



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:50 AM UTC

PDB ID : 5I4E / pdb_00005i4e
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 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

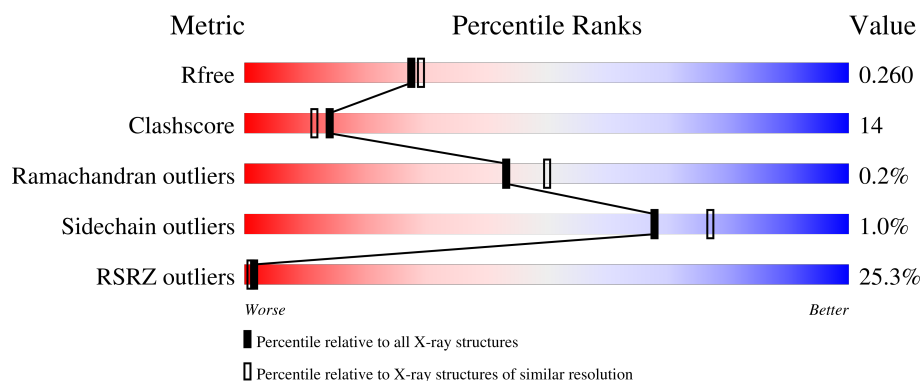
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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}	180053	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (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 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	980	25% 77% 19% ..

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.

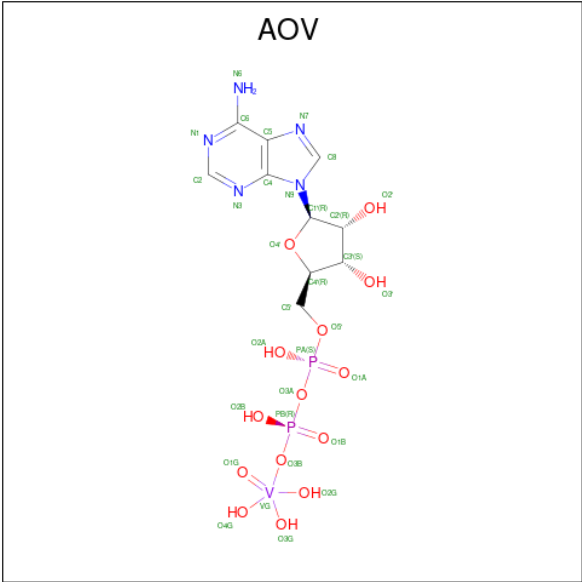
- Molecule 1 is a protein called Myosin-14,Alpha-actinin A.

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 (CCD ID: 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 (CCD ID: MG) (formula: Mg).

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

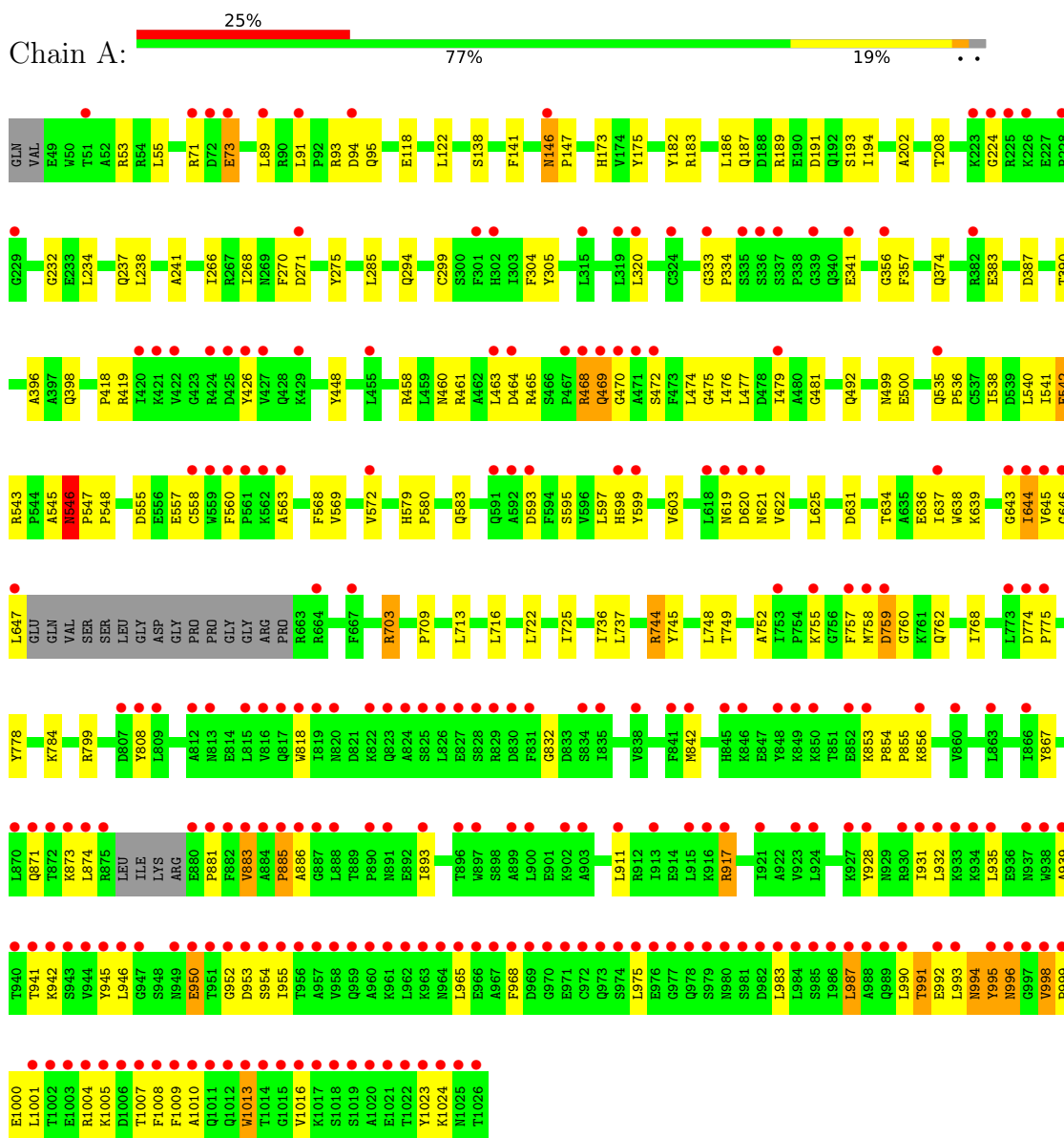
- Molecule 4 is water.

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

3 Residue-property plots

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-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) 99.6 (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 0.241 , 0.260	Depositor DCC
R_{free} test set	3792 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)	0.30 , 63.5	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: MG, AOV

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	0.93	4/7844 (0.1%)	1.37	51/10583 (0.5%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	266	ILE	C-O	-5.53	1.18	1.24
1	A	492	GLN	C-O	-5.28	1.17	1.24
1	A	268	ILE	C-O	-5.07	1.18	1.24
1	A	469	GLN	CA-C	-5.06	1.45	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	541	ILE	N-CA-C	9.92	119.85	110.53
1	A	333	GLY	CA-C-N	9.05	129.10	119.78
1	A	333	GLY	C-N-CA	9.05	129.10	119.78
1	A	950	GLU	N-CA-C	8.07	121.68	109.41
1	A	546	ASN	N-CA-C	-7.95	92.25	109.81
1	A	998	VAL	CA-C-N	7.46	126.98	118.85
1	A	998	VAL	C-N-CA	7.46	126.98	118.85
1	A	886	ALA	N-CA-C	7.41	120.80	108.73
1	A	546	ASN	CA-C-N	-7.39	112.77	120.38
1	A	546	ASN	C-N-CA	-7.39	112.77	120.38
1	A	285	LEU	N-CA-C	7.38	121.43	111.24
1	A	950	GLU	N-CA-CB	-7.22	99.94	111.43
1	A	146	ASN	CA-C-N	7.17	126.67	118.85
1	A	146	ASN	C-N-CA	7.17	126.67	118.85
1	A	356	GLY	N-CA-C	7.17	122.36	114.40
1	A	468	ARG	N-CA-C	-7.04	101.81	110.61
1	A	357	PHE	N-CA-C	6.91	120.40	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	987	LEU	O-C-N	6.71	129.23	122.12
1	A	759	ASP	N-CA-C	6.61	119.17	108.32
1	A	991	THR	N-CA-C	6.59	119.89	108.76
1	A	995	TYR	CB-CA-C	6.16	120.44	110.96
1	A	542	GLU	N-CA-C	6.12	120.90	113.38
1	A	744	ARG	N-CA-C	6.08	117.99	111.36
1	A	237	GLN	CA-C-N	6.03	128.64	120.38
1	A	237	GLN	C-N-CA	6.03	128.64	120.38
1	A	759	ASP	CB-CA-C	-5.92	99.88	109.89
1	A	832	GLY	N-CA-C	5.86	122.76	114.85
1	A	543	ARG	CA-C-N	5.75	125.12	118.85
1	A	543	ARG	C-N-CA	5.75	125.12	118.85
1	A	469	GLN	N-CA-C	-5.62	101.59	109.96
1	A	643	GLY	N-CA-C	5.61	121.72	112.30
1	A	885	PRO	CA-N-CD	5.58	119.81	112.00
1	A	755	LYS	CB-CA-C	-5.51	110.20	116.54
1	A	71	ARG	N-CA-C	5.44	117.02	111.14
1	A	545	ALA	N-CA-C	5.44	115.58	108.07
1	A	716	LEU	CA-C-N	5.37	127.93	120.63
1	A	716	LEU	C-N-CA	5.37	127.93	120.63
1	A	304	PHE	CA-C-N	5.36	127.73	120.44
1	A	304	PHE	C-N-CA	5.36	127.73	120.44
1	A	1024	LYS	CB-CA-C	-5.28	110.05	117.23
1	A	73	GLU	N-CA-C	5.26	117.64	108.76
1	A	1013	TRP	N-CA-C	-5.26	105.20	111.03
1	A	448	TYR	CA-C-N	5.25	127.63	120.54
1	A	448	TYR	C-N-CA	5.25	127.63	120.54
1	A	398	GLN	N-CA-C	-5.16	105.57	111.14
1	A	941	THR	N-CA-C	-5.14	106.52	112.89
1	A	481	GLY	N-CA-C	5.13	119.11	112.54
1	A	946	LEU	N-CA-C	5.12	116.86	111.28
1	A	398	GLN	CA-C-N	5.09	127.05	120.44
1	A	398	GLN	C-N-CA	5.09	127.05	120.44
1	A	893	ILE	N-CA-C	-5.02	105.65	110.72

There are no chirality outliers.

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	7697	0	7667	221	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	221	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 (221) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HH11	1:A:93:ARG:HG2	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:HZ	1:A:762:GLN:HB3	1.55	0.70
1:A:757:PHE:CZ	1:A:762:GLN:HB3	2.27	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: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:89:LEU:CD2	1:A:91:LEU:HD23	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:871:GLN:HE22	1:A:883:VAL:HG13	1.62	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
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:138:SER:HB2	1:A:725:ILE:HD11	1.81	0.61
1:A:468:ARG:HG3	1:A:468:ARG:O	2.00	0.61
1:A:952:GLY:O	1:A:953:ASP:HB3	2.00	0.61
1:A:146:ASN:CG	2:A:1500:AOV:C8	2.73	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:942:LYS:HZ3	1:A:965:LEU:HD23	1.67	0.58
1:A:73:GLU:OE2	1:A:93:ARG:HD2	2.04	0.58
1:A:737:LEU:HD23	1:A:784:LYS:HG2	1.86	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: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:500:GLU:CD	1:A:599:TYR:HD2	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:818:TRP:CH2	1:A:856:LYS:HG3	2.42	0.54
1:A:853:LYS:N	1:A:854:PRO:HD2	2.21	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
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:N	1:A:855:PRO:CD	2.72	0.52
1:A:854:PRO:HD2	1:A:855:PRO:HD2	1.91	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:942:LYS:HZ1	1:A:965:LEU:HD23	1.75	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:644:ILE:N	1:A:644:ILE:CD1	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: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:HG2	1:A:703:ARG:HH11	1.77	0.50
1:A:645:VAL:HG12	1:A:646:GLY:N	2.26	0.49
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:942:LYS:HZ3	1:A:965:LEU:CD2	2.26	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:853:LYS:C	1:A:855:PRO:HD2	2.40	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
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:759:ASP:OD1	1:A:759:ASP:C	2.58	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:NH1	1:A:93:ARG:CG	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:TYR:HD1	1:A:995:TYR:HA	1.47	0.42
1:A:928:TYR:OH	1:A:999:PRO:HG3	2.18	0.42
1:A:1004:ARG:O	1:A:1007:THR:OG1	2.35	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: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:O	1:A:758:MET:CG	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
1:A:294:GLN:HG2	1:A:299:CYS:C	2.45	0.41
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:993:LEU:C	1:A:995:TYR:N	2.77	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: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:995:TYR:O	1:A:996:ASN:C	2.62	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%)	43	50

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	546	ASN
1	A	885	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	827/844 (98%)	819 (99%)	8 (1%)	68	77

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	465	ARG
1	A	644	ILE
1	A	703	ARG
1	A	883	VAL
1	A	917	ARG
1	A	994	ASN
1	A	996	ASN
1	A	1023	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	173	HIS
1	A	340	GLN
1	A	359	HIS
1	A	374	GLN
1	A	398	GLN
1	A	508	HIS
1	A	587	HIS
1	A	621	ASN
1	A	845	HIS
1	A	980	ASN

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
2	AOV	A	1500	3	32,34,34	2.28	5 (15%)	42,56,56	2.96	16 (38%)

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	-	1/16/39/39	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	AOV	O1G-VG	9.55	1.78	1.61
2	A	1500	AOV	C5-C4	4.72	1.47	1.39
2	A	1500	AOV	PB-O3A	3.78	1.63	1.59
2	A	1500	AOV	C5-C6	2.84	1.48	1.41
2	A	1500	AOV	C8-N7	2.81	1.37	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	AOV	N3-C4-N9	8.96	142.41	127.17
2	A	1500	AOV	C4-N9-C8	6.81	112.89	105.74
2	A	1500	AOV	C5-C4-N3	-6.75	117.42	126.72
2	A	1500	AOV	C5-C4-N9	-5.18	100.17	105.81
2	A	1500	AOV	O4'-C1'-N9	4.98	117.65	108.09
2	A	1500	AOV	C2-N3-C4	4.78	123.49	111.83
2	A	1500	AOV	C2'-C3'-C4'	-3.93	95.01	102.61
2	A	1500	AOV	N3-C2-N1	-3.70	122.98	128.58
2	A	1500	AOV	C3'-C2'-C1'	3.67	108.40	101.46
2	A	1500	AOV	O2A-PA-O1A	3.21	127.39	112.44
2	A	1500	AOV	O3'-C3'-C4'	-3.00	102.48	111.08
2	A	1500	AOV	O4'-C4'-C3'	2.73	110.57	105.15
2	A	1500	AOV	O3A-PA-O1A	-2.63	102.80	110.70
2	A	1500	AOV	C2'-C1'-N9	-2.45	107.22	113.30
2	A	1500	AOV	N9-C8-N7	-2.31	110.66	113.94
2	A	1500	AOV	C4-C5-N7	2.29	113.20	110.58

There are no chirality outliers.

All (1) torsion outliers are listed below:

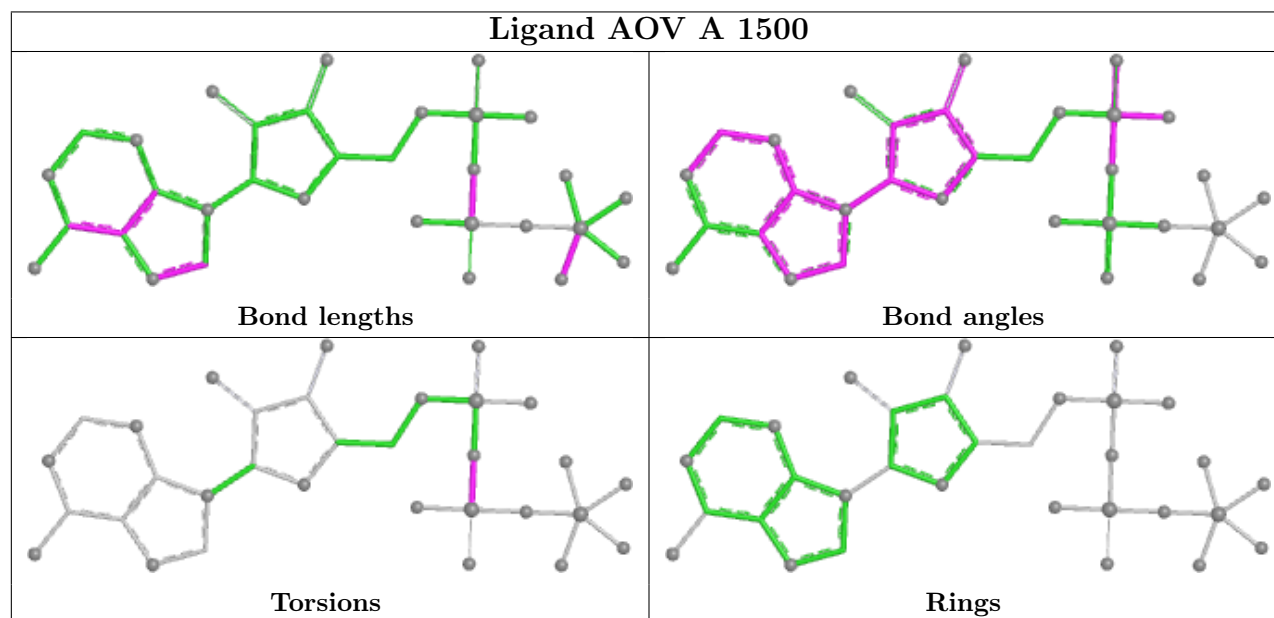
Mol	Chain	Res	Type	Atoms
2	A	1500	AOV	PA-O3A-PB-O2B

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%)	1.22	243 (25%) 1 1	28, 55, 180, 215	0

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1013	TRP	8.0
1	A	647	LEU	7.0
1	A	971	GLU	6.6
1	A	1002	THR	6.3
1	A	942	LYS	6.1
1	A	935	LEU	6.1
1	A	819	ILE	6.0
1	A	471	ALA	5.7
1	A	464	ASP	5.6
1	A	913	ILE	5.6
1	A	938	TRP	5.5
1	A	826	LEU	5.5
1	A	959	GLN	5.4
1	A	1009	PHE	5.3
1	A	962	LEU	5.3
1	A	1016	VAL	5.3
1	A	967	ALA	5.2
1	A	831	PHE	5.1
1	A	224	GLY	5.1
1	A	1006	ASP	5.1
1	A	958	VAL	5.1
1	A	955	ILE	5.0
1	A	931	ILE	5.0
1	A	945	TYR	5.0
1	A	883	VAL	5.0
1	A	957	ALA	4.8
1	A	558	CYS	4.8

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Mol	Chain	Res	Type	RSRZ
1	A	644	ILE	4.8
1	A	470	GLY	4.7
1	A	944	VAL	4.6
1	A	667	PHE	4.6
1	A	1022	THR	4.6
1	A	934	LYS	4.6
1	A	226	LYS	4.5
1	A	1014	THR	4.5
1	A	923	VAL	4.4
1	A	968	PHE	4.4
1	A	964	ASN	4.4
1	A	970	GLY	4.3
1	A	956	THR	4.3
1	A	822	LYS	4.3
1	A	1010	ALA	4.3
1	A	932	LEU	4.3
1	A	818	TRP	4.3
1	A	998	VAL	4.2
1	A	951	THR	4.2
1	A	984	LEU	4.2
1	A	1020	ALA	4.2
1	A	757	PHE	4.2
1	A	1017	LYS	4.1
1	A	975	LEU	4.1
1	A	73	GLU	4.1
1	A	816	VAL	4.1
1	A	972	CYS	4.0
1	A	886	ALA	4.0
1	A	559	TRP	4.0
1	A	645	VAL	4.0
1	A	983	LEU	4.0
1	A	993	LEU	4.0
1	A	882	PHE	4.0
1	A	835	ILE	3.9
1	A	888	LEU	3.9
1	A	646	GLY	3.9
1	A	960	ALA	3.9
1	A	985	SER	3.8
1	A	535	GLN	3.8
1	A	223	LYS	3.8
1	A	987	LEU	3.8
1	A	979	SER	3.8

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Mol	Chain	Res	Type	RSRZ
1	A	881	PRO	3.8
1	A	643	GLY	3.8
1	A	977	GLY	3.7
1	A	427	VAL	3.7
1	A	965	LEU	3.7
1	A	846	LYS	3.7
1	A	880	GLU	3.6
1	A	621	ASN	3.6
1	A	1024	LYS	3.6
1	A	874	LEU	3.6
1	A	969	ASP	3.6
1	A	228	PRO	3.6
1	A	824	ALA	3.6
1	A	838	VAL	3.6
1	A	1008	PHE	3.5
1	A	225	ARG	3.5
1	A	875	ARG	3.5
1	A	848	TYR	3.5
1	A	820	ASN	3.5
1	A	988	ALA	3.5
1	A	758	MET	3.5
1	A	426	TYR	3.5
1	A	812	ALA	3.5
1	A	893	ILE	3.5
1	A	146	ASN	3.5
1	A	953	ASP	3.5
1	A	980	ASN	3.5
1	A	829	ARG	3.4
1	A	885	PRO	3.4
1	A	989	GLN	3.4
1	A	999	PRO	3.4
1	A	963	LYS	3.3
1	A	986	ILE	3.3
1	A	320	LEU	3.3
1	A	562	LYS	3.3
1	A	823	GLN	3.3
1	A	939	ALA	3.3
1	A	952	GLY	3.3
1	A	897	TRP	3.2
1	A	941	THR	3.2
1	A	1005	LYS	3.2
1	A	72	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	973	GLN	3.2
1	A	1007	THR	3.2
1	A	335	SER	3.1
1	A	356	GLY	3.1
1	A	982	ASP	3.1
1	A	469	GLN	3.1
1	A	815	LEU	3.1
1	A	890	PRO	3.1
1	A	992	GLU	3.1
1	A	572	VAL	3.1
1	A	463	LEU	3.1
1	A	940	THR	3.1
1	A	825	SER	3.1
1	A	887	GLY	3.1
1	A	902	LYS	3.1
1	A	1004	ARG	3.0
1	A	1021	GLU	3.0
1	A	834	SER	3.0
1	A	995	TYR	2.9
1	A	324	CYS	2.9
1	A	339	GLY	2.9
1	A	774	ASP	2.9
1	A	637	ILE	2.9
1	A	229	GLY	2.9
1	A	808	TYR	2.9
1	A	899	ALA	2.9
1	A	974	SER	2.8
1	A	981	SER	2.8
1	A	978	GLN	2.8
1	A	841	PHE	2.8
1	A	1026	THR	2.8
1	A	930	ARG	2.8
1	A	863	LEU	2.8
1	A	71	ARG	2.8
1	A	1023	TYR	2.8
1	A	1025	ASN	2.7
1	A	337	SER	2.7
1	A	773	LEU	2.7
1	A	591	GLN	2.7
1	A	620	ASP	2.7
1	A	828	SER	2.7
1	A	976	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	961	LYS	2.7
1	A	990	LEU	2.7
1	A	1001	LEU	2.7
1	A	301	PHE	2.7
1	A	860	VAL	2.7
1	A	619	ASN	2.7
1	A	333	GLY	2.7
1	A	947	GLY	2.7
1	A	997	GLY	2.7
1	A	341	GLU	2.7
1	A	472	SER	2.7
1	A	946	LEU	2.7
1	A	884	ALA	2.6
1	A	916	LYS	2.6
1	A	382	ARG	2.6
1	A	455	LEU	2.6
1	A	873	LYS	2.6
1	A	842	MET	2.6
1	A	852	GLU	2.6
1	A	561	PRO	2.6
1	A	809	LEU	2.6
1	A	1003	GLU	2.6
1	A	420	ILE	2.6
1	A	845	HIS	2.6
1	A	900	LEU	2.5
1	A	759	ASP	2.5
1	A	807	ASP	2.5
1	A	1015	GLY	2.5
1	A	1011	GLN	2.5
1	A	479	ILE	2.5
1	A	599	TYR	2.5
1	A	563	ALA	2.5
1	A	996	ASN	2.5
1	A	422	VAL	2.5
1	A	424	ARG	2.5
1	A	468	ARG	2.5
1	A	924	LEU	2.5
1	A	849	LYS	2.5
1	A	921	ILE	2.4
1	A	315	LEU	2.4
1	A	319	LEU	2.4
1	A	853	LYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	856	LYS	2.4
1	A	830	ASP	2.4
1	A	827	GLU	2.4
1	A	950	GLU	2.4
1	A	1019	SER	2.4
1	A	89	LEU	2.4
1	A	949	ASN	2.4
1	A	1018	SER	2.4
1	A	911	LEU	2.4
1	A	755	LYS	2.3
1	A	891	ASN	2.3
1	A	421	LYS	2.3
1	A	429	LYS	2.3
1	A	336	SER	2.3
1	A	937	ASN	2.3
1	A	817	GLN	2.3
1	A	94	ASP	2.2
1	A	850	LYS	2.2
1	A	903	ALA	2.2
1	A	425	ASP	2.2
1	A	813	ASN	2.2
1	A	933	LYS	2.2
1	A	51	THR	2.2
1	A	664	ARG	2.1
1	A	618	LEU	2.1
1	A	775	PRO	2.1
1	A	598	HIS	2.1
1	A	592	ALA	2.1
1	A	872	THR	2.1
1	A	896	THR	2.1
1	A	593	ASP	2.1
1	A	943	SER	2.1
1	A	954	SER	2.1
1	A	870	LEU	2.1
1	A	271	ASP	2.1
1	A	302	HIS	2.1
1	A	966	GLU	2.1
1	A	1012	GLN	2.1
1	A	928	TYR	2.1
1	A	917	ARG	2.1
1	A	927	LYS	2.0
1	A	91	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	467	PRO	2.0
1	A	560	PHE	2.0
1	A	871	GLN	2.0
1	A	915	LEU	2.0
1	A	753	ILE	2.0
1	A	866	ILE	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](#)

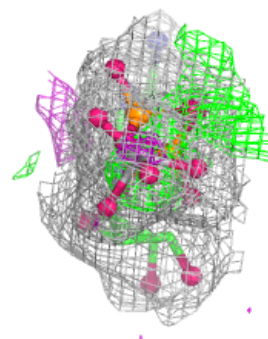
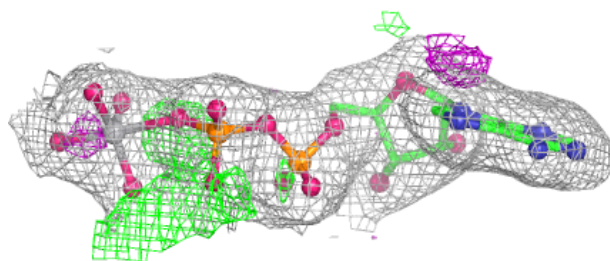
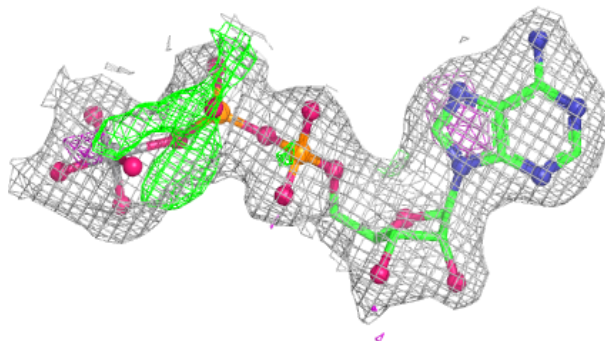
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
3	MG	A	1501	1/1	0.94	0.05	23,23,23,23	0
2	AOV	A	1500	32/32	0.97	0.07	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.

Electron density around AOV A 1500:

$2mF_o-DF_c$ (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.