



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 23, 2018 – 10:19 PM EST

PDB ID : 1D0Y
Title : DICTYOSTELIUM MYOSIN S1DC (MOTOR DOMAIN FRAGMENT)
COMPLEXED WITH O-NITROPHENYL AMINOETHYLDIPHOSPHATE
BERYLLIUM FLUORIDE.
Authors : Gulick, A.M.; Bauer, C.B.; Thoden, J.B.; Pate, E.; Yount, R.G.; Rayment, I.
Deposited on : 1999-09-15
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

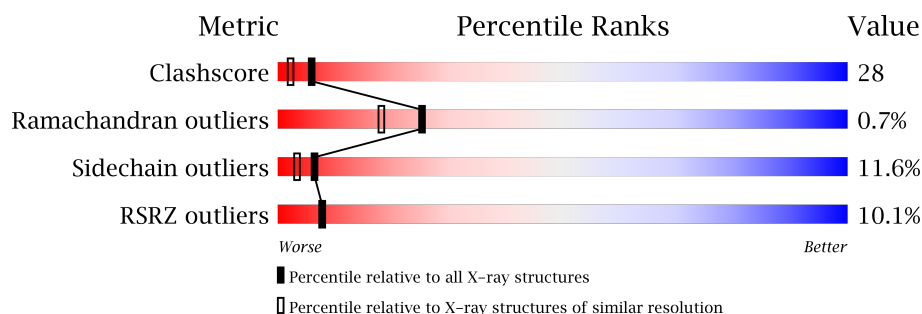
1 Overall quality at a glance

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	112137	7775 (2.00-2.00)
Ramachandran outliers	110173	7679 (2.00-2.00)
Sidechain outliers	110143	7678 (2.00-2.00)
RSRZ outliers	101464	6696 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	761	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6623 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called MYOSIN S1DC MOTOR DOMAIN.

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

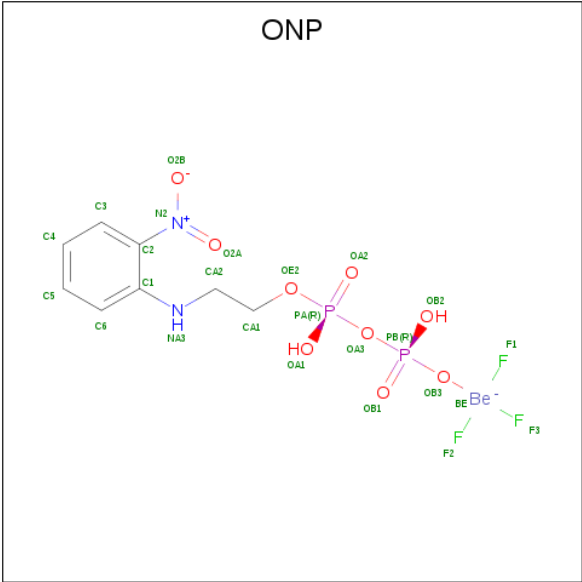
There are 3 discrepancies between the modelled and reference sequences:

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

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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



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

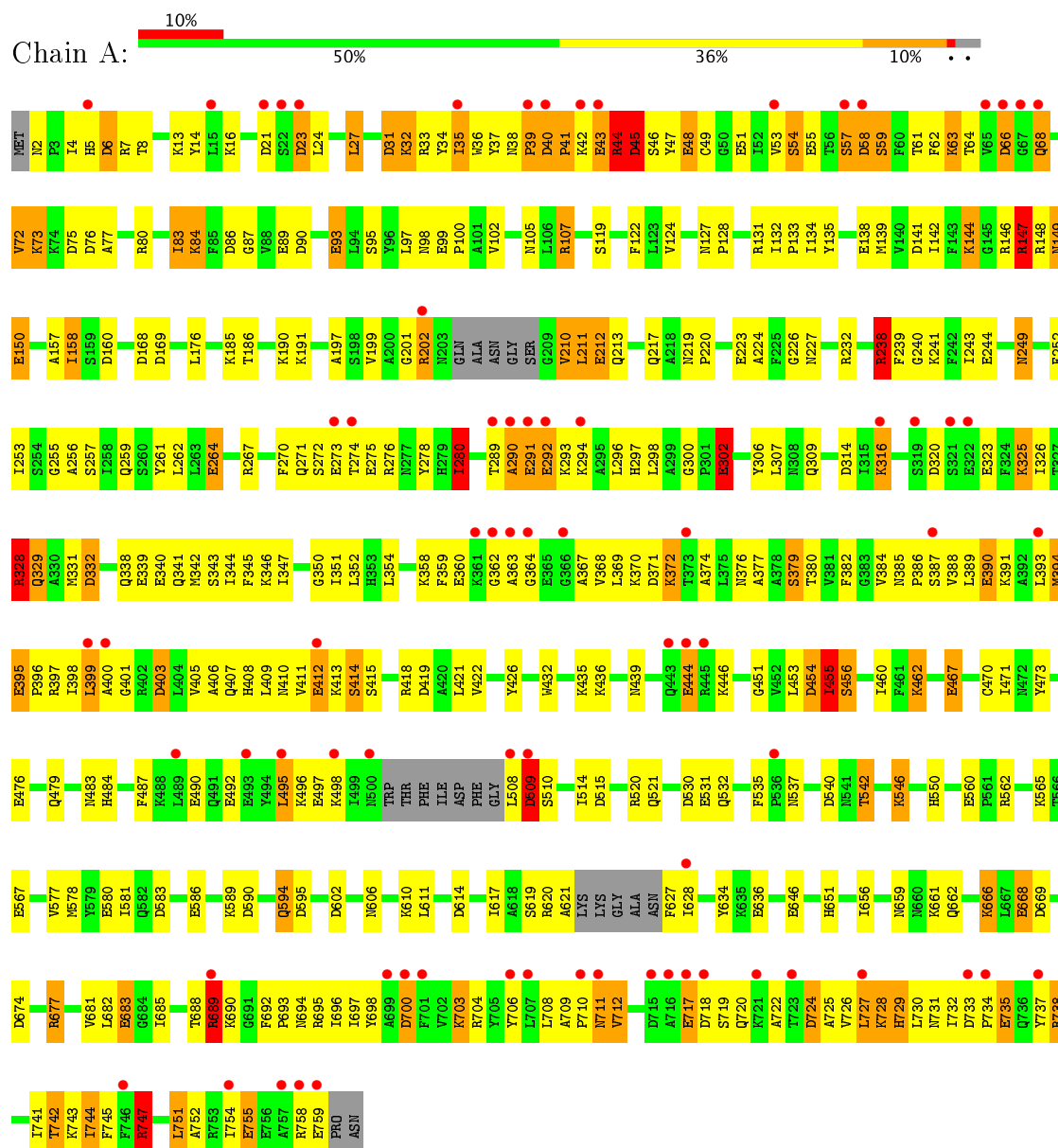
- Molecule 4 is water.

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

3 Residue-property plots

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

• Molecule 1: MYOSIN S1DC MOTOR DOMAIN



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	103.80 Å 180.30 Å 54.00 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 19.95 – 2.01	Depositor EDS
% Data completeness (in resolution range)	86.6 (25.00-2.00) 84.6 (19.95-2.01)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.60 (at 2.01 Å)	Xtriage
Refinement program	TNT 5E	Depositor
R, R_{free}	0.178 , (Not available) 0.191 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	21.8	Xtriage
Anisotropy	0.275	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 121.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6623	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	36/6001 (0.6%)	1.51	98/8102 (1.2%)

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

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

All (36) bond length outliers are listed below:

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

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

All (98) bond angle outliers are listed below:

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

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

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

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	45	ASP	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5889	0	5792	323	0
2	A	1	0	0	0	0
3	A	25	0	9	1	0
4	A	708	0	0	40	0
All	All	6623	0	5801	324	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 28.

All (324) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:THR:HG23	1:A:68:GLN:O	1.97	0.65
1:A:484:HIS:O	1:A:487:PHE:HB3	1.97	0.64
1:A:627:PHE:N	4:A:1426:HOH:O	2.30	0.64
1:A:185:LYS:HE3	1:A:456:SER:HA	1.79	0.64
1:A:241:LYS:H	1:A:455:ILE:HD12	1.63	0.64
1:A:202:ARG:HH11	1:A:202:ARG:HG3	1.62	0.63
1:A:38:ASN:C	1:A:40:ASP:H	2.01	0.63
1:A:344:ILE:HD11	1:A:432:TRP:HZ3	1.63	0.62
1:A:698:TYR:CZ	1:A:720:GLN:HG2	2.33	0.62
1:A:59:SER:HB2	1:A:72:VAL:O	1.99	0.62
1:A:202:ARG:NH1	1:A:252:PHE:CB	2.62	0.62
1:A:462:LYS:HG2	4:A:1572:HOH:O	1.99	0.62
1:A:35:ILE:CD1	1:A:77:ALA:HB1	2.17	0.62
1:A:138:GLU:O	1:A:142:ILE:HD12	1.99	0.61
1:A:331:MET:CE	1:A:345:PHE:HZ	2.14	0.61
1:A:453:LEU:CD1	1:A:455:ILE:HD13	2.30	0.61
1:A:47:TYR:CE1	1:A:100:PRO:HG3	2.35	0.61
1:A:58:ASP:HA	4:A:1238:HOH:O	2.00	0.61
1:A:238:ARG:HD3	1:A:264:GLU:OE2	2.01	0.61
1:A:724:ASP:OD2	1:A:728:LYS:HD2	2.01	0.61
1:A:138:GLU:HB3	4:A:1632:HOH:O	2.00	0.60
1:A:224:ALA:O	1:A:280:ILE:HG13	2.00	0.60
1:A:290:ALA:CA	1:A:293:LYS:HD2	2.29	0.60
1:A:594:GLN:HE21	1:A:594:GLN:CA	2.13	0.60
1:A:698:TYR:CE1	1:A:720:GLN:HG3	2.37	0.60
1:A:62:PHE:CE2	1:A:72:VAL:CG2	2.81	0.60
1:A:14:TYR:CE2	1:A:133:PRO:HG2	2.37	0.60
1:A:158:ILE:HD11	1:A:651:HIS:HB3	1.83	0.59
1:A:40:ASP:HB3	1:A:42:LYS:H	1.67	0.59
1:A:147:ARG:O	1:A:150:GLU:HB2	2.01	0.59
1:A:202:ARG:HG3	1:A:202:ARG:NH1	2.16	0.59
1:A:432:TRP:CZ2	1:A:436:LYS:HE2	2.37	0.58
1:A:191:LYS:CA	1:A:191:LYS:HE2	2.33	0.58
1:A:397:ARG:C	1:A:398:ILE:HD12	2.23	0.58
1:A:139:MET:HA	1:A:142:ILE:HD12	1.86	0.58
1:A:399:LEU:HD12	1:A:400:ALA:N	2.19	0.57
1:A:331:MET:CE	1:A:345:PHE:CZ	2.87	0.57
1:A:280:ILE:HD12	1:A:280:ILE:N	2.18	0.57
1:A:677:ARG:HG3	1:A:682:LEU:HD12	1.86	0.57
1:A:316:LYS:HB2	1:A:316:LYS:NZ	2.16	0.57
1:A:149:ASN:ND2	1:A:150:GLU:N	2.52	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:999:ONP:NA3	3:A:999:ONP:O2B	2.38	0.56
1:A:40:ASP:OD2	1:A:42:LYS:HG3	2.05	0.56
1:A:741:ILE:HG22	1:A:742:THR:HG22	1.88	0.56
1:A:710:PRO:HG3	1:A:729:HIS:CE1	2.40	0.56
1:A:391:LYS:HE3	4:A:1613:HOH:O	2.06	0.56
1:A:379:SER:HB2	1:A:386:PRO:HG3	1.87	0.56
1:A:32:LYS:HB3	1:A:34:TYR:CE2	2.40	0.56
1:A:496:LYS:HG3	4:A:1353:HOH:O	2.06	0.56
1:A:124:VAL:HG13	1:A:656:ILE:CD1	2.36	0.56
1:A:550:HIS:HD2	4:A:1076:HOH:O	1.89	0.56
1:A:621:ALA:HB2	1:A:628:ILE:HG12	1.88	0.56
1:A:399:LEU:HD12	1:A:399:LEU:C	2.25	0.56
1:A:40:ASP:CG	1:A:42:LYS:HB2	2.27	0.56
1:A:398:ILE:HD13	1:A:407:GLN:CG	2.36	0.55
1:A:710:PRO:HD3	1:A:729:HIS:CG	2.40	0.55
1:A:758:ARG:HA	4:A:1236:HOH:O	2.05	0.55
1:A:331:MET:HE3	1:A:345:PHE:CZ	2.42	0.55
1:A:362:GLY:HA3	4:A:1567:HOH:O	2.06	0.55
1:A:385:ASN:HB3	1:A:388:VAL:HG23	1.87	0.55
1:A:698:TYR:CD1	1:A:720:GLN:HG3	2.42	0.55
1:A:2:ASN:CB	1:A:5:HIS:HD2	2.13	0.54
1:A:733:ASP:OD2	1:A:734:PRO:HD2	2.07	0.54
1:A:83:ILE:HD11	4:A:1421:HOH:O	2.08	0.54
1:A:532:GLN:OE1	1:A:542:THR:HB	2.06	0.54
1:A:692:PHE:CD1	1:A:747:ARG:HG2	2.42	0.54
1:A:399:LEU:HD13	1:A:403:ASP:O	2.08	0.54
1:A:201:GLY:HA2	1:A:212:GLU:OE2	2.06	0.54
1:A:385:ASN:HB3	1:A:388:VAL:HB	1.90	0.54
1:A:84:LYS:HG3	1:A:704:ARG:NH2	2.23	0.54
1:A:737:TYR:O	1:A:738:ARG:NE	2.36	0.53
1:A:202:ARG:N	1:A:212:GLU:OE2	2.37	0.53
1:A:202:ARG:HH11	1:A:202:ARG:CG	2.20	0.53
1:A:259:GLN:HG2	1:A:261:TYR:CZ	2.43	0.53
1:A:219:ASN:HD21	1:A:243:ILE:CD1	2.22	0.53
1:A:197:ALA:HA	1:A:253:ILE:HD11	1.91	0.53
1:A:372:LYS:O	1:A:376:ASN:ND2	2.42	0.53
1:A:217:GLN:NE2	4:A:1451:HOH:O	2.26	0.53
1:A:302:GLU:HG2	4:A:1651:HOH:O	2.09	0.53
1:A:385:ASN:HB3	1:A:388:VAL:CB	2.38	0.53
1:A:734:PRO:HA	1:A:737:TYR:CE2	2.43	0.53
1:A:95:SER:HB3	1:A:752:ALA:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ASN:C	1:A:695:ARG:HG3	2.29	0.53
1:A:149:ASN:HD22	1:A:150:GLU:H	1.55	0.53
1:A:331:MET:HE1	1:A:345:PHE:HZ	1.73	0.53
1:A:186:THR:HG22	1:A:190:LYS:HE3	1.91	0.53
1:A:367:ALA:O	1:A:408:HIS:HE1	1.91	0.52
1:A:399:LEU:HD11	1:A:401:GLY:C	2.30	0.52
1:A:6:ASP:OD1	1:A:8:THR:HG23	2.09	0.52
1:A:219:ASN:CB	4:A:1642:HOH:O	2.45	0.52
1:A:540:ASP:HB3	1:A:581:ILE:HG23	1.90	0.52
1:A:698:TYR:CZ	1:A:720:GLN:CG	2.91	0.52
1:A:359:PHE:HB3	1:A:411:VAL:HG22	1.91	0.52
1:A:730:LEU:HB2	1:A:732:ILE:HG12	1.91	0.52
1:A:34:TYR:HB3	1:A:49:CYS:SG	2.50	0.52
1:A:219:ASN:HD21	1:A:243:ILE:HD13	1.75	0.52
1:A:436:LYS:O	1:A:439:ASN:HB2	2.10	0.51
1:A:132:ILE:HG22	1:A:134:ILE:HG23	1.91	0.51
1:A:410:ASN:O	1:A:414:SER:HB2	2.10	0.51
1:A:41:PRO:C	1:A:43:GLU:H	2.07	0.51
1:A:2:ASN:HD21	1:A:146:ARG:NH2	2.08	0.51
1:A:309:GLN:HB2	4:A:1174:HOH:O	2.09	0.51
1:A:226:GLY:HA3	1:A:239:PHE:CE2	2.47	0.50
1:A:210:VAL:CG2	1:A:211:LEU:N	2.74	0.50
1:A:2:ASN:ND2	1:A:5:HIS:NE2	2.60	0.50
1:A:710:PRO:O	1:A:711:ASN:ND2	2.44	0.50
1:A:384:VAL:O	1:A:386:PRO:HD3	2.11	0.50
1:A:296:LEU:O	1:A:297:HIS:HB2	2.12	0.50
1:A:273:GLU:O	1:A:274:THR:OG1	2.15	0.49
1:A:342:MET:HA	1:A:342:MET:CE	2.42	0.49
1:A:62:PHE:HD1	1:A:63:LYS:O	1.95	0.49
1:A:709:ALA:HB2	1:A:726:VAL:HA	1.94	0.49
1:A:331:MET:HE1	1:A:345:PHE:CZ	2.47	0.49
1:A:2:ASN:CB	1:A:5:HIS:CD2	2.91	0.49
1:A:398:ILE:HD12	1:A:398:ILE:N	2.27	0.49
1:A:698:TYR:CE2	1:A:720:GLN:HG2	2.46	0.49
1:A:710:PRO:CG	1:A:729:HIS:CE1	2.95	0.49
1:A:38:ASN:O	1:A:40:ASP:N	2.45	0.49
1:A:708:LEU:HD23	1:A:759:GLU:HA	1.94	0.49
1:A:241:LYS:N	1:A:455:ILE:CD1	2.75	0.49
1:A:698:TYR:CE1	1:A:720:GLN:CG	2.95	0.49
1:A:403:ASP:HB3	1:A:405:VAL:HG23	1.94	0.49
1:A:508:LEU:O	1:A:509:ASP:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:521:GLN:OE1	4:A:1671:HOH:O	2.20	0.49
1:A:683:GLU:HG3	4:A:1181:HOH:O	2.12	0.49
1:A:107:ARG:NE	4:A:1187:HOH:O	2.39	0.49
1:A:668:GLU:OE1	4:A:1666:HOH:O	2.20	0.48
1:A:688:THR:HG22	1:A:693:PRO:HB3	1.95	0.48
1:A:238:ARG:CD	1:A:264:GLU:OE2	2.61	0.48
1:A:243:ILE:O	1:A:451:GLY:HA2	2.13	0.48
1:A:2:ASN:N	4:A:1362:HOH:O	2.46	0.48
1:A:496:LYS:NZ	1:A:496:LYS:CB	2.77	0.48
1:A:390:GLU:HG2	1:A:394:MET:CE	2.44	0.48
1:A:535:PHE:N	1:A:535:PHE:CD2	2.82	0.48
1:A:36:TRP:CZ2	1:A:80:ARG:HG3	2.49	0.48
1:A:367:ALA:O	1:A:408:HIS:CE1	2.67	0.48
1:A:23:ASP:OD1	1:A:23:ASP:N	2.45	0.48
1:A:697:ILE:O	1:A:700:ASP:HB2	2.13	0.48
1:A:289:THR:O	1:A:292:GLU:N	2.46	0.47
1:A:496:LYS:HB3	1:A:496:LYS:HZ3	1.78	0.47
1:A:710:PRO:HD3	1:A:729:HIS:CE1	2.48	0.47
1:A:212:GLU:OE2	4:A:1175:HOH:O	2.20	0.47
1:A:692:PHE:CE1	1:A:747:ARG:CG	2.97	0.47
1:A:316:LYS:HB2	1:A:316:LYS:HE3	1.65	0.47
1:A:241:LYS:N	1:A:455:ILE:HD12	2.29	0.47
1:A:240:GLY:HA3	1:A:455:ILE:HG13	1.97	0.47
1:A:323:GLU:O	1:A:326:ILE:HB	2.15	0.47
1:A:127:ASN:OD1	1:A:128:PRO:HD2	2.15	0.47
1:A:730:LEU:O	1:A:731:ASN:HB3	2.14	0.47
1:A:202:ARG:NH2	4:A:1461:HOH:O	2.48	0.47
1:A:619:SER:HB3	1:A:627:PHE:CD2	2.49	0.47
1:A:36:TRP:CZ3	1:A:49:CYS:HB2	2.49	0.46
1:A:666:LYS:NZ	4:A:1182:HOH:O	2.47	0.46
1:A:454:ASP:O	1:A:455:ILE:HD12	2.15	0.46
1:A:259:GLN:HG2	1:A:261:TYR:OH	2.15	0.46
1:A:38:ASN:ND2	1:A:46:SER:O	2.43	0.46
1:A:737:TYR:C	1:A:737:TYR:CD1	2.88	0.46
1:A:744:ILE:HD13	1:A:745:PHE:N	2.31	0.46
1:A:255:GLY:O	1:A:256:ALA:HB2	2.15	0.46
1:A:36:TRP:CE2	1:A:80:ARG:HG3	2.50	0.46
1:A:280:ILE:HD11	1:A:426:TYR:OH	2.15	0.46
1:A:726:VAL:O	1:A:730:LEU:HG	2.16	0.46
1:A:16:LYS:HE3	1:A:16:LYS:HB3	1.83	0.45
1:A:479:GLN:HE21	1:A:483:ASN:ND2	2.13	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:MET:HE2	1:A:578:MET:HB3	1.72	0.45
1:A:83:ILE:CD1	1:A:86:ASP:OD1	2.64	0.45
1:A:510:SER:O	1:A:514:ILE:HG13	2.17	0.45
1:A:210:VAL:HG13	1:A:210:VAL:H	1.31	0.45
1:A:352:LEU:HA	1:A:352:LEU:HD23	1.82	0.45
1:A:379:SER:CB	1:A:386:PRO:HG3	2.46	0.45
1:A:710:PRO:HD3	1:A:729:HIS:CD2	2.51	0.45
1:A:27:LEU:HA	1:A:27:LEU:HD12	1.77	0.45
1:A:37:TYR:O	1:A:47:TYR:HA	2.17	0.45
1:A:351:ILE:HG23	1:A:422:VAL:HG13	1.99	0.45
1:A:594:GLN:HB2	4:A:1664:HOH:O	2.17	0.45
1:A:90:ASP:HB3	1:A:93:GLU:HG3	1.99	0.44
1:A:144:LYS:HD2	1:A:199:VAL:HG12	1.99	0.44
1:A:724:ASP:OD2	1:A:728:LYS:HE2	2.17	0.44
1:A:410:ASN:OD1	1:A:413:LYS:N	2.47	0.44
1:A:34:TYR:CD1	1:A:49:CYS:SG	3.10	0.44
1:A:149:ASN:N	1:A:149:ASN:HD22	2.14	0.44
1:A:470:CYS:O	1:A:473:TYR:HB3	2.18	0.44
1:A:54:SER:OG	1:A:61:THR:HB	2.17	0.44
1:A:201:GLY:CA	1:A:212:GLU:OE2	2.66	0.43
1:A:354:LEU:O	1:A:418:ARG:HD3	2.17	0.43
1:A:4:ILE:CG2	1:A:4:ILE:O	2.65	0.43
1:A:362:GLY:C	1:A:364:GLY:N	2.70	0.43
1:A:619:SER:HB3	1:A:627:PHE:CE2	2.53	0.43
1:A:68:GLN:HB3	1:A:68:GLN:HE21	1.60	0.43
1:A:409:LEU:HB3	1:A:413:LYS:HB3	2.00	0.43
1:A:698:TYR:HB3	1:A:719:SER:HB3	1.99	0.43
1:A:191:LYS:CE	1:A:191:LYS:CA	2.96	0.43
1:A:59:SER:CB	1:A:72:VAL:O	2.65	0.43
1:A:202:ARG:CG	1:A:202:ARG:NH1	2.82	0.43
1:A:498:LYS:HG2	1:A:498:LYS:O	2.18	0.43
1:A:611:LEU:HA	1:A:617:ILE:HG21	2.01	0.43
1:A:24:LEU:HD23	1:A:24:LEU:N	2.34	0.43
1:A:389:LEU:O	1:A:393:LEU:HG	2.19	0.43
1:A:692:PHE:CE1	1:A:747:ARG:HG2	2.53	0.43
1:A:751:LEU:HD23	1:A:751:LEU:HA	1.84	0.43
1:A:44:ARG:O	1:A:45:ASP:OD2	2.37	0.43
1:A:45:ASP:OD1	1:A:677:ARG:NH2	2.49	0.43
1:A:460:ILE:HG12	1:A:577:VAL:HG22	2.01	0.43
1:A:158:ILE:CD1	1:A:651:HIS:HB3	2.47	0.43
1:A:690:LYS:NZ	4:A:1198:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASN:O	1:A:102:VAL:HG23	2.18	0.42
1:A:379:SER:HB3	1:A:386:PRO:HD3	2.01	0.42
1:A:399:LEU:HD12	1:A:401:GLY:N	2.34	0.42
1:A:453:LEU:HD12	1:A:455:ILE:HD13	2.00	0.42
1:A:471:ILE:HA	1:A:471:ILE:HD12	1.85	0.42
1:A:396:PRO:HG2	1:A:398:ILE:HD11	2.01	0.42
1:A:610:LYS:HA	1:A:610:LYS:HD2	1.76	0.42
1:A:289:THR:O	1:A:291:GLU:N	2.51	0.42
1:A:325:LYS:HA	1:A:325:LYS:HD3	1.76	0.42
1:A:374:ALA:O	1:A:377:ALA:HB3	2.19	0.42
1:A:217:GLN:C	1:A:220:PRO:HD2	2.39	0.42
1:A:35:ILE:HD13	4:A:1251:HOH:O	2.20	0.42
1:A:144:LYS:NZ	4:A:1593:HOH:O	2.53	0.42
1:A:710:PRO:CD	1:A:729:HIS:CE1	3.02	0.42
1:A:87:GLY:H	1:A:105:ASN:HD21	1.65	0.42
1:A:190:LYS:HE2	1:A:223:GLU:OE2	2.20	0.42
1:A:453:LEU:HD11	1:A:455:ILE:HD13	2.00	0.42
1:A:369:LEU:HA	1:A:369:LEU:HD12	1.85	0.42
1:A:467:GLU:H	1:A:467:GLU:CD	2.22	0.42
1:A:692:PHE:O	1:A:695:ARG:NE	2.38	0.42
1:A:249:ASN:ND2	1:A:249:ASN:N	2.63	0.42
1:A:350:GLY:HA3	1:A:382:PHE:CZ	2.55	0.42
1:A:39:PRO:HG3	1:A:48:GLU:HG2	2.02	0.42
1:A:73:LYS:HA	1:A:73:LYS:HD2	1.49	0.42
1:A:289:THR:O	1:A:289:THR:OG1	2.37	0.41
1:A:300:GLY:HA3	1:A:302:GLU:OE2	2.20	0.41
1:A:737:TYR:HE1	4:A:1460:HOH:O	1.88	0.41
1:A:354:LEU:HD13	1:A:421:LEU:HD23	2.02	0.41
1:A:537:ASN:HB2	4:A:1282:HOH:O	2.19	0.41
1:A:59:SER:HB2	1:A:73:LYS:HD2	2.03	0.41
1:A:681:VAL:O	1:A:685:ILE:HG13	2.20	0.41
1:A:696:ILE:O	1:A:743:LYS:HB3	2.20	0.41
1:A:223:GLU:O	1:A:227:ASN:HB2	2.20	0.41
1:A:306:TYR:O	1:A:307:LEU:HD23	2.20	0.41
1:A:316:LYS:NZ	1:A:316:LYS:CB	2.78	0.41
1:A:627:PHE:CA	4:A:1426:HOH:O	2.68	0.41
1:A:99:GLU:HB2	1:A:100:PRO:HD3	2.03	0.41
1:A:270:PHE:C	1:A:271:GLN:HG3	2.41	0.41
1:A:293:LYS:O	1:A:297:HIS:N	2.53	0.41
1:A:706:TYR:HE1	4:A:1676:HOH:O	2.03	0.41
1:A:138:GLU:OE2	1:A:138:GLU:N	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:GLN:O	1:A:332:ASP:HB2	2.21	0.41
1:A:741:ILE:C	1:A:742:THR:CG2	2.87	0.41
1:A:344:ILE:HD11	1:A:432:TRP:CZ3	2.50	0.41
1:A:696:ILE:N	1:A:696:ILE:HD12	2.35	0.41
1:A:147:ARG:HG3	1:A:150:GLU:CD	2.39	0.41
1:A:341:GLN:O	1:A:345:PHE:CD2	2.74	0.41
1:A:727:LEU:HD12	1:A:727:LEU:HA	1.65	0.41
1:A:415:SER:O	1:A:418:ARG:HB3	2.21	0.41
1:A:197:ALA:HA	1:A:253:ILE:CD1	2.50	0.40
1:A:278:TYR:HB3	1:A:280:ILE:HD11	2.03	0.40
1:A:415:SER:OG	1:A:418:ARG:NH2	2.45	0.40
1:A:659:ASN:OD1	1:A:661:LYS:N	2.52	0.40
1:A:754:ILE:HG22	1:A:755:GLU:N	2.36	0.40
1:A:134:ILE:HA	1:A:139:MET:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	733/761 (96%)	690 (94%)	38 (5%)	5 (1%)	25	18

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	363	ALA
1	A	711	ASN
1	A	290	ALA
1	A	41	PRO
1	A	39	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	631/665 (95%)	558 (88%)	73 (12%)	6 3

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

Mol	Chain	Res	Type
1	A	13	LYS
1	A	27	LEU
1	A	31	ASP
1	A	32	LYS
1	A	35	ILE
1	A	40	ASP
1	A	44	ARG
1	A	54	SER
1	A	57	SER
1	A	59	SER
1	A	63	LYS
1	A	66	ASP
1	A	68	GLN
1	A	72	VAL
1	A	73	LYS
1	A	83	ILE
1	A	84	LYS
1	A	144	LYS
1	A	147	ARG
1	A	149	ASN
1	A	150	GLU
1	A	158	ILE
1	A	202	ARG
1	A	210	VAL
1	A	211	LEU
1	A	213	GLN
1	A	238	ARG
1	A	257	SER
1	A	262	LEU
1	A	272	SER

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Mol	Chain	Res	Type
1	A	280	ILE
1	A	294	LYS
1	A	302	GLU
1	A	316	LYS
1	A	325	LYS
1	A	328	ARG
1	A	329	GLN
1	A	338	GLN
1	A	358	LYS
1	A	368	VAL
1	A	370	LYS
1	A	372	LYS
1	A	379	SER
1	A	380	THR
1	A	387	SER
1	A	394	MET
1	A	399	LEU
1	A	412	GLU
1	A	414	SER
1	A	444	GLU
1	A	446	LYS
1	A	455	ILE
1	A	456	SER
1	A	462	LYS
1	A	495	LEU
1	A	509	ASP
1	A	542	THR
1	A	546	LYS
1	A	565	LYS
1	A	589	LYS
1	A	594	GLN
1	A	666	LYS
1	A	689	ARG
1	A	703	LYS
1	A	712	VAL
1	A	717	GLU
1	A	727	LEU
1	A	728	LYS
1	A	738	ARG
1	A	742	THR
1	A	744	ILE
1	A	747	ARG

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Mol	Chain	Res	Type
1	A	751	LEU

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

Mol	Chain	Res	Type
1	A	68	GLN
1	A	105	ASN
1	A	149	ASN
1	A	219	ASN
1	A	234	ASN
1	A	249	ASN
1	A	259	GLN
1	A	283	GLN
1	A	376	ASN
1	A	408	HIS
1	A	439	ASN
1	A	483	ASN
1	A	491	GLN
1	A	521	GLN
1	A	550	HIS
1	A	594	GLN
1	A	711	ASN
1	A	729	HIS

5.3.3 RNA [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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	ONP	A	999	2	20,25,25	1.01	1 (5%)	20,37,37	1.59	2 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ONP	A	999	2	-	0/17/24/24	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	999	ONP	C6-C1	-2.13	1.36	1.39

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	999	ONP	CA2-NA3-C1	-4.80	110.89	123.25
3	A	999	ONP	C3-C2-N2	3.17	120.57	116.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	741/761 (97%)	0.33	75 (10%) 8 8	14, 36, 80, 100	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	364	GLY	6.4
1	A	737	TYR	5.9
1	A	362	GLY	5.6
1	A	444	GLU	5.6
1	A	294	LYS	5.5
1	A	443	GLN	5.0
1	A	42	LYS	4.7
1	A	710	PRO	4.6
1	A	319	SER	4.6
1	A	711	ASN	4.6
1	A	289	THR	4.5
1	A	53	VAL	4.5
1	A	508	LEU	4.4
1	A	707	LEU	4.3
1	A	757	ALA	4.3
1	A	43	GLU	4.3
1	A	316	LYS	3.9
1	A	23	ASP	3.8
1	A	290	ALA	3.8
1	A	66	ASP	3.7
1	A	5	HIS	3.6
1	A	495	LEU	3.6
1	A	291	GLU	3.5
1	A	759	GLU	3.5
1	A	35	ILE	3.4
1	A	65	VAL	3.4
1	A	717	GLU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	400	ALA	3.3
1	A	412	GLU	3.2
1	A	202	ARG	3.2
1	A	363	ALA	3.2
1	A	500	ASN	3.1
1	A	40	ASP	3.0
1	A	689	ARG	2.9
1	A	67	GLY	2.9
1	A	68	GLN	2.9
1	A	322	GLU	2.8
1	A	445	ARG	2.8
1	A	493	GLU	2.8
1	A	718	ASP	2.8
1	A	746	PHE	2.7
1	A	292	GLU	2.7
1	A	321	SER	2.7
1	A	273	GLU	2.6
1	A	536	PRO	2.6
1	A	758	ARG	2.6
1	A	733	ASP	2.6
1	A	723	THR	2.6
1	A	15	LEU	2.6
1	A	399	LEU	2.6
1	A	715	ASP	2.5
1	A	39	PRO	2.5
1	A	489	LEU	2.5
1	A	706	TYR	2.5
1	A	701	PHE	2.5
1	A	58	ASP	2.4
1	A	700	ASP	2.3
1	A	387	SER	2.3
1	A	721	LYS	2.3
1	A	727	LEU	2.3
1	A	716	ALA	2.3
1	A	509	ASP	2.2
1	A	754	ILE	2.2
1	A	498	LYS	2.2
1	A	361	LYS	2.2
1	A	699	ALA	2.1
1	A	393	LEU	2.1
1	A	734	PRO	2.1
1	A	628	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	373	THR	2.1
1	A	366	GLY	2.1
1	A	274	THR	2.0
1	A	22	SER	2.0
1	A	21	ASP	2.0
1	A	57	SER	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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	ONP	A	999	25/25	0.98	0.09	-0.49	12,20,35,79	0
2	MG	A	998	1/1	0.99	0.05	-1.84	19,19,19,19	0

6.5 Other polymers [i](#)

There are no such residues in this entry.