



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:52 PM UTC

PDB ID : 1D1C / pdb_00001d1c
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH N-METHYL-O-NITROPHENYL AMINOETHYL
DIPHOSPHATE 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 : 2.30 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

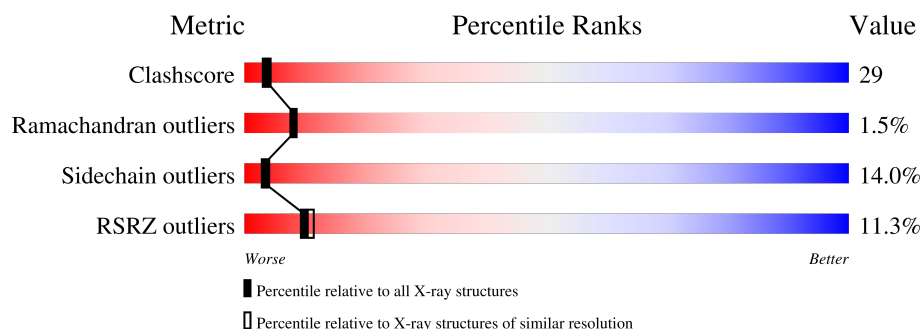
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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 6528 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	744	Total	C	N	O	S	0	0	0
			5910	3759	1017	1118	16			

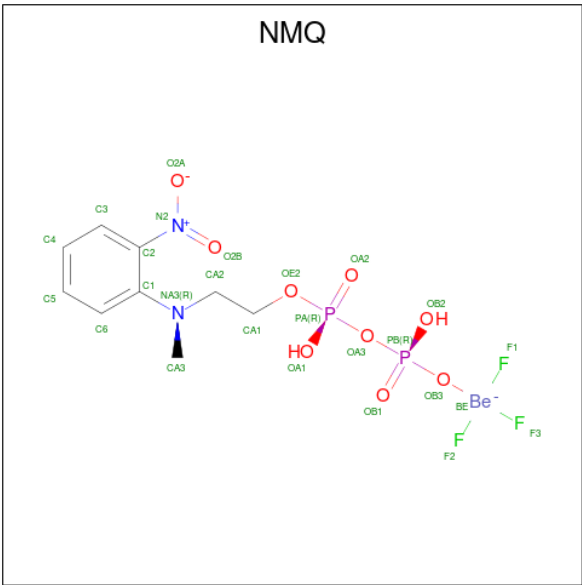
There are 3 discrepancies between the modelled and reference sequences:

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 N-METHYL O-NITROPHENYL AMINOETHYLDIPHOSPHATE BERYLLIUM TRIFLUORIDE (CCD ID: NMQ) (formula: C₉H₁₃BeF₃N₂O₉P₂).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	Be	C	F	N	O	P		
3	A	1	26	1	9	3	2	9	2	0	0

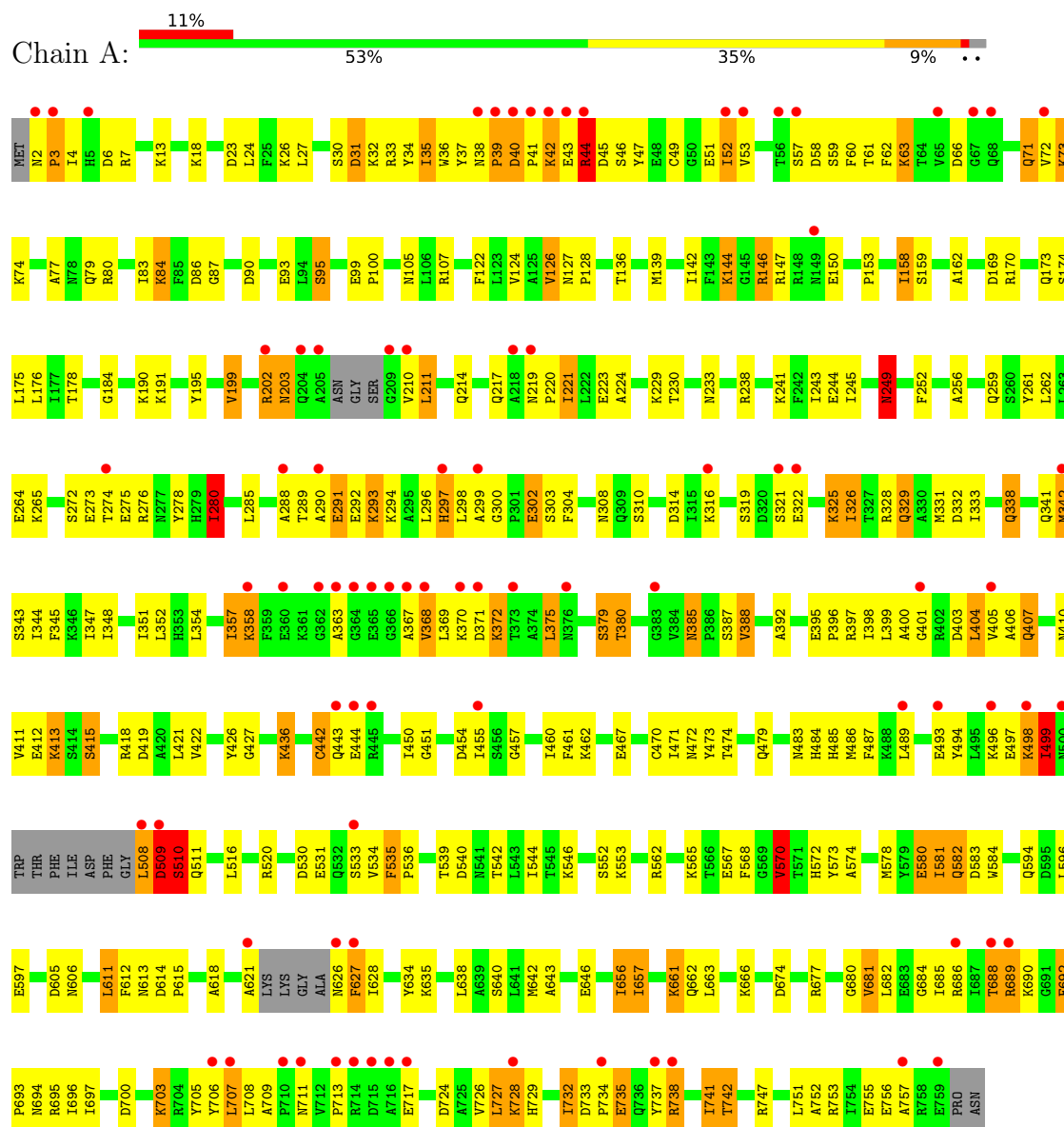
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	591	Total	O	0	0
			591	591		

3 Residue-property plots [i](#)

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	103.90Å 180.90Å 54.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.30 25.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	90.9 (25.00-2.30) 87.9 (25.00-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.75 (at 2.31Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.181 , (Not available) 0.194 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	15.7	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 105.7	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	0.92	EDS
Total number of atoms	6528	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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: NMQ, 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	1.11	7/6022 (0.1%)	1.51	42/8131 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	737	TYR	C-N	8.59	1.44	1.33
1	A	508	LEU	C-N	7.93	1.44	1.33
1	A	509	ASP	CA-C	7.41	1.62	1.52
1	A	509	ASP	N-CA	6.55	1.54	1.46
1	A	510	SER	N-CA	5.71	1.53	1.46
1	A	580	GLU	CD-OE2	5.64	1.36	1.25
1	A	457	GLY	C-N	-5.07	1.26	1.33

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	535	PHE	CA-CB-CG	-10.95	102.85	113.80
1	A	737	TYR	O-C-N	8.77	133.78	123.17
1	A	729	HIS	CA-CB-CG	-7.88	105.92	113.80
1	A	627	PHE	N-CA-CB	7.69	121.36	110.36
1	A	280	ILE	CB-CA-C	-7.48	101.13	112.05
1	A	510	SER	N-CA-C	7.34	121.50	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	509	ASP	CA-CB-CG	7.24	119.84	112.60
1	A	509	ASP	N-CA-C	7.22	126.18	110.80
1	A	509	ASP	O-C-N	-7.01	113.27	122.59
1	A	606	ASN	N-CA-C	6.90	119.83	111.82
1	A	233	ASN	CA-CB-CG	6.77	119.37	112.60
1	A	280	ILE	N-CA-CB	6.44	120.65	110.54
1	A	570	VAL	N-CA-CB	6.32	121.81	111.44
1	A	657	ILE	CB-CA-C	6.21	117.92	110.78
1	A	681	VAL	N-CA-C	6.20	116.38	110.42
1	A	385	ASN	CA-C-O	6.17	123.30	119.29
1	A	606	ASN	CA-CB-CG	-6.14	106.46	112.60
1	A	52	ILE	CB-CA-C	-6.08	104.73	111.35
1	A	450	ILE	CA-C-N	-5.80	117.18	122.80
1	A	450	ILE	C-N-CA	-5.80	117.18	122.80
1	A	692	PHE	CA-C-N	5.77	125.46	119.05
1	A	692	PHE	C-N-CA	5.77	125.46	119.05
1	A	122	PHE	CA-CB-CG	5.76	119.56	113.80
1	A	202	ARG	CB-CA-C	5.76	120.79	111.05
1	A	442	CYS	N-CA-C	5.45	118.13	110.23
1	A	606	ASN	N-CA-CB	5.45	118.72	110.28
1	A	42	LYS	N-CA-C	-5.44	105.45	111.71
1	A	380	THR	N-CA-CB	5.44	117.89	110.01
1	A	304	PHE	CA-C-N	5.34	127.44	120.28
1	A	304	PHE	C-N-CA	5.34	127.44	120.28
1	A	95	SER	N-CA-CB	5.27	117.82	110.07
1	A	461	PHE	CA-C-N	5.25	127.62	120.54
1	A	461	PHE	C-N-CA	5.25	127.62	120.54
1	A	249	ASN	CA-CB-CG	-5.24	107.36	112.60
1	A	367	ALA	N-CA-C	5.20	117.83	110.50
1	A	419	ASP	CA-CB-CG	-5.18	107.42	112.60
1	A	472	ASN	CA-CB-CG	-5.15	107.45	112.60
1	A	626	ASN	CA-CB-CG	5.14	117.75	112.60
1	A	511	GLN	N-CA-C	5.09	117.72	111.82
1	A	245	ILE	N-CA-CB	5.05	117.52	111.31
1	A	297	HIS	CA-CB-CG	-5.05	108.75	113.80
1	A	41	PRO	N-CA-CB	5.04	108.23	103.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	606	ASN	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	5910	0	5820	333	0
2	A	1	0	0	0	0
3	A	26	0	11	5	0
4	A	591	0	0	30	0
All	All	6528	0	5831	336	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (336) 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:147:ARG:HB2	1:A:150:GLU:HG3	1.30	1.12
1:A:4:ILE:HD11	1:A:142:ILE:HG23	1.19	1.12
1:A:707:LEU:HD23	1:A:707:LEU:H	1.17	1.08
1:A:385:ASN:HB3	1:A:388:VAL:HG21	1.38	1.04
1:A:410:ASN:H	1:A:413:LYS:HZ3	0.99	0.98
1:A:686:ARG:HA	1:A:689:ARG:HH12	1.25	0.98
1:A:385:ASN:HB3	1:A:388:VAL:CG2	1.94	0.97
1:A:707:LEU:H	1:A:707:LEU:CD2	1.81	0.94
1:A:202:ARG:HH11	1:A:252:PHE:HB2	1.31	0.93
1:A:741:ILE:HG22	1:A:742:THR:CG2	1.99	0.93
1:A:35:ILE:HD11	1:A:77:ALA:HB1	1.52	0.90
1:A:621:ALA:HB2	1:A:628:ILE:HG12	1.53	0.90
1:A:707:LEU:HD23	1:A:707:LEU:N	1.89	0.88
1:A:40:ASP:OD2	1:A:42:LYS:HB2	1.76	0.86
1:A:410:ASN:H	1:A:413:LYS:NZ	1.74	0.86
1:A:45:ASP:CG	1:A:677:ARG:HH22	1.83	0.85
1:A:273:GLU:O	1:A:274:THR:OG1	1.95	0.85
1:A:249:ASN:ND2	1:A:249:ASN:H	1.71	0.84
1:A:59:SER:HB2	1:A:72:VAL:O	1.77	0.84
1:A:741:ILE:HG22	1:A:742:THR:HG23	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ARG:HH11	1:A:252:PHE:CB	1.89	0.84
1:A:290:ALA:HA	1:A:293:LYS:HD2	1.61	0.82
1:A:686:ARG:HA	1:A:689:ARG:NH1	1.95	0.82
1:A:398:ILE:HD13	1:A:407:GLN:CG	2.10	0.82
1:A:289:THR:OG1	1:A:292:GLU:HG3	1.79	0.81
1:A:735:GLU:HA	1:A:738:ARG:HH22	1.46	0.81
1:A:4:ILE:HD11	1:A:142:ILE:CG2	2.07	0.81
1:A:43:GLU:HA	4:A:1110:HOH:O	1.81	0.80
1:A:497:GLU:C	1:A:741:ILE:HD12	2.08	0.79
1:A:84:LYS:HE3	4:A:1251:HOH:O	1.83	0.78
1:A:44:ARG:HH21	1:A:677:ARG:CZ	1.96	0.78
1:A:62:PHE:HE2	1:A:72:VAL:HG23	1.50	0.77
1:A:158:ILE:HD13	1:A:159:SER:N	1.99	0.77
1:A:689:ARG:HH11	1:A:689:ARG:HB3	1.50	0.77
1:A:176:LEU:N	1:A:176:LEU:HD12	2.01	0.76
1:A:497:GLU:O	1:A:741:ILE:HD12	1.85	0.76
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.68	0.76
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.66	0.75
1:A:289:THR:HB	1:A:291:GLU:OE2	1.87	0.75
1:A:290:ALA:HA	1:A:293:LYS:CD	2.17	0.75
1:A:510:SER:HB2	4:A:1438:HOH:O	1.88	0.74
1:A:241:LYS:HD2	1:A:243:ILE:HD11	1.69	0.74
1:A:302:GLU:H	1:A:302:GLU:CD	1.94	0.74
1:A:397:ARG:HD2	1:A:404:LEU:CD1	2.17	0.73
1:A:436:LYS:HZ3	1:A:436:LYS:HB3	1.53	0.73
1:A:398:ILE:HD13	1:A:407:GLN:HG3	1.68	0.73
1:A:62:PHE:HE2	1:A:72:VAL:CG2	2.02	0.72
1:A:540:ASP:HB3	1:A:581:ILE:HG23	1.71	0.71
1:A:53:VAL:HG11	1:A:63:LYS:CG	2.20	0.71
1:A:191:LYS:HA	1:A:191:LYS:HE2	1.71	0.71
1:A:344:ILE:O	1:A:348:ILE:HG12	1.91	0.71
1:A:735:GLU:OE2	1:A:747:ARG:NH2	2.22	0.71
1:A:682:LEU:O	1:A:686:ARG:HG3	1.91	0.71
1:A:4:ILE:CD1	1:A:142:ILE:HG23	2.09	0.71
1:A:202:ARG:NH1	1:A:252:PHE:HB2	2.06	0.71
1:A:396:PRO:HG2	1:A:398:ILE:HD11	1.72	0.70
1:A:24:LEU:N	1:A:24:LEU:HD23	2.05	0.70
1:A:289:THR:HG23	1:A:292:GLU:OE2	1.91	0.69
1:A:574:ALA:HA	4:A:1258:HOH:O	1.93	0.69
1:A:321:SER:O	1:A:325:LYS:HE3	1.93	0.69
1:A:343:SER:HB3	1:A:605:ASP:OD1	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLN:HE21	1:A:407:GLN:HA	1.56	0.69
1:A:706:TYR:CE2	1:A:707:LEU:HD22	2.28	0.68
1:A:395:GLU:HA	1:A:407:GLN:O	1.93	0.68
1:A:399:LEU:HD13	1:A:401:GLY:H	1.59	0.68
1:A:224:ALA:O	1:A:280:ILE:HG13	1.92	0.68
1:A:689:ARG:HH11	1:A:689:ARG:CB	2.06	0.68
1:A:642:MET:O	1:A:646:GLU:HG2	1.92	0.67
1:A:509:ASP:O	1:A:509:ASP:OD2	2.12	0.67
1:A:44:ARG:NH2	1:A:677:ARG:NE	2.43	0.67
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.29	0.67
1:A:689:ARG:HH11	1:A:689:ARG:CG	2.08	0.67
1:A:290:ALA:CA	1:A:293:LYS:HD2	2.25	0.67
1:A:415:SER:OG	1:A:418:ARG:NH2	2.27	0.67
1:A:582:GLN:NE2	4:A:1057:HOH:O	2.29	0.66
1:A:396:PRO:O	1:A:398:ILE:HD12	1.94	0.66
3:A:999:NMQ:OE2	3:A:999:NMQ:HA33	1.96	0.66
1:A:23:ASP:OD2	1:A:23:ASP:N	2.28	0.66
1:A:498:LYS:C	1:A:499:ILE:HG12	2.20	0.66
1:A:2:ASN:ND2	4:A:1336:HOH:O	2.30	0.65
1:A:238:ARG:HD3	1:A:264:GLU:OE2	1.96	0.65
1:A:392:ALA:HB1	1:A:596:LEU:HD23	1.79	0.65
1:A:735:GLU:HA	1:A:738:ARG:NH2	2.10	0.65
1:A:219:ASN:N	1:A:220:PRO:HD2	2.12	0.65
1:A:331:MET:HE1	1:A:345:PHE:HZ	1.62	0.65
1:A:385:ASN:O	1:A:388:VAL:HG23	1.97	0.65
1:A:316:LYS:NZ	4:A:1428:HOH:O	2.30	0.64
1:A:296:LEU:HB3	1:A:298:LEU:HD21	1.80	0.64
1:A:44:ARG:NH1	4:A:1311:HOH:O	2.30	0.63
1:A:397:ARG:HA	1:A:406:ALA:HA	1.81	0.63
1:A:508:LEU:HG	1:A:509:ASP:H	1.64	0.62
1:A:398:ILE:HD13	1:A:407:GLN:HG2	1.81	0.62
1:A:485:HIS:NE2	1:A:489:LEU:HD11	2.13	0.62
1:A:147:ARG:CB	1:A:150:GLU:HG3	2.20	0.62
1:A:329:GLN:O	1:A:332:ASP:HB2	1.99	0.62
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.81	0.62
1:A:38:ASN:ND2	1:A:46:SER:O	2.31	0.62
1:A:53:VAL:HG11	1:A:63:LYS:HG2	1.81	0.61
1:A:410:ASN:OD1	1:A:413:LYS:HB2	2.01	0.61
1:A:436:LYS:HB3	1:A:436:LYS:NZ	2.16	0.61
1:A:289:THR:HB	1:A:291:GLU:CD	2.26	0.60
1:A:44:ARG:HH21	1:A:677:ARG:NE	1.99	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:407:GLN:HE21	1:A:407:GLN:CA	2.14	0.60
1:A:661:LYS:HD3	1:A:663:LEU:HD12	1.83	0.60
1:A:399:LEU:HD22	1:A:400:ALA:N	2.16	0.60
1:A:399:LEU:HD22	1:A:403:ASP:O	2.02	0.60
1:A:358:LYS:HZ2	1:A:358:LYS:HA	1.67	0.60
1:A:43:GLU:O	1:A:44:ARG:HB3	2.02	0.59
1:A:191:LYS:HE2	1:A:191:LYS:CA	2.32	0.59
1:A:621:ALA:CB	1:A:628:ILE:HG12	2.29	0.59
1:A:62:PHE:CE2	1:A:72:VAL:HG23	2.34	0.59
1:A:289:THR:C	1:A:293:LYS:HD2	2.28	0.59
1:A:410:ASN:N	1:A:413:LYS:HZ3	1.84	0.59
1:A:733:ASP:OD2	1:A:734:PRO:HD2	2.03	0.59
1:A:44:ARG:NH2	1:A:677:ARG:CZ	2.66	0.58
1:A:280:ILE:HD11	1:A:426:TYR:OH	2.02	0.58
1:A:300:GLY:HA3	1:A:302:GLU:OE2	2.04	0.58
1:A:436:LYS:HE2	4:A:1494:HOH:O	2.03	0.58
1:A:243:ILE:O	1:A:451:GLY:HA2	2.04	0.58
1:A:144:LYS:HE2	4:A:1134:HOH:O	2.03	0.58
1:A:706:TYR:CD2	1:A:707:LEU:HD22	2.38	0.58
1:A:347:ILE:O	1:A:351:ILE:HG13	2.04	0.57
1:A:38:ASN:C	1:A:40:ASP:H	2.10	0.57
1:A:83:ILE:HD12	1:A:86:ASP:OD1	2.04	0.57
1:A:184:GLY:HA2	3:A:999:NMQ:PA	2.45	0.57
1:A:375:LEU:O	1:A:379:SER:OG	2.21	0.57
1:A:293:LYS:O	1:A:297:HIS:N	2.37	0.57
1:A:37:TYR:O	1:A:47:TYR:HA	2.05	0.56
1:A:34:TYR:CE1	1:A:51:GLU:HB2	2.40	0.56
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.86	0.56
1:A:202:ARG:NH1	1:A:252:PHE:CB	2.64	0.56
1:A:368:VAL:HG22	1:A:369:LEU:H	1.70	0.56
1:A:124:VAL:HG13	1:A:656:ILE:CD1	2.36	0.56
1:A:399:LEU:HD21	1:A:401:GLY:O	2.06	0.55
1:A:735:GLU:CA	1:A:738:ARG:HH22	2.17	0.55
1:A:158:ILE:HD13	1:A:158:ILE:C	2.29	0.55
1:A:176:LEU:N	1:A:176:LEU:CD1	2.69	0.55
1:A:398:ILE:CD1	1:A:407:GLN:HG2	2.35	0.55
1:A:535:PHE:N	1:A:535:PHE:CD2	2.74	0.55
1:A:685:ILE:HA	1:A:688:THR:OG1	2.07	0.55
1:A:61:THR:HA	1:A:71:GLN:HG2	1.88	0.55
1:A:285:LEU:HD22	1:A:299:ALA:O	2.06	0.55
1:A:338:GLN:HB2	4:A:1279:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:TYR:CE2	1:A:199:VAL:HG11	2.41	0.55
1:A:697:ILE:HB	1:A:700:ASP:OD1	2.06	0.55
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.43	0.55
1:A:407:GLN:HA	1:A:407:GLN:NE2	2.22	0.54
1:A:732:ILE:N	1:A:732:ILE:HD13	2.21	0.54
1:A:392:ALA:CB	1:A:596:LEU:HD23	2.37	0.54
1:A:486:MET:CE	1:A:688:THR:HG23	2.37	0.54
1:A:288:ALA:O	1:A:293:LYS:NZ	2.34	0.54
1:A:611:LEU:O	1:A:618:ALA:HB2	2.07	0.54
1:A:60:PHE:CE1	1:A:74:LYS:HG2	2.43	0.54
1:A:735:GLU:CD	1:A:747:ARG:HH21	2.16	0.53
1:A:635:LYS:NZ	4:A:1195:HOH:O	2.35	0.53
1:A:61:THR:OG1	1:A:71:GLN:OE1	2.27	0.53
1:A:87:GLY:H	1:A:105:ASN:ND2	2.06	0.53
1:A:238:ARG:CD	1:A:264:GLU:OE2	2.56	0.53
1:A:689:ARG:NH2	4:A:1282:HOH:O	2.42	0.53
1:A:38:ASN:C	1:A:40:ASP:N	2.65	0.53
1:A:153:PRO:HD3	4:A:1037:HOH:O	2.09	0.53
1:A:397:ARG:HD2	1:A:404:LEU:HD11	1.90	0.53
1:A:83:ILE:HD11	4:A:1397:HOH:O	2.08	0.52
1:A:175:LEU:C	1:A:176:LEU:HD12	2.35	0.52
1:A:296:LEU:HB2	1:A:298:LEU:HD11	1.90	0.52
1:A:124:VAL:HG13	1:A:656:ILE:HD12	1.92	0.52
1:A:368:VAL:HG22	1:A:369:LEU:N	2.25	0.52
1:A:2:ASN:HD21	1:A:146:ARG:HH22	1.56	0.52
1:A:474:THR:HG23	1:A:638:LEU:HD13	1.92	0.52
1:A:684:GLY:O	1:A:688:THR:OG1	2.24	0.52
1:A:708:LEU:HD13	1:A:757:ALA:HB3	1.93	0.51
1:A:753:ARG:O	1:A:756:GLU:HB2	2.10	0.51
1:A:328:ARG:HA	1:A:331:MET:HE3	1.92	0.51
1:A:38:ASN:O	1:A:40:ASP:N	2.43	0.51
1:A:534:VAL:O	1:A:536:PRO:HD3	2.11	0.51
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.30	0.51
1:A:184:GLY:HA2	3:A:999:NMQ:OA1	2.10	0.51
1:A:296:LEU:HB2	1:A:298:LEU:HG	1.91	0.51
1:A:39:PRO:O	1:A:40:ASP:HB3	2.10	0.51
1:A:238:ARG:HB2	1:A:278:TYR:HE1	1.75	0.51
1:A:484:HIS:O	1:A:487:PHE:HB3	2.11	0.51
1:A:30:SER:O	4:A:1462:HOH:O	2.19	0.50
1:A:53:VAL:HG11	1:A:63:LYS:HG3	1.92	0.50
1:A:210:VAL:O	1:A:214:GLN:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:265:LYS:HD3	1:A:427:GLY:HA3	1.93	0.50
1:A:689:ARG:NH1	1:A:689:ARG:HG2	2.27	0.50
1:A:689:ARG:HH11	1:A:689:ARG:HG2	1.76	0.50
1:A:493:GLU:OE1	1:A:493:GLU:HA	2.11	0.50
1:A:58:ASP:OD1	1:A:73:LYS:NZ	2.25	0.50
1:A:392:ALA:N	4:A:1566:HOH:O	2.43	0.50
1:A:2:ASN:O	1:A:4:ILE:N	2.45	0.50
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.46	0.50
1:A:568:PHE:CA	1:A:578:MET:HE1	2.40	0.50
1:A:467:GLU:CD	1:A:467:GLU:H	2.19	0.50
1:A:568:PHE:N	1:A:578:MET:HE1	2.27	0.50
1:A:692:PHE:CE1	1:A:747:ARG:HG2	2.46	0.50
1:A:147:ARG:HG3	1:A:150:GLU:OE1	2.11	0.50
1:A:643:ALA:O	1:A:646:GLU:HB2	2.12	0.50
1:A:338:GLN:O	1:A:342:MET:SD	2.70	0.49
1:A:44:ARG:HG2	1:A:45:ASP:OD2	2.12	0.49
1:A:202:ARG:HH11	1:A:252:PHE:HB3	1.76	0.49
1:A:486:MET:HE3	1:A:688:THR:HG23	1.94	0.49
3:A:999:NMQ:CA2	3:A:999:NMQ:O2B	2.60	0.49
1:A:18:LYS:HB2	4:A:1375:HOH:O	2.12	0.49
1:A:244:GLU:O	1:A:256:ALA:HA	2.12	0.49
1:A:296:LEU:HB2	1:A:298:LEU:CD1	2.42	0.49
1:A:341:GLN:O	1:A:345:PHE:CD2	2.65	0.49
1:A:662:GLN:NE2	4:A:1070:HOH:O	2.45	0.49
1:A:59:SER:HB3	1:A:73:LYS:HD3	1.95	0.49
1:A:18:LYS:HG3	4:A:1086:HOH:O	2.12	0.49
1:A:259:GLN:CG	1:A:261:TYR:CZ	2.97	0.48
1:A:399:LEU:HD13	1:A:399:LEU:C	2.38	0.48
1:A:147:ARG:HB2	1:A:150:GLU:CG	2.22	0.48
1:A:35:ILE:HD11	1:A:77:ALA:CB	2.33	0.48
1:A:535:PHE:HA	1:A:536:PRO:HD2	1.78	0.48
1:A:7:ARG:NH2	4:A:1576:HOH:O	2.34	0.48
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.14	0.48
1:A:621:ALA:HB3	1:A:628:ILE:H	1.77	0.48
1:A:371:ASP:OD2	1:A:372:LYS:N	2.47	0.47
1:A:705:TYR:O	1:A:706:TYR:C	2.57	0.47
1:A:661:LYS:HB2	1:A:663:LEU:HG	1.96	0.47
1:A:169:ASP:C	1:A:170:ARG:HG2	2.38	0.47
1:A:479:GLN:HE21	1:A:483:ASN:ND2	2.13	0.47
1:A:3:PRO:HA	1:A:6:ASP:HB3	1.97	0.47
1:A:190:LYS:HE3	1:A:223:GLU:OE2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:707:LEU:HA	4:A:1525:HOH:O	2.14	0.47
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.55	0.47
1:A:724:ASP:O	1:A:728:LYS:HB2	2.14	0.47
1:A:202:ARG:O	1:A:203:ASN:O	2.33	0.47
1:A:694:ASN:C	1:A:695:ARG:HG3	2.39	0.47
1:A:703:LYS:O	1:A:703:LYS:HG3	2.09	0.47
1:A:442:CYS:SG	1:A:443:GLN:N	2.88	0.46
1:A:162:ALA:O	1:A:173:GLN:HG3	2.15	0.46
1:A:229:LYS:HE2	1:A:274:THR:O	2.16	0.46
1:A:357:ILE:HB	1:A:418:ARG:NH1	2.30	0.46
1:A:552:SER:O	1:A:553:LYS:HB2	2.16	0.46
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.50	0.46
1:A:72:VAL:HG12	1:A:73:LYS:O	2.16	0.46
1:A:369:LEU:HD12	1:A:369:LEU:HA	1.80	0.46
1:A:352:LEU:HD23	1:A:352:LEU:HA	1.75	0.46
1:A:45:ASP:OD2	1:A:677:ARG:NH2	2.48	0.46
1:A:520:ARG:HD3	4:A:1561:HOH:O	2.16	0.46
1:A:126:VAL:HG13	1:A:656:ILE:HG22	1.98	0.45
1:A:407:GLN:CA	1:A:407:GLN:NE2	2.79	0.45
1:A:72:VAL:HG12	1:A:73:LYS:N	2.31	0.45
1:A:342:MET:SD	1:A:342:MET:N	2.89	0.45
1:A:83:ILE:CD1	1:A:86:ASP:OD1	2.64	0.45
1:A:568:PHE:C	1:A:578:MET:CE	2.90	0.45
1:A:24:LEU:HD11	4:A:1523:HOH:O	2.16	0.45
1:A:238:ARG:HH11	1:A:264:GLU:CD	2.24	0.45
1:A:696:ILE:HG22	1:A:697:ILE:N	2.30	0.45
1:A:35:ILE:HG12	1:A:79:GLN:HA	1.99	0.45
1:A:302:GLU:CD	1:A:302:GLU:N	2.67	0.45
1:A:328:ARG:HA	1:A:331:MET:CE	2.46	0.45
1:A:290:ALA:N	1:A:293:LYS:HD2	2.31	0.45
1:A:689:ARG:HA	1:A:693:PRO:HG3	1.98	0.45
1:A:689:ARG:NH1	1:A:689:ARG:CG	2.71	0.45
1:A:99:GLU:HB2	1:A:100:PRO:HD3	1.99	0.44
1:A:219:ASN:N	1:A:220:PRO:CD	2.80	0.44
1:A:272:SER:O	1:A:310:SER:HB2	2.18	0.44
1:A:289:THR:O	1:A:293:LYS:HD2	2.17	0.44
1:A:73:LYS:HD3	1:A:73:LYS:HA	1.61	0.44
1:A:289:THR:C	1:A:291:GLU:N	2.74	0.44
1:A:388:VAL:HG23	1:A:388:VAL:H	1.29	0.44
1:A:158:ILE:HD13	1:A:159:SER:H	1.78	0.44
1:A:338:GLN:NE2	4:A:1496:HOH:O	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:HE3	1:A:372:LYS:HB2	1.70	0.44
1:A:573:TYR:OH	1:A:680:GLY:HA2	2.17	0.44
1:A:530:ASP:O	1:A:533:SER:HB2	2.18	0.44
1:A:296:LEU:HB2	1:A:298:LEU:CG	2.46	0.44
1:A:494:TYR:HE2	1:A:695:ARG:NH2	2.16	0.44
1:A:567:GLU:HB3	1:A:578:MET:HE2	2.00	0.44
1:A:290:ALA:HA	1:A:293:LYS:HD3	1.95	0.43
1:A:474:THR:OG1	1:A:634:TYR:OH	2.34	0.43
1:A:596:LEU:HD23	1:A:596:LEU:HA	1.77	0.43
1:A:60:PHE:N	1:A:72:VAL:O	2.41	0.43
1:A:259:GLN:HG3	1:A:261:TYR:CZ	2.53	0.43
1:A:273:GLU:O	1:A:274:THR:CB	2.65	0.43
1:A:326:ILE:O	1:A:329:GLN:HB3	2.18	0.43
1:A:508:LEU:O	1:A:509:ASP:CB	2.67	0.43
1:A:567:GLU:HB3	1:A:578:MET:CE	2.49	0.43
1:A:62:PHE:CD1	1:A:62:PHE:C	2.96	0.43
1:A:249:ASN:OD1	4:A:1146:HOH:O	2.21	0.43
1:A:298:LEU:N	1:A:298:LEU:HD23	2.33	0.43
3:A:999:NMQ:O2B	3:A:999:NMQ:HA22	2.19	0.43
1:A:178:THR:HG22	1:A:455:ILE:O	2.19	0.43
1:A:174:SER:C	1:A:175:LEU:HD12	2.44	0.42
1:A:299:ALA:HB3	1:A:303:SER:OG	2.19	0.42
1:A:329:GLN:O	1:A:333:ILE:CD1	2.68	0.42
1:A:230:THR:HB	1:A:275:GLU:OE2	2.19	0.42
1:A:421:LEU:HB2	1:A:596:LEU:HD13	2.01	0.42
1:A:436:LYS:NZ	1:A:436:LYS:CB	2.78	0.42
1:A:697:ILE:O	1:A:700:ASP:HB2	2.20	0.42
1:A:733:ASP:OD2	1:A:733:ASP:C	2.63	0.42
1:A:217:GLN:O	1:A:221:ILE:HG13	2.19	0.42
1:A:147:ARG:H	1:A:150:GLU:CD	2.28	0.42
1:A:399:LEU:CD2	1:A:403:ASP:O	2.66	0.42
1:A:211:LEU:HD23	1:A:211:LEU:HA	1.67	0.42
1:A:752:ALA:O	1:A:755:GLU:HB3	2.20	0.42
1:A:139:MET:HA	1:A:142:ILE:HD12	2.02	0.42
1:A:31:ASP:OD2	1:A:31:ASP:N	2.53	0.41
1:A:107:ARG:NE	4:A:1409:HOH:O	2.39	0.41
1:A:127:ASN:OD1	1:A:128:PRO:HD2	2.19	0.41
1:A:485:HIS:NE2	1:A:489:LEU:CD1	2.81	0.41
1:A:319:SER:OG	1:A:322:GLU:CG	2.68	0.41
1:A:354:LEU:HD13	1:A:421:LEU:HD23	2.02	0.41
1:A:296:LEU:CB	1:A:298:LEU:HD11	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:520:ARG:HB2	4:A:1227:HOH:O	2.19	0.41
1:A:733:ASP:OD2	1:A:734:PRO:CD	2.68	0.41
1:A:144:LYS:HD3	4:A:1134:HOH:O	2.20	0.41
1:A:470:CYS:O	1:A:473:TYR:HB3	2.21	0.41
1:A:681:VAL:HG13	4:A:1130:HOH:O	2.18	0.41
1:A:570:VAL:HG22	1:A:572:HIS:CD2	2.55	0.41
1:A:614:ASP:OD1	1:A:614:ASP:C	2.63	0.41
1:A:90:ASP:O	1:A:93:GLU:HB2	2.20	0.41
1:A:276:ARG:HH11	1:A:314:ASP:HA	1.86	0.41
1:A:709:ALA:HB2	1:A:726:VAL:HA	2.02	0.41
1:A:33:ARG:HB3	1:A:52:ILE:HD12	2.03	0.41
1:A:35:ILE:CD1	1:A:77:ALA:HB1	2.37	0.41
1:A:539:THR:OG1	1:A:542:THR:HG23	2.21	0.41
1:A:597:GLU:OE1	1:A:612:PHE:HD2	2.03	0.41
1:A:190:LYS:CE	1:A:223:GLU:OE2	2.69	0.41
1:A:308:ASN:OD1	1:A:308:ASN:C	2.63	0.41
1:A:467:GLU:CD	1:A:467:GLU:N	2.79	0.41
1:A:454:ASP:C	1:A:455:ILE:HG23	2.45	0.40
1:A:727:LEU:HA	1:A:727:LEU:HD12	1.65	0.40
1:A:136:THR:OG1	1:A:139:MET:HG2	2.22	0.40
1:A:613:ASN:O	1:A:615:PRO:HD3	2.21	0.40
1:A:296:LEU:CB	1:A:298:LEU:HG	2.52	0.40
1:A:471:ILE:HA	1:A:471:ILE:HD12	1.78	0.40
1:A:59:SER:CB	1:A:72:VAL:O	2.60	0.40
1:A:195:TYR:CZ	1:A:199:VAL:HG11	2.55	0.40
1:A:273:GLU:C	1:A:274:THR:HG23	2.47	0.40
1:A:296:LEU:O	1:A:297:HIS:HB2	2.21	0.40
1:A:580:GLU:OE1	1:A:582:GLN:HB3	2.21	0.40
1:A:583:ASP:O	1:A:584:TRP:C	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	736/761 (97%)	692 (94%)	33 (4%)	11 (2%)	8 8

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	ASN
1	A	363	ALA
1	A	44	ARG
1	A	509	ASP
1	A	711	ASN
1	A	498	LYS
1	A	499	ILE
1	A	713	PRO
1	A	3	PRO
1	A	40	ASP
1	A	39	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	634/665 (95%)	545 (86%)	89 (14%)	3 3

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LYS
1	A	26	LYS
1	A	27	LEU
1	A	31	ASP
1	A	32	LYS
1	A	35	ILE
1	A	44	ARG
1	A	57	SER
1	A	63	LYS
1	A	66	ASP

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Mol	Chain	Res	Type
1	A	71	GLN
1	A	73	LYS
1	A	84	LYS
1	A	95	SER
1	A	126	VAL
1	A	144	LYS
1	A	146	ARG
1	A	158	ILE
1	A	199	VAL
1	A	211	LEU
1	A	221	ILE
1	A	249	ASN
1	A	262	LEU
1	A	280	ILE
1	A	291	GLU
1	A	293	LYS
1	A	294	LYS
1	A	302	GLU
1	A	325	LYS
1	A	326	ILE
1	A	329	GLN
1	A	338	GLN
1	A	342	MET
1	A	357	ILE
1	A	358	LYS
1	A	368	VAL
1	A	370	LYS
1	A	372	LYS
1	A	375	LEU
1	A	379	SER
1	A	380	THR
1	A	387	SER
1	A	388	VAL
1	A	404	LEU
1	A	405	VAL
1	A	407	GLN
1	A	411	VAL
1	A	412	GLU
1	A	413	LYS
1	A	415	SER
1	A	436	LYS
1	A	444	GLU

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Mol	Chain	Res	Type
1	A	460	ILE
1	A	462	LYS
1	A	496	LYS
1	A	499	ILE
1	A	510	SER
1	A	516	LEU
1	A	531	GLU
1	A	544	ILE
1	A	546	LYS
1	A	562	ARG
1	A	565	LYS
1	A	570	VAL
1	A	581	ILE
1	A	582	GLN
1	A	594	GLN
1	A	611	LEU
1	A	627	PHE
1	A	640	SER
1	A	656	ILE
1	A	657	ILE
1	A	661	LYS
1	A	666	LYS
1	A	674	ASP
1	A	688	THR
1	A	689	ARG
1	A	690	LYS
1	A	703	LYS
1	A	707	LEU
1	A	717	GLU
1	A	727	LEU
1	A	728	LYS
1	A	732	ILE
1	A	735	GLU
1	A	738	ARG
1	A	741	ILE
1	A	742	THR
1	A	751	LEU

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	2	ASN

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Mol	Chain	Res	Type
1	A	5	HIS
1	A	19	GLN
1	A	78	ASN
1	A	105	ASN
1	A	149	ASN
1	A	217	GLN
1	A	234	ASN
1	A	249	ASN
1	A	259	GLN
1	A	407	GLN
1	A	408	HIS
1	A	439	ASN
1	A	479	GLN
1	A	484	HIS
1	A	491	GLN
1	A	582	GLN
1	A	594	GLN
1	A	649	ASN
1	A	662	GLN
1	A	720	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	NMQ	A	999	2	24,26,26	1.54	4 (16%)	24,39,39	1.77	5 (20%)

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	NMQ	A	999	2	-	2/19/27/27	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	NMQ	C1-NA3	-3.72	1.33	1.41
3	A	999	NMQ	CA3-NA3	-3.63	1.40	1.46
3	A	999	NMQ	C4-C5	2.56	1.43	1.38
3	A	999	NMQ	O2A-N2	-2.11	1.21	1.35

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	999	NMQ	C6-C1-NA3	-5.49	114.69	121.96
3	A	999	NMQ	CA3-NA3-C1	-3.12	107.59	116.03
3	A	999	NMQ	CA1-CA2-NA3	-2.99	106.59	112.44
3	A	999	NMQ	CA2-NA3-C1	-2.37	107.54	117.16
3	A	999	NMQ	OA1-PA-OA3	2.12	113.00	107.27

There are no chirality outliers.

All (2) torsion outliers are listed below:

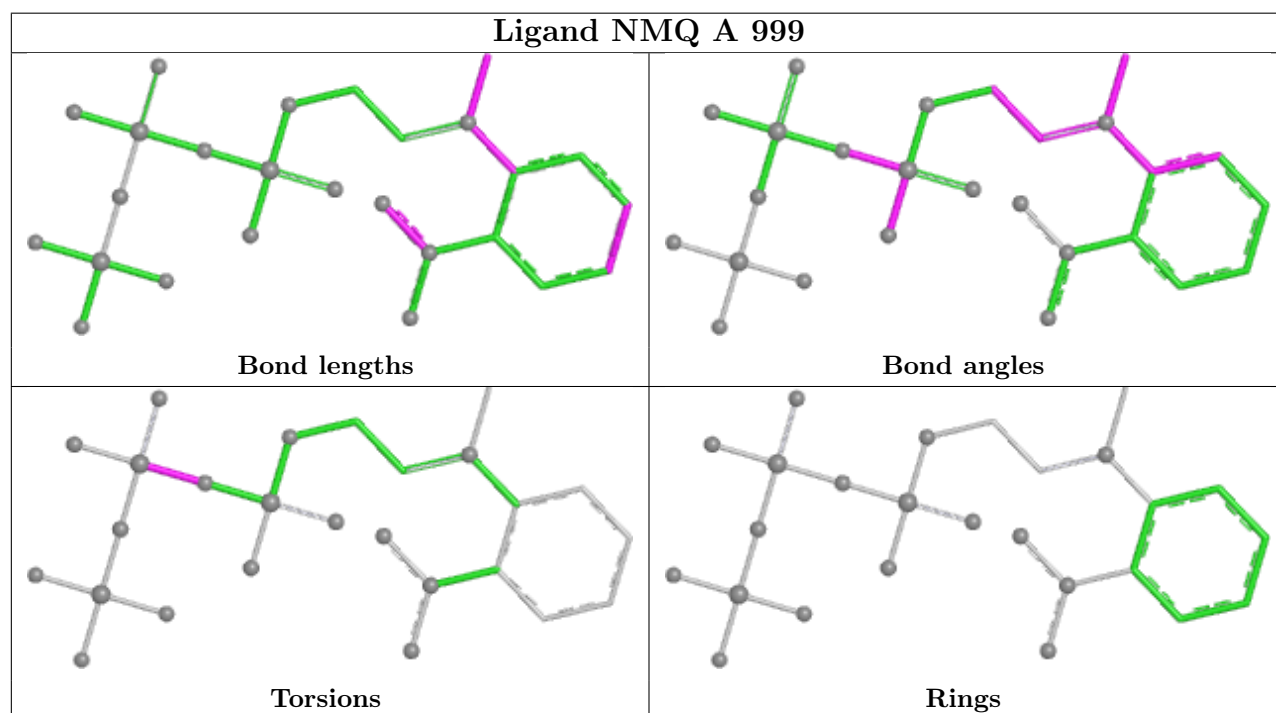
Mol	Chain	Res	Type	Atoms
3	A	999	NMQ	PA-OA3-PB-OB2
3	A	999	NMQ	PA-OA3-PB-OB1

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	999	NMQ	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	744/761 (97%)	0.55	84 (11%) 10 11	9, 31, 75, 100	0

All (84) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	500	ASN	5.9
1	A	366	GLY	5.1
1	A	367	ALA	4.9
1	A	508	LEU	4.8
1	A	364	GLY	4.6
1	A	621	ALA	4.6
1	A	362	GLY	4.5
1	A	710	PRO	4.5
1	A	363	ALA	4.4
1	A	715	ASP	4.3
1	A	72	VAL	4.3
1	A	509	ASP	4.2
1	A	455	ILE	4.1
1	A	401	GLY	4.1
1	A	210	VAL	4.0
1	A	368	VAL	4.0
1	A	707	LEU	3.9
1	A	443	GLN	3.9
1	A	39	PRO	3.9
1	A	322	GLU	3.8
1	A	713	PRO	3.8
1	A	42	LYS	3.7
1	A	405	VAL	3.7
1	A	371	ASP	3.6
1	A	737	TYR	3.5
1	A	358	LYS	3.4
1	A	65	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	219	ASN	3.2
1	A	493	GLU	3.2
1	A	209	GLY	3.0
1	A	3	PRO	3.0
1	A	489	LEU	3.0
1	A	370	LYS	3.0
1	A	711	ASN	3.0
1	A	299	ALA	2.9
1	A	43	GLU	2.9
1	A	342	MET	2.9
1	A	498	LYS	2.8
1	A	627	PHE	2.7
1	A	360	GLU	2.7
1	A	717	GLU	2.7
1	A	728	LYS	2.7
1	A	274	THR	2.7
1	A	365	GLU	2.7
1	A	626	ASN	2.6
1	A	57	SER	2.6
1	A	56	THR	2.6
1	A	290	ALA	2.5
1	A	149	ASN	2.5
1	A	321	SER	2.5
1	A	41	PRO	2.5
1	A	686	ARG	2.5
1	A	376	ASN	2.5
1	A	44	ARG	2.4
1	A	759	GLU	2.4
1	A	688	THR	2.4
1	A	202	ARG	2.4
1	A	68	GLN	2.4
1	A	205	ALA	2.3
1	A	288	ALA	2.3
1	A	316	LYS	2.3
1	A	496	LYS	2.3
1	A	67	GLY	2.3
1	A	218	ALA	2.3
1	A	373	THR	2.3
1	A	689	ARG	2.3
1	A	706	TYR	2.3
1	A	716	ALA	2.3
1	A	2	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	533	SER	2.3
1	A	40	ASP	2.2
1	A	444	GLU	2.2
1	A	38	ASN	2.2
1	A	383	GLY	2.2
1	A	445	ARG	2.2
1	A	738	ARG	2.2
1	A	714	ARG	2.1
1	A	297	HIS	2.1
1	A	5	HIS	2.1
1	A	204	GLN	2.1
1	A	52	ILE	2.1
1	A	757	ALA	2.0
1	A	53	VAL	2.0
1	A	734	PRO	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](#)

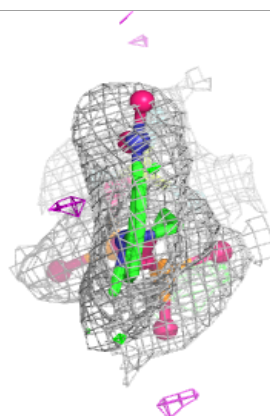
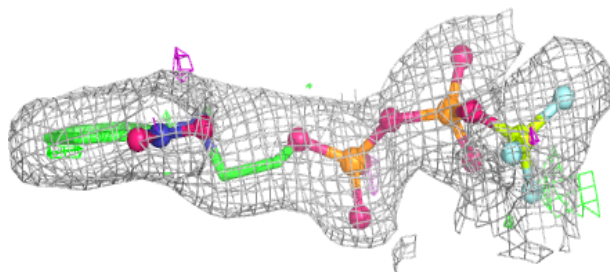
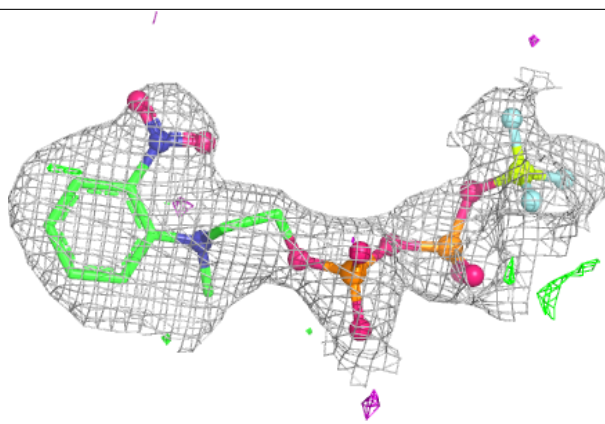
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	0.95	0.09	21,21,21,21	0
3	NMQ	A	999	26/26	0.97	0.10	8,24,52,100	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.

Electron density around NMQ A 999:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.