



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:48 AM UTC

PDB ID : 4RWT / pdb_00004rwt
Title : Structure of actin-Lmod complex
Authors : Chen, X.; Ni, F.; Wang, Q.
Deposited on : 2014-12-05
Resolution : 2.98 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

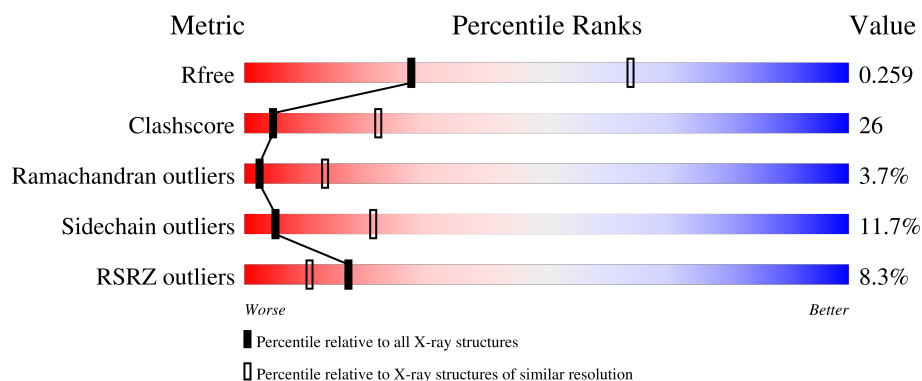
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	384	3% 56% 34% 6% . .
1	B	384	2% 58% 33% 5% . .
2	C	506	2% 16% 13% . . 67%
2	D	506	15% 23% 25% 6% . 45%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9317 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 Actin-5C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	369	Total	C	N	O	S	0	0	0
			2873	1817	485	550	21			
1	B	369	Total	C	N	O	S	0	0	0
			2871	1815	485	550	21			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	291	GLU	LYS	engineered mutation	UNP P10987
A	322	LYS	PRO	engineered mutation	UNP P10987
A	376	ALA	-	expression tag	UNP P10987
A	377	SER	-	expression tag	UNP P10987
A	378	HIS	-	expression tag	UNP P10987
A	379	HIS	-	expression tag	UNP P10987
A	380	HIS	-	expression tag	UNP P10987
A	381	HIS	-	expression tag	UNP P10987
A	382	HIS	-	expression tag	UNP P10987
A	383	HIS	-	expression tag	UNP P10987
B	291	GLU	LYS	engineered mutation	UNP P10987
B	322	LYS	PRO	engineered mutation	UNP P10987
B	376	ALA	-	expression tag	UNP P10987
B	377	SER	-	expression tag	UNP P10987
B	378	HIS	-	expression tag	UNP P10987
B	379	HIS	-	expression tag	UNP P10987
B	380	HIS	-	expression tag	UNP P10987
B	381	HIS	-	expression tag	UNP P10987
B	382	HIS	-	expression tag	UNP P10987
B	383	HIS	-	expression tag	UNP P10987

- Molecule 2 is a protein called Leiomodin-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	168	Total 1338	C 829	N 242	O 259	S 8	0	0	0
2	D	280	Total 2171	C 1340	N 398	O 423	S 10	0	0	0

There are 142 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	expression tag	UNP Q6P5Q4
C	-9	ALA	-	expression tag	UNP Q6P5Q4
C	-8	HIS	-	expression tag	UNP Q6P5Q4
C	-7	HIS	-	expression tag	UNP Q6P5Q4
C	-6	HIS	-	expression tag	UNP Q6P5Q4
C	-5	HIS	-	expression tag	UNP Q6P5Q4
C	-4	HIS	-	expression tag	UNP Q6P5Q4
C	-3	HIS	-	expression tag	UNP Q6P5Q4
C	-2	VAL	-	expression tag	UNP Q6P5Q4
C	-1	GLY	-	expression tag	UNP Q6P5Q4
C	0	THR	-	expression tag	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	SER	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	LEU	deletion	UNP Q6P5Q4
C	?	-	ILE	deletion	UNP Q6P5Q4
C	?	-	PHE	deletion	UNP Q6P5Q4
C	?	-	THR	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	SER	deletion	UNP Q6P5Q4
C	?	-	ASN	deletion	UNP Q6P5Q4
C	?	-	SER	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	VAL	deletion	UNP Q6P5Q4
C	?	-	SER	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	VAL	deletion	UNP Q6P5Q4
C	?	-	TYR	deletion	UNP Q6P5Q4
C	?	-	THR	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4

Continued on next page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	SER	deletion	UNP Q6P5Q4
C	?	-	GLN	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	GLU	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	SER	deletion	UNP Q6P5Q4
C	?	-	SER	deletion	UNP Q6P5Q4
C	?	-	GLN	deletion	UNP Q6P5Q4
C	?	-	ARG	deletion	UNP Q6P5Q4
C	?	-	LEU	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	?	-	PRO	deletion	UNP Q6P5Q4
C	426	GLY	LYS	engineered mutation	UNP Q6P5Q4
C	427	SER	LYS	engineered mutation	UNP Q6P5Q4
C	428	GLY	LYS	engineered mutation	UNP Q6P5Q4
C	429	SER	LYS	engineered mutation	UNP Q6P5Q4
C	431	GLY	LYS	engineered mutation	UNP Q6P5Q4
C	432	SER	LYS	engineered mutation	UNP Q6P5Q4
C	434	GLY	LYS	engineered mutation	UNP Q6P5Q4
C	435	SER	LYS	engineered mutation	UNP Q6P5Q4
D	-10	MET	-	expression tag	UNP Q6P5Q4
D	-9	ALA	-	expression tag	UNP Q6P5Q4
D	-8	HIS	-	expression tag	UNP Q6P5Q4
D	-7	HIS	-	expression tag	UNP Q6P5Q4
D	-6	HIS	-	expression tag	UNP Q6P5Q4
D	-5	HIS	-	expression tag	UNP Q6P5Q4



Continued from previous page...

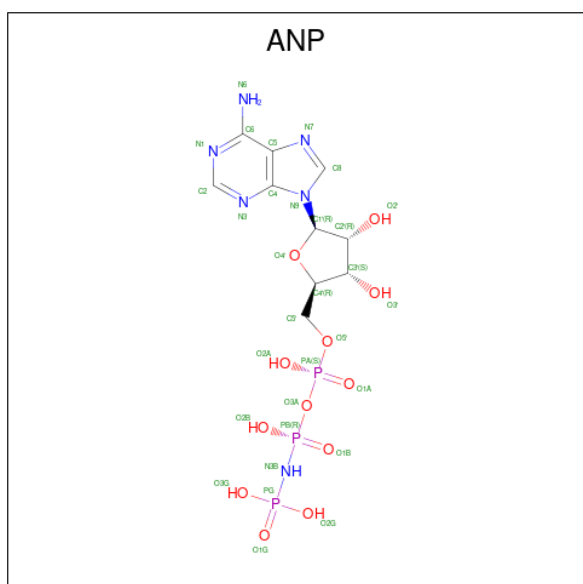
Chain	Residue	Modelled	Actual	Comment	Reference
D	-4	HIS	-	expression tag	UNP Q6P5Q4
D	-3	HIS	-	expression tag	UNP Q6P5Q4
D	-2	VAL	-	expression tag	UNP Q6P5Q4
D	-1	GLY	-	expression tag	UNP Q6P5Q4
D	0	THR	-	expression tag	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	SER	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	LEU	deletion	UNP Q6P5Q4
D	?	-	ILE	deletion	UNP Q6P5Q4
D	?	-	PHE	deletion	UNP Q6P5Q4
D	?	-	THR	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	SER	deletion	UNP Q6P5Q4
D	?	-	ASN	deletion	UNP Q6P5Q4
D	?	-	SER	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	VAL	deletion	UNP Q6P5Q4
D	?	-	SER	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	VAL	deletion	UNP Q6P5Q4
D	?	-	TYR	deletion	UNP Q6P5Q4
D	?	-	THR	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	SER	deletion	UNP Q6P5Q4
D	?	-	GLN	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	GLU	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	SER	deletion	UNP Q6P5Q4
D	?	-	SER	deletion	UNP Q6P5Q4
D	?	-	GLN	deletion	UNP Q6P5Q4
D	?	-	ARG	deletion	UNP Q6P5Q4
D	?	-	LEU	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	?	-	PRO	deletion	UNP Q6P5Q4
D	426	GLY	LYS	engineered mutation	UNP Q6P5Q4
D	427	SER	LYS	engineered mutation	UNP Q6P5Q4
D	428	GLY	LYS	engineered mutation	UNP Q6P5Q4
D	429	SER	LYS	engineered mutation	UNP Q6P5Q4
D	431	GLY	LYS	engineered mutation	UNP Q6P5Q4
D	432	SER	LYS	engineered mutation	UNP Q6P5Q4
D	434	GLY	LYS	engineered mutation	UNP Q6P5Q4
D	435	SER	LYS	engineered mutation	UNP Q6P5Q4

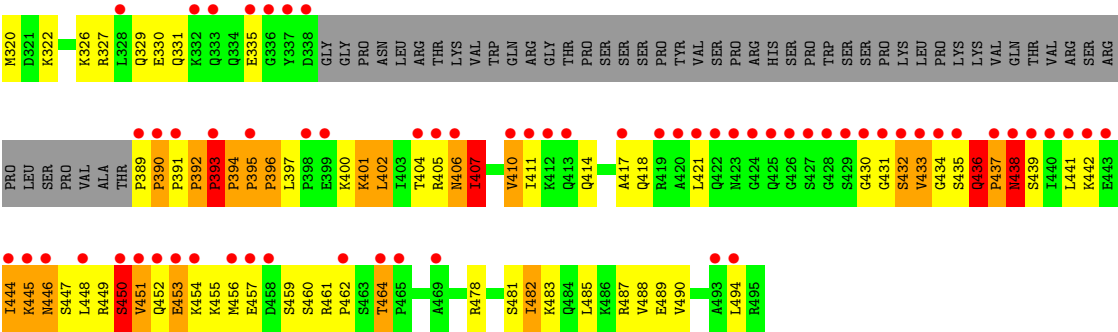
- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	65.35Å 65.65Å 81.92Å 101.29° 90.94° 107.97°	Depositor
Resolution (Å)	51.07 – 2.98 51.07 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.5 (51.07-2.98) 97.4 (51.07-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.77 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.248 , 0.257 0.249 , 0.259	Depositor DCC
R_{free} test set	1288 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	54.0	Xtriage
Anisotropy	0.157	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.2	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	0.89	EDS
Total number of atoms	9317	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 16.29% 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, ANP

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	0.59	1/2934 (0.0%)	0.96	12/3973 (0.3%)
1	B	0.62	1/2932 (0.0%)	0.95	11/3970 (0.3%)
2	C	0.56	0/1352	0.88	2/1823 (0.1%)
2	D	0.75	1/2199 (0.0%)	1.06	12/2966 (0.4%)
All	All	0.64	3/9417 (0.0%)	0.97	37/12732 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	MET	C-O	-6.77	1.15	1.24
2	D	430	GLY	C-O	6.11	1.29	1.23
1	A	47	MET	C-O	-5.10	1.15	1.23

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	389	PRO	CA-C-N	12.80	133.56	120.38
2	D	389	PRO	C-N-CA	12.80	133.56	120.38
2	D	394	PRO	N-CA-C	7.39	119.72	110.70
1	A	44	MET	CA-C-N	-7.00	109.36	121.97
1	A	44	MET	C-N-CA	-7.00	109.36	121.97
1	B	47	MET	N-CA-C	6.93	120.97	112.23
1	A	39	ARG	CA-C-N	-6.67	111.45	122.39
1	A	39	ARG	C-N-CA	-6.67	111.45	122.39
2	D	407	ILE	N-CA-C	-6.63	106.33	112.43
1	A	44	MET	N-CA-C	6.52	124.69	110.80
2	D	436	GLN	CA-C-N	-6.39	111.85	119.84
2	D	436	GLN	C-N-CA	-6.39	111.85	119.84
1	B	44	MET	CA-C-N	-6.33	110.58	121.97
1	B	44	MET	C-N-CA	-6.33	110.58	121.97

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	46	GLY	N-CA-C	-6.05	105.03	112.77
1	B	43	VAL	CA-C-N	-6.04	110.00	121.54
1	B	43	VAL	C-N-CA	-6.04	110.00	121.54
2	C	305	LEU	CA-C-N	6.03	125.58	119.19
2	C	305	LEU	C-N-CA	6.03	125.58	119.19
1	A	42	GLY	CA-C-N	-5.90	113.01	120.56
1	A	42	GLY	C-N-CA	-5.90	113.01	120.56
2	D	393	PRO	N-CA-C	5.78	117.75	110.70
1	A	332	PRO	CA-C-N	5.61	125.28	119.56
1	A	332	PRO	C-N-CA	5.61	125.28	119.56
1	B	47	MET	CA-C-N	-5.58	116.07	121.31
1	B	47	MET	C-N-CA	-5.58	116.07	121.31
2	D	392	PRO	CA-C-N	5.51	126.06	120.38
2	D	392	PRO	C-N-CA	5.51	126.06	120.38
2	D	402	LEU	N-CA-C	5.39	117.19	108.41
1	A	97	ALA	CA-C-N	5.26	124.97	119.82
1	A	97	ALA	C-N-CA	5.26	124.97	119.82
1	A	163	VAL	N-CA-C	5.20	113.30	108.15
1	B	332	PRO	CA-C-N	5.17	126.31	119.84
1	B	332	PRO	C-N-CA	5.17	126.31	119.84
2	D	451	VAL	N-CA-C	5.13	115.08	108.82
2	D	450	SER	N-CA-C	5.08	121.61	110.80
1	B	323	SER	N-CA-C	5.00	117.38	111.33

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	2873	0	2842	128	2
1	B	2871	0	2834	140	0
2	C	1338	0	1364	93	0
2	D	2171	0	2190	207	2
3	A	31	0	13	2	0
3	B	31	0	13	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	9317	0	9256	478	2

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 26.

All (478) 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:44:MET:O	1:A:46:GLY:N	1.76	1.19
1:A:121:GLN:NE2	2:D:320:MET:HB3	1.59	1.18
2:D:390:PRO:HB2	2:D:391:PRO:CD	1.77	1.14
2:C:187:ASN:HD22	1:B:49:GLN:HA	0.93	1.08
2:C:193:THR:HB	2:C:196:THR:HB	1.11	1.07
2:C:187:ASN:ND2	1:B:49:GLN:HA	1.70	1.06
1:A:44:MET:O	1:A:45:VAL:C	2.00	1.03
1:A:125:GLU:OE2	2:D:327:ARG:NH2	1.91	1.01
2:C:310:MET:HB3	2:D:448:LEU:HB2	1.37	1.01
1:A:196:ARG:HG2	1:A:196:ARG:HH11	1.18	1.01
1:A:351:THR:HB	2:D:411:ILE:CG2	1.93	0.99
2:D:448:LEU:HD21	2:D:452:GLN:HB2	1.43	0.99
2:C:187:ASN:HD22	1:B:49:GLN:CA	1.76	0.98
2:D:257:MET:HE1	2:D:290:LEU:HD11	1.45	0.98
1:A:345:ILE:HG22	2:D:402:LEU:HD13	1.43	0.97
2:D:435:SER:C	2:D:437:PRO:HD3	1.90	0.96
2:D:390:PRO:HB2	2:D:391:PRO:HD3	1.46	0.96
1:B:44:MET:HB3	1:B:64:ILE:HD12	1.46	0.96
1:A:60:SER:HB2	2:D:390:PRO:HD2	1.46	0.95
2:D:299:LEU:HD22	2:D:312:MET:HE2	1.48	0.95
1:A:38:PRO:HB3	1:A:43:VAL:HG11	1.44	0.95
1:B:43:VAL:HG23	1:B:43:VAL:O	1.64	0.95
1:B:227:MET:HE1	1:B:256:ARG:HD2	1.47	0.95
2:D:435:SER:HA	1:B:270:GLU:HG2	1.46	0.95
2:D:434:GLY:HA2	1:B:271:ALA:HB2	1.49	0.94
2:C:278:MET:HE2	2:C:278:MET:HA	1.50	0.93
1:B:39:ARG:O	1:B:40:HIS:HB2	1.70	0.91
1:A:121:GLN:HE22	2:D:320:MET:HB3	1.20	0.91
2:C:311:SER:OG	2:D:452:GLN:HG3	1.74	0.87
2:C:193:THR:CB	2:C:196:THR:HB	2.02	0.87
2:D:218:THR:O	2:D:220:ALA:N	2.07	0.86

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:THR:HB	2:D:411:ILE:HG21	1.58	0.86
2:D:261:GLN:NE2	2:D:292:GLU:OE1	2.09	0.85
2:D:433:VAL:O	1:B:270:GLU:HG3	1.76	0.84
2:C:309:ARG:O	2:C:313:THR:HG22	1.77	0.84
2:C:310:MET:HG2	2:D:448:LEU:H	1.42	0.84
2:D:250:GLY:HA3	2:D:282:VAL:HG11	1.59	0.84
2:D:257:MET:HE1	2:D:290:LEU:CD1	2.10	0.81
2:D:457:GLU:HG2	1:B:113:LYS:HZ2	1.46	0.81
2:C:202:GLU:HA	2:C:205:LYS:HB2	1.63	0.80
2:C:192:ILE:O	2:C:193:THR:OG1	1.99	0.80
2:D:243:VAL:CG1	2:D:243:VAL:O	2.31	0.79
2:D:264:THR:HA	2:D:295:THR:HG21	1.65	0.79
1:A:227:MET:HE1	1:A:256:ARG:HD2	1.64	0.79
2:D:294:THR:CG2	2:D:322:LYS:HD2	2.14	0.78
1:B:191:LYS:O	1:B:195:GLU:HG2	1.84	0.78
2:D:457:GLU:HB2	1:B:371:HIS:CD2	2.18	0.78
1:A:196:ARG:HH11	1:A:196:ARG:CG	1.97	0.77
2:D:390:PRO:HB2	2:D:391:PRO:HD2	1.64	0.77
2:D:232:LEU:HD11	2:D:266:LEU:HD22	1.67	0.77
1:A:351:THR:HB	2:D:411:ILE:HG22	1.67	0.77
2:D:457:GLU:HB3	1:B:113:LYS:HD3	1.64	0.77
1:A:39:ARG:HG3	1:A:64:ILE:C	2.11	0.75
2:C:189:ILE:HG13	2:C:191:ASN:HB2	1.68	0.75
2:D:435:SER:HA	1:B:270:GLU:CG	2.17	0.75
1:A:121:GLN:NE2	2:D:320:MET:CB	2.47	0.74
2:D:457:GLU:HG2	1:B:113:LYS:NZ	2.03	0.74
2:D:405:ARG:HG2	2:D:406:ASN:H	1.52	0.73
2:C:271:PHE:HE2	2:C:299:LEU:HD21	1.54	0.73
1:B:39:ARG:O	1:B:40:HIS:CB	2.37	0.73
2:D:451:VAL:HG12	2:D:452:GLN:H	1.55	0.72
1:B:248:ILE:HG12	1:B:249:THR:N	2.05	0.72
2:D:277:ILE:HG12	2:D:279:GLY:H	1.55	0.72
2:D:294:THR:HG23	2:D:322:LYS:HD2	1.72	0.72
2:D:167:ILE:HD11	2:D:189:ILE:HG21	1.72	0.72
2:C:328:LEU:O	2:C:332:LYS:HB2	1.90	0.71
1:B:38:PRO:HD3	1:B:47:MET:HE1	1.70	0.71
2:D:166:VAL:HG12	2:D:167:ILE:H	1.55	0.71
2:D:485:LEU:HD11	1:B:345:ILE:HG13	1.71	0.71
1:A:60:SER:O	2:D:390:PRO:CG	2.38	0.71
1:A:64:ILE:HG22	1:A:64:ILE:O	1.91	0.71
2:D:459:SER:HB3	1:B:372:ARG:HE	1.56	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ARG:N	1:B:64:ILE:O	2.24	0.70
2:C:326:LYS:O	2:C:329:GLN:HG2	1.90	0.70
1:A:351:THR:CG2	2:D:411:ILE:HG22	2.22	0.70
2:D:435:SER:CA	1:B:270:GLU:HG2	2.19	0.70
1:A:284:LYS:NZ	1:A:284:LYS:HB2	2.06	0.69
2:D:234:VAL:HG12	2:D:234:VAL:O	1.92	0.69
2:D:393:PRO:O	2:D:395:PRO:HD3	1.93	0.69
1:B:43:VAL:O	1:B:43:VAL:CG2	2.35	0.69
1:A:196:ARG:HG2	1:A:196:ARG:NH1	1.99	0.69
2:C:193:THR:HB	2:C:196:THR:CB	2.06	0.69
2:C:251:LYS:HD2	2:C:251:LYS:N	2.08	0.69
2:D:309:ARG:O	2:D:313:THR:HG22	1.92	0.69
1:A:221:LEU:HD21	1:A:311:ASP:HB2	1.73	0.69
1:A:148:THR:OG1	2:D:410:VAL:HG21	1.92	0.68
1:A:349:LEU:HD11	2:D:407:ILE:HG23	1.75	0.68
1:A:40:HIS:O	1:A:41:GLN:HB2	1.94	0.68
2:C:187:ASN:O	2:C:189:ILE:N	2.26	0.68
1:B:43:VAL:O	1:B:45:VAL:N	2.27	0.68
1:A:47:MET:HE1	1:A:53:TYR:CE1	2.28	0.68
1:A:205:GLU:O	1:A:208:ILE:HG13	1.92	0.68
2:D:253:ILE:O	2:D:257:MET:HG2	1.94	0.68
1:B:64:ILE:O	1:B:64:ILE:HG12	1.92	0.68
2:D:236:GLU:HA	2:D:265:VAL:HG21	1.73	0.68
1:A:39:ARG:N	1:A:64:ILE:O	2.27	0.68
2:D:438:ASN:O	2:D:442:LYS:HG2	1.94	0.67
1:B:180:LEU:HD13	1:B:267:LEU:HD12	1.77	0.67
1:A:10:VAL:HB	1:A:105:LEU:CD2	2.25	0.67
2:D:390:PRO:CB	2:D:391:PRO:HD3	2.23	0.67
2:C:324:ARG:HA	2:C:327:ARG:NH1	2.10	0.67
2:C:275:ARG:HG3	2:C:276:HIS:H	1.60	0.67
2:C:310:MET:HE1	1:B:115:ASN:OD1	1.94	0.67
2:D:457:GLU:CG	1:B:113:LYS:HZ2	2.07	0.67
1:B:370:VAL:O	1:B:374:CYS:HB2	1.94	0.67
1:A:180:LEU:HD21	1:A:261:LEU:HD23	1.77	0.66
2:C:230:GLU:HG3	2:C:233:LYS:HE3	1.78	0.66
2:D:390:PRO:CB	2:D:391:PRO:CD	2.63	0.66
1:A:163:VAL:HG13	1:A:175:ILE:CD1	2.26	0.65
2:D:267:THR:HG23	2:D:268:GLU:HG3	1.78	0.65
2:D:435:SER:CB	2:D:437:PRO:HD3	2.26	0.65
2:C:196:THR:O	2:C:200:PHE:HD1	1.77	0.65
1:A:121:GLN:HE21	2:D:320:MET:HB3	1.56	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:215:LEU:HD11	2:D:243:VAL:HG22	1.78	0.65
1:A:148:THR:HG21	1:A:167:GLU:OE2	1.97	0.65
1:B:171:LEU:HB3	1:B:173:HIS:CE1	2.31	0.65
2:D:257:MET:CE	2:D:290:LEU:HG	2.26	0.65
1:A:60:SER:HB2	2:D:390:PRO:CD	2.26	0.64
2:C:257:MET:HE3	2:C:257:MET:HA	1.80	0.64
1:B:39:ARG:HB2	1:B:64:ILE:O	1.96	0.64
1:A:220:ALA:O	1:A:312:ARG:HD2	1.98	0.64
2:C:257:MET:HB3	2:C:289:LEU:HD13	1.77	0.64
1:A:306:TYR:CE2	3:A:401:ANP:H2	2.32	0.64
1:A:219:VAL:HG11	1:A:262:PHE:CE1	2.32	0.64
2:D:431:GLY:HA3	1:B:176:LEU:HD22	1.80	0.64
1:A:276:GLU:HG2	1:A:320:LEU:HD11	1.79	0.64
1:B:250:ILE:HD12	1:B:254:ARG:HG2	1.80	0.64
2:D:241:VAL:HG23	2:D:266:LEU:HD11	1.79	0.63
2:D:459:SER:HB3	1:B:372:ARG:NE	2.12	0.63
2:D:437:PRO:O	2:D:441:LEU:HG	1.99	0.63
1:A:64:ILE:O	1:A:64:ILE:CG2	2.46	0.63
2:D:243:VAL:O	2:D:243:VAL:HG12	1.97	0.63
1:A:351:THR:CB	2:D:411:ILE:HG22	2.28	0.63
1:A:25:ASP:HB2	2:D:401:LYS:H	1.64	0.63
2:D:432:SER:O	2:D:434:GLY:N	2.29	0.63
2:D:457:GLU:CB	1:B:371:HIS:CD2	2.82	0.63
1:B:220:ALA:O	1:B:312:ARG:HD3	1.98	0.63
1:A:218:TYR:OH	1:A:226:GLU:OE1	2.15	0.63
1:A:242:LEU:HB3	1:A:243:PRO:HD2	1.80	0.63
1:B:191:LYS:O	1:B:195:GLU:CG	2.46	0.62
1:B:219:VAL:HG11	1:B:262:PHE:CE1	2.33	0.62
1:B:44:MET:HE3	1:B:64:ILE:HB	1.80	0.62
2:C:302:HIS:HB2	1:B:78:ASN:HD22	1.63	0.62
1:A:47:MET:HE1	1:A:53:TYR:CD1	2.35	0.62
2:C:327:ARG:NH2	1:B:363:ASP:OD1	2.33	0.62
2:C:291:LYS:O	2:C:318:ARG:NH2	2.28	0.62
2:C:258:ARG:HG3	2:C:289:LEU:HD21	1.83	0.61
2:C:231:MET:HE2	2:C:232:LEU:HD23	1.82	0.61
2:C:243:VAL:O	2:C:271:PHE:HA	2.00	0.61
2:D:275:ARG:HG3	2:D:276:HIS:H	1.64	0.61
2:D:219:HIS:O	2:D:219:HIS:ND1	2.34	0.61
2:C:217:ASN:OD1	1:B:43:VAL:HG12	2.00	0.61
2:D:457:GLU:HB2	1:B:371:HIS:HD2	1.66	0.61
2:C:193:THR:CG2	2:C:196:THR:H	2.13	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:310:MET:CE	1:B:115:ASN:OD1	2.49	0.60
1:B:284:LYS:HB2	1:B:284:LYS:NZ	2.15	0.60
2:C:287:VAL:HG11	2:C:311:SER:HB2	1.84	0.60
1:A:162:THR:HG21	1:A:277:THR:O	2.01	0.60
1:A:286:ASP:HA	1:B:195:GLU:O	2.02	0.60
2:D:454:LYS:H	2:D:454:LYS:HD3	1.65	0.60
2:D:239:THR:HB	2:D:267:THR:HG22	1.83	0.60
1:A:125:GLU:CD	2:D:327:ARG:HH21	2.06	0.60
2:C:236:GLU:HA	2:C:265:VAL:HG21	1.83	0.60
2:C:287:VAL:HG11	2:C:311:SER:CB	2.31	0.60
1:A:257:CYS:HB3	1:A:258:PRO:HD3	1.84	0.60
1:A:156:GLY:HA2	3:A:401:ANP:O1A	2.02	0.59
1:A:363:ASP:OD1	2:D:327:ARG:NH1	2.20	0.59
2:C:278:MET:HA	2:C:278:MET:CE	2.29	0.59
2:C:325:GLN:O	2:C:328:LEU:HB3	2.01	0.59
2:D:457:GLU:H	1:B:113:LYS:HZ2	1.49	0.59
1:A:43:VAL:HG13	1:A:64:ILE:HG21	1.85	0.59
2:D:434:GLY:CA	1:B:271:ALA:HB2	2.29	0.59
2:D:464:THR:HG22	2:D:464:THR:O	2.02	0.59
2:D:435:SER:HB3	2:D:437:PRO:HD3	1.85	0.59
2:D:451:VAL:HG12	2:D:452:GLN:N	2.17	0.59
1:B:230:ALA:HB2	1:B:236:LEU:HD23	1.85	0.59
2:C:310:MET:CB	2:D:448:LEU:HB2	2.25	0.58
2:D:257:MET:HE2	2:D:286:ILE:HG23	1.84	0.58
2:D:431:GLY:O	2:D:432:SER:C	2.47	0.58
2:C:263:ASN:OD1	2:C:263:ASN:C	2.46	0.58
2:D:435:SER:C	2:D:437:PRO:CD	2.73	0.58
2:D:222:ASP:OD1	2:D:249:THR:OG1	2.19	0.58
1:A:78:ASN:ND2	2:D:302:HIS:HB2	2.18	0.58
2:D:258:ARG:O	2:D:261:GLN:HB2	2.03	0.58
2:D:410:VAL:O	2:D:414:GLN:N	2.37	0.57
1:B:147:ARG:NH2	1:B:330:ILE:HG12	2.19	0.57
2:D:258:ARG:HG3	2:D:289:LEU:HD21	1.87	0.57
2:D:194:THR:CG2	2:D:223:SER:OG	2.53	0.57
2:C:193:THR:HG22	2:C:196:THR:H	1.70	0.57
1:B:322:LYS:HE2	1:B:325:MET:HE2	1.85	0.57
2:C:285:GLU:O	2:C:289:LEU:HB2	2.05	0.57
2:C:257:MET:HE2	2:C:290:LEU:HD11	1.87	0.57
1:B:104:LEU:HD12	1:B:133:TYR:HB3	1.87	0.56
1:A:284:LYS:HB2	1:A:284:LYS:HZ2	1.69	0.56
2:C:217:ASN:CG	1:B:43:VAL:HG12	2.30	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:VAL:HG13	1:A:175:ILE:HD11	1.87	0.56
2:D:405:ARG:HG2	2:D:406:ASN:N	2.18	0.56
1:B:136:ILE:HB	1:B:139:VAL:HG13	1.86	0.56
2:D:439:SER:O	2:D:445:LYS:NZ	2.31	0.56
1:A:151:ILE:HD11	1:A:162:THR:OG1	2.06	0.56
2:C:306:PRO:HB2	2:D:446:ASN:O	2.05	0.56
1:B:39:ARG:HB2	1:B:64:ILE:C	2.31	0.56
2:D:299:LEU:CD2	2:D:312:MET:HE2	2.29	0.56
2:D:407:ILE:HD13	2:D:407:ILE:O	2.06	0.55
1:B:161:HIS:CE1	1:B:177:ARG:HG3	2.40	0.55
2:C:305:LEU:HB3	2:C:308:PRO:HG2	1.88	0.55
2:D:449:ARG:O	2:D:451:VAL:N	2.39	0.55
1:B:358:SER:HB2	1:B:361:GLU:HG3	1.88	0.55
2:D:294:THR:HG23	2:D:322:LYS:NZ	2.22	0.55
2:D:435:SER:HA	1:B:270:GLU:CD	2.32	0.55
1:B:41:GLN:O	1:B:43:VAL:N	2.38	0.55
2:C:261:GLN:NE2	2:C:292:GLU:OE2	2.39	0.55
1:A:230:ALA:HB2	1:A:236:LEU:HD12	1.89	0.55
2:D:193:THR:HB	2:D:196:THR:H	1.71	0.55
2:D:431:GLY:CA	1:B:176:LEU:HD22	2.37	0.54
1:B:136:ILE:HB	1:B:139:VAL:CG1	2.38	0.54
1:B:296:ASN:O	1:B:298:VAL:HG23	2.07	0.54
1:B:186:THR:OG1	1:B:213:LYS:NZ	2.35	0.54
1:A:25:ASP:HB2	2:D:400:LYS:H	1.72	0.54
2:D:166:VAL:N	2:D:169:ASP:OD2	2.40	0.54
2:D:258:ARG:HG3	2:D:289:LEU:HD11	1.90	0.54
2:D:327:ARG:O	2:D:331:GLN:HB3	2.07	0.54
1:B:257:CYS:HB3	1:B:258:PRO:HD3	1.89	0.54
2:C:245:SER:HA	2:C:273:ASN:O	2.08	0.54
1:A:299:LEU:HD12	1:A:331:ALA:HB2	1.89	0.54
1:A:353:GLN:O	1:A:356:TRP:HD1	1.91	0.54
2:C:251:LYS:N	2:C:251:LYS:CD	2.71	0.54
1:B:149:THR:OG1	1:B:167:GLU:OE2	2.23	0.54
2:D:400:LYS:O	2:D:401:LYS:HB2	2.08	0.53
1:B:177:ARG:NH1	1:B:179:ASP:OD1	2.41	0.53
1:B:120:THR:HG23	1:B:132:MET:HE1	1.89	0.53
1:B:198:TYR:HB2	1:B:200:PHE:CE1	2.44	0.53
2:D:243:VAL:O	2:D:243:VAL:HG13	2.06	0.53
1:A:43:VAL:O	1:A:44:MET:C	2.50	0.53
1:A:187:ASP:OD1	1:A:206:ARG:NH2	2.36	0.53
2:D:457:GLU:CD	1:B:113:LYS:HD3	2.34	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:LEU:O	1:A:145:SER:OG	2.25	0.53
1:A:358:SER:HB2	1:A:361:GLU:HG3	1.91	0.53
1:A:60:SER:O	2:D:390:PRO:HG3	2.09	0.53
1:A:163:VAL:HG13	1:A:175:ILE:HD13	1.90	0.53
2:D:294:THR:HG23	2:D:322:LYS:HZ2	1.73	0.53
2:D:455:LYS:HE3	1:B:112:PRO:HB3	1.91	0.53
2:D:457:GLU:OE1	1:B:371:HIS:CG	2.62	0.53
2:D:481:SER:C	2:D:483:LYS:H	2.16	0.53
1:A:10:VAL:HB	1:A:105:LEU:HD23	1.90	0.52
2:D:239:THR:O	2:D:267:THR:HG22	2.09	0.52
2:D:494:LEU:HB3	1:B:56:ASP:CG	2.34	0.52
1:B:37:ARG:NH2	1:B:81:ASP:OD2	2.43	0.52
1:A:283:MET:HA	1:A:283:MET:HE2	1.91	0.52
1:A:335:ARG:HA	1:A:338:SER:HB3	1.92	0.52
1:A:190:MET:HG3	1:A:209:VAL:HG11	1.91	0.52
2:D:478:ARG:HG3	1:B:148:THR:HG22	1.91	0.52
2:D:490:VAL:HG21	1:B:30:VAL:CG2	2.40	0.52
1:B:198:TYR:CD2	1:B:198:TYR:N	2.71	0.52
2:D:202:GLU:HA	2:D:205:LYS:HB2	1.91	0.52
2:D:294:THR:O	2:D:294:THR:HG22	2.10	0.52
2:D:444:ILE:HG13	2:D:445:LYS:N	2.23	0.52
1:B:131:ALA:HA	1:B:357:ILE:O	2.10	0.52
1:A:163:VAL:HG22	1:A:175:ILE:HD13	1.91	0.52
1:B:241:GLU:HG2	1:B:247:VAL:HG22	1.90	0.52
1:A:221:LEU:HD21	1:A:311:ASP:CB	2.41	0.51
2:C:234:VAL:HG12	2:C:234:VAL:O	2.10	0.51
2:D:243:VAL:HG13	2:D:248:ILE:HD12	1.92	0.51
1:A:237:GLU:HG2	1:A:238:LYS:N	2.25	0.51
1:A:47:MET:HE3	1:A:65:LEU:HD21	1.91	0.51
2:C:188:ASN:HA	2:C:217:ASN:HB3	1.93	0.51
1:A:26:ALA:HB1	1:A:27:PRO:HD2	1.93	0.51
1:B:103:VAL:HG12	1:B:105:LEU:CD1	2.40	0.51
1:B:198:TYR:CE2	1:B:248:ILE:HD12	2.45	0.51
1:A:194:THR:HA	1:A:198:TYR:O	2.11	0.51
1:B:180:LEU:HD13	1:B:267:LEU:CD1	2.40	0.51
1:A:47:MET:CE	1:A:53:TYR:CE1	2.93	0.51
1:B:9:VAL:HG21	1:B:344:SER:HA	1.93	0.51
2:D:257:MET:CE	2:D:290:LEU:CG	2.89	0.51
1:A:43:VAL:HB	2:D:217:ASN:HD21	1.76	0.51
1:A:106:THR:HB	1:A:137:GLN:HG3	1.92	0.51
2:D:455:LYS:HD2	1:B:113:LYS:HB2	1.91	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:231:MET:HE1	2:C:238:ILE:HD12	1.92	0.50
2:C:306:PRO:CB	2:D:446:ASN:O	2.59	0.50
2:D:454:LYS:H	2:D:454:LYS:CD	2.24	0.50
2:D:331:GLN:HA	2:D:335:GLU:OE1	2.11	0.50
2:D:435:SER:OG	1:B:269:MET:HA	2.10	0.50
1:B:194:THR:HA	1:B:198:TYR:O	2.12	0.50
1:B:107:GLU:OE1	1:B:116:ARG:HG2	2.11	0.50
1:A:233:SER:OG	1:A:234:SER:N	2.45	0.50
2:C:187:ASN:C	2:C:189:ILE:H	2.18	0.50
2:D:178:ASP:C	2:D:180:ASP:H	2.20	0.50
1:B:131:ALA:HB1	1:B:356:TRP:HB3	1.94	0.50
1:A:317:ILE:HG22	1:A:317:ILE:O	2.12	0.50
1:A:372:ARG:HH12	1:A:373:LYS:HG2	1.77	0.50
2:C:243:VAL:O	2:C:243:VAL:HG23	2.12	0.50
1:B:335:ARG:HA	1:B:338:SER:HB3	1.92	0.50
2:D:451:VAL:CG1	2:D:452:GLN:H	2.24	0.50
1:B:242:LEU:HB3	1:B:243:PRO:HD2	1.93	0.50
2:D:229:ALA:O	2:D:232:LEU:HB2	2.12	0.50
2:C:188:ASN:OD1	2:C:217:ASN:ND2	2.45	0.49
2:D:257:MET:HE1	2:D:290:LEU:CG	2.41	0.49
2:D:457:GLU:CG	1:B:113:LYS:NZ	2.70	0.49
1:B:64:ILE:O	1:B:64:ILE:CG1	2.61	0.49
1:A:60:SER:O	2:D:390:PRO:HG2	2.10	0.49
2:D:194:THR:HG23	2:D:223:SER:OG	2.10	0.49
1:B:170:ALA:O	1:B:172:PRO:HD3	2.13	0.49
1:A:78:ASN:HD22	2:D:302:HIS:HB2	1.77	0.49
1:A:131:ALA:HA	1:A:357:ILE:O	2.11	0.49
2:C:189:ILE:O	2:C:190:GLU:C	2.54	0.49
2:D:258:ARG:CG	2:D:289:LEU:HD21	2.43	0.49
1:B:42:GLY:O	1:B:43:VAL:C	2.54	0.49
1:B:248:ILE:CG1	1:B:249:THR:N	2.74	0.49
2:D:432:SER:C	2:D:434:GLY:N	2.71	0.49
1:B:284:LYS:HB2	1:B:284:LYS:HZ2	1.77	0.49
2:C:258:ARG:CG	2:C:289:LEU:HD21	2.42	0.49
2:C:314:SER:HB3	2:D:453:GLU:OE1	2.13	0.49
2:D:447:SER:OG	1:B:112:PRO:HG3	2.13	0.49
1:A:41:GLN:O	1:A:43:VAL:N	2.45	0.48
1:B:37:ARG:HB3	1:B:38:PRO:HD2	1.95	0.48
1:A:170:ALA:O	1:A:172:PRO:HD3	2.12	0.48
2:C:185:ASN:OD1	2:C:187:ASN:HB3	2.12	0.48
2:D:485:LEU:HD13	1:B:24:ASP:O	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:8:LEU:HD13	1:B:101:HIS:HB3	1.96	0.48
2:D:201:ALA:O	2:D:231:MET:HG3	2.14	0.48
2:D:442:LYS:HE2	2:D:445:LYS:HD2	1.96	0.48
1:A:186:THR:OG1	1:A:213:LYS:NZ	2.43	0.48
2:C:207:ASN:OD1	2:C:208:THR:N	2.46	0.48
2:D:405:ARG:CG	2:D:406:ASN:H	2.25	0.48
1:B:282:ILE:O	1:B:285:CYS:HB2	2.13	0.48
2:D:196:THR:O	2:D:200:PHE:HD1	1.97	0.48
2:D:435:SER:OG	1:B:270:GLU:N	2.45	0.48
1:A:295:ALA:HA	1:A:328:LYS:H	1.78	0.48
2:D:436:GLN:N	2:D:437:PRO:CD	2.77	0.48
1:B:185:LEU:CD2	1:B:260:ALA:HB3	2.43	0.48
1:A:132:MET:HE3	1:A:357:ILE:HD12	1.95	0.47
1:A:282:ILE:O	1:A:285:CYS:HB2	2.14	0.47
2:D:195:GLN:HA	2:D:198:THR:HB	1.95	0.47
1:B:140:LEU:O	1:B:342:GLY:HA3	2.13	0.47
1:A:148:THR:CG2	1:A:167:GLU:OE2	2.62	0.47
2:D:221:ASP:C	2:D:221:ASP:OD1	2.56	0.47
1:A:137:GLN:HG2	1:A:339:VAL:HG11	1.95	0.47
2:D:280:SER:HA	2:D:283:GLU:HB2	1.96	0.47
2:D:460:SER:HB2	1:B:372:ARG:HD3	1.96	0.47
2:D:254:LEU:HD22	2:D:285:GLU:HG2	1.97	0.47
1:A:200:PHE:HA	1:A:205:GLU:CD	2.39	0.47
2:C:264:THR:HA	2:C:295:THR:HG21	1.97	0.47
2:D:294:THR:CG2	2:D:322:LYS:NZ	2.78	0.47
2:D:457:GLU:H	1:B:113:LYS:NZ	2.13	0.47
2:C:166:VAL:HB	2:C:169:ASP:HB3	1.96	0.47
2:D:166:VAL:HG12	2:D:167:ILE:N	2.25	0.47
1:B:286:ASP:HB3	1:B:289:ILE:HG12	1.96	0.47
1:B:327:ILE:HD12	1:B:327:ILE:N	2.29	0.47
2:C:230:GLU:HA	2:C:233:LYS:HE2	1.97	0.46
1:A:140:LEU:O	1:A:342:GLY:HA3	2.16	0.46
2:C:283:GLU:OE1	2:C:301:TYR:OH	2.32	0.46
2:C:254:LEU:HB3	2:C:258:ARG:HH21	1.81	0.46
2:D:329:GLN:HG3	2:D:330:GLU:N	2.30	0.46
2:D:234:VAL:O	2:D:234:VAL:CG1	2.62	0.46
2:D:435:SER:CA	2:D:437:PRO:HD3	2.44	0.46
1:A:50:LYS:HD2	1:A:53:TYR:CE2	2.51	0.46
1:A:361:GLU:O	1:A:365:SER:OG	2.33	0.46
2:C:187:ASN:HD22	1:B:49:GLN:CB	2.27	0.46
2:D:417:ALA:O	2:D:418:GLN:HG2	2.15	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ARG:NH2	1:A:330:ILE:HG12	2.31	0.45
1:A:284:LYS:NZ	1:A:284:LYS:CB	2.76	0.45
1:A:286:ASP:HB3	1:A:289:ILE:HG12	1.96	0.45
1:A:185:LEU:CD2	1:A:260:ALA:HB3	2.47	0.45
2:D:208:THR:HA	2:D:237:HIS:CD2	2.51	0.45
1:B:21:PHE:O	1:B:24:ASP:HB2	2.16	0.45
2:C:187:ASN:O	2:C:187:ASN:OD1	2.35	0.45
2:D:172:ASP:O	2:D:176:SER:HB2	2.17	0.45
1:B:213:LYS:HA	1:B:217:CYS:SG	2.56	0.45
1:A:196:ARG:CG	1:A:196:ARG:NH1	2.64	0.45
2:D:487:ARG:NH1	1:B:25:ASP:OD2	2.50	0.45
1:A:112:PRO:HB3	1:B:224:GLU:OE1	2.16	0.45
2:C:182:THR:HA	2:C:209:VAL:O	2.17	0.45
1:A:209:VAL:HA	1:A:212:ILE:HD12	1.97	0.45
1:A:279:TYR:HD1	1:A:294:TYR:HH	1.64	0.45
2:D:481:SER:C	2:D:483:LYS:N	2.74	0.45
1:B:8:LEU:HD13	1:B:101:HIS:CB	2.47	0.45
2:D:396:PRO:HB2	2:D:397:LEU:H	1.63	0.45
2:C:253:ILE:HG13	2:C:278:MET:SD	2.57	0.45
2:D:257:MET:CE	2:D:290:LEU:CD1	2.89	0.45
1:B:49:GLN:H	1:B:49:GLN:HG2	1.68	0.45
1:A:34:ILE:HG22	1:A:69:TYR:CE2	2.52	0.45
2:D:224:ALA:O	2:D:227:ALA:HB3	2.17	0.45
2:D:232:LEU:CD1	2:D:266:LEU:HD22	2.43	0.45
1:B:66:THR:HG22	1:B:68:LYS:HE2	1.98	0.45
1:B:295:ALA:HA	1:B:328:LYS:H	1.82	0.45
2:C:284:MET:HE3	2:C:308:PRO:HD3	2.00	0.44
2:D:194:THR:HG21	2:D:223:SER:OG	2.17	0.44
2:D:225:ALA:O	2:D:229:ALA:N	2.45	0.44
2:D:243:VAL:CG1	2:D:248:ILE:HD12	2.47	0.44
2:D:305:LEU:HA	2:D:306:PRO:HD3	1.86	0.44
2:D:461:ARG:O	2:D:461:ARG:HG3	2.16	0.44
1:B:180:LEU:CD1	1:B:267:LEU:CD1	2.94	0.44
1:A:43:VAL:HB	2:D:217:ASN:ND2	2.31	0.44
2:C:264:THR:C	2:C:265:VAL:HG22	2.41	0.44
1:A:64:ILE:HD13	1:A:64:ILE:HA	1.88	0.44
1:A:202:THR:O	1:A:205:GLU:HG2	2.17	0.44
2:D:261:GLN:HE22	2:D:292:GLU:CD	2.26	0.44
2:C:281:GLN:O	2:C:285:GLU:HG2	2.16	0.44
2:D:260:LEU:HA	2:D:263:ASN:HB3	1.97	0.44
2:D:457:GLU:CB	1:B:113:LYS:HD3	2.43	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:MET:HG3	1:B:209:VAL:HG21	1.98	0.44
1:A:244:ASP:OD1	1:A:244:ASP:N	2.47	0.44
2:C:326:LYS:C	2:C:328:LEU:N	2.74	0.44
2:C:186:LEU:HB3	2:C:191:ASN:HD22	1.83	0.43
2:D:249:THR:CG2	2:D:275:ARG:HH21	2.30	0.43
1:B:259:GLU:CD	1:B:312:ARG:HH12	2.27	0.43
1:A:201:THR:H	1:A:205:GLU:CD	2.23	0.43
2:C:195:GLN:HA	2:C:198:THR:HB	2.01	0.43
2:D:435:SER:N	1:B:270:GLU:HG2	2.33	0.43
1:A:219:VAL:HG22	1:A:258:PRO:HB2	2.00	0.43
1:A:242:LEU:HB3	1:A:243:PRO:CD	2.46	0.43
2:C:204:LEU:HA	2:C:207:ASN:HB2	2.00	0.43
2:C:213:PHE:CZ	2:C:215:LEU:HD22	2.53	0.43
2:C:312:MET:HE3	2:C:312:MET:HA	1.99	0.43
2:D:288:LYS:HG3	2:D:289:LEU:N	2.33	0.43
2:D:490:VAL:HG21	1:B:30:VAL:HG21	2.00	0.43
1:A:221:LEU:CD2	1:A:311:ASP:HB2	2.46	0.43
2:C:254:LEU:HA	2:C:257:MET:HB2	2.00	0.43
2:C:271:PHE:CE2	2:C:299:LEU:HD21	2.44	0.43
2:D:294:THR:HG23	2:D:322:LYS:CD	2.46	0.43
2:C:175:LYS:H	2:C:175:LYS:HG2	1.60	0.43
2:C:247:PHE:CD2	2:C:275:ARG:HB3	2.54	0.43
1:B:332:PRO:O	1:B:335:ARG:NH1	2.49	0.43
1:A:70:PRO:HG3	1:A:81:ASP:HB3	2.00	0.42
2:D:226:MET:O	2:D:230:GLU:HG2	2.20	0.42
2:D:235:ASN:OD1	2:D:236:GLU:N	2.52	0.42
2:D:243:VAL:HG13	2:D:248:ILE:CD1	2.49	0.42
2:D:442:LYS:NZ	1:B:73:HIS:CD2	2.88	0.42
1:A:305:MET:HA	1:A:335:ARG:NH2	2.34	0.42
1:B:39:ARG:CB	1:B:64:ILE:O	2.65	0.42
2:D:178:ASP:HA	2:D:179:PRO:HD3	1.88	0.42
2:D:457:GLU:CD	1:B:371:HIS:HB3	2.44	0.42
1:A:31:PHE:CD2	1:A:93:GLU:HG2	2.55	0.42
1:B:218:TYR:C	1:B:218:TYR:CD2	2.98	0.42
1:A:210:ARG:NH1	1:A:214:GLU:OE2	2.52	0.42
2:D:192:ILE:HG22	2:D:197:LEU:HG	2.02	0.42
2:D:236:GLU:O	2:D:265:VAL:HG11	2.18	0.42
1:B:291:GLU:HG3	1:B:325:MET:SD	2.60	0.42
1:A:41:GLN:HB3	1:A:42:GLY:H	1.68	0.42
2:D:282:VAL:O	2:D:286:ILE:HG13	2.20	0.42
1:A:351:THR:HG22	2:D:411:ILE:HG22	1.99	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:257:MET:HE3	2:D:290:LEU:HG	1.99	0.42
1:B:218:TYR:CE2	1:B:255:PHE:HB3	2.55	0.42
2:D:432:SER:CB	1:B:178:LEU:HD12	2.49	0.41
1:A:303:THR:CG2	1:A:303:THR:O	2.67	0.41
2:C:250:GLY:O	2:C:254:LEU:HG	2.19	0.41
2:D:193:THR:HG22	2:D:194:THR:N	2.34	0.41
2:D:199:ARG:HA	2:D:199:ARG:HD3	1.85	0.41
2:D:254:LEU:HD22	2:D:285:GLU:CG	2.50	0.41
1:B:286:ASP:OD1	1:B:287:VAL:N	2.53	0.41
2:C:252:GLY:O	2:C:255:ALA:HB3	2.21	0.41
1:B:134:VAL:O	1:B:134:VAL:HG13	2.20	0.41
1:A:120:THR:HG23	1:A:132:MET:HE2	2.02	0.41
2:D:442:LYS:CE	2:D:445:LYS:HB3	2.51	0.41
1:A:131:ALA:HB1	1:A:356:TRP:HB3	2.01	0.41
2:D:247:PHE:O	2:D:275:ARG:HD3	2.20	0.41
2:D:322:LYS:O	2:D:326:LYS:HB2	2.21	0.41
2:D:490:VAL:O	2:D:490:VAL:HG22	2.21	0.41
2:D:482:ILE:HG22	2:D:482:ILE:O	2.21	0.41
1:A:69:TYR:HA	1:A:70:PRO:HD3	1.95	0.41
2:C:251:LYS:CD	2:C:251:LYS:H	2.34	0.41
2:C:287:VAL:HG11	2:C:311:SER:HB3	1.99	0.41
2:D:243:VAL:HG13	2:D:246:ASN:HD22	1.85	0.41
1:A:202:THR:HG23	1:A:205:GLU:OE2	2.21	0.41
1:A:282:ILE:HG23	1:A:293:LEU:HD23	2.03	0.41
1:A:313:MET:HB3	1:A:329:ILE:CD1	2.51	0.41
2:D:271:PHE:CD2	2:D:271:PHE:N	2.89	0.41
1:B:38:PRO:HG3	1:B:47:MET:SD	2.61	0.41
1:B:162:THR:HG21	1:B:278:THR:HA	2.03	0.41
2:C:327:ARG:NH1	1:B:125:GLU:OE2	2.51	0.41
2:D:444:ILE:HG21	1:B:72:GLU:OE1	2.21	0.40
2:C:217:ASN:HD21	1:B:43:VAL:HA	1.86	0.40
1:A:284:LYS:HB2	1:A:284:LYS:HZ3	1.85	0.40
2:C:306:PRO:O	2:C:310:MET:HB2	2.21	0.40
2:C:324:ARG:HA	2:C:327:ARG:HH12	1.84	0.40
1:B:34:ILE:HD13	1:B:67:LEU:HD13	2.03	0.40
1:B:213:LYS:O	1:B:217:CYS:HB2	2.20	0.40
1:A:47:MET:CE	1:A:53:TYR:HE1	2.32	0.40

All (2) 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:225:GLN:OE1	2:D:447:SER:O[1_665]	2.15	0.05
1:A:232:SER:O	2:D:432:SER:O[1_665]	2.16	0.04

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	367/384 (96%)	341 (93%)	18 (5%)	8 (2%)	5	24
1	B	367/384 (96%)	346 (94%)	14 (4%)	7 (2%)	6	27
2	C	166/506 (33%)	137 (82%)	23 (14%)	6 (4%)	2	14
2	D	276/506 (54%)	210 (76%)	43 (16%)	23 (8%)	0	3
All	All	1176/1780 (66%)	1034 (88%)	98 (8%)	44 (4%)	2	13

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	39	ARG
1	A	45	VAL
2	C	193	THR
2	C	265	VAL
2	D	219	HIS
2	D	390	PRO
2	D	393	PRO
2	D	406	ASN
2	D	436	GLN
2	D	450	SER
1	B	40	HIS
1	B	42	GLY
1	B	43	VAL
1	B	45	VAL
1	A	42	GLY
1	A	44	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	182	GLY
2	D	392	PRO
2	D	396	PRO
2	D	401	LYS
2	D	432	SER
2	D	433	VAL
2	D	444	ILE
2	D	446	ASN
1	B	182	GLY
1	A	15	GLY
2	C	191	ASN
2	D	489	GLU
1	A	41	GLN
2	C	275	ARG
2	D	394	PRO
2	D	395	PRO
2	D	421	LEU
2	D	437	PRO
2	D	488	VAL
1	B	15	GLY
1	B	356	TRP
1	A	356	TRP
2	C	188	ASN
2	D	464	THR
2	D	482	ILE
2	D	438	ASN
2	D	462	PRO
2	C	308	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	311/325 (96%)	272 (88%)	39 (12%)	4	19
1	B	310/325 (95%)	280 (90%)	30 (10%)	8	29
2	C	152/451 (34%)	128 (84%)	24 (16%)	2	12

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	241/451 (53%)	215 (89%)	26 (11%)	6	24
All	All	1014/1552 (65%)	895 (88%)	119 (12%)	5	21

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	CYS
1	A	18	LYS
1	A	40	HIS
1	A	44	MET
1	A	49	GLN
1	A	54	VAL
1	A	84	LYS
1	A	132	MET
1	A	155	SER
1	A	162	THR
1	A	169	TYR
1	A	175	ILE
1	A	180	LEU
1	A	195	GLU
1	A	196	ARG
1	A	202	THR
1	A	203	THR
1	A	207	GLU
1	A	208	ILE
1	A	210	ARG
1	A	225	GLN
1	A	229	THR
1	A	233	SER
1	A	235	SER
1	A	237	GLU
1	A	281	SER
1	A	284	LYS
1	A	287	VAL
1	A	288	ASP
1	A	293	LEU
1	A	312	ARG
1	A	322	LYS
1	A	329	ILE
1	A	334	GLU
1	A	350	SER
1	A	351	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	354	GLN
1	A	365	SER
1	A	368	SER
2	C	181	THR
2	C	190	GLU
2	C	196	THR
2	C	198	THR
2	C	215	LEU
2	C	236	GLU
2	C	249	THR
2	C	257	MET
2	C	262	HIS
2	C	265	VAL
2	C	267	THR
2	C	270	ARG
2	C	275	ARG
2	C	281	GLN
2	C	288	LYS
2	C	289	LEU
2	C	292	GLU
2	C	295	THR
2	C	299	LEU
2	C	305	LEU
2	C	310	MET
2	C	313	THR
2	C	318	ARG
2	C	326	LYS
2	D	177	ASN
2	D	206	ASP
2	D	215	LEU
2	D	232	LEU
2	D	243	VAL
2	D	262	HIS
2	D	277	ILE
2	D	280	SER
2	D	282	VAL
2	D	284	MET
2	D	287	VAL
2	D	288	LYS
2	D	289	LEU
2	D	292	GLU
2	D	295	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	D	311	SER
2	D	313	THR
2	D	318	ARG
2	D	404	THR
2	D	407	ILE
2	D	410	VAL
2	D	438	ASN
2	D	445	LYS
2	D	450	SER
2	D	453	GLU
2	D	456	MET
1	B	17	CYS
1	B	34	ILE
1	B	40	HIS
1	B	45	VAL
1	B	49	GLN
1	B	57	GLU
1	B	64	ILE
1	B	84	LYS
1	B	139	VAL
1	B	140	LEU
1	B	141	SER
1	B	148	THR
1	B	151	ILE
1	B	190	MET
1	B	193	LEU
1	B	198	TYR
1	B	201	THR
1	B	210	ARG
1	B	236	LEU
1	B	237	GLU
1	B	248	ILE
1	B	284	LYS
1	B	287	VAL
1	B	288	ASP
1	B	303	THR
1	B	336	LYS
1	B	339	VAL
1	B	351	THR
1	B	368	SER
1	B	372	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	ASN
1	A	173	HIS
1	A	263	GLN
2	C	187	ASN
2	C	261	GLN
2	C	302	HIS
2	D	185	ASN
2	D	207	ASN
2	D	246	ASN
2	D	261	GLN
2	D	406	ASN
2	D	413	GLN
1	B	73	HIS
1	B	128	ASN
1	B	161	HIS
1	B	354	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	ANP	B	401	4	33,33,33	2.10	9 (27%)	45,52,52	2.02	14 (31%)
3	ANP	A	401	4	33,33,33	2.08	9 (27%)	45,52,52	1.95	11 (24%)

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	ANP	B	401	4	-	6/18/38/38	0/3/3/3
3	ANP	A	401	4	-	5/18/38/38	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	ANP	C5-C4	4.67	1.47	1.39
3	B	401	ANP	PG-N3B	4.60	1.75	1.63
3	A	401	ANP	PB-N3B	4.46	1.75	1.63
3	B	401	ANP	PB-N3B	4.46	1.75	1.63
3	A	401	ANP	PG-N3B	4.41	1.74	1.63
3	B	401	ANP	C5-C4	4.35	1.46	1.39
3	B	401	ANP	PB-O1B	3.73	1.51	1.46
3	B	401	ANP	PG-O1G	3.65	1.51	1.46
3	B	401	ANP	PA-O3A	3.62	1.63	1.59
3	A	401	ANP	PG-O1G	3.55	1.51	1.46
3	B	401	ANP	PB-O3A	3.46	1.63	1.59
3	A	401	ANP	PB-O1B	3.39	1.51	1.46
3	A	401	ANP	PA-O3A	3.32	1.63	1.59
3	A	401	ANP	PB-O3A	3.11	1.62	1.59
3	B	401	ANP	C5-C6	2.55	1.48	1.41
3	A	401	ANP	C8-N7	2.51	1.36	1.31
3	A	401	ANP	C5-C6	2.48	1.47	1.41
3	B	401	ANP	C8-N7	2.37	1.36	1.31

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ANP	C5-C4-N3	-5.43	119.25	126.72
3	B	401	ANP	C5-C4-N3	-5.24	119.50	126.72
3	B	401	ANP	O1G-PG-N3B	-5.17	104.16	111.77
3	A	401	ANP	O1G-PG-N3B	-4.98	104.43	111.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	401	ANP	N3-C4-N9	4.54	134.89	127.17
3	A	401	ANP	N3-C4-N9	4.47	134.77	127.17
3	B	401	ANP	N3-C2-N1	-3.72	122.95	128.58
3	B	401	ANP	C2-N3-C4	3.65	120.75	111.83
3	A	401	ANP	C2-N3-C4	3.49	120.36	111.83
3	B	401	ANP	O2B-PB-O1B	3.44	117.25	109.87
3	A	401	ANP	N3-C2-N1	-3.27	123.63	128.58
3	A	401	ANP	O2B-PB-O1B	3.26	116.86	109.87
3	A	401	ANP	O1B-PB-N3B	-3.25	106.99	111.77
3	B	401	ANP	C4-N9-C8	3.20	109.10	105.74
3	B	401	ANP	C4-C5-N7	-2.88	107.29	110.58
3	A	401	ANP	C4-C5-N7	-2.82	107.35	110.58
3	B	401	ANP	C5-N7-C8	2.50	107.37	103.45
3	B	401	ANP	O1B-PB-N3B	-2.42	108.21	111.77
3	A	401	ANP	C4-N9-C8	2.37	108.22	105.74
3	B	401	ANP	N9-C8-N7	-2.33	110.63	113.94
3	A	401	ANP	C5-N7-C8	2.28	107.03	103.45
3	B	401	ANP	C6-C5-N7	2.17	136.28	132.09
3	B	401	ANP	O2G-PG-O3G	2.07	113.16	107.59
3	A	401	ANP	O2G-PG-O3G	2.07	113.15	107.59
3	B	401	ANP	C2-N1-C6	2.02	122.05	118.73

There are no chirality outliers.

All (11) torsion outliers are listed below:

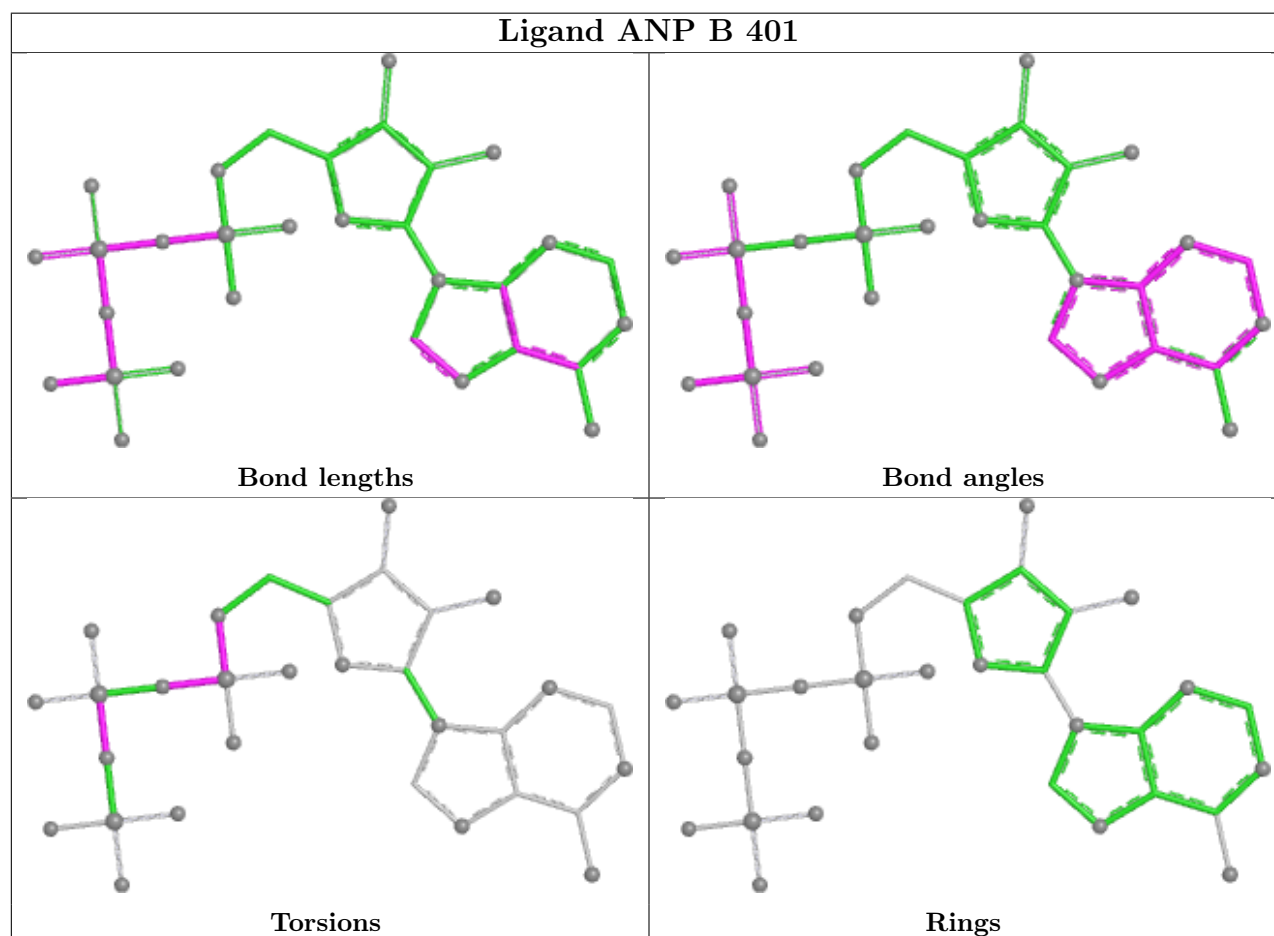
Mol	Chain	Res	Type	Atoms
3	A	401	ANP	PA-O3A-PB-O2B
3	A	401	ANP	O4'-C4'-C5'-O5'
3	B	401	ANP	C5'-O5'-PA-O2A
3	B	401	ANP	C5'-O5'-PA-O3A
3	A	401	ANP	C3'-C4'-C5'-O5'
3	A	401	ANP	C5'-O5'-PA-O1A
3	B	401	ANP	C5'-O5'-PA-O1A
3	B	401	ANP	PB-O3A-PA-O2A
3	A	401	ANP	PA-O3A-PB-O1B
3	B	401	ANP	PG-N3B-PB-O3A
3	B	401	ANP	PB-O3A-PA-O1A

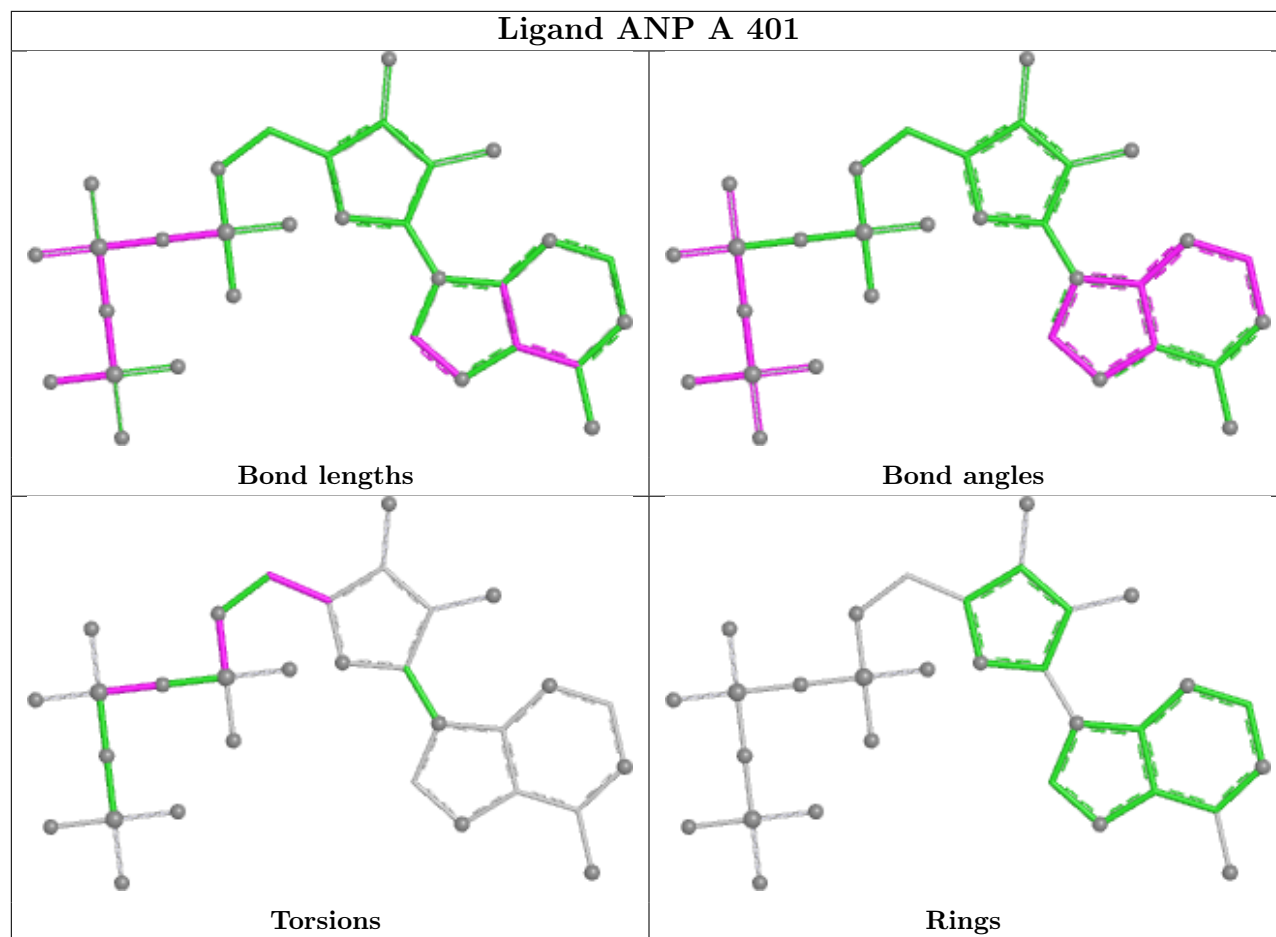
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	401	ANP	2	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	369/384 (96%)	0.31	10 (2%) 56 37	22, 39, 61, 94	0
1	B	369/384 (96%)	0.29	7 (1%) 66 47	22, 38, 63, 82	0
2	C	168/506 (33%)	0.60	8 (4%) 35 22	34, 54, 83, 150	0
2	D	280/506 (55%)	1.40	74 (26%) 1 1	34, 61, 184, 280	0
All	All	1186/1780 (66%)	0.60	99 (8%) 17 11	22, 46, 82, 280	0

All (99) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	430	GLY	7.9
2	D	429	SER	7.6
2	D	428	GLY	7.2
2	D	427	SER	6.5
2	D	451	VAL	6.0
2	D	431	GLY	5.9
2	D	494	LEU	5.7
2	D	433	VAL	5.5
2	D	440	ILE	5.5
2	D	422	GLN	5.2
2	D	426	GLY	5.2
2	D	423	ASN	5.1
2	D	424	GLY	5.0
2	D	389	PRO	4.5
2	D	439	SER	4.5
2	D	432	SER	4.4
2	C	197	LEU	4.3
2	D	457	GLU	4.3
2	D	404	THR	4.2
2	D	425	GLN	4.2
2	D	420	ALA	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	435	SER	4.0
2	D	434	GLY	3.9
1	A	168	GLY	3.9
2	D	393	PRO	3.7
2	D	406	ASN	3.7
2	D	441	LEU	3.6
2	D	193	THR	3.6
2	D	337	TYR	3.6
2	D	336	GLY	3.5
2	C	188	ASN	3.4
1	A	42	GLY	3.4
2	D	458	ASP	3.4
1	B	100	GLU	3.2
1	B	45	VAL	3.2
2	D	465	PRO	3.2
1	A	336	LYS	3.1
1	A	337	TYR	3.1
2	D	189	ILE	3.1
2	D	448	LEU	3.1
2	C	332	LYS	3.0
2	D	450	SER	3.0
2	D	446	ASN	3.0
2	D	391	PRO	3.0
1	B	41	GLN	2.9
2	D	413	GLN	2.9
2	C	193	THR	2.9
2	D	437	PRO	2.9
2	D	335	GLU	2.9
2	D	421	LEU	2.9
1	A	166	TYR	2.9
2	D	412	LYS	2.8
2	D	170	ALA	2.8
2	D	332	LYS	2.8
2	D	390	PRO	2.8
2	D	411	ILE	2.7
2	C	170	ALA	2.7
2	D	438	ASN	2.7
2	D	410	VAL	2.7
2	D	453	GLU	2.7
2	D	338	ASP	2.7
2	D	462	PRO	2.6
2	D	395	PRO	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	328	LEU	2.5
1	A	248	ILE	2.5
2	D	192	ILE	2.5
2	D	399	GLU	2.5
2	C	187	ASN	2.5
1	A	169	TYR	2.4
2	D	398	PRO	2.4
2	D	493	ALA	2.4
2	D	464	THR	2.4
2	D	194	THR	2.4
1	A	44	MET	2.4
2	D	197	LEU	2.4
2	D	276	HIS	2.4
2	C	220	ALA	2.3
2	D	196	THR	2.3
1	A	46	GLY	2.3
1	B	47	MET	2.3
2	D	417	ALA	2.3
2	C	191	ASN	2.3
2	D	454	LYS	2.2
2	D	219	HIS	2.2
2	D	444	ILE	2.2
1	B	201	THR	2.2
2	D	442	LYS	2.2
2	D	275	ARG	2.2
1	A	41	GLN	2.2
2	D	405	ARG	2.1
2	D	419	ARG	2.1
2	D	456	MET	2.1
2	D	452	GLN	2.1
2	D	445	LYS	2.1
1	B	183	ARG	2.1
2	D	443	GLU	2.1
2	D	333	GLN	2.0
2	D	469	ALA	2.0
1	B	44	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

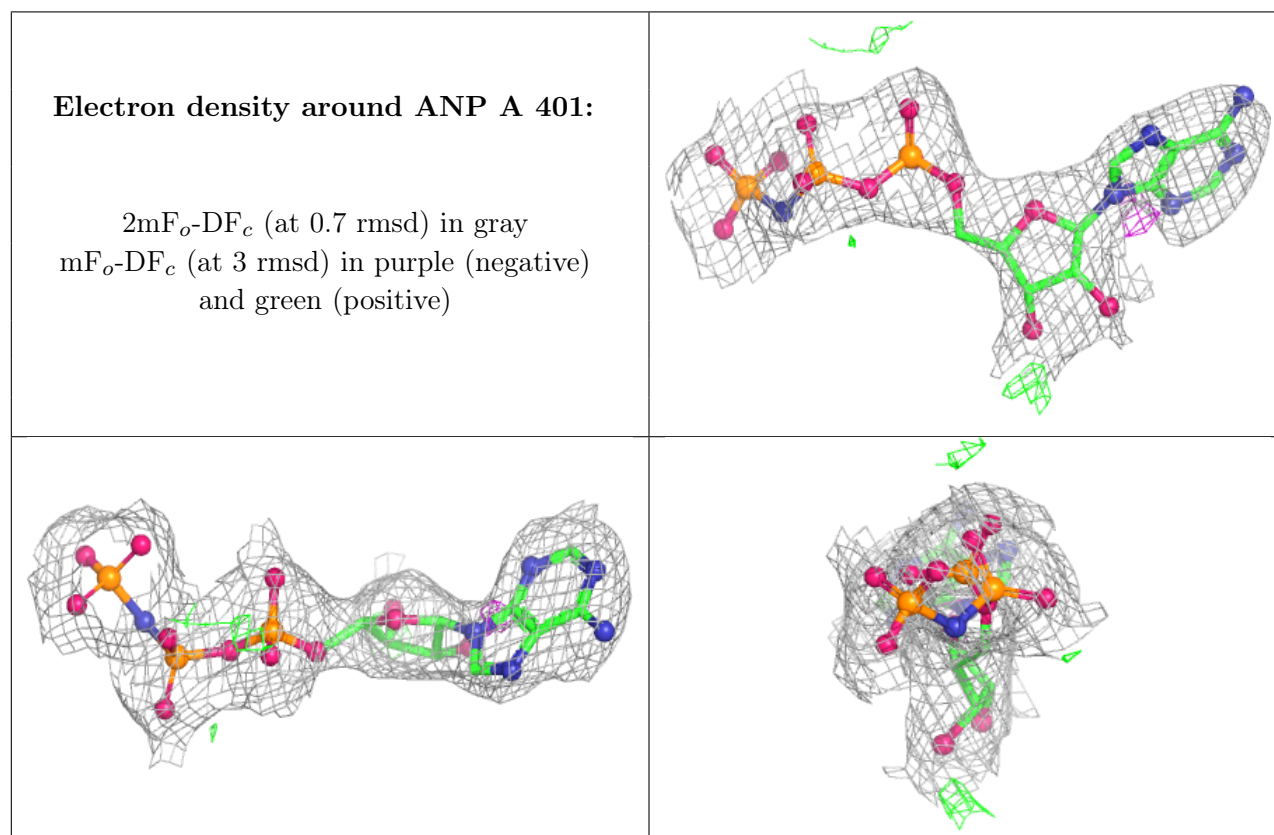
There are no oligosaccharides in this entry.

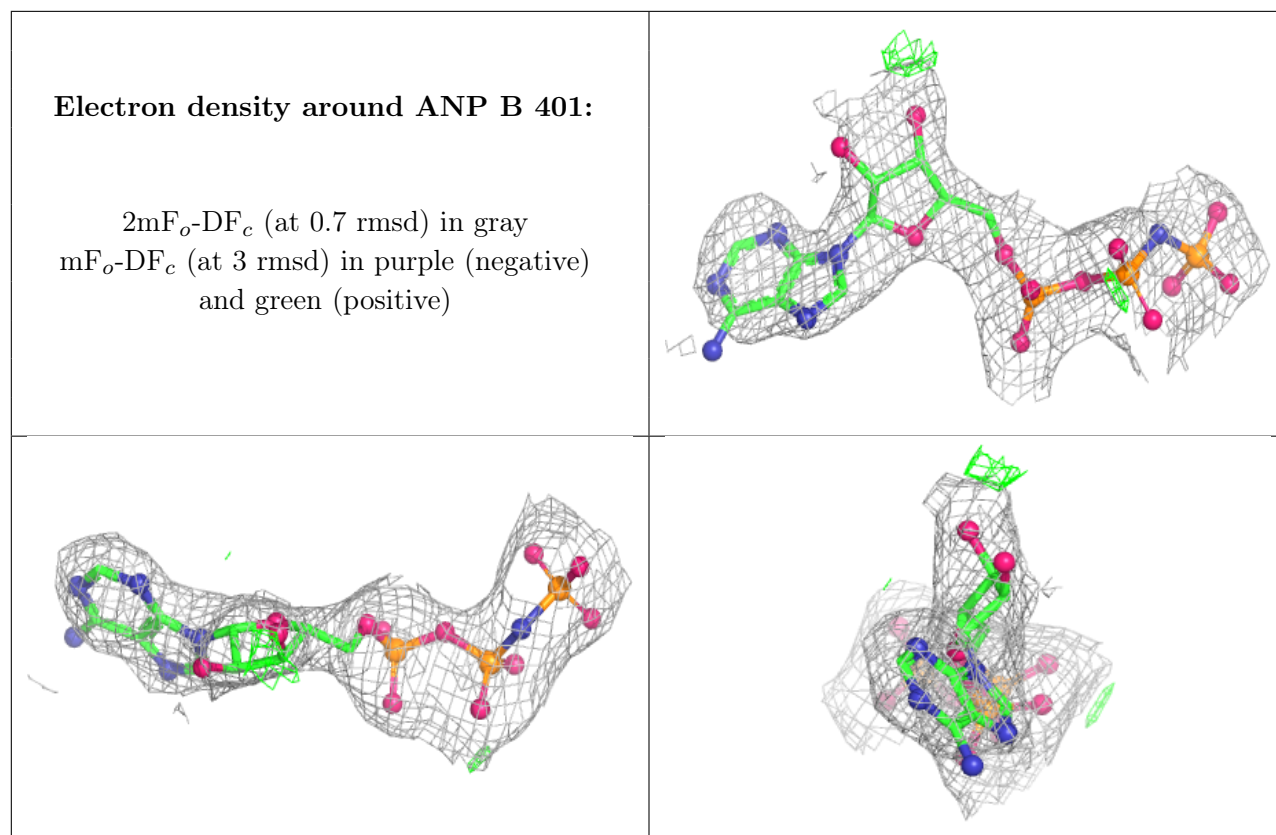
6.4 Ligands [i](#)

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
4	MG	A	402	1/1	0.78	0.21	44,44,44,44	0
4	MG	B	402	1/1	0.84	0.10	39,39,39,39	0
3	ANP	A	401	31/31	0.88	0.10	34,43,55,59	0
3	ANP	B	401	31/31	0.88	0.11	40,50,60,64	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.