



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:01 PM UTC

PDB ID : 2IOA / pdb_00002ioa
Title : E. coli Bifunctional glutathionylspermidine synthetase/amidase Incomplex with Mg²⁺ and ADP and phosphinate inhibitor
Authors : Pai, C.H.; Chiang, B.Y.; Ko, T.P.; Chou, C.C.; Chong, C.M.; Yen, F.J.; Coward, J.K.; Wang, A.H.-J.; Lin, C.H.
Deposited on : 2006-10-10
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

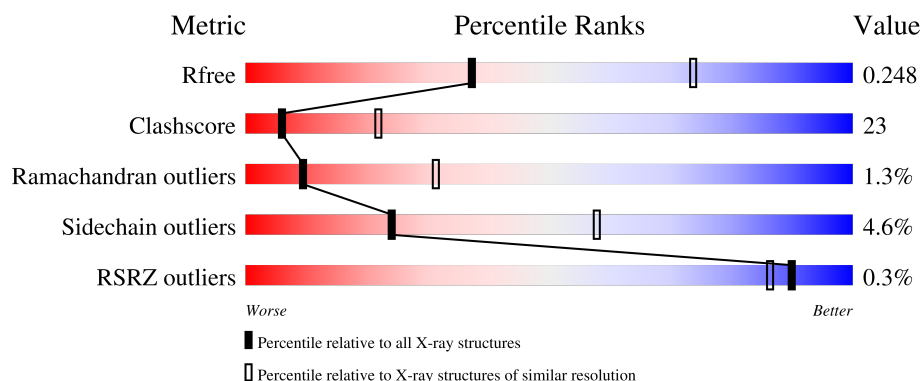
1 Overall quality at a glance

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	
1	B	619	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 10089 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.

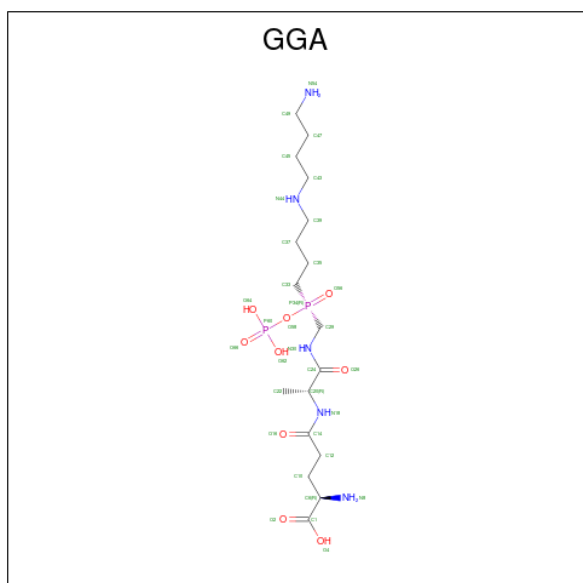
- Molecule 1 is a protein called Bifunctional glutathionylspermidine synthetase/amidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4755	3051	813	872	19			
1	B	589	Total	C	N	O	S	0	0	0
			4753	3048	813	873	19			

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

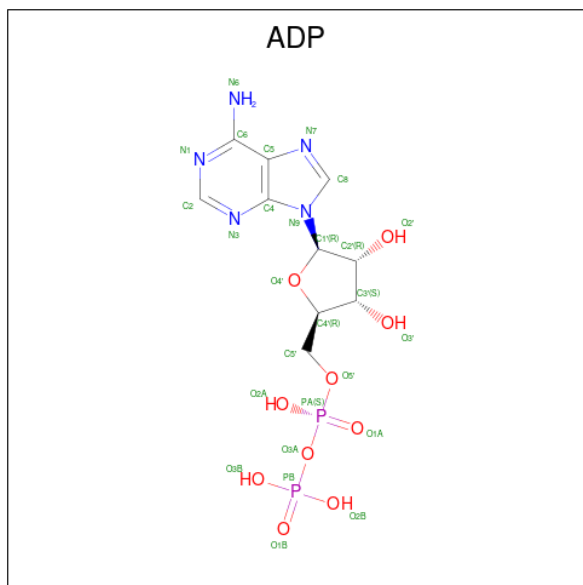
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Mg	0	0
			2	2		
2	B	2	Total	Mg	0	0
			2	2		

- Molecule 3 is D-GAMMA-GLUTAMYL-N-[(R)-{4-[(4-AMINOBTUTYL)AMINO]BUTYL}(PHOSPHONOOXY)PHOSPHORYL]METHYL}-D-ALANINAMIDE (CCD ID: GGA) (formula: C₁₇H₃₇N₅O₉P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			33	17	5	9	2		
3	B	1	Total	C	N	O	P	0	0
			33	17	5	9	2		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

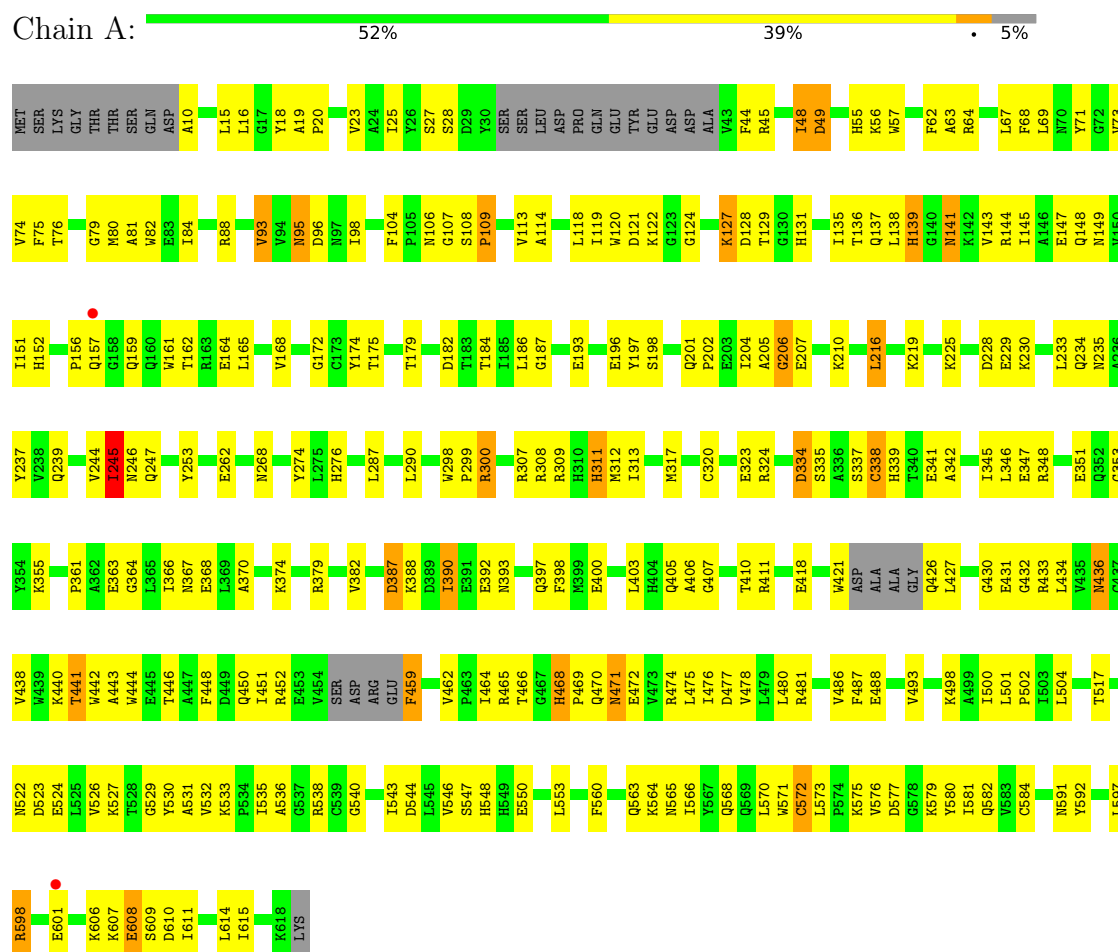
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	236	Total	O	0	0
			236	236		
5	B	221	Total	O	0	0
			221	221		

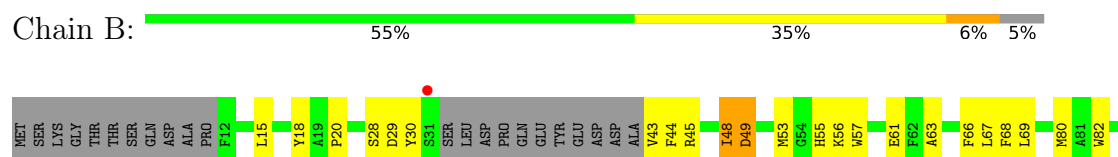
3 Residue-property plots

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: Bifunctional glutathionylspermidine synthetase/amidase



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P534	F85	E166	Y274	R377	Y454	P534
I535	F89	Y174	L275	A378	SER	I535
R538	L90	I185	H276	R379	ASP	R538
D544	R91	I186	K280	P380	GLU	D544
S547	E92	G187	W281	F381	F459	S547
E551	V93	W188	L282	V382	A460	E551
V552	N95	M189	W298	H383	A461	V552
K555	D96	T195	P299	I384	V462	K555
F560	N97	E196	R300	M385	R465	F560
Q563	Q102	Y197	D387	Q386	T466	Q563
K564	A103	S198	K301	D388	G467	K564
N565	F104	Y199	L302	D389	H468	N565
I566	P105	L200	L303	I390	P469	I566
Y567	N106	Q201	R307	N393	Q470	Y567
Q568	G107	L204	R308	Q397	R474	Q568
L570	R110	A205	R309	F398	V476	L570
V571	A111	G206	H310	P399	R481	V571
C572	P112	E207	H311	E400	P482	C572
D577	L117	L208	M312	Q401	E483	D577
I581	L118	R215	T314	E409	V484	I581
C584	I119	K219	G315	T410	L485	C584
T587	W120	G220	R316	R411	V486	T587
Y592	D121	Q221	C320	L412	F487	Y592
C596	K122	L227	M321	L413	E488	C596
L597	F126	D231	D322	D417	P489	L597
R598	K127	P232	R323	E418	L490	R598
S601	D128	L233	R324	L419	V493	S601
S602	T129	Q234	ASP	G420	I494	S602
L603	G130	N235	ALA	W421	K498	L603
R607	H131	A236	G425	L427	I503	R607
S609	V132	Y237	Q426	E430	L504	S609
D610	A133	V238	L427	E431	S506	D610
L611	I134	Q239	H339	V438	R512	L611
L614	T136	A240	T340	W439	Y513	L614
V616	Q137	N241	E341	K440	L514	V616
V617	L138	G242	A342	T441	L515	V617
K618	H139	Q243	G343	W444	V521	K618
LYS	K142	V244	L344	E445	D523	LYS
	V143	I245	I345	T446	E524	
	R144	N246	L346	A447	L525	
	I145	Q247	E347	F448	V526	
	A146	Y250	R348	D449	K527	
	E147	H251	E351	Q450	T528	
	V150	T254	Q352	I451	G529	
	I151	Q261	N360	R452	Y530	
	Q160	E262	P361	V532	A531	
	W161	N268	L365	K533	R533	
	E164	E269	A370			
	L165					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.03Å 75.29Å 84.66Å 70.09° 74.06° 77.55°	Depositor
Resolution (Å)	30.00 – 2.80 30.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 94.7 (30.00-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.23 (at 2.68Å)	Xtriage
Refinement program	CNS, XTALVIEW	Depositor
R, R_{free}	0.173 , 0.243 0.182 , 0.248	Depositor DCC
R_{free} test set	3491 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	32.8	Xtriage
Anisotropy	0.415	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 62.7	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	0.94	EDS
Total number of atoms	10089	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% 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: ADP, MG, GGA

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	0.51	0/4877	1.03	29/6621 (0.4%)
1	B	0.50	0/4874	1.03	31/6615 (0.5%)
All	All	0.51	0/9751	1.03	60/13236 (0.5%)

There are no bond length outliers.

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	441	THR	N-CA-C	-10.09	100.45	113.17
1	B	93	VAL	N-CA-C	9.75	120.56	110.62
1	A	93	VAL	N-CA-C	9.25	122.62	111.05
1	B	441	THR	N-CA-C	-8.88	102.18	113.72
1	A	245	ILE	N-CA-C	-8.34	105.03	111.62
1	A	438	VAL	N-CA-C	8.09	119.76	108.12
1	A	486	VAL	N-CA-C	7.74	119.62	108.48
1	A	219	LYS	N-CA-C	-7.69	101.96	112.03
1	B	347	GLU	N-CA-C	-7.24	102.99	111.03
1	A	598	ARG	N-CA-C	-6.99	97.57	109.24
1	A	529	GLY	N-CA-C	-6.97	104.49	112.29
1	B	451	ILE	N-CA-C	-6.92	105.86	111.81
1	A	244	VAL	N-CA-C	6.85	117.39	108.35
1	A	451	ILE	N-CA-C	-6.77	105.98	111.81
1	A	119	ILE	N-CA-C	6.74	118.30	108.53
1	B	617	VAL	N-CA-C	6.66	117.43	108.11
1	A	245	ILE	CB-CA-C	-6.60	105.18	111.05
1	B	130	GLY	N-CA-C	-6.60	100.91	112.53
1	A	572	CYS	N-CA-C	6.52	119.93	110.28
1	A	139	HIS	N-CA-C	6.47	114.96	108.75
1	B	106	ASN	N-CA-C	-6.45	101.15	110.24
1	B	119	ILE	N-CA-C	6.37	117.02	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	468	HIS	CA-C-N	6.33	125.82	119.24
1	A	468	HIS	C-N-CA	6.33	125.82	119.24
1	B	438	VAL	N-CA-C	6.29	117.83	108.46
1	B	417	ASP	N-CA-C	6.26	118.10	111.28
1	A	198	SER	N-CA-C	6.18	118.89	110.55
1	A	387	ASP	N-CA-C	-6.15	102.60	110.53
1	B	409	GLU	N-CA-C	-6.14	100.89	110.42
1	B	342	ALA	N-CA-C	5.84	117.73	111.36
1	B	486	VAL	N-CA-C	5.83	116.88	108.48
1	B	207	GLU	N-CA-C	5.80	118.38	111.71
1	B	447	ALA	N-CA-C	-5.71	104.67	111.69
1	A	139	HIS	CB-CA-C	-5.66	108.22	116.53
1	A	48	ILE	N-CA-C	-5.61	97.95	106.42
1	A	106	ASN	N-CA-C	-5.59	101.77	110.10
1	B	48	ILE	N-CA-C	-5.56	97.78	109.34
1	A	109	PRO	N-CA-C	-5.50	107.26	114.03
1	A	530	TYR	N-CA-C	5.45	117.13	108.79
1	B	572	CYS	N-CA-C	5.45	118.34	110.28
1	A	23	VAL	N-CA-C	5.44	116.19	107.98
1	A	406	ALA	N-CA-C	-5.42	106.70	113.15
1	A	466	THR	N-CA-C	-5.39	105.00	113.02
1	B	261	GLN	N-CA-C	-5.37	105.32	111.07
1	A	216	LEU	N-CA-C	-5.37	102.10	110.42
1	B	382	VAL	N-CA-C	5.36	115.57	107.75
1	B	610	ASP	N-CA-C	5.35	117.43	110.53
1	B	129	THR	N-CA-C	5.35	117.19	111.36
1	B	370	ALA	N-CA-C	-5.32	105.59	111.71
1	B	107	GLY	N-CA-C	-5.30	100.62	113.18
1	B	462	VAL	N-CA-C	-5.29	103.76	108.95
1	B	314	THR	N-CA-C	5.29	117.11	108.76
1	A	311	HIS	N-CA-C	5.27	119.86	113.38
1	B	529	GLY	N-CA-C	-5.25	106.12	112.48
1	B	398	PHE	N-CA-C	-5.22	105.27	111.69
1	B	352	GLN	N-CA-C	5.11	119.78	113.50
1	A	193	GLU	N-CA-C	-5.04	106.98	113.23
1	B	566	ILE	N-CA-C	-5.02	100.67	108.95
1	B	530	TYR	N-CA-C	5.01	116.67	108.76
1	B	563	GLN	N-CA-C	5.01	116.99	110.43

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	4755	0	4641	226	0
1	B	4753	0	4637	210	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	33	0	35	7	0
3	B	33	0	34	2	0
4	A	27	0	11	2	0
4	B	27	0	11	0	0
5	A	236	0	0	18	0
5	B	221	0	0	8	0
All	All	10089	0	9369	434	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 (434) 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:245:ILE:O	5:A:4192:HOH:O	1.73	1.03
1:A:210:LYS:HD3	1:A:323:GLU:HB3	1.40	1.02
1:A:64:ARG:HG3	1:A:74:VAL:HG23	1.43	0.96
1:A:311:HIS:ND1	5:A:4195:HOH:O	1.97	0.96
1:A:341:GLU:HG2	1:A:611:ILE:HG13	1.48	0.93
1:B:608:GLU:CD	1:B:608:GLU:H	1.79	0.91
1:B:268:ASN:HD21	1:B:592:TYR:H	1.24	0.83
1:A:311:HIS:CE1	5:A:4195:HOH:O	2.32	0.83
1:B:607:LYS:O	3:B:6002:GGA:H432	1.79	0.83
1:B:465:ARG:HG3	1:B:474:ARG:HH21	1.42	0.82
1:B:233:LEU:HD12	1:B:401:GLN:OE1	1.80	0.81
1:A:607:LYS:O	3:A:6001:GGA:H432	1.82	0.80
1:B:337:SER:O	1:B:338:CYS:HB2	1.81	0.80
1:A:121:ASP:HB2	1:A:186:LEU:HD21	1.62	0.80
1:A:28:SER:HB3	1:A:57:TRP:HB2	1.63	0.79
1:B:341:GLU:HG2	1:B:611:ILE:HG13	1.65	0.79
1:B:384:ILE:HG23	1:B:439:TRP:HE3	1.49	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLU:HG3	1:B:430:GLY:H	1.49	0.77
1:A:311:HIS:O	1:A:313:ILE:HD12	1.86	0.75
1:A:442:TRP:HE3	3:A:6001:GGA:O2	1.67	0.75
1:A:96:ASP:CG	1:A:309:ARG:HH21	1.96	0.74
1:A:498:LYS:HB3	1:A:566:ILE:HD13	1.70	0.74
1:A:390:ILE:H	1:A:390:ILE:HD12	1.51	0.74
1:B:245:ILE:HG13	1:B:246:ASN:H	1.52	0.74
1:A:157:GLN:CD	1:A:157:GLN:H	1.96	0.73
1:A:540:GLY:HA2	1:A:543:ILE:HD12	1.71	0.72
1:B:361:PRO:HG3	1:B:614:LEU:HD23	1.71	0.72
1:A:79:GLY:O	1:A:80:MET:HE2	1.90	0.72
1:B:138:LEU:HD12	1:B:143:VAL:HG12	1.71	0.72
1:A:337:SER:O	1:A:338:CYS:HB2	1.88	0.72
1:A:138:LEU:HD12	1:A:143:VAL:HG12	1.71	0.72
1:B:522:ASN:C	1:B:522:ASN:HD22	1.98	0.71
1:A:137:GLN:HG2	1:A:144:ARG:HB2	1.72	0.71
1:A:421:TRP:H	1:A:471:ASN:HD21	1.38	0.71
1:A:442:TRP:CE3	3:A:6001:GGA:O2	2.44	0.71
1:B:204:ILE:HD13	1:B:205:ALA:N	2.05	0.71
1:A:151:ILE:HD12	1:A:162:THR:HB	1.72	0.70
1:B:301:LEU:HD13	1:B:494:ILE:HD11	1.73	0.70
1:A:48:ILE:HD13	1:A:69:LEU:HD21	1.74	0.69
1:A:137:GLN:HE21	1:A:139:HIS:CE1	2.10	0.69
1:A:268:ASN:HD21	1:A:592:TYR:H	1.40	0.69
1:A:320:CYS:HG	1:A:571:TRP:CD1	2.11	0.69
1:A:20:PRO:HG2	1:A:136:THR:HB	1.74	0.69
1:A:448:PHE:O	1:A:452:ARG:HG3	1.93	0.69
1:A:579:LYS:HD2	5:A:4086:HOH:O	1.92	0.68
1:A:201:GLN:HG3	1:A:202:PRO:HD2	1.73	0.68
1:A:82:TRP:HD1	1:A:129:THR:O	1.77	0.68
1:B:413:LEU:HD23	1:B:418:GLU:OE1	1.94	0.68
1:B:532:VAL:HB	1:B:544:ASP:HB2	1.74	0.68
1:B:245:ILE:HG13	1:B:246:ASN:N	2.08	0.67
1:A:379:ARG:HH12	1:A:436:ASN:HB2	1.60	0.67
1:A:575:LYS:HD2	1:A:580:TYR:CZ	2.29	0.67
1:B:122:LYS:HB2	1:B:127:LYS:O	1.95	0.67
1:B:137:GLN:CD	1:B:144:ARG:HD2	2.20	0.67
1:A:337:SER:OG	3:A:6001:GGA:H372	1.95	0.66
1:A:418:GLU:HG2	1:A:418:GLU:O	1.94	0.66
1:A:527:LYS:O	1:A:548:HIS:HB3	1.95	0.66
1:B:233:LEU:HD11	1:B:398:PHE:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLU:CG	1:B:430:GLY:H	2.09	0.65
1:B:598:ARG:NH1	5:B:4308:HOH:O	2.28	0.65
1:A:535:ILE:HG22	1:A:566:ILE:HG23	1.79	0.65
1:A:540:GLY:HA2	1:A:543:ILE:CD1	2.27	0.65
1:A:135:ILE:HD13	1:A:145:ILE:HG22	1.78	0.65
1:B:522:ASN:HD21	1:B:525:LEU:H	1.43	0.65
1:A:341:GLU:CG	1:A:611:ILE:HG13	2.24	0.64
1:A:210:LYS:HD3	1:A:323:GLU:CB	2.22	0.64
1:A:95:ASN:N	1:A:95:ASN:HD22	1.94	0.64
1:A:137:GLN:CD	1:A:144:ARG:HD2	2.23	0.64
1:B:227:LEU:HD23	1:B:348:ARG:HG2	1.78	0.64
1:A:64:ARG:CG	1:A:74:VAL:HG23	2.21	0.64
1:B:320:CYS:HG	1:B:571:TRP:CD1	2.16	0.64
1:A:15:LEU:HD21	1:A:18:TYR:CZ	2.33	0.63
1:A:426:GLN:N	5:A:4229:HOH:O	2.30	0.63
1:B:102:GLN:NE2	1:B:195:THR:HG22	2.14	0.63
1:B:215:ARG:HD3	5:B:4401:HOH:O	1.98	0.63
1:B:303:LEU:HD13	1:B:307:ARG:NH2	2.14	0.63
1:B:384:ILE:HG23	1:B:439:TRP:CE3	2.34	0.63
1:A:411:ARG:NE	1:A:418:GLU:OE1	2.28	0.62
1:A:579:LYS:HE3	1:A:601:GLU:OE2	1.98	0.62
1:B:105:PRO:HD3	1:B:199:LEU:HG	1.79	0.62
1:B:164:GLU:O	1:B:165:LEU:HD23	1.99	0.62
1:A:210:LYS:NZ	1:A:323:GLU:HG2	2.13	0.62
1:B:102:GLN:CD	1:B:195:THR:HG22	2.24	0.62
1:B:298:TRP:HB2	1:B:299:PRO:HD3	1.81	0.62
1:A:390:ILE:HD12	1:A:390:ILE:N	2.15	0.61
1:B:498:LYS:HB2	1:B:535:ILE:HA	1.80	0.61
1:A:124:GLY:HA3	1:A:182:ASP:O	2.00	0.61
1:B:418:GLU:HG3	1:B:430:GLY:N	2.14	0.61
1:A:144:ARG:HD3	1:A:161:TRP:CD1	2.35	0.61
1:B:204:ILE:HD13	1:B:205:ALA:H	1.63	0.61
1:A:462:VAL:HG12	1:A:464:ILE:HG23	1.81	0.61
1:A:400:GLU:HG3	1:A:410:THR:OG1	2.01	0.60
1:B:166:GLU:HB3	5:B:4283:HOH:O	2.00	0.60
1:A:121:ASP:HB2	1:A:186:LEU:CD2	2.32	0.60
1:A:390:ILE:H	1:A:390:ILE:CD1	2.12	0.60
1:B:246:ASN:HB2	5:B:4468:HOH:O	2.02	0.60
1:B:498:LYS:HB3	1:B:566:ILE:HD13	1.84	0.60
1:A:298:TRP:HB2	1:A:299:PRO:HD3	1.84	0.60
1:A:474:ARG:NH2	1:A:477:ASP:OD2	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ILE:HA	1:B:145:ILE:HG22	1.82	0.60
1:B:465:ARG:HG3	1:B:474:ARG:NH2	2.16	0.59
1:B:522:ASN:O	1:B:526:VAL:HG23	2.02	0.59
1:B:247:GLN:HG3	5:B:4468:HOH:O	2.03	0.59
1:A:120:TRP:HB2	1:A:131:HIS:HB3	1.84	0.58
1:A:104:PHE:O	1:A:187:GLY:HA3	2.02	0.58
1:A:341:GLU:HG2	1:A:611:ILE:CG1	2.29	0.58
1:A:573:LEU:HD22	1:A:581:ILE:O	2.04	0.58
1:B:382:VAL:HB	1:B:410:THR:HG22	1.84	0.58
1:B:238:VAL:O	1:B:242:GLY:N	2.32	0.58
1:B:82:TRP:HD1	1:B:129:THR:O	1.86	0.58
1:B:523:ASP:O	1:B:526:VAL:HB	2.04	0.58
1:B:251:HIS:HE1	1:B:577:ASP:OD2	1.86	0.58
1:B:48:ILE:O	1:B:49:ASP:HB2	2.04	0.57
1:A:137:GLN:HE21	1:A:139:HIS:HE1	1.50	0.57
1:A:235:ASN:O	1:A:239:GLN:HG2	2.04	0.57
1:A:361:PRO:HG3	1:A:614:LEU:HD23	1.86	0.57
1:A:387:ASP:OD1	1:A:388:LYS:N	2.36	0.57
1:A:121:ASP:CB	1:A:186:LEU:HD21	2.33	0.57
1:B:235:ASN:O	1:B:239:GLN:HG2	2.05	0.57
1:B:538:ARG:NH1	1:B:560:PHE:HZ	2.03	0.57
1:B:341:GLU:CG	1:B:611:ILE:HG13	2.34	0.57
1:A:403:LEU:HD13	1:A:410:THR:HG21	1.87	0.56
1:A:312:MET:HA	1:A:488:GLU:OE2	2.06	0.56
1:A:351:GLU:O	1:A:351:GLU:HG2	2.05	0.56
1:A:538:ARG:NH1	1:A:560:PHE:HZ	2.02	0.56
1:B:282:LEU:HD21	1:B:494:ILE:CD1	2.35	0.56
1:B:468:HIS:CG	1:B:469:PRO:HD2	2.40	0.56
1:A:164:GLU:O	1:A:165:LEU:HD23	2.05	0.56
1:B:94:VAL:HG13	5:B:4347:HOH:O	2.05	0.56
1:B:322:ASP:OD2	1:B:324:ARG:HB2	2.05	0.56
1:A:502:PRO:HG3	1:A:517:THR:HG22	1.88	0.56
1:B:303:LEU:HD13	1:B:307:ARG:HH21	1.70	0.56
1:B:522:ASN:ND2	1:B:525:LEU:H	2.02	0.56
1:A:131:HIS:HE1	1:A:147:GLU:OE2	1.89	0.55
1:A:347:GLU:OE2	1:A:363:GLU:HB3	2.06	0.55
1:A:335:SER:HB2	5:A:4005:HOH:O	2.05	0.55
1:B:44:PHE:HD2	1:B:55:HIS:HE1	1.54	0.55
1:A:95:ASN:N	1:A:95:ASN:ND2	2.52	0.55
1:A:151:ILE:CD1	1:A:162:THR:HB	2.35	0.55
1:A:225:LYS:HE2	1:A:229:GLU:OE2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:MET:SD	1:A:129:THR:HG22	2.46	0.55
1:B:112:PRO:HB3	1:B:188:TRP:CD2	2.41	0.55
1:B:127:LYS:HB3	1:B:128:ASP:OD1	2.07	0.55
1:A:307:ARG:HD3	1:B:49:ASP:OD2	2.07	0.55
1:B:63:ALA:O	1:B:67:LEU:HG	2.07	0.55
1:A:107:GLY:HA2	1:A:174:TYR:O	2.07	0.55
1:A:465:ARG:NH2	1:A:472:GLU:O	2.38	0.55
1:A:137:GLN:NE2	1:A:144:ARG:HD2	2.22	0.54
1:A:426:GLN:HG3	5:A:4381:HOH:O	2.06	0.54
1:A:44:PHE:HB3	1:A:55:HIS:CE1	2.42	0.54
1:A:114:ALA:HB1	1:B:460:ALA:HB2	1.88	0.54
1:A:597:LEU:HD11	1:A:614:LEU:HD13	1.89	0.54
1:B:481:ARG:NH1	1:B:483:GLU:OE1	2.39	0.54
1:A:113:VAL:HG22	1:A:114:ALA:N	2.22	0.54
1:B:572:CYS:HB3	1:B:603:LEU:HD22	1.90	0.54
1:B:80:MET:SD	1:B:129:THR:HG22	2.47	0.54
1:B:89:PHE:CE2	1:B:269:GLU:HG3	2.42	0.54
1:B:301:LEU:HD23	1:B:490:LEU:HG	1.89	0.54
1:A:345:ILE:HD12	1:A:345:ILE:N	2.23	0.54
1:A:427:LEU:HD21	1:A:478:VAL:HG22	1.90	0.54
1:B:601:GLU:CD	1:B:601:GLU:H	2.16	0.54
1:A:335:SER:OG	3:A:6001:GGA:H223	2.07	0.54
1:A:608:GLU:H	1:A:608:GLU:CD	2.15	0.54
1:A:608:GLU:O	1:A:609:SER:C	2.51	0.54
1:A:433:ARG:HG2	1:A:434:LEU:N	2.23	0.54
1:A:436:ASN:HD22	1:A:436:ASN:C	2.15	0.53
1:A:71:TYR:HB2	1:A:73:VAL:HG22	1.89	0.53
1:A:546:VAL:O	1:A:570:LEU:HD22	2.08	0.53
1:A:540:GLY:CA	1:A:543:ILE:HD12	2.36	0.53
1:A:450:GLN:OE1	1:A:475:LEU:HB3	2.09	0.53
1:A:96:ASP:OD1	1:A:309:ARG:NH2	2.38	0.53
1:B:45:ARG:NH2	5:B:4203:HOH:O	2.33	0.53
1:B:254:THR:HA	1:B:615:ILE:O	2.08	0.53
1:B:311:HIS:N	1:B:311:HIS:CD2	2.76	0.53
1:A:342:ALA:HA	1:A:346:LEU:HD12	1.91	0.52
1:A:532:VAL:HB	1:A:544:ASP:HB2	1.89	0.52
1:A:207:GLU:HA	1:A:207:GLU:OE2	2.09	0.52
1:A:364:GLY:C	5:A:4456:HOH:O	2.51	0.52
1:A:45:ARG:O	1:A:56:LYS:HE3	2.10	0.52
1:B:268:ASN:ND2	1:B:592:TYR:H	2.01	0.52
1:A:81:ALA:O	1:A:84:ILE:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:ASP:OD1	1:A:309:ARG:NE	2.40	0.52
1:B:44:PHE:HD2	1:B:55:HIS:CE1	2.26	0.52
1:B:150:VAL:C	1:B:151:ILE:HD12	2.34	0.52
1:B:236:ALA:CB	1:B:397:GLN:HE22	2.22	0.52
1:B:533:LYS:NZ	1:B:568:GLN:HE22	2.08	0.52
1:A:98:ILE:HD12	1:A:98:ILE:N	2.25	0.52
1:A:122:LYS:HB2	1:A:127:LYS:O	2.09	0.52
1:B:527:LYS:HE2	1:B:528:THR:HG22	1.92	0.52
1:A:95:ASN:HD22	1:A:95:ASN:H	1.56	0.52
1:A:196:GLU:O	1:A:197:TYR:HB2	2.10	0.52
1:B:339:HIS:CD2	1:B:339:HIS:H	2.27	0.52
1:A:57:TRP:HB3	1:A:148:GLN:NE2	2.24	0.52
1:B:96:ASP:CG	1:B:309:ARG:HH21	2.18	0.52
1:A:48:ILE:O	1:A:49:ASP:HB2	2.08	0.51
1:B:254:THR:HG22	1:B:615:ILE:HG22	1.91	0.51
1:A:210:LYS:HZ2	1:A:323:GLU:HG2	1.73	0.51
1:B:57:TRP:HZ3	1:B:61:GLU:OE1	1.93	0.51
1:B:139:HIS:HB2	1:B:142:LYS:O	2.10	0.51
1:B:342:ALA:HA	1:B:346:LEU:HD12	1.92	0.51
1:B:126:PHE:O	1:B:127:LYS:O	2.28	0.51
1:B:341:GLU:CB	1:B:611:ILE:HG13	2.41	0.51
1:B:144:ARG:HD3	1:B:161:TRP:CD1	2.45	0.51
1:B:534:PRO:HB2	1:B:563:GLN:NE2	2.26	0.51
1:A:370:ALA:O	1:A:374:LYS:HG3	2.11	0.51
1:A:548:HIS:C	1:A:550:GLU:H	2.19	0.51
1:B:328:VAL:HG12	1:B:513:TYR:O	2.11	0.51
1:B:385:MET:HE3	1:B:419:LEU:HD11	1.93	0.51
1:A:118:LEU:HD22	1:A:135:ILE:HD11	1.91	0.51
1:A:564:LYS:HG2	1:A:565:ASN:N	2.26	0.51
1:B:15:LEU:HD21	1:B:18:TYR:OH	2.10	0.51
1:B:522:ASN:C	1:B:522:ASN:ND2	2.68	0.50
1:A:113:VAL:CG2	1:A:114:ALA:N	2.74	0.50
1:A:538:ARG:HG3	1:A:538:ARG:HH11	1.77	0.50
1:B:43:VAL:N	5:B:4183:HOH:O	2.43	0.50
1:B:527:LYS:HE2	1:B:528:THR:CG2	2.41	0.50
1:A:228:ASP:OD2	1:A:230:LYS:N	2.45	0.50
1:A:614:LEU:O	1:A:615:ILE:HD12	2.12	0.50
1:B:112:PRO:HB2	1:B:135:ILE:HD13	1.93	0.50
1:B:240:ALA:CB	1:B:390:ILE:HG13	2.41	0.50
1:B:131:HIS:HE1	1:B:147:GLU:OE1	1.95	0.49
1:B:137:GLN:HG2	1:B:144:ARG:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:4487:HOH:O	1:B:160:GLN:HG2	2.12	0.49
1:B:48:ILE:HD13	1:B:69:LEU:HD21	1.93	0.49
1:B:137:GLN:CG	1:B:144:ARG:HB2	2.42	0.49
1:B:236:ALA:HB2	1:B:397:GLN:HE22	1.78	0.49
1:B:313:ILE:HD13	1:B:487:PHE:HD2	1.77	0.49
1:A:233:LEU:HD21	1:A:398:PHE:HD1	1.77	0.49
1:A:443:ALA:HB3	3:A:6001:GGA:O4	2.12	0.49
1:B:608:GLU:O	1:B:609:SER:C	2.54	0.49
1:A:246:ASN:HB2	5:A:4392:HOH:O	2.12	0.49
1:B:327:LYS:HG3	1:B:515:LEU:HD21	1.93	0.49
1:B:341:GLU:HB3	1:B:611:ILE:HG13	1.94	0.49
1:B:468:HIS:HE1	1:B:470:GLN:HB2	1.76	0.49
1:A:459:PHE:HD1	1:A:459:PHE:O	1.96	0.49
1:B:104:PHE:O	1:B:187:GLY:HA3	2.11	0.49
1:B:233:LEU:HD13	1:B:344:LEU:HD22	1.95	0.49
1:B:215:ARG:HH11	1:B:215:ARG:HG3	1.77	0.49
1:A:82:TRP:CD1	1:A:129:THR:O	2.63	0.48
1:B:120:TRP:NE1	1:B:185:ILE:HD11	2.28	0.48
1:A:311:HIS:CG	5:A:4195:HOH:O	2.58	0.48
1:A:598:ARG:HD2	1:A:611:ILE:HD13	1.94	0.48
1:B:533:LYS:NZ	1:B:568:GLN:NE2	2.60	0.48
1:A:137:GLN:NE2	1:A:144:ARG:NH1	2.61	0.48
1:A:366:ILE:HG23	1:A:367:ASN:N	2.27	0.48
1:A:430:GLY:C	1:A:432:GLY:H	2.21	0.48
1:B:43:VAL:HG12	1:B:43:VAL:O	2.12	0.48
1:A:109:PRO:HB2	1:A:197:TYR:CE1	2.48	0.48
1:A:474:ARG:NH1	1:A:476:ILE:HD11	2.29	0.48
1:B:44:PHE:HB3	1:B:55:HIS:CE1	2.49	0.48
1:A:568:GLN:HG2	4:A:3001:ADP:HN61	1.78	0.48
1:B:418:GLU:HG3	1:B:430:GLY:CA	2.43	0.48
1:A:247:GLN:HG2	5:A:4392:HOH:O	2.13	0.48
1:A:364:GLY:O	1:A:368:GLU:HB2	2.14	0.48
1:B:53:MET:HE2	1:B:53:MET:HA	1.95	0.48
1:B:524:GLU:O	1:B:527:LYS:HG3	2.13	0.48
1:B:127:LYS:HB3	1:B:128:ASP:H	1.46	0.48
1:A:392:GLU:OE1	1:A:441:THR:OG1	2.31	0.47
1:B:262:GLU:OE1	1:B:262:GLU:HA	2.14	0.47
1:A:165:LEU:CD2	1:A:179:THR:HG23	2.44	0.47
1:A:287:LEU:HA	1:A:290:LEU:HD12	1.96	0.47
1:B:196:GLU:O	1:B:197:TYR:HB2	2.13	0.47
1:B:150:VAL:HG12	1:B:151:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:581:ILE:CG2	1:B:597:LEU:HD22	2.44	0.47
1:A:538:ARG:HH11	1:A:538:ARG:CG	2.28	0.47
1:B:427:LEU:HD21	1:B:478:VAL:HG22	1.97	0.47
1:B:95:ASN:O	1:B:97:ASN:N	2.48	0.47
1:B:274:TYR:CE1	1:B:504:LEU:HD11	2.49	0.47
1:A:522:ASN:O	1:A:526:VAL:HG23	2.14	0.47
1:B:547:SER:OG	1:B:551:GLU:HG2	2.15	0.47
1:A:274:TYR:CZ	1:A:504:LEU:HD11	2.50	0.46
1:A:575:LYS:HE2	5:A:4254:HOH:O	2.15	0.46
1:B:316:ARG:HD2	1:B:584:CYS:HB3	1.97	0.46
1:B:608:GLU:CD	1:B:608:GLU:N	2.58	0.46
1:B:400:GLU:HG3	1:B:410:THR:OG1	2.15	0.46
1:B:601:GLU:CD	1:B:601:GLU:N	2.73	0.46
1:A:98:ILE:HD13	1:A:276:HIS:CD2	2.50	0.46
1:B:104:PHE:CE2	1:B:110:ARG:HG2	2.49	0.46
1:B:85:PHE:HA	1:B:189:MET:CE	2.45	0.46
1:A:137:GLN:HE22	1:A:144:ARG:NH1	2.13	0.46
1:B:121:ASP:O	1:B:130:GLY:HA2	2.16	0.46
1:B:339:HIS:CD2	1:B:339:HIS:N	2.84	0.46
1:A:421:TRP:HE3	1:A:471:ASN:HD22	1.64	0.46
1:B:131:HIS:CG	1:B:132:VAL:N	2.83	0.46
1:A:547:SER:HB3	1:A:553:LEU:HD11	1.97	0.46
1:B:48:ILE:CG2	1:B:68:PHE:HE2	2.29	0.46
1:B:240:ALA:HB2	1:B:390:ILE:HG13	1.98	0.46
1:B:117:LEU:O	1:B:188:TRP:HA	2.16	0.46
1:B:221:GLN:OE1	1:B:250:TYR:HE2	1.99	0.46
1:B:379:ARG:HE	1:B:485:LEU:HB2	1.81	0.46
1:B:418:GLU:HG3	1:B:430:GLY:HA3	1.98	0.46
1:B:552:VAL:HG11	1:B:555:LYS:HE3	1.98	0.46
1:A:138:LEU:HD12	1:A:143:VAL:CG1	2.42	0.46
1:B:85:PHE:HA	1:B:189:MET:SD	2.56	0.46
1:B:66:PHE:CE2	1:B:134:ILE:HG21	2.51	0.46
1:A:268:ASN:ND2	1:A:592:TYR:H	2.11	0.45
1:A:498:LYS:C	1:A:500:ILE:H	2.24	0.45
1:A:405:GLN:C	1:A:407:GLY:H	2.24	0.45
1:B:324:ARG:NH2	1:B:572:CYS:O	2.45	0.45
1:B:348:ARG:NH1	1:B:351:GLU:OE2	2.48	0.45
1:A:313:ILE:HD13	1:A:487:PHE:HD2	1.81	0.45
1:B:347:GLU:HA	1:B:347:GLU:OE1	2.15	0.45
1:B:459:PHE:N	1:B:459:PHE:CD2	2.82	0.45
1:A:174:TYR:CD1	1:A:174:TYR:N	2.84	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ASP:OD2	1:B:322:ASP:C	2.60	0.45
1:A:498:LYS:HB2	1:A:535:ILE:HA	1.99	0.45
1:B:303:LEU:O	1:B:307:ARG:HG2	2.17	0.45
1:B:379:ARG:H	1:B:379:ARG:HD3	1.82	0.45
1:B:449:ASP:OD1	1:B:452:ARG:NH2	2.40	0.45
1:A:379:ARG:NH1	1:A:436:ASN:HB2	2.29	0.45
1:B:386:GLN:NE2	1:B:387:ASP:O	2.50	0.44
3:A:6001:GGA:H491	5:A:4176:HOH:O	2.17	0.44
1:B:120:TRP:NE1	1:B:185:ILE:CD1	2.80	0.44
1:A:204:ILE:HG21	1:A:262:GLU:HG2	1.99	0.44
1:B:112:PRO:HB2	1:B:135:ILE:CD1	2.48	0.44
1:B:138:LEU:HD12	1:B:143:VAL:CG1	2.43	0.44
1:A:56:LYS:HA	1:A:57:TRP:HA	1.61	0.44
1:B:28:SER:HB2	1:B:57:TRP:O	2.17	0.44
1:B:444:TRP:HB2	1:B:493:VAL:HG12	1.99	0.44
1:A:25:ILE:HG12	1:A:62:PHE:CE1	2.52	0.44
1:A:300:ARG:NH1	5:A:4196:HOH:O	2.50	0.44
1:A:533:LYS:NZ	1:A:568:GLN:NE2	2.66	0.44
1:B:387:ASP:HB2	3:B:6002:GGA:HN81	1.81	0.44
1:A:63:ALA:O	1:A:67:LEU:HG	2.18	0.44
1:A:346:LEU:HD23	1:A:346:LEU:HA	1.80	0.44
1:B:468:HIS:HE1	1:B:470:GLN:HE21	1.66	0.44
1:A:430:GLY:O	1:A:432:GLY:N	2.49	0.44
1:B:584:CYS:HB2	1:B:596:CYS:SG	2.58	0.44
1:A:10:ALA:N	5:A:4348:HOH:O	2.50	0.44
1:B:360:ASN:OD1	1:B:361:PRO:HD2	2.18	0.44
1:A:151:ILE:HD12	1:A:162:THR:CB	2.44	0.44
1:B:56:LYS:HA	1:B:57:TRP:HA	1.66	0.44
1:B:311:HIS:O	1:B:313:ILE:HD12	2.18	0.44
1:A:68:PHE:HE1	1:A:93:VAL:HG11	1.82	0.43
1:A:137:GLN:CG	1:A:144:ARG:HB2	2.46	0.43
1:A:421:TRP:HE3	1:A:471:ASN:ND2	2.16	0.43
1:A:421:TRP:HA	1:A:426:GLN:O	2.18	0.43
1:A:109:PRO:HA	1:A:172:GLY:O	2.17	0.43
1:B:521:VAL:HG22	1:B:567:TYR:CD1	2.53	0.43
1:B:529:GLY:C	1:B:570:LEU:HB2	2.43	0.43
1:B:535:ILE:HG23	1:B:564:LYS:O	2.18	0.43
1:A:109:PRO:HB2	1:A:197:TYR:CD1	2.53	0.43
1:A:411:ARG:HA	5:A:4313:HOH:O	2.19	0.43
1:B:20:PRO:HD3	1:B:160:GLN:O	2.17	0.43
1:B:120:TRP:HB2	1:B:131:HIS:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:308:ARG:HG3	1:A:308:ARG:HH11	1.83	0.43
1:B:512:ARG:HG2	1:B:512:ARG:HH11	1.82	0.43
1:A:411:ARG:HH21	1:A:418:GLU:CD	2.26	0.43
1:B:444:TRP:CB	1:B:493:VAL:HG12	2.49	0.43
1:A:74:VAL:HG22	1:A:75:PHE:N	2.34	0.43
1:A:205:ALA:O	1:A:207:GLU:N	2.52	0.43
1:B:48:ILE:O	1:B:49:ASP:CB	2.66	0.43
1:A:10:ALA:N	1:A:152:HIS:O	2.52	0.43
1:A:15:LEU:HD21	1:A:18:TYR:CE1	2.53	0.43
1:A:201:GLN:CG	1:A:202:PRO:HD2	2.47	0.43
1:A:205:ALA:O	1:A:206:GLY:C	2.60	0.43
1:A:348:ARG:HD2	1:A:351:GLU:OE1	2.19	0.43
1:B:131:HIS:CE1	1:B:150:VAL:HG21	2.54	0.43
1:B:337:SER:O	1:B:338:CYS:CB	2.58	0.43
1:B:481:ARG:HH11	1:B:483:GLU:CD	2.26	0.43
1:B:314:THR:HA	1:B:587:THR:O	2.18	0.43
1:B:490:LEU:O	1:B:493:VAL:HG13	2.18	0.43
1:A:234:GLN:O	1:A:237:TYR:HB3	2.19	0.42
1:A:468:HIS:HA	1:A:469:PRO:HD2	1.85	0.42
1:A:481:ARG:NH2	5:A:4229:HOH:O	2.52	0.42
1:B:45:ARG:O	1:B:56:LYS:HE3	2.19	0.42
1:B:503:ILE:O	1:B:506:SER:HB3	2.19	0.42
1:A:62:PHE:HB2	1:A:148:GLN:HB2	2.01	0.42
1:A:107:GLY:CA	1:A:174:TYR:O	2.66	0.42
1:B:44:PHE:O	1:B:56:LYS:HG3	2.20	0.42
1:A:337:SER:O	1:A:338:CYS:CB	2.60	0.42
1:A:245:ILE:HG23	1:A:345:ILE:HG21	2.01	0.42
1:A:533:LYS:HZ3	1:A:568:GLN:NE2	2.18	0.42
1:B:560:PHE:HB3	1:B:563:GLN:CD	2.44	0.42
1:A:88:ARG:HG3	1:A:201:GLN:HB2	2.02	0.42
1:A:141:ASN:HD22	1:A:141:ASN:H	1.67	0.42
1:A:168:VAL:CG2	1:A:175:THR:HB	2.49	0.42
1:A:317:MET:O	1:A:584:CYS:HA	2.19	0.42
1:A:536:ALA:H	1:A:563:GLN:NE2	2.18	0.42
1:B:431:GLU:OE2	1:B:431:GLU:HA	2.19	0.42
1:A:334:ASP:OD2	1:A:444:TRP:HB2	2.20	0.42
1:B:111:ALA:HB2	1:B:174:TYR:CZ	2.55	0.42
1:A:501:LEU:HD23	1:A:504:LEU:HD12	2.01	0.42
1:A:582:GLN:NE2	4:A:3001:ADP:O3'	2.53	0.42
1:B:532:VAL:HG22	1:B:567:TYR:CD1	2.55	0.42
1:A:339:HIS:HB3	1:A:398:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:LYS:HE3	1:B:219:LYS:HB3	1.89	0.42
1:A:108:SER:HA	1:A:109:PRO:HD3	1.93	0.42
1:A:465:ARG:HD3	1:A:474:ARG:NH2	2.34	0.42
1:A:16:LEU:HD21	1:A:27:SER:HB2	2.02	0.41
1:A:137:GLN:CG	1:A:144:ARG:HD2	2.50	0.41
1:B:151:ILE:HD12	1:B:151:ILE:N	2.35	0.41
1:B:533:LYS:HZ1	1:B:568:GLN:NE2	2.18	0.41
1:A:324:ARG:NH2	1:A:572:CYS:O	2.49	0.41
1:A:382:VAL:HB	1:A:410:THR:HG22	2.00	0.41
1:A:576:VAL:HG12	1:A:577:ASP:OD1	2.20	0.41
1:B:244:VAL:CG1	1:B:245:ILE:N	2.83	0.41
1:B:276:HIS:CE1	1:B:280:LYS:HE2	2.55	0.41
1:B:381:PHE:CD1	1:B:409:GLU:HB2	2.56	0.41
1:A:19:ALA:O	1:A:20:PRO:C	2.63	0.41
1:A:121:ASP:CG	1:A:186:LEU:HD21	2.46	0.41
1:A:379:ARG:HH11	1:A:379:ARG:HG3	1.85	0.41
1:A:440:LYS:HE2	1:A:444:TRP:CD1	2.55	0.41
1:B:29:ASP:O	1:B:30:TYR:CG	2.73	0.41
1:B:131:HIS:CG	1:B:132:VAL:H	2.39	0.41
1:B:231:ASP:CB	1:B:234:GLN:HE21	2.33	0.41
1:B:245:ILE:HG13	1:B:246:ASN:OD1	2.20	0.41
1:B:418:GLU:CG	1:B:418:GLU:O	2.68	0.41
1:B:515:LEU:HD12	1:B:568:GLN:OE1	2.21	0.41
1:A:268:ASN:ND2	1:A:591:ASN:HA	2.36	0.41
1:B:119:ILE:N	1:B:119:ILE:HD12	2.36	0.41
1:A:18:TYR:CG	1:B:466:THR:HG21	2.56	0.41
1:A:237:TYR:CE2	1:A:345:ILE:HG12	2.55	0.41
1:A:598:ARG:HA	1:A:610:ASP:O	2.21	0.41
1:A:253:TYR:CZ	1:A:581:ILE:HD11	2.56	0.41
1:B:204:ILE:HD11	1:B:208:LEU:HD12	2.03	0.41
1:A:313:ILE:HD13	1:A:487:PHE:CD2	2.56	0.41
1:A:606:LYS:O	1:A:607:LYS:C	2.64	0.41
1:B:95:ASN:O	1:B:96:ASP:C	2.63	0.41
1:B:196:GLU:HG2	1:B:197:TYR:CD1	2.55	0.41
1:B:470:GLN:HB2	1:B:470:GLN:HE21	1.71	0.41
1:B:312:MET:HA	1:B:488:GLU:OE2	2.20	0.41
1:A:216:LEU:HD13	1:A:353:GLY:O	2.21	0.40
1:A:527:LYS:O	1:A:548:HIS:CB	2.66	0.40
1:B:144:ARG:HD3	1:B:161:TRP:CG	2.56	0.40
1:A:15:LEU:HD21	1:A:18:TYR:OH	2.20	0.40
1:A:462:VAL:HG11	1:A:480:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:564:LYS:HG2	1:B:565:ASN:N	2.36	0.40
1:A:498:LYS:C	1:A:500:ILE:N	2.77	0.40
1:A:531:ALA:HA	1:A:544:ASP:O	2.21	0.40
1:B:560:PHE:CD1	1:B:560:PHE:N	2.89	0.40
1:A:156:PRO:O	1:A:159:GLN:HB2	2.21	0.40
1:B:105:PRO:O	1:B:106:ASN:C	2.64	0.40
1:B:597:LEU:HD11	1:B:614:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	581/619 (94%)	534 (92%)	40 (7%)	7 (1%)	10	34
1	B	581/619 (94%)	526 (90%)	47 (8%)	8 (1%)	9	30
All	All	1162/1238 (94%)	1060 (91%)	87 (8%)	15 (1%)	9	31

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	127	LYS
1	A	334	ASP
1	B	96	ASP
1	B	127	LYS
1	B	334	ASP
1	A	431	GLU
1	B	49	ASP
1	B	338	CYS
1	A	49	ASP
1	A	338	CYS

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Mol	Chain	Res	Type
1	B	95	ASN
1	B	365	LEU
1	B	522	ASN
1	A	206	GLY

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	505/530 (95%)	485 (96%)	20 (4%)	28	63
1	B	505/530 (95%)	479 (95%)	26 (5%)	21	54
All	All	1010/1060 (95%)	964 (95%)	46 (5%)	24	58

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	95	ASN
1	A	128	ASP
1	A	141	ASN
1	A	149	ASN
1	A	184	THR
1	A	245	ILE
1	A	300	ARG
1	A	355	LYS
1	A	390	ILE
1	A	393	ASN
1	A	397	GLN
1	A	436	ASN
1	A	446	THR
1	A	459	PHE
1	A	470	GLN
1	A	471	ASN
1	A	493	VAL
1	A	523	ASP
1	A	524	GLU

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Mol	Chain	Res	Type
1	A	608	GLU
1	B	91	ARG
1	B	127	LYS
1	B	128	ASP
1	B	147	GLU
1	B	201	GLN
1	B	204	ILE
1	B	233	LEU
1	B	247	GLN
1	B	261	GLN
1	B	352	GLN
1	B	377	ARG
1	B	379	ARG
1	B	386	GLN
1	B	389	ASP
1	B	393	ASN
1	B	412	ILE
1	B	426	GLN
1	B	446	THR
1	B	459	PHE
1	B	466	THR
1	B	470	GLN
1	B	522	ASN
1	B	524	GLU
1	B	527	LYS
1	B	560	PHE
1	B	615	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	70	ASN
1	A	95	ASN
1	A	131	HIS
1	A	137	GLN
1	A	139	HIS
1	A	141	ASN
1	A	149	ASN
1	A	201	GLN
1	A	241	ASN
1	A	261	GLN

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Mol	Chain	Res	Type
1	A	268	ASN
1	A	276	HIS
1	A	310	HIS
1	A	339	HIS
1	A	352	GLN
1	A	383	HIS
1	A	386	GLN
1	A	405	GLN
1	A	436	ASN
1	A	471	ASN
1	A	549	HIS
1	A	563	GLN
1	A	565	ASN
1	A	568	GLN
1	B	55	HIS
1	B	70	ASN
1	B	102	GLN
1	B	131	HIS
1	B	139	HIS
1	B	157	GLN
1	B	201	GLN
1	B	234	GLN
1	B	235	ASN
1	B	251	HIS
1	B	268	ASN
1	B	286	ASN
1	B	310	HIS
1	B	339	HIS
1	B	357	ASN
1	B	367	ASN
1	B	375	HIS
1	B	395	HIS
1	B	397	GLN
1	B	426	GLN
1	B	468	HIS
1	B	470	GLN
1	B	471	ASN
1	B	522	ASN
1	B	563	GLN
1	B	565	ASN
1	B	568	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
4	ADP	A	3001	2	28,29,29	1.83	5 (17%)	43,45,45	1.09	2 (4%)
4	ADP	B	3002	2	28,29,29	1.93	5 (17%)	43,45,45	1.12	3 (6%)
3	GGA	B	6002	2	26,32,32	2.75	5 (19%)	29,42,42	1.83	8 (27%)
3	GGA	A	6001	2	26,32,32	2.57	5 (19%)	29,42,42	1.61	7 (24%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ADP	A	3001	2	-	2/16/32/32	0/3/3/3
4	ADP	B	3002	2	-	2/16/32/32	0/3/3/3
3	GGA	B	6002	2	-	10/36/40/40	-
3	GGA	A	6001	2	-	5/36/40/40	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	6002	GGA	P34-O56	-9.55	1.32	1.49
3	A	6001	GGA	P34-O56	-9.03	1.33	1.49
4	B	3002	ADP	O3'-C3'	-7.51	1.24	1.43
4	A	3001	ADP	O3'-C3'	-7.34	1.24	1.43
3	B	6002	GGA	O2-C1	6.96	1.42	1.22
3	B	6002	GGA	P60-O64	-5.36	1.34	1.54
3	A	6001	GGA	P60-O64	-5.28	1.35	1.54
3	A	6001	GGA	O2-C1	5.25	1.37	1.22
3	A	6001	GGA	O4-C1	4.29	1.44	1.30
4	B	3002	ADP	C2-N1	3.40	1.40	1.33
3	B	6002	GGA	O4-C1	-3.32	1.20	1.30
4	A	3001	ADP	C2-N1	3.30	1.39	1.33
3	B	6002	GGA	C14-N18	2.92	1.40	1.34
4	B	3002	ADP	C1'-N9	2.62	1.53	1.46
4	B	3002	ADP	C5-N7	-2.53	1.34	1.39
4	B	3002	ADP	PA-O3A	-2.45	1.56	1.59
3	A	6001	GGA	C14-N18	2.35	1.39	1.34
4	A	3001	ADP	PA-O3A	-2.24	1.57	1.59
4	A	3001	ADP	C6-N6	-2.14	1.28	1.34
4	A	3001	ADP	C5-N7	-2.13	1.35	1.39

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	6002	GGA	C20-N18-C14	4.32	127.69	121.13
3	B	6002	GGA	C22-C20-N18	4.23	118.15	110.38
3	A	6001	GGA	C22-C20-N18	4.19	118.08	110.38
3	A	6001	GGA	C20-N18-C14	3.53	126.50	121.13
3	B	6002	GGA	O26-C24-C20	-3.52	112.81	120.57
4	B	3002	ADP	N3-C2-N1	-3.39	123.44	128.58
4	A	3001	ADP	N3-C2-N1	-3.22	123.71	128.58
3	A	6001	GGA	O26-C24-C20	-3.13	113.67	120.57
3	B	6002	GGA	C20-C24-N30	2.72	122.75	116.47
4	A	3001	ADP	C2-N1-C6	2.68	123.14	118.73
4	B	3002	ADP	C2-N1-C6	2.66	123.09	118.73
3	A	6001	GGA	C37-C39-N44	-2.57	105.18	112.07
3	B	6002	GGA	O4-C1-O2	-2.51	118.39	124.08
3	B	6002	GGA	C37-C39-N44	-2.40	105.63	112.07
3	B	6002	GGA	O62-P60-O58	2.32	112.41	104.64
3	A	6001	GGA	O62-P60-O58	2.21	112.05	104.64
3	B	6002	GGA	C12-C10-C6	-2.20	108.81	113.86
3	A	6001	GGA	O64-P60-O58	2.15	111.85	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	3002	ADP	O2A-PA-O5'	2.03	116.78	107.57
3	A	6001	GGA	C20-C24-N30	2.01	121.11	116.47

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	6001	GGA	C22-C20-C24-O26
3	B	6002	GGA	C12-C10-C6-C1
3	B	6002	GGA	C22-C20-C24-O26
4	A	3001	ADP	PA-O3A-PB-O3B
4	B	3002	ADP	PA-O3A-PB-O3B
3	A	6001	GGA	C22-C20-C24-N30
3	B	6002	GGA	C22-C20-C24-N30
3	B	6002	GGA	C22-C20-N18-C14
3	A	6001	GGA	C22-C20-N18-C14
3	B	6002	GGA	O4-C1-C6-C10
3	A	6001	GGA	C33-C35-C37-C39
3	B	6002	GGA	C33-C35-C37-C39
3	B	6002	GGA	O2-C1-C6-C10
3	B	6002	GGA	O4-C1-C6-N8
3	B	6002	GGA	O2-C1-C6-N8
3	A	6001	GGA	N30-C29-P34-C33
3	B	6002	GGA	N30-C29-P34-C33
4	A	3001	ADP	PA-O3A-PB-O2B
4	B	3002	ADP	PA-O3A-PB-O2B

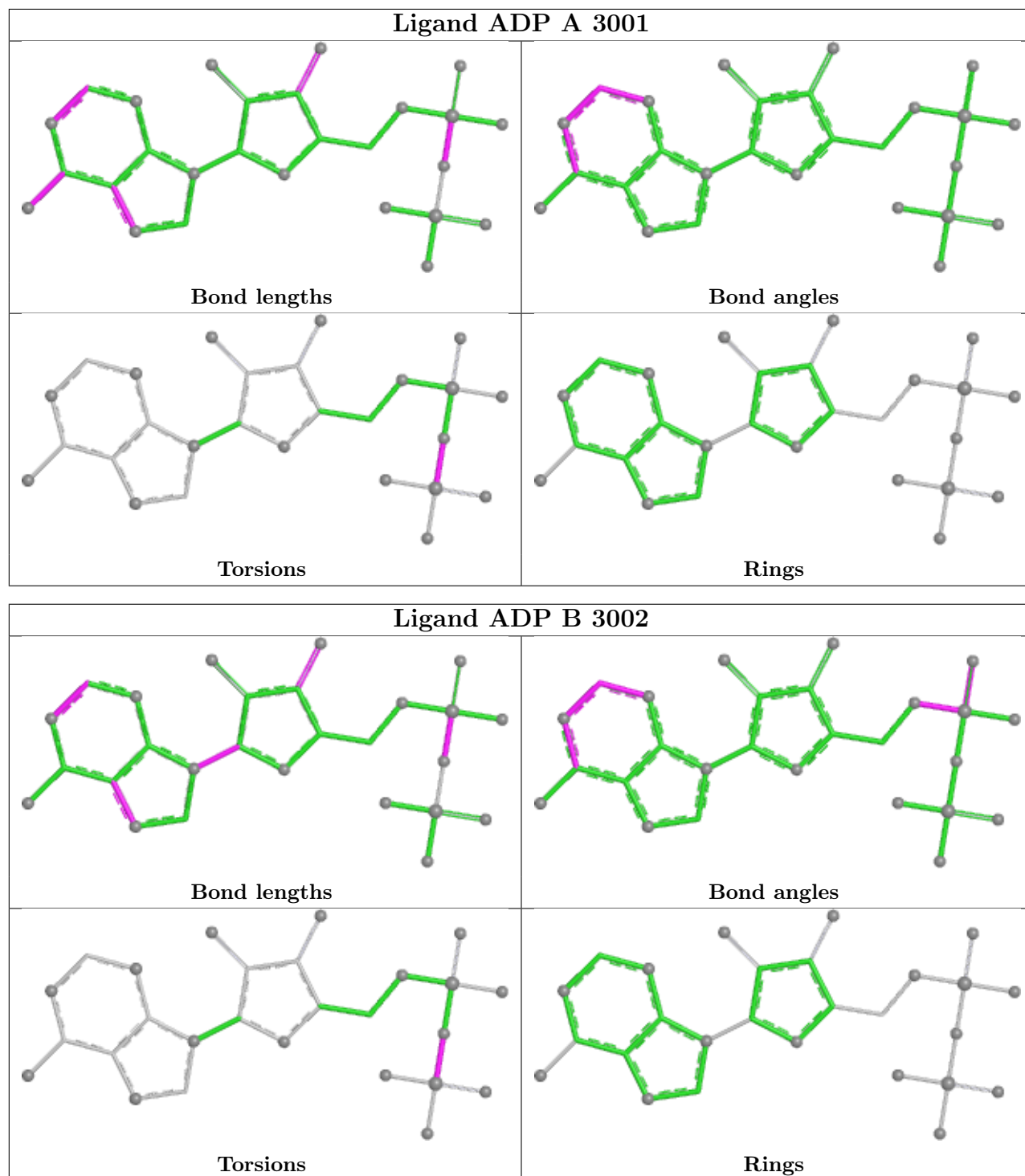
There are no ring outliers.

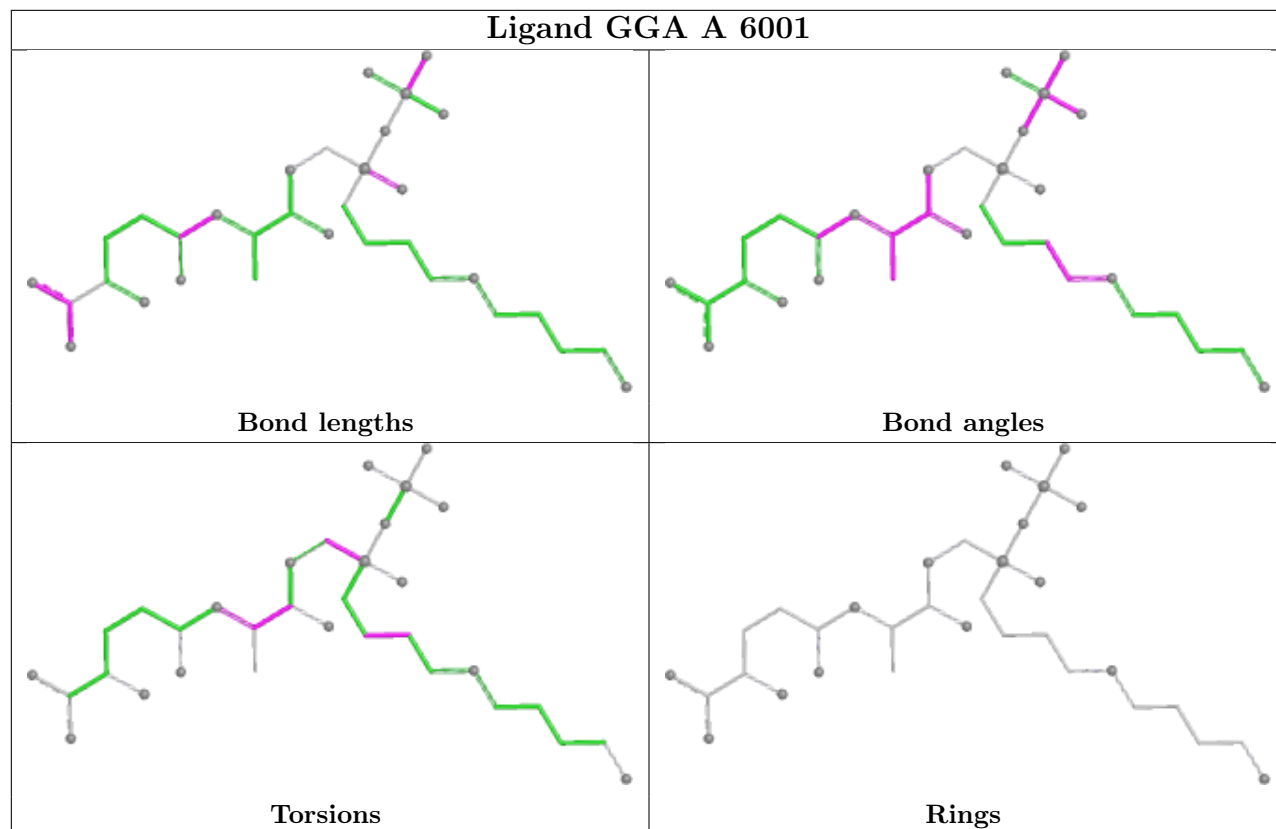
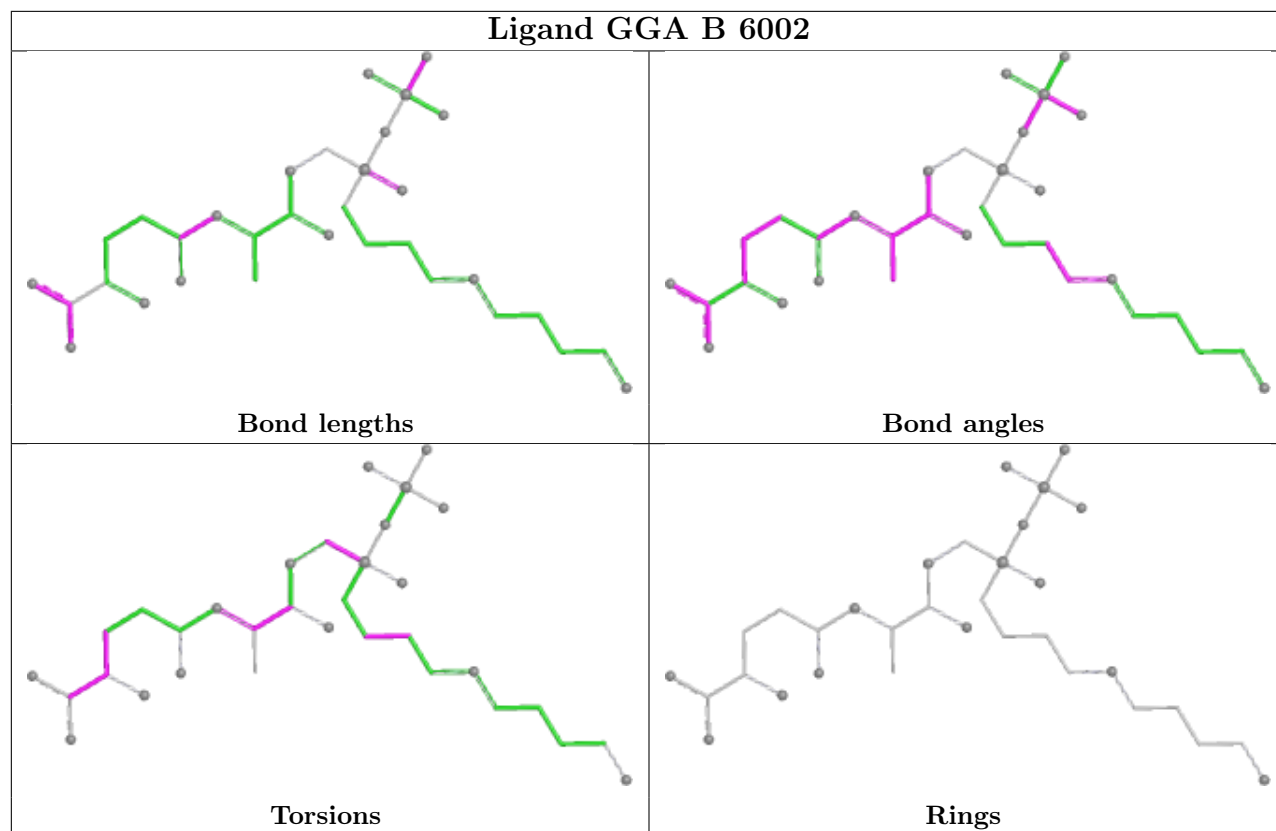
3 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	3001	ADP	2	0
3	B	6002	GGA	2	0
3	A	6001	GGA	7	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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	589/619 (95%)	-0.23	2 (0%) 90 86	7, 27, 48, 63	0
1	B	589/619 (95%)	-0.23	2 (0%) 90 86	8, 29, 48, 67	0
All	All	1178/1238 (95%)	-0.23	4 (0%) 90 86	7, 28, 48, 67	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	31	SER	3.0
1	B	454	VAL	2.9
1	A	157	GLN	2.1
1	A	601	GLU	2.1

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	GGA	A	6001	33/33	0.94	0.12	22,31,45,49	0

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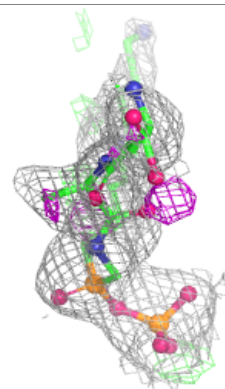
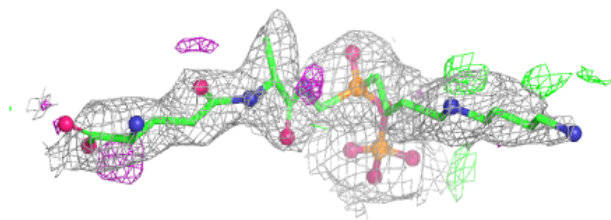
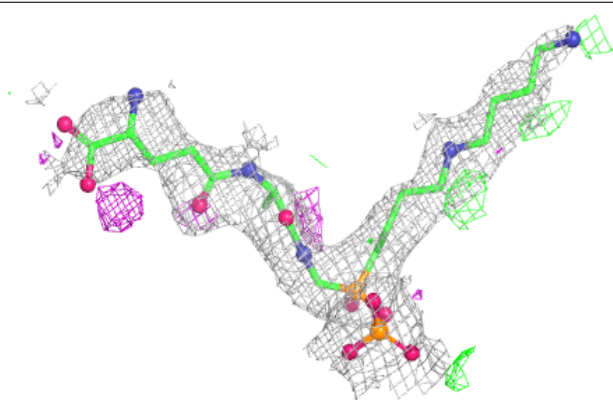
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GGA	B	6002	33/33	0.94	0.12	22,37,54,56	0
2	MG	A	5002	1/1	0.97	0.05	8,8,8,8	0
2	MG	A	5001	1/1	0.98	0.03	8,8,8,8	0
4	ADP	A	3001	27/27	0.98	0.06	1,18,21,23	0
4	ADP	B	3002	27/27	0.98	0.05	6,18,20,21	0
2	MG	B	5003	1/1	0.99	0.02	10,10,10,10	0
2	MG	B	5004	1/1	0.99	0.03	12,12,12,12	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.

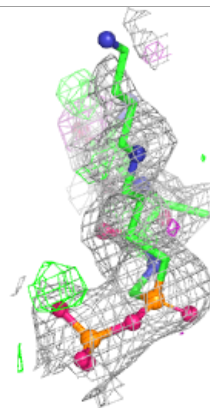
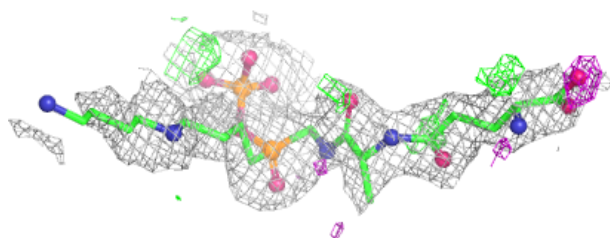
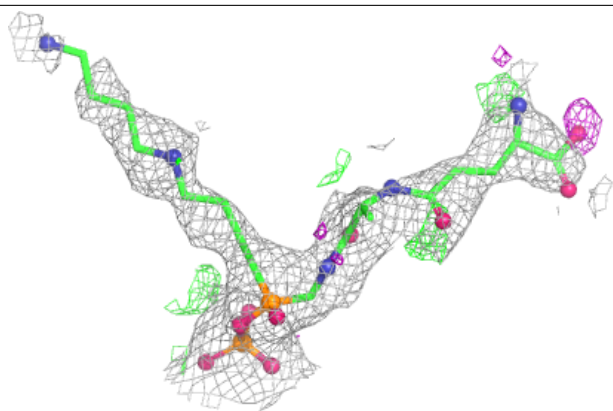
Electron density around GGA A 6001:

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

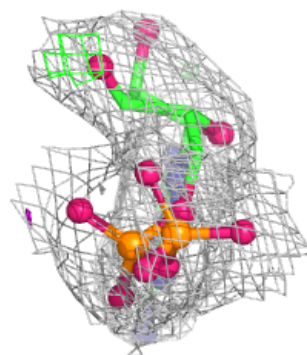
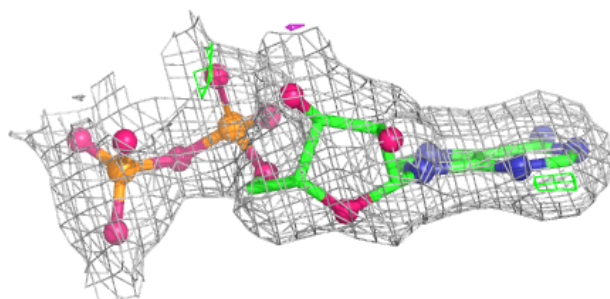
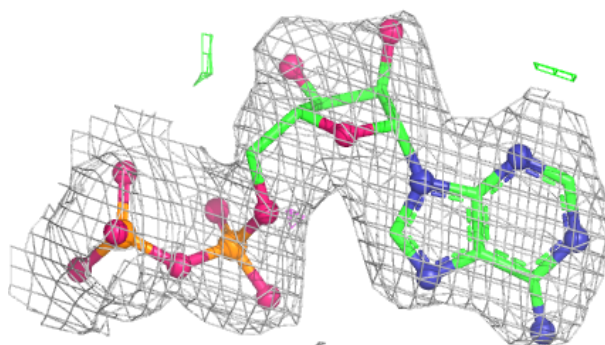


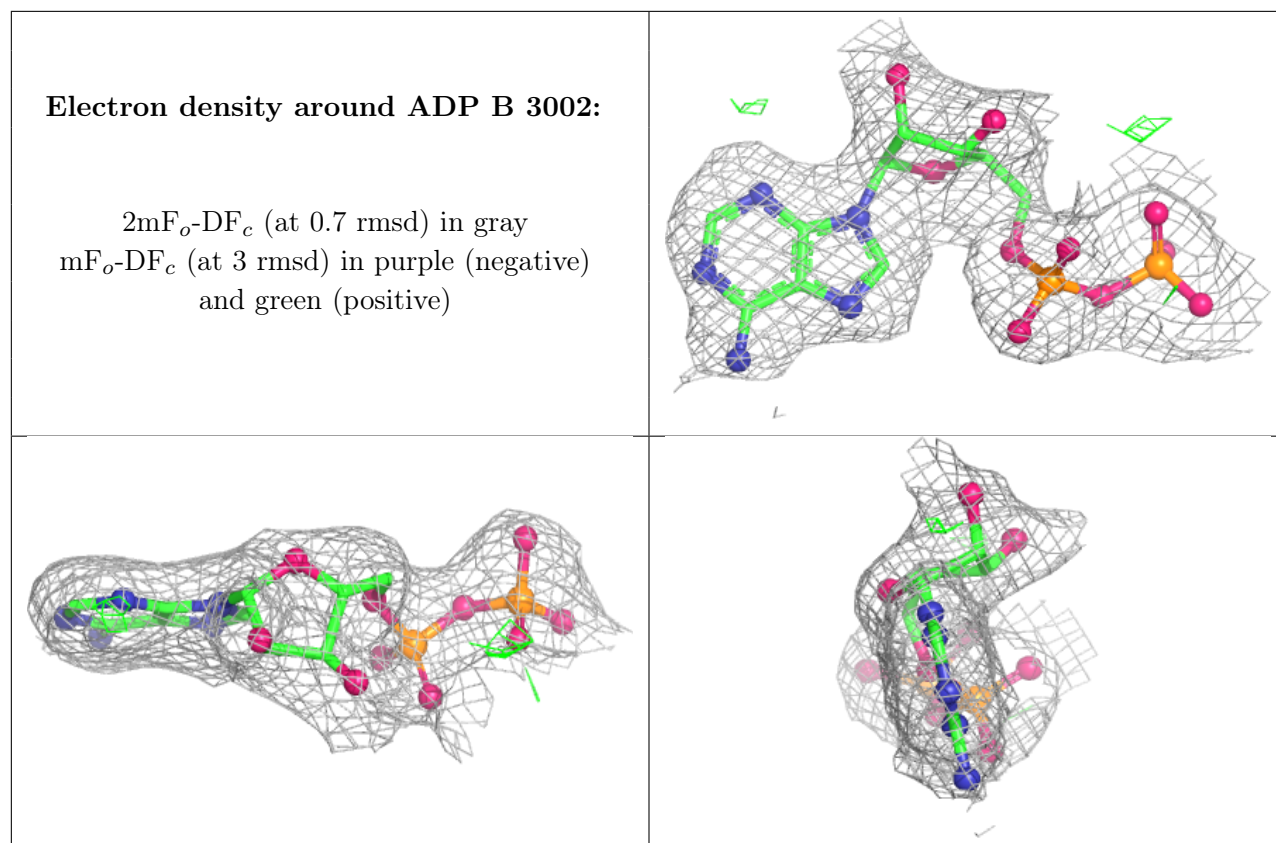
Electron density around GGA B 6002:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.