



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:17 AM UTC

PDB ID : 4LQQ / pdb_00004lqq
Title : Crystal structure of the Cbk1(T743E)-Mob2 kinase-coactivator complex in crystal form B
Authors : Gogl, G.; Remenyi, A.
Deposited on : 2013-07-19
Resolution : 3.60 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

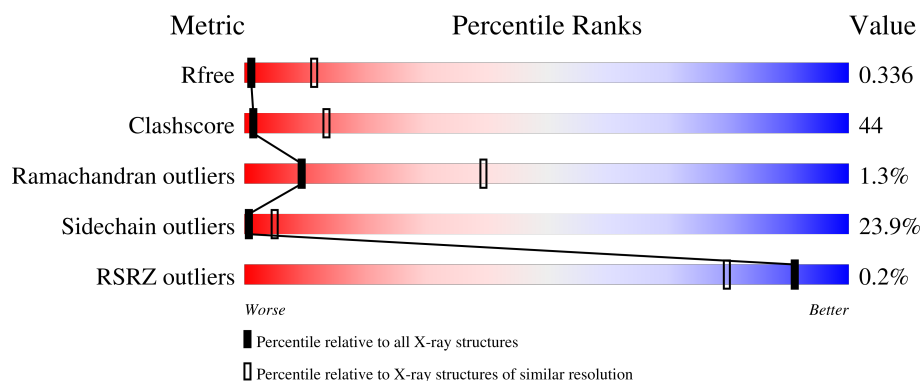
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

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	508	
1	D	508	
2	B	244	
2	E	244	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	ANP	A	801	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7498 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 Serine/threonine-protein kinase CBK1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	S	0	0	0
			2956	1889	513	542	12			
1	D	329	Total	C	N	O	S	0	0	0
			2520	1616	429	464	11			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	249	GLY	-	expression tag	UNP P53894
A	250	SER	-	expression tag	UNP P53894
A	475	ALA	ASP	engineered mutation	UNP P53894
A	743	GLU	THR	engineered mutation	UNP P53894
D	249	GLY	-	expression tag	UNP P53894
D	250	SER	-	expression tag	UNP P53894
D	475	ALA	ASP	engineered mutation	UNP P53894
D	743	GLU	THR	engineered mutation	UNP P53894

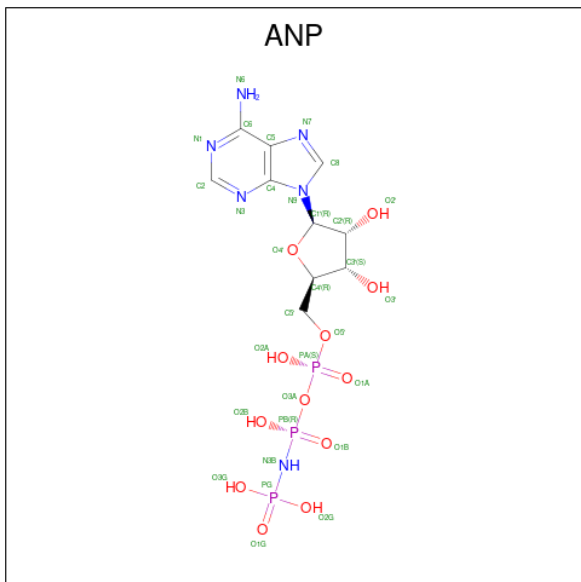
- Molecule 2 is a protein called CBK1 kinase activator protein MOB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O		0	0	0
			1004	651	170	183				
2	E	137	Total	C	N	O	S	0	0	0
			987	645	163	178	1			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	44	GLY	-	expression tag	UNP P43563
B	45	SER	-	expression tag	UNP P43563
E	44	GLY	-	expression tag	UNP P43563
E	45	SER	-	expression tag	UNP P43563

- Molecule 3 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $\text{C}_{10}\text{H}_{17}\text{N}_6\text{O}_{12}\text{P}_3$).

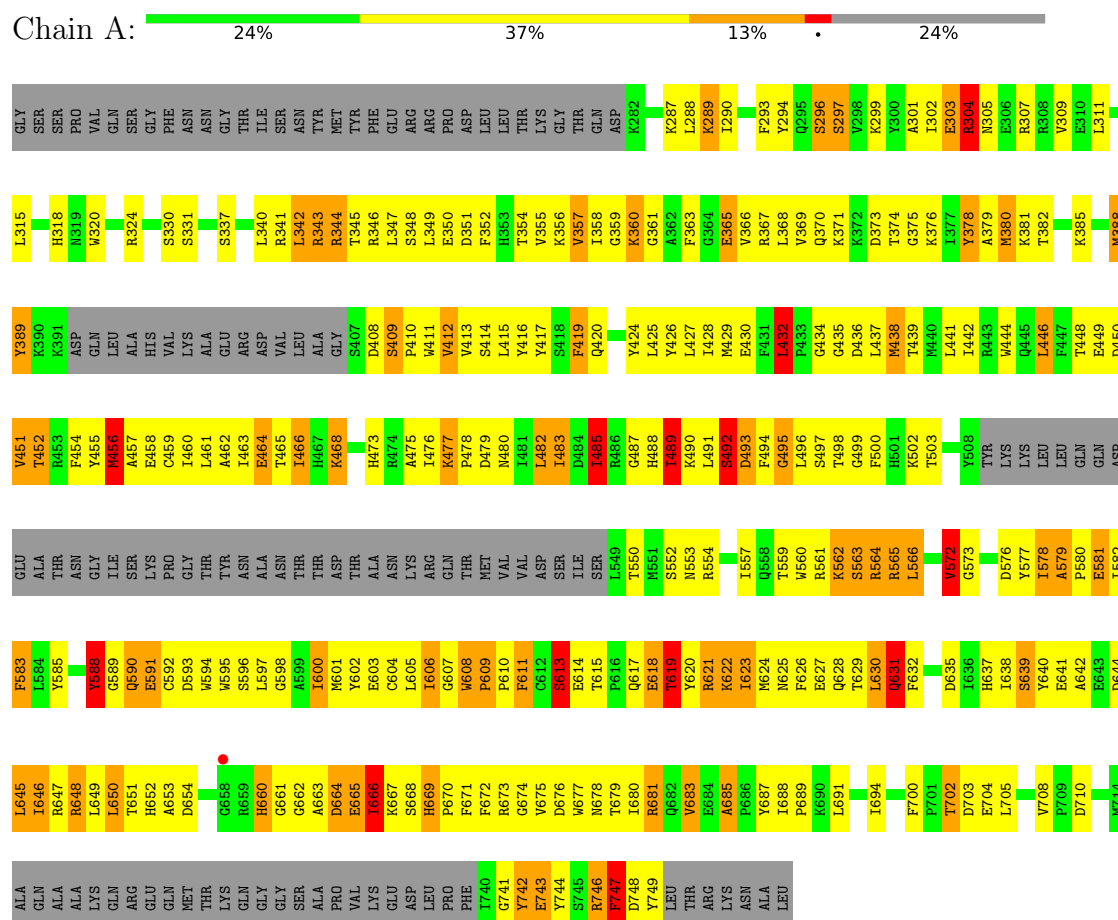


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total 31	C 10	N 6	O 12	P 3	0	0

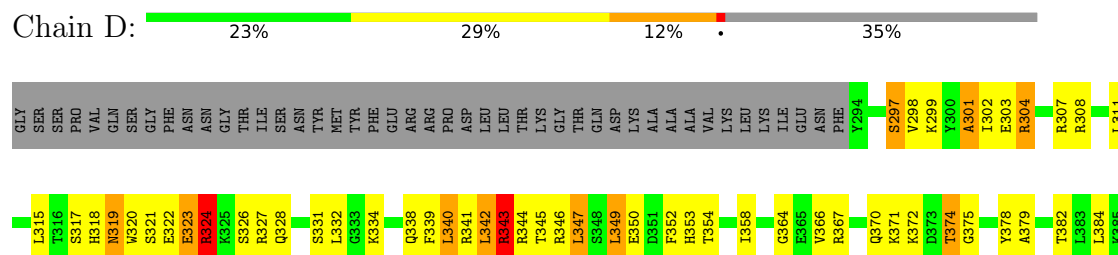
3 Residue-property plots

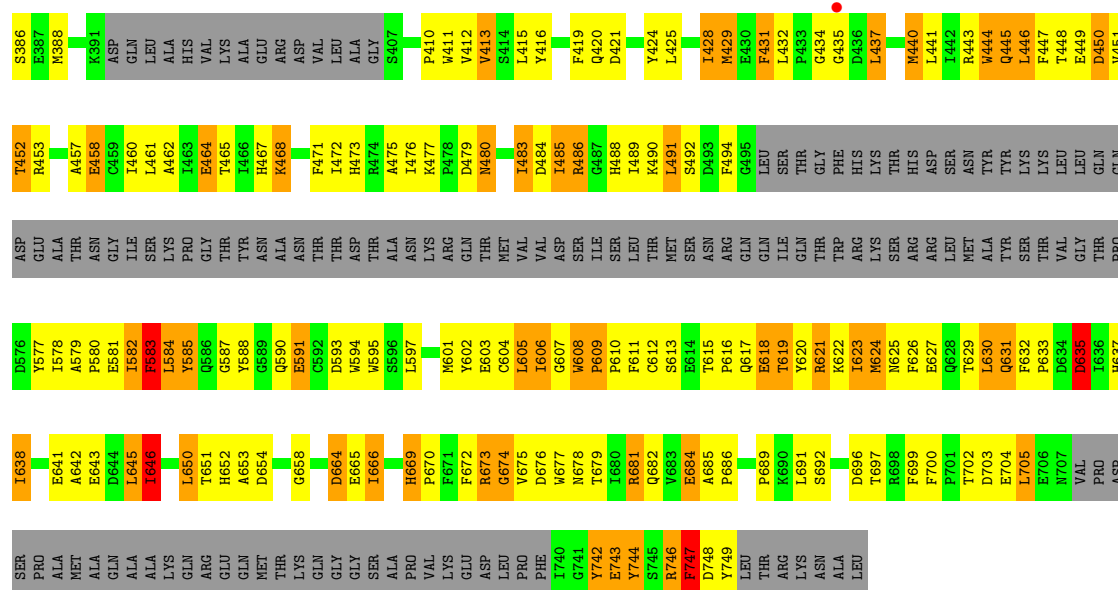
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Serine/threonine-protein kinase CBK1

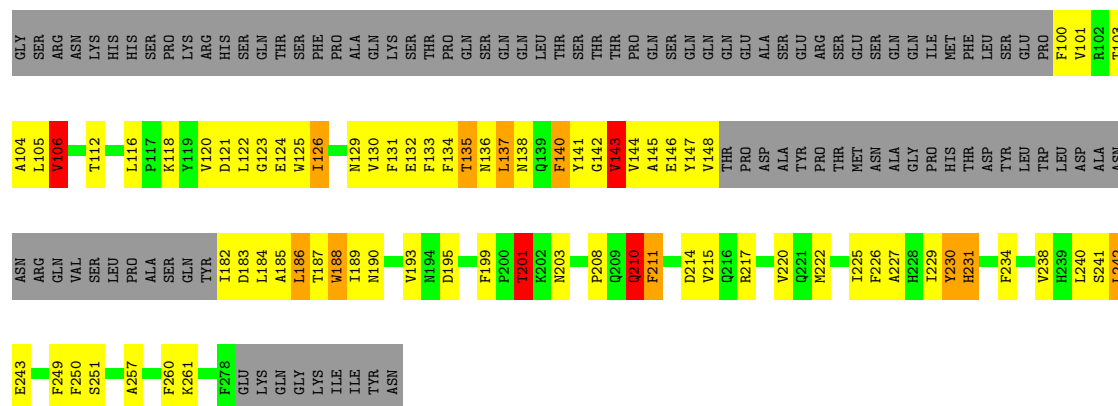
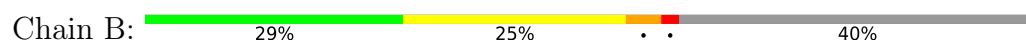


• Molecule 1: Serine/threonine-protein kinase CBK1

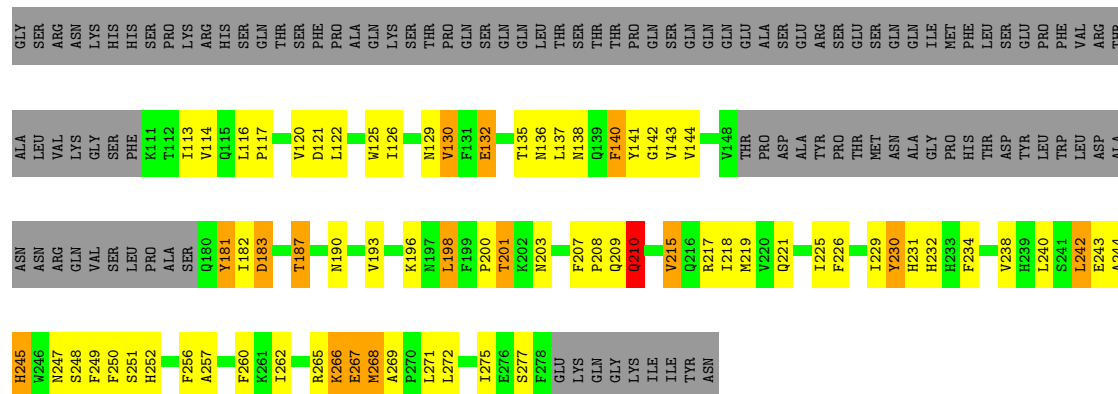
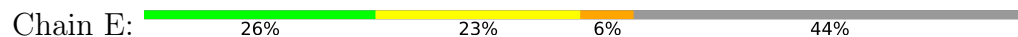




- Molecule 2: CBK1 kinase activator protein MOB2



- Molecule 2: CBK1 kinase activator protein MOB2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	79.74Å 139.06Å 187.58Å 90.00° 90.09° 90.00°	Depositor
Resolution (Å)	46.49 – 3.60 46.49 – 3.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.49-3.60) 98.6 (46.49-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 3.57Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.258 , 0.319 0.255 , 0.336	Depositor DCC
R_{free} test set	1207 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	115.9	Xtriage
Anisotropy	0.239	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 435.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.027 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.026 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.023 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.026 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.428 for h,-k,-l	Xtriage
Reported twinning fraction	0.490 for h,-k,-l	Depositor
Outliers	2 of 23527 reflections (0.009%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7498	wwPDB-VP
Average B, all atoms (Å ²)	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.73	1/3027 (0.0%)	1.40	48/4111 (1.2%)
1	D	0.63	0/2581	1.31	34/3508 (1.0%)
2	B	0.74	1/1033 (0.1%)	1.28	11/1428 (0.8%)
2	E	0.58	0/1014	1.16	11/1395 (0.8%)
All	All	0.68	2/7655 (0.0%)	1.32	104/10442 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
1	D	0	3
2	B	0	2
2	E	0	1
All	All	0	12

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	466	ILE	CA-CB	-5.56	1.48	1.54
2	B	106	VAL	N-CA	5.14	1.52	1.46

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	495	GLY	N-CA-C	11.84	128.77	114.69
1	D	742	TYR	N-CA-C	10.77	126.78	112.88
1	A	742	TYR	N-CA-C	10.38	124.55	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	409	SER	CA-C-N	9.47	129.72	119.87
1	A	409	SER	C-N-CA	9.47	129.72	119.87
1	A	669	HIS	CA-C-N	9.39	129.03	119.82
1	A	669	HIS	C-N-CA	9.39	129.03	119.82
1	A	351	ASP	N-CA-C	-8.80	102.24	113.16
1	D	747	PHE	N-CA-C	8.80	123.40	109.50
2	B	103	THR	N-CA-C	8.79	120.28	107.88
1	A	432	LEU	CA-C-N	8.66	128.38	119.19
1	A	432	LEU	C-N-CA	8.66	128.38	119.19
1	D	579	ALA	CA-C-N	-8.62	109.07	119.84
1	D	579	ALA	C-N-CA	-8.62	109.07	119.84
1	A	741	GLY	N-CA-C	8.48	125.30	110.80
1	A	466	ILE	CB-CA-C	-7.93	101.90	111.81
1	A	653	ALA	N-CA-C	-7.83	103.84	113.15
1	A	491	LEU	N-CA-C	7.61	122.75	113.17
1	D	646	ILE	CB-CA-C	-7.51	102.26	111.88
1	D	331	SER	N-CA-C	-7.45	100.06	110.35
1	A	347	LEU	N-CA-C	7.45	118.38	107.88
1	D	669	HIS	CA-C-N	7.20	126.88	119.82
1	D	669	HIS	C-N-CA	7.20	126.88	119.82
1	D	658	GLY	N-CA-C	-7.18	100.20	110.46
1	A	683	VAL	N-CA-C	-6.96	99.17	108.35
2	B	210	GLN	N-CA-C	-6.89	104.88	113.28
1	D	301	ALA	N-CA-C	-6.83	103.44	111.03
1	D	588	TYR	CB-CA-C	-6.81	108.72	116.63
1	D	635	ASP	N-CA-C	-6.81	96.00	107.99
1	A	609	PRO	CA-C-N	6.77	127.04	119.32
1	A	609	PRO	C-N-CA	6.77	127.04	119.32
1	A	485	ILE	CB-CA-C	-6.63	103.39	111.88
1	A	664	ASP	N-CA-C	-6.47	99.99	109.18
1	D	491	LEU	N-CA-C	6.46	121.33	113.38
1	A	666	ILE	N-CA-C	-6.40	103.62	113.16
1	D	583	PHE	N-CA-C	-6.37	100.47	109.96
1	A	337	SER	N-CA-C	6.36	116.97	108.38
1	A	380	MET	CA-C-N	-6.36	114.57	122.84
1	A	380	MET	C-N-CA	-6.36	114.57	122.84
1	A	702	THR	N-CA-C	-6.35	103.28	111.02
1	D	618	GLU	N-CA-C	-6.32	105.67	113.19
1	A	685	ALA	CA-C-N	6.31	126.79	119.47
1	A	685	ALA	C-N-CA	6.31	126.79	119.47
2	B	203	ASN	N-CA-C	6.30	117.32	108.00
1	A	613	SER	N-CA-C	6.29	121.12	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	579	ALA	CA-C-N	-6.29	111.98	119.84
1	A	579	ALA	C-N-CA	-6.29	111.98	119.84
1	D	588	TYR	N-CA-C	6.23	118.60	108.08
1	D	685	ALA	CA-C-N	6.22	126.41	119.32
1	D	685	ALA	C-N-CA	6.22	126.41	119.32
1	D	324	ARG	N-CA-C	6.14	118.70	111.02
1	D	342	LEU	N-CA-C	-6.14	100.71	108.45
1	A	493	ASP	N-CA-C	6.14	117.56	108.60
2	B	143	VAL	CB-CA-C	-6.14	104.02	112.24
2	B	186	LEU	N-CA-C	-6.09	104.72	111.36
2	E	215	VAL	N-CA-C	6.09	116.73	110.82
1	A	609	PRO	O-C-N	6.05	124.09	121.31
1	A	588	TYR	N-CA-C	6.01	116.90	108.00
2	E	203	ASN	N-CA-C	5.97	116.83	108.00
2	E	210	GLN	N-CA-C	-5.96	106.01	113.28
1	D	331	SER	CA-C-N	5.95	132.41	121.70
1	D	331	SER	C-N-CA	5.95	132.41	121.70
1	A	747	PHE	N-CA-C	5.90	119.17	109.85
1	D	587	GLY	N-CA-C	5.88	120.31	111.42
1	A	378	TYR	N-CA-C	5.85	118.75	108.75
1	D	432	LEU	CA-C-N	5.84	125.46	119.56
1	D	432	LEU	C-N-CA	5.84	125.46	119.56
1	A	631	GLN	N-CA-C	5.83	118.40	108.02
2	B	201	THR	N-CA-C	-5.82	104.12	111.11
1	D	343	ARG	N-CA-C	5.80	117.34	108.52
1	A	482	LEU	N-CA-C	5.76	118.29	108.90
1	A	489	ILE	N-CA-C	5.75	116.15	107.75
1	A	608	TRP	CA-C-N	5.75	123.86	119.66
1	A	608	TRP	C-N-CA	5.75	123.86	119.66
2	B	211	PHE	N-CA-C	-5.73	105.11	111.36
1	D	608	TRP	CA-C-N	5.72	123.78	119.66
1	D	608	TRP	C-N-CA	5.72	123.78	119.66
1	A	361	GLY	N-CA-C	-5.64	100.14	110.97
2	B	188	TRP	N-CA-C	-5.63	105.29	111.82
2	E	196	LYS	N-CA-C	5.59	118.22	111.40
1	A	611	PHE	N-CA-C	5.56	119.75	112.92
2	E	267	GLU	N-CA-C	-5.54	105.34	111.71
2	E	183	ASP	N-CA-C	-5.50	104.93	111.69
1	A	662	GLY	N-CA-C	5.47	122.45	112.27
2	E	201	THR	N-CA-C	-5.46	105.49	111.82
1	A	304	ARG	N-CA-C	-5.46	106.60	113.20
2	E	232	HIS	N-CA-C	5.43	118.37	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	252	HIS	N-CA-C	-5.40	105.31	111.14
1	D	347	LEU	N-CA-C	5.37	115.33	108.24
2	B	104	ALA	N-CA-C	5.36	117.18	110.91
2	B	222	MET	N-CA-C	5.31	118.22	111.69
1	A	360	LYS	N-CA-C	5.30	117.24	109.24
2	E	121	ASP	N-CA-C	-5.27	102.11	109.96
1	D	609	PRO	O-C-N	5.26	123.62	121.15
1	A	344	ARG	N-CA-C	-5.24	106.89	113.28
2	B	203	ASN	CB-CA-C	-5.24	109.01	116.34
1	A	492	SER	N-CA-C	5.23	117.81	109.02
2	E	203	ASN	CB-CA-C	-5.17	109.10	116.34
1	A	451	VAL	CB-CA-C	-5.16	105.26	112.02
1	A	385	LYS	N-CA-C	-5.15	101.71	109.60
1	D	674	GLY	N-CA-C	-5.15	103.81	112.77
1	D	472	ILE	N-CA-C	5.14	115.30	108.11
1	D	384	LEU	N-CA-C	5.08	117.45	108.75
1	D	664	ASP	N-CA-C	-5.08	99.97	110.80

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	289	LYS	Peptide
1	A	550	THR	Peptide
1	A	572	VAL	Peptide
1	A	618	GLU	Peptide
1	A	619	THR	Peptide
1	A	635	ASP	Peptide
2	B	105	LEU	Peptide
2	B	106	VAL	Peptide
1	D	447	PHE	Peptide
1	D	582	ILE	Peptide
1	D	635	ASP	Peptide
2	E	181	TYR	Peptide

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	2956	0	2671	285	0
1	D	2520	0	2280	211	0
2	B	1004	0	774	74	0
2	E	987	0	827	69	0
3	A	31	0	13	12	0
All	All	7498	0	6565	619	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (619) 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:665:GLU:HA	1:A:668:SER:HB3	1.43	1.00
1:A:675:VAL:HG13	1:A:677:TRP:H	1.22	1.00
1:A:366:VAL:HA	1:A:381:LYS:HA	1.46	0.96
1:D:613:SER:HB2	1:D:618:GLU:HB3	1.47	0.95
1:D:446:LEU:HB2	1:D:448:THR:HG23	1.47	0.95
1:A:413:VAL:HG22	1:A:432:LEU:HD13	1.50	0.92
1:A:628:GLN:O	1:A:631:GLN:NE2	2.05	0.89
1:A:664:ASP:C	1:A:666:ILE:H	1.74	0.88
1:A:343:ARG:HG3	1:A:345:THR:H	1.33	0.88
1:A:448:THR:HA	1:A:451:VAL:HB	1.55	0.88
2:E:268:MET:O	2:E:272:LEU:N	2.05	0.88
1:A:297:SER:HB2	2:B:143:VAL:HG22	1.57	0.87
2:B:125:TRP:O	2:B:129:ASN:ND2	2.08	0.86
1:D:413:VAL:HB	1:D:492:SER:HA	1.54	0.86
1:A:465:THR:HA	1:A:468:LYS:HE2	1.57	0.86
1:A:464:GLU:HG2	1:A:663:ALA:HB1	1.56	0.86
2:E:208:PRO:HB2	2:E:210:GLN:HG3	1.56	0.85
2:E:243:GLU:O	2:E:247:ASN:N	2.10	0.85
1:D:448:THR:HB	1:D:452:THR:HB	1.58	0.84
2:B:185:ALA:O	2:B:189:ILE:N	2.10	0.83
1:D:339:PHE:HB3	1:D:341:ARG:HD3	1.59	0.83
2:E:240:LEU:HB3	2:E:242:LEU:HD12	1.61	0.83
1:D:580:PRO:HA	1:D:583:PHE:HE2	1.42	0.81
2:E:181:TYR:O	2:E:183:ASP:N	2.13	0.81
1:D:448:THR:HA	1:D:451:VAL:HB	1.61	0.81
1:A:438:MET:HB2	1:A:478:PRO:HB2	1.62	0.81
1:D:622:LYS:O	1:D:626:PHE:N	2.12	0.81
1:D:610:PRO:HB3	1:D:630:LEU:HD21	1.64	0.80
2:B:184:LEU:O	2:B:188:TRP:N	2.14	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:609:PRO:HG2	1:D:612:CYS:HB2	1.61	0.80
2:E:138:ASN:O	2:E:142:GLY:N	2.13	0.80
1:D:298:VAL:HG22	2:E:240:LEU:HD21	1.64	0.79
1:A:371:LYS:HE2	1:A:373:ASP:HB3	1.63	0.79
1:A:664:ASP:OD2	1:A:665:GLU:N	2.15	0.78
3:A:801:ANP:O3A	3:A:801:ANP:O2G	1.99	0.78
1:A:577:TYR:HB2	1:A:596:SER:HA	1.66	0.77
1:A:592:CYS:O	1:A:596:SER:OG	2.02	0.77
1:D:297:SER:HB3	2:E:143:VAL:HG13	1.67	0.77
1:D:477:LYS:HB2	1:D:480:ASN:HB2	1.65	0.77
1:A:367:ARG:N	1:A:380:MET:O	2.18	0.77
1:D:349:LEU:HD22	1:D:350:GLU:H	1.49	0.77
1:D:601:MET:HE1	1:D:645:LEU:HB3	1.64	0.77
2:E:137:LEU:O	2:E:141:TYR:N	2.16	0.77
2:E:265:ARG:HA	2:E:268:MET:SD	2.24	0.77
1:D:342:LEU:O	1:D:343:ARG:NH2	2.19	0.76
1:D:602:TYR:OH	1:D:631:GLN:O	2.02	0.76
1:A:603:GLU:O	1:A:607:GLY:N	2.18	0.75
2:B:240:LEU:HD23	2:B:242:LEU:HG	1.67	0.75
1:D:486:ARG:HH22	1:D:682:GLN:HB3	1.51	0.75
1:A:294:TYR:HE1	2:B:145:ALA:HB3	1.51	0.75
2:B:241:SER:HA	2:B:243:GLU:OE1	1.86	0.75
1:A:436:ASP:OD2	1:A:439:THR:N	2.14	0.75
2:E:200:PRO:HG2	2:E:207:PHE:HA	1.69	0.75
1:A:610:PRO:HB3	1:A:630:LEU:HD21	1.69	0.74
1:A:652:HIS:CE1	1:D:486:ARG:HH21	2.04	0.74
1:D:343:ARG:HG3	1:D:345:THR:H	1.50	0.74
1:A:436:ASP:HA	1:A:482:LEU:HD23	1.70	0.74
1:D:580:PRO:HA	1:D:583:PHE:CE2	2.21	0.74
1:A:432:LEU:HD21	1:A:490:LYS:HD2	1.68	0.73
1:D:616:PRO:O	1:D:619:THR:OG1	2.06	0.73
2:B:187:THR:HA	2:B:190:ASN:HB2	1.69	0.73
1:D:457:ALA:O	1:D:461:LEU:N	2.18	0.73
1:A:379:ALA:HB3	1:A:429:MET:HB2	1.69	0.73
1:A:646:ILE:O	1:A:650:LEU:N	2.22	0.72
1:A:664:ASP:C	1:A:666:ILE:N	2.46	0.72
1:D:742:TYR:O	1:D:744:TYR:N	2.23	0.71
1:A:646:ILE:HA	1:A:649:LEU:HB2	1.72	0.71
1:A:354:THR:HA	1:A:369:VAL:HG12	1.73	0.71
1:D:374:THR:OG1	1:D:375:GLY:O	2.08	0.71
1:A:647:ARG:O	1:A:651:THR:N	2.24	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:374:THR:OG1	1:A:375:GLY:N	2.23	0.70
3:A:801:ANP:PA	3:A:801:ANP:H8	2.31	0.70
2:E:132:GLU:O	2:E:135:THR:N	2.24	0.70
1:A:439:THR:HA	1:A:442:ILE:HD12	1.72	0.70
1:A:475:ALA:HA	1:A:577:TYR:OH	1.90	0.69
1:A:675:VAL:HG22	1:A:676:ASP:H	1.55	0.69
1:A:460:ILE:O	1:A:464:GLU:N	2.20	0.69
1:A:611:PHE:CZ	1:A:626:PHE:HB3	2.27	0.69
1:A:358:ILE:HB	1:A:366:VAL:HG13	1.74	0.69
1:A:480:ASN:ND2	3:A:801:ANP:O2A	2.23	0.69
2:B:240:LEU:HB3	2:B:242:LEU:HD12	1.75	0.69
1:A:345:THR:OG1	1:A:346:ARG:N	2.26	0.68
1:D:675:VAL:HG13	1:D:677:TRP:H	1.58	0.68
1:A:343:ARG:HG3	1:A:345:THR:N	2.07	0.68
1:A:687:TYR:CE1	1:A:689:PRO:HA	2.29	0.68
1:D:611:PHE:CZ	1:D:626:PHE:HB3	2.28	0.68
1:D:603:GLU:O	1:D:607:GLY:N	2.21	0.68
1:D:673:ARG:HD3	1:D:674:GLY:H	1.59	0.68
1:A:341:ARG:H	2:B:120:VAL:HG13	1.59	0.68
2:E:137:LEU:HG	2:E:249:PHE:HE2	1.59	0.68
1:A:477:LYS:HG3	1:A:480:ASN:HB2	1.75	0.67
1:A:652:HIS:C	1:A:654:ASP:H	2.00	0.67
1:A:413:VAL:HG21	1:A:482:LEU:HD12	1.77	0.67
1:A:413:VAL:HB	1:A:492:SER:HA	1.76	0.67
1:A:626:PHE:HB2	1:A:630:LEU:HB2	1.77	0.67
2:B:210:GLN:O	2:B:214:ASP:N	2.25	0.67
2:B:186:LEU:O	2:B:190:ASN:N	2.23	0.66
1:D:467:HIS:ND1	1:D:590:GLN:HB2	2.10	0.66
2:B:227:ALA:O	2:B:231:HIS:N	2.20	0.66
1:A:437:LEU:HA	1:A:483:ILE:HD11	1.76	0.66
1:D:615:THR:OG1	1:D:617:GLN:NE2	2.26	0.66
1:A:456:MET:HA	1:A:459:CYS:SG	2.35	0.66
1:A:611:PHE:HZ	1:A:626:PHE:HB3	1.61	0.66
2:B:116:LEU:HD22	2:B:122:LEU:HD13	1.77	0.65
1:D:486:ARG:HH11	1:D:486:ARG:HB2	1.62	0.65
1:A:566:LEU:HD23	1:A:566:LEU:H	1.62	0.65
2:B:183:ASP:O	2:B:187:THR:OG1	2.13	0.65
1:D:323:GLU:OE1	1:D:324:ARG:N	2.25	0.65
1:A:626:PHE:O	1:A:629:THR:N	2.22	0.65
1:D:484:ASP:OD1	1:D:488:HIS:N	2.30	0.65
1:D:689:PRO:HB2	1:D:691:LEU:HD21	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:215:VAL:O	2:E:219:MET:N	2.30	0.64
2:E:141:TYR:CD1	2:E:144:VAL:HB	2.32	0.64
1:D:621:ARG:O	1:D:625:ASN:N	2.30	0.64
1:A:435:GLY:HA2	1:A:700:PHE:CZ	2.32	0.63
1:D:620:TYR:HA	1:D:623:ILE:HG23	1.79	0.63
1:A:708:VAL:O	1:A:710:ASP:N	2.31	0.63
1:A:438:MET:HA	1:A:441:LEU:HD12	1.81	0.63
1:A:476:ILE:HB	1:A:596:SER:HB3	1.81	0.63
1:A:495:GLY:N	1:A:496:LEU:HA	2.13	0.63
1:A:613:SER:HB3	1:A:618:GLU:HB3	1.80	0.63
1:A:462:ALA:O	1:A:466:ILE:HG13	1.98	0.62
1:A:645:LEU:O	1:A:649:LEU:N	2.31	0.62
1:D:353:HIS:N	1:D:370:GLN:O	2.28	0.62
1:D:613:SER:C	1:D:615:THR:H	2.07	0.62
1:A:624:MET:HE2	1:D:679:THR:HA	1.81	0.62
1:D:491:LEU:HD23	1:D:491:LEU:H	1.63	0.62
1:A:592:CYS:SG	1:A:593:ASP:N	2.72	0.62
1:D:332:LEU:C	1:D:334:LYS:H	2.08	0.62
1:A:345:THR:HB	2:B:201:THR:HG23	1.82	0.62
1:A:483:ILE:HG22	1:A:487:GLY:HA2	1.82	0.62
1:A:494:PHE:O	1:A:497:SER:N	2.33	0.62
1:D:458:GLU:HA	1:D:461:LEU:HB2	1.83	0.61
1:A:582:ILE:HA	1:A:588:TYR:CD1	2.36	0.61
1:A:340:LEU:N	1:A:341:ARG:HA	2.16	0.61
2:E:181:TYR:C	2:E:183:ASP:H	2.07	0.60
1:A:742:TYR:O	1:A:744:TYR:N	2.34	0.60
1:D:577:TYR:O	1:D:595:TRP:NE1	2.28	0.60
1:A:363:PHE:CE2	1:A:497:SER:HA	2.36	0.60
2:E:243:GLU:OE1	2:E:243:GLU:N	2.29	0.60
2:E:114:VAL:HB	2:E:256:PHE:HD1	1.66	0.60
1:A:748:ASP:HB3	1:A:749:TYR:HD2	1.67	0.60
2:B:141:TYR:O	2:B:145:ALA:N	2.34	0.60
1:D:635:ASP:OD1	1:D:635:ASP:N	2.35	0.60
2:E:268:MET:HB2	2:E:272:LEU:HG	1.83	0.59
2:E:218:ILE:HA	2:E:221:GLN:HG2	1.84	0.59
1:A:687:TYR:CZ	1:A:689:PRO:HA	2.38	0.59
1:A:479:ASP:HB2	3:A:801:ANP:O3'	2.02	0.59
1:A:577:TYR:H	1:A:577:TYR:HD2	1.49	0.59
1:A:619:THR:HG22	1:A:623:ILE:HB	1.84	0.59
1:A:625:ASN:O	1:A:627:GLU:HG2	2.02	0.59
3:A:801:ANP:O2A	3:A:801:ANP:H3'	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:326:SER:C	1:D:328:GLN:H	2.10	0.59
2:E:140:PHE:O	2:E:144:VAL:HG23	2.01	0.59
2:E:198:LEU:HA	2:E:208:PRO:HG3	1.84	0.59
1:A:675:VAL:HG13	1:A:677:TRP:N	2.06	0.59
1:D:307:ARG:HH22	1:D:311:LEU:HD22	1.66	0.59
1:D:613:SER:HB3	1:D:619:THR:HG23	1.84	0.59
1:A:358:ILE:HD11	1:A:368:LEU:HB2	1.85	0.59
1:A:415:LEU:HD12	1:A:428:ILE:O	2.02	0.59
2:E:266:LYS:HD3	2:E:267:GLU:N	2.18	0.59
2:E:141:TYR:HA	2:E:144:VAL:HG23	1.84	0.58
2:B:134:PHE:HE1	2:B:186:LEU:HB2	1.68	0.58
2:E:137:LEU:HA	2:E:140:PHE:HB2	1.83	0.58
1:A:425:LEU:HD22	1:A:426:TYR:H	1.67	0.58
1:D:462:ALA:O	1:D:465:THR:OG1	2.19	0.58
1:A:348:SER:OG	1:A:349:LEU:N	2.35	0.58
2:E:245:HIS:H	2:E:245:HIS:CD2	2.20	0.58
1:A:307:ARG:HH12	1:A:311:LEU:HD22	1.69	0.58
1:A:603:GLU:HG3	1:A:608:TRP:N	2.19	0.58
1:D:379:ALA:HB2	1:D:431:PHE:HB2	1.85	0.58
1:A:294:TYR:HD2	2:B:147:TYR:HH	1.50	0.57
1:A:344:ARG:O	1:A:742:TYR:HD2	1.87	0.57
1:D:379:ALA:N	1:D:429:MET:O	2.23	0.57
1:A:617:GLN:CD	1:A:617:GLN:H	2.12	0.57
2:E:229:ILE:O	2:E:234:PHE:N	2.37	0.57
1:A:365:GLU:O	1:A:382:THR:N	2.38	0.56
1:D:613:SER:HB2	1:D:618:GLU:CB	2.29	0.56
1:D:689:PRO:HA	1:D:699:PHE:HZ	1.70	0.56
1:D:601:MET:HE3	1:D:646:ILE:HG12	1.86	0.56
1:A:446:LEU:HB2	1:A:448:THR:CG2	2.36	0.56
1:A:494:PHE:CE1	1:A:496:LEU:HD22	2.40	0.56
1:A:502:LYS:HB2	1:A:503:THR:HA	1.86	0.56
1:A:557:ILE:O	1:A:561:ARG:HG3	2.05	0.56
2:B:134:PHE:CE1	2:B:186:LEU:HB2	2.39	0.56
1:D:416:TYR:HD2	1:D:428:ILE:HG22	1.71	0.56
1:D:645:LEU:HG	1:D:669:HIS:CE1	2.40	0.56
2:E:268:MET:O	2:E:271:LEU:N	2.38	0.56
1:A:342:LEU:HD11	1:A:344:ARG:HE	1.71	0.56
1:A:454:PHE:HZ	1:A:488:HIS:CE1	2.21	0.56
1:A:648:ARG:O	1:A:651:THR:HG22	2.06	0.56
1:D:308:ARG:HH22	2:E:249:PHE:HD1	1.53	0.56
1:A:381:LYS:N	1:A:427:LEU:O	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:LEU:HD22	1:A:426:TYR:N	2.20	0.56
2:B:229:ILE:O	2:B:234:PHE:N	2.39	0.56
1:D:307:ARG:O	1:D:307:ARG:NH1	2.32	0.56
1:D:340:LEU:N	1:D:341:ARG:HA	2.20	0.56
1:A:369:VAL:HG23	1:A:378:TYR:HB2	1.88	0.56
2:B:100:PHE:CB	2:B:101:VAL:HA	2.36	0.56
1:D:437:LEU:HD12	1:D:441:LEU:HG	1.87	0.56
1:A:601:MET:HE3	1:A:646:ILE:HG12	1.87	0.56
2:B:126:ILE:HG21	2:B:215:VAL:HG21	1.88	0.56
1:D:420:GLN:HB3	1:D:425:LEU:HA	1.86	0.55
1:D:464:GLU:OE1	1:D:468:LYS:NZ	2.33	0.55
1:A:434:GLY:HA3	1:A:483:ILE:HB	1.87	0.55
1:D:343:ARG:HB3	1:D:345:THR:HG23	1.88	0.55
1:D:437:LEU:HD11	1:D:446:LEU:HD21	1.87	0.55
1:D:491:LEU:O	1:D:492:SER:OG	2.22	0.55
1:A:619:THR:HA	1:A:620:TYR:O	2.07	0.55
1:A:663:ALA:O	1:A:667:LYS:HG3	2.06	0.55
1:A:452:THR:O	1:A:456:MET:HB2	2.06	0.55
1:A:577:TYR:CG	1:A:578:ILE:N	2.72	0.55
1:A:371:LYS:HB3	1:A:375:GLY:H	1.72	0.55
1:A:463:ILE:HA	1:A:466:ILE:HD12	1.86	0.55
1:D:651:THR:OG1	1:D:652:HIS:N	2.40	0.55
1:A:297:SER:HB2	2:B:143:VAL:CG2	2.35	0.54
1:A:603:GLU:O	1:A:606:ILE:N	2.40	0.54
2:B:116:LEU:N	2:B:260:PHE:HZ	2.05	0.54
2:E:257:ALA:O	2:E:262:ILE:N	2.35	0.54
1:A:457:ALA:O	1:A:460:ILE:N	2.40	0.54
1:A:638:ILE:HG22	1:A:639:SER:O	2.07	0.54
2:B:126:ILE:O	2:B:130:VAL:HG13	2.07	0.54
1:D:388:MET:HE3	1:D:388:MET:HA	1.87	0.54
2:B:195:ASP:O	2:B:199:PHE:HB2	2.08	0.54
1:A:611:PHE:CD2	1:A:623:ILE:HG12	2.42	0.54
1:D:299:LYS:HA	1:D:302:ILE:HG12	1.90	0.54
1:D:585:TYR:H	1:D:585:TYR:HD2	1.54	0.54
1:A:632:PHE:HE1	1:A:647:ARG:HE	1.54	0.54
1:A:746:ARG:HH21	1:A:747:PHE:C	2.15	0.54
1:D:486:ARG:HB2	1:D:486:ARG:NH1	2.22	0.54
1:D:673:ARG:CD	1:D:674:GLY:H	2.21	0.54
2:E:238:VAL:HA	2:E:243:GLU:OE1	2.07	0.54
1:A:498:THR:OG1	1:A:499:GLY:N	2.29	0.54
2:B:125:TRP:CD1	2:B:126:ILE:HD13	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ASP:HA	1:A:667:LYS:H	1.73	0.54
1:D:410:PRO:HB2	1:D:681:ARG:NH2	2.23	0.54
1:D:591:GLU:CD	1:D:591:GLU:H	2.15	0.53
1:A:330:SER:OG	1:A:331:SER:N	2.41	0.53
1:A:581:GLU:HG3	1:A:588:TYR:HA	1.89	0.53
1:D:343:ARG:HA	1:D:343:ARG:NE	2.23	0.53
1:A:414:SER:H	1:A:430:GLU:HG2	1.72	0.53
1:A:424:TYR:HB2	1:A:426:TYR:CZ	2.44	0.53
1:A:618:GLU:HG3	1:A:622:LYS:HE2	1.89	0.53
2:E:244:ALA:HA	2:E:247:ASN:HB2	1.90	0.53
2:B:120:VAL:HG12	2:B:121:ASP:O	2.08	0.53
2:B:134:PHE:HD2	2:B:135:THR:HG23	1.72	0.53
2:B:142:GLY:HA2	2:B:145:ALA:HB2	1.89	0.53
1:D:619:THR:HG22	1:D:623:ILE:HG22	1.90	0.53
1:A:380:MET:HE1	1:A:426:TYR:HB3	1.91	0.53
1:D:342:LEU:HB2	1:D:747:PHE:CZ	2.43	0.53
1:A:297:SER:CB	2:B:143:VAL:HG22	2.36	0.53
1:A:299:LYS:O	1:A:303:GLU:HB3	2.08	0.53
2:B:230:TYR:HE2	2:B:250:PHE:CD2	2.26	0.53
1:D:301:ALA:O	1:D:304:ARG:N	2.40	0.53
1:D:697:THR:O	1:D:700:PHE:HD2	1.91	0.53
1:D:315:LEU:HG	1:D:318:HIS:NE2	2.23	0.53
1:D:307:ARG:HH11	1:D:307:ARG:C	2.14	0.53
1:A:446:LEU:HB2	1:A:448:THR:HG22	1.90	0.52
1:A:448:THR:HB	1:A:452:THR:HB	1.90	0.52
2:B:217:ARG:O	2:B:220:VAL:HG22	2.09	0.52
2:B:193:VAL:HA	2:B:199:PHE:CD2	2.45	0.52
1:A:381:LYS:NZ	3:A:801:ANP:O1A	2.28	0.52
1:A:601:MET:HA	1:A:604:CYS:SG	2.50	0.52
1:D:411:TRP:HZ2	1:D:461:LEU:HD13	1.74	0.52
1:A:676:ASP:OD1	1:A:679:THR:OG1	2.16	0.52
2:B:122:LEU:HD12	2:B:125:TRP:HD1	1.74	0.52
2:E:226:PHE:CE1	2:E:250:PHE:HA	2.45	0.52
1:D:602:TYR:CG	1:D:610:PRO:HG3	2.45	0.52
1:A:560:TRP:O	1:A:563:SER:OG	2.26	0.52
1:A:610:PRO:HB2	1:A:611:PHE:CD2	2.44	0.52
1:A:652:HIS:C	1:A:654:ASP:N	2.67	0.52
1:A:594:TRP:HA	1:A:594:TRP:CE3	2.45	0.52
1:D:379:ALA:HB2	1:D:431:PHE:CB	2.40	0.52
2:E:208:PRO:C	2:E:210:GLN:H	2.17	0.52
1:A:370:GLN:HG3	1:A:376:LYS:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:THR:HA	1:A:620:TYR:C	2.35	0.52
1:D:602:TYR:O	1:D:606:ILE:HB	2.08	0.52
1:A:475:ALA:HA	1:A:577:TYR:CZ	2.44	0.51
1:A:490:LYS:HG3	1:A:681:ARG:HH22	1.74	0.51
1:A:448:THR:OG1	1:A:449:GLU:N	2.44	0.51
2:B:257:ALA:O	2:B:261:LYS:N	2.43	0.51
1:A:315:LEU:O	1:A:318:HIS:HB2	2.09	0.51
2:B:121:ASP:CG	2:B:124:GLU:H	2.19	0.51
1:A:304:ARG:HA	1:A:307:ARG:HB3	1.93	0.51
1:A:580:PRO:HD3	1:A:595:TRP:CZ2	2.46	0.51
1:A:613:SER:HB3	1:A:618:GLU:CB	2.40	0.51
1:A:742:TYR:C	1:A:744:TYR:H	2.19	0.51
1:A:598:GLY:CA	1:A:649:LEU:HD13	2.39	0.51
1:A:459:CYS:O	1:A:463:ILE:HG13	2.11	0.50
2:B:122:LEU:O	2:B:126:ILE:N	2.32	0.50
1:D:320:TRP:HZ2	1:D:341:ARG:HH22	1.58	0.50
1:D:460:ILE:HG23	1:D:594:TRP:HZ3	1.75	0.50
1:A:315:LEU:HG	1:A:318:HIS:ND1	2.26	0.50
1:A:564:ARG:O	1:A:565:ARG:HD2	2.12	0.50
1:A:660:HIS:N	1:A:661:GLY:HA3	2.26	0.50
2:B:122:LEU:HD12	2:B:125:TRP:CD1	2.47	0.50
2:B:134:PHE:CD2	2:B:135:THR:HG23	2.45	0.50
2:B:137:LEU:HG	2:B:249:PHE:HE2	1.75	0.50
2:E:238:VAL:HA	2:E:243:GLU:HB3	1.93	0.50
1:A:613:SER:HB3	1:A:618:GLU:C	2.35	0.50
2:B:122:LEU:HG	2:B:126:ILE:HG12	1.93	0.50
2:B:146:GLU:C	2:B:148:VAL:H	2.19	0.50
1:D:467:HIS:NE2	1:D:593:ASP:OD2	2.43	0.50
1:D:619:THR:HA	1:D:620:TYR:C	2.36	0.50
2:E:122:LEU:O	2:E:126:ILE:HG12	2.11	0.50
2:B:193:VAL:HA	2:B:199:PHE:CG	2.46	0.50
1:D:692:SER:OG	1:D:696:ASP:OD1	2.18	0.50
1:D:343:ARG:HA	1:D:343:ARG:CZ	2.42	0.50
1:A:344:ARG:HB3	1:A:742:TYR:HB2	1.93	0.50
1:A:594:TRP:HA	1:A:594:TRP:HE3	1.76	0.50
2:E:221:GLN:O	2:E:225:ILE:HD12	2.11	0.50
1:D:346:ARG:NH2	2:E:193:VAL:O	2.44	0.50
1:D:349:LEU:CD2	1:D:350:GLU:H	2.21	0.50
1:D:638:ILE:HG21	1:D:643:GLU:HB2	1.92	0.50
1:A:349:LEU:HD23	1:A:350:GLU:N	2.26	0.50
1:D:342:LEU:O	1:D:343:ARG:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:602:TYR:CE1	1:D:606:ILE:HG21	2.47	0.50
1:A:663:ALA:H	1:A:666:ILE:HD12	1.77	0.49
1:D:326:SER:C	1:D:328:GLN:N	2.70	0.49
1:D:346:ARG:HH21	2:E:193:VAL:HG23	1.77	0.49
1:A:371:LYS:CE	1:A:373:ASP:HB3	2.40	0.49
1:A:601:MET:O	1:A:605:LEU:HG	2.12	0.49
1:A:611:PHE:CG	1:A:623:ILE:HG12	2.48	0.49
2:E:247:ASN:O	2:E:250:PHE:HB3	2.12	0.49
1:A:606:ILE:HG22	1:A:608:TRP:H	1.77	0.49
1:D:621:ARG:N	1:D:624:MET:HB2	2.28	0.49
1:A:356:LYS:O	1:A:367:ARG:HG2	2.13	0.49
1:A:420:GLN:HB3	1:A:425:LEU:HA	1.94	0.49
2:E:141:TYR:HA	2:E:144:VAL:CG2	2.43	0.49
1:A:626:PHE:N	1:A:629:THR:OG1	2.46	0.49
3:A:801:ANP:O1A	3:A:801:ANP:O1B	2.31	0.49
1:D:346:ARG:HG2	1:D:347:LEU:N	2.28	0.49
1:A:425:LEU:CD1	1:A:427:LEU:HG	2.43	0.49
1:A:461:LEU:O	1:A:465:THR:HG23	2.13	0.49
1:A:598:GLY:HA2	1:A:649:LEU:HD13	1.93	0.49
1:D:606:ILE:HG13	1:D:633:PRO:HD2	1.93	0.49
2:B:133:PHE:HA	2:B:136:ASN:OD1	2.13	0.48
1:D:412:VAL:HG12	1:D:413:VAL:O	2.13	0.48
1:A:429:MET:SD	3:A:801:ANP:N6	2.86	0.48
1:A:498:THR:HG1	1:A:499:GLY:H	1.60	0.48
2:B:118:LYS:O	2:B:120:VAL:HG23	2.13	0.48
2:E:117:PRO:HD2	2:E:125:TRP:CD2	2.49	0.48
2:B:135:THR:HA	2:B:138:ASN:OD1	2.12	0.48
2:B:225:ILE:O	2:B:229:ILE:HG13	2.13	0.48
1:D:742:TYR:C	1:D:744:TYR:H	2.22	0.48
1:A:572:VAL:CB	1:A:573:GLY:HA2	2.43	0.48
1:A:582:ILE:HA	1:A:588:TYR:HD1	1.77	0.48
1:D:473:HIS:CE1	1:D:475:ALA:HB3	2.47	0.48
2:E:245:HIS:CD2	2:E:245:HIS:N	2.80	0.48
1:A:603:GLU:OE2	1:A:609:PRO:HD3	2.13	0.48
2:B:131:PHE:O	2:B:134:PHE:HB3	2.14	0.48
1:D:435:GLY:HA2	1:D:700:PHE:CE1	2.49	0.48
1:A:301:ALA:O	1:A:304:ARG:NH1	2.47	0.48
1:A:380:MET:SD	1:A:426:TYR:HB3	2.54	0.48
1:A:582:ILE:HA	1:A:588:TYR:CE1	2.49	0.47
1:A:642:ALA:HB2	1:A:671:PHE:CE2	2.49	0.47
2:B:241:SER:HA	2:B:243:GLU:CD	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:307:ARG:NH1	1:D:308:ARG:HD3	2.28	0.47
1:D:317:SER:O	1:D:320:TRP:CG	2.67	0.47
1:A:359:GLY:HA3	3:A:801:ANP:H4'	1.95	0.47
1:A:579:ALA:HB2	1:A:595:TRP:HB3	1.95	0.47
3:A:801:ANP:H8	3:A:801:ANP:O5'	2.15	0.47
1:D:346:ARG:NH2	2:E:193:VAL:HG23	2.29	0.47
1:D:608:TRP:HE3	1:D:609:PRO:O	1.97	0.47
1:A:417:TYR:CZ	1:A:428:ILE:HG21	2.48	0.47
1:A:460:ILE:H	1:A:460:ILE:HG13	1.43	0.47
1:A:594:TRP:HZ2	1:A:663:ALA:HB2	1.79	0.47
2:E:116:LEU:H	2:E:260:PHE:HZ	1.61	0.47
2:E:125:TRP:O	2:E:129:ASN:ND2	2.48	0.47
1:A:644:ASP:OD2	1:A:648:ARG:NH2	2.24	0.47
1:A:646:ILE:CA	1:A:649:LEU:HB2	2.42	0.47
1:A:664:ASP:HB2	1:A:667:LYS:HE3	1.95	0.47
2:B:121:ASP:OD1	2:B:123:GLY:N	2.47	0.47
1:D:675:VAL:HG22	1:D:676:ASP:H	1.79	0.47
2:E:129:ASN:HA	2:E:132:GLU:CD	2.40	0.47
2:E:183:ASP:O	2:E:187:THR:OG1	2.33	0.47
1:D:332:LEU:C	1:D:334:LYS:N	2.73	0.47
1:D:477:LYS:O	1:D:480:ASN:N	2.46	0.47
2:E:116:LEU:HD22	2:E:122:LEU:HD13	1.96	0.47
2:E:226:PHE:HE1	2:E:250:PHE:HA	1.80	0.47
1:D:623:ILE:O	1:D:623:ILE:HG12	2.14	0.47
1:D:748:ASP:HA	1:D:749:TYR:HA	1.53	0.47
2:B:116:LEU:H	2:B:260:PHE:HZ	1.61	0.47
1:D:350:GLU:O	1:D:372:LYS:HD2	2.15	0.47
1:D:617:GLN:C	1:D:619:THR:N	2.72	0.47
1:A:427:LEU:HD23	1:A:427:LEU:HA	1.62	0.47
1:A:624:MET:HE3	1:D:682:GLN:NE2	2.30	0.47
1:A:665:GLU:CA	1:A:668:SER:HB3	2.29	0.47
2:B:182:ILE:HD12	2:B:225:ILE:HG13	1.95	0.47
1:D:582:ILE:HG22	1:D:583:PHE:N	2.30	0.47
1:A:297:SER:HB2	2:B:143:VAL:HG13	1.97	0.46
1:D:344:ARG:O	1:D:742:TYR:HD2	1.98	0.46
1:D:673:ARG:HD3	1:D:674:GLY:N	2.29	0.46
2:E:120:VAL:HG11	2:E:125:TRP:HB2	1.97	0.46
1:D:332:LEU:O	1:D:334:LYS:N	2.37	0.46
1:D:366:VAL:HG22	1:D:367:ARG:H	1.80	0.46
1:D:595:TRP:CD1	1:D:595:TRP:C	2.93	0.46
2:E:141:TYR:HD1	2:E:144:VAL:HB	1.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:198:LEU:HD23	2:E:208:PRO:HG3	1.97	0.46
1:A:590:GLN:HG3	1:A:591:GLU:N	2.29	0.46
2:B:185:ALA:HA	2:B:188:TRP:HB3	1.97	0.46
1:A:360:LYS:O	3:A:801:ANP:O2G	2.33	0.46
1:A:379:ALA:O	1:A:428:ILE:HA	2.15	0.46
1:A:448:THR:HG21	1:A:605:LEU:HD23	1.97	0.46
1:D:749:TYR:N	1:D:749:TYR:CD2	2.84	0.46
1:A:304:ARG:HH11	1:A:304:ARG:HB3	1.80	0.46
1:A:380:MET:HA	1:A:427:LEU:O	2.16	0.46
2:E:230:TYR:HD1	2:E:230:TYR:HA	1.54	0.46
1:A:580:PRO:HD2	1:A:581:GLU:OE1	2.16	0.46
1:A:638:ILE:HG22	1:A:639:SER:N	2.31	0.46
2:B:183:ASP:O	2:B:186:LEU:HG	2.16	0.46
2:E:137:LEU:HA	2:E:137:LEU:HD23	1.65	0.46
1:A:294:TYR:CD2	2:B:147:TYR:CZ	3.04	0.46
1:A:624:MET:CE	1:D:679:THR:HA	2.44	0.46
1:D:411:TRP:HA	1:D:411:TRP:CE3	2.51	0.46
1:A:409:SER:HA	1:A:410:PRO:HD3	1.63	0.46
1:D:646:ILE:CG2	1:D:650:LEU:HD22	2.46	0.46
2:E:226:PHE:HD1	2:E:250:PHE:HD1	1.63	0.46
1:A:645:LEU:HD23	1:A:645:LEU:HA	1.65	0.46
1:A:664:ASP:HA	1:A:667:LYS:HG3	1.98	0.46
1:A:666:ILE:O	1:A:672:PHE:HE1	1.99	0.46
1:D:446:LEU:HB2	1:D:448:THR:CG2	2.30	0.46
1:D:450:ASP:HA	1:D:453:ARG:HH12	1.81	0.46
1:D:669:HIS:HB3	1:D:672:PHE:CE1	2.51	0.46
1:A:411:TRP:CE3	1:A:411:TRP:HA	2.51	0.45
1:A:585:TYR:OH	1:D:684:GLU:HG2	2.16	0.45
1:A:293:PHE:O	1:A:294:TYR:HB2	2.17	0.45
1:D:326:SER:O	1:D:328:GLN:N	2.37	0.45
2:E:266:LYS:C	2:E:269:ALA:H	2.23	0.45
1:A:580:PRO:HD3	1:A:595:TRP:CE2	2.51	0.45
2:E:190:ASN:O	2:E:193:VAL:HG22	2.15	0.45
1:A:602:TYR:OH	1:A:631:GLN:O	2.34	0.45
1:D:434:GLY:HA3	1:D:483:ILE:HB	1.99	0.45
1:D:445:GLN:CD	1:D:445:GLN:H	2.24	0.45
1:A:588:TYR:HB2	1:A:589:GLY:H	1.46	0.45
1:D:416:TYR:CD2	1:D:428:ILE:HG22	2.51	0.45
1:D:626:PHE:CZ	1:D:652:HIS:CE1	3.04	0.45
1:A:289:LYS:HA	1:A:290:ILE:HA	1.81	0.45
1:A:412:VAL:C	1:A:490:LYS:HB3	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:301:ALA:HB1	2:E:245:HIS:CE1	2.51	0.45
1:D:319:ASN:OD1	1:D:319:ASN:N	2.49	0.45
1:D:652:HIS:C	1:D:654:ASP:H	2.23	0.45
1:D:743:GLU:OE2	1:D:743:GLU:HA	2.14	0.45
1:D:307:ARG:NH1	1:D:308:ARG:HA	2.32	0.45
1:A:342:LEU:HD12	1:A:343:ARG:N	2.32	0.45
1:A:371:LYS:O	1:A:375:GLY:HA2	2.16	0.45
1:D:352:PHE:N	1:D:372:LYS:HG3	2.32	0.45
1:A:646:ILE:O	1:A:650:LEU:HB2	2.17	0.44
1:D:301:ALA:HB1	2:E:245:HIS:HE1	1.82	0.44
1:D:645:LEU:HG	1:D:669:HIS:CG	2.52	0.44
1:D:744:TYR:H	1:D:744:TYR:HD2	1.63	0.44
1:A:452:THR:HG23	1:A:456:MET:SD	2.57	0.44
1:D:297:SER:CB	2:E:143:VAL:HG13	2.42	0.44
1:D:386:SER:HA	1:D:388:MET:N	2.32	0.44
1:D:602:TYR:CE1	1:D:610:PRO:HA	2.53	0.44
1:A:304:ARG:NH1	1:A:304:ARG:HB3	2.32	0.44
1:A:350:GLU:C	1:A:352:PHE:H	2.22	0.44
2:B:234:PHE:O	2:B:238:VAL:HG23	2.18	0.44
1:D:378:TYR:HB3	1:D:428:ILE:HG23	1.98	0.44
1:D:444:TRP:N	1:D:444:TRP:CD1	2.85	0.44
1:D:450:ASP:HA	1:D:453:ARG:NH1	2.33	0.44
1:A:344:ARG:HH21	1:A:344:ARG:HG3	1.83	0.44
1:A:359:GLY:O	1:A:366:VAL:HG12	2.17	0.44
1:D:646:ILE:HG22	1:D:650:LEU:HD22	2.00	0.44
2:B:185:ALA:HA	2:B:188:TRP:CB	2.48	0.44
1:D:358:ILE:HG13	1:D:367:ARG:HA	2.00	0.44
1:D:457:ALA:H	1:D:460:ILE:HD12	1.83	0.44
1:A:446:LEU:C	1:A:448:THR:HG23	2.43	0.44
1:A:485:ILE:O	1:A:689:PRO:HG2	2.17	0.44
1:A:602:TYR:O	1:A:606:ILE:HB	2.17	0.44
1:A:685:ALA:HB3	1:A:688:ILE:HD13	2.00	0.44
1:A:476:ILE:HG22	1:A:600:ILE:HD12	1.99	0.44
1:A:601:MET:HE1	1:A:645:LEU:HD13	2.00	0.44
1:D:581:GLU:OE1	1:D:653:ALA:HB2	2.18	0.44
1:A:487:GLY:HA3	1:A:687:TYR:O	2.18	0.43
1:A:676:ASP:HB2	1:A:679:THR:H	1.83	0.43
2:B:226:PHE:O	2:B:230:TYR:HB2	2.18	0.43
1:D:364:GLY:HA3	1:D:382:THR:O	2.19	0.43
1:D:604:CYS:SG	1:D:605:LEU:N	2.91	0.43
1:D:619:THR:HA	1:D:620:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:ILE:HG13	1:A:368:LEU:N	2.34	0.43
1:A:641:GLU:O	1:A:669:HIS:HE1	2.02	0.43
1:D:344:ARG:HB3	1:D:742:TYR:HB2	2.00	0.43
1:D:349:LEU:HD23	1:D:352:PHE:HD2	1.83	0.43
1:D:473:HIS:CE1	1:D:494:PHE:HA	2.53	0.43
1:D:620:TYR:O	1:D:623:ILE:N	2.48	0.43
1:A:287:LYS:CB	1:A:288:LEU:HA	2.49	0.43
1:A:494:PHE:O	1:A:497:SER:OG	2.20	0.43
1:A:626:PHE:HA	1:A:630:LEU:N	2.33	0.43
1:A:669:HIS:CG	1:A:670:PRO:HD2	2.53	0.43
1:A:703:ASP:OD1	1:A:704:GLU:N	2.52	0.43
1:A:606:ILE:HG22	1:A:608:TRP:N	2.33	0.43
1:A:613:SER:C	1:A:615:THR:H	2.26	0.43
2:B:141:TYR:CD1	2:B:144:VAL:HB	2.54	0.43
2:B:208:PRO:C	2:B:210:GLN:H	2.27	0.43
2:B:226:PHE:HD1	2:B:250:PHE:HD1	1.66	0.43
1:D:410:PRO:O	1:D:490:LYS:NZ	2.49	0.43
1:A:315:LEU:HG	1:A:318:HIS:CE1	2.53	0.43
1:D:449:GLU:O	1:D:452:THR:HG22	2.18	0.43
2:B:129:ASN:HA	2:B:132:GLU:CD	2.42	0.43
1:D:580:PRO:HD3	1:D:595:TRP:CZ2	2.52	0.43
1:D:669:HIS:O	1:D:672:PHE:HD1	2.02	0.43
1:A:416:TYR:OH	1:A:430:GLU:HB3	2.18	0.43
2:B:242:LEU:C	2:B:242:LEU:HD13	2.43	0.43
1:D:489:ILE:HD13	1:D:489:ILE:HA	1.83	0.43
2:E:242:LEU:HD22	2:E:242:LEU:O	2.19	0.43
1:A:664:ASP:CA	1:A:667:LYS:H	2.32	0.43
2:B:225:ILE:HD12	2:B:225:ILE:H	1.83	0.43
1:D:475:ALA:O	1:D:476:ILE:HD13	2.19	0.43
1:D:626:PHE:O	1:D:629:THR:HG23	2.18	0.43
2:E:126:ILE:O	2:E:130:VAL:HG13	2.19	0.43
1:A:668:SER:O	1:A:668:SER:OG	2.35	0.43
2:E:141:TYR:O	2:E:144:VAL:N	2.51	0.43
1:A:294:TYR:C	1:A:296:SER:H	2.26	0.42
1:A:621:ARG:HB3	1:A:622:LYS:H	1.61	0.42
1:D:321:SER:OG	1:D:322:GLU:N	2.52	0.42
1:A:454:PHE:CZ	1:A:488:HIS:CE1	3.06	0.42
1:A:665:GLU:C	1:A:668:SER:H	2.27	0.42
1:A:460:ILE:HG23	1:A:594:TRP:CH2	2.54	0.42
1:A:579:ALA:CB	1:A:592:CYS:HA	2.49	0.42
1:A:602:TYR:CD1	1:A:602:TYR:C	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:638:ILE:HG22	1:D:642:ALA:HB3	2.02	0.42
1:D:674:GLY:HA3	1:D:675:VAL:HA	1.75	0.42
1:D:703:ASP:OD1	1:D:704:GLU:N	2.52	0.42
2:E:248:SER:O	2:E:251:SER:N	2.52	0.42
1:D:437:LEU:HD13	1:D:437:LEU:HA	1.94	0.42
1:D:664:ASP:C	1:D:666:ILE:H	2.26	0.42
1:D:705:LEU:HD13	1:D:705:LEU:HA	1.90	0.42
1:A:494:PHE:C	1:A:497:SER:H	2.26	0.42
1:A:582:ILE:HG13	1:A:588:TYR:CD1	2.54	0.42
1:A:664:ASP:O	1:A:666:ILE:N	2.42	0.42
2:B:211:PHE:O	2:B:215:VAL:HG13	2.19	0.42
1:D:583:PHE:HA	1:D:584:LEU:HA	1.72	0.42
1:D:669:HIS:CG	1:D:670:PRO:HD2	2.55	0.42
1:A:479:ASP:O	3:A:801:ANP:H2'	2.20	0.42
1:A:580:PRO:HA	1:A:583:PHE:HE2	1.83	0.42
1:D:601:MET:SD	1:D:646:ILE:HG12	2.59	0.42
1:D:632:PHE:HA	1:D:633:PRO:HD3	1.81	0.42
1:A:294:TYR:CD2	2:B:147:TYR:OH	2.71	0.42
1:A:305:ASN:O	1:A:309:VAL:HG23	2.20	0.42
1:A:341:ARG:HG3	1:A:342:LEU:HD23	2.02	0.42
1:A:630:LEU:HD22	1:A:631:GLN:H	1.85	0.42
1:D:457:ALA:H	1:D:460:ILE:CD1	2.33	0.42
2:B:187:THR:HA	2:B:190:ASN:CB	2.43	0.42
1:D:670:PRO:C	1:D:672:PHE:H	2.28	0.42
1:A:389:TYR:HD2	1:A:498:THR:HG23	1.86	0.41
1:A:748:ASP:HA	1:A:749:TYR:HA	1.65	0.41
1:D:371:LYS:O	1:D:375:GLY:HA2	2.20	0.41
1:D:746:ARG:HG3	1:D:746:ARG:HH11	1.85	0.41
1:A:581:GLU:HB2	1:A:588:TYR:H	1.85	0.41
2:B:126:ILE:HD13	2:B:126:ILE:HA	1.72	0.41
1:D:341:ARG:HD2	1:D:341:ARG:C	2.46	0.41
2:E:132:GLU:H	2:E:132:GLU:HG3	1.68	0.41
1:A:457:ALA:HA	1:A:460:ILE:HD12	2.02	0.41
1:A:483:ILE:HA	1:A:488:HIS:O	2.21	0.41
1:A:676:ASP:C	1:A:678:ASN:H	2.28	0.41
1:D:298:VAL:HG12	1:D:301:ALA:HB3	2.02	0.41
1:D:411:TRP:O	1:D:491:LEU:HD23	2.19	0.41
1:D:645:LEU:HG	1:D:669:HIS:CD2	2.55	0.41
1:A:419:PHE:O	1:A:426:TYR:HB2	2.19	0.41
1:A:432:LEU:HD21	1:A:490:LYS:HB2	2.02	0.41
1:D:304:ARG:HB3	1:D:304:ARG:NH1	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:611:PHE:CD1	1:D:622:LYS:HB2	2.56	0.41
1:D:617:GLN:OE1	1:D:617:GLN:N	2.51	0.41
2:E:275:ILE:C	2:E:277:SER:H	2.29	0.41
1:A:411:TRP:CH2	1:A:458:GLU:HB2	2.55	0.41
1:A:489:ILE:HD13	1:A:489:ILE:HA	1.76	0.41
1:A:609:PRO:HA	1:A:610:PRO:HD3	1.85	0.41
1:A:674:GLY:HA3	1:A:675:VAL:HA	1.76	0.41
1:D:307:ARG:HH12	1:D:311:LEU:CB	2.34	0.41
1:A:365:GLU:HG2	1:A:382:THR:HB	2.03	0.41
1:A:425:LEU:HD11	1:A:427:LEU:HG	2.02	0.41
1:A:559:THR:O	1:A:562:LYS:HB2	2.21	0.41
1:A:652:HIS:CE1	1:D:486:ARG:NH2	2.81	0.41
1:D:458:GLU:OE2	1:D:489:ILE:N	2.34	0.41
1:D:676:ASP:C	1:D:678:ASN:H	2.28	0.41
2:E:136:ASN:O	2:E:140:PHE:N	2.38	0.41
1:A:494:PHE:CD1	1:A:496:LEU:HB3	2.56	0.41
1:A:502:LYS:CB	1:A:503:THR:HA	2.49	0.41
1:D:379:ALA:HB3	1:D:429:MET:SD	2.61	0.41
1:D:410:PRO:O	1:D:490:LYS:HG2	2.19	0.41
1:D:421:ASP:OD2	1:D:424:TYR:HB2	2.21	0.41
2:E:217:ARG:O	2:E:221:GLN:NE2	2.28	0.41
1:A:357:VAL:HA	1:A:367:ARG:CG	2.51	0.41
1:A:367:ARG:NH2	1:A:382:THR:OG1	2.54	0.41
1:A:371:LYS:HG3	1:A:374:THR:H	1.86	0.41
1:A:494:PHE:HD1	1:A:496:LEU:HB3	1.86	0.41
1:A:566:LEU:H	1:A:566:LEU:CD2	2.32	0.41
1:A:626:PHE:HA	1:A:629:THR:C	2.46	0.41
1:A:679:THR:O	1:A:683:VAL:HG23	2.21	0.41
2:B:193:VAL:HG12	2:B:199:PHE:CE2	2.56	0.41
1:D:641:GLU:CD	1:D:641:GLU:H	2.28	0.41
1:D:746:ARG:HH21	1:D:748:ASP:N	2.19	0.41
1:A:632:PHE:HE1	1:A:647:ARG:NE	2.19	0.41
2:B:137:LEU:HD23	2:B:140:PHE:HB2	2.02	0.41
1:D:621:ARG:HB3	1:D:622:LYS:H	1.46	0.41
1:A:363:PHE:CE1	1:A:388:MET:HE2	2.55	0.40
1:A:454:PHE:CD2	1:A:454:PHE:C	2.99	0.40
1:A:380:MET:HE1	1:A:419:PHE:HE1	1.86	0.40
1:A:675:VAL:HG22	1:A:676:ASP:N	2.31	0.40
1:D:650:LEU:HA	1:D:650:LEU:HD12	1.63	0.40
1:A:355:VAL:HG23	1:A:369:VAL:HA	2.02	0.40
1:A:603:GLU:HB2	1:A:609:PRO:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:669:HIS:CE1	1:A:670:PRO:HG2	2.56	0.40
1:A:455:TYR:HD1	1:A:455:TYR:HA	1.66	0.40
1:D:415:LEU:HA	1:D:429:MET:HB3	2.03	0.40
1:D:440:MET:HE3	1:D:440:MET:HB2	1.82	0.40
1:D:485:ILE:HG13	1:D:486:ARG:H	1.87	0.40
1:D:664:ASP:O	1:D:666:ILE:HG13	2.22	0.40
1:A:628:GLN:HG3	1:A:629:THR:HG23	2.04	0.40
1:A:640:TYR:HD1	1:A:640:TYR:HA	1.73	0.40
1:A:694:ILE:HD12	1:A:694:ILE:HA	1.88	0.40
2:B:186:LEU:HD12	2:B:187:THR:HG23	2.03	0.40
1:D:303:GLU:OE2	1:D:307:ARG:HB2	2.21	0.40
1:D:307:ARG:NH1	1:D:311:LEU:HB2	2.37	0.40
1:D:591:GLU:CD	1:D:591:GLU:N	2.78	0.40
1:D:613:SER:HB3	1:D:622:LYS:HE3	2.04	0.40
1:D:621:ARG:O	1:D:625:ASN:HB2	2.22	0.40
1:D:622:LYS:HA	1:D:629:THR:HG21	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	380/508 (75%)	298 (78%)	74 (20%)	8 (2%)	5	31
1	D	321/508 (63%)	247 (77%)	71 (22%)	3 (1%)	14	46
2	B	142/244 (58%)	121 (85%)	20 (14%)	1 (1%)	18	51
2	E	133/244 (54%)	120 (90%)	12 (9%)	1 (1%)	16	49
All	All	976/1504 (65%)	786 (80%)	177 (18%)	13 (1%)	9	39

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	572	VAL
2	B	106	VAL
2	E	182	ILE
1	A	743	GLU
1	D	743	GLU
1	A	552	SER
1	A	553	ASN
1	A	576	ASP
1	D	327	ARG
1	A	456	MET
1	A	645	LEU
1	A	578	ILE
1	D	578	ILE

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	277/449 (62%)	205 (74%)	72 (26%)	0	4
1	D	239/449 (53%)	176 (74%)	63 (26%)	0	3
2	B	76/223 (34%)	64 (84%)	12 (16%)	2	15
2	E	85/223 (38%)	70 (82%)	15 (18%)	2	12
All	All	677/1344 (50%)	515 (76%)	162 (24%)	1	5

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	296	SER
1	A	297	SER
1	A	302	ILE
1	A	303	GLU
1	A	304	ARG
1	A	320	TRP
1	A	324	ARG
1	A	342	LEU
1	A	343	ARG

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Mol	Chain	Res	Type
1	A	357	VAL
1	A	365	GLU
1	A	388	MET
1	A	389	TYR
1	A	408	ASP
1	A	412	VAL
1	A	419	PHE
1	A	432	LEU
1	A	438	MET
1	A	444	TRP
1	A	446	LEU
1	A	450	ASP
1	A	452	THR
1	A	456	MET
1	A	464	GLU
1	A	468	LYS
1	A	473	HIS
1	A	477	LYS
1	A	483	ILE
1	A	485	ILE
1	A	489	ILE
1	A	492	SER
1	A	493	ASP
1	A	500	PHE
1	A	554	ARG
1	A	562	LYS
1	A	563	SER
1	A	564	ARG
1	A	565	ARG
1	A	566	LEU
1	A	581	GLU
1	A	583	PHE
1	A	588	TYR
1	A	590	GLN
1	A	591	GLU
1	A	597	LEU
1	A	600	ILE
1	A	606	ILE
1	A	613	SER
1	A	614	GLU
1	A	619	THR
1	A	621	ARG

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Mol	Chain	Res	Type
1	A	622	LYS
1	A	623	ILE
1	A	630	LEU
1	A	631	GLN
1	A	637	HIS
1	A	639	SER
1	A	646	ILE
1	A	648	ARG
1	A	650	LEU
1	A	660	HIS
1	A	665	GLU
1	A	666	ILE
1	A	673	ARG
1	A	680	ILE
1	A	681	ARG
1	A	691	LEU
1	A	702	THR
1	A	705	LEU
1	A	743	GLU
1	A	746	ARG
1	A	747	PHE
2	B	112	THR
2	B	126	ILE
2	B	135	THR
2	B	137	LEU
2	B	140	PHE
2	B	143	VAL
2	B	201	THR
2	B	210	GLN
2	B	230	TYR
2	B	231	HIS
2	B	242	LEU
2	B	251	SER
1	D	297	SER
1	D	304	ARG
1	D	319	ASN
1	D	323	GLU
1	D	324	ARG
1	D	338	GLN
1	D	340	LEU
1	D	343	ARG
1	D	349	LEU

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Mol	Chain	Res	Type
1	D	354	THR
1	D	374	THR
1	D	413	VAL
1	D	419	PHE
1	D	428	ILE
1	D	429	MET
1	D	431	PHE
1	D	437	LEU
1	D	440	MET
1	D	443	ARG
1	D	444	TRP
1	D	445	GLN
1	D	446	LEU
1	D	450	ASP
1	D	452	THR
1	D	458	GLU
1	D	464	GLU
1	D	468	LYS
1	D	471	PHE
1	D	479	ASP
1	D	480	ASN
1	D	483	ILE
1	D	485	ILE
1	D	486	ARG
1	D	583	PHE
1	D	584	LEU
1	D	585	TYR
1	D	591	GLU
1	D	597	LEU
1	D	605	LEU
1	D	606	ILE
1	D	619	THR
1	D	621	ARG
1	D	623	ILE
1	D	624	MET
1	D	627	GLU
1	D	630	LEU
1	D	631	GLN
1	D	637	HIS
1	D	638	ILE
1	D	645	LEU
1	D	646	ILE

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Mol	Chain	Res	Type
1	D	650	LEU
1	D	665	GLU
1	D	666	ILE
1	D	673	ARG
1	D	681	ARG
1	D	684	GLU
1	D	686	PRO
1	D	702	THR
1	D	705	LEU
1	D	744	TYR
1	D	746	ARG
1	D	747	PHE
2	E	113	ILE
2	E	130	VAL
2	E	132	GLU
2	E	140	PHE
2	E	187	THR
2	E	198	LEU
2	E	201	THR
2	E	209	GLN
2	E	210	GLN
2	E	230	TYR
2	E	231	HIS
2	E	242	LEU
2	E	245	HIS
2	E	266	LYS
2	E	268	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	338	GLN
1	A	480	ASN
1	A	655	GLN
1	A	660	HIS
2	B	129	ASN
2	B	197	ASN
1	D	420	GLN
1	D	682	GLN
2	E	245	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is modelled in this entry.

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	A	801	-	33,33,33	2.61	9 (27%)	45,52,52	3.07	20 (44%)

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	A	801	-	-	9/18/38/38	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ANP	PB-O1B	10.07	1.61	1.46
3	A	801	ANP	PB-N3B	4.55	1.75	1.63
3	A	801	ANP	C2'-C3'	-4.41	1.41	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	ANP	C6-N6	4.29	1.45	1.34
3	A	801	ANP	O4'-C4'	-3.32	1.37	1.45
3	A	801	ANP	PG-O1G	2.83	1.50	1.46
3	A	801	ANP	C2'-C1'	-2.53	1.45	1.53
3	A	801	ANP	O2'-C2'	-2.27	1.37	1.43
3	A	801	ANP	O3'-C3'	-2.09	1.37	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	ANP	O1B-PB-N3B	-12.55	93.29	111.77
3	A	801	ANP	O2B-PB-O1B	6.31	123.40	109.87
3	A	801	ANP	N3-C2-N1	-5.03	120.97	128.58
3	A	801	ANP	O2B-PB-O3A	4.60	120.01	104.64
3	A	801	ANP	C5-C4-N3	-4.49	120.53	126.72
3	A	801	ANP	C2'-C1'-N9	4.02	123.29	113.30
3	A	801	ANP	O5'-C5'-C4'	3.87	122.17	108.99
3	A	801	ANP	C4-C5-N7	-3.70	106.35	110.58
3	A	801	ANP	C2-N3-C4	3.62	120.66	111.83
3	A	801	ANP	N9-C8-N7	-3.42	109.08	113.94
3	A	801	ANP	C5-N7-C8	3.39	108.78	103.45
3	A	801	ANP	O3A-PB-N3B	-3.01	98.23	106.59
3	A	801	ANP	C4-N9-C1'	-2.68	120.37	126.63
3	A	801	ANP	N3-C4-N9	2.53	131.47	127.17
3	A	801	ANP	C6-C5-N7	2.40	136.72	132.09
3	A	801	ANP	O4'-C1'-N9	2.30	112.50	108.09
3	A	801	ANP	O5'-PA-O1A	2.25	117.85	108.94
3	A	801	ANP	O3G-PG-O1G	-2.21	107.92	113.45
3	A	801	ANP	C1'-N9-C8	2.12	131.81	127.09
3	A	801	ANP	C5-C4-N9	2.01	108.00	105.81

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	ANP	PB-N3B-PG-O1G
3	A	801	ANP	PG-N3B-PB-O1B
3	A	801	ANP	PG-N3B-PB-O3A
3	A	801	ANP	PA-O3A-PB-O2B
3	A	801	ANP	PB-O3A-PA-O1A
3	A	801	ANP	PB-O3A-PA-O2A
3	A	801	ANP	C4'-C5'-O5'-PA

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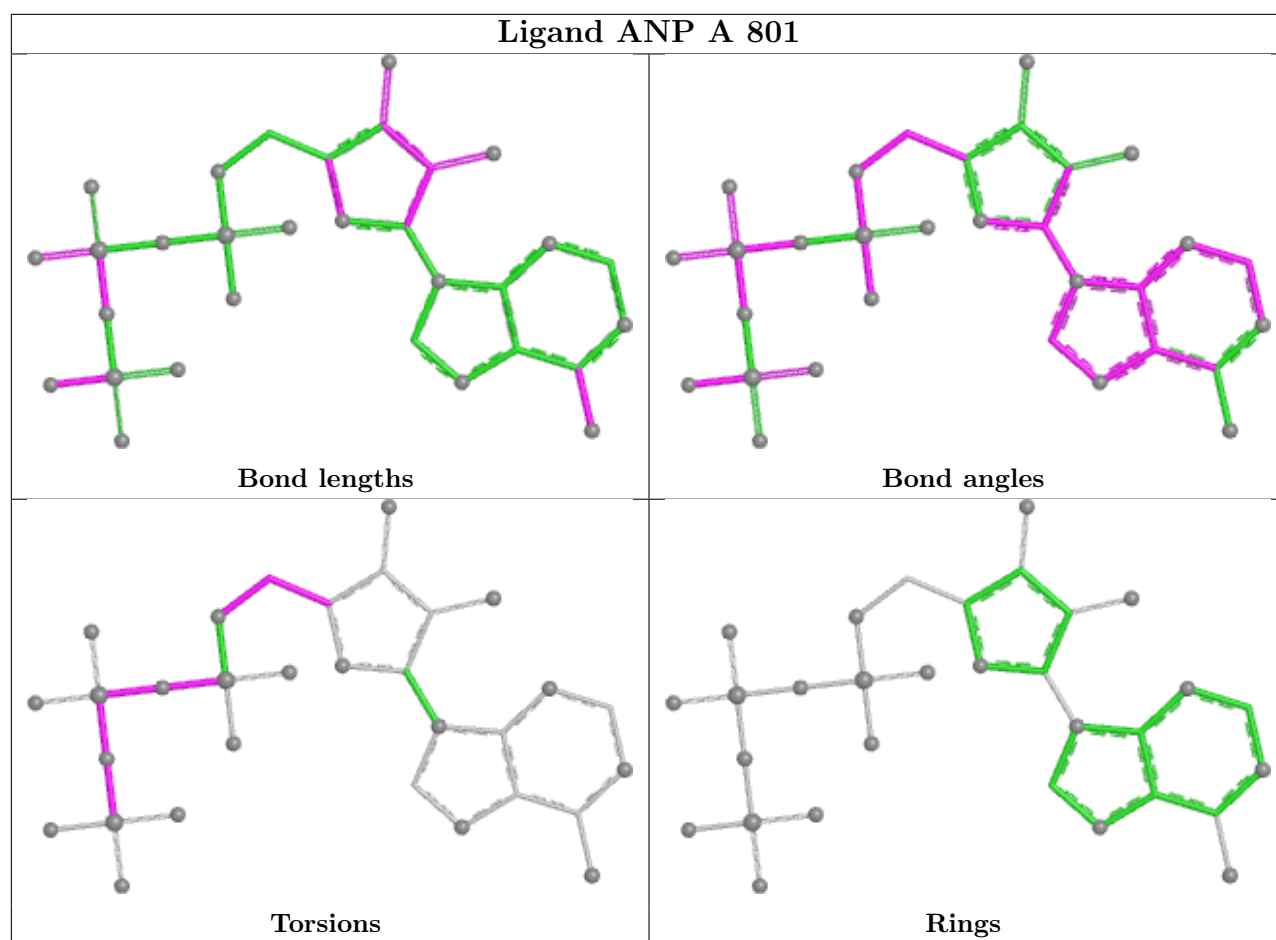
Mol	Chain	Res	Type	Atoms
3	A	801	ANP	O4'-C4'-C5'-O5'
3	A	801	ANP	PA-O3A-PB-O1B

There are no ring outliers.

1 monomer is involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	ANP	12	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	388/508 (76%)	-0.95	1 (0%) 90 75	37, 93, 161, 237	0
1	D	329/508 (64%)	-0.85	1 (0%) 90 75	57, 107, 198, 273	0
2	B	146/244 (59%)	-1.00	0 100 100	67, 119, 201, 244	0
2	E	137/244 (56%)	-0.96	0 100 100	60, 128, 234, 266	0
All	All	1000/1504 (66%)	-0.92	2 (0%) 91 80	37, 106, 192, 273	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	658	GLY	2.3
1	D	435	GLY	2.3

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](#)

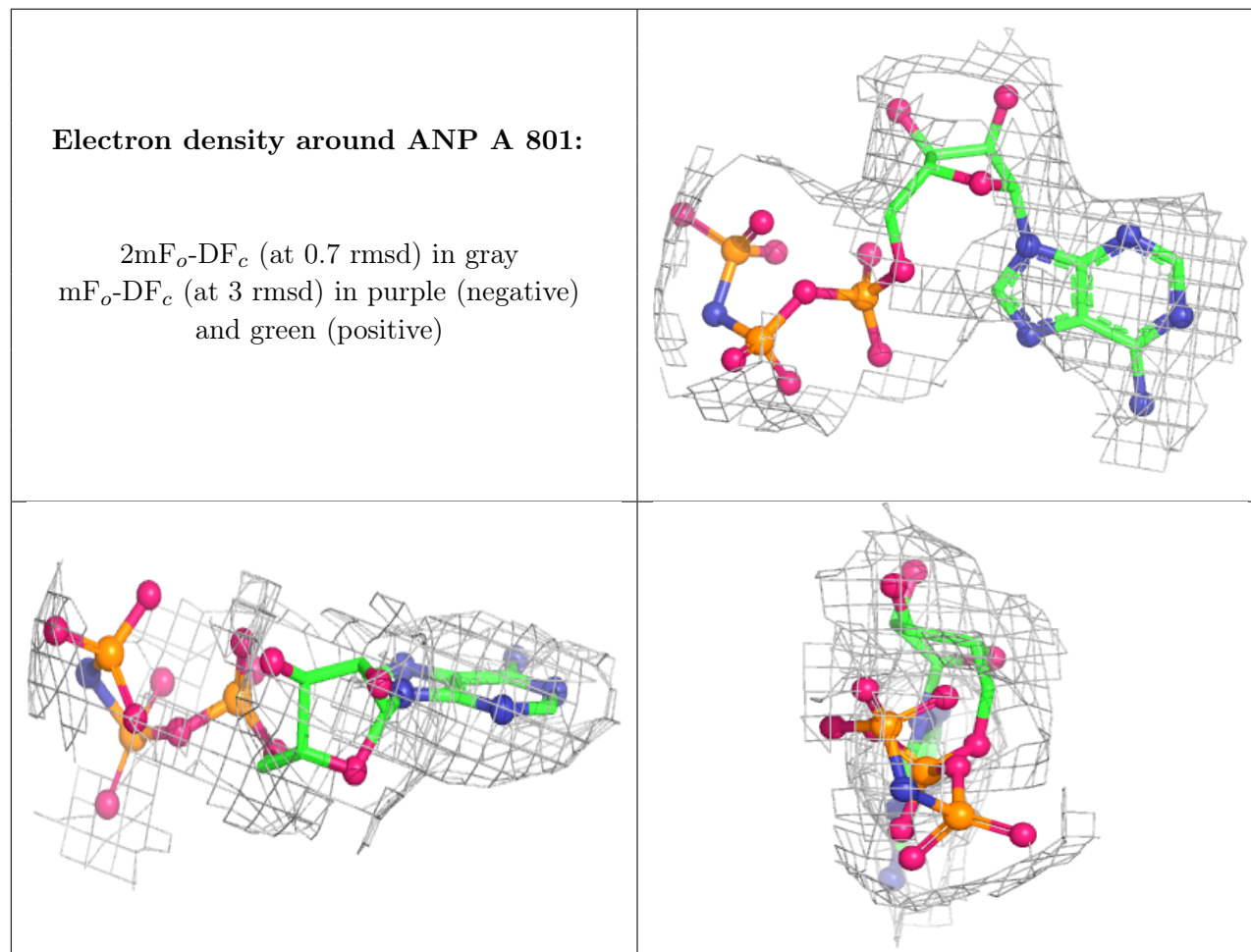
There are no oligosaccharides in this entry.

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	ANP	A	801	31/31	0.99	0.04	24,60,84,100	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers ⓘ

There are no such residues in this entry.