



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:47 AM EDT

PDB ID : 1D0Y / pdb_00001d0y
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH O-NITROPHENYL AMINOETHYLDIPHOSPHA
TE BERYLLIUM 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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

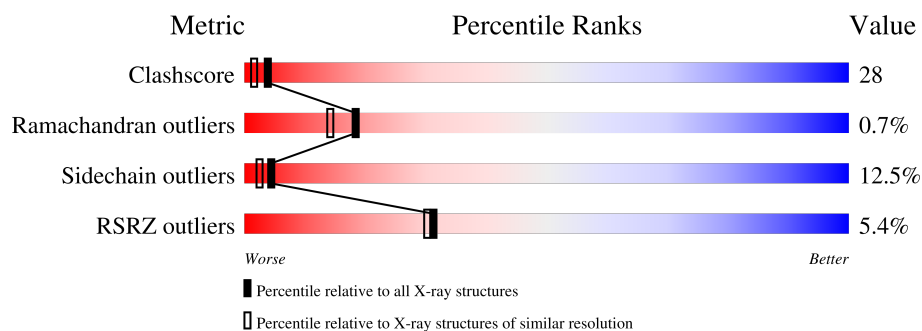
1 Overall quality at a glance

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	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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 6623 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 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			

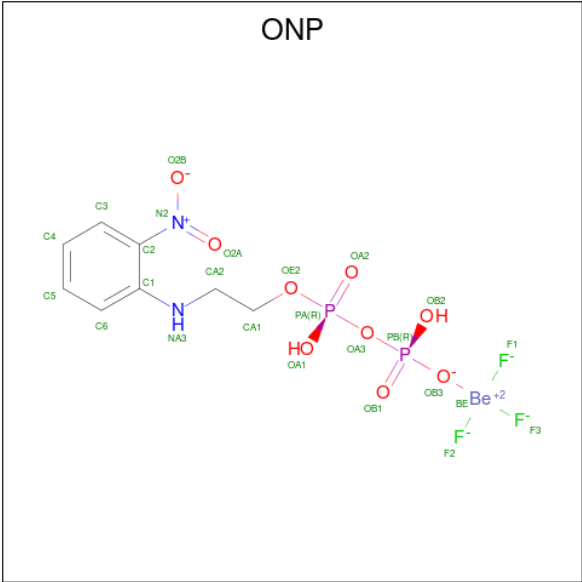
There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is O-NITROPHENYL AMINOETHYLDIPHOSPHATE BERYLLIUM TRIFLUORIDE (CCD ID: ONP) (formula: $C_8H_{11}BeF_3N_2O_9P_2$).



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

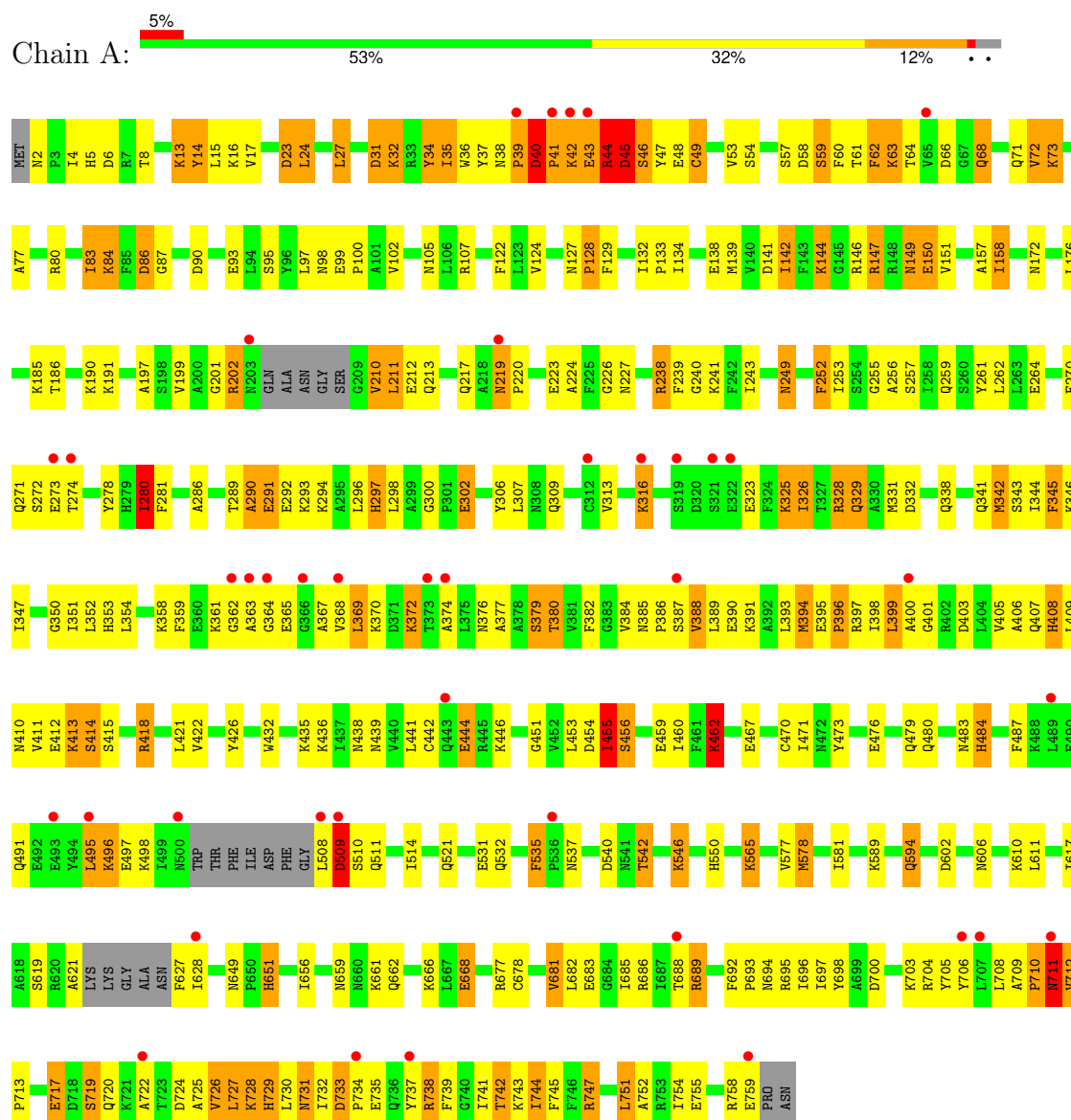
- Molecule 4 is water.

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

3 Residue-property plots

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

• Molecule 1: MYOSIN S1DC MOTOR DOMAIN



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 25.00 – 2.01	Depositor EDS
% Data completeness (in resolution range)	86.6 (25.00-2.00) 84.0 (25.00-2.01)	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 5E	Depositor
R, R_{free}	0.178 , (Not available) 0.190 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
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 , 147.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.25	7/6001 (0.1%)	1.82	97/8102 (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 (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	361	LYS	CA-C	-7.44	1.49	1.53
1	A	44	ARG	N-CA	7.08	1.53	1.46
1	A	480	GLN	CA-C	5.45	1.60	1.52
1	A	668	GLU	CD-OE2	5.37	1.35	1.25
1	A	531	GLU	CD-OE2	5.32	1.35	1.25
1	A	46	SER	N-CA	-5.29	1.39	1.46
1	A	238	ARG	CD-NE	-5.26	1.38	1.46

All (97) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	249	ASN	CA-CB-CG	-12.18	100.42	112.60
1	A	729	HIS	CA-CB-CG	-10.82	102.98	113.80
1	A	43	GLU	O-C-N	-10.75	113.74	123.41
1	A	42	LYS	N-CA-C	-9.61	102.17	112.93
1	A	535	PHE	CA-CB-CG	-9.44	104.36	113.80
1	A	711	ASN	CA-CB-CG	9.40	122.00	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	ASN	CA-CB-CG	-8.90	103.70	112.60
1	A	31	ASP	CA-CB-CG	8.81	121.41	112.60
1	A	484	HIS	CA-CB-CG	-8.57	105.23	113.80
1	A	441	LEU	N-CA-C	8.23	120.33	111.36
1	A	280	ILE	CB-CA-C	-8.11	101.41	112.04
1	A	49	CYS	CA-C-N	-7.96	114.86	122.66
1	A	49	CYS	C-N-CA	-7.96	114.86	122.66
1	A	705	TYR	N-CA-C	7.54	122.61	112.88
1	A	455	ILE	CA-CB-CG2	7.41	123.09	110.50
1	A	712	VAL	N-CA-C	7.38	124.82	108.88
1	A	129	PHE	CA-CB-CG	-7.34	106.46	113.80
1	A	678	CYS	N-CA-C	7.27	120.25	111.82
1	A	408	HIS	CA-CB-CG	-7.21	106.59	113.80
1	A	45	ASP	O-C-N	7.21	129.95	122.09
1	A	219	ASN	O-C-N	-7.13	113.12	121.32
1	A	45	ASP	CA-C-N	-7.00	113.06	122.72
1	A	45	ASP	C-N-CA	-7.00	113.06	122.72
1	A	361	LYS	O-C-N	6.99	127.45	121.65
1	A	157	ALA	N-CA-CB	6.88	119.99	110.01
1	A	345	PHE	CA-CB-CG	-6.86	106.94	113.80
1	A	703	LYS	CB-CA-C	6.82	123.68	110.46
1	A	62	PHE	CA-CB-CG	-6.73	107.07	113.80
1	A	34	TYR	N-CA-C	6.51	119.71	110.14
1	A	711	ASN	CA-C-N	6.48	134.12	122.13
1	A	711	ASN	C-N-CA	6.48	134.12	122.13
1	A	14	TYR	N-CA-C	6.38	121.15	113.23
1	A	717	GLU	N-CA-CB	6.33	120.05	110.30
1	A	380	THR	N-CA-CB	6.20	119.00	110.01
1	A	40	ASP	O-C-N	-6.10	114.31	121.32
1	A	535	PHE	O-C-N	6.06	126.93	121.35
1	A	361	LYS	CB-CA-C	-6.02	107.68	116.53
1	A	509	ASP	CB-CA-C	-5.99	98.97	110.65
1	A	281	PHE	CA-CB-CG	-5.94	107.86	113.80
1	A	122	PHE	CB-CA-C	-5.88	99.55	109.83
1	A	476	GLU	CB-CA-C	-5.87	100.87	110.85
1	A	435	LYS	CB-CA-C	5.81	120.73	110.85
1	A	462	LYS	N-CA-C	-5.80	104.86	111.07
1	A	606	ASN	CB-CA-C	5.63	121.48	110.67
1	A	606	ASN	N-CA-CB	5.56	118.89	110.28
1	A	365	GLU	CA-C-N	5.55	127.63	120.64
1	A	365	GLU	C-N-CA	5.55	127.63	120.64
1	A	739	PHE	CA-C-N	-5.55	115.66	122.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	739	PHE	C-N-CA	-5.55	115.66	122.15
1	A	651	HIS	CA-CB-CG	-5.54	108.26	113.80
1	A	31	ASP	CA-C-N	5.53	128.95	121.05
1	A	31	ASP	C-N-CA	5.53	128.95	121.05
1	A	733	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	649	ASN	N-CA-C	-5.49	98.81	108.69
1	A	17	VAL	N-CA-C	-5.49	101.65	108.89
1	A	297	HIS	CA-CB-CG	-5.46	108.34	113.80
1	A	388	VAL	N-CA-CB	-5.44	102.41	110.58
1	A	141	ASP	N-CA-C	5.44	117.21	111.28
1	A	442	CYS	N-CA-C	5.40	118.06	109.96
1	A	151	VAL	N-CA-CB	-5.37	105.00	112.52
1	A	733	ASP	CA-C-N	5.36	125.43	119.32
1	A	733	ASP	C-N-CA	5.36	125.43	119.32
1	A	731	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	280	ILE	N-CA-CB	5.35	117.15	110.47
1	A	24	LEU	CB-CA-C	5.34	118.30	109.70
1	A	128	PRO	CB-CA-C	-5.32	102.79	111.56
1	A	511	GLN	N-CA-C	5.30	117.47	111.11
1	A	286	ALA	CA-C-N	5.28	126.99	120.34
1	A	286	ALA	C-N-CA	5.28	126.99	120.34
1	A	444	GLU	N-CA-C	-5.27	106.85	113.28
1	A	15	LEU	CA-C-N	-5.26	113.96	122.81
1	A	15	LEU	C-N-CA	-5.26	113.96	122.81
1	A	353	HIS	CA-CB-CG	-5.26	108.54	113.80
1	A	418	ARG	CD-NE-CZ	-5.26	117.04	124.40
1	A	438	ASN	CA-CB-CG	-5.23	107.37	112.60
1	A	60	PHE	CA-CB-CG	5.22	119.02	113.80
1	A	713	PRO	N-CA-CB	5.21	108.72	103.25
1	A	476	GLU	N-CA-C	-5.18	105.71	111.36
1	A	602	ASP	CA-CB-CG	5.18	117.78	112.60
1	A	142	ILE	CB-CA-C	-5.16	103.91	112.26
1	A	710	PRO	N-CA-CB	5.16	106.16	102.65
1	A	535	PHE	CA-C-N	5.13	125.17	119.32
1	A	535	PHE	C-N-CA	5.13	125.17	119.32
1	A	565	LYS	CB-CA-C	-5.12	101.51	110.17
1	A	313	VAL	N-CA-C	-5.12	108.13	113.10
1	A	365	GLU	N-CA-C	-5.11	107.08	113.72
1	A	396	PRO	CB-CA-C	-5.11	104.29	110.98
1	A	681	VAL	N-CA-C	5.09	115.31	110.42
1	A	491	GLN	CB-CG-CD	-5.07	103.98	112.60
1	A	13	LYS	CA-C-O	5.07	126.14	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	719	SER	N-CA-C	5.05	117.17	111.11
1	A	86	ASP	CA-CB-CG	-5.05	107.55	112.60
1	A	726	VAL	O-C-N	5.05	126.99	121.94
1	A	280	ILE	N-CA-C	5.02	116.34	110.62
1	A	509	ASP	CA-CB-CG	5.02	117.62	112.60
1	A	238	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	A	252	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	ASP	Mainchain

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	5889	0	5792	332	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	333	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 28.

All (333) 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: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:40:ASP:C	1:A:42:LYS:H	1.67	1.00
1:A:342:MET:HG3	1:A:346:LYS:HE3	1.44	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.00	0.95
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.72	0.95
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: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:HA	1:A:594:GLN:HE21	1.43	0.83
1:A:147:ARG:HG3	1:A:150:GLU:OE1	1.80	0.82
1:A:342:MET:HE3	1:A:342:MET:HA	1.59	0.82
1:A:191:LYS:HA	1:A:191:LYS:HE2	1.62	0.82
1:A:331:MET:HE1	1:A:345:PHE:HZ	1.44	0.80
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:40:ASP:C	1:A:42:LYS:N	2.40	0.75
1:A:147:ARG:HB2	1:A:149:ASN:HD21	1.51	0.74
1:A:302:GLU:H	1:A:302:GLU:CD	1.95	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:99:GLU:OE2	4:A:1390:HOH:O	2.10	0.69
1:A:546:LYS:NZ	4:A:1507:HOH:O	2.25	0.69
1:A:495:LEU:HD12	4:A:1223:HOH:O	1.92	0.69
1:A:176:LEU:N	1:A:176:LEU:HD12	2.09	0.68
1:A:202:ARG:HG3	4:A:1175:HOH:O	1.91	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:38:ASN:C	1:A:40:ASP:H	2.01	0.67
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.76	0.67
1:A:249:ASN:ND2	1:A:249:ASN:H	1.91	0.67
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
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:397:ARG:C	1:A:398:ILE:HD12	2.23	0.63
1:A:41:PRO:C	1:A:43:GLU:H	2.07	0.62
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:GLU:HB3	4:A:1632:HOH:O	2.00	0.60
1:A:40:ASP:CG	1:A:42:LYS:HB2	2.27	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:399:LEU:C	1:A:399:LEU:HD12	2.25	0.59
1:A:147:ARG:O	1:A:150:GLU:HB2	2.01	0.59
1:A:202:ARG:NH1	1:A:202:ARG:HG3	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: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:694:ASN:C	1:A:695:ARG:HG3	2.29	0.57
1:A:280:ILE:N	1:A:280:ILE:HD12	2.18	0.57
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.86	0.57
1:A:316:LYS:HB2	1:A:316:LYS:NZ	2.16	0.57
1:A:399:LEU:HD11	1:A:401:GLY:C	2.30	0.57
1:A:149:ASN:ND2	1:A:150:GLU:N	2.52	0.57
1:A:331:MET:CE	1:A:345:PHE:HZ	2.14	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
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:32:LYS:HB3	1:A:34:TYR:CE2	2.40	0.56
1:A:496:LYS:HG3	4:A:1353:HOH:O	2.06	0.56
1:A:124:VAL:HG13	1:A:656:ILE:CD1	2.36	0.56
1:A:550:HIS:HD2	4:A:1076:HOH:O	1.89	0.56
1:A:621:ALA:HB2	1:A:628:ILE:HG12	1.88	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:362:GLY:HA3	4:A:1567:HOH:O	2.06	0.55
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.87	0.55
1:A:698:TYR:CD1	1:A:720:GLN:HG3	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:197:ALA:HA	1:A:253:ILE:HD11	1.91	0.53
1:A:219:ASN:HD21	1:A:243:ILE:CD1	2.22	0.53
1:A:372:LYS:O	1:A:376:ASN:ND2	2.42	0.53
1:A:95:SER:HB3	1:A:752:ALA:HB2	1.90	0.53
1:A:217:GLN:NE2	4:A:1451:HOH:O	2.26	0.53
1:A:302:GLU:HG2	4:A:1651:HOH:O	2.09	0.53
1:A:385:ASN:HB3	1:A:388:VAL:CB	2.38	0.53
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.43	0.53
1:A:149:ASN:HD22	1:A:150:GLU:H	1.55	0.53
1:A:186:THR:HG22	1:A:190:LYS:HE3	1.91	0.53
1:A:6:ASP:OD1	1:A:8:THR:HG23	2.09	0.52
1:A:367:ALA:O	1:A:408:HIS:HE1	1.91	0.52
1:A:219:ASN:CB	4:A:1642:HOH:O	2.45	0.52
1:A:540:ASP:HB3	1:A:581:ILE:HG23	1.90	0.52
1:A:698:TYR:CZ	1:A:720:GLN:CG	2.91	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:38:ASN:C	1:A:40:ASP:N	2.69	0.51
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:737:TYR:CD1	1:A:737:TYR:C	2.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:62:PHE:HD1	1:A:63:LYS:O	1.95	0.49
1:A:273:GLU:O	1:A:274:THR:OG1	2.15	0.49
1:A:709:ALA:HB2	1:A:726:VAL:HA	1.94	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:668:GLU:OE1	4:A:1666:HOH:O	2.20	0.48
1:A:688:THR:HG22	1:A:693:PRO:HB3	1.95	0.48
1:A:2:ASN:N	4:A:1362:HOH:O	2.46	0.48
1:A:238:ARG:CD	1:A:264:GLU:OE2	2.61	0.48
1:A:243:ILE:O	1:A:451:GLY:HA2	2.13	0.48
1:A:496:LYS:NZ	1:A:496:LYS:CB	2.77	0.48
1:A:362:GLY:C	1:A:364:GLY:N	2.70	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:23:ASP:OD1	1:A:23:ASP:N	2.45	0.48
1:A:697:ILE:O	1:A:700:ASP:HB2	2.13	0.48
1:A:289:THR:O	1:A:292:GLU:N	2.46	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:240:GLY:HA3	1:A:455:ILE:HG13	1.97	0.47
1:A:241:LYS:N	1:A:455:ILE:HD12	2.29	0.47
1:A:316:LYS:HB2	1:A:316:LYS:HE3	1.65	0.47
1:A:467:GLU:CD	1:A:467:GLU:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASN:OD1	1:A:128:PRO:HD2	2.15	0.47
1:A:217:GLN:C	1:A:220:PRO:HD2	2.39	0.47
1:A:323:GLU:O	1:A:326:ILE:HB	2.15	0.47
1:A:730:LEU:O	1:A:731:ASN:HB3	2.14	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:741:ILE:C	1:A:742:THR:CG2	2.87	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:578:MET:HE2	1:A:578:MET:HB3	1.71	0.46
1:A:38:ASN:ND2	1:A:46:SER:O	2.43	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:270:PHE:C	1:A:271:GLN:HG3	2.41	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:147:ARG:HG3	1:A:150:GLU:CD	2.39	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:510:SER:O	1:A:514:ILE:HG13	2.17	0.45
1:A:496:LYS:HB3	1:A:496:LYS:HZ3	1.79	0.45
1:A:210:VAL:H	1:A:210:VAL:HG13	1.31	0.45
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.82	0.45
1:A:379:SER:CB	1:A:386:PRO:HG3	2.46	0.45
1:A:710:PRO:HD3	1:A:729:HIS:CD2	2.51	0.45
1:A:27:LEU:HD12	1:A:27:LEU:HA	1.77	0.45
1:A:37:TYR:O	1:A:47:TYR:HA	2.17	0.45
1:A:241:LYS:NZ	4:A:1221:HOH:O	2.46	0.45
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.99	0.45
1:A:390:GLU:HG2	1:A:394:MET:HE3	1.99	0.45
1:A:594:GLN:HB2	4:A:1664:HOH:O	2.17	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:54:SER:OG	1:A:61:THR:HB	2.17	0.44
1:A:149:ASN:HD22	1:A:149:ASN:N	2.14	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:CYS:O	1:A:473:TYR:HB3	2.18	0.44
1:A:744:ILE:HD13	1:A:744:ILE:C	2.43	0.44
1:A:4:ILE:O	1:A:4:ILE:CG2	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:68:GLN:HE21	1:A:68:GLN:HB3	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:CA	1:A:191:LYS:CE	2.96	0.43
1:A:149:ASN:ND2	1:A:149:ASN:C	2.76	0.43
1:A:59:SER:CB	1:A:72:VAL:O	2.65	0.43
1:A:459:GLU:C	1:A:460:ILE:HG13	2.43	0.43
1:A:202:ARG:NH1	1:A:202:ARG:CG	2.82	0.43
1:A:611:LEU:HA	1:A:617:ILE:HG21	2.01	0.43
1:A:24:LEU:N	1:A:24:LEU:HD23	2.34	0.43
1:A:389:LEU:O	1:A:393:LEU:HG	2.19	0.43
1:A:467:GLU:CD	1:A:467:GLU:N	2.76	0.43
1:A:692:PHE:CE1	1:A:747:ARG:HG2	2.53	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:289:THR:C	1:A:291:GLU:N	2.74	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:379:SER:HB3	1:A:386:PRO:HD3	2.01	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:471:ILE:HD12	1:A:471:ILE:HA	1.85	0.42
1:A:396:PRO:HG2	1:A:398:ILE:HD11	2.01	0.42
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:87:GLY:H	1:A:105:ASN:HD21	1.65	0.42
1:A:144:LYS:NZ	4:A:1593:HOH:O	2.53	0.42
1:A:710:PRO:CD	1:A:729:HIS:CE1	3.02	0.42
1:A:190:LYS:HE2	1:A:223:GLU:OE2	2.20	0.42
1:A:325:LYS:NZ	4:A:1402:HOH:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:LEU:HD11	1:A:455:ILE:HD13	2.00	0.42
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.85	0.42
1:A:498:LYS:O	1:A:498:LYS:HG2	2.18	0.42
1:A:692:PHE:O	1:A:695:ARG:NE	2.38	0.42
1:A:741:ILE:C	1:A:742:THR:HG22	2.45	0.42
1:A:39:PRO:HG3	1:A:48:GLU:HG2	2.02	0.42
1:A:73:LYS:HD2	1:A:73:LYS:HA	1.49	0.42
1:A:249:ASN:ND2	1:A:249:ASN:N	2.63	0.42
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.55	0.42
1:A:289:THR:O	1:A:289:THR:OG1	2.37	0.41
1:A:300:GLY:HA3	1:A:302:GLU:OE2	2.20	0.41
1:A:737:TYR:HE1	4:A:1460:HOH:O	1.88	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:685:ILE:O	1:A:686:ARG:C	2.62	0.41
1:A:696:ILE:O	1:A:743:LYS:HB3	2.20	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:316:LYS:NZ	1:A:316:LYS:CB	2.78	0.41
1:A:627:PHE:CA	4:A:1426:HOH:O	2.68	0.41
1:A:99:GLU:HB2	1:A:100:PRO:HD3	2.03	0.41
1:A:293:LYS:O	1:A:297:HIS:N	2.53	0.41
1:A:706:TYR:HE1	4:A:1676:HOH:O	2.03	0.41
1:A:138:GLU:OE2	1:A:138:GLU:N	2.49	0.41
1:A:329:GLN:O	1:A:332:ASP:HB2	2.21	0.41
1:A:342:MET:HA	1:A:342:MET:CE	2.42	0.41
1:A:341:GLN:O	1:A:345:PHE:CD2	2.74	0.41
1:A:344:ILE:HD11	1:A:432:TRP:CZ3	2.50	0.41
1:A:696:ILE:N	1:A:696:ILE:HD12	2.35	0.41
1:A:727:LEU:HA	1:A:727:LEU:HD12	1.65	0.41
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:497:GLU:C	1:A:741:ILE:HD12	2.46	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
1:A:289:THR:O	1:A:290:ALA:C	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	733/761 (96%)	690 (94%)	38 (5%)	5 (1%)	18 14

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 [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	631/665 (95%)	552 (88%)	79 (12%)	4 2

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	23	ASP
1	A	27	LEU

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Mol	Chain	Res	Type
1	A	31	ASP
1	A	32	LYS
1	A	35	ILE
1	A	40	ASP
1	A	44	ARG
1	A	57	SER
1	A	59	SER
1	A	63	LYS
1	A	66	ASP
1	A	68	GLN
1	A	71	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	257	SER
1	A	262	LEU
1	A	272	SER
1	A	280	ILE
1	A	291	GLU
1	A	294	LYS
1	A	302	GLU
1	A	316	LYS
1	A	325	LYS
1	A	326	ILE
1	A	328	ARG
1	A	329	GLN
1	A	338	GLN
1	A	342	MET
1	A	358	LYS
1	A	368	VAL
1	A	369	LEU
1	A	370	LYS

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Mol	Chain	Res	Type
1	A	372	LYS
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	413	LYS
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	496	LYS
1	A	509	ASP
1	A	542	THR
1	A	546	LYS
1	A	565	LYS
1	A	578	MET
1	A	589	LYS
1	A	594	GLN
1	A	666	LYS
1	A	689	ARG
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	78	ASN
1	A	105	ASN
1	A	149	ASN

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Mol	Chain	Res	Type
1	A	188	ASN
1	A	194	GLN
1	A	217	GLN
1	A	219	ASN
1	A	234	ASN
1	A	249	ASN
1	A	259	GLN
1	A	283	GLN
1	A	376	ASN
1	A	385	ASN
1	A	408	HIS
1	A	439	ASN
1	A	479	GLN
1	A	480	GLN
1	A	491	GLN
1	A	511	GLN
1	A	521	GLN
1	A	550	HIS
1	A	594	GLN
1	A	649	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 oligosaccharides 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	ONP	A	999	2	23,25,25	1.20	2 (8%)	22,37,37	1.69	3 (13%)

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	-	2/16/24/24	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	ONP	C6-C1	-2.30	1.36	1.39
3	A	999	ONP	PB-OA3	2.11	1.61	1.59

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	ONP	CA2-NA3-C1	-5.14	110.89	123.35
3	A	999	ONP	C3-C2-N2	3.83	120.57	116.47
3	A	999	ONP	O2A-N2-C2	-2.07	115.49	119.03

There are no chirality outliers.

All (2) torsion outliers are listed below:

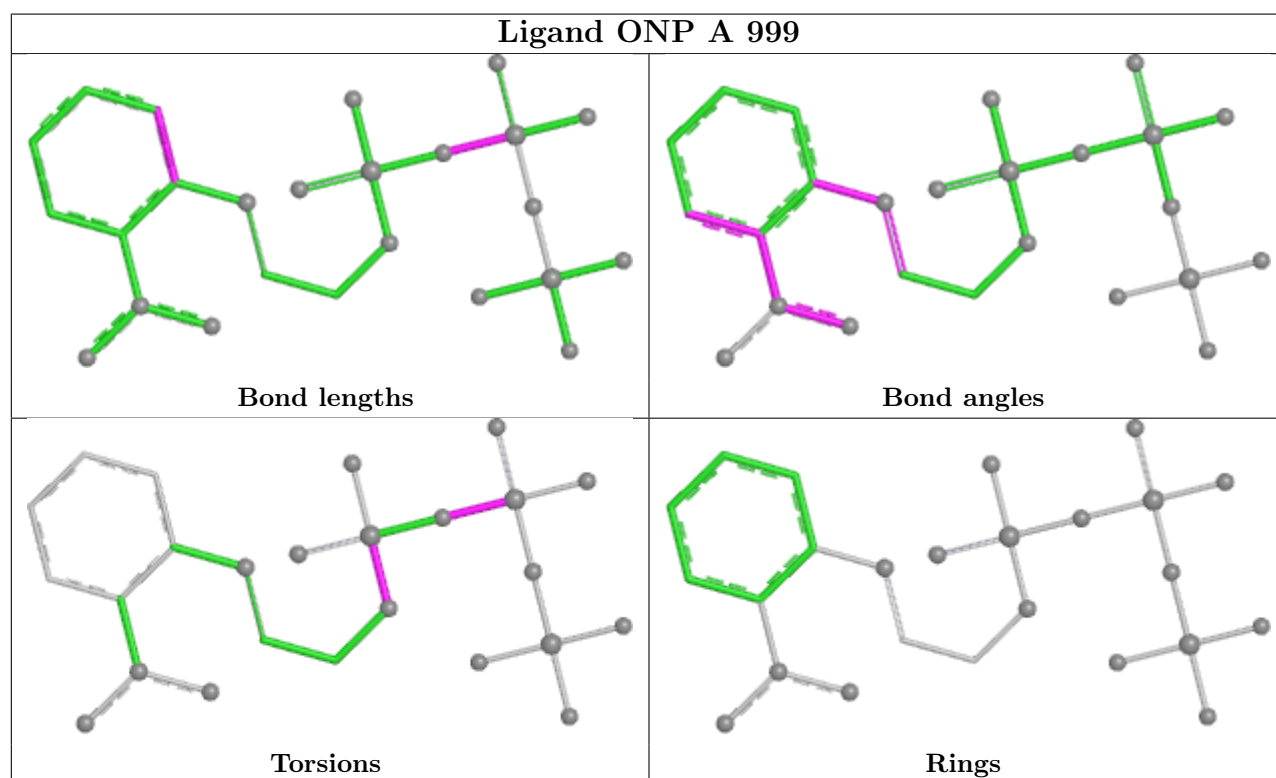
Mol	Chain	Res	Type	Atoms
3	A	999	ONP	PA-OA3-PB-OB2
3	A	999	ONP	CA1-OE2-PA-OA2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	ONP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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%)	0.01	40 (5%) 31 30	14, 36, 80, 100	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	7.6
1	A	443	GLN	5.0
1	A	707	LEU	4.7
1	A	319	SER	4.4
1	A	273	GLU	4.0
1	A	493	GLU	4.0
1	A	43	GLU	3.8
1	A	322	GLU	3.5
1	A	41	PRO	3.2
1	A	366	GLY	3.2
1	A	711	ASN	3.1
1	A	489	LEU	3.1
1	A	362	GLY	3.0
1	A	536	PRO	3.0
1	A	364	GLY	2.9
1	A	321	SER	2.9
1	A	508	LEU	2.9
1	A	734	PRO	2.8
1	A	495	LEU	2.7
1	A	400	ALA	2.6
1	A	500	ASN	2.6
1	A	316	LYS	2.6
1	A	274	THR	2.6
1	A	363	ALA	2.5
1	A	374	ALA	2.5
1	A	628	ILE	2.4
1	A	65	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	706	TYR	2.3
1	A	39	PRO	2.3
1	A	688	THR	2.3
1	A	722	ALA	2.2
1	A	759	GLU	2.2
1	A	219	ASN	2.2
1	A	387	SER	2.1
1	A	368	VAL	2.1
1	A	203	ASN	2.1
1	A	42	LYS	2.1
1	A	312	CYS	2.0
1	A	509	ASP	2.0
1	A	373	THR	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](#)

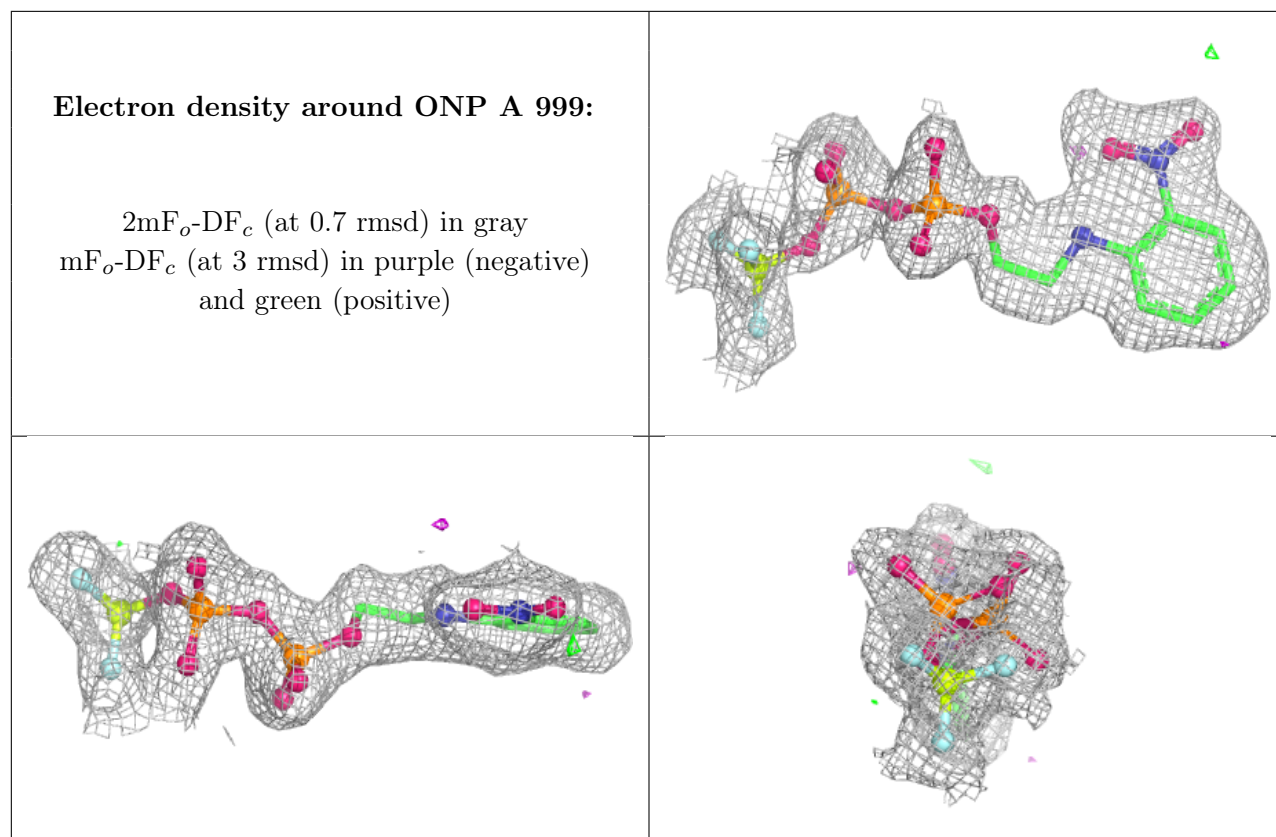
There are no oligosaccharides in this entry.

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	A	998	1/1	0.99	0.01	19,19,19,19	0
3	ONP	A	999	25/25	0.99	0.05	12,20,35,79	0

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



6.5 Other polymers [i](#)

There are no such residues in this entry.