



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:00 PM UTC

PDB ID : 1D1B / pdb_00001d1b
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH O,P-DINITROPHENYL AMINOPROPYLDIPHOS
PHATE BERYLLIUM TRIFLUORIDE.
Authors : Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Pate, E.; Yount, R.G.; Rayment, I.
Deposited on : 1999-09-15
Resolution : 2.00 Å(reported)

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

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

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

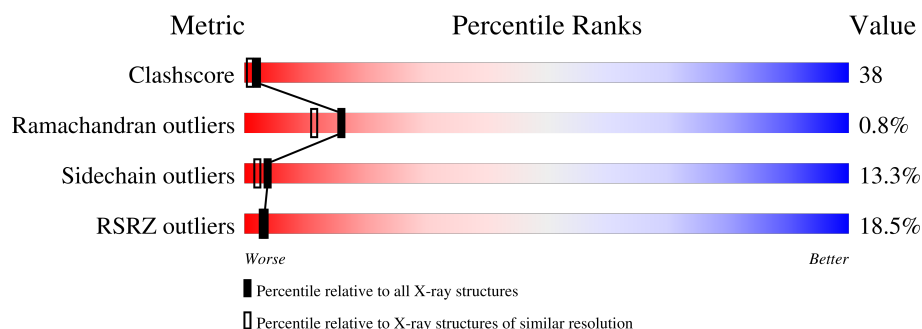
1 Overall quality at a glance

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 6374 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called MYOSIN.

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

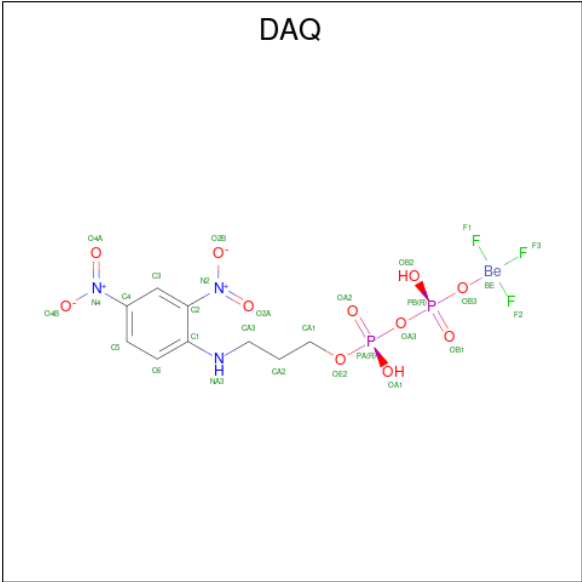
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	312	CYS	TYR	SEE REMARK 999	UNP P08799
A	760	PRO	GLN	engineered 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 AMINOPROPYLDIPHOSPHATE BERYLLIUM TRIFLUORIDE (CCD ID: DAQ) (formula: C₉H₁₂BeF₃N₃O₁₁P₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Be	C	F	N	O	P		
3	A	1	29	1	9	3	3	11	2	0	0

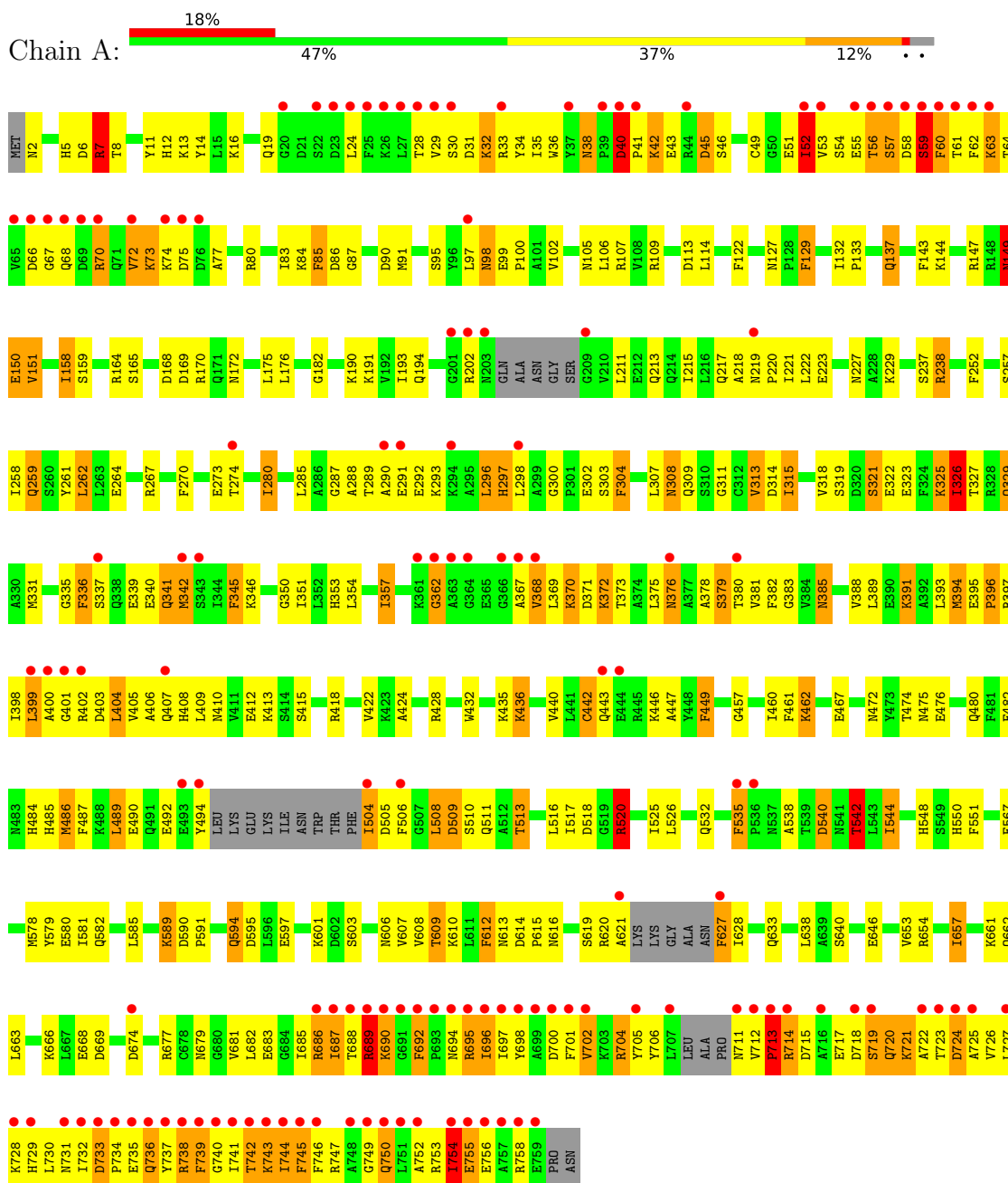
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	541	Total	O	0	0
			541	541		

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



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.88Å 180.46Å 54.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 25.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (25.00-2.00) 97.0 (25.00-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.32 (at 2.00Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.204 , (Not available) 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.5	Xtriage
Anisotropy	0.435	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 136.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6374	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.13% 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: DAQ, MG

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	2.21	27/5914 (0.5%)	1.92	112/7992 (1.4%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	40	ASP	CG-OD2	97.16	3.10	1.25
1	A	40	ASP	CG-OD1	61.10	2.41	1.25
1	A	40	ASP	CB-CG	45.15	2.65	1.52
1	A	657	ILE	CG1-CD1	38.06	3.00	1.51
1	A	480	GLN	CA-C	7.24	1.62	1.52
1	A	326	ILE	CA-CB	-6.38	1.47	1.54
1	A	657	ILE	CA-C	6.05	1.59	1.52
1	A	132	ILE	CA-CB	-6.04	1.49	1.54
1	A	440	VAL	N-CA	-5.79	1.39	1.46
1	A	520	ARG	CA-C	5.79	1.59	1.52
1	A	638	LEU	CA-CB	5.62	1.62	1.53
1	A	550	HIS	CA-C	-5.57	1.44	1.52
1	A	308	ASN	CA-C	-5.43	1.46	1.53
1	A	308	ASN	N-CA	-5.33	1.39	1.46
1	A	202	ARG	CA-C	5.30	1.58	1.53
1	A	663	LEU	C-N	5.30	1.39	1.33
1	A	578	MET	CA-CB	5.30	1.60	1.53
1	A	548	HIS	ND1-CE1	5.24	1.37	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	548	HIS	CA-C	5.22	1.59	1.52
1	A	689	ARG	NE-CZ	5.21	1.38	1.33
1	A	267	ARG	CA-C	-5.18	1.45	1.52
1	A	165	SER	C-N	-5.16	1.27	1.33
1	A	551	PHE	CA-CB	5.07	1.61	1.54
1	A	653	VAL	CA-C	5.05	1.59	1.52
1	A	526	LEU	CA-C	5.05	1.59	1.52
1	A	513	THR	CA-C	-5.04	1.46	1.52
1	A	122	PHE	CA-C	5.01	1.59	1.52

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	657	ILE	CB-CG1-CD1	-25.67	59.90	113.80
1	A	40	ASP	CB-CG-OD1	-20.31	71.69	118.40
1	A	40	ASP	CA-CB-CG	20.27	132.87	112.60
1	A	535	PHE	CA-CB-CG	-13.48	100.32	113.80
1	A	713	PRO	N-CA-CB	11.50	115.32	103.25
1	A	345	PHE	CA-CB-CG	-10.16	103.64	113.80
1	A	540	ASP	CA-CB-CG	9.50	122.10	112.60
1	A	45	ASP	CA-CB-CG	-9.13	103.47	112.60
1	A	72	VAL	CB-CA-C	-8.89	99.44	111.80
1	A	627	PHE	CA-CB-CG	8.87	122.67	113.80
1	A	40	ASP	CA-C-N	8.80	129.03	119.87
1	A	40	ASP	C-N-CA	8.80	129.03	119.87
1	A	484	HIS	CA-CB-CG	-8.55	105.25	113.80
1	A	402	ARG	N-CA-C	-8.34	102.88	113.72
1	A	40	ASP	CB-CG-OD2	-8.28	99.37	118.40
1	A	12	HIS	CA-CB-CG	-7.37	106.43	113.80
1	A	518	ASP	N-CA-C	7.32	122.39	113.17
1	A	724	ASP	N-CA-C	-7.24	103.47	111.36
1	A	341	GLN	N-CA-C	7.02	118.93	111.28
1	A	542	THR	N-CA-CB	-7.02	99.83	110.01
1	A	90	ASP	CA-CB-CG	7.00	119.60	112.60
1	A	692	PHE	O-C-N	6.99	127.56	121.34
1	A	149	ASN	CA-C-N	-6.97	111.17	122.26
1	A	149	ASN	C-N-CA	-6.97	111.17	122.26
1	A	238	ARG	NE-CZ-NH2	-6.84	113.05	119.20
1	A	85	PHE	CA-CB-CG	6.82	120.62	113.80
1	A	318	VAL	N-CA-C	6.80	117.91	108.12
1	A	475	ASN	CA-CB-CG	-6.79	105.81	112.60
1	A	724	ASP	CA-CB-CG	6.75	119.35	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	HIS	CA-CB-CG	-6.72	107.08	113.80
1	A	606	ASN	N-CA-C	6.51	119.37	111.82
1	A	692	PHE	CA-C-N	6.45	126.95	119.47
1	A	692	PHE	C-N-CA	6.45	126.95	119.47
1	A	525	ILE	N-CA-C	6.36	116.52	110.42
1	A	508	LEU	CA-C-N	6.31	129.03	120.38
1	A	508	LEU	C-N-CA	6.31	129.03	120.38
1	A	238	ARG	NE-CZ-NH1	6.24	127.74	121.50
1	A	717	GLU	N-CA-C	6.23	120.88	113.28
1	A	11	TYR	N-CA-C	-6.19	104.45	111.07
1	A	75	ASP	CB-CA-C	6.19	120.42	109.65
1	A	405	VAL	N-CA-C	6.18	116.76	108.11
1	A	696	ILE	N-CA-C	6.16	118.00	109.80
1	A	729	HIS	CA-C-N	6.15	129.13	120.28
1	A	729	HIS	C-N-CA	6.15	129.13	120.28
1	A	280	ILE	N-CA-C	6.07	117.53	110.62
1	A	449	PHE	CA-CB-CG	-6.07	107.73	113.80
1	A	755	GLU	N-CA-C	-6.04	104.81	111.82
1	A	494	TYR	N-CA-CB	6.04	120.77	110.50
1	A	29	VAL	CB-CA-C	5.96	119.84	111.08
1	A	612	PHE	CA-CB-CG	-5.81	107.99	113.80
1	A	73	LYS	N-CA-CB	5.80	118.81	110.06
1	A	14	TYR	N-CA-C	5.69	120.29	113.23
1	A	262	LEU	N-CA-CB	-5.68	103.50	111.62
1	A	237	SER	CA-C-O	-5.66	113.92	120.49
1	A	314	ASP	N-CA-C	5.62	117.95	109.23
1	A	535	PHE	CA-C-N	5.62	125.46	119.28
1	A	535	PHE	C-N-CA	5.62	125.46	119.28
1	A	335	GLY	CA-C-N	-5.60	113.49	121.50
1	A	335	GLY	C-N-CA	-5.60	113.49	121.50
1	A	315	ILE	N-CA-CB	5.59	118.91	111.64
1	A	336	PHE	CA-CB-CG	5.56	119.36	113.80
1	A	98	ASN	CA-CB-CG	5.56	118.16	112.60
1	A	702	VAL	N-CA-C	5.53	115.73	110.42
1	A	509	ASP	N-CA-C	5.52	118.01	111.33
1	A	538	ALA	N-CA-CB	5.45	118.73	110.45
1	A	129	PHE	N-CA-CB	5.44	120.35	112.13
1	A	511	GLN	N-CA-C	5.43	117.20	111.28
1	A	326	ILE	N-CA-CB	-5.38	104.97	110.62
1	A	59	SER	CA-C-N	-5.38	113.41	123.03
1	A	59	SER	C-N-CA	-5.38	113.41	123.03
1	A	739	PHE	N-CA-CB	5.38	118.54	109.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	ILE	CB-CA-C	5.37	118.53	111.33
1	A	229	LYS	CA-CB-CG	-5.36	103.38	114.10
1	A	137	GLN	CA-CB-CG	-5.33	103.43	114.10
1	A	447	ALA	N-CA-CB	5.33	118.45	110.19
1	A	144	LYS	N-CA-C	5.32	118.28	110.30
1	A	457	GLY	N-CA-C	-5.31	102.40	112.27
1	A	740	GLY	N-CA-C	-5.30	103.01	111.18
1	A	252	PHE	CA-CB-CG	-5.29	108.51	113.80
1	A	151	VAL	CA-CB-CG1	5.28	119.37	110.40
1	A	304	PHE	CA-CB-CG	5.25	119.05	113.80
1	A	472	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	33	ARG	N-CA-CB	5.24	117.93	110.44
1	A	442	CYS	N-CA-C	5.23	118.02	110.28
1	A	516	LEU	CA-C-O	5.22	126.08	120.55
1	A	758	ARG	N-CA-C	5.21	117.84	110.50
1	A	122	PHE	CA-CB-CG	5.19	118.99	113.80
1	A	396	PRO	CB-CA-C	-5.18	105.20	111.46
1	A	353	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	307	LEU	CA-C-N	-5.16	114.37	122.79
1	A	307	LEU	C-N-CA	-5.16	114.37	122.79
1	A	24	LEU	CB-CA-C	5.16	118.28	109.72
1	A	435	LYS	CA-C-O	5.15	125.88	120.42
1	A	308	ASN	CA-C-N	-5.13	112.67	122.53
1	A	308	ASN	C-N-CA	-5.13	112.67	122.53
1	A	113	ASP	CA-CB-CG	5.10	117.70	112.60
1	A	194	GLN	CB-CA-C	-5.09	102.88	110.88
1	A	168	ASP	N-CA-CB	5.08	117.78	110.20
1	A	474	THR	CA-C-O	5.08	126.34	120.90
1	A	215	ILE	N-CA-C	-5.08	105.03	110.36
1	A	385	ASN	CA-C-N	5.07	125.35	119.47
1	A	385	ASN	C-N-CA	5.07	125.35	119.47
1	A	476	GLU	CB-CA-C	-5.05	102.26	110.85
1	A	542	THR	N-CA-C	-5.04	105.68	111.07
1	A	606	ASN	CB-CA-C	5.04	120.34	110.67
1	A	754	ILE	N-CA-C	-5.04	105.63	110.72
1	A	262	LEU	CB-CA-C	-5.03	104.40	111.95
1	A	394	MET	CA-C-N	-5.03	117.14	122.28
1	A	394	MET	C-N-CA	-5.03	117.14	122.28
1	A	143	PHE	CA-CB-CG	-5.02	108.78	113.80
1	A	461	PHE	CA-CB-CG	-5.01	108.79	113.80
1	A	238	ARG	CD-NE-CZ	5.01	131.42	124.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	40	ASP	Sidechain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5803	0	5638	434	0
2	A	1	0	0	0	0
3	A	29	0	10	5	0
4	A	541	0	0	31	0
All	All	6374	0	5648	435	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 (435) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:THR:HB	1:A:292:GLU:OE2	1.38	1.19
1:A:532:GLN:OE1	1:A:542:THR:HG22	1.38	1.19
1:A:289:THR:HG22	1:A:291:GLU:H	1.05	1.14
1:A:62:PHE:HE2	1:A:72:VAL:CG2	1.61	1.12
1:A:686:ARG:HH11	1:A:686:ARG:HB2	0.95	1.10
1:A:63:LYS:HE2	1:A:67:GLY:HA2	1.32	1.09
1:A:7:ARG:HG3	1:A:7:ARG:HH11	1.08	1.08
1:A:342:MET:HE2	1:A:342:MET:HA	1.33	1.08
1:A:398:ILE:HD12	1:A:407:GLN:HG3	1.34	1.05
1:A:296:LEU:HB3	1:A:298:LEU:CD1	1.89	1.03
1:A:686:ARG:HH11	1:A:686:ARG:CB	1.72	1.02
1:A:62:PHE:HE2	1:A:72:VAL:HG23	1.23	1.01
1:A:734:PRO:HA	1:A:737:TYR:CZ	1.94	1.01
1:A:35:ILE:HD11	1:A:77:ALA:HB1	1.44	0.99
1:A:750:GLN:HE21	1:A:754:ILE:HD12	1.28	0.99
1:A:686:ARG:HB2	1:A:686:ARG:NH1	1.77	0.98
1:A:409:LEU:HD22	1:A:413:LYS:HE3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:PHE:CE1	1:A:486:MET:HE2	2.01	0.95
1:A:273:GLU:O	1:A:274:THR:OG1	1.85	0.94
1:A:62:PHE:CE2	1:A:72:VAL:HG23	2.02	0.94
1:A:62:PHE:CE2	1:A:72:VAL:CG2	2.52	0.93
1:A:706:TYR:CD1	1:A:713:PRO:HA	2.03	0.93
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.04	0.93
1:A:80:ARG:NH2	1:A:83:ILE:HD11	1.83	0.92
1:A:753:ARG:HA	1:A:756:GLU:HB2	1.51	0.91
1:A:289:THR:HG22	1:A:291:GLU:N	1.84	0.91
1:A:697:ILE:HB	1:A:700:ASP:HB2	1.54	0.90
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.79	0.90
1:A:80:ARG:CZ	1:A:83:ILE:HD11	2.01	0.90
1:A:55:GLU:HG2	1:A:56:THR:O	1.73	0.89
1:A:737:TYR:HB3	1:A:746:PHE:CE1	2.09	0.88
1:A:487:PHE:CE2	1:A:505:ASP:HB2	2.10	0.87
1:A:432:TRP:CZ2	1:A:436:LYS:HD2	2.08	0.87
1:A:296:LEU:HB3	1:A:298:LEU:HD13	1.57	0.86
1:A:296:LEU:HB3	1:A:298:LEU:HD11	1.55	0.86
1:A:60:PHE:CE1	1:A:74:LYS:HA	2.10	0.85
1:A:35:ILE:HD11	1:A:77:ALA:CB	2.07	0.85
1:A:736:GLN:HB3	1:A:750:GLN:HG2	1.57	0.83
1:A:219:ASN:HB3	1:A:220:PRO:HD3	1.59	0.83
1:A:84:LYS:HD2	1:A:84:LYS:C	2.04	0.83
1:A:487:PHE:CD2	1:A:505:ASP:HB2	2.12	0.83
1:A:695:ARG:HA	1:A:744:ILE:O	1.79	0.82
1:A:191:LYS:HA	1:A:191:LYS:HE2	1.60	0.82
1:A:43:GLU:OE1	1:A:43:GLU:HA	1.74	0.81
1:A:40:ASP:OD1	1:A:42:LYS:HG2	1.80	0.81
1:A:99:GLU:HG2	1:A:686:ARG:HH21	1.46	0.81
1:A:289:THR:O	1:A:293:LYS:HD2	1.79	0.81
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.15	0.81
1:A:99:GLU:HG2	1:A:686:ARG:NH2	1.97	0.80
1:A:399:LEU:HD23	1:A:403:ASP:O	1.80	0.80
1:A:97:LEU:HB2	1:A:689:ARG:HD3	1.63	0.80
1:A:342:MET:HA	1:A:342:MET:CE	2.12	0.79
1:A:398:ILE:HD12	1:A:407:GLN:CG	2.12	0.79
1:A:34:TYR:CD1	1:A:51:GLU:HA	2.18	0.78
1:A:7:ARG:HG3	1:A:7:ARG:NH1	1.85	0.78
1:A:289:THR:CB	1:A:292:GLU:OE2	2.27	0.78
1:A:319:SER:OG	1:A:322:GLU:HG2	1.83	0.78
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:ILE:HG22	1:A:742:THR:CG2	2.14	0.77
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.67	0.77
1:A:371:ASP:OD2	1:A:373:THR:N	2.15	0.77
1:A:398:ILE:CD1	1:A:407:GLN:HG3	2.14	0.76
1:A:706:TYR:HD1	1:A:713:PRO:HA	1.49	0.76
1:A:482:PHE:HE1	1:A:486:MET:HE2	1.48	0.76
1:A:687:ILE:HG22	1:A:688:THR:N	1.97	0.76
1:A:87:GLY:H	1:A:105:ASN:ND2	1.82	0.76
1:A:695:ARG:HD3	1:A:745:PHE:CE2	2.20	0.75
1:A:219:ASN:HA	4:A:1403:HOH:O	1.87	0.75
1:A:337:SER:O	1:A:341:GLN:HG3	1.87	0.74
1:A:668:GLU:OE1	4:A:1203:HOH:O	2.06	0.74
1:A:735:GLU:HA	1:A:738:ARG:HH21	1.53	0.74
1:A:391:LYS:HB3	1:A:391:LYS:NZ	2.03	0.73
1:A:296:LEU:CB	1:A:298:LEU:HD13	2.18	0.73
1:A:750:GLN:HE21	1:A:754:ILE:CD1	2.01	0.72
1:A:385:ASN:HB3	1:A:388:VAL:CG2	2.19	0.72
3:A:999:DAQ:HA22	4:A:1509:HOH:O	1.90	0.72
1:A:513:THR:O	1:A:517:ILE:HD12	1.88	0.71
1:A:504:ILE:O	1:A:504:ILE:HG13	1.89	0.71
1:A:63:LYS:HE2	1:A:67:GLY:CA	2.17	0.71
1:A:698:TYR:CZ	1:A:720:GLN:HG2	2.25	0.71
1:A:692:PHE:HB3	1:A:745:PHE:HB3	1.71	0.71
1:A:354:LEU:O	1:A:418:ARG:HD3	1.90	0.70
1:A:540:ASP:OD2	4:A:1264:HOH:O	2.09	0.70
1:A:682:LEU:HB3	1:A:686:ARG:HH22	1.55	0.70
1:A:40:ASP:CG	1:A:40:ASP:CB	2.64	0.70
1:A:321:SER:O	1:A:325:LYS:HE2	1.92	0.70
1:A:382:PHE:O	1:A:603:SER:OG	2.09	0.70
1:A:63:LYS:CE	1:A:67:GLY:HA2	2.18	0.70
1:A:391:LYS:HZ2	1:A:395:GLU:HB2	1.58	0.69
1:A:273:GLU:O	4:A:1523:HOH:O	2.11	0.69
1:A:694:ASN:C	1:A:695:ARG:HG2	2.18	0.68
1:A:399:LEU:HD22	1:A:401:GLY:H	1.58	0.68
1:A:137:GLN:HG3	1:A:137:GLN:O	1.94	0.67
1:A:147:ARG:HG3	1:A:147:ARG:HH11	1.59	0.67
1:A:331:MET:HE1	1:A:345:PHE:HZ	1.56	0.67
1:A:368:VAL:HG12	1:A:369:LEU:H	1.60	0.67
1:A:734:PRO:HA	1:A:737:TYR:CE1	2.29	0.67
1:A:336:PHE:O	1:A:341:GLN:NE2	2.26	0.67
1:A:737:TYR:HB3	1:A:746:PHE:HE1	1.58	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ASN:HD21	3:A:999:DAQ:HA21	1.59	0.66
1:A:97:LEU:HD13	1:A:685:ILE:HG23	1.77	0.66
1:A:219:ASN:HB3	1:A:220:PRO:CD	2.24	0.66
1:A:298:LEU:N	1:A:298:LEU:HD12	2.09	0.66
1:A:367:ALA:HB3	1:A:394:MET:HG2	1.78	0.66
1:A:34:TYR:HE1	1:A:51:GLU:HB2	1.61	0.66
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.28	0.66
1:A:752:ALA:O	1:A:756:GLU:N	2.29	0.66
1:A:532:GLN:OE1	1:A:542:THR:CG2	2.31	0.66
1:A:736:GLN:NE2	1:A:753:ARG:HH22	1.93	0.66
1:A:396:PRO:HD2	1:A:407:GLN:O	1.96	0.65
1:A:367:ALA:O	1:A:408:HIS:NE2	2.27	0.65
1:A:736:GLN:HG3	1:A:750:GLN:OE1	1.97	0.65
1:A:56:THR:CG2	1:A:57:SER:N	2.59	0.65
1:A:60:PHE:HE1	1:A:74:LYS:HA	1.60	0.65
1:A:682:LEU:O	1:A:686:ARG:NH1	2.30	0.64
1:A:35:ILE:CD1	1:A:77:ALA:HB1	2.23	0.64
1:A:302:GLU:H	1:A:302:GLU:CD	2.05	0.64
1:A:62:PHE:HE2	1:A:72:VAL:HG21	1.60	0.64
1:A:327:THR:HG22	1:A:331:MET:HE2	1.79	0.64
1:A:60:PHE:O	1:A:72:VAL:N	2.30	0.64
1:A:322:GLU:O	1:A:325:LYS:HB2	1.96	0.64
1:A:489:LEU:N	1:A:489:LEU:HD23	2.06	0.64
1:A:56:THR:HG23	1:A:57:SER:H	1.63	0.63
1:A:682:LEU:HD22	1:A:686:ARG:NH2	2.12	0.63
1:A:741:ILE:C	1:A:742:THR:HG23	2.23	0.63
1:A:409:LEU:HD22	1:A:413:LYS:CE	2.25	0.63
1:A:692:PHE:O	1:A:695:ARG:NE	2.31	0.63
1:A:40:ASP:OD1	1:A:40:ASP:CG	2.41	0.63
1:A:16:LYS:NZ	4:A:1014:HOH:O	2.31	0.63
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.34	0.63
1:A:695:ARG:HA	1:A:745:PHE:HA	1.81	0.63
1:A:371:ASP:OD2	1:A:372:LYS:N	2.32	0.63
1:A:399:LEU:CD2	1:A:400:ALA:N	2.62	0.62
1:A:687:ILE:O	1:A:690:LYS:HG3	1.99	0.62
1:A:681:VAL:O	1:A:685:ILE:HG13	1.99	0.62
1:A:696:ILE:O	1:A:743:LYS:HB3	2.00	0.62
1:A:727:LEU:O	1:A:731:ASN:HA	2.00	0.62
1:A:300:GLY:O	1:A:303:SER:HB2	2.00	0.62
1:A:72:VAL:HG12	1:A:73:LYS:N	2.14	0.61
1:A:60:PHE:N	1:A:72:VAL:O	2.31	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:O	1:A:376:ASN:ND2	2.33	0.61
1:A:621:ALA:HB3	1:A:627:PHE:HA	1.82	0.61
1:A:409:LEU:CD2	1:A:413:LYS:HE3	2.27	0.61
1:A:378:ALA:O	1:A:381:VAL:HG22	2.01	0.60
1:A:64:THR:HG23	1:A:68:GLN:O	2.00	0.60
1:A:176:LEU:N	1:A:176:LEU:HD12	2.17	0.60
1:A:724:ASP:O	1:A:728:LYS:N	2.34	0.60
1:A:391:LYS:HB3	1:A:391:LYS:HZ1	1.65	0.60
1:A:621:ALA:HB2	1:A:628:ILE:HG23	1.84	0.60
1:A:535:PHE:N	1:A:535:PHE:CD2	2.69	0.60
1:A:91:MET:HE1	1:A:106:LEU:HG	1.84	0.59
1:A:742:THR:OG1	1:A:743:LYS:HG3	2.02	0.59
1:A:56:THR:HG22	1:A:58:ASP:H	1.68	0.59
1:A:87:GLY:H	1:A:105:ASN:HD21	1.48	0.59
1:A:56:THR:CG2	1:A:57:SER:H	2.15	0.59
1:A:62:PHE:CE2	1:A:72:VAL:HG21	2.35	0.59
1:A:30:SER:HA	4:A:1282:HOH:O	2.03	0.58
1:A:298:LEU:CD1	1:A:298:LEU:N	2.66	0.58
1:A:415:SER:O	1:A:418:ARG:HB3	2.03	0.58
1:A:218:ALA:O	1:A:221:ILE:HB	2.04	0.58
1:A:695:ARG:HB3	1:A:745:PHE:CD1	2.38	0.58
1:A:544:ILE:O	1:A:544:ILE:HG13	2.03	0.58
1:A:217:GLN:O	1:A:220:PRO:HD2	2.03	0.58
1:A:706:TYR:HB2	1:A:712:VAL:O	2.03	0.58
1:A:357:ILE:HG22	1:A:357:ILE:O	2.03	0.57
1:A:735:GLU:CB	1:A:738:ARG:HH21	2.17	0.57
1:A:219:ASN:CB	1:A:220:PRO:CD	2.80	0.57
1:A:590:ASP:N	1:A:591:PRO:HD3	2.20	0.57
1:A:704:ARG:NH2	1:A:755:GLU:OE1	2.33	0.57
1:A:399:LEU:HD22	1:A:400:ALA:N	2.20	0.57
1:A:2:ASN:ND2	1:A:5:HIS:CE1	2.73	0.56
1:A:83:ILE:HG13	1:A:86:ASP:OD1	2.05	0.56
1:A:722:ALA:O	1:A:726:VAL:HG23	2.05	0.56
1:A:213:GLN:O	1:A:217:GLN:HG2	2.05	0.56
1:A:290:ALA:HA	1:A:293:LYS:HD2	1.87	0.56
1:A:753:ARG:O	1:A:756:GLU:O	2.24	0.56
1:A:410:ASN:OD1	1:A:413:LYS:HB2	2.06	0.56
1:A:399:LEU:HD21	1:A:401:GLY:O	2.04	0.56
1:A:736:GLN:CB	1:A:750:GLN:HG2	2.34	0.56
1:A:290:ALA:HA	1:A:293:LYS:CD	2.35	0.56
1:A:585:LEU:O	1:A:589:LYS:HD3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:686:ARG:HH11	1:A:686:ARG:CG	2.18	0.55
1:A:397:ARG:HB3	1:A:404:LEU:HD22	1.87	0.55
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.41	0.55
1:A:311:GLY:N	4:A:1083:HOH:O	2.15	0.55
1:A:718:ASP:O	1:A:721:LYS:N	2.40	0.55
1:A:308:ASN:OD1	1:A:309:GLN:NE2	2.40	0.55
1:A:698:TYR:HB3	1:A:719:SER:HB3	1.87	0.55
1:A:133:PRO:HB2	4:A:1225:HOH:O	2.06	0.55
1:A:323:GLU:HA	1:A:326:ILE:HG13	1.88	0.54
1:A:662:GLN:NE2	4:A:1397:HOH:O	2.39	0.54
1:A:706:TYR:HB2	1:A:712:VAL:HG12	1.90	0.54
1:A:61:THR:HA	1:A:70:ARG:O	2.07	0.54
1:A:217:GLN:C	1:A:220:PRO:HD2	2.33	0.54
1:A:505:ASP:O	1:A:508:LEU:HD23	2.07	0.54
1:A:749:GLY:O	1:A:753:ARG:HG3	2.07	0.54
1:A:750:GLN:NE2	1:A:754:ILE:HD12	2.10	0.54
1:A:238:ARG:CD	1:A:264:GLU:OE2	2.56	0.54
1:A:190:LYS:O	4:A:1242:HOH:O	2.18	0.54
1:A:259:GLN:OE1	4:A:1413:HOH:O	2.17	0.54
1:A:219:ASN:OD1	1:A:220:PRO:N	2.42	0.53
1:A:654:ARG:NH2	1:A:679:ASN:O	2.38	0.53
1:A:331:MET:CE	1:A:345:PHE:HZ	2.21	0.53
1:A:442:CYS:SG	1:A:443:GLN:N	2.82	0.53
1:A:697:ILE:CB	1:A:700:ASP:HB2	2.33	0.53
1:A:323:GLU:HA	1:A:323:GLU:OE1	2.08	0.53
1:A:389:LEU:HG	1:A:393:LEU:HD12	1.90	0.53
1:A:219:ASN:N	1:A:220:PRO:HD2	2.22	0.53
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.91	0.53
1:A:695:ARG:HB3	1:A:745:PHE:CG	2.44	0.53
1:A:399:LEU:HD22	1:A:401:GLY:N	2.23	0.53
1:A:745:PHE:CD1	1:A:745:PHE:N	2.76	0.53
1:A:399:LEU:HD23	1:A:400:ALA:H	1.73	0.53
1:A:628:ILE:HD11	1:A:633:GLN:HB2	1.91	0.53
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.48	0.53
1:A:506:PHE:O	1:A:509:ASP:HB2	2.08	0.53
1:A:695:ARG:CD	1:A:745:PHE:CE2	2.91	0.52
1:A:741:ILE:HG22	1:A:742:THR:HG23	1.89	0.52
1:A:102:VAL:HG21	1:A:685:ILE:HD12	1.92	0.52
1:A:701:PHE:CD1	1:A:705:TYR:CD2	2.97	0.52
1:A:391:LYS:NZ	1:A:395:GLU:HB2	2.23	0.52
1:A:2:ASN:HD22	1:A:5:HIS:CE1	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:666:LYS:HE3	4:A:1208:HOH:O	2.10	0.52
1:A:694:ASN:O	1:A:745:PHE:HA	2.10	0.52
1:A:399:LEU:HD23	1:A:400:ALA:N	2.25	0.52
1:A:323:GLU:O	1:A:326:ILE:HB	2.09	0.52
1:A:147:ARG:HB2	1:A:149:ASN:ND2	2.25	0.51
1:A:749:GLY:C	1:A:753:ARG:NH1	2.69	0.51
1:A:695:ARG:NE	1:A:745:PHE:CD2	2.79	0.51
1:A:732:ILE:HG22	1:A:733:ASP:N	2.25	0.51
1:A:308:ASN:OD1	1:A:308:ASN:C	2.54	0.51
1:A:504:ILE:HG12	1:A:506:PHE:CE1	2.46	0.51
1:A:619:SER:HB3	1:A:627:PHE:CE2	2.46	0.51
1:A:745:PHE:N	1:A:745:PHE:HD1	2.09	0.51
1:A:2:ASN:O	1:A:5:HIS:N	2.34	0.51
1:A:238:ARG:HH11	1:A:264:GLU:CD	2.18	0.51
1:A:722:ALA:O	1:A:725:ALA:HB3	2.11	0.51
1:A:172:ASN:HB2	4:A:1439:HOH:O	2.10	0.51
1:A:646:GLU:OE1	4:A:1195:HOH:O	2.19	0.51
1:A:59:SER:HB2	1:A:72:VAL:O	2.12	0.50
1:A:72:VAL:CG1	1:A:73:LYS:N	2.73	0.50
1:A:409:LEU:CD2	1:A:413:LYS:CE	2.89	0.50
1:A:695:ARG:O	1:A:743:LYS:HD3	2.11	0.50
1:A:695:ARG:CA	1:A:744:ILE:O	2.56	0.50
1:A:701:PHE:CE1	1:A:705:TYR:CD2	2.99	0.50
1:A:292:GLU:O	1:A:296:LEU:HB2	2.12	0.50
1:A:84:LYS:HD2	1:A:84:LYS:O	2.12	0.50
1:A:406:ALA:C	1:A:407:GLN:HG2	2.36	0.50
1:A:52:ILE:HD12	1:A:52:ILE:C	2.36	0.49
1:A:389:LEU:HG	1:A:393:LEU:CD1	2.42	0.49
1:A:391:LYS:NZ	1:A:395:GLU:CB	2.75	0.49
1:A:702:VAL:HG21	1:A:722:ALA:HB3	1.94	0.49
1:A:735:GLU:CA	1:A:738:ARG:HH21	2.24	0.49
1:A:292:GLU:O	1:A:293:LYS:C	2.54	0.49
1:A:59:SER:CB	1:A:72:VAL:O	2.60	0.49
1:A:679:ASN:HB2	4:A:1117:HOH:O	2.12	0.49
1:A:567:GLU:HA	1:A:579:TYR:O	2.12	0.49
1:A:734:PRO:CA	1:A:737:TYR:CZ	2.84	0.49
1:A:147:ARG:HH11	1:A:147:ARG:CG	2.25	0.49
1:A:297:HIS:C	1:A:298:LEU:HD12	2.38	0.49
1:A:315:ILE:HD13	4:A:1416:HOH:O	2.13	0.49
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.95	0.49
1:A:238:ARG:HD3	1:A:264:GLU:OE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:LEU:HD22	1:A:686:ARG:HH21	1.76	0.48
1:A:289:THR:C	1:A:291:GLU:H	2.20	0.48
1:A:389:LEU:HD11	1:A:393:LEU:HD11	1.95	0.48
1:A:397:ARG:HA	1:A:406:ALA:HA	1.94	0.48
1:A:97:LEU:H	1:A:689:ARG:NE	2.12	0.48
1:A:683:GLU:CG	1:A:687:ILE:HD12	2.42	0.48
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.45	0.48
1:A:702:VAL:HG13	1:A:712:VAL:HG11	1.96	0.48
1:A:654:ARG:NH1	4:A:1200:HOH:O	2.05	0.48
1:A:698:TYR:CE1	1:A:720:GLN:HG2	2.48	0.48
1:A:736:GLN:HB3	1:A:750:GLN:CG	2.38	0.48
1:A:127:ASN:OD1	3:A:999:DAQ:O2A	2.31	0.48
1:A:697:ILE:HD13	1:A:743:LYS:HG2	1.96	0.48
1:A:56:THR:HG22	1:A:57:SER:N	2.28	0.48
1:A:38:ASN:C	1:A:40:ASP:H	2.22	0.48
1:A:147:ARG:CB	1:A:149:ASN:ND2	2.76	0.48
1:A:590:ASP:N	1:A:591:PRO:CD	2.76	0.47
1:A:191:LYS:HE2	1:A:191:LYS:CA	2.37	0.47
1:A:594:GLN:O	1:A:594:GLN:HG3	2.14	0.47
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.49	0.47
1:A:273:GLU:C	1:A:274:THR:OG1	2.56	0.47
1:A:313:VAL:HG23	1:A:313:VAL:O	2.13	0.47
1:A:375:LEU:HD12	1:A:389:LEU:HD23	1.96	0.47
1:A:686:ARG:CB	1:A:686:ARG:NH1	2.57	0.47
1:A:737:TYR:CD1	1:A:737:TYR:C	2.92	0.47
1:A:98:ASN:OD1	1:A:100:PRO:HD2	2.15	0.47
1:A:741:ILE:C	1:A:742:THR:CG2	2.88	0.47
1:A:191:LYS:HA	1:A:191:LYS:CE	2.38	0.47
1:A:289:THR:C	1:A:291:GLU:N	2.71	0.47
1:A:410:ASN:OD1	1:A:410:ASN:C	2.57	0.47
1:A:504:ILE:O	1:A:504:ILE:HG23	2.15	0.47
1:A:621:ALA:HB2	1:A:628:ILE:H	1.79	0.47
1:A:698:TYR:CE2	1:A:720:GLN:HG2	2.49	0.47
1:A:40:ASP:OD1	1:A:42:LYS:CG	2.59	0.47
1:A:345:PHE:HD1	1:A:345:PHE:HA	1.57	0.47
1:A:172:ASN:ND2	4:A:1439:HOH:O	2.27	0.46
1:A:80:ARG:NE	1:A:83:ILE:HD11	2.30	0.46
1:A:289:THR:CG2	1:A:290:ALA:N	2.78	0.46
1:A:285:LEU:HD11	1:A:304:PHE:CE1	2.51	0.46
1:A:380:THR:HG22	1:A:381:VAL:N	2.29	0.46
1:A:683:GLU:HG3	1:A:687:ILE:HD12	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:697:ILE:HG22	1:A:700:ASP:H	1.80	0.46
1:A:147:ARG:CG	1:A:147:ARG:NH1	2.78	0.46
1:A:219:ASN:CB	1:A:220:PRO:HD3	2.36	0.46
1:A:520:ARG:HD3	4:A:1146:HOH:O	2.16	0.46
1:A:609:THR:OG1	4:A:1267:HOH:O	2.20	0.46
1:A:696:ILE:C	1:A:743:LYS:HB3	2.40	0.46
1:A:368:VAL:HG12	1:A:369:LEU:N	2.28	0.46
1:A:72:VAL:HG12	1:A:73:LYS:O	2.15	0.46
1:A:449:PHE:C	1:A:449:PHE:CD2	2.94	0.46
1:A:601:LYS:O	1:A:613:ASN:OD1	2.34	0.46
1:A:59:SER:HB2	1:A:73:LYS:HA	1.98	0.46
1:A:109:ARG:HB3	1:A:114:LEU:HB2	1.97	0.46
1:A:692:PHE:CE1	1:A:747:ARG:HG2	2.50	0.46
1:A:107:ARG:NH2	4:A:1031:HOH:O	2.37	0.46
1:A:223:GLU:O	1:A:227:ASN:HB2	2.15	0.46
1:A:273:GLU:C	1:A:274:THR:HG1	2.13	0.46
1:A:372:LYS:HB3	1:A:376:ASN:HD21	1.81	0.46
1:A:296:LEU:HD12	1:A:296:LEU:HA	1.65	0.45
1:A:692:PHE:CE1	1:A:747:ARG:CG	2.99	0.45
1:A:399:LEU:CD2	1:A:399:LEU:C	2.89	0.45
1:A:219:ASN:C	1:A:221:ILE:N	2.74	0.45
1:A:727:LEU:O	1:A:731:ASN:CA	2.65	0.45
1:A:321:SER:O	1:A:325:LYS:CE	2.63	0.45
1:A:395:GLU:HA	1:A:407:GLN:O	2.16	0.45
1:A:399:LEU:HD21	1:A:401:GLY:C	2.42	0.45
1:A:706:TYR:CD1	1:A:713:PRO:CA	2.90	0.45
1:A:692:PHE:CD1	1:A:747:ARG:HG2	2.52	0.45
1:A:34:TYR:CD1	1:A:51:GLU:CA	2.96	0.45
1:A:38:ASN:OD1	1:A:38:ASN:N	2.50	0.45
1:A:685:ILE:HG22	1:A:686:ARG:HD3	1.99	0.45
1:A:732:ILE:HG21	1:A:750:GLN:CD	2.42	0.45
1:A:695:ARG:HB3	1:A:745:PHE:CE1	2.52	0.45
1:A:701:PHE:O	1:A:705:TYR:HD2	1.99	0.45
1:A:730:LEU:HA	1:A:730:LEU:HD23	1.59	0.45
1:A:750:GLN:OE1	1:A:753:ARG:NH2	2.50	0.45
1:A:339:GLU:HB3	1:A:340:GLU:H	1.63	0.45
1:A:486:MET:HE3	1:A:486:MET:HB3	1.73	0.45
1:A:490:GLU:OE1	1:A:490:GLU:HA	2.17	0.45
1:A:698:TYR:CE1	1:A:720:GLN:CG	3.00	0.44
1:A:698:TYR:O	1:A:702:VAL:HG23	2.17	0.44
1:A:372:LYS:HB3	1:A:372:LYS:HE2	1.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:HB2	1:A:150:GLU:HB2	1.99	0.44
1:A:262:LEU:HB3	4:A:1411:HOH:O	2.17	0.44
1:A:595:ASP:HB3	4:A:1461:HOH:O	2.17	0.44
1:A:193:ILE:HG21	1:A:193:ILE:HD13	1.75	0.44
1:A:375:LEU:CD1	1:A:389:LEU:HD23	2.48	0.44
1:A:694:ASN:HB2	1:A:746:PHE:HB2	2.00	0.44
1:A:325:LYS:O	1:A:329:GLN:HB2	2.18	0.44
1:A:40:ASP:HA	1:A:41:PRO:HD3	1.78	0.44
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.44	0.44
1:A:686:ARG:NH1	1:A:686:ARG:CG	2.81	0.44
1:A:754:ILE:HG22	1:A:755:GLU:N	2.32	0.44
1:A:191:LYS:CA	1:A:191:LYS:CE	2.95	0.43
1:A:270:PHE:CD1	1:A:270:PHE:C	2.96	0.43
1:A:607:VAL:O	1:A:608:VAL:C	2.60	0.43
1:A:85:PHE:HE2	4:A:1285:HOH:O	2.00	0.43
1:A:182:GLY:HA2	3:A:999:DAQ:HA11	2.00	0.43
1:A:309:GLN:NE2	4:A:1456:HOH:O	2.49	0.43
1:A:341:GLN:O	1:A:345:PHE:CD2	2.71	0.43
1:A:325:LYS:HA	1:A:325:LYS:HD3	1.49	0.43
1:A:744:ILE:C	1:A:745:PHE:HD1	2.27	0.43
1:A:129:PHE:CE1	1:A:662:GLN:HA	2.53	0.43
1:A:190:LYS:HE3	1:A:223:GLU:OE2	2.18	0.43
1:A:337:SER:OG	1:A:339:GLU:HB3	2.19	0.43
1:A:64:THR:OG1	1:A:68:GLN:N	2.52	0.43
1:A:692:PHE:O	1:A:695:ARG:CZ	2.67	0.43
1:A:175:LEU:HD12	1:A:175:LEU:N	2.34	0.42
1:A:362:GLY:HA3	1:A:368:VAL:CG2	2.49	0.42
1:A:467:GLU:CD	1:A:467:GLU:H	2.26	0.42
1:A:738:ARG:HA	1:A:738:ARG:HD3	1.48	0.42
1:A:64:THR:CG2	1:A:68:GLN:O	2.67	0.42
1:A:149:ASN:ND2	1:A:150:GLU:OE1	2.52	0.42
1:A:485:HIS:ND1	4:A:1136:HOH:O	2.14	0.42
1:A:508:LEU:N	1:A:508:LEU:CD2	2.81	0.42
1:A:735:GLU:CB	1:A:738:ARG:NH2	2.81	0.42
1:A:594:GLN:HA	1:A:594:GLN:HE21	1.84	0.42
1:A:719:SER:O	1:A:723:THR:N	2.52	0.42
1:A:99:GLU:CD	1:A:682:LEU:HD13	2.45	0.42
1:A:169:ASP:C	1:A:170:ARG:HG2	2.43	0.42
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.19	0.42
1:A:704:ARG:HG3	1:A:704:ARG:O	2.18	0.42
1:A:415:SER:OG	1:A:418:ARG:NH2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:GLN:N	4:A:1258:HOH:O	2.39	0.42
1:A:342:MET:O	1:A:346:LYS:N	2.48	0.42
1:A:379:SER:O	1:A:383:GLY:N	2.48	0.42
1:A:293:LYS:O	1:A:297:HIS:N	2.53	0.42
1:A:296:LEU:C	1:A:298:LEU:CD1	2.93	0.42
1:A:350:GLY:HA2	1:A:381:VAL:HG21	2.02	0.42
1:A:753:ARG:C	1:A:756:GLU:H	2.27	0.42
1:A:158:ILE:HG23	1:A:158:ILE:HD13	1.71	0.41
1:A:164:ARG:HA	1:A:164:ARG:HD3	1.81	0.41
1:A:412:GLU:HG2	1:A:413:LYS:N	2.34	0.41
1:A:424:ALA:O	1:A:428:ARG:HB2	2.20	0.41
1:A:462:LYS:HE3	1:A:462:LYS:HB2	1.71	0.41
1:A:614:ASP:O	1:A:616:ASN:N	2.53	0.41
1:A:45:ASP:OD1	1:A:677:ARG:NH1	2.49	0.41
1:A:342:MET:O	1:A:346:LYS:HG3	2.21	0.41
1:A:682:LEU:CB	1:A:686:ARG:HH22	2.28	0.41
1:A:399:LEU:HA	1:A:403:ASP:O	2.21	0.41
1:A:706:TYR:CD1	1:A:714:ARG:N	2.88	0.41
1:A:706:TYR:CB	1:A:712:VAL:HG12	2.49	0.41
1:A:280:ILE:O	1:A:280:ILE:HG13	2.20	0.41
1:A:724:ASP:HA	1:A:739:PHE:HZ	1.84	0.41
1:A:342:MET:HE2	1:A:342:MET:CA	2.24	0.41
1:A:508:LEU:HD13	4:A:1376:HOH:O	2.21	0.41
1:A:669:ASP:HB3	4:A:1271:HOH:O	2.20	0.41
1:A:51:GLU:O	1:A:53:VAL:HG23	2.20	0.41
1:A:127:ASN:ND2	3:A:999:DAQ:HA21	2.32	0.41
1:A:391:LYS:HZ3	1:A:395:GLU:HB3	1.84	0.41
1:A:581:ILE:O	1:A:582:GLN:C	2.60	0.41
1:A:370:LYS:HB3	1:A:370:LYS:HE2	1.84	0.41
1:A:597:GLU:OE1	1:A:612:PHE:CD2	2.74	0.41
1:A:34:TYR:CE1	1:A:51:GLU:CB	2.89	0.41
1:A:51:GLU:OE1	1:A:53:VAL:HG22	2.21	0.41
1:A:288:ALA:O	1:A:293:LYS:HE3	2.20	0.41
1:A:290:ALA:HA	1:A:293:LYS:HD3	2.02	0.41
1:A:367:ALA:CB	1:A:394:MET:HG2	2.49	0.41
1:A:620:ARG:O	4:A:1316:HOH:O	2.22	0.41
1:A:219:ASN:CG	1:A:220:PRO:N	2.77	0.41
1:A:238:ARG:HD2	1:A:264:GLU:OE2	2.20	0.41
1:A:287:GLY:O	1:A:325:LYS:NZ	2.54	0.41
1:A:734:PRO:O	1:A:737:TYR:O	2.39	0.41
1:A:219:ASN:N	1:A:220:PRO:CD	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:222:LEU:HA	1:A:222:LEU:HD23	1.80	0.40
1:A:391:LYS:HZ2	1:A:395:GLU:CB	2.30	0.40
1:A:610:LYS:HD2	1:A:610:LYS:HA	1.64	0.40
1:A:697:ILE:CG2	1:A:698:TYR:N	2.84	0.40
1:A:6:ASP:C	1:A:8:THR:H	2.29	0.40
1:A:399:LEU:CD2	1:A:401:GLY:N	2.84	0.40
1:A:102:VAL:HG21	1:A:685:ILE:CD1	2.51	0.40
1:A:614:ASP:O	1:A:615:PRO: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	726/761 (95%)	679 (94%)	41 (6%)	6 (1%)	16	11

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	714	ARG
1	A	719	SER
1	A	7	ARG
1	A	362	GLY
1	A	32	LYS
1	A	713	PRO

5.3.2 Protein sidechains [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	615/665 (92%)	533 (87%)	82 (13%)	4 2

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	13	LYS
1	A	28	THR
1	A	31	ASP
1	A	32	LYS
1	A	38	ASN
1	A	42	LYS
1	A	46	SER
1	A	52	ILE
1	A	54	SER
1	A	56	THR
1	A	57	SER
1	A	59	SER
1	A	60	PHE
1	A	63	LYS
1	A	66	ASP
1	A	70	ARG
1	A	95	SER
1	A	149	ASN
1	A	150	GLU
1	A	151	VAL
1	A	158	ILE
1	A	159	SER
1	A	211	LEU
1	A	257	SER
1	A	258	ILE
1	A	259	GLN
1	A	296	LEU
1	A	313	VAL
1	A	321	SER
1	A	325	LYS
1	A	326	ILE
1	A	329	GLN
1	A	342	MET
1	A	357	ILE

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Mol	Chain	Res	Type
1	A	368	VAL
1	A	370	LYS
1	A	372	LYS
1	A	376	ASN
1	A	379	SER
1	A	391	LYS
1	A	399	LEU
1	A	404	LEU
1	A	436	LYS
1	A	446	LYS
1	A	460	ILE
1	A	462	LYS
1	A	486	MET
1	A	489	LEU
1	A	492	GLU
1	A	504	ILE
1	A	510	SER
1	A	520	ARG
1	A	542	THR
1	A	544	ILE
1	A	580	GLU
1	A	589	LYS
1	A	594	GLN
1	A	609	THR
1	A	640	SER
1	A	657	ILE
1	A	661	LYS
1	A	674	ASP
1	A	686	ARG
1	A	687	ILE
1	A	689	ARG
1	A	690	LYS
1	A	695	ARG
1	A	704	ARG
1	A	711	ASN
1	A	715	ASP
1	A	720	GLN
1	A	721	LYS
1	A	733	ASP
1	A	736	GLN
1	A	738	ARG
1	A	742	THR

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Mol	Chain	Res	Type
1	A	743	LYS
1	A	744	ILE
1	A	745	PHE
1	A	750	GLN
1	A	754	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	HIS
1	A	105	ASN
1	A	149	ASN
1	A	188	ASN
1	A	217	GLN
1	A	234	ASN
1	A	283	GLN
1	A	309	GLN
1	A	329	GLN
1	A	338	GLN
1	A	376	ASN
1	A	479	GLN
1	A	480	GLN
1	A	491	GLN
1	A	511	GLN
1	A	594	GLN
1	A	606	ASN
1	A	613	ASN
1	A	649	ASN
1	A	662	GLN
1	A	736	GLN

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 [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	DAQ	A	999	2	27,29,29	1.49	4 (14%)	26,43,43	1.53	2 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DAQ	A	999	2	-	4/19/29/29	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	DAQ	C2-N2	4.45	1.53	1.45
3	A	999	DAQ	PA-OA3	2.85	1.62	1.59
3	A	999	DAQ	C1-NA3	2.54	1.44	1.37
3	A	999	DAQ	F3-BE	-2.04	1.49	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	DAQ	C3-C4-N4	4.54	122.65	118.74
3	A	999	DAQ	C3-C2-C1	-2.85	118.94	121.55

There are no chirality outliers.

All (4) torsion outliers are listed below:

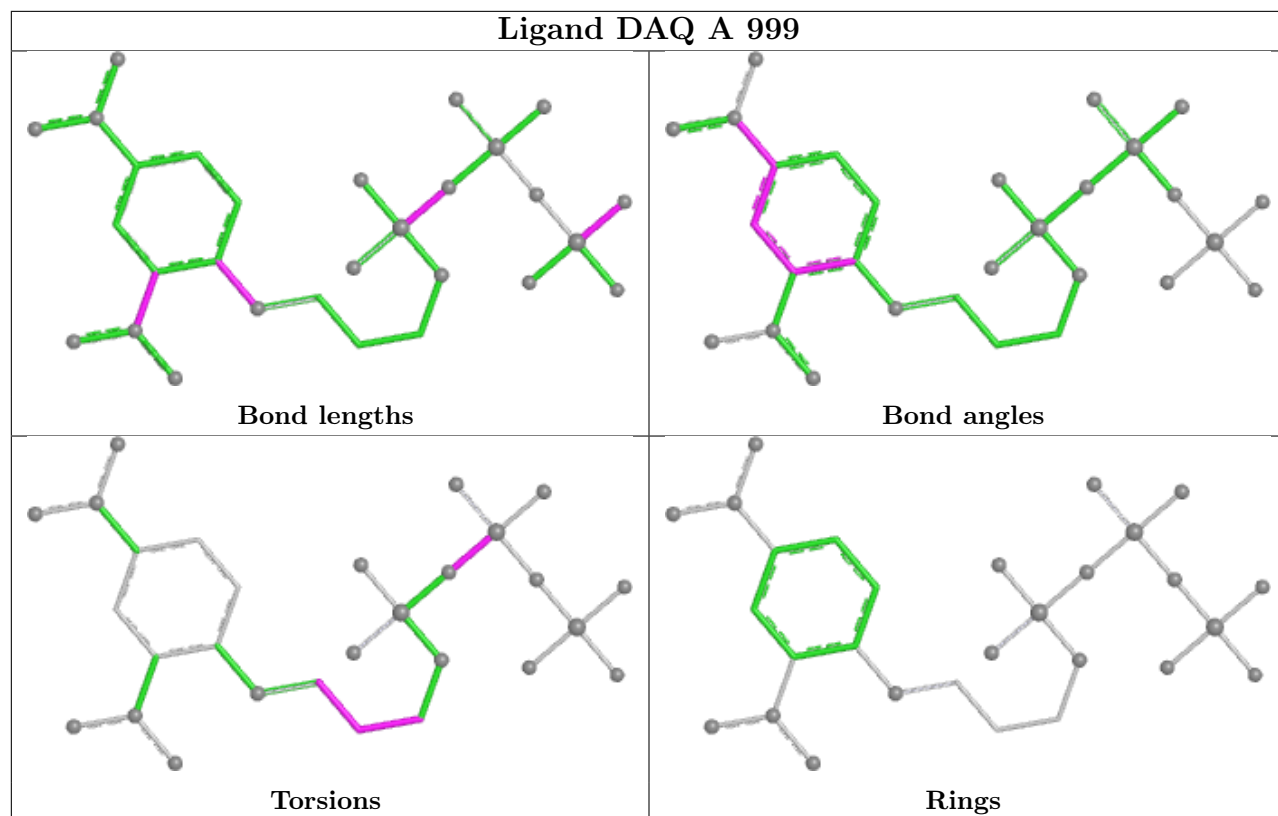
Mol	Chain	Res	Type	Atoms
3	A	999	DAQ	CA1-CA2-CA3-NA3
3	A	999	DAQ	PA-OA3-PB-OB2
3	A	999	DAQ	OE2-CA1-CA2-CA3
3	A	999	DAQ	PA-OA3-PB-OB1

There are no ring outliers.

1 monomer is involved in 5 short contacts:

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

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	736/761 (96%)	0.57	136 (18%) 3 3	11, 36, 88, 100	0

All (136) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	737	TYR	10.7
1	A	65	VAL	6.9
1	A	364	GLY	5.0
1	A	27	LEU	5.0
1	A	59	SER	4.7
1	A	363	ALA	4.5
1	A	734	PRO	4.4
1	A	621	ALA	4.1
1	A	493	GLU	4.1
1	A	728	LYS	4.0
1	A	759	GLU	4.0
1	A	25	PHE	4.0
1	A	53	VAL	4.0
1	A	722	ALA	3.9
1	A	723	THR	3.9
1	A	536	PRO	3.8
1	A	368	VAL	3.8
1	A	56	THR	3.7
1	A	29	VAL	3.7
1	A	716	ALA	3.6
1	A	697	ILE	3.6
1	A	732	ILE	3.6
1	A	707	LEU	3.6
1	A	294	LYS	3.6
1	A	701	PHE	3.6
1	A	494	TYR	3.5
1	A	757	ALA	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	758	ARG	3.4
1	A	274	THR	3.4
1	A	713	PRO	3.4
1	A	366	GLY	3.3
1	A	694	ASN	3.3
1	A	733	ASP	3.3
1	A	209	GLY	3.2
1	A	52	ILE	3.2
1	A	74	LYS	3.2
1	A	741	ILE	3.2
1	A	744	ILE	3.2
1	A	506	PHE	3.2
1	A	361	LYS	3.2
1	A	731	ASN	3.2
1	A	725	ALA	3.1
1	A	201	GLY	3.1
1	A	202	ARG	3.1
1	A	24	LEU	3.1
1	A	40	ASP	3.0
1	A	28	THR	3.0
1	A	751	LEU	3.0
1	A	62	PHE	3.0
1	A	739	PHE	3.0
1	A	705	TYR	3.0
1	A	696	ILE	2.9
1	A	689	ARG	2.9
1	A	698	TYR	2.9
1	A	367	ALA	2.9
1	A	695	ARG	2.8
1	A	714	ARG	2.8
1	A	39	PRO	2.8
1	A	755	GLU	2.8
1	A	68	GLN	2.8
1	A	362	GLY	2.8
1	A	699	ALA	2.8
1	A	754	ILE	2.8
1	A	60	PHE	2.8
1	A	746	PHE	2.8
1	A	749	GLY	2.8
1	A	688	THR	2.8
1	A	700	ASP	2.8
1	A	693	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	23	ASP	2.7
1	A	687	ILE	2.7
1	A	627	PHE	2.7
1	A	41	PRO	2.7
1	A	752	ALA	2.6
1	A	745	PHE	2.6
1	A	719	SER	2.6
1	A	702	VAL	2.6
1	A	66	ASP	2.6
1	A	738	ARG	2.6
1	A	736	GLN	2.6
1	A	33	ARG	2.6
1	A	718	ASP	2.6
1	A	97	LEU	2.6
1	A	376	ASN	2.5
1	A	402	ARG	2.5
1	A	400	ALA	2.5
1	A	69	ASP	2.5
1	A	342	MET	2.5
1	A	70	ARG	2.5
1	A	727	LEU	2.5
1	A	72	VAL	2.4
1	A	76	ASP	2.4
1	A	743	LYS	2.4
1	A	692	PHE	2.4
1	A	740	GLY	2.4
1	A	686	ARG	2.4
1	A	748	ALA	2.4
1	A	729	HIS	2.4
1	A	401	GLY	2.4
1	A	61	THR	2.4
1	A	298	LEU	2.4
1	A	22	SER	2.4
1	A	742	THR	2.4
1	A	203	ASN	2.3
1	A	535	PHE	2.3
1	A	337	SER	2.3
1	A	407	GLN	2.3
1	A	399	LEU	2.3
1	A	380	THR	2.3
1	A	724	ASP	2.3
1	A	55	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	444	GLU	2.3
1	A	20	GLY	2.3
1	A	291	GLU	2.2
1	A	711	ASN	2.2
1	A	674	ASP	2.2
1	A	63	LYS	2.2
1	A	712	VAL	2.2
1	A	75	ASP	2.2
1	A	756	GLU	2.2
1	A	735	GLU	2.2
1	A	290	ALA	2.2
1	A	343	SER	2.1
1	A	26	LYS	2.1
1	A	30	SER	2.1
1	A	44	ARG	2.1
1	A	67	GLY	2.1
1	A	691	GLY	2.1
1	A	219	ASN	2.1
1	A	58	ASP	2.1
1	A	37	TYR	2.1
1	A	504	ILE	2.1
1	A	57	SER	2.1
1	A	750	GLN	2.0
1	A	443	GLN	2.0
1	A	690	LYS	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 ⓘ

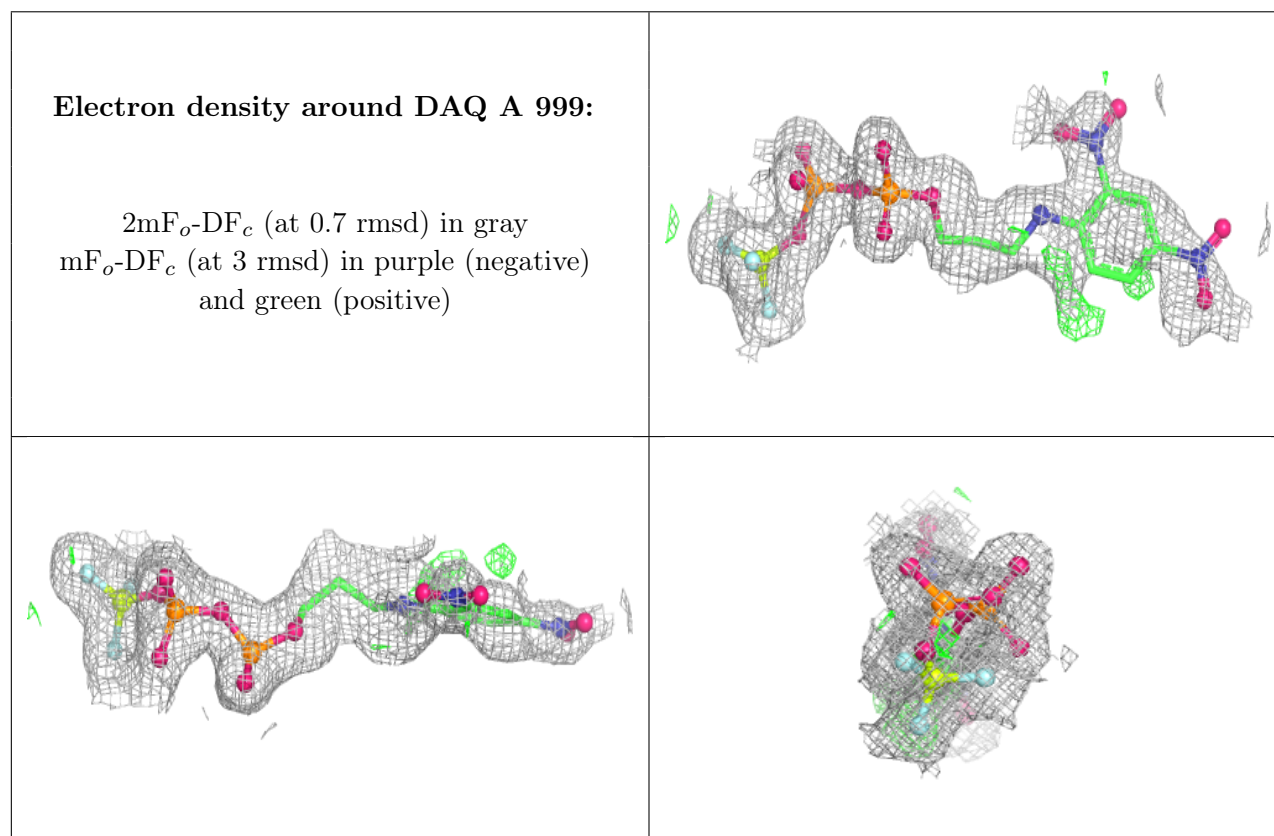
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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	DAQ	A	999	29/29	0.97	0.12	3,23,100,100	12
2	MG	A	998	1/1	1.00	0.02	18,18,18,18	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.