



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:13 AM UTC

PDB ID : 4YIY / pdb_00004yiy
Title : Structure of MRB1590 bound to AMP-PNP
Authors : Shaw, P.L.R.; Schumacher, M.A.
Deposited on : 2015-03-02
Resolution : 3.02 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

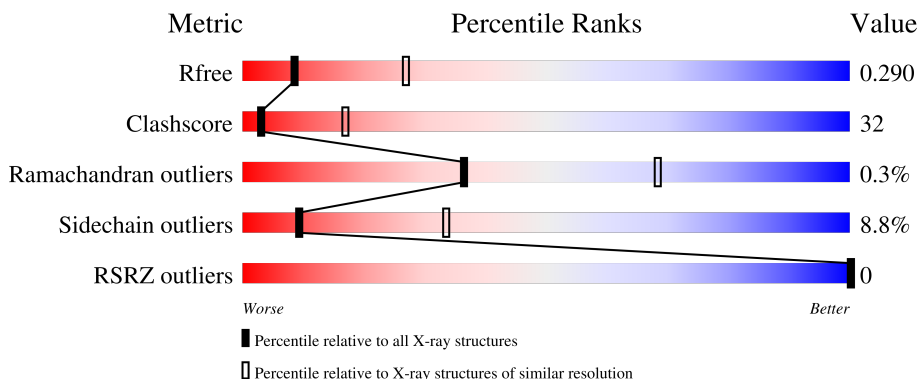
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.02 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	3131 (3.04-3.00)
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (3.04-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	680	
1	B	680	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 8916 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 kRNA Editing A6 Specific Protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	577	Total	C	N	O	S	0	0	0
			4416	2763	782	845	26			
1	A	577	Total	C	N	O	S	0	0	0
			4418	2763	783	846	26			

There are 46 discrepancies between the modelled and reference sequences:

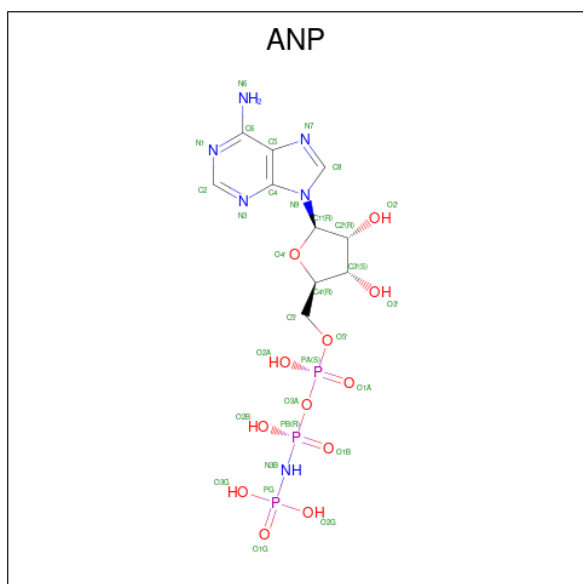
Chain	Residue	Modelled	Actual	Comment	Reference
B	-11	MET	-	initiating methionine	UNP Q57ZF2
B	-10	HIS	-	expression tag	UNP Q57ZF2
B	-9	HIS	-	expression tag	UNP Q57ZF2
B	-8	HIS	-	expression tag	UNP Q57ZF2
B	-7	HIS	-	expression tag	UNP Q57ZF2
B	-6	HIS	-	expression tag	UNP Q57ZF2
B	-5	HIS	-	expression tag	UNP Q57ZF2
B	-4	SER	-	expression tag	UNP Q57ZF2
B	-3	SER	-	expression tag	UNP Q57ZF2
B	-2	GLY	-	expression tag	UNP Q57ZF2
B	-1	VAL	-	expression tag	UNP Q57ZF2
B	0	ASP	-	expression tag	UNP Q57ZF2
B	1	LEU	-	expression tag	UNP Q57ZF2
B	2	GLY	-	expression tag	UNP Q57ZF2
B	3	THR	-	expression tag	UNP Q57ZF2
B	4	GLU	-	expression tag	UNP Q57ZF2
B	5	ASN	-	expression tag	UNP Q57ZF2
B	6	LEU	-	expression tag	UNP Q57ZF2
B	7	TYR	-	expression tag	UNP Q57ZF2
B	8	PHE	-	expression tag	UNP Q57ZF2
B	9	GLN	-	expression tag	UNP Q57ZF2
B	10	SER	-	expression tag	UNP Q57ZF2
B	242	GLU	VAL	conflict	UNP Q57ZF2
A	-11	MET	-	initiating methionine	UNP Q57ZF2
A	-10	HIS	-	expression tag	UNP Q57ZF2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	HIS	-	expression tag	UNP Q57ZF2
A	-8	HIS	-	expression tag	UNP Q57ZF2
A	-7	HIS	-	expression tag	UNP Q57ZF2
A	-6	HIS	-	expression tag	UNP Q57ZF2
A	-5	HIS	-	expression tag	UNP Q57ZF2
A	-4	SER	-	expression tag	UNP Q57ZF2
A	-3	SER	-	expression tag	UNP Q57ZF2
A	-2	GLY	-	expression tag	UNP Q57ZF2
A	-1	VAL	-	expression tag	UNP Q57ZF2
A	0	ASP	-	expression tag	UNP Q57ZF2
A	1	LEU	-	expression tag	UNP Q57ZF2
A	2	GLY	-	expression tag	UNP Q57ZF2
A	3	THR	-	expression tag	UNP Q57ZF2
A	4	GLU	-	expression tag	UNP Q57ZF2
A	5	ASN	-	expression tag	UNP Q57ZF2
A	6	LEU	-	expression tag	UNP Q57ZF2
A	7	TYR	-	expression tag	UNP Q57ZF2
A	8	PHE	-	expression tag	UNP Q57ZF2
A	9	GLN	-	expression tag	UNP Q57ZF2
A	10	SER	-	expression tag	UNP Q57ZF2
A	242	GLU	VAL	conflict	UNP Q57ZF2

- Molecule 2 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Mg	0	0
			2	2		
3	A	2	Total	Mg	0	0
			2	2		

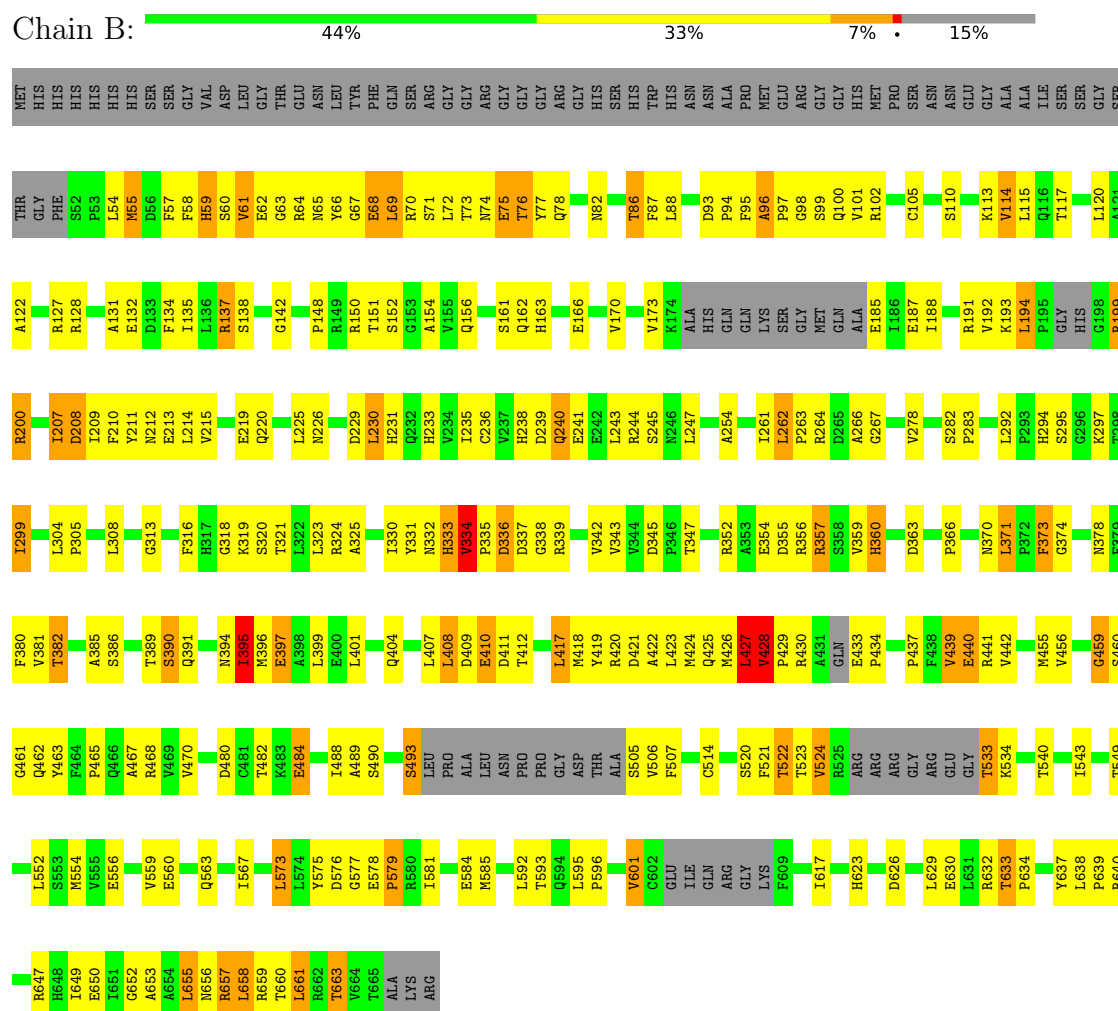
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	12	Total	O	0	0
			12	12		
4	A	4	Total	O	0	0
			4	4		

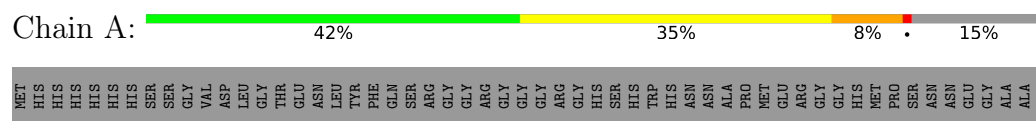
3 Residue-property plots

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: kRNA Editing A6 Specific Protein



• Molecule 1: kRNA Editing A6 Specific Protein



L631	ARG	L445	T368	H294	E200	V114	THR
G632	GLY	L445	T368	H294	E200	V114	GLY
T633	ARG	L445	T368	H294	E200	V114	PHE
P634	GLU	N448	T378	G296	G203	G126	S52
G635	GLY	H449	T378	K297	H204	R127	P53
C636	T633	L445	T378	G301	G205	L54	L54
L637	K534	S452	T379	G301	A206	A130	M55
L638	L543	S453	T381	P305	T207	A131	S55
P639	E556	L454	T382	L308	D208	E132	F57
G640	E556	M455	A383	T309	D133	F58	F58
G641	V559	V456	D384	L310	F210	F134	H59
P642	E560	I457	A385	L310	Y211	F134	S60
T643	E561	G458	S386	G313	M212	L136	V61
G644	G562	G459	G387	G313	E213	R137	S61
G645	G562	S460	G388	G314	L214	G62	G63
G646	G563	G461	T389	F316	Y215	I147	R64
R647	I567	Q462	S390	F316	P216	P148	N65
H648	A568	Q463	S391	H317	L217	R149	Y66
I649	Q569	Q463	Q391	H317	L217	R150	G87
G652	G569	Q466	T395	G318	Q220	G68	E88
A653	L573	L467	T395	K319	Q221	A154	R69
A654	L574	R468	E397	S320	V222	V155	L70
L655	Y575	V469	A398	L322	G225	Q156	S71
M656	D576	V470	L399	L323	L225	R159	L72
G657	G577	E400	E400	R324	M226	P160	T73
L658	E578	Y476	L401	G328	E227	S161	M74
R659	PRO	Q480	L405	V328	L230	H163	T76
T660	C880	D480	L406	G329	H230	Q162	Y77
L661	I581	C481	L406	L330	H231	H163	Q78
R662	V582	T482	L407	T331	Q232	V164	Q78
T663	P583	L408	L408	N332	H233	L165	I79
V664	E584	A485	D409	H333	V234	G69	S80
T665	M585	E584	E410	P335	T235	V170	N82
ALA	T586	I488	D411	P335	C236	G171	V83
LYS	T587	T412	T412	D337	V237	L172	R84
ARG	K588	S493	L417	D337	H238	V173	C85
L592	L592	L592	L417	G338	D239	K174	T86
L595	L595	L595	N418	R339	Q240	ALA	F87
P596	P596	P596	Y419	R339	E241	HIS	F87
V601	V601	V601	ALA	V342	E242	GLN	L88
C602	C602	C602	ASN	V343	L243	GLN	S89
GLU	GLU	GLU	PRO	V344	R244	LYS	I90
ILE	ILE	ILE	PRO	D345	S245	SER	Q91
GLN	GLN	ALA	R430	V344	M246	GLY	S92
ARG	ARG	S505	R431	D345	L247	MET	D93
GLY	GLY	V506	A431	R352	L248	GLN	P94
LYS	LYS	N512	F431	R352	L248	ALA	F95
F609	F609	N512	E431	R352	Y252	E185	A96
F613	F613	S520	E431	R352	L261	I188	G98
S614	S614	F521	T435	R356	P263	R191	R102
H623	H623	T522	T435	R356	L262	V192	L103
K627	K627	V524	F438	R356	P263	K193	V104
F630	F630	R525	V439	R356	S285	L194	C105
F630	F630	R525	E440	R356	L286	P195	P106
F630	F630	R525	E440	R356	E287	GLY	P106
F630	F630	R525	E440	R356	E287	HIS	S110
F630	F630	R525	E440	R356	E287	G198	F112
F630	F630	R525	E440	R356	E287	G198	F112

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	103.18Å 71.52Å 103.54Å 90.00° 120.03° 90.00°	Depositor
Resolution (Å)	44.82 – 3.02 44.82 – 3.02	Depositor EDS
% Data completeness (in resolution range)	97.6 (44.82-3.02) 97.6 (44.82-3.02)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 3.01Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.233 , 0.297 0.251 , 0.290	Depositor DCC
R_{free} test set	2004 reflections (7.87%)	wwPDB-VP
Wilson B-factor (Å ²)	51.2	Xtriage
Anisotropy	0.781	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.036 for l,k,-h-l 0.036 for -h-l,k,h 0.047 for h,-k,-h-l 0.378 for l,-k,h 0.044 for -h-l,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8916	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.19% 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, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.10	7/4495 (0.2%)	1.27	53/6091 (0.9%)
1	B	1.10	9/4494 (0.2%)	1.20	46/6091 (0.8%)
All	All	1.10	16/8989 (0.2%)	1.24	99/12182 (0.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	634	PRO	N-CD	-13.46	1.28	1.47
1	B	199	ARG	CA-C	6.90	1.62	1.52
1	A	659	ARG	CA-C	6.59	1.62	1.52
1	B	262	LEU	C-N	6.09	1.40	1.33
1	B	355	ASP	CA-C	-5.88	1.45	1.52
1	B	428	VAL	C-N	5.83	1.40	1.33
1	A	395	ILE	C-O	-5.49	1.18	1.24
1	A	93	ASP	CA-C	-5.21	1.47	1.52
1	B	299	ILE	C-O	-5.14	1.18	1.24
1	B	333	HIS	CA-C	-5.11	1.46	1.52
1	A	248	LEU	CA-C	-5.07	1.45	1.52
1	A	391	GLN	CA-C	-5.04	1.46	1.52
1	B	390	SER	C-O	-5.03	1.18	1.24
1	A	345	ASP	C-O	-5.03	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	395	ILE	C-O	-5.02	1.18	1.24
1	B	429	PRO	N-CD	5.00	1.54	1.47

All (99) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	631	LEU	N-CA-C	-18.12	83.70	110.52
1	B	408	LEU	N-CA-C	11.08	126.92	109.07
1	B	592	LEU	N-CA-C	10.88	127.52	109.46
1	A	201	ILE	N-CA-C	10.75	121.59	110.62
1	B	657	ARG	CB-CA-C	-10.74	93.84	111.13
1	A	317	HIS	N-CA-C	10.71	125.61	112.54
1	A	88	LEU	N-CA-C	10.22	125.56	112.89
1	A	247	LEU	N-CA-C	9.88	121.81	111.14
1	A	581	ILE	N-CA-C	9.84	123.38	111.09
1	B	658	LEU	N-CA-C	-9.55	97.04	110.50
1	B	86	THR	N-CA-C	9.54	123.96	108.41
1	A	75	GLU	N-CA-C	-9.32	93.99	109.46
1	B	404	GLN	N-CA-C	9.21	124.82	113.50
1	A	389	THR	N-CA-C	8.88	120.96	111.28
1	A	88	LEU	CA-C-O	8.65	130.03	119.31
1	A	533	THR	N-CA-CB	-8.40	97.22	111.50
1	A	94	PRO	N-CA-C	8.23	126.02	113.75
1	B	247	LEU	N-CA-C	8.18	119.97	111.14
1	A	408	LEU	N-CA-C	8.15	121.81	108.52
1	B	69	LEU	N-CA-C	-7.83	103.61	113.01
1	A	319	LYS	N-CA-C	7.75	120.41	111.11
1	B	333	HIS	N-CA-C	7.43	121.76	109.95
1	B	199	ARG	CA-C-O	7.37	128.20	119.28
1	B	245	SER	N-CA-C	-7.29	103.36	111.82
1	A	631	LEU	CB-CA-C	7.24	122.50	109.83
1	A	86	THR	N-CA-C	7.23	120.19	108.41
1	B	334	VAL	N-CA-C	-7.21	101.03	108.96
1	A	634	PRO	N-CA-C	6.90	122.96	113.65
1	B	200	ARG	N-CA-C	-6.87	100.11	110.28
1	B	59	HIS	N-CA-C	-6.66	104.02	111.28
1	A	243	LEU	N-CA-C	-6.58	105.07	113.23
1	B	657	ARG	CA-C-O	6.46	128.37	120.55
1	B	404	GLN	CA-C-O	6.46	126.25	119.14
1	A	658	LEU	N-CA-C	-6.38	100.39	109.96
1	A	659	ARG	CA-C-O	6.34	126.95	119.28
1	A	397	GLU	N-CA-C	-6.25	104.47	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	357	ARG	N-CA-C	-6.24	101.70	110.50
1	A	357	ARG	N-CA-C	-6.21	101.75	110.50
1	B	633	THR	N-CA-C	-6.13	102.04	109.83
1	B	262	LEU	CA-C-N	-6.06	114.37	120.31
1	B	262	LEU	C-N-CA	-6.06	114.37	120.31
1	B	278	VAL	CA-C-N	6.05	125.99	119.76
1	B	278	VAL	C-N-CA	6.05	125.99	119.76
1	B	428	VAL	CA-C-N	-6.05	114.04	120.03
1	B	428	VAL	C-N-CA	-6.05	114.04	120.03
1	A	93	ASP	N-CA-C	6.04	115.09	108.14
1	A	59	HIS	CA-C-N	6.04	128.87	120.29
1	A	59	HIS	C-N-CA	6.04	128.87	120.29
1	B	427	LEU	N-CA-C	-5.99	104.66	111.07
1	B	199	ARG	CB-CA-C	-5.96	99.29	110.01
1	A	657	ARG	CB-CA-C	-5.92	101.92	111.28
1	A	370	ASN	N-CA-C	5.88	117.59	109.54
1	B	318	GLY	N-CA-C	5.87	124.20	115.64
1	B	374	GLY	N-CA-C	-5.73	106.08	114.90
1	A	321	THR	CA-C-N	5.71	127.87	120.44
1	A	321	THR	C-N-CA	5.71	127.87	120.44
1	A	354	GLU	N-CA-C	-5.70	99.01	108.75
1	A	390	SER	CB-CA-C	-5.67	99.78	110.67
1	A	385	ALA	N-CA-C	5.64	118.17	110.55
1	A	524	VAL	CB-CA-C	5.56	118.19	111.13
1	A	248	LEU	N-CA-C	-5.51	106.40	113.23
1	B	78	GLN	N-CA-CB	5.47	119.14	110.55
1	A	583	PRO	CA-N-CD	-5.45	104.37	112.00
1	B	162	GLN	N-CA-C	-5.43	106.62	113.20
1	B	62	GLU	CB-CA-C	-5.43	100.58	110.63
1	A	69	LEU	N-CA-C	5.42	119.39	112.34
1	B	593	THR	CB-CA-C	5.42	119.15	109.29
1	A	263	PRO	CA-N-CD	-5.37	104.48	112.00
1	A	633	THR	CA-C-N	-5.33	113.41	119.28
1	A	633	THR	C-N-CA	-5.33	113.41	119.28
1	A	92	SER	N-CA-C	5.33	117.09	111.28
1	B	459	GLY	N-CA-C	5.30	125.74	113.18
1	A	636	CYS	N-CA-C	5.29	118.56	110.20
1	A	580	ARG	N-CA-C	5.29	119.45	112.89
1	A	435	ILE	N-CA-C	5.27	116.20	109.30
1	A	96	ALA	N-CA-C	-5.25	102.84	110.08
1	A	388	SER	N-CA-C	5.23	116.78	111.14
1	B	408	LEU	N-CA-CB	-5.21	102.39	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	626	ASP	CB-CA-C	-5.21	102.14	110.79
1	B	630	GLU	N-CA-C	5.21	118.66	107.67
1	B	633	THR	CA-C-N	5.17	124.83	119.56
1	B	633	THR	C-N-CA	5.17	124.83	119.56
1	A	592	LEU	N-CA-C	5.17	117.78	110.50
1	B	192	VAL	N-CA-C	5.13	115.86	108.48
1	B	593	THR	N-CA-C	-5.11	107.22	113.50
1	A	63	GLY	N-CA-C	5.11	119.31	112.77
1	A	284	LYS	N-CA-C	5.11	116.85	111.28
1	A	574	LEU	N-CA-C	-5.09	105.73	111.28
1	A	580	ARG	CA-C-N	5.09	128.65	120.30
1	A	580	ARG	C-N-CA	5.09	128.65	120.30
1	B	292	LEU	CA-C-N	5.07	124.68	119.05
1	B	292	LEU	C-N-CA	5.07	124.68	119.05
1	A	659	ARG	N-CA-C	5.07	119.45	113.16
1	B	360	HIS	N-CA-C	5.06	115.67	107.23
1	B	522	THR	N-CA-C	5.05	116.47	111.07
1	A	63	GLY	CA-C-O	5.05	126.01	120.66
1	B	373	PHE	N-CA-C	5.01	118.70	112.58
1	B	655	LEU	N-CA-C	-5.01	105.82	111.28
1	A	67	GLY	N-CA-C	-5.00	106.68	113.24

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	336	ASP	Peptide
1	B	336	ASP	Peptide
1	B	96	ALA	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	4418	0	4382	262	50
1	B	4416	0	4381	317	50
2	A	31	0	13	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	31	0	13	7	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	4	0	0	3	0
4	B	12	0	0	4	0
All	All	8916	0	8789	558	50

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 32.

All (558) 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:B:114:VAL:HG23	1:B:115:LEU:CD1	1.70	1.21
1:B:576:ASP:OD2	1:B:634:PRO:HD2	1.03	1.19
1:A:57:PHE:O	1:A:60:SER:HB2	1.38	1.17
1:A:244:ARG:NH2	1:A:332:ASN:OD1	1.78	1.16
1:B:430:ARG:HA	1:B:433:GLU:HB3	1.25	1.14
1:A:204:HIS:O	1:A:207:ILE:HG22	1.44	1.13
1:B:576:ASP:OD2	1:B:634:PRO:CD	1.97	1.13
1:B:244:ARG:HG2	1:B:343:VAL:HB	1.30	1.11
1:B:244:ARG:HH22	1:B:332:ASN:ND2	1.48	1.11
1:B:244:ARG:NH2	1:B:332:ASN:HD21	1.48	1.08
1:B:114:VAL:HG23	1:B:115:LEU:HD13	1.11	1.05
1:B:366:PRO:HG2	1:B:396:MET:CE	1.86	1.05
1:A:93:ASP:HB3	1:A:94:PRO:CD	1.87	1.05
1:B:54:LEU:HD11	1:B:58:PHE:CE2	1.93	1.03
1:B:137:ARG:NH1	1:B:334:VAL:HB	1.74	1.02
1:A:93:ASP:CB	1:A:94:PRO:HD2	1.86	1.00
1:B:66:TYR:OH	1:B:194:LEU:O	1.78	0.98
1:B:576:ASP:CG	1:B:634:PRO:HD2	1.87	0.98
1:A:88:LEU:HD13	1:A:640:ARG:HD3	1.44	0.97
1:A:613:PHE:CZ	1:A:655:LEU:HD23	1.99	0.97
1:A:344:VAL:HG13	1:A:405:LEU:CD2	1.95	0.96
1:A:93:ASP:HB3	1:A:94:PRO:HD2	0.98	0.96
1:B:163:HIS:CE1	1:B:333:HIS:HE1	1.83	0.94
1:B:459:GLY:HA2	1:A:424:MET:HG2	1.46	0.94
1:B:244:ARG:NH2	1:B:332:ASN:ND2	2.12	0.93
1:B:114:VAL:CG2	1:B:115:LEU:HD13	1.98	0.92
1:B:366:PRO:HG2	1:B:396:MET:HE1	1.50	0.92
1:B:66:TYR:CE2	1:B:94:PRO:HG3	2.04	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:244:ARG:HH12	1:B:332:ASN:HD22	1.16	0.90
1:A:368:ILE:HD13	1:A:389:THR:HG22	1.52	0.90
1:A:460:SER:HB3	4:A:803:HOH:O	1.70	0.90
1:A:55:MET:HG3	1:A:207:ILE:HD11	1.52	0.90
1:B:653:ALA:HB1	1:B:657:ARG:HH12	1.36	0.89
1:B:244:ARG:HH22	1:B:332:ASN:HD21	1.04	0.89
1:B:370:ASN:O	1:B:371:LEU:HD23	1.72	0.88
1:B:66:TYR:HE2	1:B:94:PRO:HG3	1.38	0.88
1:B:137:ARG:HH12	1:B:334:VAL:HB	1.37	0.88
1:B:334:VAL:HG23	1:B:335:PRO:HD2	1.56	0.87
1:B:430:ARG:CA	1:B:433:GLU:HB3	2.04	0.87
1:B:163:HIS:CE1	1:B:333:HIS:CE1	2.62	0.86
1:B:58:PHE:O	1:B:61:VAL:HG23	1.75	0.86
1:B:638:LEU:HD23	1:B:639:PRO:HD2	1.57	0.85
1:A:344:VAL:CG1	1:A:405:LEU:HD23	2.06	0.85
1:B:88:LEU:HD13	1:B:640:ARG:HD3	1.56	0.85
1:A:396:MET:HE3	1:A:399:LEU:HD12	1.59	0.84
1:B:524:VAL:HG21	1:B:575:TYR:HE1	1.42	0.84
1:B:163:HIS:HE1	1:B:333:HIS:HE1	1.23	0.83
1:A:127:ARG:HH21	1:A:294:HIS:HD2	1.24	0.83
1:B:386:SER:O	1:B:390:SER:OG	1.96	0.83
1:B:370:ASN:OD1	1:B:371:LEU:N	2.13	0.82
1:B:638:LEU:HD23	1:B:639:PRO:CD	2.09	0.82
1:B:460:SER:HB3	4:B:803:HOH:O	1.78	0.82
1:B:460:SER:O	4:B:801:HOH:O	1.95	0.82
1:B:128:ARG:HH11	1:B:128:ARG:HG2	1.45	0.81
1:A:344:VAL:CG1	1:A:405:LEU:CD2	2.59	0.81
2:B:701:ANP:O2A	1:A:386:SER:HB2	1.80	0.81
1:B:357:ARG:NH2	1:B:657:ARG:HG2	1.95	0.81
1:B:230:LEU:O	1:B:230:LEU:HD12	1.79	0.81
1:B:244:ARG:HG2	1:B:343:VAL:CB	2.10	0.81
1:B:93:ASP:CG	1:B:94:PRO:HD2	2.05	0.81
1:B:210:PHE:O	1:B:215:VAL:HG23	1.81	0.80
1:B:356:ARG:HA	1:B:385:ALA:H	1.47	0.80
2:B:701:ANP:O1G	1:A:386:SER:OG	1.98	0.80
1:A:98:GLY:HA3	1:A:191:ARG:HG2	1.63	0.80
1:A:352:ARG:NH1	1:A:556:GLU:OE2	2.15	0.80
1:B:244:ARG:HH12	1:B:332:ASN:ND2	1.79	0.79
1:A:313:GLY:O	1:A:319:LYS:NZ	2.16	0.78
1:B:313:GLY:HA3	1:B:319:LYS:HE2	1.64	0.78
1:A:580:ARG:O	1:A:583:PRO:HD2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:TYR:CD2	1:B:212:ASN:OD1	2.37	0.78
1:B:243:LEU:HD12	1:B:243:LEU:O	1.84	0.78
1:B:366:PRO:HG2	1:B:396:MET:HE3	1.66	0.78
1:B:647:ARG:NH2	1:B:650:GLU:OE2	2.18	0.77
1:B:152:SER:OG	1:B:213:GLU:OE1	2.02	0.77
1:B:490:SER:O	1:B:493:SER:O	2.02	0.77
1:A:441:ARG:O	1:A:445:LEU:HD12	1.85	0.77
1:B:114:VAL:C	1:B:115:LEU:HD12	2.11	0.76
2:B:701:ANP:O3'	1:A:384:ASP:O	2.02	0.76
1:A:206:ALA:HA	1:A:209:ILE:HD12	1.67	0.76
1:B:334:VAL:CG2	1:B:335:PRO:HD2	2.16	0.75
1:B:321:THR:OG1	2:B:701:ANP:H5'2	1.87	0.75
1:B:573:LEU:HA	1:B:633:THR:HG21	1.68	0.75
1:B:524:VAL:HG21	1:B:575:TYR:CE1	2.22	0.75
1:A:417:LEU:HB3	1:A:418:MET:HE2	1.69	0.74
1:B:430:ARG:HA	1:B:433:GLU:CB	2.12	0.74
1:B:386:SER:HB2	1:B:389:THR:HB	1.69	0.74
1:B:61:VAL:HA	1:B:64:ARG:HD2	1.70	0.74
1:B:244:ARG:NH1	1:B:332:ASN:ND2	2.34	0.74
1:A:208:ASP:OD1	1:A:212:ASN:ND2	2.20	0.73
1:B:354:GLU:O	1:B:390:SER:CB	2.37	0.73
1:A:248:LEU:HD12	1:A:252:TYR:O	1.88	0.73
1:B:117:THR:HG21	1:B:122:ALA:HB3	1.70	0.73
1:B:61:VAL:O	1:B:64:ARG:HB2	1.89	0.72
1:B:533:THR:OG1	1:B:534:LYS:N	2.20	0.72
1:B:73:THR:O	1:B:75:GLU:N	2.23	0.72
1:A:520:SER:O	1:A:660:THR:HG23	1.89	0.72
1:B:96:ALA:HB1	1:B:97:PRO:HD3	1.72	0.72
1:A:243:LEU:HD12	1:A:243:LEU:O	1.88	0.72
1:B:354:GLU:O	1:B:390:SER:HB2	1.90	0.71
1:A:613:PHE:CE2	1:A:655:LEU:HD23	2.25	0.71
1:A:137:ARG:HH12	1:A:334:VAL:HB	1.55	0.71
1:A:427:LEU:HG	1:A:428:VAL:HG13	1.70	0.71
1:A:72:LEU:N	1:A:72:LEU:HD12	2.06	0.71
1:A:57:PHE:O	1:A:60:SER:CB	2.30	0.71
1:A:173:VAL:O	1:A:185:GLU:N	2.24	0.70
1:B:66:TYR:HE2	1:B:94:PRO:CG	2.04	0.70
1:B:73:THR:HG22	1:B:74:ASN:OD1	1.91	0.70
1:B:244:ARG:CZ	1:B:332:ASN:ND2	2.54	0.70
1:A:368:ILE:HD13	1:A:389:THR:CG2	2.21	0.70
1:B:420:ARG:HH22	1:B:430:ARG:NH1	1.89	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:ILE:HD11	1:A:83:VAL:HG11	1.74	0.70
1:A:397:GLU:HG3	1:A:656:ASN:ND2	2.06	0.70
1:B:93:ASP:CG	1:B:94:PRO:CD	2.64	0.69
1:B:244:ARG:NH1	1:B:332:ASN:HD22	1.88	0.69
1:B:230:LEU:HD12	1:B:230:LEU:C	2.14	0.69
1:A:582:VAL:O	1:A:586:THR:OG1	2.08	0.69
1:A:194:LEU:HD12	1:A:194:LEU:N	2.08	0.69
1:B:397:GLU:HG3	1:B:656:ASN:ND2	2.08	0.69
1:A:127:ARG:HH21	1:A:294:HIS:CD2	2.10	0.69
1:A:581:ILE:HG23	1:A:585:MET:HG2	1.75	0.68
1:A:170:VAL:HG22	1:A:188:ILE:HG12	1.76	0.68
1:A:313:GLY:O	1:A:319:LYS:CE	2.41	0.68
1:B:396:MET:HE1	1:B:507:PHE:CD1	2.29	0.67
1:A:576:ASP:OD2	1:A:634:PRO:HD2	1.94	0.67
1:B:54:LEU:CD1	1:B:58:PHE:CE2	2.76	0.67
1:B:236:CYS:O	1:B:240:GLN:HB2	1.94	0.67
1:B:267:GLY:HA2	1:A:384:ASP:OD2	1.95	0.67
1:B:244:ARG:CG	1:B:343:VAL:CG1	2.73	0.67
1:A:520:SER:O	1:A:660:THR:CG2	2.42	0.67
1:A:408:LEU:HB2	1:A:455:MET:HB2	1.77	0.66
1:A:410:GLU:OE1	1:A:457:ILE:HA	1.95	0.66
1:B:244:ARG:CZ	1:B:332:ASN:HD21	2.09	0.66
1:B:244:ARG:HG3	1:B:343:VAL:CG1	2.25	0.66
1:B:424:MET:HG3	1:A:459:GLY:HA2	1.78	0.66
1:A:368:ILE:CD1	1:A:389:THR:HG22	2.24	0.66
1:A:370:ASN:H	1:A:434:PRO:HB3	1.61	0.66
1:B:114:VAL:HG23	1:B:115:LEU:HD12	1.73	0.65
1:B:357:ARG:CZ	1:B:657:ARG:HG2	2.26	0.65
1:A:149:ARG:C	1:A:150:ARG:HG2	2.19	0.65
1:A:386:SER:HB3	1:A:389:THR:OG1	1.97	0.65
1:B:380:PHE:CZ	1:B:389:THR:CG2	2.79	0.65
1:B:366:PRO:CD	1:B:396:MET:HE3	2.26	0.65
1:B:522:THR:HG23	1:B:523:THR:N	2.12	0.65
1:B:522:THR:HG23	1:B:523:THR:HG23	1.79	0.65
1:B:523:THR:O	1:B:524:VAL:HG13	1.97	0.65
1:B:127:ARG:HH21	1:B:294:HIS:CD2	2.15	0.65
1:B:154:ALA:HB1	1:B:193:LYS:HB2	1.79	0.65
1:B:386:SER:HB3	2:A:701:ANP:O1G	1.98	0.64
1:B:366:PRO:CG	1:B:396:MET:HE3	2.27	0.64
1:A:54:LEU:HD13	1:A:77:TYR:CE2	2.31	0.64
1:A:132:GLU:OE2	1:A:172:LEU:N	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ARG:NH2	1:B:657:ARG:CG	2.61	0.64
1:B:409:ASP:O	1:B:411:ASP:N	2.31	0.64
1:B:127:ARG:CG	1:B:238:HIS:HD2	2.09	0.64
1:B:514:CYS:O	1:B:663:THR:OG1	2.15	0.64
1:A:661:LEU:O	1:A:662:ARG:NH1	2.29	0.64
1:B:360:HIS:CE1	1:B:663:THR:H	2.16	0.63
1:B:420:ARG:HH12	1:B:430:ARG:HD3	1.63	0.63
1:A:364:ILE:HD12	1:A:368:ILE:HD12	1.79	0.63
1:B:54:LEU:HD11	1:B:58:PHE:HE2	1.57	0.63
1:B:463:TYR:HD2	4:B:801:HOH:O	1.81	0.63
1:A:205:GLY:O	1:A:209:ILE:HG13	1.98	0.63
1:B:638:LEU:CD2	1:B:639:PRO:HD2	2.28	0.62
1:A:87:PHE:HD1	1:A:90:ILE:HD11	1.63	0.62
1:B:88:LEU:CD1	1:B:640:ARG:HD3	2.30	0.62
1:B:134:PHE:HB2	1:B:233:HIS:CD2	2.34	0.62
1:B:419:TYR:HH	1:A:419:TYR:HE1	1.48	0.62
1:B:419:TYR:OH	1:A:419:TYR:HE1	1.83	0.62
1:B:267:GLY:N	1:A:384:ASP:OD2	2.33	0.62
1:A:55:MET:HB2	1:A:211:TYR:CE2	2.34	0.62
1:A:134:PHE:HB2	1:A:233:HIS:CD2	2.35	0.62
1:B:137:ARG:NH1	1:B:334:VAL:CB	2.60	0.61
2:B:701:ANP:O2A	1:A:386:SER:CB	2.46	0.61
1:B:128:ARG:HG2	1:B:128:ARG:NH1	2.14	0.61
1:B:470:VAL:H	1:B:482:THR:HB	1.65	0.61
1:A:396:MET:CE	1:A:399:LEU:HD12	2.30	0.61
1:B:319:LYS:HB2	2:B:701:ANP:O1B	2.01	0.61
1:B:86:THR:HB	1:B:102:ARG:HB3	1.82	0.61
1:B:194:LEU:N	1:B:194:LEU:HD22	2.16	0.61
1:A:70:ARG:O	1:A:73:THR:HG22	2.01	0.60
1:A:408:LEU:HB2	1:A:455:MET:CB	2.31	0.60
1:B:211:TYR:HD2	1:B:212:ASN:OD1	1.81	0.60
1:B:132:GLU:OE1	4:B:802:HOH:O	2.17	0.60
1:A:133:ASP:O	1:A:137:ARG:HG2	2.02	0.60
1:B:420:ARG:HH22	1:B:430:ARG:HH11	1.47	0.60
1:A:69:LEU:O	1:A:72:LEU:HD13	2.01	0.60
1:A:76:THR:HG23	1:A:85:CYS:O	2.02	0.60
1:B:357:ARG:HH21	1:B:657:ARG:HA	1.67	0.60
1:A:88:LEU:CD1	1:A:640:ARG:HD3	2.28	0.60
1:B:170:VAL:HG22	1:B:188:ILE:HG12	1.82	0.60
1:A:578:GLU:C	1:A:580:ARG:N	2.60	0.60
1:A:149:ARG:O	1:A:150:ARG:HD3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:ASN:O	1:A:201:ILE:HD11	2.02	0.59
1:B:127:ARG:HE	1:B:238:HIS:CD2	2.21	0.59
1:B:66:TYR:CD2	1:B:94:PRO:HG3	2.38	0.59
1:B:76:THR:CG2	1:B:86:THR:OG1	2.50	0.59
1:A:73:THR:O	1:A:74:ASN:HB2	2.01	0.59
1:B:421:ASP:OD2	1:A:461:GLY:N	2.36	0.59
1:B:522:THR:HG23	1:B:523:THR:H	1.67	0.59
1:A:321:THR:OG1	2:A:701:ANP:O2A	2.11	0.59
1:B:330:ILE:HG13	1:B:331:TYR:CD2	2.38	0.59
1:B:540:THR:HG22	1:B:540:THR:O	2.02	0.59
1:A:71:SER:O	1:A:75:GLU:OE1	2.21	0.59
1:B:163:HIS:ND1	1:B:333:HIS:CE1	2.70	0.58
1:B:363:ASP:OD1	1:B:378:ASN:HA	2.02	0.58
1:B:658:LEU:HD12	1:B:659:ARG:H	1.66	0.58
1:B:73:THR:C	1:B:75:GLU:H	2.11	0.58
1:B:366:PRO:CG	1:B:396:MET:CE	2.72	0.58
1:B:199:ARG:O	1:B:199:ARG:HG2	2.01	0.58
1:A:308:LEU:HD23	1:A:467:ALA:HA	1.85	0.58
1:A:368:ILE:HD11	1:A:389:THR:HA	1.86	0.58
1:B:128:ARG:HH11	1:B:128:ARG:CG	2.16	0.58
1:A:72:LEU:HD12	1:A:72:LEU:H	1.65	0.58
1:A:581:ILE:HG23	1:A:585:MET:CG	2.33	0.58
1:B:127:ARG:HH21	1:B:294:HIS:HD2	1.49	0.58
1:B:366:PRO:HD2	1:B:396:MET:HE3	1.86	0.57
1:B:173:VAL:O	1:B:185:GLU:N	2.37	0.57
1:B:231:HIS:O	1:B:235:ILE:HG13	2.03	0.57
1:B:267:GLY:CA	1:A:384:ASP:OD2	2.52	0.57
1:A:569:GLN:HE22	1:A:630:GLU:HA	1.68	0.57
1:B:395:ILE:O	1:B:399:LEU:HG	2.04	0.57
1:B:421:ASP:OD2	1:A:460:SER:HA	2.05	0.57
1:A:365:SER:N	1:A:366:PRO:CD	2.67	0.57
1:B:262:LEU:HD22	1:B:325:ALA:CB	2.35	0.57
1:B:267:GLY:CA	1:A:356:ARG:HB3	2.35	0.57
1:A:439:VAL:HG23	1:A:466:GLN:HG3	1.87	0.57
1:B:357:ARG:HH21	1:B:657:ARG:HG2	1.70	0.56
1:A:72:LEU:O	1:A:75:GLU:HB2	2.05	0.56
1:A:560:GLU:HB2	1:A:563:GLN:HG3	1.86	0.56
1:A:237:VAL:O	1:A:240:GLN:HB2	2.06	0.56
1:B:489:ALA:O	1:B:493:SER:HB2	2.06	0.56
1:B:576:ASP:CB	1:B:634:PRO:HD2	2.36	0.56
1:A:293:PRO:HG2	1:A:294:HIS:ND1	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLY:O	1:A:319:LYS:HE3	2.05	0.56
1:B:267:GLY:HA2	1:A:356:ARG:HB3	1.87	0.56
1:B:396:MET:HE1	1:B:507:PHE:HD1	1.70	0.56
1:B:577:GLY:O	1:B:581:ILE:HB	2.06	0.55
1:A:92:SER:O	1:A:93:ASP:OD1	2.24	0.55
1:A:350:LYS:NZ	1:A:556:GLU:OE1	2.39	0.55
1:B:244:ARG:HG3	1:B:343:VAL:HG11	1.89	0.55
1:B:54:LEU:HD13	1:B:77:TYR:CE2	2.41	0.55
1:B:370:ASN:OD1	1:B:371:LEU:O	2.23	0.55
1:A:114:VAL:O	1:A:127:ARG:NH1	2.40	0.55
1:A:363:ASP:OD1	1:A:378:ASN:HA	2.06	0.55
1:A:295:SER:HB2	1:A:297:LYS:HD3	1.89	0.55
1:B:408:LEU:HD23	1:B:418:MET:HE3	1.89	0.55
1:A:91:GLN:HG3	1:A:98:GLY:O	2.07	0.54
1:A:659:ARG:HG2	1:A:659:ARG:O	2.07	0.54
1:A:72:LEU:H	1:A:72:LEU:CD1	2.20	0.54
1:B:61:VAL:O	1:B:64:ARG:N	2.39	0.54
1:B:93:ASP:OD2	1:B:94:PRO:HD2	2.07	0.54
1:B:57:PHE:C	1:B:57:PHE:CD2	2.85	0.54
1:A:316:PHE:CZ	2:A:701:ANP:H4'	2.43	0.54
1:A:439:VAL:O	1:A:442:VAL:HG12	2.07	0.54
1:A:585:MET:HE1	1:A:623:HIS:ND1	2.22	0.54
1:A:86:THR:HB	1:A:102:ARG:HB3	1.89	0.53
1:A:334:VAL:HG23	1:A:335:PRO:HD2	1.89	0.53
1:A:401:LEU:HD13	1:A:649:ILE:HA	1.89	0.53
1:B:134:PHE:C	1:B:134:PHE:CD2	2.86	0.53
1:B:420:ARG:HH12	1:B:430:ARG:CD	2.21	0.53
1:B:243:LEU:HD22	1:B:299:ILE:HD11	1.89	0.53
1:B:319:LYS:HD2	1:B:456:VAL:HG13	1.90	0.53
1:A:147:ILE:HB	1:A:148:PRO:HD3	1.90	0.53
1:B:87:PHE:HA	1:B:101:VAL:HG12	1.91	0.53
1:B:330:ILE:HD11	1:B:331:TYR:CE2	2.44	0.53
1:B:82:ASN:HB2	1:B:219:GLU:OE1	2.09	0.53
1:A:630:GLU:OE2	1:A:641:GLY:N	2.41	0.53
1:B:137:ARG:HH11	1:B:334:VAL:HB	1.70	0.53
1:A:72:LEU:O	1:A:75:GLU:CB	2.57	0.53
1:A:210:PHE:O	1:A:215:VAL:HG23	2.09	0.53
1:A:154:ALA:HB1	1:A:193:LYS:HB2	1.91	0.53
1:A:512:ASN:HB3	1:A:665:THR:OG1	2.09	0.53
1:A:639:PRO:HB2	1:A:642:PHE:CD1	2.43	0.53
1:A:54:LEU:HD13	1:A:77:TYR:HE2	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:334:VAL:CG2	1:A:335:PRO:HD2	2.39	0.52
1:A:653:ALA:HB1	1:A:657:ARG:HH12	1.74	0.52
1:B:360:HIS:HA	1:B:381:VAL:HG22	1.91	0.52
1:A:79:ILE:HD12	1:A:215:VAL:HG22	1.91	0.52
1:A:155:VAL:HG11	1:A:214:LEU:HD21	1.90	0.52
1:A:449:HIS:ND1	1:A:609:PHE:HE1	2.07	0.52
1:A:194:LEU:N	1:A:194:LEU:CD1	2.73	0.52
1:B:57:PHE:CE2	1:B:61:VAL:HG21	2.43	0.52
1:B:337:ASP:OD2	1:B:339:ARG:NE	2.33	0.52
1:A:244:ARG:NH1	4:A:801:HOH:O	2.42	0.52
1:B:409:ASP:C	1:B:411:ASP:N	2.66	0.52
1:B:137:ARG:HH12	1:B:334:VAL:CB	2.16	0.52
1:B:210:PHE:CD1	1:B:214:LEU:HD12	2.45	0.52
1:A:161:SER:OG	1:A:162:GLN:N	2.42	0.52
1:B:58:PHE:HA	1:B:61:VAL:CG2	2.40	0.51
1:B:408:LEU:HB2	1:B:455:MET:HB3	1.92	0.51
1:A:283:PRO:HG2	1:A:286:LEU:HD12	1.92	0.51
1:A:613:PHE:CE2	1:A:655:LEU:CD2	2.93	0.51
1:B:67:GLY:O	1:B:69:LEU:N	2.43	0.51
1:B:439:VAL:O	1:B:442:VAL:HG12	2.11	0.51
1:A:476:TYR:HB3	2:A:701:ANP:N6	2.26	0.51
1:B:420:ARG:NH1	1:B:430:ARG:HD3	2.24	0.51
1:A:533:THR:OG1	1:A:534:LYS:N	2.41	0.51
1:A:72:LEU:N	1:A:72:LEU:CD1	2.73	0.51
1:A:113:LYS:HE2	1:A:227:GLU:OE2	2.11	0.51
1:B:76:THR:HG23	1:B:86:THR:HA	1.93	0.51
1:A:231:HIS:O	1:A:235:ILE:HG13	2.11	0.50
1:A:632:ARG:O	1:A:633:THR:C	2.53	0.50
1:B:61:VAL:HG12	1:B:68:GLU:OE1	2.10	0.50
1:A:623:HIS:CD2	1:A:627:LYS:HE2	2.47	0.50
1:B:424:MET:HE3	1:A:459:GLY:H	1.76	0.50
1:B:484:GLU:O	1:B:488:ILE:HG12	2.11	0.50
1:B:115:LEU:HD12	1:B:115:LEU:N	2.21	0.50
1:B:127:ARG:HG3	1:B:238:HIS:HD2	1.74	0.50
1:B:424:MET:HG3	1:A:459:GLY:CA	2.41	0.50
1:A:206:ALA:O	1:A:209:ILE:N	2.44	0.50
1:B:54:LEU:O	1:B:57:PHE:HB3	2.11	0.50
1:B:66:TYR:HE1	1:B:69:LEU:HD22	1.76	0.50
1:B:313:GLY:CA	1:B:319:LYS:HE2	2.40	0.50
1:B:397:GLU:HG3	1:B:656:ASN:HD22	1.77	0.50
1:A:78:GLN:HG3	1:A:84:ARG:HG3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ARG:HE	1:A:160:PRO:HB2	1.76	0.50
1:B:115:LEU:CD1	1:B:115:LEU:N	2.75	0.49
1:B:82:ASN:HB2	1:B:219:GLU:OE2	2.12	0.49
1:B:408:LEU:HB2	1:B:455:MET:CB	2.42	0.49
1:A:130:ALA:HB2	1:A:237:VAL:HG11	1.93	0.49
1:B:334:VAL:CG2	1:B:335:PRO:CD	2.89	0.49
1:A:54:LEU:HB2	1:A:77:TYR:CD2	2.47	0.49
1:A:391:GLN:HE22	1:A:418:MET:CE	2.24	0.49
1:B:396:MET:HE1	1:B:507:PHE:CE1	2.48	0.49
1:B:655:LEU:O	1:B:661:LEU:HD13	2.13	0.49
1:A:61:VAL:O	1:A:61:VAL:HG12	2.13	0.49
1:A:357:ARG:HH21	1:A:657:ARG:HG2	1.77	0.49
1:A:470:VAL:H	1:A:482:THR:HB	1.77	0.49
1:A:354:GLU:O	1:A:390:SER:OG	2.27	0.49
1:A:400:GLU:OE2	1:A:613:PHE:HB3	2.13	0.49
1:A:66:TYR:CE1	1:A:94:PRO:HD3	2.48	0.49
1:A:313:GLY:N	1:A:319:LYS:HD3	2.28	0.49
1:B:426:MET:O	1:B:427:LEU:C	2.56	0.49
1:A:344:VAL:HG13	1:A:405:LEU:HD21	1.88	0.49
1:B:336:ASP:O	1:B:337:ASP:C	2.57	0.48
1:B:58:PHE:HA	1:B:61:VAL:HG23	1.94	0.48
1:B:520:SER:HA	1:B:660:THR:O	2.13	0.48
1:B:59:HIS:O	1:B:60:SER:C	2.51	0.48
1:B:194:LEU:N	1:B:194:LEU:CD2	2.76	0.48
1:A:310:LEU:HD11	1:A:463:TYR:HB3	1.96	0.48
1:B:82:ASN:HB2	1:B:219:GLU:CD	2.38	0.48
1:B:225:LEU:HD21	1:B:230:LEU:CD2	2.43	0.48
1:B:652:GLY:O	1:B:656:ASN:HB2	2.13	0.48
1:B:76:THR:HG23	1:B:86:THR:CA	2.43	0.48
1:B:225:LEU:CD2	1:B:230:LEU:HD23	2.44	0.48
1:A:221:CYS:O	1:A:225:LEU:HD13	2.14	0.48
1:A:242:GLU:O	1:A:246:ASN:CG	2.57	0.48
1:A:131:ALA:O	1:A:135:ILE:HG13	2.14	0.47
1:B:73:THR:HG22	1:B:74:ASN:CG	2.39	0.47
1:B:128:ARG:O	1:B:132:GLU:HG3	2.14	0.47
1:A:368:ILE:CD1	1:A:389:THR:HA	2.44	0.47
1:A:485:ALA:O	1:A:488:ILE:N	2.47	0.47
1:B:66:TYR:CE2	1:B:94:PRO:CG	2.85	0.47
1:B:76:THR:HG23	1:B:86:THR:OG1	2.13	0.47
1:B:352:ARG:NH1	1:B:556:GLU:OE2	2.47	0.47
1:B:543:ILE:O	1:B:549:THR:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:VAL:HA	1:A:231:HIS:HD2	1.79	0.47
1:A:261:ILE:N	1:A:338:GLY:O	2.48	0.47
1:B:241:GLU:HG2	1:B:601:VAL:HG21	1.97	0.47
1:B:67:GLY:C	1:B:69:LEU:H	2.23	0.47
1:B:337:ASP:CG	1:B:339:ARG:HH21	2.23	0.47
1:B:357:ARG:HH21	1:B:657:ARG:CA	2.27	0.47
1:B:459:GLY:H	1:A:424:MET:HE2	1.80	0.47
1:B:573:LEU:CA	1:B:633:THR:HG21	2.38	0.47
1:B:578:GLU:N	1:B:579:PRO:HD2	2.30	0.47
1:A:79:ILE:HD11	1:A:83:VAL:CG1	2.44	0.47
1:A:82:ASN:OD1	1:A:82:ASN:N	2.48	0.47
1:B:439:VAL:HG13	1:B:440:GLU:HG2	1.95	0.47
1:A:54:LEU:HD11	1:A:58:PHE:CE2	2.49	0.47
1:A:287:GLU:HA	1:A:301:GLY:O	2.14	0.47
1:A:317:HIS:O	1:A:476:TYR:HD1	1.96	0.47
1:A:337:ASP:OD1	1:A:339:ARG:NH2	2.48	0.47
1:A:360:HIS:HB3	1:A:661:LEU:HD23	1.96	0.47
1:B:240:GLN:OE1	1:B:332:ASN:HB3	2.13	0.47
1:B:305:PRO:HG2	1:B:468:ARG:HG2	1.97	0.47
1:A:577:GLY:HA3	1:A:581:ILE:HD12	1.97	0.47
1:B:137:ARG:NH2	1:B:161:SER:O	2.48	0.47
1:B:409:ASP:O	1:B:410:GLU:C	2.58	0.47
1:A:192:VAL:O	1:A:194:LEU:CD1	2.63	0.47
1:B:226:ASN:OD1	1:B:229:ASP:OD2	2.32	0.46
1:B:391:GLN:HB3	1:B:417:LEU:HD12	1.97	0.46
1:A:79:ILE:HD12	1:A:215:VAL:CG2	2.46	0.46
1:A:337:ASP:OD2	1:A:339:ARG:NE	2.32	0.46
1:B:409:ASP:C	1:B:411:ASP:H	2.22	0.46
1:B:441:ARG:HB3	1:B:507:PHE:HZ	1.81	0.46
1:B:225:LEU:HD23	1:B:226:ASN:N	2.30	0.46
1:B:308:LEU:HD23	1:B:467:ALA:HA	1.98	0.46
1:B:373:PHE:N	1:B:373:PHE:CD1	2.79	0.46
1:A:581:ILE:HA	1:A:584:GLU:HB3	1.96	0.46
1:B:163:HIS:HD1	1:B:333:HIS:CE1	2.34	0.46
1:B:244:ARG:CG	1:B:343:VAL:HB	2.22	0.46
1:B:370:ASN:C	1:B:371:LEU:HD23	2.38	0.46
1:A:344:VAL:HG13	1:A:405:LEU:HD22	1.92	0.46
1:A:357:ARG:NH2	1:A:657:ARG:HG2	2.30	0.46
1:A:505:SER:OG	1:A:506:VAL:N	2.49	0.46
1:B:480:ASP:OD1	1:B:482:THR:HG22	2.15	0.46
1:A:93:ASP:CB	1:A:94:PRO:CD	2.61	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:ARG:HG3	1:A:238:HIS:HD2	1.80	0.46
1:A:127:ARG:NH2	1:A:294:HIS:HD2	2.02	0.46
1:B:352:ARG:HD3	1:B:554:MET:HB3	1.98	0.46
1:A:149:ARG:O	1:A:150:ARG:HG2	2.15	0.46
1:A:448:ASN:HD22	1:A:505:SER:HB2	1.80	0.46
1:A:521:PHE:CE2	1:A:575:TYR:HA	2.50	0.46
1:A:58:PHE:O	1:A:62:GLU:N	2.49	0.46
1:A:69:LEU:HA	1:A:72:LEU:HD13	1.96	0.46
1:B:76:THR:HG21	1:B:86:THR:OG1	2.15	0.46
1:B:380:PHE:CZ	1:B:389:THR:HG21	2.48	0.46
1:B:156:GLN:HB3	1:B:191:ARG:HB3	1.97	0.46
1:B:391:GLN:O	1:B:394:ASN:HB2	2.16	0.46
1:A:73:THR:C	1:A:75:GLU:H	2.24	0.46
1:A:573:LEU:HD11	1:A:581:ILE:HD13	1.98	0.46
1:B:386:SER:HB2	1:B:389:THR:CB	2.43	0.45
1:A:449:HIS:ND1	1:A:609:PHE:CE1	2.84	0.45
1:A:339:ARG:O	1:A:342:VAL:HG13	2.16	0.45
1:B:96:ALA:O	1:B:98:GLY:N	2.50	0.45
1:B:262:LEU:HD22	1:B:325:ALA:HB2	1.97	0.45
1:A:114:VAL:HG23	1:A:115:LEU:HD13	1.99	0.45
1:B:95:PHE:O	1:B:95:PHE:CD1	2.70	0.45
1:B:113:LYS:HE3	1:B:231:HIS:ND1	2.31	0.45
1:B:127:ARG:NH2	1:B:294:HIS:HD2	2.14	0.45
1:A:344:VAL:HG12	1:A:345:ASP:N	2.32	0.45
1:B:57:PHE:CZ	1:B:72:LEU:HD11	2.52	0.45
1:B:127:ARG:HG3	1:B:238:HIS:CD2	2.51	0.45
1:B:131:ALA:O	1:B:135:ILE:HG13	2.16	0.45
1:B:382:THR:HG21	1:A:316:PHE:HZ	1.82	0.45
1:B:96:ALA:HB1	1:B:97:PRO:CD	2.44	0.45
1:B:244:ARG:HH22	1:B:332:ASN:CG	2.17	0.45
1:B:263:PRO:O	1:B:263:PRO:HG2	2.16	0.45
1:B:461:GLY:N	1:A:421:ASP:OD2	2.46	0.45
1:A:165:LEU:HD21	1:A:563:GLN:NE2	2.32	0.45
1:A:344:VAL:O	1:A:345:ASP:C	2.56	0.45
1:A:360:HIS:CD2	1:A:663:THR:N	2.85	0.45
1:A:417:LEU:O	1:A:437:PRO:HA	2.17	0.45
1:B:57:PHE:O	1:B:60:SER:HB2	2.17	0.45
1:B:142:GLY:O	1:B:148:PRO:HD3	2.17	0.45
1:A:429:PRO:HB2	1:A:432:GLN:HG2	1.99	0.45
1:A:192:VAL:O	1:A:194:LEU:HD12	2.17	0.45
1:B:254:ALA:HB3	1:B:304:LEU:HD12	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:355:ASP:C	1:A:356:ARG:HG3	2.43	0.44
1:A:360:HIS:HA	1:A:381:VAL:HG22	1.99	0.44
1:B:422:ALA:HB1	1:B:426:MET:HE2	2.00	0.44
1:A:244:ARG:NH1	1:A:343:VAL:HG12	2.31	0.44
1:B:336:ASP:O	1:B:338:GLY:N	2.50	0.44
1:A:351:ILE:HG13	1:A:406:LEU:HD22	1.98	0.44
1:A:309:THR:HB	1:A:454:ILE:HG23	2.00	0.44
1:B:55:MET:HB2	1:B:207:ILE:HG12	2.00	0.44
1:B:505:SER:OG	1:B:506:VAL:N	2.49	0.44
1:A:54:LEU:O	1:A:57:PHE:HB3	2.18	0.44
1:A:523:THR:HG21	1:A:660:THR:OG1	2.18	0.44
1:B:210:PHE:HD1	1:B:214:LEU:HD12	1.82	0.44
1:B:199:ARG:NH1	1:A:199:ARG:HD3	2.32	0.44
1:B:261:ILE:O	1:B:264:ARG:NH2	2.51	0.44
1:B:266:ALA:C	1:A:384:ASP:OD2	2.61	0.44
1:B:521:PHE:O	1:B:524:VAL:HG22	2.18	0.43
1:B:244:ARG:CG	1:B:343:VAL:HG12	2.46	0.43
1:B:420:ARG:O	1:B:420:ARG:HG3	2.18	0.43
1:A:156:GLN:HB3	1:A:191:ARG:HB3	1.99	0.43
1:A:231:HIS:CE1	1:A:235:ILE:HD11	2.53	0.43
1:B:128:ARG:NH1	1:B:128:ARG:CG	2.73	0.43
1:B:354:GLU:O	1:B:390:SER:HB3	2.15	0.43
1:A:159:ARG:HA	1:A:160:PRO:HD2	1.72	0.43
1:A:163:HIS:CE1	1:A:333:HIS:HD1	2.35	0.43
1:A:367:PHE:CE2	1:A:395:ILE:HG21	2.53	0.43
1:A:395:ILE:O	1:A:399:LEU:HG	2.18	0.43
1:B:333:HIS:HB3	1:B:337:ASP:CB	2.48	0.43
1:B:401:LEU:HD13	1:B:649:ILE:HA	2.00	0.43
1:B:617:ILE:HD13	1:B:617:ILE:HA	1.89	0.43
1:B:653:ALA:HB1	1:B:657:ARG:NH1	2.17	0.43
1:A:61:VAL:HG12	1:A:201:ILE:HD12	2.00	0.43
1:A:148:PRO:C	1:A:150:ARG:N	2.74	0.43
1:A:206:ALA:O	1:A:209:ILE:HB	2.18	0.43
1:A:233:HIS:O	1:A:237:VAL:HG23	2.19	0.43
1:A:430:ARG:HH22	1:A:436:THR:HG23	1.84	0.43
1:B:225:LEU:HD21	1:B:230:LEU:HD23	1.99	0.43
1:A:380:PHE:O	1:A:381:VAL:HG23	2.19	0.43
1:A:480:ASP:OD1	1:A:482:THR:HG22	2.18	0.43
1:B:523:THR:O	1:B:523:THR:OG1	2.33	0.43
1:B:560:GLU:HB2	1:B:563:GLN:HG3	2.00	0.43
1:A:54:LEU:HD13	1:A:77:TYR:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PRO:HG2	1:A:95:PHE:HD2	1.84	0.43
1:A:222:VAL:O	1:A:225:LEU:HD22	2.18	0.43
1:A:660:THR:HG23	1:A:660:THR:O	2.18	0.43
1:A:62:GLU:CD	1:A:62:GLU:C	2.87	0.43
1:A:324:ARG:O	1:A:328:VAL:HG22	2.19	0.43
1:A:659:ARG:O	1:A:659:ARG:CG	2.66	0.43
1:A:308:LEU:O	1:A:468:ARG:HB3	2.19	0.42
1:A:330:ILE:HD12	1:A:647:ARG:HD3	2.00	0.42
1:A:400:GLU:O	1:A:614:SER:HB2	2.19	0.42
1:A:428:VAL:O	1:A:428:VAL:HG23	2.18	0.42
1:B:166:GLU:HG2	1:B:629:LEU:HD11	2.00	0.42
1:A:636:CYS:SG	1:A:638:LEU:HB2	2.59	0.42
1:B:244:ARG:HG3	1:B:343:VAL:HG12	1.99	0.42
1:B:407:LEU:C	1:B:408:LEU:HD12	2.44	0.42
1:B:423:LEU:HD12	1:A:461:GLY:C	2.45	0.42
1:B:437:PRO:HB2	1:B:439:VAL:HG12	2.02	0.42
1:A:82:ASN:O	1:A:106:PRO:HD2	2.19	0.42
1:A:305:PRO:HG2	1:A:468:ARG:HG2	2.00	0.42
1:A:401:LEU:HD11	1:A:652:GLY:HA3	2.01	0.42
1:B:337:ASP:OD1	1:B:339:ARG:NH2	2.52	0.42
1:A:562:GLY:C	1:A:644:SER:H	2.27	0.42
1:A:360:HIS:HD2	1:A:663:THR:HB	1.85	0.42
1:B:397:GLU:CG	1:B:656:ASN:ND2	2.81	0.42
1:B:434:PRO:HD2	1:A:314:GLY:O	2.20	0.42
1:B:356:ARG:O	1:B:659:ARG:NH2	2.47	0.42
1:B:370:ASN:HB3	1:B:434:PRO:HB3	2.02	0.42
1:B:595:LEU:HD23	1:B:596:PRO:HD2	2.01	0.42
1:A:203:GLY:O	1:A:207:ILE:HB	2.20	0.42
1:A:360:HIS:CD2	1:A:663:THR:H	2.37	0.42
1:A:366:PRO:O	1:A:441:ARG:NE	2.52	0.42
1:A:405:LEU:HA	1:A:452:SER:O	2.20	0.42
1:B:295:SER:OG	1:B:297:LYS:HB2	2.20	0.42
1:B:543:ILE:HG13	1:B:552:LEU:HD11	2.02	0.42
1:B:585:MET:HE1	1:B:623:HIS:ND1	2.35	0.42
1:B:57:PHE:CE2	1:B:72:LEU:HD11	2.55	0.41
1:B:208:ASP:O	1:B:209:ILE:C	2.60	0.41
1:B:425:GLN:O	1:B:428:VAL:O	2.36	0.41
1:A:126:CYS:HB2	1:A:601:VAL:HG23	2.01	0.41
1:B:97:PRO:HD2	1:B:98:GLY:H	1.85	0.41
1:B:235:ILE:O	1:B:239:ASP:HB2	2.20	0.41
1:A:433:GLU:HA	1:A:434:PRO:HD3	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:SER:HA	1:B:283:PRO:HD2	1.89	0.41
1:B:323:LEU:HD22	1:B:456:VAL:HG23	2.02	0.41
1:B:419:TYR:HB2	1:B:462:GLN:OE1	2.19	0.41
1:A:364:ILE:C	1:A:366:PRO:HD2	2.45	0.41
1:B:150:ARG:HG2	1:B:212:ASN:HB3	2.03	0.41
1:B:354:GLU:HG2	1:B:357:ARG:HB3	2.03	0.41
1:B:357:ARG:NH2	1:B:657:ARG:HA	2.35	0.41
1:A:82:ASN:O	1:A:105:CYS:HB2	2.20	0.41
1:A:573:LEU:N	1:A:633:THR:HG21	2.35	0.41
1:B:170:VAL:HA	1:B:187:GLU:O	2.20	0.41
1:A:73:THR:C	1:A:75:GLU:N	2.79	0.41
1:A:313:GLY:H	1:A:319:LYS:HD3	1.85	0.41
1:B:58:PHE:C	1:B:61:VAL:HG23	2.41	0.41
1:B:67:GLY:C	1:B:69:LEU:N	2.78	0.41
1:B:100:GLN:H	1:B:100:GLN:HG3	1.67	0.41
1:B:320:SER:O	1:B:324:ARG:HG3	2.20	0.41
1:B:345:ASP:OD1	1:B:347:THR:OG1	2.32	0.41
1:B:424:MET:CE	1:A:459:GLY:H	2.34	0.41
1:B:638:LEU:HD23	1:B:639:PRO:HD3	1.95	0.41
1:A:220:GLN:NE2	4:A:802:HOH:O	2.51	0.41
1:A:354:GLU:O	1:A:390:SER:CB	2.68	0.41
1:A:421:ASP:HB3	1:A:424:MET:HB2	2.03	0.41
1:A:595:LEU:HD23	1:A:596:PRO:HD2	2.03	0.41
1:A:638:LEU:HA	1:A:639:PRO:HD3	1.92	0.41
1:A:148:PRO:HG3	1:A:217:LEU:HG	2.02	0.41
1:B:54:LEU:HD13	1:B:77:TYR:CD2	2.56	0.40
1:B:396:MET:O	1:B:397:GLU:C	2.63	0.40
1:B:408:LEU:HD12	1:B:408:LEU:N	2.36	0.40
1:B:647:ARG:HE	1:B:647:ARG:HB2	1.72	0.40
1:B:658:LEU:HD12	1:B:659:ARG:N	2.36	0.40
1:A:62:GLU:OE1	1:A:63:GLY:N	2.54	0.40
1:B:462:GLN:O	1:B:465:PRO:HD2	2.21	0.40
1:A:102:ARG:HG2	1:A:104:VAL:HG23	2.03	0.40
1:A:323:LEU:HD12	1:A:323:LEU:HA	1.96	0.40
1:B:316:PHE:N	2:B:701:ANP:O2B	2.54	0.40
1:A:149:ARG:C	1:A:150:ARG:CG	2.91	0.40
1:B:357:ARG:NE	1:B:657:ARG:HG2	2.36	0.40
1:B:359:VAL:O	1:B:381:VAL:HA	2.22	0.40

All (50) 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:B:63:GLY:C	1:A:580:ARG:NH1[2_455]	0.27	1.93
1:B:69:LEU:C	1:A:632:ARG:NH2[2_455]	0.39	1.81
1:B:70:ARG:CA	1:A:632:ARG:NE[2_455]	0.55	1.65
1:B:584:GLU:CD	1:A:64:ARG:NE[2_455]	0.57	1.63
1:B:584:GLU:CG	1:A:64:ARG:NH2[2_455]	0.63	1.57
1:B:64:ARG:N	1:A:580:ARG:CZ[2_455]	0.89	1.31
1:B:584:GLU:CD	1:A:64:ARG:CZ[2_455]	0.93	1.27
1:B:70:ARG:C	1:A:632:ARG:CD[2_455]	0.97	1.23
1:B:63:GLY:O	1:A:580:ARG:NH1[2_455]	1.07	1.13
1:B:70:ARG:O	1:A:632:ARG:CD[2_455]	1.09	1.11
1:B:70:ARG:N	1:A:632:ARG:NH2[2_455]	1.12	1.08
1:B:584:GLU:OE1	1:A:64:ARG:NE[2_455]	1.12	1.08
1:B:584:GLU:OE2	1:A:64:ARG:NE[2_455]	1.14	1.06
1:B:70:ARG:N	1:A:632:ARG:CZ[2_455]	1.17	1.03
1:B:584:GLU:OE1	1:A:64:ARG:NH1[2_455]	1.55	0.65
1:B:69:LEU:O	1:A:632:ARG:NH2[2_455]	1.59	0.61
1:B:70:ARG:CB	1:A:632:ARG:NE[2_455]	1.64	0.56
1:B:63:GLY:O	1:A:580:ARG:CZ[2_455]	1.65	0.55
1:B:70:ARG:NH1	1:A:634:PRO:CB[2_455]	1.68	0.52
1:B:71:SER:N	1:A:632:ARG:CZ[2_455]	1.68	0.52
1:B:70:ARG:C	1:A:632:ARG:CZ[2_455]	1.70	0.50
1:B:64:ARG:C	1:A:580:ARG:NE[2_455]	1.72	0.48
1:B:69:LEU:O	1:A:632:ARG:CZ[2_455]	1.77	0.43
1:B:70:ARG:C	1:A:632:ARG:NH1[2_455]	1.79	0.41
1:B:70:ARG:C	1:A:632:ARG:CG[2_455]	1.79	0.41
1:B:70:ARG:O	1:A:632:ARG:CG[2_455]	1.79	0.41
1:B:64:ARG:CB	1:A:580:ARG:NH2[2_455]	1.80	0.40
1:B:64:ARG:C	1:A:580:ARG:CZ[2_455]	1.81	0.39
1:B:72:LEU:N	1:A:632:ARG:NH1[2_455]	1.83	0.37
1:B:584:GLU:CD	1:A:64:ARG:NH2[2_455]	1.83	0.37
1:B:64:ARG:C	1:A:580:ARG:NH2[2_455]	1.86	0.34
1:B:61:VAL:O	1:A:580:ARG:NH2[2_455]	1.91	0.29
1:B:584:GLU:CD	1:A:64:ARG:CD[2_455]	1.94	0.26
1:B:70:ARG:CB	1:A:632:ARG:CD[2_455]	1.95	0.25
1:B:69:LEU:O	1:A:632:ARG:NH1[2_455]	2.00	0.20
1:B:64:ARG:N	1:A:580:ARG:NE[2_455]	2.02	0.18
1:B:71:SER:N	1:A:632:ARG:NE[2_455]	2.02	0.18
1:B:69:LEU:N	1:A:632:ARG:NH2[2_455]	2.03	0.17
1:B:584:GLU:CD	1:A:64:ARG:NH1[2_455]	2.03	0.17
1:B:584:GLU:CG	1:A:64:ARG:NE[2_455]	2.04	0.16
1:B:584:GLU:CG	1:A:64:ARG:NH1[2_455]	2.04	0.16
1:B:63:GLY:O	1:A:580:ARG:NE[2_455]	2.07	0.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:SER:N	1:A:632:ARG:CG[2_455]	2.07	0.13
1:B:71:SER:CA	1:A:632:ARG:NH1[2_455]	2.09	0.11
1:B:64:ARG:O	1:A:580:ARG:CZ[2_455]	2.10	0.10
1:B:584:GLU:OE2	1:A:64:ARG:CZ[2_455]	2.11	0.09
1:B:64:ARG:O	1:A:580:ARG:NH2[2_455]	2.12	0.08
1:B:75:GLU:OE2	1:A:640:ARG:NH1[2_455]	2.14	0.06
1:B:71:SER:N	1:A:632:ARG:CD[2_455]	2.15	0.05
1:B:584:GLU:OE2	1:A:64:ARG:CD[2_455]	2.19	0.01

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	563/680 (83%)	535 (95%)	28 (5%)	0	100	100
1	B	563/680 (83%)	534 (95%)	26 (5%)	3 (0%)	24	59
All	All	1126/1360 (83%)	1069 (95%)	54 (5%)	3 (0%)	36	68

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	GLU
1	B	410	GLU
1	B	579	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	491/567 (87%)	449 (91%)	42 (9%)	10	34
1	B	491/567 (87%)	447 (91%)	44 (9%)	9	32
All	All	982/1134 (87%)	896 (91%)	86 (9%)	9	33

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	55	MET
1	B	61	VAL
1	B	65	ASN
1	B	75	GLU
1	B	76	THR
1	B	99	SER
1	B	105	CYS
1	B	110	SER
1	B	114	VAL
1	B	120	LEU
1	B	137	ARG
1	B	138	SER
1	B	151	THR
1	B	194	LEU
1	B	200	ARG
1	B	207	ILE
1	B	208	ASP
1	B	220	GLN
1	B	230	LEU
1	B	240	GLN
1	B	334	VAL
1	B	342	VAL
1	B	371	LEU
1	B	382	THR
1	B	395	ILE
1	B	397	GLU
1	B	412	THR
1	B	417	LEU
1	B	427	LEU
1	B	428	VAL
1	B	439	VAL
1	B	440	GLU
1	B	484	GLU
1	B	493	SER
1	B	524	VAL

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Mol	Chain	Res	Type
1	B	533	THR
1	B	559	VAL
1	B	567	ILE
1	B	573	LEU
1	B	601	VAL
1	B	632	ARG
1	B	637	TYR
1	B	661	LEU
1	B	663	THR
1	A	75	GLU
1	A	77	TYR
1	A	81	GLU
1	A	82	ASN
1	A	103	LEU
1	A	110	SER
1	A	115	LEU
1	A	199	ARG
1	A	207	ILE
1	A	225	LEU
1	A	227	GLU
1	A	230	LEU
1	A	248	LEU
1	A	333	HIS
1	A	343	VAL
1	A	357	ARG
1	A	368	ILE
1	A	369	ASN
1	A	382	THR
1	A	384	ASP
1	A	396	MET
1	A	397	GLU
1	A	400	GLU
1	A	412	THR
1	A	417	LEU
1	A	432	GLN
1	A	435	ILE
1	A	439	VAL
1	A	445	LEU
1	A	457	ILE
1	A	469	VAL
1	A	493	SER
1	A	512	ASN

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Mol	Chain	Res	Type
1	A	533	THR
1	A	559	VAL
1	A	567	ILE
1	A	574	LEU
1	A	588	LYS
1	A	630	GLU
1	A	638	LEU
1	A	660	THR
1	A	663	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	124	ASN
1	B	163	HIS
1	B	226	ASN
1	B	238	HIS
1	B	281	GLN
1	B	332	ASN
1	B	333	HIS
1	B	656	ASN
1	A	91	GLN
1	A	162	GLN
1	A	231	HIS
1	A	240	GLN
1	A	391	GLN
1	A	448	ASN
1	A	612	ASN
1	A	625	HIS
1	A	656	ASN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 4 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
2	ANP	B	701	3	33,33,33	2.04	11 (33%)	45,52,52	2.06	13 (28%)
2	ANP	A	701	3	33,33,33	2.20	11 (33%)	45,52,52	2.83	15 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ANP	B	701	3	-	6/18/38/38	0/3/3/3
2	ANP	A	701	3	-	7/18/38/38	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	701	ANP	C5-C4	4.70	1.47	1.39
2	B	701	ANP	PG-N3B	4.66	1.75	1.63
2	A	701	ANP	PB-O2B	-4.62	1.44	1.56
2	B	701	ANP	PB-N3B	4.61	1.75	1.63
2	A	701	ANP	PG-O3G	-4.41	1.45	1.56
2	A	701	ANP	C5-N7	-4.27	1.31	1.39
2	A	701	ANP	C4-N9	-3.63	1.30	1.37
2	A	701	ANP	C5-C4	3.59	1.45	1.39
2	B	701	ANP	PB-O1B	3.51	1.51	1.46
2	B	701	ANP	PG-O1G	3.42	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	ANP	O4'-C4'	-3.14	1.38	1.45
2	A	701	ANP	PG-O2G	-2.96	1.48	1.56
2	A	701	ANP	C8-N9	-2.88	1.32	1.37
2	A	701	ANP	PG-N3B	2.79	1.70	1.63
2	B	701	ANP	C5-C6	2.76	1.48	1.41
2	B	701	ANP	C8-N7	2.38	1.36	1.31
2	B	701	ANP	C5-N7	-2.22	1.35	1.39
2	A	701	ANP	PA-O2A	-2.15	1.45	1.55
2	A	701	ANP	C2'-C3'	-2.05	1.47	1.53
2	B	701	ANP	PG-O3G	-2.03	1.51	1.56
2	B	701	ANP	PB-O2B	-2.02	1.51	1.56
2	B	701	ANP	PG-O2G	-2.02	1.51	1.56

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	ANP	O1G-PG-N3B	-11.17	95.32	111.77
2	A	701	ANP	O2B-PB-O1B	6.83	124.52	109.87
2	B	701	ANP	C5-C4-N3	-5.81	118.71	126.72
2	A	701	ANP	C5-C4-N3	-5.43	119.24	126.72
2	A	701	ANP	N3-C4-N9	5.30	136.18	127.17
2	B	701	ANP	O1G-PG-N3B	-4.83	104.65	111.77
2	B	701	ANP	N3-C4-N9	4.59	134.97	127.17
2	A	701	ANP	O1B-PB-N3B	-4.49	105.15	111.77
2	B	701	ANP	O2B-PB-O1B	3.98	118.41	109.87
2	A	701	ANP	O2A-PA-O3A	3.82	117.59	107.27
2	B	701	ANP	C2-N3-C4	3.68	120.82	111.83
2	B	701	ANP	C4-C5-N7	-3.46	106.63	110.58
2	B	701	ANP	N3-C2-N1	-3.22	123.71	128.58
2	A	701	ANP	C2-N3-C4	3.17	119.56	111.83
2	A	701	ANP	O3A-PB-N3B	3.03	115.00	106.59
2	A	701	ANP	N3-C2-N1	-2.91	124.18	128.58
2	B	701	ANP	C4-N9-C8	2.60	108.47	105.74
2	A	701	ANP	N6-C6-N1	2.58	124.13	118.38
2	B	701	ANP	C3'-C2'-C1'	2.53	106.26	101.46
2	B	701	ANP	C5-N7-C8	2.53	107.43	103.45
2	B	701	ANP	O1B-PB-N3B	-2.52	108.06	111.77
2	A	701	ANP	C4-N9-C8	2.42	108.28	105.74
2	B	701	ANP	O2G-PG-O3G	2.33	113.84	107.59
2	A	701	ANP	O3'-C3'-C2'	-2.24	104.62	111.82
2	A	701	ANP	O2G-PG-O3G	2.23	113.60	107.59
2	A	701	ANP	O3'-C3'-C4'	-2.16	104.86	111.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	701	ANP	C6-C5-N7	2.06	136.07	132.09
2	A	701	ANP	C2-N1-C6	2.03	122.07	118.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

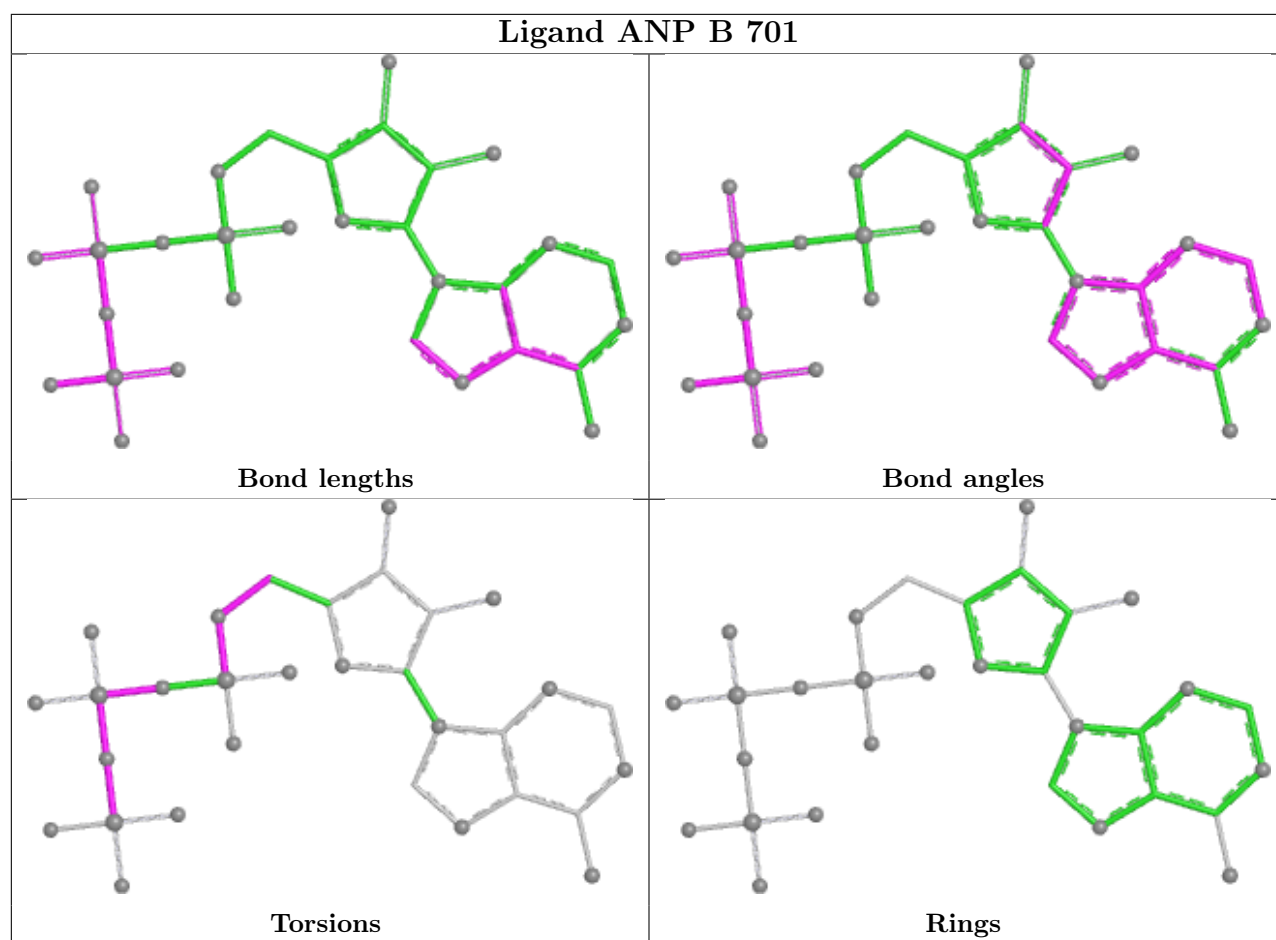
Mol	Chain	Res	Type	Atoms
2	B	701	ANP	PB-N3B-PG-O1G
2	B	701	ANP	PG-N3B-PB-O1B
2	B	701	ANP	C5'-O5'-PA-O2A
2	B	701	ANP	C5'-O5'-PA-O3A
2	A	701	ANP	PB-N3B-PG-O1G
2	A	701	ANP	PG-N3B-PB-O1B
2	A	701	ANP	PA-O3A-PB-O1B
2	A	701	ANP	C5'-O5'-PA-O1A
2	A	701	ANP	C5'-O5'-PA-O3A
2	A	701	ANP	C5'-O5'-PA-O2A
2	B	701	ANP	C4'-C5'-O5'-PA
2	A	701	ANP	O4'-C4'-C5'-O5'
2	B	701	ANP	PA-O3A-PB-O1B

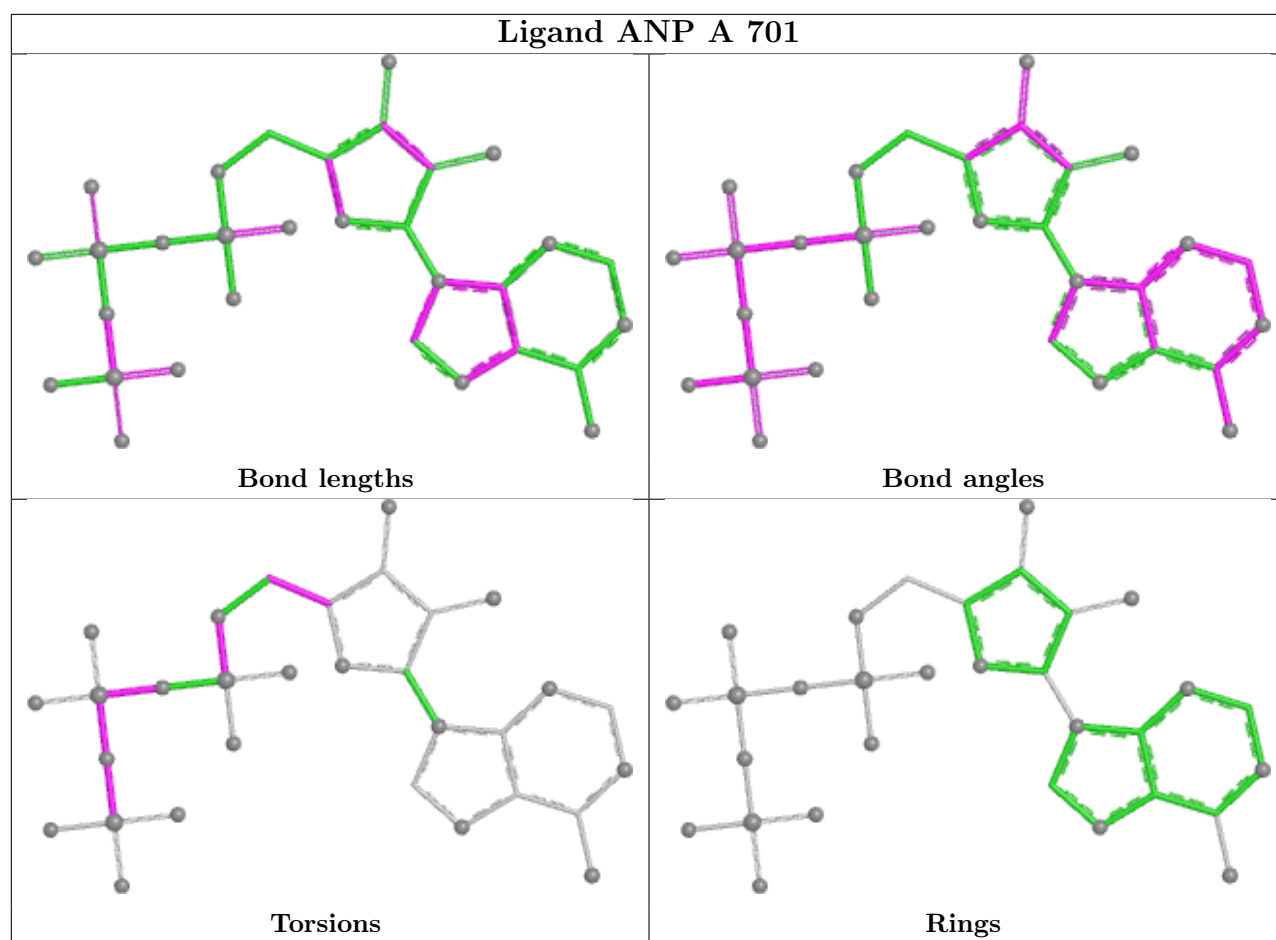
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	701	ANP	7	0
2	A	701	ANP	4	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	577/680 (84%)	-1.36	0 100 100	26, 43, 72, 80	0
1	B	577/680 (84%)	-1.31	0 100 100	26, 42, 74, 81	0
All	All	1154/1360 (84%)	-1.34	0 100 100	26, 42, 73, 81	0

There are no RSRZ outliers to report.

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](#)

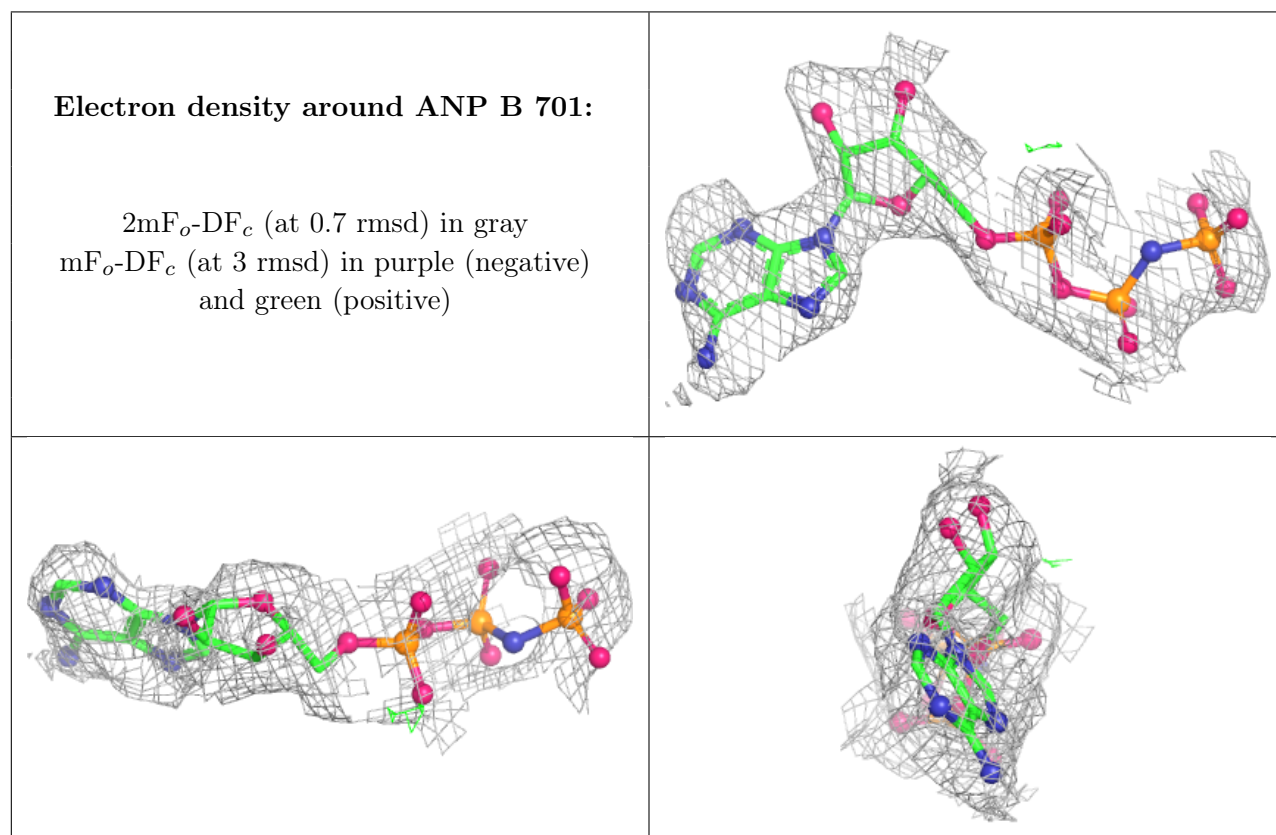
There are no oligosaccharides in this entry.

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.

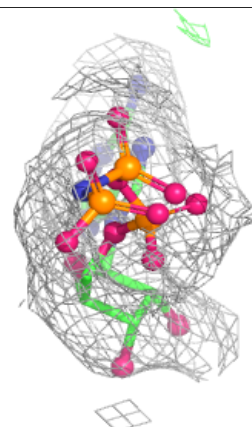
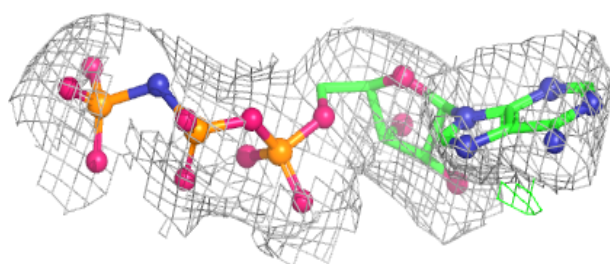
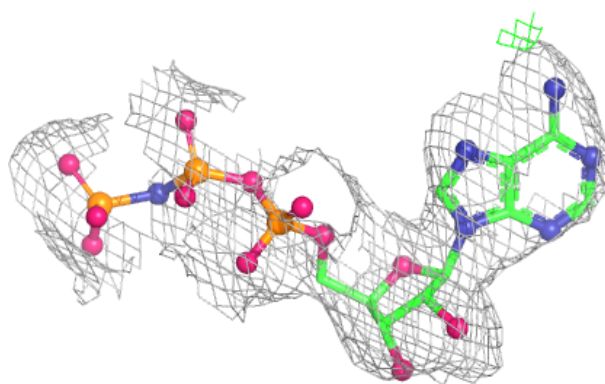
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	A	703	1/1	0.97	0.05	79,79,79,79	0
3	MG	A	702	1/1	0.98	0.05	45,45,45,45	0
2	ANP	B	701	31/31	0.99	0.04	36,37,40,40	0
3	MG	B	703	1/1	1.00	0.03	37,37,37,37	0
2	ANP	A	701	31/31	1.00	0.03	36,40,44,45	0
3	MG	B	702	1/1	1.00	0.05	43,43,43,43	0

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



Electron density around ANP A 701:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.