASN:CB	1:A:5:HIS:CD2	2.91	0.49
1:A:398:ILE:HD12	1:A:398:ILE:N	2.27	0.49
1:A:698:TYR:CE2	1:A:720:GLN:HG2	2.46	0.49
1:A:710:PRO:CG	1:A:729:HIS:CE1	2.95	0.49
1:A:38:ASN:O	1:A:40:ASP:N	2.45	0.49
1:A:708:LEU:HD23	1:A:759:GLU:HA	1.94	0.49
1:A:241:LYS:N	1:A:455:ILE:CD1	2.75	0.49
1:A:698:TYR:CE1	1:A:720:GLN:CG	2.95	0.49
1:A:403:ASP:HB3	1:A:405:VAL:HG23	1.94	0.49
1:A:508:LEU:O	1:A:509:ASP:HB2	2.12	0.49
1:A:521:GLN:OE1	4:A:1671:HOH:O	2.20	0.49
1:A:683:GLU:HG3	4:A:1181:HOH:O	2.12	0.49
1:A:107:ARG:NE	4:A:1187:HOH:O	2.39	0.49
1:A:688:THR:HG22	1:A:693:PRO:HB3	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:668:GLU:OE1	4:A:1666:HOH:O	2.20	0.48
1:A:2:ASN:N	4:A:1362:HOH:O	2.46	0.48
1:A:243:ILE:O	1:A:451:GLY:HA2	2.13	0.48
1:A:238:ARG:CD	1:A:264:GLU:OE2	2.61	0.48
1:A:496:LYS:NZ	1:A:496:LYS:CB	2.77	0.48
1:A:390:GLU:HG2	1:A:394:MET:CE	2.44	0.48
1:A:535:PHE:N	1:A:535:PHE:CD2	2.82	0.48
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.49	0.48
1:A:367:ALA:O	1:A:408:HIS:CE1	2.67	0.48
1:A:697:ILE:O	1:A:700:ASP:HB2	2.13	0.48
1:A:23:ASP:OD1	1:A:23:ASP:N	2.45	0.48
1:A:289:THR:O	1:A:292:GLU:N	2.46	0.47
1:A:496:LYS:HB3	1:A:496:LYS:HZ3	1.78	0.47
1:A:710:PRO:HD3	1:A:729:HIS:CE1	2.48	0.47
1:A:212:GLU:OE2	4:A:1175:HOH:O	2.20	0.47
1:A:692:PHE:CE1	1:A:747:ARG:CG	2.97	0.47
1:A:241:LYS:N	1:A:455:ILE:HD12	2.29	0.47
1:A:240:GLY:HA3	1:A:455:ILE:HG13	1.97	0.47
1:A:316:LYS:HB2	1:A:316:LYS:HE3	1.65	0.47
1:A:730:LEU:O	1:A:731:ASN:HB3	2.14	0.47
1:A:323:GLU:O	1:A:326:ILE:HB	2.15	0.47
1:A:127:ASN:OD1	1:A:128:PRO:HD2	2.15	0.47
1:A:202:ARG:NH2	4:A:1461:HOH:O	2.48	0.47
1:A:619:SER:HB3	1:A:627:PHE:CD2	2.49	0.47
1:A:36:TRP:CZ3	1:A:49:CYS:HB2	2.49	0.46
1:A:666:LYS:NZ	4:A:1182:HOH:O	2.47	0.46
1:A:454:ASP:O	1:A:455:ILE:HD12	2.15	0.46
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.15	0.46
1:A:38:ASN:ND2	1:A:46:SER:O	2.43	0.46
1:A:737:TYR:C	1:A:737:TYR:CD1	2.88	0.46
1:A:744:ILE:HD13	1:A:745:PHE:N	2.31	0.46
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.50	0.46
1:A:255:GLY:O	1:A:256:ALA:HB2	2.15	0.46
1:A:280:ILE:HD11	1:A:426:TYR:OH	2.15	0.46
1:A:726:VAL:O	1:A:730:LEU:HG	2.16	0.46
1:A:16:LYS:HB3	1:A:16:LYS:HE3	1.83	0.45
1:A:479:GLN:HE21	1:A:483:ASN:ND2	2.13	0.45
1:A:83:ILE:CD1	1:A:86:ASP:OD1	2.64	0.45
1:A:578:MET:HE2	1:A:578:MET:HB3	1.72	0.45
1:A:510:SER:O	1:A:514:ILE:HG13	2.17	0.45
1:A:710:PRO:HD3	1:A:729:HIS:CD2	2.51	0.45
1:A:379:SER:CB	1:A:386:PRO:HG3	2.46	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:210:VAL:HG13	1:A:210:VAL:H	1.31	0.45
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.82	0.45
1:A:37:TYR:O	1:A:47:TYR:HA	2.17	0.45
1:A:27:LEU:HA	1:A:27:LEU:HD12	1.77	0.45
1:A:594:GLN:HB2	4:A:1664:HOH:O	2.17	0.45
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.99	0.45
1:A:90:ASP:HB3	1:A:93:GLU:HG3	1.99	0.44
1:A:144:LYS:HD2	1:A:199:VAL:HG12	1.99	0.44
1:A:724:ASP:OD2	1:A:728:LYS:HE2	2.17	0.44
1:A:410:ASN:OD1	1:A:413:LYS:N	2.47	0.44
1:A:34:TYR:CD1	1:A:49:CYS:SG	3.10	0.44
1:A:149:ASN:N	1:A:149:ASN:HD22	2.14	0.44
1:A:54:SER:OG	1:A:61:THR:HB	2.17	0.44
1:A:470:CYS:O	1:A:473:TYR:HB3	2.18	0.44
1:A:4:ILE:CG2	1:A:4:ILE:O	2.65	0.43
1:A:201:GLY:CA	1:A:212:GLU:OE2	2.66	0.43
1:A:354:LEU:O	1:A:418:ARG:HD3	2.17	0.43
1:A:362:GLY:C	1:A:364:GLY:N	2.70	0.43
1:A:68:GLN:HB3	1:A:68:GLN:HE21	1.60	0.43
1:A:619:SER:HB3	1:A:627:PHE:CE2	2.53	0.43
1:A:409:LEU:HB3	1:A:413:LYS:HB3	2.00	0.43
1:A:698:TYR:HB3	1:A:719:SER:HB3	1.99	0.43
1:A:191:LYS:CE	1:A:191:LYS:CA	2.96	0.43
1:A:59:SER:CB	1:A:72:VAL:O	2.65	0.43
1:A:202:ARG:CG	1:A:202:ARG:NH1	2.82	0.43
1:A:498:LYS:HG2	1:A:498:LYS:O	2.18	0.43
1:A:611:LEU:HA	1:A:617:ILE:HG21	2.01	0.43
1:A:692:PHE:CE1	1:A:747:ARG:HG2	2.53	0.43
1:A:389:LEU:O	1:A:393:LEU:HG	2.19	0.43
1:A:24:LEU:HD23	1:A:24:LEU:N	2.34	0.43
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.84	0.43
1:A:44:ARG:O	1:A:45:ASP:OD2	2.37	0.43
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.49	0.43
1:A:158:ILE:CD1	1:A:651:HIS:HB3	2.47	0.43
1:A:690:LYS:NZ	4:A:1198:HOH:O	2.51	0.43
1:A:460:ILE:HG12	1:A:577:VAL:HG22	2.01	0.43
1:A:98:ASN:O	1:A:102:VAL:HG23	2.18	0.42
1:A:399:LEU:HD12	1:A:401:GLY:N	2.34	0.42
1:A:453:LEU:HD12	1:A:455:ILE:HD13	2.00	0.42
1:A:379:SER:HB3	1:A:386:PRO:HD3	2.01	0.42
1:A:471:ILE:HA	1:A:471:ILE:HD12	1.85	0.42
1:A:396:PRO:HG2	1:A:398:ILE:HD11	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:610:LYS:HA	1:A:610:LYS:HD2	1.76	0.42
1:A:289:THR:O	1:A:291:GLU:N	2.51	0.42
1:A:325:LYS:HA	1:A:325:LYS:HD3	1.76	0.42
1:A:374:ALA:O	1:A:377:ALA:HB3	2.19	0.42
1:A:35:ILE:HD13	4:A:1251:HOH:O	2.20	0.42
1:A:217:GLN:C	1:A:220:PRO:HD2	2.39	0.42
1:A:144:LYS:NZ	4:A:1593:HOH:O	2.53	0.42
1:A:87:GLY:H	1:A:105:ASN:HD21	1.65	0.42
1:A:710:PRO:CD	1:A:729:HIS:CE1	3.02	0.42
1:A:453:LEU:HD11	1:A:455:ILE:HD13	2.00	0.42
1:A:190:LYS:HE2	1:A:223:GLU:OE2	2.20	0.42
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.85	0.42
1:A:692:PHE:O	1:A:695:ARG:NE	2.38	0.42
1:A:467:GLU:H	1:A:467:GLU:CD	2.22	0.42
1:A:73:LYS:HA	1:A:73:LYS:HD2	1.49	0.42
1:A:249:ASN:N	1:A:249:ASN:ND2	2.63	0.42
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.55	0.42
1:A:39:PRO:HG3	1:A:48:GLU:HG2	2.02	0.42
1:A:289:THR:O	1:A:289:THR:OG1	2.37	0.41
1:A:737:TYR:HE1	4:A:1460:HOH:O	1.88	0.41
1:A:300:GLY:HA3	1:A:302:GLU:OE2	2.20	0.41
1:A:59:SER:HB2	1:A:73:LYS:HD2	2.03	0.41
1:A:354:LEU:HD13	1:A:421:LEU:HD23	2.02	0.41
1:A:537:ASN:HB2	4:A:1282:HOH:O	2.19	0.41
1:A:681:VAL:O	1:A:685:ILE:HG13	2.20	0.41
1:A:696:ILE:O	1:A:743:LYS:HB3	2.20	0.41
1:A:627:PHE:CA	4:A:1426:HOH:O	2.68	0.41
1:A:316:LYS:NZ	1:A:316:LYS:CB	2.78	0.41
1:A:223:GLU:O	1:A:227:ASN:HB2	2.20	0.41
1:A:306:TYR:O	1:A:307:LEU:HD23	2.20	0.41
1:A:293:LYS:O	1:A:297:HIS:N	2.53	0.41
1:A:99:GLU:HB2	1:A:100:PRO:HD3	2.03	0.41
1:A:706:TYR:HE1	4:A:1676:HOH:O	2.03	0.41
1:A:270:PHE:C	1:A:271:GLN:HG3	2.41	0.41
1:A:138:GLU:OE2	1:A:138:GLU:N	2.49	0.41
1:A:741:ILE:C	1:A:742:THR:CG2	2.87	0.41
1:A:329:GLN:O	1:A:332:ASP:HB2	2.21	0.41
1:A:147:ARG:HG3	1:A:150:GLU:CD	2.39	0.41
1:A:344:ILE:HD11	1:A:432:TRP:CZ3	2.50	0.41
1:A:341:GLN:O	1:A:345:PHE:CD2	2.74	0.41
1:A:696:ILE:N	1:A:696:ILE:HD12	2.35	0.41
1:A:727:LEU:HD12	1:A:727:LEU:HA	1.65	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:415:SER:O	1:A:418:ARG:HB3	2.21	0.41
1:A:197:ALA:HA	1:A:253:ILE:CD1	2.50	0.40
1:A:278:TYR:HB3	1:A:280:ILE:HD11	2.03	0.40
1:A:415:SER:OG	1:A:418:ARG:NH2	2.45	0.40
1:A:659:ASN:OD1	1:A:661:LYS:N	2.52	0.40
1:A:754:ILE:HG22	1:A:755:GLU:N	2.36	0.40
1:A:134:ILE:HA	1:A:139:MET:HG3	2.03	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	733/761 (96%)	690 (94%)	38 (5%)	5 (1%)	30	20

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	ALA
1	A	711	ASN
1	A	290	ALA
1	A	41	PRO
1	A	39	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	631/665 (95%)	558 (88%)	73 (12%)	8	4

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	27	LEU
1	A	31	ASP
1	A	32	LYS
1	A	35	ILE
1	A	40	ASP
1	A	44	ARG
1	A	54	SER
1	A	57	SER
1	A	59	SER
1	A	63	LYS
1	A	66	ASP
1	A	68	GLN
1	A	72	VAL
1	A	73	LYS
1	A	83	ILE
1	A	84	LYS
1	A	144	LYS
1	A	147	ARG
1	A	149	ASN
1	A	150	GLU
1	A	158	ILE
1	A	202	ARG
1	A	210	VAL
1	A	211	LEU
1	A	213	GLN
1	A	238	ARG
1	A	257	SER
1	A	262	LEU
1	A	272	SER
1	A	280	ILE
1	A	294	LYS
1	A	302	GLU
1	A	316	LYS
1	A	325	LYS
1	A	328	ARG
1	A	329	GLN
1	A	338	GLN
1	A	358	LYS
1	A	368	VAL
1	A	370	LYS
1	A	372	LYS

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Mol	Chain	Res	Type
1	A	379	SER
1	A	380	THR
1	A	387	SER
1	A	394	MET
1	A	399	LEU
1	A	412	GLU
1	A	414	SER
1	A	444	GLU
1	A	446	LYS
1	A	455	ILE
1	A	456	SER
1	A	462	LYS
1	A	495	LEU
1	A	509	ASP
1	A	542	THR
1	A	546	LYS
1	A	565	LYS
1	A	589	LYS
1	A	594	GLN
1	A	666	LYS
1	A	689	ARG
1	A	703	LYS
1	A	712	VAL
1	A	717	GLU
1	A	727	LEU
1	A	728	LYS
1	A	738	ARG
1	A	742	THR
1	A	744	ILE
1	A	747	ARG
1	A	751	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	105	ASN
1	A	149	ASN
1	A	219	ASN
1	A	234	ASN
1	A	249	ASN
1	A	259	GLN

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Mol	Chain	Res	Type
1	A	283	GLN
1	A	376	ASN
1	A	408	HIS
1	A	439	ASN
1	A	483	ASN
1	A	491	GLN
1	A	521	GLN
1	A	550	HIS
1	A	594	GLN
1	A	711	ASN
1	A	729	HIS

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	ONP	A	999	2	24,25,25	1.53	4 (16%)	30,37,37	1.42	3 (10%)

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	ONP	A	999	2	-	0/18/24/24	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ONP	PB-OB3	4.85	1.61	1.51
3	A	999	ONP	F2-BE	-2.72	1.49	1.55
3	A	999	ONP	F1-BE	-2.12	1.50	1.55
3	A	999	ONP	C6-C1	-2.05	1.36	1.39

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	ONP	CA2-NA3-C1	-4.55	110.89	122.95
3	A	999	ONP	O2B-N2-O2A	3.04	127.51	121.35
3	A	999	ONP	C3-C2-N2	2.75	120.57	116.61

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, 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	741/761 (97%)	-0.31	26 (3%)	42 41	14, 36, 80, 100	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	5.6
1	A	707	LEU	4.0
1	A	508	LEU	3.9
1	A	364	GLY	3.8
1	A	443	GLN	3.6
1	A	444	GLU	3.4
1	A	362	GLY	3.3
1	A	319	SER	3.2
1	A	42	LYS	3.1
1	A	399	LEU	2.9
1	A	294	LYS	2.8
1	A	290	ALA	2.8
1	A	710	PRO	2.7
1	A	53	VAL	2.7
1	A	711	ASN	2.7
1	A	489	LEU	2.5
1	A	321	SER	2.4
1	A	291	GLU	2.3
1	A	757	ALA	2.3
1	A	43	GLU	2.2
1	A	273	GLU	2.2
1	A	23	ASP	2.2
1	A	493	GLU	2.1
1	A	289	THR	2.0
1	A	66	ASP	2.0
1	A	400	ALA	2.0

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	ONP	A	999	25/25	0.07	-0.36	12,20,35,79	0
2	MG	A	998	1/1	0.03	-1.80	19,19,19,19	0

6.5 Other polymers

There are no such residues in this entry.