



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:05 AM UTC

PDB ID : 3O98 / pdb_00003o98
Title : Glutathionylspermidine synthetase/amidase C59A complex with ADP and Gsp
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Deposited on : 2010-08-04
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

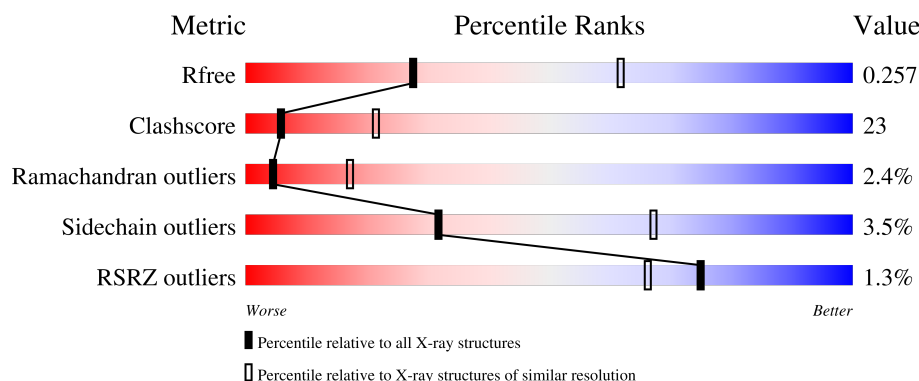
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	619	54% 37% 5% .
1	B	619	57% 37% . .

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
2	TS5	A	620	X	X	-	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9968 atoms, of which 3 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.

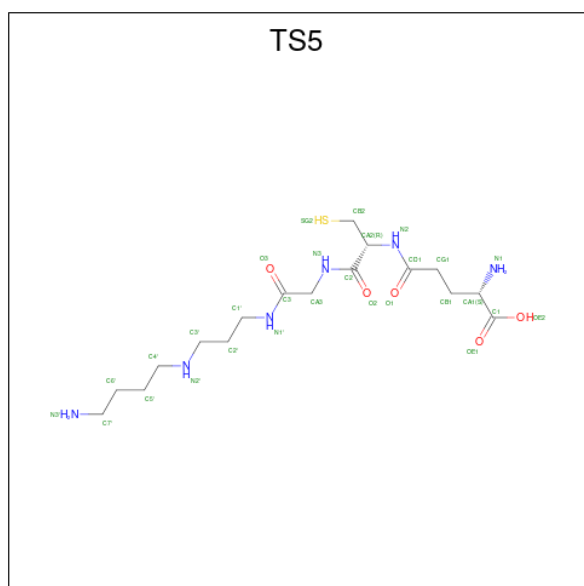
- Molecule 1 is a protein called Bifunctional glutathionylspermidine synthetase/amidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	599	Total	C	H	N	O	S	0	0	0
			4823	3087	2	826	890	18			
1	B	603	Total	C	H	N	O	S	0	0	0
			4852	3104	1	830	899	18			

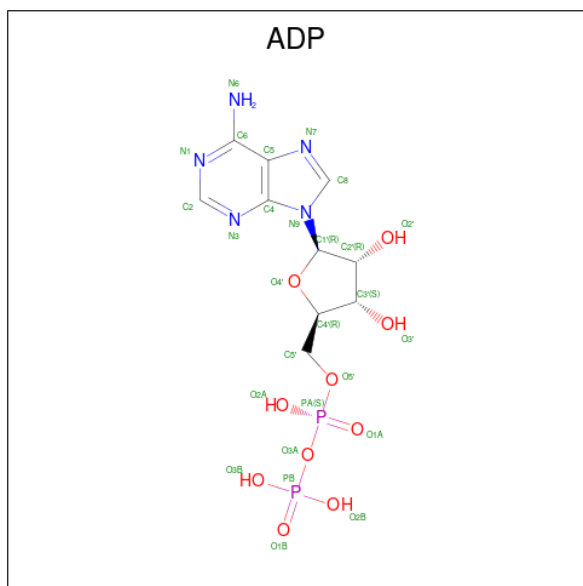
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ALA	CYS	engineered mutation	UNP P0AES0
B	59	ALA	CYS	engineered mutation	UNP P0AES0

- Molecule 2 is GLUTATHIONYLSPERMIDINE (CCD ID: TS5) (formula: $C_{17}H_{34}N_6O_5S$).



- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

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

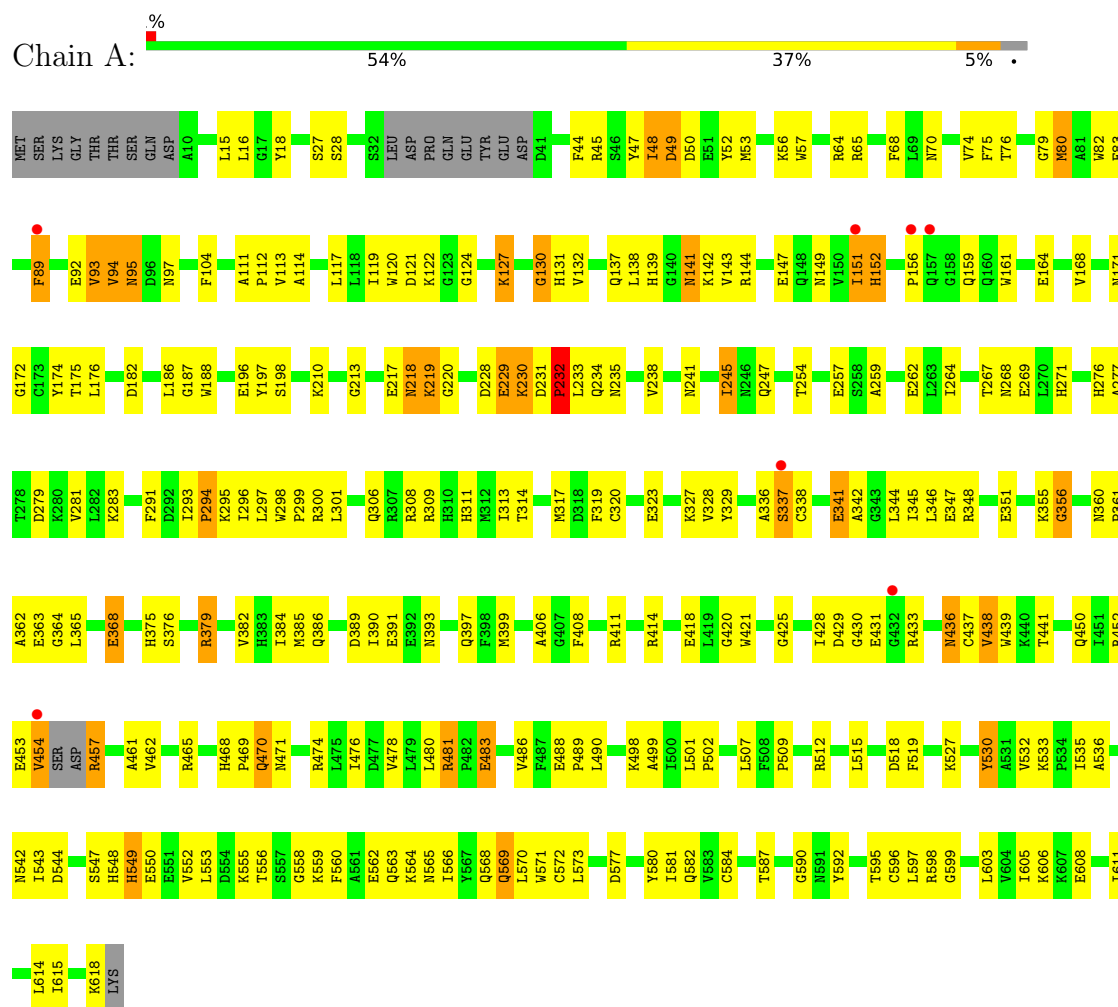
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	113	Total	O	0	0
			113	113		
5	B	93	Total	O	0	0
			93	93		

3 Residue-property plots [i](#)

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: Bifunctional glutathionylspermidine synthetase/amidase



D96	G172	I366	Q470	T556
N97	G173	N367	N471	A561
I98	Y174	E368	L475	E562
L99		H375	L476	Q563
F104	D178	M273	D477	T566
P105	T179	I384	V478	T567
M106	F180	F385	L479	Q568
G107	D181	Q386	L480	Q569
S108	D182	D387	R481	L570
P109	T183	K388	P482	V571
R110	T184	D389	E483	D577
A111	L185	I390	V484	
P112	L186	E391	L485	Y580
V113	G187	E392	V486	I581
	W188	N393	F487	Q582
L117	D194	K295	E488	N583
L118	T195	I296	P489	C584
I119	E196	L301	L490	T587
W120	Y197	R302	V491	
D121		L303	T492	Q590
K122	Q201	Q306	N497	N591
G123	I204	R307	L501	V592
G124	A205	R308	P502	T595
E125		R309		C596
	G213	I313	H511	L597
T129	A214	T314	Y513	N598
G130	R215			Q599
H131		F319	T517	D600
V132	N218	C320	D518	E601
V133	K219	M321	F519	S602
A133	G220	D322	T520	L603
I134	Q221	L326	V521	
Q137	K230	K327	N522	K606
L138		V328	D523	R607
H139		D334	E524	E608
K142	L233		L525	
V143	Q234		V526	
R144	N235			
	V238	D337	V532	
E147	Q239	C338		L614
Q148		H339	T535	I615
N149	G242	F340	A536	V616
V150		E341	G537	W617
H151	I245	A342	R538	K618
H152	N246	I345		LYS
	Q247	L346	N542	
L155		E347	I543	
	Y250		D544	
W161	I255	Q358	S547	
T162		F359		
R163	A259	A362	E551	
E164	P260	E363	V552	
L165	Q261	G364	L553	
F166	E262	L365	D554	
H167	L263		K555	
V168	I264			
V169				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.38Å 76.20Å 84.22Å 70.81° 74.37° 78.64°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.82	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 90.3 (30.00-2.82)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.54 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.220 , 0.262 0.211 , 0.257	Depositor DCC
R_{free} test set	1554 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	49.5	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 45.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9968	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 6.47% 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: TS5, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.55	2/4944 (0.0%)	0.91	17/6713 (0.3%)
1	B	0.51	0/4975	0.89	9/6757 (0.1%)
All	All	0.53	2/9919 (0.0%)	0.90	26/13470 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	VAL	C-O	9.72	1.43	1.23
1	A	453	GLU	C-N	6.71	1.42	1.33

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	THR	N-CA-C	-11.04	99.84	113.97
1	B	441	THR	N-CA-C	-9.49	101.38	113.72
1	A	453	GLU	O-C-N	-9.03	112.55	122.12
1	B	93	VAL	N-CA-C	8.04	118.59	110.23
1	B	486	VAL	N-CA-C	6.90	118.41	108.48
1	A	438	VAL	N-CA-C	6.64	117.86	108.17
1	A	219	LYS	N-CA-C	-6.61	105.29	113.15
1	B	219	LYS	N-CA-C	-6.59	105.98	112.97
1	A	549	HIS	N-CA-C	-6.45	105.38	113.18
1	B	481	ARG	CA-C-N	6.09	127.45	119.84
1	B	481	ARG	C-N-CA	6.09	127.45	119.84
1	B	581	ILE	N-CA-C	5.99	116.23	107.37
1	A	376	SER	N-CA-C	-5.95	102.52	110.55
1	A	48	ILE	N-CA-C	-5.88	97.11	109.34
1	A	453	GLU	CA-C-N	5.64	131.86	121.70
1	A	453	GLU	C-N-CA	5.64	131.86	121.70
1	B	48	ILE	N-CA-C	-5.60	96.65	106.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	230	LYS	N-CA-C	-5.49	105.38	111.36
1	A	119	ILE	N-CA-C	5.44	116.14	108.36
1	A	481	ARG	CA-C-N	5.41	126.60	119.84
1	A	481	ARG	C-N-CA	5.41	126.60	119.84
1	A	530	TYR	N-CA-C	5.25	115.47	108.38
1	A	486	VAL	N-CA-C	5.24	116.83	108.87
1	A	245	ILE	N-CA-C	-5.11	107.85	112.96
1	A	562	GLU	N-CA-C	5.10	119.56	113.23
1	A	130	GLY	N-CA-C	-5.05	103.42	112.22

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4821	2	4697	247	0
1	B	4851	1	4722	201	0
2	A	29	0	31	6	0
3	A	27	0	12	2	0
3	B	27	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	113	0	0	1	0
5	B	93	0	0	3	0
All	All	9965	3	9474	444	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 23.

All (444) 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:536:ALA:H	1:A:563:GLN:NE2	1.55	1.02
1:A:355:LYS:HD2	1:A:356:GLY:N	1.75	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ALA:HA	1:B:346:LEU:HD12	1.46	0.97
1:A:89:PHE:HE1	1:A:269:GLU:HG3	1.32	0.94
1:A:355:LYS:HD2	1:A:356:GLY:H	1.29	0.91
1:A:341:GLU:HG2	1:A:611:ILE:HG21	1.54	0.89
1:A:421:TRP:H	1:A:471:ASN:HD21	1.20	0.88
1:A:536:ALA:H	1:A:563:GLN:HE22	1.20	0.88
1:A:149:ASN:O	2:A:620:TS5:H2'2	1.77	0.84
1:B:80:MET:HE3	1:B:129:THR:HA	1.62	0.82
1:A:28:SER:HB3	1:A:57:TRP:HB2	1.62	0.81
1:A:28:SER:OG	1:A:149:ASN:OD1	1.97	0.81
1:B:110:ARG:HA	1:B:110:ARG:HH11	1.45	0.81
1:B:268:ASN:HD21	1:B:592:TYR:H	1.29	0.80
1:A:536:ALA:N	1:A:563:GLN:HE22	1.79	0.80
1:A:296:ILE:HD11	1:A:461:ALA:HA	1.64	0.79
1:B:389:ASP:HB3	1:B:391:GLU:HG2	1.67	0.77
1:B:462:VAL:HG11	1:B:480:LEU:HD13	1.65	0.77
1:A:436:ASN:HD22	1:A:436:ASN:H	1.30	0.76
1:A:138:LEU:HD12	1:A:143:VAL:HG12	1.68	0.74
1:A:151:ILE:HD13	1:A:151:ILE:H	1.52	0.73
1:A:89:PHE:CE1	1:A:269:GLU:HG3	2.22	0.73
1:B:121:ASP:HB2	1:B:186:LEU:HD21	1.70	0.72
1:A:363:GLU:HG3	1:A:364:GLY:H	1.54	0.72
1:B:590:GLY:N	5:B:8220:HOH:O	2.16	0.72
1:B:213:GLY:HA3	1:B:577:ASP:OD2	1.89	0.72
1:A:245:ILE:HB	1:A:611:ILE:HD11	1.70	0.72
1:A:611:ILE:HD12	1:A:611:ILE:O	1.90	0.71
1:A:122:LYS:HB2	1:A:127:LYS:O	1.90	0.71
1:B:31:SER:C	1:B:33:LEU:H	1.98	0.71
1:A:483:GLU:CD	1:A:483:GLU:H	2.00	0.69
1:A:498:LYS:HB2	1:A:535:ILE:HA	1.74	0.69
1:A:598:ARG:HG3	1:A:598:ARG:HH11	1.57	0.69
1:A:64:ARG:NH1	2:A:620:TS5:OE2	2.20	0.69
1:A:347:GLU:OE1	1:A:363:GLU:HB3	1.92	0.68
1:A:320:CYS:HG	1:A:571:TRP:CD1	2.11	0.68
1:A:137:GLN:HE21	1:A:139:HIS:HE1	1.40	0.68
1:A:141:ASN:ND2	1:A:142:LYS:HG2	2.09	0.68
1:A:390:ILE:HD12	1:A:391:GLU:HG3	1.76	0.68
1:A:48:ILE:O	1:A:49:ASP:HB2	1.94	0.67
1:A:80:MET:HE2	2:A:620:TS5:HB22	1.75	0.67
1:B:131:HIS:HE1	1:B:147:GLU:OE1	1.76	0.67
1:A:229:GLU:O	1:A:235:ASN:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:ILE:HG13	1:B:246:ASN:N	2.10	0.66
1:B:421:TRP:H	1:B:471:ASN:HD21	1.44	0.66
1:A:342:ALA:HA	1:A:346:LEU:HD12	1.78	0.66
1:B:542:ASN:ND2	1:B:561:ALA:HB2	2.11	0.66
1:B:338:CYS:HA	1:B:341:GLU:OE1	1.97	0.65
1:A:89:PHE:C	1:A:89:PHE:HD2	2.05	0.65
1:A:89:PHE:C	1:A:89:PHE:CD2	2.75	0.65
1:B:110:ARG:HA	1:B:110:ARG:NH1	2.12	0.65
1:B:522:ASN:HD22	1:B:523:ASP:N	1.95	0.64
1:B:522:ASN:O	1:B:526:VAL:HG23	1.96	0.64
1:B:367:ASN:ND2	1:B:405:GLN:HE22	1.96	0.64
1:A:137:GLN:NE2	1:A:144:ARG:HD2	2.13	0.63
1:B:544:ASP:OD1	1:B:555:LYS:HG3	1.98	0.63
1:B:121:ASP:HB2	1:B:186:LEU:CD2	2.28	0.63
1:A:501:LEU:HB2	1:A:502:PRO:HD3	1.80	0.63
1:B:109:PRO:HA	1:B:172:GLY:O	1.98	0.63
1:B:427:LEU:HD21	1:B:478:VAL:HG22	1.80	0.63
1:A:465:ARG:HD3	1:A:474:ARG:NH2	2.14	0.62
1:B:296:ILE:HD11	1:B:461:ALA:HA	1.81	0.62
1:A:64:ARG:HG3	1:A:74:VAL:HG23	1.80	0.62
1:A:436:ASN:HD22	1:A:436:ASN:N	1.95	0.62
1:A:393:ASN:O	1:A:397:GLN:HG3	1.99	0.62
1:A:268:ASN:HD21	1:A:592:TYR:H	1.47	0.62
1:A:536:ALA:HB3	1:A:563:GLN:HE22	1.64	0.62
1:A:121:ASP:HB2	1:A:186:LEU:HD21	1.80	0.62
1:B:31:SER:HB3	1:B:34:ASP:OD2	2.00	0.62
2:A:620:TS5:O3	2:A:620:TS5:H2'1	2.00	0.62
1:A:542:ASN:OD1	1:A:558:GLY:HA3	2.00	0.62
1:B:131:HIS:CD2	1:B:132:VAL:H	2.18	0.62
1:B:29:ASP:HB2	1:B:152:HIS:CD2	2.35	0.61
1:A:210:LYS:HD3	1:A:323:GLU:HB3	1.82	0.61
1:A:230:LYS:NZ	1:A:230:LYS:HB3	2.15	0.61
1:A:462:VAL:HG11	1:A:480:LEU:HD13	1.84	0.60
1:A:64:ARG:CG	1:A:74:VAL:HG23	2.31	0.60
1:A:196:GLU:HG2	1:A:197:TYR:CD2	2.37	0.60
1:A:141:ASN:HD22	1:A:141:ASN:H	1.50	0.60
1:B:53:MET:HE2	1:B:53:MET:HA	1.82	0.60
1:A:213:GLY:HA3	1:A:577:ASP:OD2	2.02	0.59
1:A:418:GLU:HG2	1:A:430:GLY:H	1.67	0.59
1:A:68:PHE:CE1	1:A:93:VAL:HG21	2.37	0.59
1:A:536:ALA:CA	1:A:563:GLN:HE22	2.14	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:501:LEU:HB2	1:B:502:PRO:HD3	1.84	0.59
1:A:499:ALA:O	1:A:502:PRO:HD2	2.02	0.59
1:B:328:VAL:HG12	1:B:513:TYR:O	2.02	0.59
1:A:92:GLU:HB3	1:A:95:ASN:HD21	1.66	0.59
1:A:151:ILE:H	1:A:151:ILE:CD1	2.16	0.58
1:A:168:VAL:CG2	1:A:175:THR:HB	2.32	0.58
1:A:390:ILE:HD12	1:A:391:GLU:N	2.17	0.58
1:B:536:ALA:H	1:B:563:GLN:NE2	2.01	0.58
1:B:536:ALA:H	1:B:563:GLN:HE22	1.50	0.58
1:A:113:VAL:HG22	1:A:114:ALA:N	2.18	0.58
1:A:411:ARG:HG3	1:A:411:ARG:HH11	1.68	0.58
1:A:598:ARG:HG3	1:A:598:ARG:NH1	2.17	0.58
1:B:95:ASN:OD1	1:B:97:ASN:HB3	2.03	0.58
1:A:457:ARG:HG2	1:A:457:ARG:HH11	1.68	0.58
1:B:428:ILE:HG22	1:B:434:LEU:HD23	1.84	0.58
1:B:518:ASP:OD2	1:B:519:PHE:N	2.36	0.58
1:A:418:GLU:HG3	1:A:430:GLY:HA3	1.84	0.58
1:B:475:LEU:HD11	1:B:479:LEU:HD11	1.85	0.58
1:B:301:LEU:HD23	1:B:490:LEU:HG	1.86	0.58
1:B:314:THR:HA	1:B:587:THR:O	2.04	0.58
1:B:341:GLU:HG2	1:B:611:ILE:HG13	1.85	0.58
1:B:23:VAL:HG13	1:B:69:LEU:HD12	1.86	0.57
1:B:139:HIS:HB2	1:B:142:LYS:O	2.02	0.57
1:B:400:GLU:HG3	1:B:410:THR:OG1	2.04	0.57
1:A:301:LEU:HD23	1:A:490:LEU:HG	1.87	0.57
1:B:367:ASN:HD22	1:B:405:GLN:HE22	1.51	0.57
1:A:314:THR:HA	1:A:587:THR:O	2.04	0.57
1:B:320:CYS:HG	1:B:571:TRP:CD1	2.22	0.57
1:A:536:ALA:N	1:A:563:GLN:NE2	2.35	0.57
1:B:554:ASP:OD2	1:B:555:LYS:N	2.37	0.57
1:A:421:TRP:N	1:A:471:ASN:HD21	1.99	0.57
1:B:120:TRP:HB2	1:B:131:HIS:HB3	1.87	0.57
1:B:524:GLU:OE1	1:B:524:GLU:N	2.38	0.56
1:A:549:HIS:O	1:A:550:GLU:HB2	2.05	0.56
1:B:45:ARG:HD2	1:B:375:HIS:NE2	2.20	0.56
1:B:580:TYR:O	1:B:599:GLY:HA2	2.05	0.56
1:B:601:GLU:CD	1:B:601:GLU:H	2.14	0.56
1:A:536:ALA:CB	1:A:563:GLN:HE22	2.18	0.56
1:A:542:ASN:HA	1:A:556:THR:O	2.04	0.56
1:B:42:ALA:HB1	1:B:375:HIS:CE1	2.40	0.56
1:B:147:GLU:HG3	1:B:150:VAL:HG11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:THR:O	1:B:522:ASN:N	2.39	0.55
1:A:15:LEU:HD21	1:A:18:TYR:CZ	2.41	0.55
1:A:418:GLU:HG2	1:A:430:GLY:N	2.21	0.55
1:A:559:LYS:HE2	1:A:560:PHE:CZ	2.42	0.55
1:B:319:PHE:CD2	1:B:326:LEU:HD11	2.42	0.55
1:A:95:ASN:HD22	1:A:95:ASN:H	1.55	0.55
1:A:306:GLN:OE1	1:B:94:VAL:HA	2.07	0.55
1:A:342:ALA:HB2	1:A:596:CYS:HB3	1.87	0.55
1:B:120:TRP:NE1	1:B:185:ILE:HG12	2.22	0.55
1:A:382:VAL:HG22	1:A:437:CYS:SG	2.46	0.55
1:B:30:TYR:O	1:B:31:SER:HB2	2.07	0.54
1:A:279:ASP:O	1:A:283:LYS:HG3	2.08	0.54
1:A:597:LEU:HD11	1:A:614:LEU:HD13	1.87	0.54
1:A:16:LEU:HD21	1:A:27:SER:HB2	1.88	0.54
1:A:124:GLY:HA3	1:A:182:ASP:O	2.07	0.54
1:B:89:PHE:HB2	1:B:99:LEU:O	2.07	0.54
1:B:233:LEU:HD12	1:B:401:GLN:OE1	2.08	0.54
1:A:535:ILE:HG22	1:A:566:ILE:HG23	1.89	0.54
1:B:309:ARG:HG3	1:B:309:ARG:HH11	1.72	0.54
1:B:42:ALA:HB1	1:B:375:HIS:HE1	1.71	0.54
1:A:298:TRP:HB2	1:A:299:PRO:HD3	1.89	0.54
1:A:454:VAL:CG1	1:A:457:ARG:HG3	2.37	0.54
1:A:336:ALA:O	1:A:337:SER:HB2	2.06	0.54
1:B:89:PHE:CD1	1:B:89:PHE:C	2.86	0.53
1:A:572:CYS:HB3	1:A:603:LEU:HD22	1.90	0.53
1:A:308:ARG:NE	1:A:311:HIS:ND1	2.50	0.53
1:A:112:PRO:HB3	1:A:188:TRP:CD2	2.43	0.53
1:A:175:THR:O	1:A:176:LEU:HD23	2.09	0.53
1:B:31:SER:C	1:B:33:LEU:N	2.65	0.53
1:B:194:ASP:OD1	1:B:196:GLU:HB3	2.08	0.53
1:A:229:GLU:HG2	1:A:235:ASN:HD22	1.72	0.53
1:A:556:THR:HG21	1:A:606:LYS:HE3	1.91	0.53
1:B:341:GLU:CG	1:B:611:ILE:HG13	2.39	0.53
1:B:532:VAL:HG22	1:B:567:TYR:CE1	2.44	0.53
1:A:218:ASN:C	1:A:220:GLY:H	2.16	0.53
1:A:568:GLN:HG2	3:A:3001:ADP:HN61	1.74	0.53
1:A:80:MET:H	1:A:83:GLU:CD	2.17	0.53
1:A:420:GLY:O	1:A:428:ILE:HG12	2.09	0.53
1:A:507:LEU:C	1:A:509:PRO:HD3	2.33	0.53
1:B:562:GLU:HB2	5:B:8151:HOH:O	2.08	0.53
1:A:512:ARG:HH11	1:A:512:ARG:HG2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:512:ARG:HG2	1:B:512:ARG:HH11	1.74	0.52
1:A:308:ARG:HG3	1:A:308:ARG:HH11	1.73	0.52
1:A:361:PRO:HG3	1:A:614:LEU:HD23	1.92	0.52
1:A:389:ASP:HB3	1:A:391:GLU:OE1	2.09	0.52
1:B:399:MET:HE3	1:B:439:TRP:CZ2	2.45	0.52
1:B:459:PHE:HD2	1:B:459:PHE:O	1.91	0.52
1:A:48:ILE:HG12	1:A:53:MET:HG3	1.90	0.52
1:A:469:PRO:HG2	1:A:470:GLN:NE2	2.25	0.52
1:A:436:ASN:H	1:A:436:ASN:ND2	2.04	0.52
1:A:341:GLU:CG	1:A:611:ILE:HG21	2.34	0.52
1:B:28:SER:HB2	1:B:57:TRP:HB2	1.92	0.52
1:B:319:PHE:CE2	1:B:328:VAL:HB	2.45	0.52
1:B:427:LEU:HD21	1:B:478:VAL:HG13	1.92	0.52
1:B:547:SER:OG	1:B:551:GLU:HG2	2.10	0.52
1:A:120:TRP:HB2	1:A:131:HIS:HB3	1.91	0.51
1:B:80:MET:HE3	1:B:129:THR:CA	2.36	0.51
1:B:167:MET:HE3	1:B:169:VAL:CG2	2.39	0.51
1:A:117:LEU:O	1:A:188:TRP:HA	2.10	0.51
1:B:522:ASN:ND2	1:B:525:LEU:H	2.08	0.51
1:B:287:LEU:O	1:B:290:LEU:HG	2.10	0.51
1:A:348:ARG:HD2	1:A:351:GLU:OE1	2.11	0.51
1:B:104:PHE:O	1:B:187:GLY:HA3	2.10	0.51
1:B:523:ASP:HB2	1:B:524:GLU:OE1	2.10	0.51
1:B:556:THR:CG2	1:B:606:LYS:HE3	2.41	0.51
1:A:137:GLN:CD	1:A:144:ARG:HD2	2.35	0.51
1:A:276:HIS:HE1	5:A:8102:HOH:O	1.94	0.51
1:B:235:ASN:O	1:B:239:GLN:HG2	2.11	0.51
1:B:319:PHE:O	1:B:582:GLN:HG3	2.11	0.51
1:A:247:GLN:OE1	1:A:247:GLN:HA	2.12	0.50
1:B:480:LEU:O	1:B:482:PRO:HD3	2.11	0.50
1:B:117:LEU:O	1:B:188:TRP:HA	2.11	0.50
1:B:204:ILE:HG12	1:B:205:ALA:N	2.27	0.50
1:B:342:ALA:O	1:B:362:ALA:HB3	2.12	0.50
1:B:125:GLU:HB3	1:B:183:THR:CG2	2.42	0.50
1:A:210:LYS:NZ	1:A:323:GLU:HG2	2.27	0.50
1:A:532:VAL:HB	1:A:544:ASP:HB2	1.92	0.50
1:A:468:HIS:CE1	1:A:470:GLN:HE21	2.30	0.50
1:B:53:MET:SD	1:B:65:ARG:HA	2.51	0.50
1:B:124:GLY:HA3	1:B:182:ASP:O	2.12	0.49
1:B:137:GLN:CG	1:B:144:ARG:HB2	2.42	0.49
1:A:465:ARG:HD3	1:A:474:ARG:HH21	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:566:ILE:C	1:A:566:ILE:HD12	2.36	0.49
1:B:48:ILE:O	1:B:49:ASP:HB2	2.12	0.49
1:A:74:VAL:HG22	1:A:75:PHE:N	2.27	0.49
1:A:137:GLN:HG2	1:A:144:ARG:HB2	1.94	0.49
1:A:436:ASN:N	1:A:436:ASN:ND2	2.59	0.49
1:B:25:ILE:HG23	1:B:148:GLN:HG3	1.95	0.49
1:B:366:ILE:HG23	1:B:367:ASN:N	2.26	0.49
1:B:581:ILE:CG2	1:B:597:LEU:HD22	2.43	0.49
1:A:399:MET:HE3	1:A:439:TRP:CZ2	2.48	0.49
1:B:268:ASN:ND2	1:B:592:TYR:H	2.04	0.49
1:A:527:LYS:O	1:A:548:HIS:HB2	2.13	0.49
1:B:71:TYR:O	1:B:73:VAL:HG13	2.13	0.49
1:B:178:ASP:HB2	1:B:185:ILE:HD11	1.94	0.49
1:B:462:VAL:HG11	1:B:480:LEU:CD1	2.40	0.49
1:B:566:ILE:HD12	1:B:566:ILE:C	2.38	0.49
1:A:141:ASN:HD21	1:A:142:LYS:HG2	1.78	0.49
1:B:255:ILE:HG23	1:B:614:LEU:HD11	1.95	0.49
1:B:468:HIS:HE1	1:B:470:GLN:HB2	1.78	0.49
1:A:257:GLU:OE2	1:A:618:LYS:HD3	2.12	0.48
1:B:359:PHE:CE2	1:B:616:VAL:HB	2.48	0.48
1:B:393:ASN:OD1	1:B:414:ARG:NH1	2.46	0.48
1:A:121:ASP:HB2	1:A:186:LEU:CD2	2.42	0.48
1:A:552:VAL:HG11	1:A:555:LYS:HE3	1.95	0.48
1:B:164:GLU:O	1:B:165:LEU:HD23	2.13	0.48
1:B:538:ARG:HB3	5:B:6001:HOH:O	2.13	0.48
1:A:45:ARG:HB3	1:A:47:TYR:CE1	2.49	0.48
1:A:64:ARG:NH2	1:A:75:PHE:CE1	2.82	0.48
1:B:387:ASP:CG	1:B:388:LYS:H	2.20	0.48
1:A:327:LYS:HG3	1:A:515:LEU:HD21	1.94	0.48
1:A:15:LEU:HD21	1:A:18:TYR:CE1	2.48	0.48
1:B:347:GLU:OE2	1:B:363:GLU:HB2	2.13	0.48
1:B:481:ARG:NH1	1:B:483:GLU:OE1	2.47	0.48
1:A:294:PRO:HD3	1:A:452:ARG:HH12	1.78	0.48
1:A:363:GLU:HG3	1:A:364:GLY:N	2.27	0.48
1:B:386:GLN:NE2	1:B:414:ARG:HD2	2.29	0.48
1:A:139:HIS:HB2	1:A:142:LYS:O	2.14	0.48
1:A:79:GLY:N	1:A:83:GLU:OE1	2.47	0.48
1:A:533:LYS:HG2	1:A:543:ILE:HD12	1.96	0.48
1:A:95:ASN:HD22	1:A:95:ASN:N	2.10	0.47
1:A:94:VAL:CG1	1:B:303:LEU:HD23	2.45	0.47
1:A:329:TYR:HE2	1:A:573:LEU:HD21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:389:ASP:C	1:A:391:GLU:H	2.21	0.47
1:B:523:ASP:O	1:B:526:VAL:HB	2.13	0.47
1:A:144:ARG:HG2	1:A:164:GLU:HG2	1.96	0.47
1:B:497:ASN:OD1	1:B:535:ILE:HB	2.15	0.47
1:B:522:ASN:HD21	1:B:525:LEU:H	1.59	0.47
1:A:295:LYS:HA	1:A:298:TRP:CD1	2.49	0.47
1:B:31:SER:O	1:B:33:LEU:N	2.48	0.47
1:B:245:ILE:HG13	1:B:246:ASN:OD1	2.14	0.47
1:B:321:MET:O	1:B:322:ASP:HB3	2.14	0.47
1:A:411:ARG:HG3	1:A:411:ARG:NH1	2.28	0.47
1:A:425:GLY:O	1:A:481:ARG:NH2	2.47	0.47
1:B:264:ILE:HG12	1:B:592:TYR:CD2	2.49	0.47
1:A:293:ILE:O	1:A:294:PRO:C	2.57	0.47
1:A:342:ALA:HB1	1:A:362:ALA:CB	2.45	0.47
1:A:389:ASP:C	1:A:391:GLU:N	2.72	0.47
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.80	0.47
1:B:259:ALA:O	1:B:262:GLU:HB3	2.15	0.47
1:B:390:ILE:N	1:B:390:ILE:HD13	2.29	0.47
1:B:109:PRO:HB2	1:B:197:TYR:CD1	2.50	0.47
1:B:270:LEU:HD23	1:B:273:MET:SD	2.55	0.47
1:A:231:ASP:O	1:A:233:LEU:N	2.48	0.47
1:A:151:ILE:HD13	1:A:151:ILE:N	2.27	0.46
1:A:544:ASP:OD1	1:A:555:LYS:HG2	2.15	0.46
1:B:104:PHE:CE2	1:B:110:ARG:HG2	2.50	0.46
1:A:418:GLU:HG2	1:A:418:GLU:O	2.15	0.46
1:A:141:ASN:HD22	1:A:141:ASN:N	2.11	0.46
1:B:147:GLU:HG3	1:B:150:VAL:CG1	2.45	0.46
1:B:137:GLN:HG3	1:B:144:ARG:HB2	1.96	0.46
1:A:210:LYS:HZ2	1:A:323:GLU:HG2	1.81	0.46
1:B:155:LEU:HD11	1:B:162:THR:HG22	1.97	0.46
1:A:231:ASP:O	1:A:232:PRO:C	2.59	0.46
1:A:342:ALA:HB1	1:A:362:ALA:HB3	1.97	0.46
1:A:535:ILE:HG13	1:A:536:ALA:N	2.30	0.46
1:B:245:ILE:HG13	1:B:246:ASN:H	1.81	0.46
1:B:429:ASP:OD2	1:B:433:ARG:HB3	2.15	0.46
1:A:137:GLN:HE21	1:A:139:HIS:CE1	2.28	0.46
1:A:429:ASP:C	1:A:431:GLU:H	2.23	0.46
1:A:53:MET:SD	1:A:65:ARG:HA	2.57	0.45
1:A:168:VAL:HG22	1:A:175:THR:HB	1.98	0.45
1:A:320:CYS:HG	1:A:571:TRP:HD1	1.60	0.45
1:B:601:GLU:CD	1:B:601:GLU:N	2.74	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:VAL:CG2	1:A:114:ALA:N	2.79	0.45
1:A:386:GLN:NE2	1:A:414:ARG:HE	2.13	0.45
1:A:556:THR:CG2	1:A:606:LYS:HE3	2.46	0.45
1:B:56:LYS:HA	1:B:57:TRP:HA	1.62	0.45
1:B:425:GLY:O	1:B:481:ARG:NH2	2.40	0.45
1:A:406:ALA:HB1	1:A:408:PHE:HE1	1.82	0.45
1:A:104:PHE:O	1:A:187:GLY:HA3	2.16	0.45
1:A:138:LEU:CD1	1:A:143:VAL:HG12	2.43	0.45
1:A:141:ASN:HD22	1:A:142:LYS:N	2.13	0.45
1:A:44:PHE:O	1:A:56:LYS:HG3	2.17	0.45
1:B:468:HIS:CE1	1:B:470:GLN:HB2	2.51	0.45
1:A:297:LEU:O	1:A:300:ARG:N	2.50	0.45
1:A:151:ILE:O	1:A:152:HIS:CG	2.70	0.45
1:B:386:GLN:HG3	1:B:387:ASP:O	2.16	0.45
1:B:418:GLU:HG2	1:B:430:GLY:N	2.32	0.45
1:B:488:GLU:HB3	1:B:492:THR:HG21	1.99	0.45
1:B:313:ILE:HB	1:B:488:GLU:OE1	2.17	0.45
1:A:344:LEU:O	1:A:347:GLU:N	2.46	0.44
1:B:512:ARG:HG2	1:B:512:ARG:NH1	2.32	0.44
1:A:277:ALA:O	1:A:281:VAL:HG23	2.18	0.44
1:A:512:ARG:HG2	1:A:512:ARG:NH1	2.32	0.44
1:B:66:PHE:CE2	1:B:134:ILE:HG21	2.52	0.44
1:B:106:ASN:HD22	1:B:185:ILE:HB	1.82	0.44
1:A:308:ARG:NH1	1:A:489:PRO:HB3	2.33	0.44
1:A:259:ALA:O	1:A:262:GLU:HB3	2.17	0.44
1:A:298:TRP:CD1	1:A:298:TRP:H	2.35	0.44
1:A:580:TYR:O	1:A:599:GLY:HA2	2.18	0.44
1:B:178:ASP:OD2	1:B:180:PHE:HD1	2.00	0.44
1:A:52:TYR:O	1:A:53:MET:HE2	2.17	0.44
1:A:291:PHE:CD1	1:A:291:PHE:N	2.85	0.44
1:A:564:LYS:HG2	1:A:565:ASN:N	2.31	0.44
1:B:112:PRO:HB3	1:B:188:TRP:CD2	2.52	0.44
1:B:307:ARG:HG3	1:B:308:ARG:HG3	2.00	0.44
1:B:320:CYS:SG	1:B:571:TRP:HD1	2.41	0.44
1:A:462:VAL:HG11	1:A:480:LEU:CD1	2.48	0.44
1:B:196:GLU:O	1:B:197:TYR:HB2	2.17	0.44
1:B:238:VAL:HG13	1:B:242:GLY:HA2	1.98	0.44
1:B:368:GLU:HA	1:B:368:GLU:OE1	2.18	0.44
1:B:430:GLY:C	1:B:432:GLY:H	2.25	0.44
1:A:264:ILE:HG12	1:A:592:TYR:CD2	2.52	0.44
1:A:295:LYS:HA	1:A:298:TRP:NE1	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:TYR:HA	1:A:570:LEU:N	2.33	0.44
1:A:568:GLN:HG2	3:A:3001:ADP:N6	2.33	0.44
1:B:568:GLN:O	1:B:569:GLN:C	2.60	0.44
1:A:94:VAL:HA	1:B:306:GLN:NE2	2.33	0.43
1:A:111:ALA:HB2	1:A:174:TYR:CZ	2.53	0.43
1:A:384:ILE:HG23	1:A:439:TRP:HE3	1.83	0.43
1:B:119:ILE:HD13	1:B:132:VAL:HG23	2.00	0.43
1:B:342:ALA:HB2	1:B:596:CYS:HB3	2.00	0.43
1:B:418:GLU:HG2	1:B:430:GLY:H	1.83	0.43
1:B:517:THR:OG1	1:B:568:GLN:HG3	2.17	0.43
1:A:56:LYS:HA	1:A:57:TRP:HA	1.61	0.43
1:A:320:CYS:HB2	1:A:329:TYR:CZ	2.53	0.43
1:B:320:CYS:HG	1:B:571:TRP:HD1	1.62	0.43
1:B:481:ARG:HH11	1:B:483:GLU:CD	2.26	0.43
1:A:470:GLN:NE2	1:A:470:GLN:N	2.66	0.43
1:B:542:ASN:HD21	1:B:561:ALA:HB2	1.82	0.43
1:B:556:THR:HG21	1:B:606:LYS:HE3	1.98	0.43
1:B:580:TYR:CE2	1:B:603:LEU:HD23	2.53	0.43
1:A:131:HIS:CG	1:A:132:VAL:N	2.86	0.43
1:A:595:THR:HG22	1:A:596:CYS:N	2.32	0.43
1:B:308:ARG:NH1	1:B:486:VAL:O	2.47	0.43
1:B:426:GLN:HA	1:B:481:ARG:NH2	2.34	0.43
1:A:80:MET:HB2	1:A:82:TRP:NE1	2.32	0.43
1:B:31:SER:HB3	1:B:34:ASP:CG	2.43	0.43
1:B:481:ARG:HH11	1:B:481:ARG:HG2	1.83	0.43
1:B:384:ILE:HG23	1:B:439:TRP:HE3	1.82	0.43
1:B:437:CYS:HA	1:B:485:LEU:O	2.17	0.43
1:B:32:SER:C	1:B:33:LEU:HD23	2.44	0.43
1:B:584:CYS:HB2	1:B:596:CYS:SG	2.59	0.43
1:A:390:ILE:HD12	1:A:390:ILE:C	2.44	0.43
1:A:144:ARG:HD3	1:A:161:TRP:CD1	2.54	0.43
1:B:89:PHE:C	1:B:89:PHE:HD1	2.26	0.43
1:B:107:GLY:HA2	1:B:174:TYR:O	2.18	0.43
1:A:94:VAL:HG13	1:B:303:LEU:HD23	2.01	0.42
1:B:358:GLY:HA3	1:B:615:ILE:CG2	2.49	0.42
1:A:234:GLN:O	1:A:238:VAL:HG23	2.19	0.42
1:A:313:ILE:HB	1:A:488:GLU:OE1	2.19	0.42
1:B:389:ASP:HB3	1:B:391:GLU:CG	2.44	0.42
1:A:45:ARG:HD2	1:A:375:HIS:NE2	2.33	0.42
1:A:271:HIS:CE1	1:A:590:GLY:HA2	2.55	0.42
1:B:386:GLN:HA	1:B:441:THR:OG1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:PRO:HD3	1:A:452:ARG:NH1	2.34	0.42
1:A:566:ILE:HD12	1:A:566:ILE:O	2.19	0.42
1:B:275:LEU:N	1:B:275:LEU:HD23	2.33	0.42
1:B:421:TRP:HA	1:B:426:GLN:O	2.20	0.42
1:B:532:VAL:HG22	1:B:567:TYR:HE1	1.82	0.42
1:B:536:ALA:N	1:B:563:GLN:HE22	2.14	0.42
1:A:229:GLU:HG2	1:A:235:ASN:ND2	2.33	0.42
1:A:230:LYS:HB3	1:A:230:LYS:HZ3	1.82	0.42
1:A:518:ASP:OD1	1:A:519:PHE:N	2.52	0.42
1:B:138:LEU:HD12	1:B:143:VAL:HG12	2.00	0.42
1:A:196:GLU:C	1:A:198:SER:H	2.27	0.42
1:A:418:GLU:CG	1:A:430:GLY:HA3	2.48	0.42
1:B:48:ILE:CG2	1:B:68:PHE:HE2	2.33	0.42
1:B:468:HIS:CG	1:B:469:PRO:HD2	2.54	0.42
1:A:80:MET:CE	2:A:620:TS5:HB22	2.48	0.42
1:A:317:MET:O	1:A:584:CYS:HA	2.19	0.42
1:A:581:ILE:CG2	1:A:597:LEU:HD22	2.50	0.42
1:A:582:GLN:OE1	1:A:605:ILE:HG13	2.19	0.42
1:A:130:GLY:O	1:A:131:HIS:HB2	2.20	0.42
1:A:308:ARG:O	1:A:309:ARG:C	2.62	0.42
1:A:122:LYS:HA	1:A:130:GLY:HA2	2.00	0.42
1:A:254:THR:HA	1:A:615:ILE:O	2.20	0.42
1:A:319:PHE:CE2	1:A:328:VAL:HB	2.55	0.42
1:B:32:SER:O	1:B:33:LEU:HD23	2.19	0.42
1:B:334:ASP:OD2	1:B:444:TRP:HB2	2.19	0.42
1:B:476:ILE:C	1:B:478:VAL:H	2.27	0.42
1:A:418:GLU:CG	1:A:430:GLY:H	2.32	0.42
1:A:429:ASP:OD2	1:A:433:ARG:N	2.52	0.42
1:B:121:ASP:O	1:B:122:LYS:C	2.63	0.42
1:B:245:ILE:HG22	1:B:345:ILE:HG21	2.02	0.42
1:B:511:HIS:HE1	1:B:513:TYR:CD2	2.37	0.42
1:A:530:TYR:CD1	1:A:530:TYR:C	2.98	0.41
1:A:230:LYS:NZ	1:A:230:LYS:CB	2.82	0.41
1:A:298:TRP:CD1	1:A:298:TRP:N	2.88	0.41
1:A:368:GLU:OE1	1:A:368:GLU:HA	2.20	0.41
1:A:95:ASN:CG	1:A:97:ASN:HB3	2.45	0.41
1:B:215:ARG:HG3	1:B:215:ARG:NH1	2.35	0.41
1:B:221:GLN:OE1	1:B:250:TYR:HE2	2.04	0.41
1:B:270:LEU:O	1:B:274:TYR:HD1	2.03	0.41
1:A:450:GLN:HE22	1:A:474:ARG:HB3	1.85	0.41
1:B:471:ASN:HD22	1:B:471:ASN:HA	1.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HB3	1:A:47:TYR:HE1	1.85	0.41
1:A:70:ASN:ND2	1:B:461:ALA:HB1	2.35	0.41
1:A:547:SER:HB3	1:A:553:LEU:HD21	2.02	0.41
1:A:309:ARG:HG3	1:A:309:ARG:HH11	1.84	0.41
1:A:217:GLU:O	1:A:219:LYS:N	2.48	0.41
1:A:347:GLU:OE1	1:A:360:ASN:HB3	2.21	0.41
1:A:476:ILE:C	1:A:478:VAL:H	2.28	0.41
1:B:595:THR:HG22	1:B:596:CYS:N	2.35	0.41
1:A:15:LEU:HD21	1:A:18:TYR:OH	2.21	0.41
1:A:295:LYS:HE2	1:A:295:LYS:HB3	1.89	0.41
1:A:342:ALA:HB2	1:A:596:CYS:CB	2.51	0.41
1:A:363:GLU:C	1:A:365:LEU:H	2.29	0.41
1:A:568:GLN:O	1:A:569:GLN:C	2.64	0.41
1:B:245:ILE:CG1	1:B:246:ASN:N	2.80	0.41
1:B:538:ARG:HA	3:B:3002:ADP:O2B	2.21	0.41
1:A:156:PRO:HB2	1:A:159:GLN:HB2	2.02	0.41
1:A:379:ARG:HB2	1:A:437:CYS:HB2	2.03	0.41
1:B:427:LEU:CD2	1:B:478:VAL:HG13	2.51	0.41
1:A:338:CYS:HA	1:A:341:GLU:OE2	2.20	0.40
1:A:344:LEU:O	1:A:345:ILE:C	2.63	0.40
1:B:161:TRP:CZ3	1:B:164:GLU:HG3	2.56	0.40
1:B:422:ASP:OD1	1:B:426:GLN:N	2.45	0.40
1:A:385:MET:HG3	1:A:438:VAL:HG13	2.03	0.40
1:B:339:HIS:CD2	1:B:395:HIS:HE1	2.39	0.40
1:A:49:ASP:HB3	1:A:50:ASP:H	1.66	0.40
1:B:121:ASP:HB2	1:B:186:LEU:CG	2.51	0.40
1:A:131:HIS:HD2	2:A:620:TS5:HN1'	1.67	0.40
1:A:469:PRO:HG2	1:A:470:GLN:HE22	1.87	0.40
1:B:366:ILE:CG2	1:B:367:ASN:N	2.85	0.40
1:A:48:ILE:HG12	1:A:53:MET:CG	2.51	0.40
1:A:92:GLU:O	1:A:95:ASN:ND2	2.55	0.40
1:B:538:ARG:HH11	1:B:538:ARG:HG3	1.87	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	593/619 (96%)	525 (88%)	54 (9%)	14 (2%)	4	17
1	B	599/619 (97%)	540 (90%)	44 (7%)	15 (2%)	4	16
All	All	1192/1238 (96%)	1065 (89%)	98 (8%)	29 (2%)	4	17

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	A	341	GLU
1	B	150	VAL
1	A	94	VAL
1	A	356	GLY
1	B	32	SER
1	B	94	VAL
1	B	218	ASN
1	B	247	GLN
1	B	521	VAL
1	A	49	ASP
1	A	228	ASP
1	A	232	PRO
1	B	31	SER
1	B	341	GLU
1	B	522	ASN
1	B	76	THR
1	B	322	ASP
1	A	152	HIS
1	A	171	ASN
1	A	337	SER
1	A	218	ASN
1	B	482	PRO
1	A	93	VAL
1	A	294	PRO
1	A	172	GLY
1	B	364	GLY
1	B	358	GLY
1	B	294	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	510/529 (96%)	490 (96%)	20 (4%)	28	64
1	B	514/529 (97%)	498 (97%)	16 (3%)	35	70
All	All	1024/1058 (97%)	988 (96%)	36 (4%)	32	67

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	80	MET
1	A	89	PHE
1	A	95	ASN
1	A	141	ASN
1	A	147	GLU
1	A	151	ILE
1	A	229	GLU
1	A	230	LYS
1	A	232	PRO
1	A	241	ASN
1	A	267	THR
1	A	368	GLU
1	A	379	ARG
1	A	436	ASN
1	A	457	ARG
1	A	470	GLN
1	A	483	GLU
1	A	569	GLN
1	A	608	GLU
1	B	76	THR
1	B	113	VAL
1	B	148	GLN
1	B	201	GLN
1	B	233	LEU
1	B	261	GLN
1	B	275	LEU

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Mol	Chain	Res	Type
1	B	279	ASP
1	B	390	ILE
1	B	438	VAL
1	B	459	PHE
1	B	470	GLN
1	B	471	ASN
1	B	482	PRO
1	B	522	ASN
1	B	608	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	70	ASN
1	A	95	ASN
1	A	137	GLN
1	A	139	HIS
1	A	141	ASN
1	A	159	GLN
1	A	235	ASN
1	A	268	ASN
1	A	276	HIS
1	A	352	GLN
1	A	383	HIS
1	A	395	HIS
1	A	397	GLN
1	A	405	GLN
1	A	436	ASN
1	A	470	GLN
1	A	471	ASN
1	A	563	GLN
1	A	568	GLN
1	B	70	ASN
1	B	102	GLN
1	B	131	HIS
1	B	152	HIS
1	B	157	GLN
1	B	159	GLN
1	B	201	GLN
1	B	234	GLN
1	B	268	ASN

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Mol	Chain	Res	Type
1	B	286	ASN
1	B	306	GLN
1	B	339	HIS
1	B	352	GLN
1	B	367	ASN
1	B	386	GLN
1	B	395	HIS
1	B	426	GLN
1	B	468	HIS
1	B	471	ASN
1	B	510	HIS
1	B	522	ASN
1	B	563	GLN
1	B	565	ASN
1	B	568	GLN
1	B	591	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ADP	A	3001	4	28,29,29	1.24	3 (10%)	43,45,45	1.04	3 (6%)
3	ADP	B	3002	4	28,29,29	1.23	3 (10%)	43,45,45	1.07	2 (4%)
2	TS5	A	620	-	27,28,28	4.57	15 (55%)	30,33,33	5.46	13 (43%)

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	ADP	A	3001	4	-	3/16/32/32	0/3/3/3
3	ADP	B	3002	4	-	3/16/32/32	0/3/3/3
2	TS5	A	620	-	1/1/6/10	11/34/34/34	-

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	620	TS5	CB2-CA2	-12.05	1.40	1.53
2	A	620	TS5	C3-N1'	11.69	1.61	1.33
2	A	620	TS5	CD1-N2	6.76	1.48	1.34
2	A	620	TS5	O3-C3	6.29	1.35	1.23
2	A	620	TS5	CA2-C2	-5.60	1.38	1.52
2	A	620	TS5	O1-CD1	5.19	1.33	1.23
2	A	620	TS5	CA3-N3	4.60	1.57	1.45
2	A	620	TS5	C3'-N2'	4.29	1.61	1.47
2	A	620	TS5	CA2-N2	3.93	1.54	1.45
2	A	620	TS5	C2'-C1'	-3.90	1.36	1.51
2	A	620	TS5	C2-N3	3.85	1.42	1.33
2	A	620	TS5	CB2-SG2	3.68	1.89	1.81
3	B	3002	ADP	C2-N1	3.34	1.39	1.33
3	A	3001	ADP	C2-N1	3.30	1.39	1.33
2	A	620	TS5	C2'-C3'	3.12	1.63	1.51
2	A	620	TS5	OE2-C1	2.75	1.39	1.30
3	B	3002	ADP	C1'-N9	2.34	1.52	1.46
3	A	3001	ADP	C1'-N9	2.34	1.52	1.46
2	A	620	TS5	CA3-C3	-2.19	1.45	1.52
3	A	3001	ADP	C5-C6	2.13	1.46	1.41
3	B	3002	ADP	C5-C6	2.00	1.46	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	620	TS5	CA2-CB2-SG2	14.55	130.56	114.16
2	A	620	TS5	CB2-CA2-C2	13.69	139.28	109.50
2	A	620	TS5	C1'-N1'-C3	-10.70	102.90	122.82
2	A	620	TS5	CB2-CA2-N2	-10.23	96.69	111.28
2	A	620	TS5	C2'-C1'-N1'	9.90	139.96	112.20
2	A	620	TS5	CG1-CB1-CA1	-5.28	101.75	113.86
2	A	620	TS5	C2'-C3'-N2'	-4.63	99.64	112.07
2	A	620	TS5	O2-C2-CA2	-4.57	110.90	120.48
2	A	620	TS5	C2-CA2-N2	4.27	122.66	111.11
2	A	620	TS5	O1-CD1-N2	-4.26	115.74	122.95
2	A	620	TS5	CA2-N2-CD1	3.84	131.32	121.68
2	A	620	TS5	O3-C3-CA3	-3.39	113.19	120.75
2	A	620	TS5	CB1-CA1-C1	-3.36	101.55	110.45
3	A	3001	ADP	N3-C2-N1	-3.07	123.94	128.58
3	B	3002	ADP	N3-C2-N1	-3.02	124.01	128.58
3	B	3002	ADP	C2-N1-C6	2.71	123.18	118.73
3	A	3001	ADP	C2-N1-C6	2.26	122.44	118.73
3	A	3001	ADP	C3'-C2'-C1'	2.08	105.41	101.46

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	620	TS5	CA2

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	620	TS5	C2-CA2-CB2-SG2
3	A	3001	ADP	PA-O3A-PB-O3B
3	B	3002	ADP	PA-O3A-PB-O3B
2	A	620	TS5	O2-C2-N3-CA3
2	A	620	TS5	C2'-C1'-N1'-C3
2	A	620	TS5	CA2-C2-N3-CA3
2	A	620	TS5	N1'-C3-CA3-N3
2	A	620	TS5	O1-CD1-N2-CA2
2	A	620	TS5	CA3-C3-N1'-C1'
2	A	620	TS5	OE2-C1-CA1-CB1
3	B	3002	ADP	C4'-C5'-O5'-PA
3	A	3001	ADP	PA-O3A-PB-O2B
3	B	3002	ADP	PA-O3A-PB-O2B
3	A	3001	ADP	C4'-C5'-O5'-PA
2	A	620	TS5	C1'-C2'-C3'-N2'
2	A	620	TS5	N1-CA1-CB1-CG1

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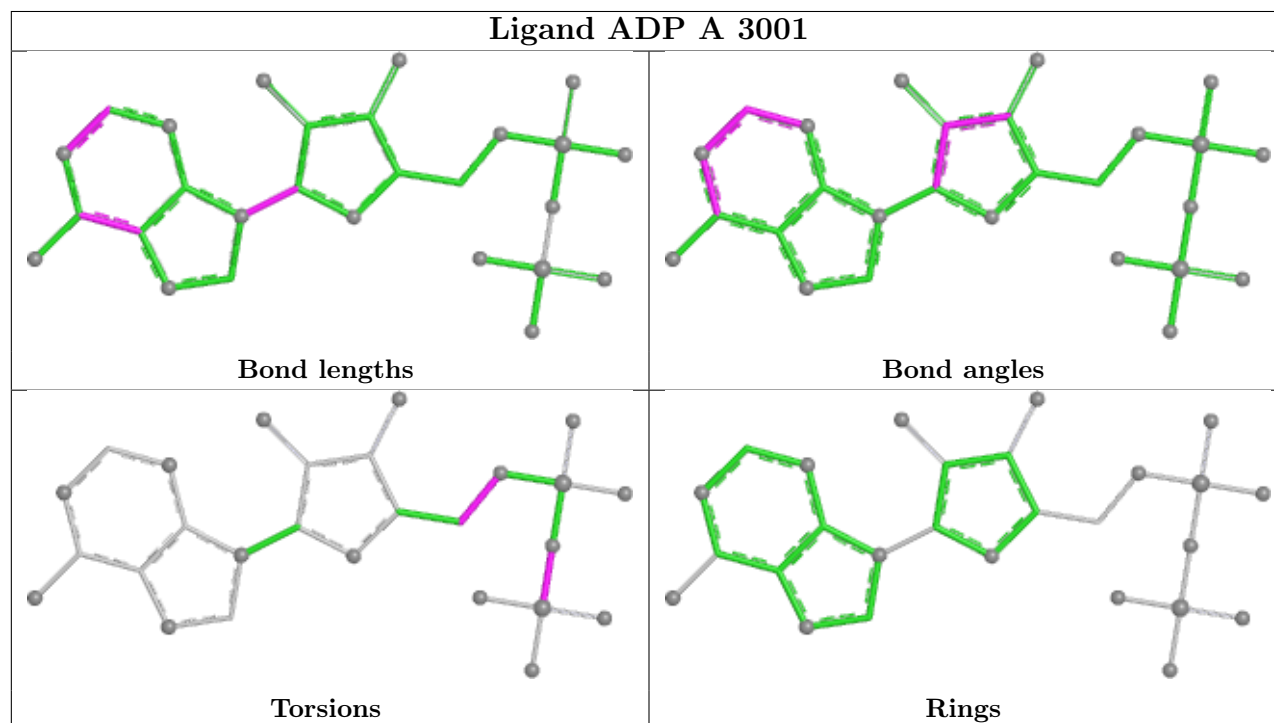
Mol	Chain	Res	Type	Atoms
2	A	620	TS5	C2'-C3'-N2'-C4'

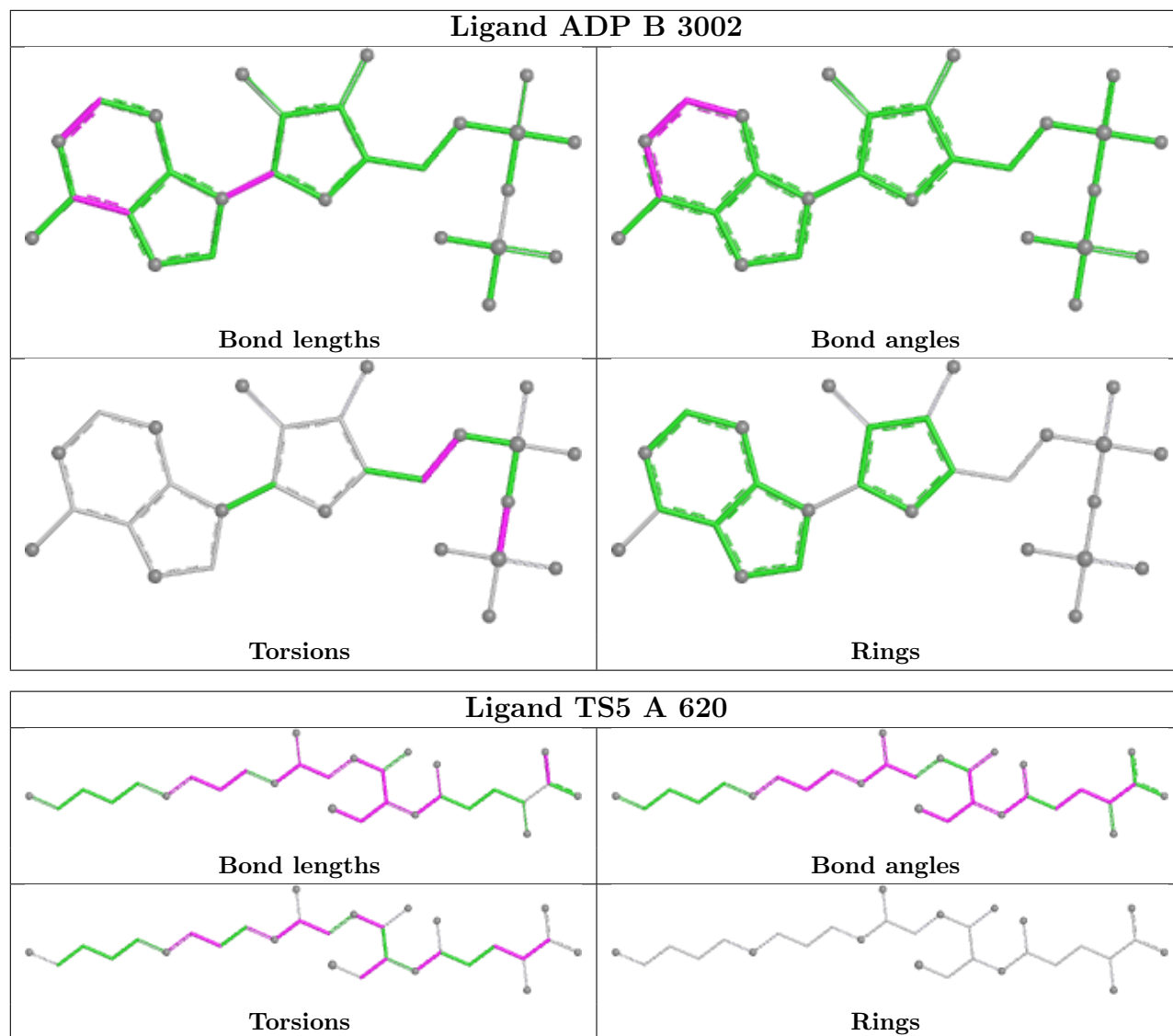
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	ADP	2	0
3	B	3002	ADP	1	0
2	A	620	TS5	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	599/619 (96%)	-0.02	7 (1%) 76 68	17, 43, 65, 84	0
1	B	603/619 (97%)	0.05	9 (1%) 72 63	19, 46, 69, 86	0
All	All	1202/1238 (97%)	0.01	16 (1%) 75 66	17, 44, 67, 86	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	33	LEU	3.8
1	A	337	SER	3.6
1	B	32	SER	3.5
1	B	553	LEU	3.1
1	B	337	SER	3.0
1	A	454	VAL	2.7
1	B	552	VAL	2.6
1	B	339	HIS	2.6
1	B	338	CYS	2.5
1	A	151	ILE	2.5
1	B	34	ASP	2.2
1	A	432	GLY	2.2
1	B	31	SER	2.2
1	A	157	GLN	2.1
1	A	156	PRO	2.1
1	A	89	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

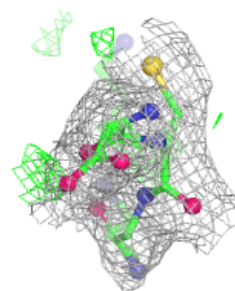
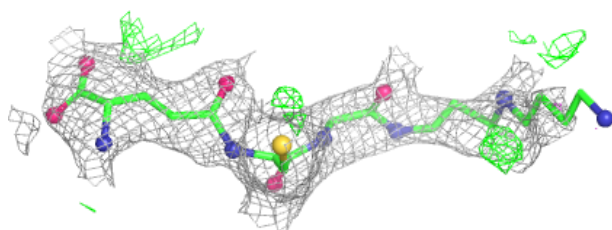
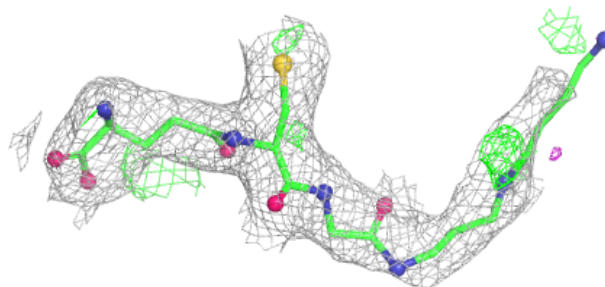
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	TS5	A	620	29/29	0.84	0.15	39,45,75,78	0
3	ADP	A	3001	27/27	0.97	0.07	30,33,34,36	0
3	ADP	B	3002	27/27	0.98	0.06	32,39,40,42	0
4	MG	A	4000	1/1	0.98	0.04	37,37,37,37	0
4	MG	B	6000	1/1	0.99	0.02	39,39,39,39	0
4	MG	A	5000	1/1	1.00	0.02	32,32,32,32	0
4	MG	B	7000	1/1	1.00	0.02	34,34,34,34	0

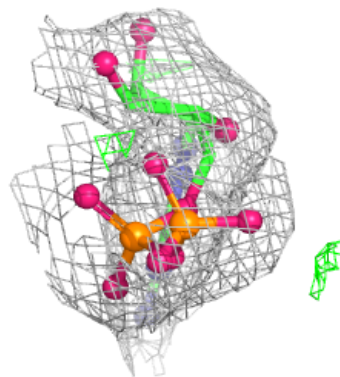
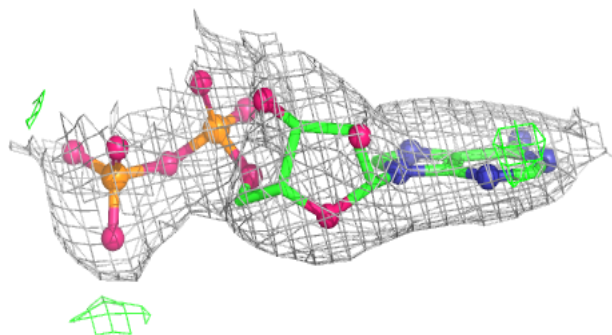
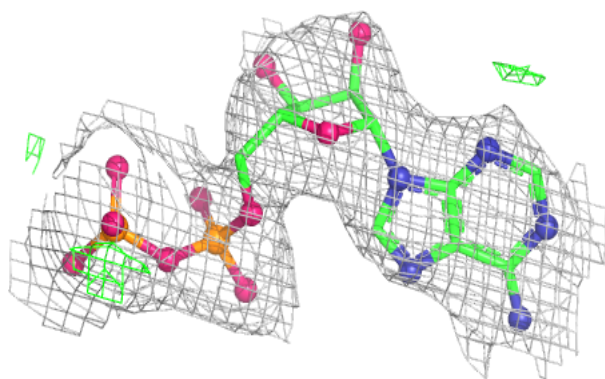
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around TS5 A 620:

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

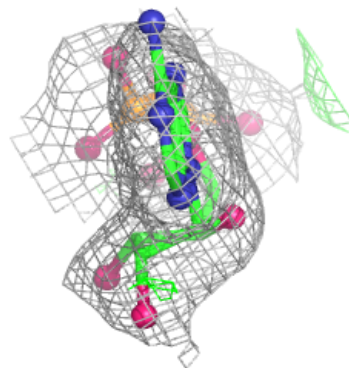
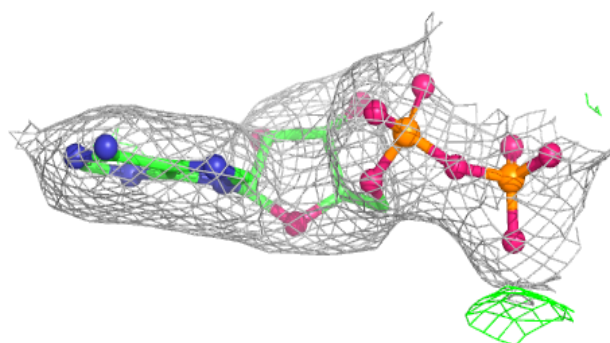
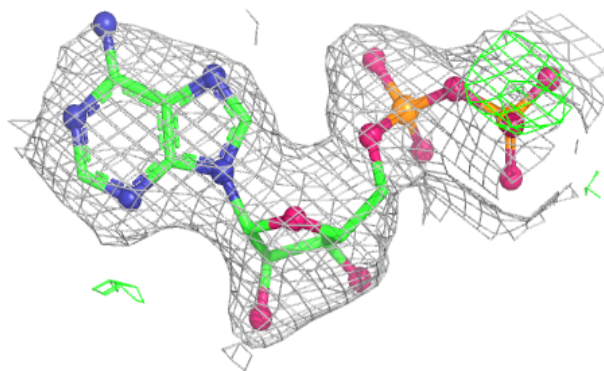
**Electron density around ADP A 3001:**

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



Electron density around ADP B 3002:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.