



Full wwPDB X-ray Structure Validation Report ⓘ

May 25, 2020 – 12:23 am BST

PDB ID : 5I4E
Title : Crystal Structure of Human Nonmuscle Myosin 2C motor domain
Authors : Chinthalapudi, K.; Heissler, S.M.; Preller, M.; Sellers, J.R.; Manstein, D.J.
Deposited on : 2016-02-11
Resolution : 2.25 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

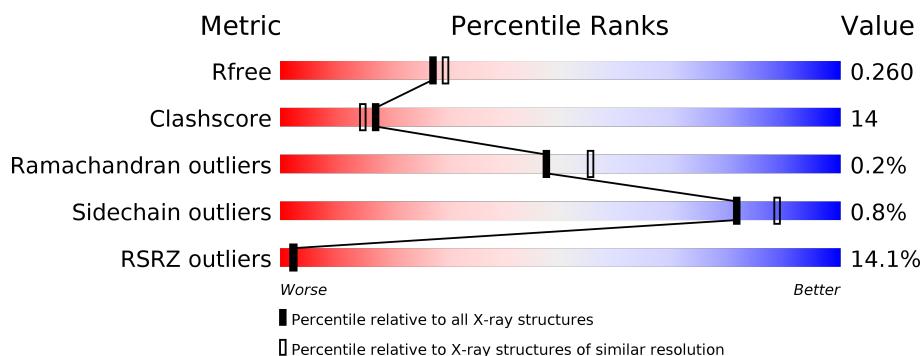
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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))
R_{free}	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 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	980	<div> <div>14%</div> <div>80%</div> <div>17%</div> <div>..</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8395 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.

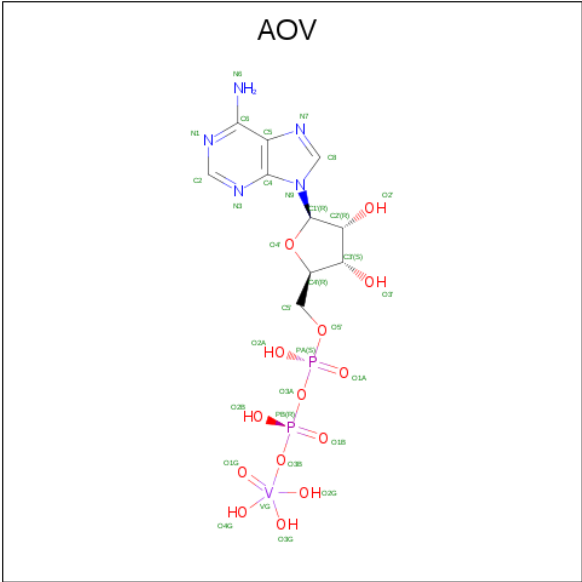
- Molecule 1 is a protein called Myosin-14,Alpha-actinin A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	959	Total	C	N	O	S	0	0	0
			7697	4858	1358	1452	29			

There are 17 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	785	ILE	-	linker	UNP Q7Z406
A	786	PHE	-	linker	UNP Q7Z406
A	787	PHE	-	linker	UNP Q7Z406
A	788	ARG	-	linker	UNP Q7Z406
A	789	ALA	-	linker	UNP Q7Z406
A	790	GLY	-	linker	UNP Q7Z406
A	791	VAL	-	linker	UNP Q7Z406
A	792	LEU	-	linker	UNP Q7Z406
A	793	ALA	-	linker	UNP Q7Z406
A	794	GLN	-	linker	UNP Q7Z406
A	795	LEU	-	linker	UNP Q7Z406
A	796	GLU	-	linker	UNP Q7Z406
A	797	GLU	-	linker	UNP Q7Z406
A	798	GLU	-	linker	UNP Q7Z406
A	799	ARG	-	linker	UNP Q7Z406
A	800	ALA	-	linker	UNP Q7Z406
A	801	SER	-	linker	UNP Q7Z406

- Molecule 2 is ADP ORTHOVANADATE (three-letter code: AOV) (formula: C₁₀H₁₇N₅O₁₄P₂V).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
2	A	1	Total	C	N	O	P	V	0	0
			32	10	5	14	2	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

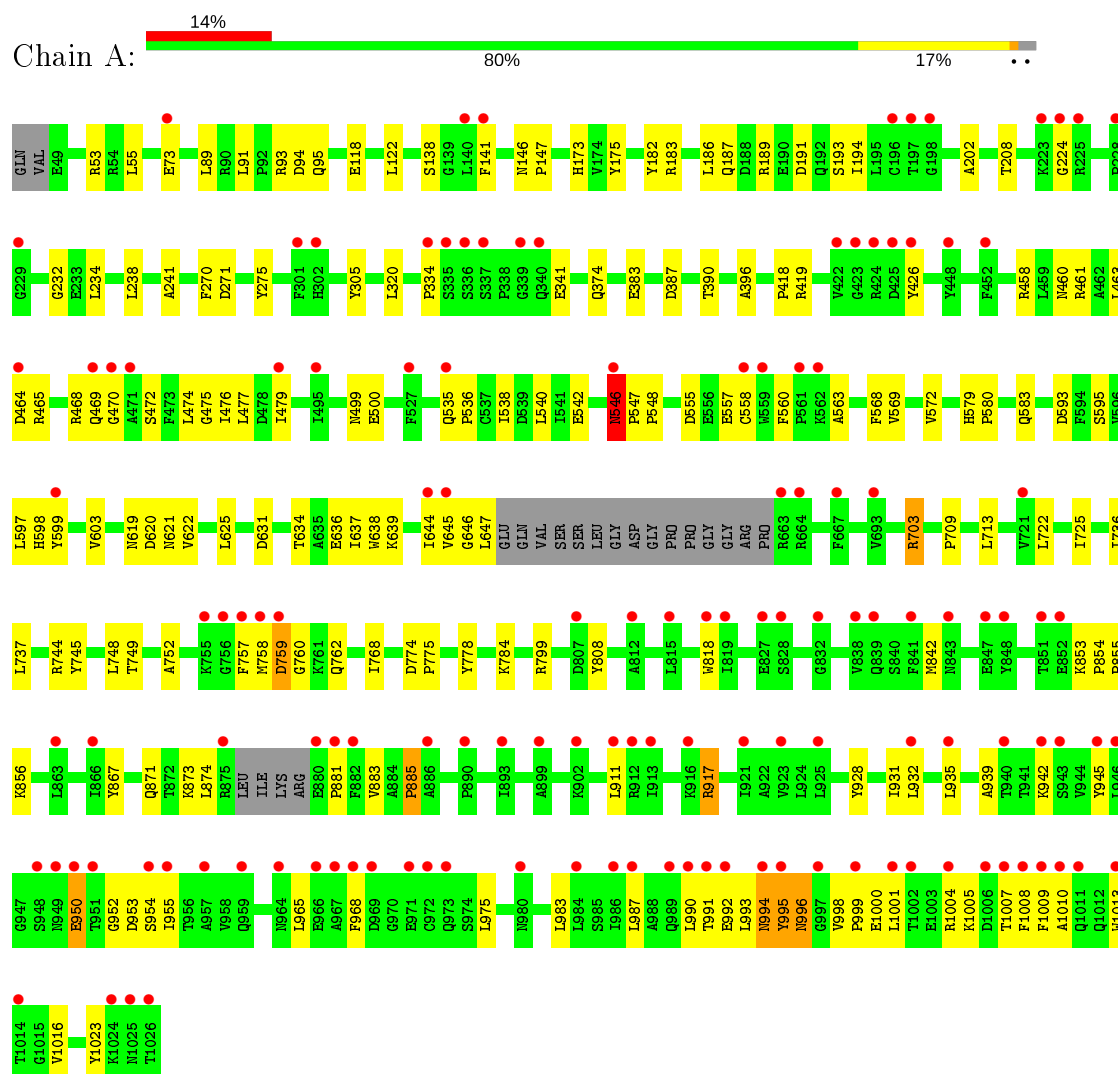
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	665	Total	O	0	0
			665	665		

3 Residue-property plots [i](#)

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-14,Alpha-actinin A



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	81.12Å 125.61Å 153.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.77 – 2.25 34.77 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.9 (34.77-2.25) 99.7 (34.77-2.25)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.72 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.220 , 0.241 0.242 , 0.260	Depositor DCC
R_{free} test set	3786 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.968	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 63.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8395	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: AOV, 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	0.58	0/7844	0.71	5/10583 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	546	ASN	N-CA-C	-6.94	92.25	111.00
1	A	950	GLU	N-CA-CB	-5.92	99.94	110.60
1	A	885	PRO	CA-N-CD	5.79	119.81	111.70
1	A	759	ASP	CB-CA-C	-5.26	99.88	110.40
1	A	995	TYR	CB-CA-C	5.02	120.44	110.40

There are no chirality outliers.

There are no planarity outliers.

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	7697	0	7667	216	1
2	A	32	0	12	6	0
3	A	1	0	0	0	0
4	A	665	0	0	8	0
All	All	8395	0	7679	216	1

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 14.

All (216) 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:757:PHE:CE2	1:A:759:ASP:HB3	1.68	1.27
1:A:987:LEU:CD2	1:A:993:LEU:HD11	1.74	1.16
1:A:987:LEU:HD21	1:A:993:LEU:HD11	1.21	1.14
1:A:931:ILE:O	1:A:935:LEU:HD13	1.48	1.14
1:A:1010:ALA:HA	1:A:1013:TRP:CD1	1.84	1.11
1:A:1010:ALA:HA	1:A:1013:TRP:HD1	0.98	1.08
1:A:917:ARG:HH12	1:A:990:LEU:HB2	1.11	1.07
1:A:774:ASP:OD1	1:A:775:PRO:HD2	1.55	1.06
1:A:546:ASN:HB3	1:A:547:PRO:CD	1.86	1.05
1:A:998:VAL:HB	1:A:999:PRO:HD3	1.40	1.04
1:A:917:ARG:NH1	1:A:990:LEU:HB2	1.77	0.97
1:A:995:TYR:O	1:A:999:PRO:HD2	1.63	0.97
1:A:995:TYR:O	1:A:999:PRO:CD	2.12	0.96
1:A:535:GLN:HG3	1:A:536:PRO:HD3	1.45	0.96
1:A:620:ASP:HB2	1:A:645:VAL:HG13	1.45	0.95
1:A:757:PHE:HZ	1:A:762:GLN:CB	1.80	0.95
1:A:987:LEU:HD21	1:A:993:LEU:CD1	1.96	0.95
1:A:757:PHE:HE2	1:A:759:ASP:HB3	1.28	0.93
1:A:535:GLN:CG	1:A:536:PRO:HD3	1.98	0.92
1:A:996:ASN:O	1:A:1000:GLU:HG2	1.70	0.92
1:A:854:PRO:HG2	1:A:855:PRO:HD3	1.49	0.92
1:A:146:ASN:OD1	2:A:1500:AOV:C8	2.18	0.91
1:A:757:PHE:CZ	1:A:762:GLN:HB2	2.06	0.91
1:A:917:ARG:HH22	1:A:990:LEU:HD22	1.38	0.88
1:A:757:PHE:CZ	1:A:762:GLN:CB	2.59	0.86
1:A:191:ASP:OD1	1:A:472:SER:HA	1.77	0.85
1:A:194:ILE:HD12	1:A:474:LEU:HD21	1.57	0.85
1:A:619:ASN:HD22	1:A:622:VAL:HG23	1.43	0.84
1:A:757:PHE:HZ	1:A:762:GLN:HB2	1.40	0.83
1:A:1010:ALA:CA	1:A:1013:TRP:HD1	1.89	0.83
1:A:965:LEU:HB3	1:A:1013:TRP:HZ3	1.40	0.82
1:A:598:HIS:HD2	1:A:603:VAL:HG23	1.43	0.82
1:A:499:ASN:HB3	1:A:599:TYR:OH	1.82	0.79
1:A:620:ASP:CB	1:A:645:VAL:HG13	2.13	0.79
1:A:990:LEU:HG	1:A:991:THR:N	1.98	0.79
1:A:500:GLU:HA	1:A:599:TYR:CE2	2.17	0.78
1:A:477:LEU:HD11	1:A:479:ILE:HG23	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:TYR:O	1:A:999:PRO:HD3	1.83	0.77
1:A:965:LEU:HB3	1:A:1013:TRP:CZ3	2.19	0.77
1:A:546:ASN:HB3	1:A:547:PRO:HD3	1.67	0.76
1:A:546:ASN:HB3	1:A:547:PRO:HD2	1.63	0.76
1:A:557:GLU:HG2	1:A:568:PHE:HB2	1.67	0.75
1:A:931:ILE:O	1:A:935:LEU:CD1	2.32	0.75
1:A:945:TYR:HB2	1:A:1016:VAL:HG21	1.69	0.74
1:A:996:ASN:O	1:A:1000:GLU:CG	2.35	0.74
1:A:942:LYS:NZ	1:A:965:LEU:HD23	2.03	0.74
1:A:118:GLU:HG2	1:A:722:LEU:HD11	1.71	0.73
1:A:189:ARG:NH2	1:A:470:GLY:O	2.21	0.73
1:A:93:ARG:HG2	1:A:93:ARG:HH11	1.54	0.72
1:A:995:TYR:O	1:A:998:VAL:N	2.22	0.72
1:A:122:LEU:HD22	1:A:713:LEU:HD21	1.71	0.72
1:A:757:PHE:CD2	1:A:759:ASP:HB3	2.24	0.72
1:A:598:HIS:HD2	1:A:603:VAL:CG2	2.03	0.71
1:A:460:ASN:O	1:A:464:ASP:HB3	1.91	0.71
1:A:644:ILE:HD12	1:A:644:ILE:N	2.05	0.70
1:A:757:PHE:CZ	1:A:762:GLN:HB3	2.27	0.70
1:A:757:PHE:HZ	1:A:762:GLN:HB3	1.55	0.70
1:A:477:LEU:HD11	1:A:479:ILE:CG2	2.21	0.69
1:A:935:LEU:HD11	1:A:975:LEU:HD22	1.75	0.69
1:A:942:LYS:HZ1	1:A:965:LEU:HD23	1.57	0.68
1:A:854:PRO:HG2	1:A:855:PRO:CD	2.23	0.67
1:A:535:GLN:HG3	1:A:536:PRO:CD	2.24	0.67
1:A:758:MET:HG2	1:A:758:MET:O	1.95	0.67
1:A:469:GLN:O	1:A:469:GLN:HG3	1.95	0.66
1:A:305:TYR:HB3	1:A:341:GLU:OE2	1.95	0.66
1:A:854:PRO:N	1:A:855:PRO:HD2	2.11	0.66
1:A:271:ASP:OD1	1:A:275:TYR:N	2.23	0.65
1:A:917:ARG:NH2	1:A:990:LEU:HD22	2.09	0.65
1:A:871:GLN:HE22	1:A:883:VAL:HG13	1.62	0.65
1:A:89:LEU:CD2	1:A:91:LEU:HD23	2.27	0.65
1:A:990:LEU:HG	1:A:991:THR:H	1.58	0.65
1:A:146:ASN:OD1	2:A:1500:AOV:N7	2.30	0.65
1:A:987:LEU:CD2	1:A:993:LEU:CD1	2.64	0.65
1:A:854:PRO:CD	1:A:855:PRO:HD2	2.26	0.64
1:A:1005:LYS:HA	1:A:1008:PHE:CD2	2.32	0.63
1:A:183:ARG:O	1:A:187:GLN:HG3	1.99	0.63
1:A:987:LEU:HD23	1:A:993:LEU:HD11	1.75	0.63
1:A:535:GLN:HG2	1:A:536:PRO:HD3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:854:PRO:CG	1:A:855:PRO:HD3	2.28	0.63
1:A:89:LEU:HD22	1:A:91:LEU:HD23	1.79	0.63
1:A:334:PRO:HG3	4:A:2235:HOH:O	1.98	0.62
1:A:138:SER:OG	1:A:141:PHE:CE2	2.53	0.62
1:A:548:PRO:HD2	4:A:1743:HOH:O	2.00	0.62
1:A:468:ARG:HG3	1:A:468:ARG:O	2.00	0.61
1:A:138:SER:HB2	1:A:725:ILE:HD11	1.81	0.61
1:A:952:GLY:O	1:A:953:ASP:HB3	2.00	0.61
1:A:173:HIS:HD2	1:A:175:TYR:H	1.48	0.61
1:A:990:LEU:CG	1:A:991:THR:H	2.14	0.61
1:A:994:ASN:OD1	1:A:994:ASN:N	2.26	0.60
1:A:990:LEU:CG	1:A:991:THR:N	2.63	0.60
1:A:854:PRO:CD	1:A:855:PRO:CD	2.80	0.60
1:A:759:ASP:OD1	1:A:760:GLY:N	2.35	0.59
1:A:598:HIS:CD2	1:A:603:VAL:CG2	2.86	0.59
1:A:458:ARG:HD3	1:A:461:ARG:HH12	1.69	0.58
1:A:477:LEU:CD1	1:A:479:ILE:HG23	2.32	0.58
1:A:854:PRO:CG	1:A:855:PRO:CD	2.82	0.58
1:A:737:LEU:HD23	1:A:784:LYS:HG2	1.86	0.58
1:A:73:GLU:OE2	1:A:93:ARG:HD2	2.04	0.58
1:A:469:GLN:O	1:A:469:GLN:CG	2.53	0.57
1:A:757:PHE:CE2	1:A:762:GLN:HB2	2.39	0.57
1:A:744:ARG:O	1:A:799:ARG:HD2	2.03	0.57
1:A:53:ARG:HE	1:A:55:LEU:HD11	1.69	0.57
1:A:540:LEU:HD22	1:A:579:HIS:HD2	1.71	0.56
1:A:146:ASN:CG	2:A:1500:AOV:C8	2.73	0.56
1:A:458:ARG:HD3	1:A:461:ARG:NH1	2.21	0.56
1:A:583:GLN:HB3	1:A:595:SER:HB2	1.87	0.56
1:A:568:PHE:CE1	1:A:572:VAL:HG21	2.41	0.56
1:A:93:ARG:HG2	1:A:93:ARG:NH1	2.17	0.56
1:A:939:ALA:HB1	1:A:1009:PHE:CD2	2.40	0.55
1:A:560:PHE:HB3	1:A:563:ALA:HB2	1.88	0.55
1:A:619:ASN:ND2	1:A:622:VAL:HG23	2.17	0.55
1:A:928:TYR:O	1:A:932:LEU:HD13	2.07	0.55
1:A:983:LEU:O	1:A:987:LEU:HG	2.07	0.55
1:A:853:LYS:N	1:A:854:PRO:HD2	2.21	0.54
1:A:818:TRP:CH2	1:A:856:LYS:HG3	2.42	0.54
1:A:874:LEU:HD13	1:A:881:PRO:O	2.06	0.54
1:A:998:VAL:CB	1:A:999:PRO:HD3	2.17	0.54
1:A:94:ASP:OD1	1:A:95:GLN:N	2.41	0.54
1:A:579:HIS:ND1	1:A:580:PRO:HD2	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:ASN:OD1	2:A:1500:AOV:C5	2.56	0.53
1:A:146:ASN:HB2	1:A:202:ALA:O	2.09	0.53
1:A:990:LEU:CD1	1:A:991:THR:H	2.22	0.53
1:A:854:PRO:HD2	1:A:855:PRO:HD2	1.91	0.52
1:A:854:PRO:N	1:A:855:PRO:CD	2.72	0.52
1:A:709:PRO:O	1:A:713:LEU:HG	2.08	0.52
1:A:745:TYR:HB3	1:A:748:LEU:HD12	1.92	0.52
1:A:468:ARG:NH2	4:A:1602:HOH:O	2.42	0.52
1:A:500:GLU:HA	1:A:599:TYR:CD2	2.45	0.52
1:A:871:GLN:NE2	1:A:883:VAL:HG13	2.25	0.52
1:A:569:VAL:HG21	1:A:593:ASP:OD2	2.09	0.52
1:A:538:ILE:O	1:A:542:GLU:HG2	2.10	0.51
1:A:500:GLU:CD	1:A:599:TYR:HD2	2.14	0.51
1:A:644:ILE:CD1	1:A:644:ILE:N	2.73	0.51
1:A:597:LEU:HD21	4:A:2086:HOH:O	2.10	0.51
1:A:1007:THR:O	1:A:1010:ALA:HB3	2.11	0.51
1:A:645:VAL:HG12	1:A:646:GLY:N	2.26	0.51
1:A:458:ARG:CD	1:A:461:ARG:NH1	2.74	0.51
1:A:621:ASN:O	1:A:625:LEU:HG	2.11	0.51
1:A:182:TYR:O	1:A:186:LEU:HG	2.12	0.50
1:A:842:MET:HG3	1:A:911:LEU:HD22	1.94	0.50
1:A:500:GLU:CA	1:A:599:TYR:HE2	2.25	0.50
1:A:703:ARG:HH11	1:A:703:ARG:HG2	1.77	0.50
1:A:965:LEU:O	1:A:968:PHE:HD1	1.96	0.49
1:A:996:ASN:OD1	1:A:996:ASN:N	2.45	0.49
1:A:146:ASN:OD1	1:A:147:PRO:HD2	2.12	0.49
1:A:757:PHE:CE2	1:A:759:ASP:CB	2.64	0.49
1:A:952:GLY:O	1:A:953:ASP:CB	2.59	0.49
1:A:917:ARG:CZ	1:A:990:LEU:HB2	2.40	0.48
1:A:194:ILE:CD1	1:A:474:LEU:HD21	2.37	0.48
1:A:634:THR:O	1:A:637:ILE:HG12	2.14	0.48
1:A:208:THR:HG23	1:A:476:ILE:CG2	2.43	0.48
1:A:555:ASP:O	1:A:558:CYS:SG	2.67	0.47
1:A:146:ASN:OD1	2:A:1500:AOV:N9	2.46	0.47
1:A:637:ILE:HG13	1:A:638:TRP:CD1	2.50	0.47
1:A:208:THR:HG23	1:A:476:ILE:HG21	1.96	0.47
1:A:631:ASP:OD1	4:A:1601:HOH:O	2.20	0.47
1:A:917:ARG:HH22	1:A:990:LEU:CD2	2.20	0.47
1:A:118:GLU:HG2	1:A:722:LEU:CD1	2.43	0.47
1:A:270:PHE:O	1:A:470:GLY:N	2.38	0.47
1:A:998:VAL:CB	1:A:999:PRO:CD	2.91	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:598:HIS:CD2	1:A:603:VAL:HG23	2.35	0.47
1:A:637:ILE:HG13	1:A:638:TRP:N	2.29	0.47
1:A:853:LYS:N	1:A:854:PRO:CD	2.78	0.47
1:A:418:PRO:HB2	1:A:621:ASN:HD22	1.79	0.47
1:A:950:GLU:HB3	1:A:954:SER:OG	2.14	0.46
1:A:460:ASN:O	1:A:464:ASP:CB	2.60	0.46
1:A:757:PHE:HE2	1:A:759:ASP:CB	2.15	0.46
1:A:500:GLU:N	1:A:599:TYR:HE2	2.13	0.46
1:A:939:ALA:HB1	1:A:1009:PHE:CE2	2.51	0.46
1:A:703:ARG:HH11	1:A:703:ARG:CG	2.28	0.45
1:A:418:PRO:HB2	1:A:621:ASN:ND2	2.31	0.45
1:A:620:ASP:HB2	1:A:645:VAL:CG1	2.32	0.45
1:A:736:ILE:O	1:A:784:LYS:HB3	2.17	0.45
1:A:939:ALA:HB1	1:A:1009:PHE:HD2	1.81	0.45
1:A:867:TYR:O	1:A:871:GLN:HG2	2.17	0.44
1:A:93:ARG:CG	1:A:93:ARG:NH1	2.79	0.44
1:A:146:ASN:HD21	2:A:1500:AOV:C1'	2.29	0.44
1:A:418:PRO:CB	1:A:621:ASN:HD22	2.30	0.44
1:A:419:ARG:HG2	1:A:426:TYR:HB3	2.00	0.44
1:A:540:LEU:HB2	1:A:579:HIS:CD2	2.52	0.44
1:A:636:GLU:O	1:A:639:LYS:HG2	2.16	0.44
1:A:873:LYS:HD2	4:A:2122:HOH:O	2.17	0.43
1:A:383:GLU:HG3	1:A:390:THR:CG2	2.49	0.43
1:A:418:PRO:CB	1:A:621:ASN:ND2	2.81	0.43
1:A:224:GLY:O	1:A:232:GLY:HA3	2.19	0.43
1:A:932:LEU:N	1:A:932:LEU:HD12	2.33	0.43
1:A:1001:LEU:O	1:A:1005:LYS:HG3	2.19	0.43
1:A:995:TYR:HD1	1:A:995:TYR:HA	1.47	0.42
1:A:1004:ARG:O	1:A:1007:THR:OG1	2.35	0.42
1:A:928:TYR:OH	1:A:999:PRO:HG3	2.18	0.42
1:A:241:ALA:HB2	1:A:463:LEU:HD11	2.01	0.42
1:A:808:TYR:CE2	1:A:867:TYR:HB2	2.54	0.42
1:A:853:LYS:C	1:A:855:PRO:HD2	2.40	0.42
1:A:89:LEU:HD21	1:A:91:LEU:HD23	2.01	0.42
1:A:645:VAL:O	1:A:647:LEU:HG	2.19	0.42
1:A:758:MET:CG	1:A:758:MET:O	2.63	0.42
1:A:540:LEU:HD22	1:A:579:HIS:CD2	2.52	0.42
1:A:644:ILE:HD12	1:A:644:ILE:H	1.80	0.42
1:A:818:TRP:CZ3	1:A:856:LYS:HG3	2.55	0.42
1:A:990:LEU:HD12	1:A:991:THR:H	1.84	0.42
1:A:193:SER:HA	1:A:475:GLY:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:GLN:HB3	4:A:1891:HOH:O	2.20	0.41
1:A:942:LYS:NZ	1:A:965:LEU:CD2	2.78	0.41
1:A:320:LEU:HD22	4:A:2145:HOH:O	2.19	0.41
1:A:374:GLN:HE21	1:A:396:ALA:HB1	1.85	0.41
1:A:749:THR:HB	1:A:752:ALA:HB2	2.02	0.41
1:A:500:GLU:CA	1:A:599:TYR:CE2	2.94	0.41
1:A:759:ASP:C	1:A:759:ASP:OD1	2.58	0.41
1:A:768:ILE:HG21	1:A:778:TYR:CZ	2.56	0.41
1:A:992:GLU:O	1:A:994:ASN:OD1	2.39	0.40
1:A:995:TYR:O	1:A:998:VAL:HB	2.21	0.40
1:A:645:VAL:CG1	1:A:646:GLY:N	2.84	0.40
1:A:535:GLN:CG	1:A:536:PRO:CD	2.85	0.40
1:A:950:GLU:OE1	1:A:955:ILE:HD13	2.21	0.40
1:A:234:LEU:O	1:A:238:LEU:HB2	2.22	0.40
1:A:138:SER:HB2	1:A:725:ILE:CD1	2.49	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:GLU:O	1:A:387:ASP:N[3_544]	2.17	0.03

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	953/980 (97%)	920 (96%)	31 (3%)	2 (0%)	47 55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	546	ASN

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Mol	Chain	Res	Type
1	A	885	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	827/844 (98%)	820 (99%)	7 (1%)	81	88

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	ARG
1	A	546	ASN
1	A	703	ARG
1	A	917	ARG
1	A	994	ASN
1	A	996	ASN
1	A	1023	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	173	HIS
1	A	374	GLN
1	A	587	HIS
1	A	619	ASN
1	A	621	ASN
1	A	871	GLN
1	A	1012	GLN

5.3.3 RNA ⓘ

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$
2	AOV	A	1500	3	27,34,34	2.11	3 (11%)	26,56,56	2.13	8 (30%)

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
2	AOV	A	1500	3	-	1/12/39/39	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	AOV	O1G-VG	9.41	1.78	1.61
2	A	1500	AOV	C5-C4	2.48	1.47	1.40
2	A	1500	AOV	C2'-C1'	-2.23	1.50	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	AOV	C3'-C2'-C1'	4.93	108.40	100.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	AOV	C2'-C3'-C4'	-3.93	95.01	102.64
2	A	1500	AOV	C4-C5-N7	3.65	113.20	109.40
2	A	1500	AOV	N3-C2-N1	-3.65	122.98	128.68
2	A	1500	AOV	O2A-PA-O1A	3.06	127.39	112.24
2	A	1500	AOV	O3'-C3'-C4'	-2.96	102.48	111.05
2	A	1500	AOV	O4'-C4'-C3'	2.76	110.57	105.11
2	A	1500	AOV	C1'-N9-C4	-2.37	122.48	126.64

There are no chirality outliers.

All (1) torsion outliers are listed below:

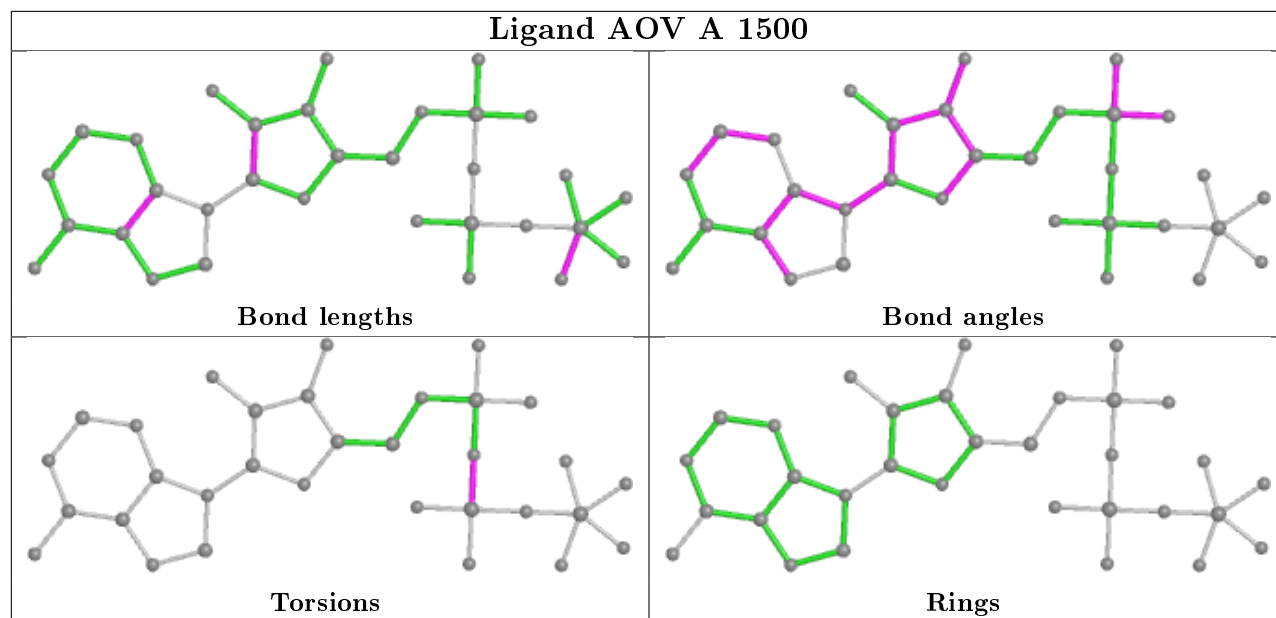
Mol	Chain	Res	Type	Atoms
2	A	1500	AOV	PA-O3A-PB-O2B

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1500	AOV	6	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	959/980 (97%)	0.69	135 (14%) 2 2	28, 55, 180, 215	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1013	TRP	10.3
1	A	945	TYR	7.9
1	A	1008	PHE	7.7
1	A	913	ILE	7.3
1	A	955	ILE	7.0
1	A	758	MET	6.8
1	A	337	SER	6.2
1	A	667	PHE	5.8
1	A	663	ARG	5.8
1	A	997	GLY	5.7
1	A	471	ALA	5.6
1	A	923	VAL	5.5
1	A	832	GLY	5.4
1	A	1002	THR	5.3
1	A	968	PHE	5.1
1	A	964	ASN	5.1
1	A	1011	GLN	5.1
1	A	949	ASN	5.0
1	A	757	PHE	4.9
1	A	1025	ASN	4.9
1	A	424	ARG	4.8
1	A	882	PHE	4.8
1	A	942	LYS	4.8
1	A	948	SER	4.7
1	A	423	GLY	4.7
1	A	1004	ARG	4.5
1	A	987	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	995	TYR	4.4
1	A	1001	LEU	4.3
1	A	645	VAL	4.2
1	A	880	GLU	4.2
1	A	991	THR	4.2
1	A	336	SER	3.9
1	A	229	GLY	3.9
1	A	875	ARG	3.8
1	A	999	PRO	3.8
1	A	664	ARG	3.8
1	A	425	ASP	3.7
1	A	969	ASP	3.7
1	A	422	VAL	3.7
1	A	986	ILE	3.6
1	A	916	LYS	3.5
1	A	893	ILE	3.5
1	A	224	GLY	3.5
1	A	470	GLY	3.5
1	A	755	LYS	3.4
1	A	932	LEU	3.4
1	A	1026	THR	3.4
1	A	1006	ASP	3.3
1	A	559	TRP	3.3
1	A	921	ILE	3.3
1	A	759	ASP	3.3
1	A	225	ARG	3.3
1	A	959	GLN	3.2
1	A	426	TYR	3.2
1	A	843	ASN	3.2
1	A	228	PRO	3.1
1	A	973	GLN	3.1
1	A	561	PRO	3.1
1	A	946	LEU	3.1
1	A	935	LEU	3.0
1	A	1024	LYS	3.0
1	A	950	GLU	3.0
1	A	828	SER	3.0
1	A	693	VAL	3.0
1	A	1010	ALA	3.0
1	A	1007	THR	3.0
1	A	971	GLU	2.9
1	A	464	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	890	PRO	2.9
1	A	1009	PHE	2.9
1	A	819	ILE	2.8
1	A	951	THR	2.8
1	A	197	THR	2.8
1	A	335	SER	2.7
1	A	546	ASN	2.7
1	A	984	LEU	2.7
1	A	994	ASN	2.7
1	A	851	THR	2.7
1	A	957	ALA	2.6
1	A	535	GLN	2.6
1	A	992	GLU	2.6
1	A	838	VAL	2.6
1	A	966	GLU	2.6
1	A	967	ALA	2.6
1	A	839	GLN	2.6
1	A	841	PHE	2.5
1	A	940	THR	2.5
1	A	818	TRP	2.5
1	A	886	ALA	2.5
1	A	334	PRO	2.5
1	A	198	GLY	2.5
1	A	925	LEU	2.5
1	A	562	LYS	2.4
1	A	972	CYS	2.4
1	A	980	ASN	2.4
1	A	911	LEU	2.4
1	A	881	PRO	2.4
1	A	495	ILE	2.4
1	A	452	PHE	2.4
1	A	73	GLU	2.3
1	A	756	GLY	2.3
1	A	866	ILE	2.3
1	A	989	GLN	2.3
1	A	141	PHE	2.3
1	A	479	ILE	2.3
1	A	943	SER	2.3
1	A	340	GLN	2.2
1	A	827	GLU	2.2
1	A	558	CYS	2.2
1	A	140	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	302	HIS	2.2
1	A	196	CYS	2.2
1	A	807	ASP	2.2
1	A	469	GLN	2.2
1	A	599	TYR	2.2
1	A	847	GLU	2.2
1	A	848	TYR	2.2
1	A	852	GLU	2.2
1	A	815	LEU	2.2
1	A	912	ARG	2.1
1	A	301	PHE	2.1
1	A	527	PHE	2.1
1	A	448	TYR	2.1
1	A	1014	THR	2.1
1	A	990	LEU	2.1
1	A	721	VAL	2.1
1	A	902	LYS	2.1
1	A	954	SER	2.1
1	A	899	ALA	2.1
1	A	339	GLY	2.0
1	A	223	LYS	2.0
1	A	644	ILE	2.0
1	A	863	LEU	2.0
1	A	812	ALA	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](#)

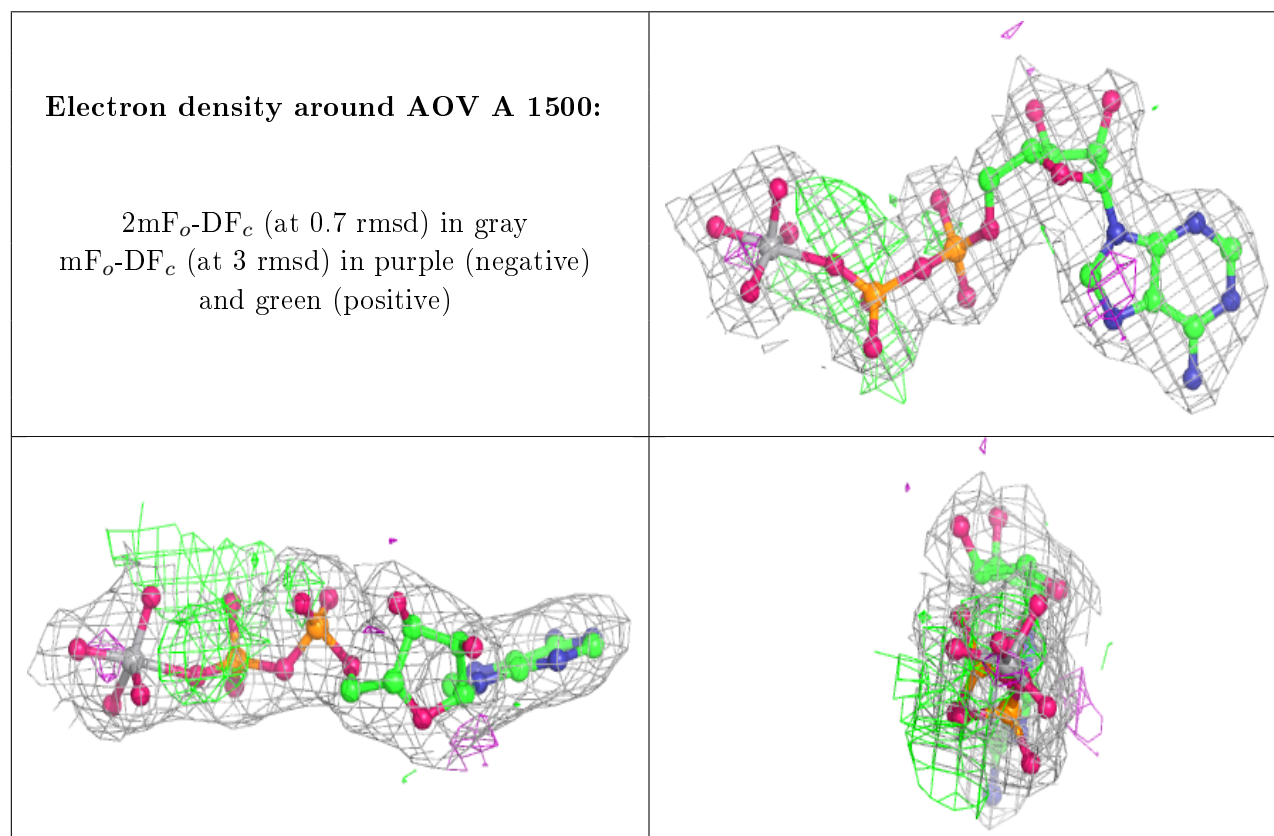
There are no carbohydrates in this entry.

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. 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(\AA^2)	Q<0.9
3	MG	A	1501	1/1	0.90	0.13	23,23,23,23	0
2	AOV	A	1500	32/32	0.96	0.15	29,36,40,43	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.