



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:13 AM UTC

PDB ID : 1D1A / pdb_00001d1a
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH O,P-DINITROPHENYL AMINOETHYLDIPHOSP
HATE BERYLLIUM TRIFLUORIDE.
Authors : Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Pate, E.; Yount, R.G.; Rayment, I.
Deposited on : 1999-09-15
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

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	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

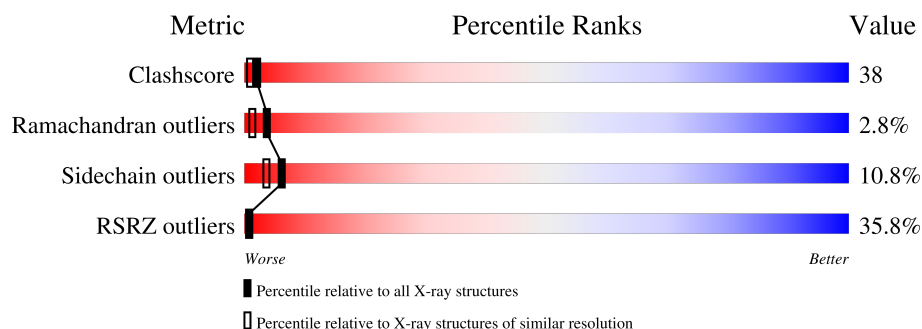
1 Overall quality at a glance

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 6235 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	745	Total	C	N	O	S	0	0	0
			5772	3660	994	1102	16			

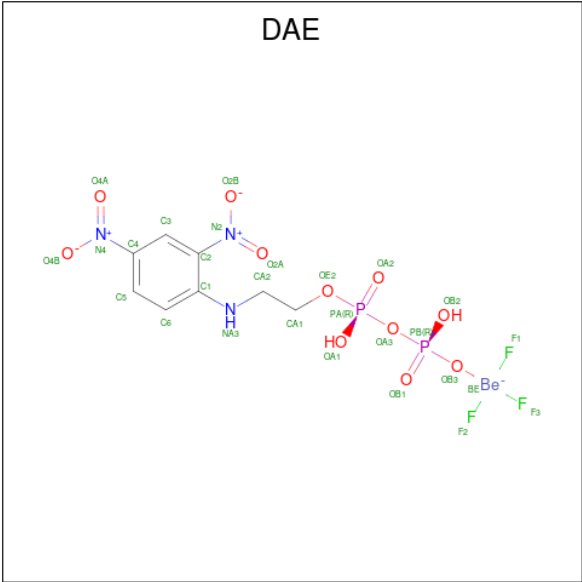
There are 3 discrepancies between the modelled and reference sequences:

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,P-DINITROPHENYL AMINOETHYLDIPHOSPHATE-BERYLLIUM TRIFLUORIDE (CCD ID: DAE) (formula: C₈H₁₀BeF₃N₃O₁₁P₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Be	C	F	N	O	P		
3	A	1	28	1	8	3	3	11	2	0	0

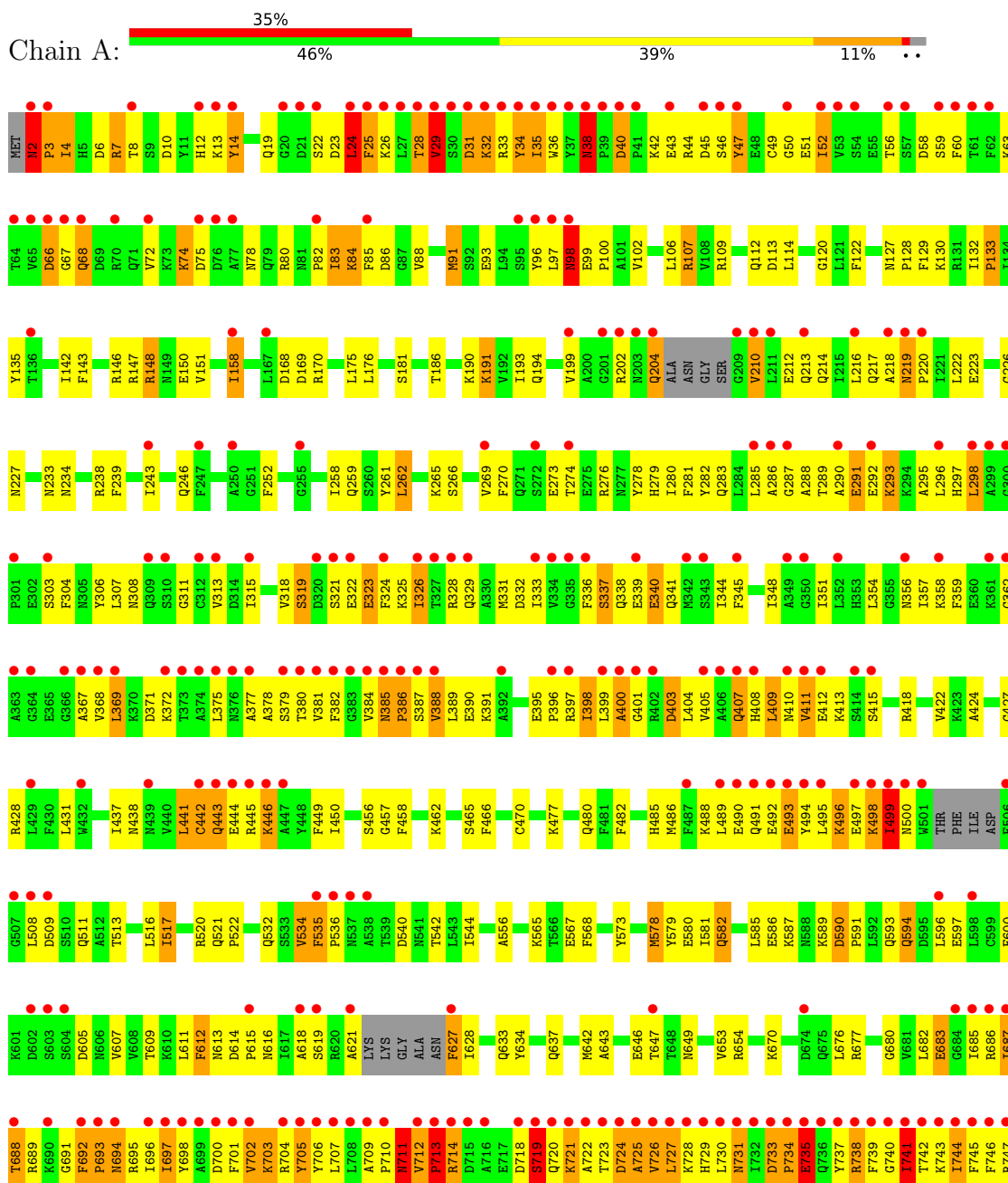
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	434	Total	O	0	0
			434	434		

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



A748	G749	Q750	L751	A752	R753	I754	E755	E756	A757	R758	E759	PRO	ASN
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.73Å 180.00Å 54.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (25.00-2.00) 96.7 (25.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.00Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.226 , (Not available) 0.252 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.3	Xtriage
Anisotropy	0.376	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 149.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6235	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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, DAE

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	1.07	2/5882 (0.0%)	1.68	79/7967 (1.0%)

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	2	0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	443	GLN	C-N	-6.46	1.24	1.33
1	A	132	ILE	CA-CB	-6.30	1.49	1.54

All (79) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	PHE	CA-CB-CG	-13.39	100.41	113.80
1	A	34	TYR	N-CA-C	11.57	126.61	109.95
1	A	25	PHE	N-CA-C	-11.01	99.86	113.18
1	A	35	ILE	N-CA-C	9.78	122.21	108.23
1	A	712	VAL	N-CA-C	9.21	117.98	108.95
1	A	233	ASN	CA-CB-CG	8.77	121.37	112.60
1	A	713	PRO	N-CA-CB	8.51	112.18	103.25
1	A	24	LEU	N-CA-C	8.37	123.03	110.64
1	A	38	ASN	CB-CA-C	-8.17	100.76	110.15
1	A	129	PHE	CA-CB-CG	-8.10	105.70	113.80
1	A	442	CYS	N-CA-C	7.80	120.96	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	403	ASP	N-CA-C	7.66	120.18	109.15
1	A	450	ILE	CA-C-N	-7.50	115.53	122.80
1	A	450	ILE	C-N-CA	-7.50	115.53	122.80
1	A	32	LYS	N-CA-C	7.45	119.75	109.18
1	A	38	ASN	CA-CB-CG	7.44	120.04	112.60
1	A	252	PHE	CA-CB-CG	-7.24	106.56	113.80
1	A	67	GLY	N-CA-C	-7.20	105.88	113.58
1	A	219	ASN	CB-CA-C	6.76	123.50	110.17
1	A	143	PHE	CA-CB-CG	-6.65	107.15	113.80
1	A	556	ALA	N-CA-C	6.44	120.24	112.38
1	A	499	ILE	CB-CA-C	6.42	121.82	111.29
1	A	385	ASN	CA-C-N	6.37	127.80	119.84
1	A	385	ASN	C-N-CA	6.37	127.80	119.84
1	A	400	ALA	N-CA-C	-6.35	102.75	110.88
1	A	493	GLU	N-CA-C	6.34	121.21	112.90
1	A	627	PHE	CA-CB-CG	6.22	120.03	113.80
1	A	194	GLN	CA-C-O	6.22	127.35	120.82
1	A	168	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	31	ASP	N-CA-C	6.19	120.69	113.20
1	A	494	TYR	O-C-N	6.19	130.43	122.39
1	A	731	ASN	CA-CB-CG	6.15	118.75	112.60
1	A	47	TYR	CB-CA-C	-6.04	99.38	110.62
1	A	14	TYR	N-CA-C	6.04	120.72	113.23
1	A	734	PRO	N-CA-CB	6.02	109.57	103.25
1	A	210	VAL	N-CA-C	5.96	116.14	110.53
1	A	66	ASP	CA-CB-CG	-5.86	106.74	112.60
1	A	721	LYS	N-CA-C	-5.84	103.71	111.24
1	A	40	ASP	CA-C-N	5.76	127.04	119.84
1	A	40	ASP	C-N-CA	5.76	127.04	119.84
1	A	318	VAL	N-CA-C	5.72	116.35	108.12
1	A	2	ASN	CA-C-N	5.70	126.96	119.84
1	A	2	ASN	C-N-CA	5.70	126.96	119.84
1	A	735	GLU	CB-CA-C	5.68	118.93	109.56
1	A	441	LEU	N-CA-C	5.65	119.35	112.23
1	A	499	ILE	N-CA-CB	5.63	120.53	111.23
1	A	612	PHE	CA-CB-CG	-5.61	108.19	113.80
1	A	735	GLU	N-CA-CB	5.59	118.97	110.42
1	A	719	SER	N-CA-C	5.55	122.63	110.80
1	A	219	ASN	N-CA-CB	5.51	120.19	110.37
1	A	24	LEU	CB-CA-C	5.50	116.57	109.80
1	A	323	GLU	CA-C-N	5.50	128.68	120.31
1	A	323	GLU	C-N-CA	5.50	128.68	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	GLU	N-CA-C	-5.49	105.45	111.82
1	A	516	LEU	CA-C-O	5.46	126.28	120.10
1	A	744	ILE	N-CA-CB	5.46	118.24	111.41
1	A	29	VAL	N-CA-C	5.45	120.68	109.34
1	A	438	ASN	CA-CB-CG	-5.44	107.16	112.60
1	A	649	ASN	N-CA-C	-5.44	100.78	109.04
1	A	24	LEU	N-CA-CB	5.43	117.56	109.19
1	A	23	ASP	CB-CA-C	-5.40	100.42	109.27
1	A	52	ILE	N-CA-C	-5.37	102.65	109.58
1	A	42	LYS	N-CA-C	-5.36	104.33	111.24
1	A	122	PHE	CB-CA-C	-5.35	100.46	109.50
1	A	411	VAL	N-CA-C	5.33	116.10	110.72
1	A	705	TYR	N-CA-C	5.27	117.60	110.06
1	A	511	GLN	N-CA-C	5.27	117.02	111.28
1	A	482	PHE	CA-CB-CG	-5.23	108.57	113.80
1	A	741	ILE	N-CA-C	5.21	120.18	109.34
1	A	409	LEU	O-C-N	5.17	129.12	123.01
1	A	279	HIS	CA-CB-CG	5.13	118.93	113.80
1	A	262	LEU	N-CA-CB	-5.12	104.29	111.62
1	A	692	PHE	CA-C-N	5.12	126.23	119.84
1	A	692	PHE	C-N-CA	5.12	126.23	119.84
1	A	133	PRO	CB-CA-C	-5.09	106.17	113.09
1	A	590	ASP	CA-C-O	5.07	123.97	120.47
1	A	466	PHE	CA-CB-CG	-5.05	108.75	113.80
1	A	711	ASN	CA-C-N	5.05	129.49	120.70
1	A	711	ASN	C-N-CA	5.05	129.49	120.70

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	219	ASN	CA
1	A	499	ILE	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	5772	0	5502	424	0
2	A	1	0	0	0	0
3	A	28	0	8	3	0
4	A	434	0	0	19	0
All	All	6235	0	5510	425	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 38.

All (425) 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:398:ILE:HD13	1:A:407:GLN:HG3	1.39	1.04
1:A:98:ASN:HB2	1:A:100:PRO:HD2	1.41	1.02
1:A:443:GLN:CG	1:A:445:ARG:O	2.07	1.00
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.46	0.97
1:A:709:ALA:HB1	1:A:729:HIS:ND1	1.81	0.96
1:A:4:ILE:HD11	1:A:142:ILE:CG2	1.96	0.93
1:A:34:TYR:HB3	1:A:51:GLU:HA	1.51	0.92
1:A:619:SER:HB3	1:A:627:PHE:CE2	2.05	0.91
1:A:711:ASN:HB2	1:A:729:HIS:CE1	2.08	0.89
1:A:619:SER:HB3	1:A:627:PHE:HE2	1.34	0.88
1:A:45:ASP:HB2	1:A:670:LYS:HG2	1.56	0.87
1:A:737:TYR:HB3	1:A:746:PHE:CE1	2.11	0.84
1:A:723:THR:HG22	1:A:739:PHE:CZ	2.11	0.84
1:A:698:TYR:CD1	1:A:720:GLN:HG2	2.13	0.83
1:A:147:ARG:HG2	1:A:150:GLU:OE1	1.79	0.82
1:A:58:ASP:O	1:A:74:LYS:HB3	1.78	0.82
1:A:289:THR:OG1	1:A:292:GLU:HG3	1.80	0.81
1:A:594:GLN:HA	1:A:594:GLN:HE21	1.45	0.81
1:A:297:HIS:C	1:A:298:LEU:HD23	2.05	0.81
1:A:443:GLN:HG2	1:A:445:ARG:O	1.79	0.80
1:A:34:TYR:CB	1:A:51:GLU:HA	2.12	0.80
1:A:723:THR:HG22	1:A:739:PHE:HZ	1.44	0.80
1:A:372:LYS:HE3	1:A:390:GLU:OE1	1.82	0.80
1:A:337:SER:O	1:A:341:GLN:HG3	1.82	0.79
1:A:80:ARG:HH12	1:A:83:ILE:HG12	1.48	0.79
1:A:621:ALA:HB2	1:A:628:ILE:HG12	1.62	0.79
1:A:480:GLN:HG3	1:A:508:LEU:HD12	1.66	0.78
1:A:336:PHE:O	1:A:341:GLN:NE2	2.15	0.78
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.66	0.78
1:A:269:VAL:HG12	1:A:306:TYR:CZ	2.20	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:GLN:HG3	1:A:508:LEU:CD1	2.14	0.77
1:A:400:ALA:HB3	1:A:403:ASP:HB2	1.67	0.76
1:A:91:MET:HE1	1:A:106:LEU:HG	1.67	0.76
1:A:4:ILE:HD11	1:A:142:ILE:HG21	1.66	0.75
1:A:43:GLU:HB2	1:A:670:LYS:HZ2	1.50	0.75
1:A:706:TYR:HB2	1:A:712:VAL:HG12	1.66	0.75
1:A:35:ILE:HG12	1:A:36:TRP:N	2.02	0.75
1:A:702:VAL:HG23	1:A:712:VAL:CG1	2.17	0.75
1:A:735:GLU:HB3	1:A:747:ARG:NH2	2.02	0.74
1:A:485:HIS:NE2	1:A:489:LEU:HD11	2.02	0.74
1:A:398:ILE:CD1	1:A:407:GLN:HG3	2.17	0.74
1:A:158:ILE:HD12	1:A:175:LEU:HD23	1.68	0.74
1:A:733:ASP:O	1:A:737:TYR:CE2	2.40	0.74
1:A:540:ASP:HB3	1:A:581:ILE:HD13	1.69	0.74
1:A:396:PRO:O	1:A:398:ILE:HD12	1.88	0.73
1:A:107:ARG:HG3	4:A:1192:HOH:O	1.89	0.72
1:A:395:GLU:HA	1:A:407:GLN:O	1.89	0.72
1:A:210:VAL:O	1:A:214:GLN:HG3	1.89	0.72
1:A:377:ALA:O	1:A:380:THR:HG22	1.89	0.72
1:A:7:ARG:HD3	1:A:12:HIS:CE1	2.25	0.71
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.25	0.71
1:A:443:GLN:HG3	1:A:445:ARG:C	2.16	0.71
1:A:709:ALA:HB2	1:A:726:VAL:HG13	1.71	0.70
1:A:443:GLN:HG3	1:A:445:ARG:O	1.92	0.70
1:A:35:ILE:HG12	1:A:36:TRP:H	1.55	0.70
1:A:582:GLN:OE1	1:A:582:GLN:N	2.20	0.70
1:A:98:ASN:CB	1:A:100:PRO:HD2	2.21	0.70
1:A:146:ARG:HD3	1:A:151:VAL:HG13	1.72	0.70
1:A:614:ASP:OD1	1:A:615:PRO:HD2	1.92	0.69
1:A:491:GLN:O	1:A:495:LEU:HD13	1.91	0.69
1:A:735:GLU:CB	1:A:747:ARG:HH21	2.05	0.69
1:A:80:ARG:HH12	1:A:83:ILE:CG1	2.06	0.69
1:A:380:THR:HG23	1:A:381:VAL:N	2.08	0.69
1:A:740:GLY:O	1:A:742:THR:N	2.25	0.68
1:A:38:ASN:OD1	1:A:44:ARG:HA	1.92	0.68
1:A:698:TYR:HH	1:A:739:PHE:HD2	1.41	0.68
1:A:753:ARG:HH21	1:A:757:ALA:HB2	1.58	0.68
1:A:80:ARG:HH12	1:A:83:ILE:CD1	2.06	0.67
1:A:702:VAL:HG23	1:A:712:VAL:HG11	1.75	0.67
1:A:293:LYS:O	1:A:296:LEU:N	2.26	0.67
1:A:325:LYS:O	1:A:329:GLN:HG3	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:738:ARG:O	1:A:744:ILE:HD12	1.95	0.67
1:A:544:ILE:HB	1:A:581:ILE:HG12	1.77	0.66
1:A:43:GLU:HB2	1:A:670:LYS:NZ	2.10	0.66
1:A:410:ASN:OD1	1:A:413:LYS:HB2	1.96	0.66
1:A:687:ILE:HG22	1:A:688:THR:N	2.07	0.66
1:A:642:MET:O	1:A:646:GLU:HG2	1.96	0.66
1:A:695:ARG:HA	1:A:745:PHE:HA	1.77	0.66
1:A:686:ARG:O	1:A:689:ARG:HB3	1.95	0.66
1:A:694:ASN:N	1:A:694:ASN:ND2	2.44	0.66
1:A:385:ASN:O	1:A:388:VAL:HG23	1.95	0.66
1:A:34:TYR:CD1	1:A:49:CYS:SG	2.89	0.65
1:A:399:LEU:HG	1:A:401:GLY:H	1.61	0.65
1:A:273:GLU:O	1:A:274:THR:OG1	2.09	0.65
1:A:711:ASN:HB2	1:A:729:HIS:HE1	1.58	0.65
1:A:443:GLN:CD	1:A:445:ARG:O	2.40	0.65
1:A:621:ALA:CB	1:A:628:ILE:HG23	2.27	0.65
1:A:283:GLN:HB3	1:A:324:PHE:HB2	1.79	0.65
1:A:586:GLU:HB2	4:A:1399:HOH:O	1.97	0.65
1:A:12:HIS:ND1	4:A:1198:HOH:O	2.28	0.65
1:A:753:ARG:O	1:A:753:ARG:NE	2.30	0.65
1:A:246:GLN:OE1	1:A:443:GLN:HB3	1.97	0.64
1:A:580:GLU:HG3	1:A:580:GLU:O	1.96	0.64
1:A:158:ILE:CD1	1:A:175:LEU:HD23	2.26	0.64
1:A:298:LEU:HD23	1:A:298:LEU:N	2.12	0.64
1:A:222:LEU:HD11	1:A:258:ILE:HD13	1.80	0.64
1:A:753:ARG:HG3	1:A:753:ARG:HH11	1.63	0.64
1:A:43:GLU:HA	1:A:670:LYS:HZ1	1.64	0.63
1:A:293:LYS:O	1:A:297:HIS:N	2.31	0.63
1:A:753:ARG:HA	1:A:756:GLU:OE2	1.99	0.63
1:A:621:ALA:HB3	1:A:628:ILE:H	1.64	0.63
1:A:753:ARG:O	1:A:756:GLU:HB2	1.98	0.63
1:A:697:ILE:HG22	1:A:700:ASP:H	1.64	0.63
1:A:35:ILE:HG22	1:A:50:GLY:O	1.99	0.62
1:A:498:LYS:CB	1:A:741:ILE:HG13	2.29	0.62
1:A:338:GLN:HB3	1:A:339:GLU:OE1	2.00	0.62
1:A:698:TYR:HE2	1:A:739:PHE:CE2	2.17	0.62
1:A:698:TYR:CG	1:A:720:GLN:HG2	2.35	0.62
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.30	0.62
1:A:382:PHE:HB2	1:A:384:VAL:HG22	1.82	0.62
1:A:686:ARG:HA	1:A:689:ARG:HB2	1.82	0.62
1:A:490:GLU:HA	1:A:490:GLU:OE1	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:VAL:O	1:A:536:PRO:HD3	2.00	0.61
1:A:375:LEU:HD23	1:A:375:LEU:C	2.25	0.61
1:A:380:THR:HG23	1:A:381:VAL:H	1.66	0.61
1:A:698:TYR:O	1:A:702:VAL:HG12	1.99	0.61
1:A:296:LEU:CB	1:A:298:LEU:HG	2.27	0.61
1:A:7:ARG:NH1	1:A:12:HIS:HE1	1.99	0.61
1:A:2:ASN:ND2	1:A:4:ILE:H	1.99	0.60
1:A:495:LEU:N	1:A:495:LEU:HD12	2.17	0.60
1:A:33:ARG:O	1:A:52:ILE:HB	2.01	0.60
1:A:34:TYR:HD1	1:A:49:CYS:SG	2.25	0.60
1:A:80:ARG:NH1	1:A:83:ILE:HG12	2.16	0.60
1:A:158:ILE:HD12	1:A:175:LEU:CD2	2.31	0.60
1:A:387:SER:O	1:A:391:LYS:HB2	2.01	0.60
1:A:130:LYS:HA	3:A:999:DAE:O4A	2.01	0.59
1:A:380:THR:CG2	1:A:381:VAL:H	2.15	0.59
1:A:24:LEU:HB3	1:A:26:LYS:CB	2.33	0.59
1:A:713:PRO:O	1:A:714:ARG:O	2.21	0.59
1:A:24:LEU:HD13	1:A:26:LYS:CB	2.32	0.59
1:A:219:ASN:N	1:A:220:PRO:HD2	2.16	0.59
1:A:611:LEU:O	1:A:618:ALA:HB2	2.02	0.59
1:A:694:ASN:N	1:A:694:ASN:HD22	1.99	0.59
1:A:399:LEU:HG	1:A:401:GLY:N	2.16	0.59
1:A:25:PHE:HA	1:A:704:ARG:NH2	2.18	0.59
1:A:289:THR:HB	1:A:291:GLU:OE1	2.03	0.58
1:A:409:LEU:HD22	1:A:413:LYS:HB3	1.84	0.58
1:A:706:TYR:CB	1:A:712:VAL:HG12	2.33	0.58
1:A:698:TYR:HE2	1:A:739:PHE:HE2	1.50	0.58
1:A:304:PHE:O	1:A:308:ASN:ND2	2.35	0.58
1:A:412:GLU:HG2	4:A:1375:HOH:O	2.02	0.58
1:A:499:ILE:HD11	1:A:745:PHE:CD1	2.39	0.58
1:A:585:LEU:O	1:A:589:LYS:HG3	2.03	0.57
1:A:213:GLN:O	1:A:217:GLN:HG2	2.04	0.57
1:A:619:SER:CB	1:A:627:PHE:HE2	2.14	0.57
1:A:45:ASP:CG	1:A:677:ARG:HH22	2.13	0.57
1:A:276:ARG:NH1	1:A:282:TYR:CG	2.72	0.57
1:A:534:VAL:HG22	1:A:535:PHE:CE2	2.39	0.57
1:A:685:ILE:HG22	1:A:686:ARG:N	2.18	0.57
1:A:509:ASP:O	4:A:1254:HOH:O	2.18	0.57
1:A:589:LYS:HB2	1:A:591:PRO:HD3	1.87	0.57
1:A:709:ALA:HB1	1:A:729:HIS:CE1	2.39	0.56
1:A:26:LYS:O	1:A:29:VAL:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:VAL:CG2	1:A:535:PHE:CE2	2.88	0.56
1:A:465:SER:OG	1:A:587:LYS:NZ	2.38	0.56
1:A:686:ARG:HA	1:A:689:ARG:CB	2.36	0.56
1:A:594:GLN:HE21	1:A:594:GLN:CA	2.10	0.56
1:A:725:ALA:O	1:A:728:LYS:N	2.39	0.56
1:A:99:GLU:H	1:A:100:PRO:CD	2.18	0.55
1:A:492:GLU:O	1:A:495:LEU:HB2	2.06	0.55
1:A:443:GLN:CG	1:A:445:ARG:C	2.75	0.55
1:A:698:TYR:OH	1:A:739:PHE:HD2	1.90	0.55
1:A:43:GLU:CB	1:A:670:LYS:HZ2	2.18	0.55
1:A:653:VAL:C	1:A:654:ARG:HE	2.14	0.55
1:A:621:ALA:HB2	1:A:628:ILE:CG1	2.36	0.55
1:A:380:THR:CG2	1:A:381:VAL:N	2.68	0.55
1:A:234:ASN:ND2	4:A:1220:HOH:O	2.40	0.55
1:A:705:TYR:O	1:A:726:VAL:HG21	2.07	0.55
1:A:377:ALA:O	1:A:381:VAL:HG22	2.07	0.54
1:A:721:LYS:O	1:A:724:ASP:HB2	2.07	0.54
1:A:486:MET:CE	1:A:687:ILE:HG21	2.37	0.54
1:A:719:SER:O	1:A:722:ALA:N	2.41	0.54
1:A:704:ARG:HB3	1:A:705:TYR:CE2	2.42	0.54
1:A:223:GLU:O	1:A:227:ASN:HB2	2.07	0.54
1:A:324:PHE:CE2	1:A:328:ARG:HD2	2.43	0.54
1:A:480:GLN:HG3	1:A:508:LEU:HD13	1.89	0.54
1:A:594:GLN:HA	1:A:594:GLN:NE2	2.17	0.53
1:A:688:THR:O	1:A:691:GLY:N	2.40	0.53
1:A:443:GLN:HG2	1:A:446:LYS:HB3	1.90	0.53
1:A:97:LEU:O	1:A:98:ASN:O	2.27	0.53
1:A:292:GLU:O	1:A:295:ALA:HB3	2.09	0.53
1:A:380:THR:HG23	1:A:381:VAL:HG13	1.91	0.53
1:A:735:GLU:HB2	1:A:747:ARG:HH21	1.72	0.53
1:A:24:LEU:HB3	1:A:26:LYS:H	1.74	0.53
1:A:63:LYS:HG3	1:A:68:GLN:O	2.09	0.53
1:A:695:ARG:CB	1:A:745:PHE:CE2	2.92	0.53
1:A:693:PRO:HD2	1:A:746:PHE:O	2.09	0.52
1:A:26:LYS:HA	1:A:29:VAL:HG13	1.90	0.52
1:A:98:ASN:O	1:A:102:VAL:HG23	2.09	0.52
1:A:344:ILE:O	1:A:348:ILE:HG12	2.10	0.52
1:A:513:THR:O	1:A:517:ILE:HD12	2.10	0.52
1:A:99:GLU:N	1:A:100:PRO:CD	2.72	0.52
1:A:219:ASN:N	1:A:220:PRO:CD	2.73	0.52
1:A:319:SER:OG	1:A:322:GLU:HB2	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ASN:ND2	1:A:694:ASN:H	2.05	0.52
1:A:4:ILE:CD1	1:A:4:ILE:N	2.72	0.51
1:A:296:LEU:O	1:A:297:HIS:HB2	2.09	0.51
1:A:735:GLU:HA	1:A:738:ARG:HH21	1.75	0.51
1:A:99:GLU:HG2	1:A:682:LEU:HD13	1.91	0.51
1:A:379:SER:HA	1:A:384:VAL:HG23	1.93	0.51
1:A:218:ALA:C	1:A:220:PRO:HD2	2.36	0.51
1:A:3:PRO:HA	1:A:6:ASP:HB3	1.93	0.51
1:A:99:GLU:H	1:A:100:PRO:HD2	1.75	0.51
1:A:437:ILE:O	1:A:441:LEU:HG	2.11	0.51
1:A:582:GLN:H	1:A:582:GLN:CD	2.16	0.51
1:A:43:GLU:O	1:A:43:GLU:HG3	2.12	0.50
1:A:408:HIS:HD2	1:A:409:LEU:N	2.09	0.50
1:A:692:PHE:CZ	1:A:747:ARG:NH1	2.80	0.50
1:A:135:TYR:CD1	1:A:191:LYS:HD2	2.46	0.50
1:A:290:ALA:N	1:A:291:GLU:OE2	2.45	0.50
1:A:354:LEU:O	1:A:418:ARG:HD3	2.12	0.50
1:A:696:ILE:O	1:A:743:LYS:HA	2.12	0.50
1:A:186:THR:HG22	1:A:190:LYS:HE3	1.93	0.50
1:A:609:THR:CG2	1:A:613:ASN:ND2	2.75	0.50
1:A:710:PRO:O	1:A:711:ASN:OD1	2.30	0.50
1:A:367:ALA:O	1:A:408:HIS:NE2	2.44	0.49
1:A:458:PHE:CZ	1:A:573:TYR:HB3	2.47	0.49
1:A:694:ASN:HB2	1:A:746:PHE:HB2	1.93	0.49
1:A:147:ARG:NH1	4:A:1215:HOH:O	2.23	0.49
1:A:102:VAL:HG21	1:A:685:ILE:HD13	1.95	0.49
1:A:737:TYR:HB3	1:A:746:PHE:HE1	1.70	0.49
1:A:47:TYR:CE1	1:A:100:PRO:HG3	2.47	0.49
1:A:497:GLU:C	1:A:741:ILE:HD12	2.38	0.49
1:A:280:ILE:HD11	1:A:345:PHE:HE1	1.77	0.49
1:A:594:GLN:O	1:A:597:GLU:HB2	2.12	0.49
1:A:358:LYS:NZ	4:A:1236:HOH:O	2.39	0.49
1:A:493:GLU:C	1:A:495:LEU:H	2.20	0.49
1:A:582:GLN:NE2	4:A:1245:HOH:O	2.27	0.49
1:A:753:ARG:HG3	1:A:753:ARG:NH1	2.27	0.49
1:A:369:LEU:O	1:A:372:LYS:NZ	2.45	0.49
1:A:621:ALA:CB	1:A:628:ILE:HG12	2.37	0.49
1:A:28:THR:HG21	1:A:84:LYS:HB2	1.96	0.48
1:A:477:LYS:NZ	4:A:1093:HOH:O	2.46	0.48
1:A:470:CYS:HB3	1:A:634:TYR:CZ	2.48	0.48
1:A:738:ARG:HB3	1:A:745:PHE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:493:GLU:C	1:A:495:LEU:N	2.68	0.48
1:A:85:PHE:O	1:A:88:VAL:HG13	2.14	0.48
1:A:442:CYS:SG	1:A:443:GLN:N	2.86	0.48
1:A:609:THR:HG23	1:A:613:ASN:ND2	2.28	0.48
1:A:226:GLY:HA3	1:A:239:PHE:CE2	2.49	0.48
1:A:707:LEU:C	1:A:709:ALA:H	2.22	0.48
1:A:286:ALA:HB1	1:A:321:SER:OG	2.13	0.48
1:A:428:ARG:O	1:A:431:LEU:HB2	2.14	0.48
1:A:99:GLU:N	1:A:100:PRO:HD2	2.29	0.48
1:A:289:THR:C	1:A:291:GLU:N	2.69	0.48
1:A:331:MET:CE	1:A:345:PHE:CZ	2.96	0.48
1:A:723:THR:CG2	1:A:739:PHE:CZ	2.91	0.48
1:A:488:LYS:C	1:A:490:GLU:H	2.21	0.48
1:A:597:GLU:OE1	1:A:612:PHE:HD2	1.97	0.48
1:A:702:VAL:O	1:A:706:TYR:HB3	2.14	0.48
1:A:722:ALA:O	1:A:725:ALA:HB3	2.13	0.48
1:A:614:ASP:C	1:A:616:ASN:N	2.72	0.47
1:A:96:TYR:CE2	1:A:749:GLY:HA2	2.49	0.47
1:A:521:GLN:HA	1:A:522:PRO:C	2.38	0.47
1:A:614:ASP:C	1:A:616:ASN:H	2.21	0.47
1:A:84:LYS:HD2	1:A:755:GLU:OE2	2.15	0.47
1:A:217:GLN:HG3	1:A:333:ILE:HD13	1.95	0.47
1:A:701:PHE:O	1:A:705:TYR:HD2	1.97	0.47
1:A:24:LEU:CD1	1:A:26:LYS:CB	2.92	0.47
1:A:499:ILE:CD1	1:A:745:PHE:CD1	2.98	0.47
1:A:288:ALA:HB1	1:A:292:GLU:HB2	1.97	0.47
1:A:311:GLY:N	4:A:1144:HOH:O	2.36	0.47
1:A:680:GLY:N	4:A:1099:HOH:O	2.45	0.47
1:A:217:GLN:HG3	1:A:333:ILE:CD1	2.45	0.47
1:A:324:PHE:O	1:A:328:ARG:HG3	2.15	0.47
1:A:695:ARG:CB	1:A:745:PHE:CD2	2.98	0.47
1:A:683:GLU:HG3	1:A:686:ARG:NH2	2.30	0.47
1:A:96:TYR:CE2	1:A:749:GLY:CA	2.97	0.46
1:A:169:ASP:C	1:A:170:ARG:HG2	2.40	0.46
1:A:614:ASP:O	1:A:616:ASN:N	2.48	0.46
1:A:31:ASP:O	1:A:32:LYS:HG2	2.14	0.46
1:A:696:ILE:O	1:A:743:LYS:CA	2.64	0.46
1:A:297:HIS:O	1:A:298:LEU:HD23	2.15	0.46
1:A:371:ASP:OD2	1:A:372:LYS:N	2.48	0.46
1:A:488:LYS:C	1:A:490:GLU:N	2.73	0.46
1:A:568:PHE:O	1:A:578:MET:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:ALA:O	1:A:647:THR:HG23	2.15	0.46
1:A:176:LEU:N	1:A:176:LEU:HD12	2.31	0.46
1:A:219:ASN:ND2	4:A:1426:HOH:O	2.38	0.46
1:A:296:LEU:O	1:A:298:LEU:HD23	2.16	0.46
1:A:357:ILE:HB	1:A:418:ARG:NH1	2.30	0.46
1:A:567:GLU:HA	1:A:579:TYR:O	2.15	0.46
1:A:219:ASN:HD21	1:A:243:ILE:HD11	1.80	0.46
1:A:726:VAL:HG12	1:A:730:LEU:CD1	2.45	0.46
1:A:6:ASP:O	1:A:8:THR:N	2.48	0.46
1:A:109:ARG:HB3	1:A:114:LEU:HB2	1.98	0.46
1:A:735:GLU:CB	1:A:747:ARG:NH2	2.68	0.46
1:A:59:SER:CB	1:A:72:VAL:O	2.64	0.46
1:A:340:GLU:O	1:A:344:ILE:HG13	2.16	0.46
1:A:456:SER:OG	1:A:457:GLY:N	2.49	0.45
1:A:534:VAL:HG22	1:A:535:PHE:CD2	2.51	0.45
1:A:727:LEU:HA	1:A:727:LEU:HD12	1.68	0.45
1:A:495:LEU:N	1:A:495:LEU:CD1	2.79	0.45
1:A:686:ARG:CB	1:A:689:ARG:CZ	2.94	0.45
1:A:654:ARG:NH1	4:A:1349:HOH:O	2.49	0.45
1:A:728:LYS:O	1:A:731:ASN:N	2.46	0.45
1:A:82:PRO:HG2	1:A:85:PHE:HE1	1.81	0.45
1:A:565:LYS:NZ	4:A:1081:HOH:O	2.49	0.45
1:A:697:ILE:HD12	1:A:743:LYS:HG2	1.99	0.45
1:A:289:THR:C	1:A:291:GLU:H	2.24	0.45
1:A:685:ILE:HG22	1:A:689:ARG:HH11	1.82	0.45
1:A:147:ARG:O	1:A:150:GLU:HB2	2.15	0.45
1:A:238:ARG:HB2	1:A:278:TYR:HE1	1.82	0.45
1:A:287:GLY:HA3	1:A:324:PHE:CD2	2.51	0.45
1:A:590:ASP:N	1:A:591:PRO:CD	2.79	0.45
1:A:259:GLN:HG3	1:A:261:TYR:CZ	2.52	0.45
1:A:578:MET:HE3	1:A:578:MET:HA	1.98	0.45
1:A:3:PRO:O	1:A:12:HIS:HD2	2.00	0.45
1:A:633:GLN:O	1:A:637:GLN:HG3	2.17	0.45
1:A:709:ALA:CB	1:A:729:HIS:ND1	2.68	0.45
1:A:733:ASP:OD2	1:A:734:PRO:HD2	2.16	0.45
1:A:38:ASN:N	1:A:38:ASN:HD22	2.15	0.44
1:A:219:ASN:HD21	1:A:243:ILE:CD1	2.30	0.44
1:A:222:LEU:CD1	1:A:258:ILE:HD13	2.47	0.44
1:A:339:GLU:N	1:A:339:GLU:CD	2.75	0.44
1:A:399:LEU:HD12	1:A:403:ASP:C	2.42	0.44
1:A:415:SER:O	1:A:418:ARG:HB3	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:GLY:O	1:A:148:ARG:NH2	2.46	0.44
1:A:2:ASN:ND2	4:A:1196:HOH:O	2.51	0.44
1:A:4:ILE:N	1:A:4:ILE:HD12	2.32	0.44
1:A:291:GLU:H	1:A:291:GLU:CD	2.26	0.44
1:A:696:ILE:O	1:A:744:ILE:N	2.45	0.44
1:A:24:LEU:C	1:A:26:LYS:N	2.71	0.44
1:A:270:PHE:CD1	1:A:270:PHE:C	2.94	0.43
1:A:297:HIS:N	1:A:297:HIS:ND1	2.66	0.43
1:A:375:LEU:HD22	1:A:386:PRO:HB3	2.00	0.43
1:A:424:ALA:O	1:A:428:ARG:HG3	2.18	0.43
1:A:605:ASP:OD1	1:A:607:VAL:N	2.49	0.43
1:A:723:THR:CG2	1:A:739:PHE:CE2	3.00	0.43
1:A:359:PHE:HB3	1:A:411:VAL:HG12	1.99	0.43
1:A:462:LYS:HG3	4:A:1243:HOH:O	2.17	0.43
1:A:686:ARG:HB3	1:A:689:ARG:CZ	2.49	0.43
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.17	0.43
1:A:351:ILE:HG23	1:A:422:VAL:HG13	2.01	0.43
1:A:686:ARG:HB3	1:A:689:ARG:NH2	2.33	0.43
1:A:692:PHE:HB3	1:A:745:PHE:HB3	2.00	0.43
1:A:375:LEU:HD23	1:A:375:LEU:O	2.19	0.43
1:A:698:TYR:CD2	1:A:720:GLN:HA	2.54	0.43
1:A:341:GLN:O	1:A:345:PHE:CD2	2.72	0.43
1:A:499:ILE:HG22	1:A:500:ASN:H	1.84	0.43
1:A:581:ILE:O	1:A:582:GLN:C	2.61	0.43
1:A:6:ASP:C	1:A:8:THR:H	2.27	0.43
1:A:36:TRP:HB2	1:A:78:ASN:HB3	2.00	0.43
1:A:289:THR:HB	1:A:291:GLU:CD	2.43	0.43
1:A:609:THR:O	1:A:613:ASN:N	2.47	0.43
1:A:49:CYS:SG	1:A:80:ARG:HD2	2.59	0.43
1:A:535:PHE:CD2	1:A:535:PHE:N	2.86	0.43
1:A:670:LYS:HG3	4:A:1199:HOH:O	2.19	0.43
1:A:532:GLN:NE2	1:A:542:THR:OG1	2.47	0.42
1:A:698:TYR:CE2	1:A:739:PHE:CE2	3.04	0.42
1:A:304:PHE:O	1:A:308:ASN:CG	2.62	0.42
1:A:697:ILE:HG22	1:A:700:ASP:N	2.31	0.42
1:A:273:GLU:C	1:A:274:THR:HG23	2.45	0.42
1:A:590:ASP:N	1:A:591:PRO:HD3	2.34	0.42
1:A:719:SER:C	1:A:721:LYS:N	2.77	0.42
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.54	0.42
1:A:368:VAL:HG22	1:A:369:LEU:N	2.35	0.42
1:A:127:ASN:OD1	1:A:128:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:PHE:O	1:A:285:LEU:HG	2.20	0.42
1:A:326:ILE:O	1:A:329:GLN:HB2	2.19	0.42
1:A:24:LEU:HA	1:A:24:LEU:HD23	1.49	0.42
1:A:91:MET:C	1:A:93:GLU:H	2.28	0.42
1:A:408:HIS:CD2	1:A:408:HIS:C	2.95	0.42
1:A:701:PHE:O	1:A:705:TYR:N	2.53	0.42
1:A:181:SER:HA	3:A:999:DAE:F1	2.10	0.42
1:A:265:LYS:HD3	1:A:427:GLY:HA3	2.01	0.42
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.79	0.42
1:A:112:GLN:O	1:A:113:ASP:HB2	2.19	0.42
1:A:7:ARG:NH1	1:A:19:GLN:OE1	2.53	0.42
1:A:304:PHE:HA	1:A:356:ASN:HD21	1.85	0.42
1:A:628:ILE:HD13	1:A:628:ILE:HG21	1.86	0.42
1:A:96:TYR:CE2	1:A:749:GLY:HA3	2.55	0.41
1:A:96:TYR:HE2	1:A:749:GLY:HA3	1.85	0.41
1:A:319:SER:OG	1:A:322:GLU:CB	2.68	0.41
1:A:493:GLU:O	1:A:496:LYS:HB2	2.19	0.41
1:A:685:ILE:HG22	1:A:689:ARG:NH1	2.35	0.41
1:A:43:GLU:HA	1:A:670:LYS:NZ	2.33	0.41
1:A:375:LEU:C	1:A:375:LEU:CD2	2.91	0.41
1:A:488:LYS:HE2	1:A:488:LYS:HB2	1.83	0.41
1:A:593:GLN:HB2	1:A:596:LEU:HD12	2.02	0.41
1:A:698:TYR:CE2	1:A:739:PHE:HE2	2.34	0.41
1:A:43:GLU:CB	1:A:670:LYS:NZ	2.79	0.41
1:A:147:ARG:H	1:A:150:GLU:CD	2.28	0.41
1:A:449:PHE:CD2	1:A:449:PHE:C	2.99	0.41
1:A:508:LEU:HD23	1:A:508:LEU:HA	1.86	0.41
1:A:609:THR:O	1:A:613:ASN:ND2	2.48	0.41
1:A:212:GLU:O	1:A:216:LEU:HG	2.21	0.41
1:A:2:ASN:ND2	1:A:2:ASN:C	2.79	0.41
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.55	0.41
1:A:193:ILE:HD13	1:A:193:ILE:HG21	1.81	0.41
1:A:397:ARG:HB3	1:A:404:LEU:HG	2.03	0.41
1:A:581:ILE:N	1:A:582:GLN:OE1	2.54	0.41
1:A:593:GLN:O	1:A:596:LEU:HB2	2.20	0.41
1:A:34:TYR:HB2	1:A:51:GLU:HA	2.00	0.41
1:A:614:ASP:HA	1:A:615:PRO:HD3	1.91	0.41
1:A:753:ARG:NE	1:A:753:ARG:C	2.78	0.41
1:A:262:LEU:HD23	1:A:262:LEU:HA	1.85	0.41
1:A:323:GLU:O	1:A:326:ILE:HB	2.21	0.41
1:A:676:LEU:HB3	1:A:682:LEU:HG	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:680:GLY:CA	4:A:1099:HOH:O	2.68	0.41
1:A:704:ARG:C	1:A:705:TYR:CG	2.99	0.41
3:A:999:DAE:H6	3:A:999:DAE:HA21	1.62	0.41
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.53	0.41
1:A:91:MET:C	1:A:93:GLU:N	2.77	0.41
1:A:202:ARG:N	1:A:212:GLU:OE2	2.51	0.41
1:A:497:GLU:O	1:A:741:ILE:HB	2.20	0.41
1:A:686:ARG:CB	1:A:689:ARG:NH2	2.84	0.41
1:A:703:LYS:O	1:A:706:TYR:HD2	2.04	0.41
1:A:738:ARG:HD3	1:A:738:ARG:HA	1.82	0.41
1:A:293:LYS:HA	1:A:298:LEU:HB2	2.02	0.41
1:A:204:GLN:H	1:A:204:GLN:HG3	1.72	0.40
1:A:280:ILE:O	1:A:280:ILE:HG13	2.21	0.40
1:A:399:LEU:HA	1:A:403:ASP:O	2.21	0.40
1:A:594:GLN:CA	1:A:594:GLN:NE2	2.74	0.40
1:A:683:GLU:CG	1:A:686:ARG:NH2	2.84	0.40
1:A:727:LEU:O	1:A:731:ASN:N	2.54	0.40
1:A:341:GLN:O	1:A:345:PHE:HD2	2.04	0.40
1:A:710:PRO:HD2	1:A:729:HIS:CG	2.56	0.40
1:A:10:ASP:O	1:A:13:LYS:HB3	2.21	0.40
1:A:212:GLU:O	1:A:216:LEU:HD12	2.22	0.40
1:A:329:GLN:O	1:A:332:ASP:HB2	2.21	0.40
1:A:378:ALA:O	1:A:381:VAL:HG22	2.22	0.40
1:A:379:SER:HB3	1:A:384:VAL:O	2.21	0.40
1:A:600:PHE:HB3	1:A:612:PHE:CE1	2.56	0.40
1:A:698:TYR:CE1	1:A:720:GLN:CD	3.00	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	737/761 (97%)	654 (89%)	62 (8%)	21 (3%)	4 1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	ASN
1	A	714	ARG
1	A	741	ILE
1	A	7	ARG
1	A	29	VAL
1	A	60	PHE
1	A	68	GLN
1	A	293	LYS
1	A	498	LYS
1	A	719	SER
1	A	386	PRO
1	A	693	PRO
1	A	711	ASN
1	A	713	PRO
1	A	725	ALA
1	A	86	ASP
1	A	718	ASP
1	A	754	ILE
1	A	703	LYS
1	A	362	GLY
1	A	3	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	594/665 (89%)	530 (89%)	64 (11%)	6 3

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	4	ILE
1	A	22	SER
1	A	24	LEU
1	A	28	THR
1	A	29	VAL
1	A	38	ASN
1	A	40	ASP
1	A	46	SER
1	A	56	THR
1	A	66	ASP
1	A	74	LYS
1	A	75	ASP
1	A	83	ILE
1	A	84	LYS
1	A	91	MET
1	A	98	ASN
1	A	107	ARG
1	A	148	ARG
1	A	158	ILE
1	A	191	LYS
1	A	199	VAL
1	A	204	GLN
1	A	266	SER
1	A	291	GLU
1	A	298	LEU
1	A	303	SER
1	A	307	LEU
1	A	313	VAL
1	A	315	ILE
1	A	319	SER
1	A	326	ILE
1	A	337	SER
1	A	369	LEU
1	A	388	VAL
1	A	389	LEU
1	A	398	ILE
1	A	405	VAL
1	A	407	GLN
1	A	444	GLU
1	A	446	LYS
1	A	496	LYS
1	A	499	ILE

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Mol	Chain	Res	Type
1	A	517	ILE
1	A	520	ARG
1	A	534	VAL
1	A	578	MET
1	A	582	GLN
1	A	594	GLN
1	A	683	GLU
1	A	687	ILE
1	A	688	THR
1	A	694	ASN
1	A	697	ILE
1	A	702	VAL
1	A	724	ASP
1	A	726	VAL
1	A	727	LEU
1	A	733	ASP
1	A	735	GLU
1	A	738	ARG
1	A	751	LEU
1	A	753	ARG
1	A	755	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2	ASN
1	A	38	ASN
1	A	219	ASN
1	A	234	ASN
1	A	259	GLN
1	A	283	GLN
1	A	329	GLN
1	A	407	GLN
1	A	439	ASN
1	A	479	GLN
1	A	594	GLN
1	A	613	ASN
1	A	649	ASN
1	A	662	GLN
1	A	694	ASN

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 oligosaccharides 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	DAE	A	999	2	26,28,28	1.11	2 (7%)	24,42,42	1.31	2 (8%)

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	DAE	A	999	2	-	5/18/28/28	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	DAE	C1-NA3	2.89	1.45	1.37
3	A	999	DAE	C2-N2	2.51	1.50	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	DAE	CA2-NA3-C1	-3.90	113.89	123.35
3	A	999	DAE	C5-C4-N4	2.22	121.28	119.34

There are no chirality outliers.

All (5) torsion outliers are listed below:

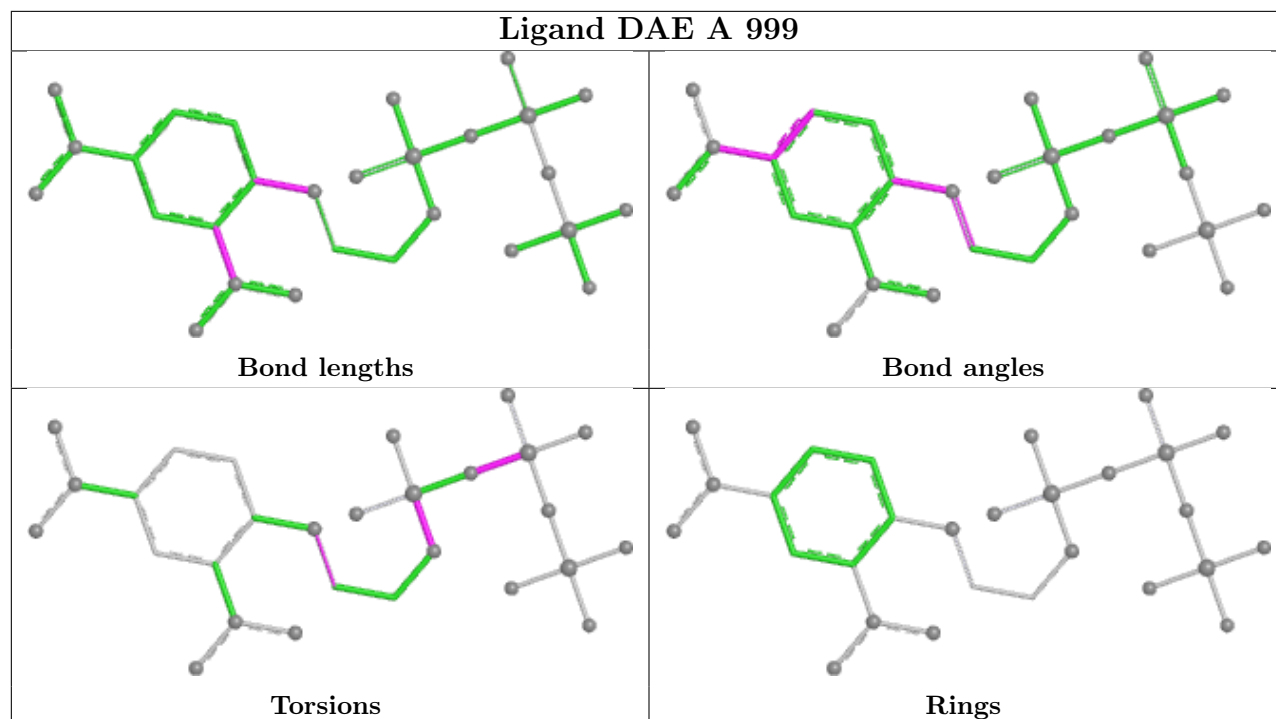
Mol	Chain	Res	Type	Atoms
3	A	999	DAE	CA1-OE2-PA-OA3
3	A	999	DAE	CA1-OE2-PA-OA1
3	A	999	DAE	CA1-CA2-NA3-C1
3	A	999	DAE	PA-OA3-PB-OB2
3	A	999	DAE	PA-OA3-PB-OB1

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	DAE	3	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 [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	745/761 (97%)	1.59	267 (35%) 1 1	17, 46, 97, 100	0

All (267) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	12.9
1	A	494	TYR	7.5
1	A	65	VAL	7.0
1	A	723	THR	6.7
1	A	443	GLN	6.6
1	A	744	ILE	6.1
1	A	734	PRO	5.5
1	A	732	ILE	5.3
1	A	27	LEU	5.2
1	A	60	PHE	5.2
1	A	727	LEU	5.2
1	A	708	LEU	5.1
1	A	300	GLY	4.8
1	A	688	THR	4.8
1	A	59	SER	4.7
1	A	72	VAL	4.6
1	A	209	GLY	4.6
1	A	745	PHE	4.6
1	A	61	THR	4.6
1	A	739	PHE	4.5
1	A	492	GLU	4.5
1	A	447	ALA	4.5
1	A	742	THR	4.4
1	A	62	PHE	4.4
1	A	406	ALA	4.3
1	A	53	VAL	4.3
1	A	362	GLY	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	381	VAL	4.3
1	A	98	ASN	4.2
1	A	721	LYS	4.2
1	A	495	LEU	4.2
1	A	498	LYS	4.1
1	A	722	ALA	4.1
1	A	30	SER	4.1
1	A	713	PRO	4.1
1	A	621	ALA	4.1
1	A	34	TYR	4.1
1	A	411	VAL	4.1
1	A	733	ASP	4.1
1	A	218	ALA	4.0
1	A	701	PHE	4.0
1	A	684	GLY	4.0
1	A	748	ALA	3.9
1	A	693	PRO	3.9
1	A	501	TRP	3.9
1	A	697	ILE	3.9
1	A	322	GLU	3.9
1	A	702	VAL	3.8
1	A	712	VAL	3.8
1	A	374	ALA	3.8
1	A	725	ALA	3.8
1	A	373	THR	3.8
1	A	741	ILE	3.7
1	A	706	TYR	3.7
1	A	299	ALA	3.7
1	A	718	ASP	3.7
1	A	615	PRO	3.7
1	A	85	PHE	3.7
1	A	535	PHE	3.7
1	A	729	HIS	3.7
1	A	25	PHE	3.7
1	A	536	PRO	3.6
1	A	50	GLY	3.6
1	A	364	GLY	3.6
1	A	383	GLY	3.6
1	A	22	SER	3.6
1	A	361	LYS	3.6
1	A	627	PHE	3.6
1	A	618	ALA	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	705	TYR	3.6
1	A	95	SER	3.6
1	A	298	LEU	3.6
1	A	445	ARG	3.6
1	A	68	GLN	3.6
1	A	56	THR	3.6
1	A	2	ASN	3.6
1	A	202	ARG	3.5
1	A	52	ILE	3.5
1	A	707	LEU	3.5
1	A	490	GLU	3.5
1	A	380	THR	3.5
1	A	39	PRO	3.5
1	A	287	GLY	3.5
1	A	508	LEU	3.5
1	A	444	GLU	3.5
1	A	746	PHE	3.4
1	A	489	LEU	3.4
1	A	497	GLU	3.4
1	A	47	TYR	3.4
1	A	730	LEU	3.4
1	A	696	ILE	3.4
1	A	386	PRO	3.4
1	A	757	ALA	3.4
1	A	698	TYR	3.3
1	A	507	GLY	3.3
1	A	740	GLY	3.3
1	A	388	VAL	3.3
1	A	500	ASN	3.3
1	A	329	GLN	3.3
1	A	67	GLY	3.3
1	A	401	GLY	3.2
1	A	537	ASN	3.2
1	A	343	SER	3.2
1	A	379	SER	3.2
1	A	692	PHE	3.2
1	A	310	SER	3.2
1	A	96	TYR	3.1
1	A	738	ARG	3.1
1	A	747	ARG	3.1
1	A	43	GLU	3.1
1	A	199	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	320	ASP	3.1
1	A	716	ALA	3.1
1	A	97	LEU	3.1
1	A	375	LEU	3.1
1	A	335	GLY	3.1
1	A	31	ASP	3.1
1	A	315	ILE	3.1
1	A	274	THR	3.1
1	A	384	VAL	3.1
1	A	603	SER	3.1
1	A	385	ASN	3.0
1	A	715	ASP	3.0
1	A	301	PRO	2.9
1	A	37	TYR	2.9
1	A	439	ASN	2.9
1	A	399	LEU	2.9
1	A	326	ILE	2.9
1	A	33	ARG	2.9
1	A	402	ARG	2.9
1	A	714	ARG	2.9
1	A	203	ASN	2.9
1	A	392	ALA	2.9
1	A	400	ALA	2.9
1	A	321	SER	2.9
1	A	24	LEU	2.8
1	A	219	ASN	2.8
1	A	749	GLY	2.8
1	A	376	ASN	2.8
1	A	324	PHE	2.8
1	A	506	PHE	2.8
1	A	349	ALA	2.8
1	A	710	PRO	2.8
1	A	13	LYS	2.8
1	A	336	PHE	2.8
1	A	358	LYS	2.8
1	A	3	PRO	2.8
1	A	368	VAL	2.8
1	A	328	ARG	2.7
1	A	54	SER	2.7
1	A	699	ALA	2.7
1	A	704	ARG	2.7
1	A	57	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	700	ASP	2.7
1	A	446	LYS	2.7
1	A	363	ALA	2.7
1	A	751	LEU	2.7
1	A	694	ASN	2.7
1	A	29	VAL	2.7
1	A	313	VAL	2.7
1	A	724	ASP	2.7
1	A	598	LEU	2.7
1	A	345	PHE	2.6
1	A	487	PHE	2.6
1	A	76	ASP	2.6
1	A	32	LYS	2.6
1	A	210	VAL	2.6
1	A	286	ALA	2.6
1	A	743	LYS	2.6
1	A	407	GLN	2.6
1	A	352	LEU	2.6
1	A	735	GLU	2.6
1	A	38	ASN	2.6
1	A	77	ALA	2.6
1	A	686	ARG	2.6
1	A	596	LEU	2.6
1	A	429	LEU	2.5
1	A	756	GLU	2.5
1	A	36	TRP	2.5
1	A	247	PHE	2.5
1	A	442	CYS	2.5
1	A	66	ASP	2.5
1	A	499	ILE	2.5
1	A	758	ARG	2.5
1	A	493	GLU	2.5
1	A	26	LYS	2.5
1	A	366	GLY	2.5
1	A	412	GLU	2.4
1	A	720	GLN	2.4
1	A	312	CYS	2.4
1	A	167	LEU	2.4
1	A	211	LEU	2.4
1	A	410	ASN	2.4
1	A	687	ILE	2.4
1	A	377	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	45	ASP	2.4
1	A	432	TRP	2.4
1	A	367	ALA	2.4
1	A	752	ALA	2.4
1	A	759	GLU	2.4
1	A	736	GLN	2.4
1	A	333	ILE	2.4
1	A	342	MET	2.3
1	A	372	LYS	2.3
1	A	309	GLN	2.3
1	A	602	ASP	2.3
1	A	674	ASP	2.3
1	A	414	SER	2.3
1	A	619	SER	2.3
1	A	719	SER	2.3
1	A	685	ILE	2.3
1	A	405	VAL	2.3
1	A	75	ASP	2.3
1	A	255	GLY	2.3
1	A	350	GLY	2.3
1	A	292	GLU	2.3
1	A	28	THR	2.3
1	A	285	LEU	2.3
1	A	296	LEU	2.3
1	A	213	GLN	2.2
1	A	269	VAL	2.2
1	A	726	VAL	2.2
1	A	70	ARG	2.2
1	A	731	ASN	2.2
1	A	35	ILE	2.2
1	A	158	ILE	2.2
1	A	243	ILE	2.2
1	A	754	ILE	2.2
1	A	509	ASP	2.2
1	A	20	GLY	2.2
1	A	216	LEU	2.2
1	A	204	GLN	2.2
1	A	136	THR	2.2
1	A	40	ASP	2.2
1	A	303	SER	2.2
1	A	397	ARG	2.2
1	A	14	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	41	PRO	2.1
1	A	755	GLU	2.1
1	A	46	SER	2.1
1	A	272	SER	2.1
1	A	415	SER	2.1
1	A	690	LYS	2.1
1	A	339	GLU	2.1
1	A	647	THR	2.1
1	A	491	GLN	2.1
1	A	408	HIS	2.1
1	A	387	SER	2.1
1	A	12	HIS	2.1
1	A	290	ALA	2.1
1	A	396	PRO	2.1
1	A	382	PHE	2.1
1	A	538	ALA	2.1
1	A	604	SER	2.1
1	A	709	ALA	2.1
1	A	356	ASN	2.0
1	A	64	THR	2.0
1	A	82	PRO	2.0
1	A	220	PRO	2.0
1	A	334	VAL	2.0
1	A	250	ALA	2.0
1	A	369	LEU	2.0
1	A	21	ASP	2.0
1	A	728	LYS	2.0
1	A	8	THR	2.0
1	A	327	THR	2.0
1	A	201	GLY	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 ⓘ

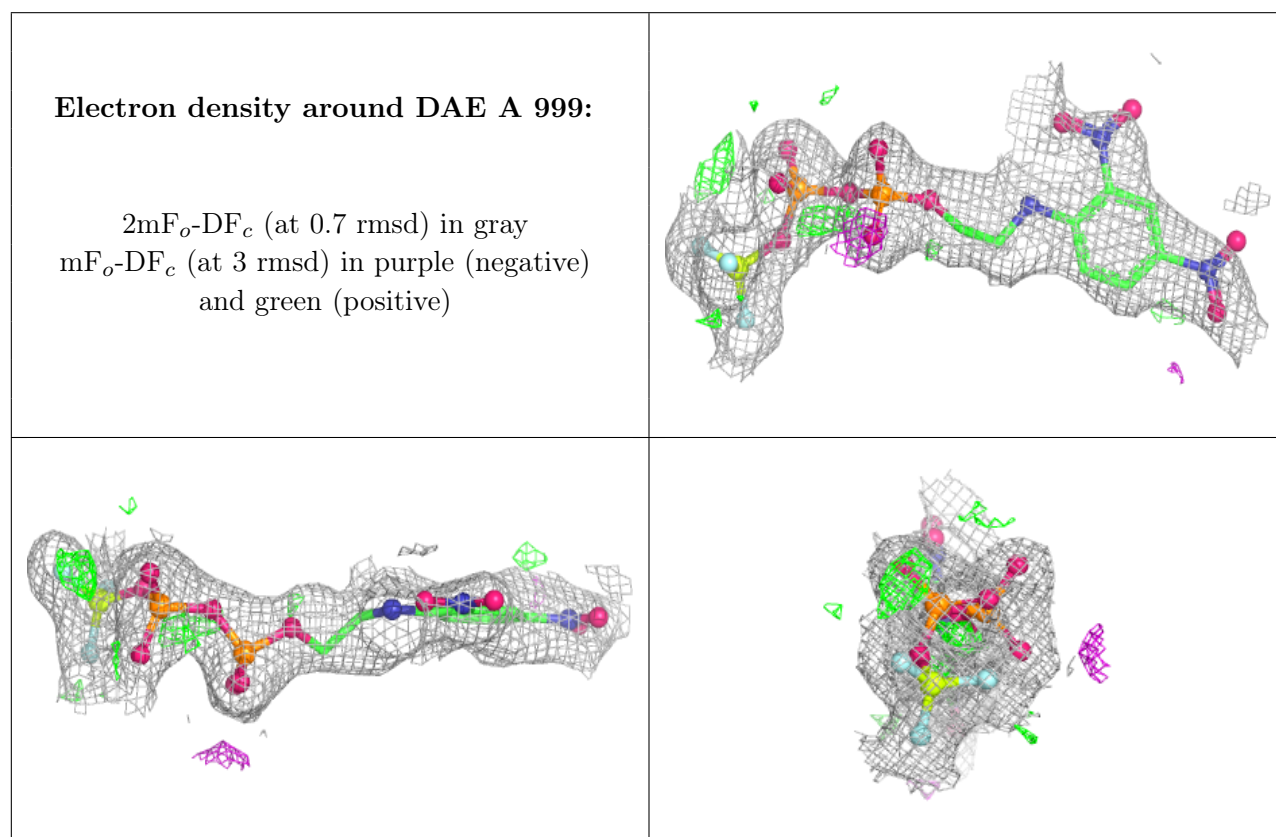
There are no oligosaccharides in this entry.

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
3	DAE	A	999	28/28	0.96	0.13	19,54,100,100	0
2	MG	A	998	1/1	0.98	0.05	25,25,25,25	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.