



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:44 PM UTC

PDB ID : 4AP0 / pdb_00004ap0
Title : The mitotic kinesin Eg5 in complex with Mg-ADP and ispinesib
Authors : Schuettelkopf, A.W.; Talapatra, S.K.; Kozielski, F.
Deposited on : 2012-03-30
Resolution : 2.59 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

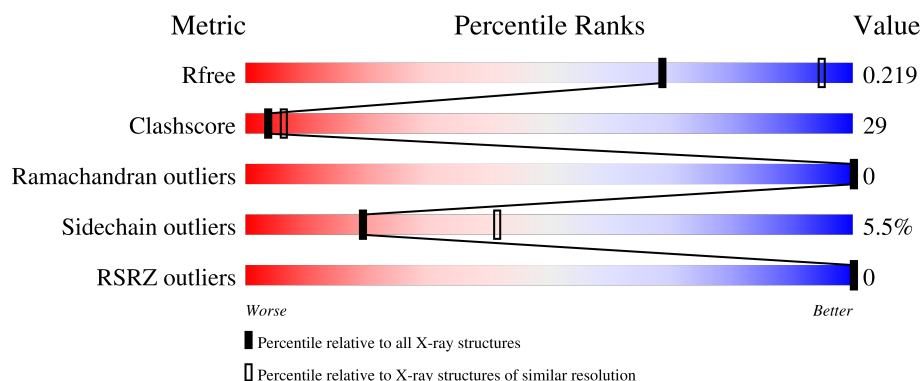
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	370	
1	B	370	
1	C	370	
1	D	370	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9849 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 KINESIN-LIKE PROTEIN KIF11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	0	0	0
			2475	1559	423	484	9			
1	B	312	Total	C	N	O	S	0	0	0
			2374	1492	407	465	10			
1	C	311	Total	C	N	O	S	0	0	0
			2347	1476	405	456	10			
1	D	309	Total	C	N	O	S	0	0	0
			2357	1486	403	459	9			

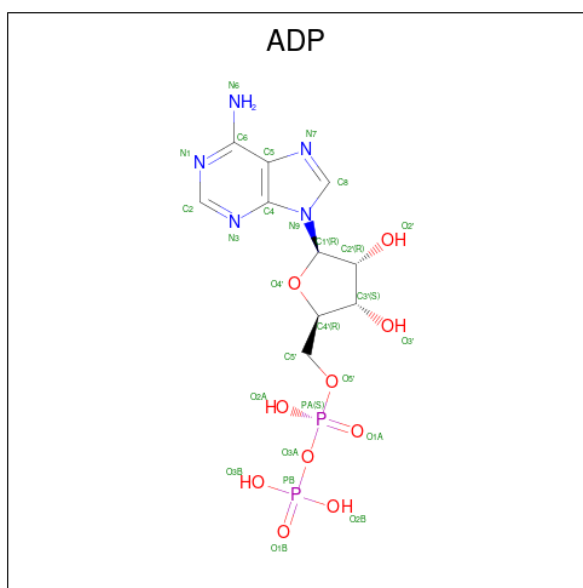
There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P52732
A	0	PRO	-	expression tag	UNP P52732
B	-1	GLY	-	expression tag	UNP P52732
B	0	PRO	-	expression tag	UNP P52732
C	-1	GLY	-	expression tag	UNP P52732
C	0	PRO	-	expression tag	UNP P52732
D	-1	GLY	-	expression tag	UNP P52732
D	0	PRO	-	expression tag	UNP P52732

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		
2	B	1	Total	Mg	0	0
			1	1		
2	C	1	Total	Mg	0	0
			1	1		
2	D	1	Total	Mg	0	0
			1	1		

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

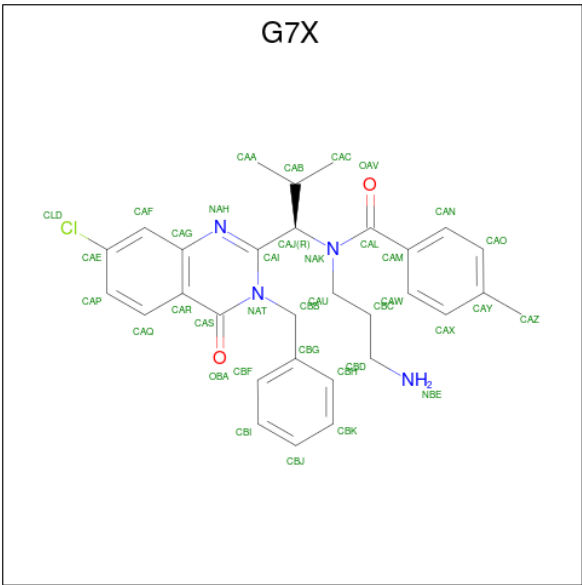


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Cl	0	0
			2	2		
4	B	3	Total	Cl	0	0
			3	3		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is ISPINESIB MESILATE (CCD ID: G7X) (formula: $C_{30}H_{33}ClN_4O_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	Cl	N	O	0	0
			34	28	1	3	2		
5	B	1	Total	C	Cl	N	O	0	0
			37	30	1	4	2		
5	C	1	Total	C	Cl	N	O	0	0
			37	30	1	4	2		
5	D	1	Total	C	Cl	N	O	0	0
			37	30	1	4	2		

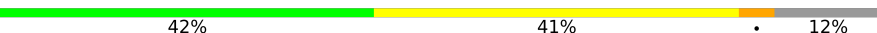
- Molecule 6 is water.

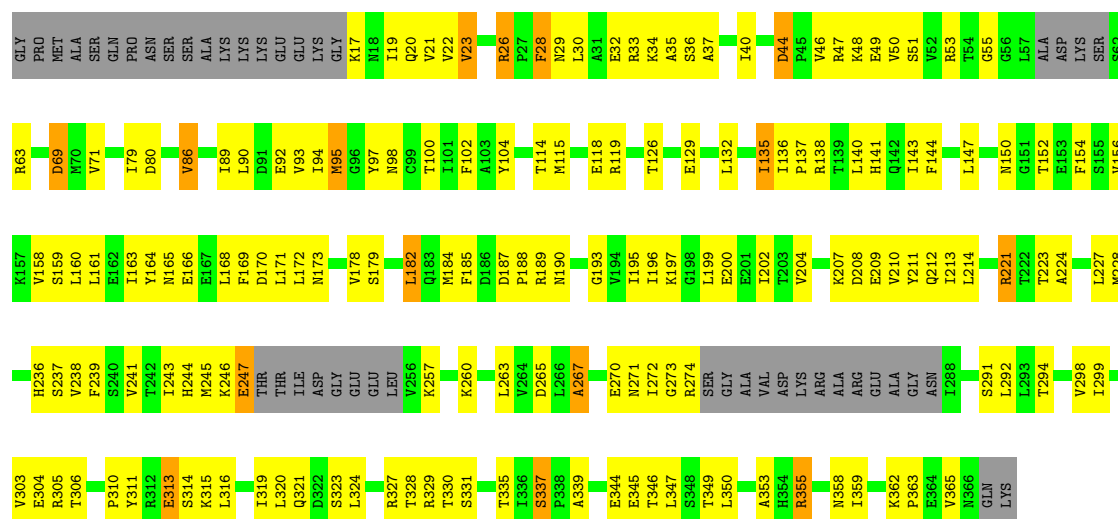
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	6	Total	O	0	0
			6	6		
6	C	10	Total	O	0	0
			10	10		
6	D	8	Total	O	0	0
			8	8		

3 Residue-property plots

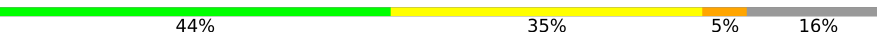
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

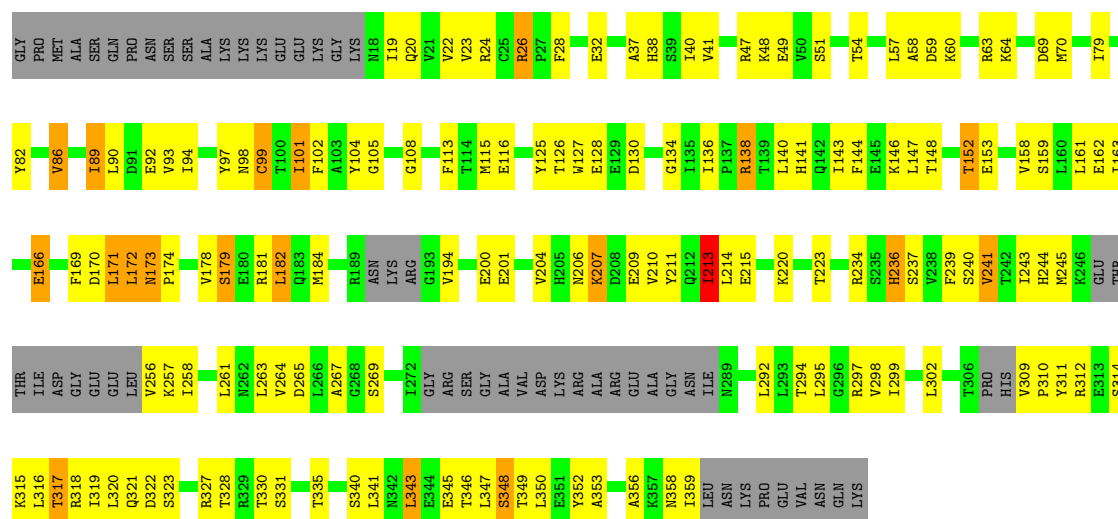
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain A: 

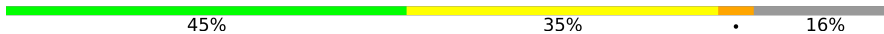


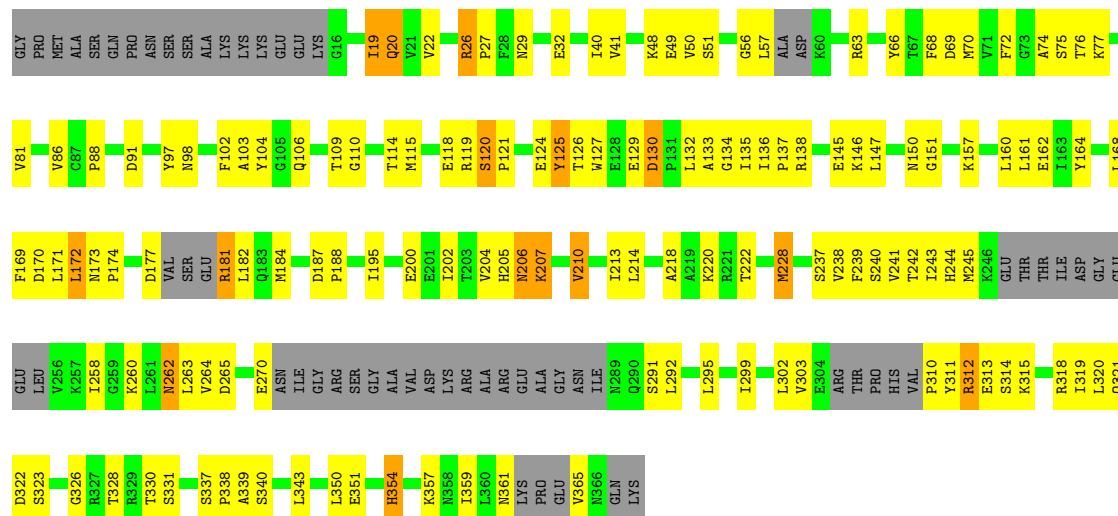
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain B: 



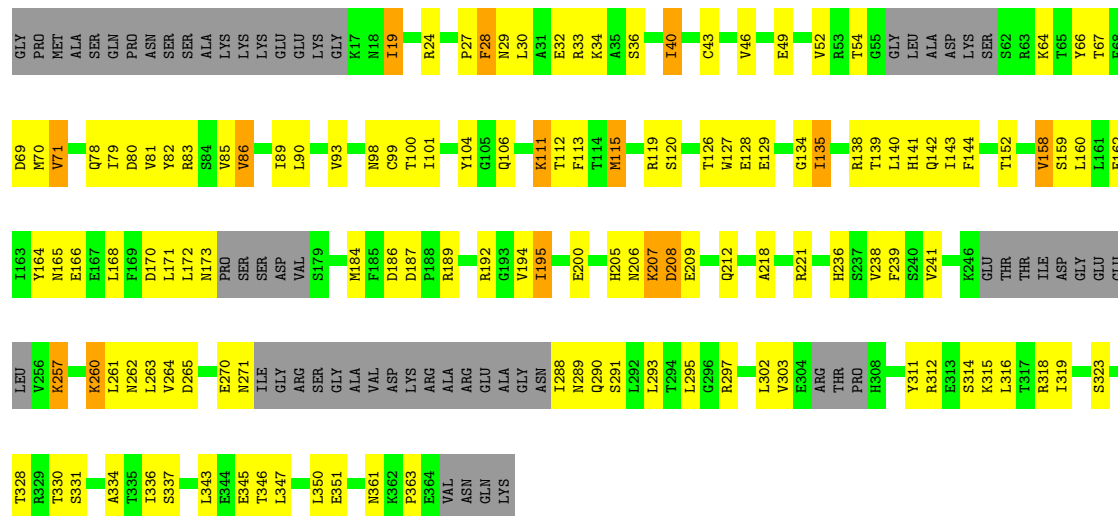
• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain C:  45% 35% 16%



• Molecule 1: KINESIN-LIKE PROTEIN KIF11

Chain D:  48% 32% 16%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.72Å 112.61Å 106.91Å 90.00° 90.02° 90.00°	Depositor
Resolution (Å)	29.86 – 2.59 29.86 – 2.59	Depositor EDS
% Data completeness (in resolution range)	95.8 (29.86-2.59) 95.8 (29.86-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 2.61Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.203 , 0.253 0.190 , 0.219	Depositor DCC
R_{free} test set	2298 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	45.3	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 19.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.019 for -h,-l,-k 0.012 for -h,l,k 0.430 for h,-k,-l	Xtriage
Reported twinning fraction	0.452 for h,-k,-l	Depositor
Outliers	1 of 45505 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	9849	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.28 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.6433e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: CL, ADP, G7X, 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	0.58	0/2512	1.10	13/3410 (0.4%)
1	B	0.57	0/2406	1.06	15/3259 (0.5%)
1	C	0.62	0/2377	1.12	14/3217 (0.4%)
1	D	0.61	0/2389	1.13	12/3237 (0.4%)
All	All	0.59	0/9684	1.10	54/13123 (0.4%)

There are no bond length outliers.

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	337	SER	CA-C-N	7.80	127.86	119.28
1	D	337	SER	C-N-CA	7.80	127.86	119.28
1	C	120	SER	CA-C-N	7.57	127.10	118.85
1	C	120	SER	C-N-CA	7.57	127.10	118.85
1	D	192	ARG	N-CA-C	-7.50	104.14	113.28
1	A	313	GLU	N-CA-C	7.43	119.38	111.28
1	D	152	THR	CB-CA-C	-7.22	108.25	116.63
1	B	130	ASP	CA-C-N	7.21	127.05	119.05
1	B	130	ASP	C-N-CA	7.21	127.05	119.05
1	C	130	ASP	CA-C-N	7.15	126.86	119.56
1	C	130	ASP	C-N-CA	7.15	126.86	119.56
1	C	124	GLU	N-CA-C	7.07	120.01	108.55
1	D	86	VAL	N-CA-C	6.95	118.58	111.00
1	C	207	LYS	N-CA-C	6.92	118.83	111.28
1	A	55	GLY	N-CA-C	6.75	120.83	112.73
1	B	173	ASN	CA-C-N	6.73	126.18	118.85
1	B	173	ASN	C-N-CA	6.73	126.18	118.85
1	A	86	VAL	N-CA-C	6.67	117.29	110.82
1	B	152	THR	CB-CA-C	-6.47	109.12	116.63
1	C	135	ILE	N-CA-C	6.44	116.61	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	135	ILE	N-CA-C	6.38	117.13	110.62
1	C	151	GLY	N-CA-C	-6.36	106.91	115.36
1	C	339	ALA	N-CA-C	6.29	119.78	110.48
1	D	71	VAL	N-CA-C	6.19	117.20	108.17
1	A	337	SER	CA-C-N	6.13	125.85	119.05
1	A	337	SER	C-N-CA	6.13	125.85	119.05
1	B	23	VAL	N-CA-C	6.10	116.90	108.12
1	D	135	ILE	N-CA-C	5.95	116.13	110.42
1	B	358	ASN	N-CA-C	5.91	118.51	111.71
1	B	99	CYS	N-CA-C	5.87	118.20	108.99
1	C	210	VAL	CB-CA-C	-5.84	104.39	112.04
1	D	135	ILE	CB-CA-C	-5.83	104.50	111.97
1	B	330	THR	N-CA-C	5.77	118.87	109.24
1	A	179	SER	N-CA-C	5.63	117.42	111.28
1	D	158	VAL	N-CA-C	5.59	115.94	108.11
1	A	26	ARG	CA-C-N	5.53	125.50	120.03
1	A	26	ARG	C-N-CA	5.53	125.50	120.03
1	B	152	THR	N-CA-C	5.52	117.41	108.08
1	C	121	PRO	N-CA-C	5.43	120.68	113.40
1	A	40	ILE	N-CA-C	5.41	117.38	112.29
1	C	86	VAL	N-CA-C	5.39	115.60	110.53
1	A	44	ASP	CA-C-N	5.38	124.72	118.85
1	A	44	ASP	C-N-CA	5.38	124.72	118.85
1	C	114	THR	N-CA-C	-5.36	105.10	111.69
1	B	138	ARG	N-CA-C	-5.21	105.49	111.07
1	A	267	ALA	N-CA-C	-5.20	103.67	110.53
1	B	213	ILE	N-CA-C	5.15	115.93	110.72
1	C	125	TYR	N-CA-C	-5.15	100.30	109.06
1	B	179	SER	N-CA-C	5.12	116.86	111.28
1	D	40	ILE	N-CA-C	5.12	117.89	112.83
1	D	111	LYS	N-CA-C	5.11	116.54	110.97
1	D	295	LEU	N-CA-C	-5.11	105.71	111.28
1	B	348	SER	N-CA-C	-5.06	105.46	110.97
1	B	125	TYR	N-CA-C	-5.06	101.39	109.23

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	2475	0	2424	160	0
1	B	2374	0	2333	137	0
1	C	2347	0	2297	128	0
1	D	2357	0	2312	117	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	2	0
3	D	27	0	12	2	0
4	A	2	0	0	0	0
4	B	3	0	0	0	0
4	D	1	0	0	0	0
5	A	34	0	25	6	0
5	B	37	0	33	14	0
5	C	37	0	33	11	0
5	D	37	0	33	11	0
6	A	9	0	0	0	0
6	B	6	0	0	0	0
6	C	10	0	0	0	0
6	D	8	0	0	0	0
All	All	9849	0	9538	559	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 29.

All (559) 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:C:312:ARG:HG2	1:C:312:ARG:HH11	1.19	1.05
1:B:148:THR:HA	1:B:152:THR:HG22	1.43	1.00
1:C:50:VAL:HG12	1:C:66:TYR:HB2	1.43	0.99
1:A:143:ILE:HD13	1:A:243:ILE:HD11	1.45	0.98
1:A:86:VAL:HG21	1:A:135:ILE:HG12	1.45	0.98
5:B:2001:G7X:HAW	5:B:2001:G7X:HBB2	1.43	0.96
5:B:2001:G7X:HBB2	5:B:2001:G7X:CAW	1.96	0.95
1:D:336:ILE:HG21	1:D:350:LEU:HD21	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:187:ASP:HA	1:C:195:ILE:HG12	1.55	0.87
1:D:54:THR:HG21	1:D:64:LYS:HE3	1.57	0.87
1:A:239:PHE:HE1	1:A:241:VAL:HG23	1.40	0.86
5:D:2001:G7X:HBB2	5:D:2001:G7X:CAW	2.06	0.86
1:B:302:LEU:HB3	1:B:359:ILE:HG12	1.58	0.85
1:C:170:ASP:HB2	1:C:182:LEU:HD11	1.57	0.84
1:C:262:ASN:HD22	1:C:262:ASN:N	1.75	0.84
1:A:214:LEU:HD22	5:A:2001:G7X:HBF	1.60	0.83
1:C:312:ARG:HH11	1:C:312:ARG:CG	1.91	0.83
1:D:173:ASN:HB2	1:D:200:GLU:HG3	1.59	0.82
1:C:243:ILE:HG22	1:C:245:MET:HG3	1.61	0.82
5:D:2001:G7X:HBB2	5:D:2001:G7X:HAW	1.63	0.81
1:B:184:MET:HE1	1:B:319:ILE:HG12	1.63	0.80
1:A:158:VAL:HG12	1:A:241:VAL:HG22	1.64	0.80
1:C:49:GLU:HA	1:C:66:TYR:O	1.82	0.80
1:C:173:ASN:HB2	1:C:200:GLU:HG3	1.63	0.79
1:C:312:ARG:HG2	1:C:312:ARG:NH1	1.83	0.79
1:B:89:ILE:HD12	1:B:101:ILE:HD11	1.62	0.79
1:A:136:ILE:HG12	1:A:263:LEU:HD13	1.64	0.78
1:C:20:GLN:HB3	1:C:331:SER:OG	1.83	0.78
1:C:322:ASP:O	1:C:326:GLY:HA3	1.85	0.76
1:D:323:SER:HA	1:D:328:THR:HB	1.66	0.76
1:C:204:VAL:HG11	1:C:210:VAL:CG2	2.16	0.76
1:B:236:HIS:CD2	1:B:267:ALA:HB2	2.20	0.76
1:A:168:LEU:HD13	1:A:196:ILE:HD12	1.67	0.75
1:C:50:VAL:CG1	1:C:66:TYR:HB2	2.16	0.75
1:A:239:PHE:CE1	1:A:241:VAL:HG23	2.22	0.75
1:B:200:GLU:HA	1:B:200:GLU:OE1	1.87	0.75
1:A:92:GLU:HG3	1:A:329:ARG:HH11	1.51	0.74
5:B:2001:G7X:HBH	5:B:2001:G7X:CAX	2.17	0.74
1:D:134:GLY:O	1:D:138:ARG:HG3	1.87	0.74
1:D:236:HIS:ND1	1:D:316:LEU:HD22	2.03	0.74
1:D:184:MET:CE	1:D:194:VAL:HG21	2.18	0.73
1:A:166:GLU:HA	1:A:166:GLU:OE1	1.87	0.73
1:D:104:TYR:O	1:D:334:ALA:HA	1.88	0.72
1:C:204:VAL:HG11	1:C:210:VAL:HG23	1.72	0.72
1:D:127:TRP:HZ2	1:D:207:LYS:HB2	1.53	0.72
1:A:30:LEU:HD22	3:D:1003:ADP:C2	2.25	0.71
1:B:184:MET:HE1	1:B:194:VAL:HG21	1.71	0.71
1:C:262:ASN:N	1:C:262:ASN:ND2	2.36	0.71
1:C:173:ASN:HD22	1:C:174:PRO:HD2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:206:ASN:C	1:C:206:ASN:OD1	2.33	0.71
1:B:158:VAL:HG12	1:B:241:VAL:HG12	1.71	0.70
5:D:2001:G7X:HBFB	5:D:2001:G7X:CAX	2.21	0.70
1:B:144:PHE:HZ	1:B:204:VAL:HG12	1.55	0.70
1:A:98:ASN:OD1	1:A:260:LYS:HB3	1.91	0.70
5:C:2001:G7X:HBB2	5:C:2001:G7X:CAW	2.22	0.70
1:D:69:ASP:O	1:D:70:MET:HG3	1.91	0.70
1:B:178:VAL:HA	1:B:220:LYS:HE3	1.74	0.70
1:A:173:ASN:HB2	1:A:200:GLU:HG3	1.73	0.69
1:B:298:VAL:O	1:B:302:LEU:HG	1.92	0.69
1:D:168:LEU:HD13	1:D:315:LYS:HZ3	1.56	0.69
1:B:172:LEU:HD11	1:B:213:ILE:HG22	1.74	0.69
1:A:246:LYS:O	1:A:247:GLU:HB2	1.90	0.69
1:A:298:VAL:HG11	1:A:324:LEU:HD13	1.75	0.68
1:A:21:VAL:HG11	1:A:353:ALA:HB1	1.75	0.68
1:C:22:VAL:HG22	1:C:70:MET:HB2	1.76	0.68
1:D:106:GLN:HG3	1:D:345:GLU:HG2	1.75	0.68
1:D:81:VAL:O	1:D:85:VAL:HB	1.93	0.68
1:A:185:PHE:CD1	1:A:197:LYS:HE3	2.29	0.67
1:A:344:GLU:OE1	1:A:344:GLU:HA	1.93	0.67
1:D:173:ASN:HB2	1:D:200:GLU:CG	2.25	0.66
1:C:323:SER:HA	1:C:328:THR:OG1	1.95	0.66
1:A:152:THR:HG23	1:A:152:THR:O	1.95	0.66
1:D:19:ILE:HG12	1:D:330:THR:HB	1.77	0.66
1:A:46:VAL:HG23	1:A:47:ARG:N	2.11	0.66
1:C:240:SER:HB3	1:C:260:LYS:HE3	1.78	0.66
1:D:184:MET:HE1	1:D:194:VAL:HG21	1.77	0.66
1:A:291:SER:HA	1:A:314:SER:HB2	1.77	0.66
1:B:101:ILE:HD13	1:B:331:SER:HB2	1.78	0.66
1:A:92:GLU:HG3	1:A:329:ARG:NH1	2.11	0.65
1:D:171:LEU:CD2	1:D:221:ARG:HB2	2.26	0.65
1:A:187:ASP:HB3	1:A:190:ASN:HB3	1.77	0.65
1:C:102:PHE:CZ	1:C:320:LEU:HD13	2.32	0.65
1:A:209:GLU:O	1:A:213:ILE:HG13	1.96	0.65
1:A:239:PHE:HE1	1:A:241:VAL:CG2	2.09	0.65
1:B:115:MET:CE	1:B:263:LEU:HB3	2.26	0.65
1:A:236:HIS:CE1	1:A:267:ALA:H	2.15	0.65
1:C:110:GLY:HA2	3:C:1003:ADP:PA	2.37	0.65
1:A:214:LEU:CD2	5:A:2001:G7X:HBFB	2.27	0.65
1:D:238:VAL:HG13	1:D:264:VAL:HG22	1.79	0.64
1:D:293:LEU:HD11	1:D:297:ARG:NH2	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:214:LEU:HD22	5:A:2001:G7X:CBF	2.26	0.64
1:B:241:VAL:CG2	1:B:261:LEU:HB3	2.27	0.64
1:B:159:SER:HA	1:B:172:LEU:HD23	1.78	0.64
1:D:49:GLU:HG2	1:D:67:THR:OG1	1.98	0.64
1:B:89:ILE:HD12	1:B:101:ILE:CD1	2.27	0.64
1:A:159:SER:HA	1:A:172:LEU:HD12	1.78	0.64
1:B:315:LYS:O	1:B:319:ILE:HG13	1.98	0.64
1:A:304:GLU:O	1:A:305:ARG:HB2	1.98	0.64
1:D:135:ILE:HG21	1:D:263:LEU:HD22	1.80	0.64
1:C:262:ASN:HD22	1:C:262:ASN:H	1.46	0.63
1:B:38:HIS:CG	1:B:57:LEU:HB3	2.34	0.63
1:B:239:PHE:CE1	1:B:241:VAL:HG13	2.34	0.63
1:D:160:LEU:HD21	5:D:2001:G7X:CLD	2.36	0.63
1:A:154:PHE:HA	1:A:244:HIS:O	1.98	0.62
1:A:299:ILE:HG23	1:A:359:ILE:HD11	1.81	0.62
1:A:114:THR:HG22	1:A:115:MET:HE2	1.81	0.62
1:A:118:GLU:O	1:A:132:LEU:HB2	2.00	0.62
1:A:141:HIS:HD2	1:A:207:LYS:HD3	1.63	0.62
1:A:291:SER:HA	1:A:314:SER:CB	2.29	0.62
1:D:218:ALA:HB2	5:D:2001:G7X:HAF	1.81	0.62
1:B:22:VAL:CG1	1:B:70:MET:HB2	2.29	0.62
1:A:92:GLU:HA	1:A:92:GLU:OE1	2.00	0.61
1:B:184:MET:CE	1:B:194:VAL:HG21	2.30	0.61
1:B:37:ALA:HB2	1:B:341:LEU:HD23	1.83	0.61
1:D:164:TYR:CD1	1:D:165:ASN:HB2	2.35	0.61
1:C:184:MET:HE3	1:C:318:ARG:CZ	2.31	0.61
1:A:246:LYS:O	1:A:247:GLU:CB	2.48	0.61
1:D:291:SER:HB3	1:D:316:LEU:CB	2.30	0.61
1:C:106:GLN:O	1:C:109:THR:HG23	2.00	0.61
1:B:244:HIS:ND1	1:B:258:ILE:HG12	2.16	0.61
1:A:159:SER:HB2	1:A:199:LEU:HD11	1.83	0.60
1:A:144:PHE:CZ	1:A:156:VAL:HG21	2.37	0.60
1:A:172:LEU:HD22	1:A:213:ILE:HG22	1.83	0.60
1:C:214:LEU:HD12	5:C:2001:G7X:HBF	1.84	0.60
1:C:330:THR:HB	1:C:361:ASN:HD21	1.66	0.60
1:A:98:ASN:C	1:A:328:THR:HG23	2.27	0.60
1:A:160:LEU:HD12	1:A:238:VAL:O	2.02	0.60
1:D:168:LEU:CD1	1:D:315:LYS:HZ3	2.13	0.60
1:B:126:THR:HB	1:B:128:GLU:OE1	2.01	0.60
1:C:303:VAL:CG2	1:C:359:ILE:HG13	2.33	0.59
1:A:184:MET:HB2	1:A:196:ILE:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:134:GLY:O	1:C:137:PRO:HG2	2.03	0.59
1:D:236:HIS:CE1	1:D:316:LEU:HD22	2.38	0.59
1:C:241:VAL:O	1:C:260:LYS:HA	2.03	0.59
1:B:159:SER:HB3	1:B:201:GLU:HG2	1.83	0.58
1:A:311:TYR:CD1	1:A:321:GLN:HG3	2.38	0.58
1:B:144:PHE:CE1	1:B:206:ASN:HA	2.37	0.58
1:A:188:PRO:HD2	1:A:195:ILE:CD1	2.33	0.58
1:B:173:ASN:HB2	1:B:200:GLU:CG	2.33	0.58
1:D:89:ILE:HD11	1:D:331:SER:OG	2.04	0.58
1:D:184:MET:HE3	1:D:194:VAL:HG21	1.84	0.58
1:C:303:VAL:HG23	1:C:359:ILE:HG13	1.86	0.58
1:D:54:THR:HG21	1:D:64:LYS:CE	2.32	0.58
1:D:127:TRP:CZ2	1:D:207:LYS:HB2	2.38	0.58
1:D:236:HIS:HD1	1:D:316:LEU:HD22	1.68	0.58
1:B:184:MET:CE	1:B:319:ILE:HG12	2.33	0.58
5:D:2001:G7X:HBD2	5:D:2001:G7X:OAV	2.03	0.58
1:A:156:VAL:HG23	1:A:204:VAL:HB	1.85	0.58
1:C:164:TYR:CE2	1:C:228:MET:HB3	2.39	0.58
1:B:22:VAL:HG12	1:B:70:MET:HB2	1.86	0.57
1:C:239:PHE:HE1	1:C:241:VAL:HG22	1.68	0.57
1:C:302:LEU:HB2	1:C:359:ILE:CD1	2.33	0.57
1:B:104:TYR:O	1:B:335:THR:N	2.35	0.57
1:B:93:VAL:HG12	1:B:243:ILE:HD12	1.86	0.57
1:C:169:PHE:CE2	1:C:228:MET:HE1	2.40	0.57
1:D:54:THR:HG21	1:D:64:LYS:HG3	1.84	0.57
1:D:186:ASP:OD2	1:D:312:ARG:NH2	2.36	0.57
1:B:244:HIS:CE1	1:B:258:ILE:HG12	2.40	0.57
1:B:294:THR:HG22	1:B:317:THR:HG21	1.86	0.57
1:C:88:PRO:O	1:C:91:ASP:HB2	2.05	0.57
1:C:354:HIS:CE1	1:C:357:LYS:HE2	2.40	0.57
1:B:57:LEU:HD12	1:B:58:ALA:N	2.20	0.57
1:C:127:TRP:CD2	5:C:2001:G7X:HBK	2.40	0.57
1:D:79:ILE:O	1:D:83:ARG:HG3	2.05	0.57
1:A:104:TYR:O	1:A:335:THR:OG1	2.23	0.56
1:A:207:LYS:O	1:A:210:VAL:HB	2.04	0.56
1:C:26:ARG:O	1:C:338:PRO:HD3	2.05	0.56
1:D:78:GLN:NE2	1:D:113:PHE:CZ	2.73	0.56
1:D:187:ASP:HA	1:D:195:ILE:HG13	1.87	0.56
1:C:204:VAL:HG11	1:C:210:VAL:HG22	1.88	0.56
1:C:239:PHE:HE1	1:C:241:VAL:CG2	2.18	0.56
1:A:185:PHE:CZ	1:A:195:ILE:HD12	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:28:PHE:CD2	1:A:33:ARG:CZ	2.89	0.56
1:A:204:VAL:HG22	1:A:213:ILE:HD12	1.88	0.56
1:B:166:GLU:OE2	1:B:314:SER:HB2	2.05	0.56
1:C:40:ILE:HD12	1:C:343:LEU:HD13	1.87	0.56
1:D:162:GLU:HG3	1:D:171:LEU:HD13	1.88	0.56
1:A:30:LEU:HD22	3:D:1003:ADP:N3	2.21	0.56
1:B:173:ASN:O	1:B:220:LYS:NZ	2.38	0.55
1:B:210:VAL:CG1	5:B:2001:G7X:HBI	2.37	0.55
1:A:327:ARG:O	1:A:363:PRO:HA	2.07	0.55
1:D:209:GLU:O	1:D:212:GLN:HG2	2.06	0.55
1:B:38:HIS:CD2	1:B:57:LEU:HB3	2.41	0.55
1:C:340:SER:O	1:C:343:LEU:HB3	2.06	0.55
1:A:304:GLU:HA	1:A:304:GLU:OE1	2.06	0.55
1:B:172:LEU:HD11	1:B:213:ILE:CG2	2.34	0.55
1:C:106:GLN:HA	1:C:270:GLU:OE1	2.07	0.55
1:C:173:ASN:ND2	1:C:174:PRO:HD2	2.21	0.55
1:B:93:VAL:CG1	1:B:243:ILE:HD12	2.37	0.55
1:D:164:TYR:CE1	1:D:165:ASN:HB2	2.41	0.55
1:C:19:ILE:CD1	1:C:359:ILE:HB	2.37	0.55
1:D:160:LEU:CD2	5:D:2001:G7X:CLD	2.92	0.55
1:D:166:GLU:OE1	1:D:291:SER:OG	2.25	0.55
1:B:170:ASP:HB2	1:B:182:LEU:HD11	1.88	0.55
1:D:98:ASN:HA	1:D:260:LYS:O	2.06	0.55
1:D:28:PHE:CE1	1:D:32:GLU:HB3	2.42	0.55
1:A:185:PHE:CE1	1:A:195:ILE:HB	2.42	0.55
5:C:2001:G7X:HBD2	5:C:2001:G7X:OAV	2.07	0.55
1:C:181:ARG:NH1	1:C:181:ARG:HG3	2.23	0.54
1:B:127:TRP:HB2	5:B:2001:G7X:CAZ	2.38	0.54
1:C:136:ILE:N	1:C:137:PRO:HD2	2.23	0.54
1:D:239:PHE:CD1	1:D:239:PHE:C	2.86	0.54
1:D:315:LYS:O	1:D:319:ILE:HG13	2.07	0.54
1:D:141:HIS:CD2	1:D:207:LYS:HD3	2.43	0.54
5:A:2001:G7X:CAN	5:A:2001:G7X:HBB2	2.37	0.54
1:D:100:THR:HG23	1:D:262:ASN:HB2	1.89	0.54
1:A:98:ASN:O	1:A:328:THR:HG23	2.08	0.54
1:A:169:PHE:CZ	1:A:228:MET:HE1	2.42	0.54
1:D:82:TYR:CD1	1:D:86:VAL:HB	2.43	0.54
1:A:19:ILE:HD12	1:A:359:ILE:HB	1.90	0.54
1:D:159:SER:HA	1:D:172:LEU:HD12	1.90	0.54
1:C:27:PRO:HG3	1:C:74:ALA:HB1	1.89	0.54
1:C:160:LEU:HD12	1:C:238:VAL:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:PHE:CE1	1:B:32:GLU:HB3	2.44	0.53
1:C:104:TYR:CD1	1:C:104:TYR:C	2.86	0.53
1:A:97:TYR:CE1	1:A:365:VAL:HB	2.44	0.53
1:B:178:VAL:HA	1:B:220:LYS:CE	2.37	0.53
1:C:103:ALA:HB2	1:C:115:MET:HE2	1.91	0.53
1:A:346:THR:O	1:A:350:LEU:HG	2.09	0.53
1:B:239:PHE:HE1	1:B:241:VAL:HG13	1.73	0.53
1:C:22:VAL:HG11	1:C:72:PHE:HE2	1.74	0.53
1:C:127:TRP:CE3	5:C:2001:G7X:HBK	2.44	0.53
1:A:21:VAL:O	1:A:69:ASP:HB2	2.09	0.53
1:C:214:LEU:HD12	5:C:2001:G7X:CBF	2.38	0.53
1:A:212:GLN:HG3	1:A:213:ILE:N	2.24	0.53
1:B:82:TYR:CD1	1:B:86:VAL:HB	2.44	0.53
1:B:127:TRP:HB2	5:B:2001:G7X:HAZ3	1.90	0.53
1:B:241:VAL:HG23	1:B:261:LEU:HB3	1.90	0.52
1:C:299:ILE:HA	1:C:359:ILE:HD11	1.90	0.52
1:B:20:GLN:HE21	1:B:70:MET:HE3	1.75	0.52
1:B:158:VAL:HG23	1:B:172:LEU:HD21	1.90	0.52
1:D:127:TRP:CE3	1:D:127:TRP:C	2.88	0.52
1:B:115:MET:HE1	1:B:263:LEU:HB3	1.90	0.52
1:B:243:ILE:O	1:B:258:ILE:HA	2.08	0.52
1:C:181:ARG:HG3	1:C:181:ARG:HH11	1.73	0.52
1:D:40:ILE:HD11	1:D:343:LEU:HA	1.92	0.52
1:A:95:MET:SD	1:A:95:MET:N	2.83	0.52
1:A:29:ASN:OD1	1:A:32:GLU:N	2.32	0.52
1:A:303:VAL:HG21	1:A:355:ARG:O	2.09	0.52
1:B:353:ALA:O	1:B:356:ALA:HB3	2.08	0.52
1:C:97:TYR:CE2	1:C:365:VAL:N	2.77	0.52
5:C:2001:G7X:HBB2	5:C:2001:G7X:HAW	1.91	0.52
1:B:40:ILE:HG13	1:B:41:VAL:HG23	1.92	0.52
1:C:291:SER:HA	1:C:314:SER:HB2	1.92	0.52
1:A:161:LEU:HD13	1:A:168:LEU:HD22	1.92	0.52
1:B:256:VAL:HG13	1:B:256:VAL:O	2.10	0.52
1:C:72:PHE:HB3	1:C:76:THR:OG1	2.10	0.52
1:D:168:LEU:N	1:D:168:LEU:HD12	2.24	0.52
1:B:138:ARG:NH1	1:B:138:ARG:HG2	2.25	0.51
1:B:236:HIS:CD2	1:B:236:HIS:N	2.78	0.51
1:A:172:LEU:HB3	1:A:202:ILE:HD12	1.92	0.51
1:C:237:SER:HB3	1:C:265:ASP:HB3	1.90	0.51
5:C:2001:G7X:NAH	5:C:2001:G7X:HAU1	2.26	0.51
1:D:361:ASN:O	1:D:363:PRO:HD3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:GLU:CD	1:D:34:LYS:HZ3	2.19	0.51
1:B:209:GLU:O	1:B:213:ILE:HG13	2.10	0.51
1:D:171:LEU:HD21	1:D:221:ARG:HB2	1.92	0.51
1:A:35:ALA:O	1:A:36:SER:HB2	2.10	0.51
1:B:166:GLU:OE1	1:B:166:GLU:HA	2.11	0.51
1:D:361:ASN:C	1:D:363:PRO:HD3	2.36	0.51
1:A:126:THR:OG1	1:A:129:GLU:HG2	2.11	0.51
1:C:50:VAL:HG11	1:C:350:LEU:HD13	1.93	0.51
1:D:141:HIS:HD2	1:D:207:LYS:HD3	1.76	0.51
1:B:311:TYR:HA	1:B:317:THR:HB	1.93	0.51
1:C:29:ASN:OD1	1:C:32:GLU:HG3	2.11	0.51
1:D:54:THR:CG2	1:D:64:LYS:HG3	2.40	0.51
1:A:119:ARG:HH22	1:A:211:TYR:HE2	1.59	0.51
1:C:136:ILE:HG12	1:C:263:LEU:HD13	1.92	0.51
1:A:310:PRO:HB2	1:A:313:GLU:HG3	1.93	0.51
1:C:202:ILE:HG21	1:C:213:ILE:HD11	1.92	0.51
1:A:209:GLU:O	1:A:212:GLN:HG2	2.10	0.51
1:C:19:ILE:HD11	1:C:359:ILE:HB	1.92	0.51
1:B:237:SER:OG	1:B:265:ASP:HB3	2.11	0.50
1:D:30:LEU:O	1:D:34:LYS:HG3	2.11	0.50
1:D:168:LEU:CD1	1:D:315:LYS:NZ	2.73	0.50
1:A:237:SER:HB3	1:A:265:ASP:HB3	1.93	0.50
1:B:20:GLN:HA	1:B:69:ASP:OD2	2.11	0.50
1:C:210:VAL:O	1:C:214:LEU:HG	2.11	0.50
1:D:69:ASP:C	1:D:70:MET:HG3	2.35	0.50
1:A:315:LYS:O	1:A:319:ILE:HG13	2.11	0.50
1:C:118:GLU:O	1:C:132:LEU:HB2	2.10	0.50
1:C:164:TYR:CD2	1:C:228:MET:SD	3.05	0.50
1:A:104:TYR:CD1	1:A:104:TYR:C	2.90	0.50
1:A:147:LEU:CD2	1:A:150:ASN:HD22	2.25	0.50
1:B:211:TYR:CE1	5:B:2001:G7X:HAA2	2.47	0.50
1:A:47:ARG:HD3	1:A:49:GLU:OE2	2.12	0.50
1:A:294:THR:HB	1:A:314:SER:OG	2.12	0.50
1:A:168:LEU:CD1	1:A:196:ILE:HD12	2.39	0.50
1:A:185:PHE:CE1	1:A:197:LYS:HE3	2.47	0.50
1:B:127:TRP:CG	5:B:2001:G7X:HBK	2.47	0.50
1:C:133:ALA:O	1:C:138:ARG:NE	2.39	0.50
1:C:311:TYR:CD1	1:C:311:TYR:N	2.78	0.50
1:D:343:LEU:O	1:D:347:LEU:HG	2.12	0.50
1:D:166:GLU:OE1	1:D:166:GLU:HA	2.11	0.49
1:B:38:HIS:O	1:B:340:SER:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:211:TYR:O	1:B:215:GLU:HB3	2.11	0.49
1:C:75:SER:O	1:C:77:LYS:HE2	2.13	0.49
1:C:98:ASN:O	1:C:328:THR:HB	2.12	0.49
1:D:291:SER:HB3	1:D:316:LEU:HB2	1.93	0.49
1:A:143:ILE:CD1	1:A:243:ILE:HD11	2.30	0.49
1:A:158:VAL:CG1	1:A:241:VAL:HG22	2.40	0.49
1:B:294:THR:OG1	1:B:314:SER:HB3	2.13	0.49
1:C:311:TYR:HD1	1:C:311:TYR:H	1.56	0.49
1:A:37:ALA:CB	1:A:339:ALA:HB1	2.43	0.49
1:A:119:ARG:NH2	1:A:211:TYR:HE2	2.11	0.49
1:A:140:LEU:HD13	1:A:210:VAL:HG13	1.93	0.49
1:B:343:LEU:O	1:B:343:LEU:HD12	2.12	0.49
1:C:161:LEU:HG	1:C:238:VAL:HB	1.94	0.49
1:B:113:PHE:CD2	3:B:1003:ADP:N7	2.81	0.48
1:B:236:HIS:NE2	1:B:267:ALA:HB2	2.27	0.48
1:C:51:SER:HB3	1:C:63:ARG:NH1	2.28	0.48
1:C:97:TYR:CE1	1:C:365:VAL:HB	2.48	0.48
1:A:104:TYR:HE1	1:A:349:THR:HA	1.78	0.48
1:B:127:TRP:CB	5:B:2001:G7X:HAZ3	2.42	0.48
1:B:207:LYS:O	1:B:210:VAL:HB	2.13	0.48
1:B:323:SER:HA	1:B:328:THR:HB	1.93	0.48
1:C:310:PRO:HB2	1:C:313:GLU:CD	2.37	0.48
1:B:243:ILE:HG22	1:B:245:MET:HG3	1.93	0.48
1:D:93:VAL:HG21	1:D:261:LEU:HB2	1.94	0.48
1:A:22:VAL:HG23	1:A:22:VAL:O	2.13	0.48
1:A:46:VAL:HG23	1:A:47:ARG:H	1.76	0.48
1:A:273:GLY:O	1:A:274:ARG:C	2.56	0.48
1:C:48:LYS:HB3	1:C:68:PHE:O	2.13	0.48
1:D:66:TYR:OH	1:D:351:GLU:HG2	2.12	0.48
1:D:111:LYS:HE2	1:D:111:LYS:HB2	1.46	0.48
1:A:214:LEU:HD23	5:A:2001:G7X:CAR	2.43	0.48
1:C:127:TRP:CE3	5:C:2001:G7X:CBK	2.95	0.48
1:B:163:ILE:HD12	1:B:316:LEU:HB2	1.95	0.48
1:A:46:VAL:CG2	1:A:47:ARG:N	2.76	0.48
1:B:153:GLU:OE1	1:B:153:GLU:HA	2.14	0.48
1:B:161:LEU:C	1:B:162:GLU:HG2	2.39	0.48
1:B:309:VAL:HB	1:B:311:TYR:CE2	2.48	0.48
1:D:115:MET:HG3	1:D:265:ASP:HB2	1.94	0.48
1:D:291:SER:HB3	1:D:316:LEU:HB3	1.95	0.48
1:C:181:ARG:HH11	1:C:181:ARG:CG	2.26	0.48
1:C:202:ILE:HG21	1:C:213:ILE:CD1	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:PRO:HD2	1:A:195:ILE:HD11	1.95	0.48
1:D:288:ILE:HG22	1:D:289:ASN:N	2.28	0.48
1:A:314:SER:O	1:A:315:LYS:C	2.57	0.47
1:C:126:THR:O	1:C:129:GLU:HG2	2.13	0.47
1:B:54:THR:HG21	1:B:64:LYS:HD2	1.97	0.47
1:C:115:MET:O	1:C:136:ILE:HG13	2.14	0.47
1:B:298:VAL:HG21	1:B:317:THR:CG2	2.44	0.47
1:B:169:PHE:HE1	1:B:179:SER:O	1.96	0.47
1:D:144:PHE:HE2	1:D:205:HIS:O	1.97	0.47
5:C:2001:G7X:NAH	5:C:2001:G7X:CAU	2.78	0.47
1:A:144:PHE:HZ	1:A:156:VAL:HG21	1.78	0.47
1:C:76:THR:CG2	1:C:81:VAL:HG23	2.45	0.47
1:C:312:ARG:CG	1:C:312:ARG:NH1	2.58	0.47
1:A:33:ARG:HG3	1:D:27:PRO:CB	2.45	0.47
5:B:2001:G7X:CAW	5:B:2001:G7X:HAJ	2.44	0.47
1:D:24:ARG:O	1:D:336:ILE:HG12	2.15	0.47
1:D:82:TYR:CE2	1:D:142:GLN:HG3	2.49	0.47
1:D:346:THR:O	1:D:350:LEU:HG	2.15	0.47
5:D:2001:G7X:HBD2	5:D:2001:G7X:CAL	2.45	0.47
1:A:173:ASN:CB	1:A:200:GLU:HG3	2.43	0.47
1:A:17:LYS:CG	1:A:17:LYS:O	2.62	0.47
1:B:173:ASN:HB2	1:B:200:GLU:HB2	1.96	0.47
1:A:51:SER:HB3	1:A:63:ARG:HE	1.79	0.47
1:A:304:GLU:HB3	1:A:306:THR:HG23	1.97	0.47
1:D:144:PHE:CE2	1:D:206:ASN:HA	2.50	0.47
1:A:136:ILE:N	1:A:137:PRO:HD2	2.30	0.46
1:B:299:ILE:O	1:B:302:LEU:HB2	2.15	0.46
5:B:2001:G7X:CAL	5:B:2001:G7X:HBD1	2.45	0.46
1:D:271:ASN:O	1:D:288:ILE:HG21	2.15	0.46
1:A:26:ARG:O	1:A:26:ARG:HG3	2.12	0.46
1:B:136:ILE:HD13	5:B:2001:G7X:HAQ	1.97	0.46
1:A:20:GLN:O	1:A:331:SER:HA	2.15	0.46
1:B:128:GLU:HG2	1:B:207:LYS:NZ	2.30	0.46
1:B:312:ARG:HA	1:B:318:ARG:HG2	1.97	0.46
1:C:146:LYS:O	1:C:150:ASN:HB2	2.16	0.46
1:D:33:ARG:HA	1:D:33:ARG:HD3	1.61	0.46
1:C:157:LYS:HE3	1:C:242:THR:HB	1.97	0.46
1:C:302:LEU:HB2	1:C:359:ILE:HG12	1.97	0.46
1:A:102:PHE:HE1	1:A:320:LEU:HD13	1.81	0.46
1:A:164:TYR:CE2	1:A:228:MET:HG2	2.50	0.46
1:A:320:LEU:O	1:A:323:SER:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:TYR:CD2	1:C:321:GLN:HG3	2.51	0.46
1:A:53:ARG:HD3	1:A:63:ARG:HH12	1.81	0.46
1:A:270:GLU:HG2	1:A:271:ASN:N	2.30	0.46
1:A:327:ARG:HA	1:A:362:LYS:O	2.16	0.46
1:B:102:PHE:HZ	1:B:320:LEU:HD13	1.80	0.46
1:A:214:LEU:HD23	5:A:2001:G7X:CAS	2.46	0.46
1:B:311:TYR:CD1	1:B:321:GLN:HG3	2.50	0.46
1:D:90:LEU:HD11	1:D:143:ILE:HG12	1.98	0.46
1:A:114:THR:HG22	1:A:135:ILE:HD12	1.97	0.46
1:A:156:VAL:CG2	1:A:204:VAL:HB	2.45	0.46
1:B:265:ASP:C	1:B:265:ASP:OD1	2.59	0.46
1:A:188:PRO:HD2	1:A:195:ILE:HD12	1.97	0.45
1:B:26:ARG:NH2	1:B:108:GLY:O	2.44	0.45
1:C:157:LYS:HE3	1:C:157:LYS:HB2	1.71	0.45
1:A:347:LEU:HA	1:A:347:LEU:HD23	1.63	0.45
1:C:19:ILE:HD11	1:C:359:ILE:CG2	2.47	0.45
1:A:161:LEU:HD12	1:A:161:LEU:O	2.16	0.45
1:A:270:GLU:HA	1:A:345:GLU:OE1	2.16	0.45
1:B:127:TRP:CD2	5:B:2001:G7X:HBK	2.52	0.45
1:B:144:PHE:CZ	1:B:204:VAL:HG12	2.43	0.45
1:B:102:PHE:CZ	1:B:320:LEU:HD13	2.52	0.45
1:B:162:GLU:HA	1:B:236:HIS:O	2.17	0.45
1:C:243:ILE:O	1:C:258:ILE:HA	2.17	0.45
1:B:345:GLU:HA	1:B:345:GLU:OE1	2.17	0.45
1:A:187:ASP:HB2	1:A:193:GLY:C	2.42	0.45
1:A:303:VAL:HG22	1:A:358:ASN:HB2	1.98	0.45
1:B:92:GLU:O	1:B:97:TYR:HB2	2.17	0.45
1:B:295:LEU:HD11	1:B:299:ILE:HD11	1.99	0.45
1:C:170:ASP:HB2	1:C:182:LEU:CD1	2.37	0.45
1:D:34:LYS:C	1:D:36:SER:H	2.25	0.45
1:D:139:THR:O	1:D:143:ILE:HG13	2.17	0.45
1:D:168:LEU:CD1	1:D:168:LEU:N	2.80	0.45
1:B:138:ARG:HG2	1:B:138:ARG:HH11	1.81	0.44
1:D:184:MET:HE3	1:D:194:VAL:CG2	2.47	0.44
1:A:115:MET:O	1:A:136:ILE:HG13	2.17	0.44
1:C:244:HIS:CE1	1:C:258:ILE:CD1	3.00	0.44
1:A:304:GLU:O	1:A:305:ARG:CB	2.63	0.44
1:B:173:ASN:HB2	1:B:200:GLU:CB	2.48	0.44
1:D:52:VAL:HG21	1:D:350:LEU:HD12	1.98	0.44
1:A:89:ILE:HD11	1:A:331:SER:OG	2.17	0.44
1:A:100:THR:HB	1:A:330:THR:HG23	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:LYS:HG3	1:A:208:ASP:N	2.32	0.44
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.72	0.44
5:B:2001:G7X:HBC1	5:B:2001:G7X:NAH	2.33	0.44
1:D:241:VAL:O	1:D:241:VAL:HG13	2.16	0.44
1:D:290:GLN:HG3	1:D:314:SER:HB3	1.99	0.44
1:A:48:LYS:C	1:A:71:VAL:HG21	2.43	0.44
1:A:79:ILE:HG23	1:A:80:ASP:N	2.33	0.44
1:C:173:ASN:O	1:C:220:LYS:NZ	2.43	0.44
1:A:44:ASP:OD1	1:A:46:VAL:HG22	2.17	0.44
1:A:272:ILE:CD1	1:A:292:LEU:HG	2.48	0.44
1:C:120:SER:HB2	1:C:125:TYR:HD2	1.82	0.44
1:D:207:LYS:O	1:D:208:ASP:C	2.59	0.44
1:D:336:ILE:HG21	1:D:350:LEU:CD2	2.37	0.44
1:B:141:HIS:HD2	1:B:207:LYS:HD2	1.83	0.44
1:B:173:ASN:HB2	1:B:200:GLU:HG3	1.99	0.44
1:C:110:GLY:HA2	3:C:1003:ADP:O3A	2.17	0.44
1:C:337:SER:OG	1:C:338:PRO:HD2	2.18	0.44
1:D:128:GLU:HG2	1:D:141:HIS:CD2	2.53	0.44
1:C:292:LEU:O	1:C:295:LEU:HB3	2.17	0.44
1:D:29:ASN:OD1	1:D:29:ASN:C	2.61	0.43
1:A:32:GLU:OE2	1:A:337:SER:OG	2.24	0.43
1:A:209:GLU:HG2	1:A:213:ILE:HD11	2.00	0.43
1:C:157:LYS:HE2	1:C:244:HIS:CD2	2.52	0.43
1:D:100:THR:OG1	1:D:328:THR:HG21	2.18	0.43
1:A:141:HIS:CD2	1:A:207:LYS:HD3	2.49	0.43
1:B:220:LYS:O	1:B:223:THR:HB	2.18	0.43
1:B:239:PHE:CD1	1:B:263:LEU:HD12	2.53	0.43
1:C:168:LEU:HD11	1:C:315:LYS:HB3	2.00	0.43
1:B:140:LEU:O	1:B:143:ILE:HB	2.19	0.43
1:B:297:ARG:HB3	1:B:310:PRO:HG3	2.00	0.43
1:C:40:ILE:CD1	1:C:343:LEU:HB2	2.49	0.43
1:C:168:LEU:HD21	1:C:319:ILE:HD11	2.00	0.43
1:D:160:LEU:HD12	1:D:238:VAL:O	2.18	0.43
1:A:265:ASP:OD1	1:A:265:ASP:C	2.62	0.43
1:C:237:SER:O	1:C:264:VAL:HA	2.18	0.43
1:D:43:CYS:HB3	1:D:71:VAL:HG12	2.00	0.43
1:D:257:LYS:HE2	1:D:257:LYS:HB2	1.65	0.43
1:A:188:PRO:O	1:A:189:ARG:CB	2.66	0.43
1:B:158:VAL:HA	1:B:240:SER:O	2.19	0.43
1:C:162:GLU:HG3	1:C:171:LEU:CD2	2.49	0.43
1:A:44:ASP:OD2	1:A:47:ARG:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ASP:HB2	1:A:182:LEU:HD11	2.00	0.43
1:A:187:ASP:OD1	1:A:188:PRO:N	2.52	0.43
1:B:352:TYR:O	1:B:356:ALA:HB2	2.19	0.43
1:C:243:ILE:HG22	1:C:245:MET:CG	2.39	0.43
5:C:2001:G7X:OAV	5:C:2001:G7X:CBD	2.66	0.43
1:D:206:ASN:O	1:D:209:GLU:HB3	2.19	0.43
1:B:59:ASP:O	1:B:60:LYS:C	2.62	0.43
1:B:102:PHE:HE1	1:B:264:VAL:HG11	1.83	0.43
1:B:347:LEU:O	1:B:348:SER:C	2.62	0.43
1:C:56:GLY:O	1:C:57:LEU:HB2	2.19	0.43
1:B:90:LEU:O	1:B:94:ILE:HG12	2.19	0.43
1:B:210:VAL:HG13	1:B:214:LEU:HD12	2.01	0.43
1:D:160:LEU:HB3	1:D:172:LEU:HG	2.01	0.43
1:A:303:VAL:HG23	1:A:359:ILE:HG13	2.00	0.42
5:D:2001:G7X:OAV	5:D:2001:G7X:CBD	2.67	0.42
1:A:138:ARG:HG2	1:A:138:ARG:HH11	1.82	0.42
1:A:224:ALA:HA	1:A:227:LEU:HB2	2.01	0.42
1:C:40:ILE:HG13	1:C:41:VAL:HG23	2.01	0.42
1:C:330:THR:HB	1:C:361:ASN:ND2	2.31	0.42
1:B:116:GLU:O	1:B:134:GLY:N	2.51	0.42
1:B:173:ASN:OD1	1:B:173:ASN:C	2.63	0.42
1:B:298:VAL:HG21	1:B:317:THR:HG21	2.01	0.42
1:C:147:LEU:HD23	1:C:147:LEU:HA	1.69	0.42
1:C:218:ALA:O	1:C:222:THR:OG1	2.33	0.42
1:C:310:PRO:HB2	1:C:313:GLU:HG3	2.01	0.42
1:A:23:VAL:HG11	1:A:50:VAL:HG21	2.01	0.42
1:A:136:ILE:HG12	1:A:263:LEU:CD1	2.43	0.42
1:B:341:LEU:C	1:B:341:LEU:HD12	2.43	0.42
1:D:312:ARG:HA	1:D:318:ARG:HG2	2.01	0.42
1:D:315:LYS:HZ2	1:D:315:LYS:HG3	1.68	0.42
1:B:166:GLU:OE1	1:B:166:GLU:CA	2.67	0.42
1:B:348:SER:O	1:B:349:THR:C	2.63	0.42
1:C:188:PRO:HD3	1:C:195:ILE:HG13	2.01	0.42
1:C:303:VAL:HG22	1:C:359:ILE:HG13	2.01	0.42
1:D:78:GLN:NE2	1:D:113:PHE:CE2	2.87	0.42
1:A:46:VAL:CG2	1:A:47:ARG:H	2.32	0.42
1:A:327:ARG:C	1:A:363:PRO:HA	2.44	0.42
5:D:2001:G7X:NAH	5:D:2001:G7X:HAU1	2.34	0.42
1:A:173:ASN:HB2	1:A:200:GLU:CG	2.46	0.42
1:A:158:VAL:O	1:A:158:VAL:HG23	2.19	0.42
1:B:148:THR:HA	1:B:152:THR:CG2	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:HA	1:B:169:PHE:O	2.20	0.42
1:C:26:ARG:HH12	1:C:32:GLU:CD	2.28	0.42
1:D:158:VAL:HG23	1:D:158:VAL:O	2.19	0.42
1:A:164:TYR:O	1:A:165:ASN:C	2.63	0.42
1:B:173:ASN:HA	1:B:174:PRO:HD3	1.83	0.42
1:C:174:PRO:O	1:C:177:ASP:OD1	2.38	0.42
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.87	0.41
1:A:178:VAL:HG21	1:A:223:THR:HG21	2.01	0.41
1:B:51:SER:HA	1:B:64:LYS:O	2.20	0.41
1:C:66:TYR:OH	1:C:351:GLU:OE2	2.34	0.41
1:C:160:LEU:HB3	1:C:172:LEU:HG	2.01	0.41
1:B:302:LEU:HD21	1:B:311:TYR:OH	2.21	0.41
1:C:119:ARG:HA	1:C:130:ASP:OD2	2.20	0.41
1:D:112:THR:OG1	1:D:265:ASP:OD2	2.37	0.41
1:D:261:LEU:HD12	1:D:262:ASN:N	2.35	0.41
1:C:40:ILE:HD13	1:C:343:LEU:HB2	2.02	0.41
1:A:294:THR:O	1:A:298:VAL:HG23	2.20	0.41
1:A:316:LEU:HG	1:A:320:LEU:HD12	2.02	0.41
1:B:102:PHE:CE1	1:B:264:VAL:HG11	2.55	0.41
1:C:69:ASP:O	1:C:70:MET:HG2	2.20	0.41
1:D:126:THR:HB	1:D:128:GLU:OE2	2.20	0.41
1:A:118:GLU:OE1	1:D:34:LYS:NZ	2.54	0.41
1:A:163:ILE:HG12	1:A:168:LEU:HD23	2.03	0.41
1:C:244:HIS:CE1	1:C:258:ILE:HD13	2.56	0.41
1:D:119:ARG:O	1:D:120:SER:C	2.62	0.41
1:D:170:ASP:OD1	1:D:170:ASP:C	2.63	0.41
1:A:94:ILE:O	1:A:245:MET:HE1	2.20	0.41
1:B:171:LEU:HD13	1:B:220:LYS:HB3	2.02	0.41
1:D:99:CYS:HA	1:D:328:THR:HG23	2.02	0.41
1:A:160:LEU:HD12	1:A:238:VAL:C	2.46	0.41
1:B:116:GLU:HG2	1:B:136:ILE:HD12	2.02	0.41
1:D:187:ASP:OD1	1:D:189:ARG:HB2	2.21	0.41
1:A:90:LEU:HD11	1:A:143:ILE:HG12	2.03	0.41
1:B:47:ARG:O	1:B:49:GLU:HG3	2.20	0.41
1:B:105:GLY:C	1:B:269:SER:HB3	2.45	0.41
1:D:171:LEU:HD22	1:D:221:ARG:HB2	2.01	0.41
1:A:163:ILE:HG12	1:A:168:LEU:CD2	2.50	0.40
1:D:293:LEU:HD11	1:D:297:ARG:HH21	1.83	0.40
1:B:90:LEU:HA	1:B:90:LEU:HD12	1.82	0.40
1:A:171:LEU:HD21	1:A:221:ARG:HG3	2.03	0.40
1:B:98:ASN:O	1:B:99:CYS:SG	2.77	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:TRP:CZ2	1:C:207:LYS:HB2	2.57	0.40
1:D:168:LEU:HD13	1:D:315:LYS:NZ	2.28	0.40
1:A:92:GLU:CG	1:A:329:ARG:NH1	2.82	0.40
1:A:303:VAL:CG2	1:A:355:ARG:O	2.70	0.40
1:B:22:VAL:HG11	1:B:70:MET:HB2	2.01	0.40
1:B:147:LEU:HD23	1:B:147:LEU:HA	1.97	0.40
1:B:320:LEU:C	1:B:322:ASP:N	2.78	0.40
1:C:19:ILE:HD12	1:C:359:ILE:HB	2.03	0.40
1:C:291:SER:HA	1:C:314:SER:CB	2.51	0.40
1:D:302:LEU:HD21	1:D:311:TYR:OH	2.22	0.40
1:A:34:LYS:HE2	1:A:34:LYS:HB2	1.88	0.40
1:B:116:GLU:C	1:B:134:GLY:HA3	2.47	0.40
1:B:346:THR:O	1:B:350:LEU:HG	2.22	0.40
1:C:205:HIS:O	1:D:46:VAL:HG22	2.21	0.40
1:D:101:ILE:HA	1:D:331:SER:O	2.22	0.40
1:D:126:THR:OG1	1:D:129:GLU:HG2	2.21	0.40
1:D:270:GLU:H	1:D:270:GLU:CD	2.27	0.40
5:D:2001:G7X:HBf	5:D:2001:G7X:CAY	2.51	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	317/370 (86%)	309 (98%)	8 (2%)	0	100	100
1	B	302/370 (82%)	295 (98%)	7 (2%)	0	100	100
1	C	297/370 (80%)	294 (99%)	3 (1%)	0	100	100
1	D	297/370 (80%)	287 (97%)	10 (3%)	0	100	100
All	All	1213/1480 (82%)	1185 (98%)	28 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	268/323 (83%)	258 (96%)	10 (4%)	30	57
1	B	257/323 (80%)	232 (90%)	25 (10%)	8	17
1	C	252/323 (78%)	241 (96%)	11 (4%)	25	50
1	D	255/323 (79%)	244 (96%)	11 (4%)	26	51
All	All	1032/1292 (80%)	975 (94%)	57 (6%)	19	41

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	VAL
1	A	28	PHE
1	A	69	ASP
1	A	93	VAL
1	A	95	MET
1	A	182	LEU
1	A	221	ARG
1	A	247	GLU
1	A	257	LYS
1	A	355	ARG
1	B	19	ILE
1	B	24	ARG
1	B	26	ARG
1	B	48	LYS
1	B	63	ARG
1	B	79	ILE
1	B	86	VAL
1	B	89	ILE
1	B	101	ILE
1	B	146	LYS
1	B	166	GLU
1	B	171	LEU
1	B	172	LEU
1	B	181	ARG

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Mol	Chain	Res	Type
1	B	182	LEU
1	B	207	LYS
1	B	213	ILE
1	B	234	ARG
1	B	236	HIS
1	B	241	VAL
1	B	257	LYS
1	B	292	LEU
1	B	317	THR
1	B	327	ARG
1	B	343	LEU
1	C	19	ILE
1	C	20	GLN
1	C	26	ARG
1	C	145	GLU
1	C	172	LEU
1	C	181	ARG
1	C	206	ASN
1	C	228	MET
1	C	262	ASN
1	C	312	ARG
1	C	354	HIS
1	D	19	ILE
1	D	28	PHE
1	D	80	ASP
1	D	115	MET
1	D	140	LEU
1	D	195	ILE
1	D	207	LYS
1	D	208	ASP
1	D	257	LYS
1	D	260	LYS
1	D	303	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	141	HIS
1	A	142	GLN
1	A	150	ASN
1	A	212	GLN

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Mol	Chain	Res	Type
1	A	229	ASN
1	A	262	ASN
1	A	308	HIS
1	A	321	GLN
1	A	354	HIS
1	B	141	HIS
1	B	229	ASN
1	B	236	HIS
1	B	262	ASN
1	B	321	GLN
1	C	18	ASN
1	C	142	GLN
1	C	173	ASN
1	C	205	HIS
1	C	244	HIS
1	C	262	ASN
1	C	321	GLN
1	C	354	HIS
1	C	361	ASN
1	D	141	HIS
1	D	206	ASN
1	D	212	GLN
1	D	229	ASN
1	D	321	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 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 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
5	G7X	C	2001	-	39,40,40	1.39	2 (5%)	50,56,56	1.47	8 (16%)
5	G7X	A	2001	-	36,37,40	1.65	4 (11%)	50,53,56	1.30	5 (10%)
3	ADP	C	1003	2	28,29,29	1.56	4 (14%)	43,45,45	2.07	12 (27%)
3	ADP	B	1003	2	28,29,29	1.57	4 (14%)	43,45,45	1.90	12 (27%)
3	ADP	A	1003	2	28,29,29	1.46	4 (14%)	43,45,45	2.01	10 (23%)
5	G7X	D	2001	-	39,40,40	1.32	3 (7%)	50,56,56	1.43	7 (14%)
3	ADP	D	1003	2	28,29,29	1.57	5 (17%)	43,45,45	1.96	11 (25%)
5	G7X	B	2001	-	39,40,40	1.41	3 (7%)	50,56,56	1.56	6 (12%)

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
5	G7X	C	2001	-	-	0/24/28/28	0/4/4/4
5	G7X	A	2001	-	-	0/20/24/28	0/4/4/4
3	ADP	C	1003	2	-	0/16/32/32	0/3/3/3
3	ADP	B	1003	2	-	1/16/32/32	0/3/3/3
3	ADP	A	1003	2	-	3/16/32/32	0/3/3/3
5	G7X	D	2001	-	-	0/24/28/28	0/4/4/4
3	ADP	D	1003	2	-	5/16/32/32	0/3/3/3
5	G7X	B	2001	-	-	2/24/28/28	0/4/4/4

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2001	G7X	CAI-NAH	6.89	1.36	1.29
5	C	2001	G7X	CAI-NAH	6.45	1.35	1.29
5	B	2001	G7X	CAI-NAH	5.87	1.35	1.29
3	D	1003	ADP	C5-C4	4.96	1.47	1.39
3	B	1003	ADP	C5-C4	4.77	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	2001	G7X	CAI-NAH	4.75	1.34	1.29
3	A	1003	ADP	C5-C4	4.32	1.46	1.39
3	C	1003	ADP	C5-C4	4.28	1.46	1.39
5	B	2001	G7X	CAR-CAS	-4.24	1.39	1.47
5	A	2001	G7X	CAR-CAS	-4.12	1.39	1.47
5	C	2001	G7X	CAR-CAS	-3.97	1.39	1.47
3	B	1003	ADP	PA-O3A	3.92	1.63	1.59
5	D	2001	G7X	CAR-CAS	-3.86	1.39	1.47
3	C	1003	ADP	PA-O3A	3.83	1.63	1.59
3	D	1003	ADP	PA-O3A	3.62	1.63	1.59
3	A	1003	ADP	C8-N7	3.21	1.37	1.31
3	C	1003	ADP	C5-C6	3.17	1.49	1.41
5	A	2001	G7X	CAI-NAT	3.16	1.43	1.38
3	A	1003	ADP	PA-O3A	3.14	1.62	1.59
3	C	1003	ADP	C8-N7	3.09	1.37	1.31
3	A	1003	ADP	C5-C6	2.95	1.49	1.41
3	B	1003	ADP	C5-C6	2.85	1.48	1.41
5	D	2001	G7X	CAG-NAH	-2.76	1.34	1.39
3	B	1003	ADP	C8-N7	2.61	1.36	1.31
3	D	1003	ADP	C5-C6	2.57	1.48	1.41
5	A	2001	G7X	CAM-CAL	2.39	1.54	1.50
3	D	1003	ADP	C8-N7	2.32	1.36	1.31
3	D	1003	ADP	C5-N7	-2.21	1.35	1.39
5	B	2001	G7X	CAI-NAT	2.15	1.41	1.38

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003	ADP	C5-C4-N3	-6.64	117.58	126.72
5	B	2001	G7X	NAT-CAI-NAH	-6.21	117.78	123.53
3	D	1003	ADP	C5-C4-N3	-6.21	118.17	126.72
3	B	1003	ADP	C5-C4-N3	-5.68	118.89	126.72
3	C	1003	ADP	C4-C5-N7	-5.35	104.47	110.58
3	C	1003	ADP	C5-C4-N3	-5.23	119.51	126.72
5	C	2001	G7X	NAT-CAI-NAH	-5.09	118.82	123.53
3	D	1003	ADP	N3-C4-N9	4.98	135.63	127.17
5	D	2001	G7X	NAT-CAI-NAH	-4.93	118.97	123.53
5	A	2001	G7X	NAT-CAI-NAH	-4.74	119.14	123.53
3	A	1003	ADP	N3-C4-N9	4.54	134.88	127.17
3	A	1003	ADP	C2-N3-C4	4.50	122.82	111.83
3	B	1003	ADP	N3-C4-N9	4.28	134.45	127.17
3	A	1003	ADP	C4-C5-N7	-4.10	105.90	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	2001	G7X	CAG-NAH-CAI	4.04	123.04	117.46
3	C	1003	ADP	C5-N7-C8	3.98	109.70	103.45
3	D	1003	ADP	C2-N3-C4	3.82	121.16	111.83
3	C	1003	ADP	N9-C8-N7	-3.74	108.63	113.94
3	B	1003	ADP	C2-N3-C4	3.73	120.94	111.83
3	C	1003	ADP	C6-C5-N7	3.67	139.16	132.09
5	D	2001	G7X	CAG-NAH-CAI	3.66	122.51	117.46
3	C	1003	ADP	C2-N3-C4	3.64	120.73	111.83
3	B	1003	ADP	C4-C5-N7	-3.62	106.44	110.58
3	D	1003	ADP	O4'-C1'-N9	3.58	114.97	108.09
3	D	1003	ADP	C4-C5-N7	-3.47	106.62	110.58
3	A	1003	ADP	N3-C2-N1	-3.44	123.38	128.58
5	D	2001	G7X	CBC-CAU-NAK	-3.36	108.16	113.25
3	B	1003	ADP	N3-C2-N1	-3.33	123.54	128.58
5	C	2001	G7X	CAG-NAH-CAI	3.27	121.97	117.46
3	C	1003	ADP	C4-N9-C8	3.14	109.04	105.74
5	A	2001	G7X	CAS-NAT-CAI	-3.13	119.81	121.38
3	D	1003	ADP	N3-C2-N1	-3.11	123.87	128.58
5	B	2001	G7X	CAR-CAS-NAT	3.09	119.78	115.26
3	A	1003	ADP	C5-N7-C8	3.09	108.30	103.45
3	C	1003	ADP	N3-C2-N1	-3.06	123.95	128.58
3	C	1003	ADP	N3-C4-N9	3.03	132.32	127.17
5	A	2001	G7X	CAR-CAS-NAT	2.80	119.37	115.26
5	A	2001	G7X	CAB-CAJ-CAI	-2.76	107.53	111.72
3	D	1003	ADP	C5-N7-C8	2.74	107.75	103.45
5	A	2001	G7X	CAG-NAH-CAI	2.72	121.22	117.46
3	A	1003	ADP	C6-C5-N7	2.68	137.26	132.09
5	D	2001	G7X	CAR-CAS-NAT	2.66	119.17	115.26
3	B	1003	ADP	O4'-C1'-N9	2.62	113.11	108.09
5	C	2001	G7X	CBC-CAU-NAK	-2.60	109.32	113.25
3	D	1003	ADP	C4-N9-C8	2.58	108.45	105.74
5	B	2001	G7X	CAB-CAJ-CAI	-2.53	107.88	111.72
5	B	2001	G7X	CAS-NAT-CAI	-2.51	120.13	121.38
3	B	1003	ADP	C5-N7-C8	2.48	107.36	103.45
3	A	1003	ADP	N9-C8-N7	-2.48	110.42	113.94
5	D	2001	G7X	CBG-CBB-NAT	-2.45	108.98	113.09
3	D	1003	ADP	C2'-C1'-N9	-2.45	107.23	113.30
5	C	2001	G7X	CAR-CAS-NAT	2.37	118.74	115.26
3	B	1003	ADP	C6-C5-N7	2.35	136.63	132.09
5	C	2001	G7X	CAW-CAM-CAN	2.34	121.54	118.57
3	B	1003	ADP	C4-N9-C8	2.31	108.16	105.74
3	B	1003	ADP	C5'-C4'-C3'	-2.28	107.01	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1003	ADP	C2'-C1'-N9	-2.21	107.81	113.30
5	D	2001	G7X	CAS-NAT-CAI	-2.21	120.27	121.38
5	B	2001	G7X	OAV-CAL-NAK	2.17	125.11	121.62
3	C	1003	ADP	C5-C4-N9	2.16	108.16	105.81
5	C	2001	G7X	CBF-CBG-CBH	2.15	121.42	118.23
3	C	1003	ADP	C4-N9-C1'	-2.14	121.62	126.63
5	C	2001	G7X	CAO-CAN-CAM	-2.13	118.52	120.80
3	D	1003	ADP	N9-C8-N7	-2.08	110.99	113.94
5	C	2001	G7X	CAR-CAG-NAH	-2.06	120.34	122.41
5	D	2001	G7X	CAR-CAG-NAH	-2.06	120.34	122.41
3	A	1003	ADP	C5'-C4'-C3'	-2.04	107.86	115.21
3	B	1003	ADP	C2-N1-C6	2.04	122.08	118.73
3	C	1003	ADP	O2'-C2'-C1'	2.03	117.10	110.10
3	A	1003	ADP	C4-N9-C8	2.01	107.85	105.74
3	D	1003	ADP	C6-C5-N7	2.00	135.95	132.09

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003	ADP	PA-O3A-PB-O3B
3	B	1003	ADP	C5'-O5'-PA-O2A
3	D	1003	ADP	C5'-O5'-PA-O1A
3	D	1003	ADP	C5'-O5'-PA-O2A
3	D	1003	ADP	C5'-O5'-PA-O3A
5	B	2001	G7X	NAK-CAU-CBC-CBD
3	A	1003	ADP	PA-O3A-PB-O2B
5	B	2001	G7X	CAU-CBC-CBD-NBE
3	A	1003	ADP	PA-O3A-PB-O1B
3	D	1003	ADP	PB-O3A-PA-O1A
3	D	1003	ADP	PB-O3A-PA-O2A

There are no ring outliers.

7 monomers are involved in 47 short contacts:

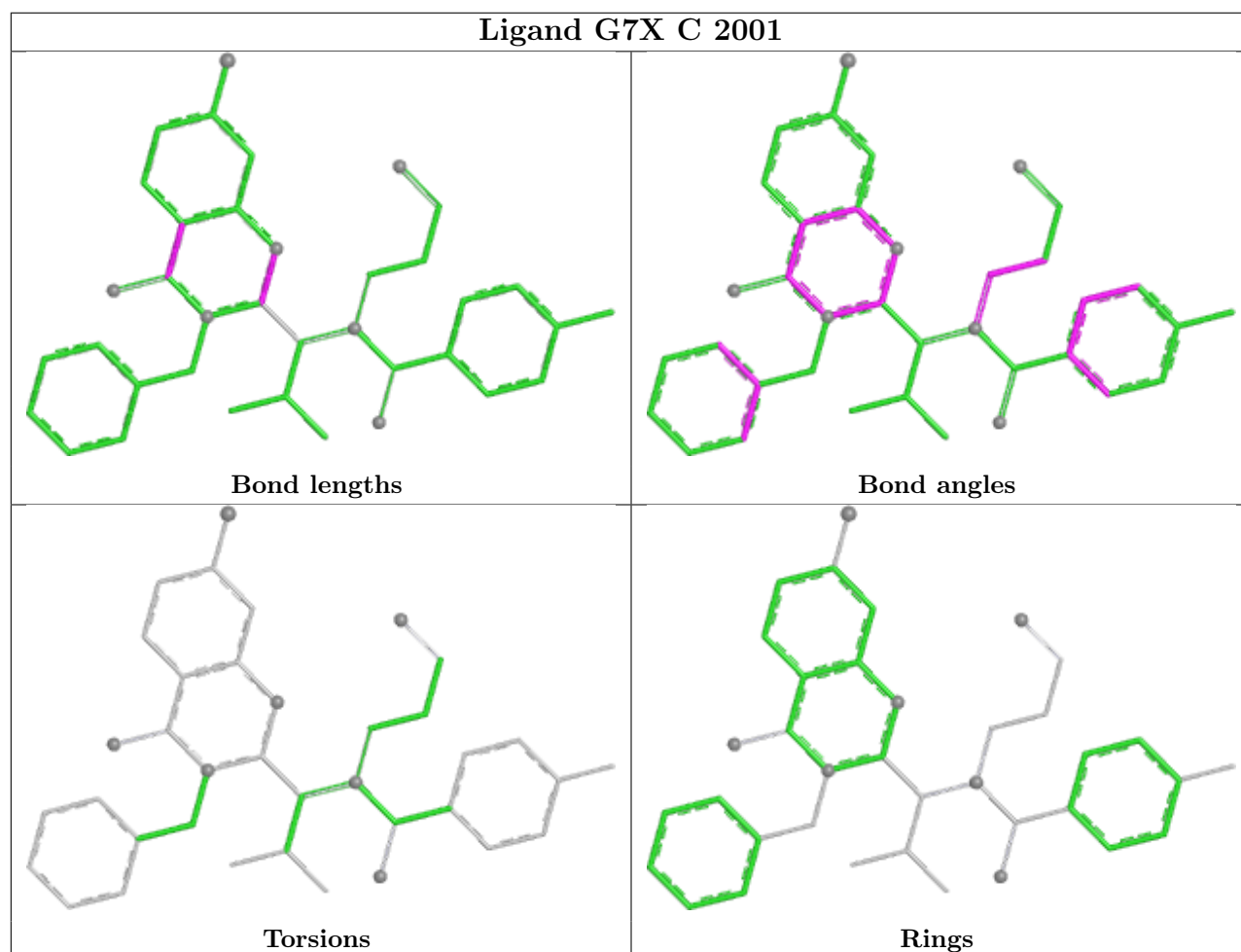
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	2001	G7X	11	0
5	A	2001	G7X	6	0
3	C	1003	ADP	2	0
3	B	1003	ADP	1	0
5	D	2001	G7X	11	0

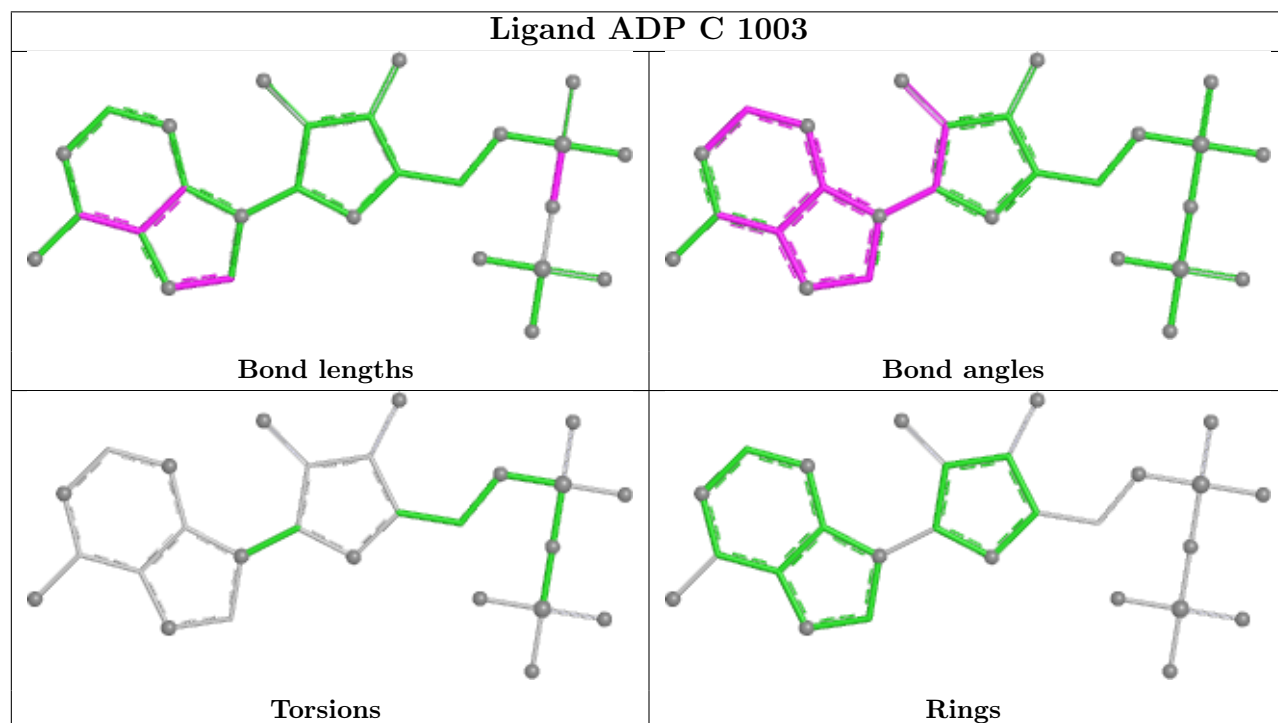
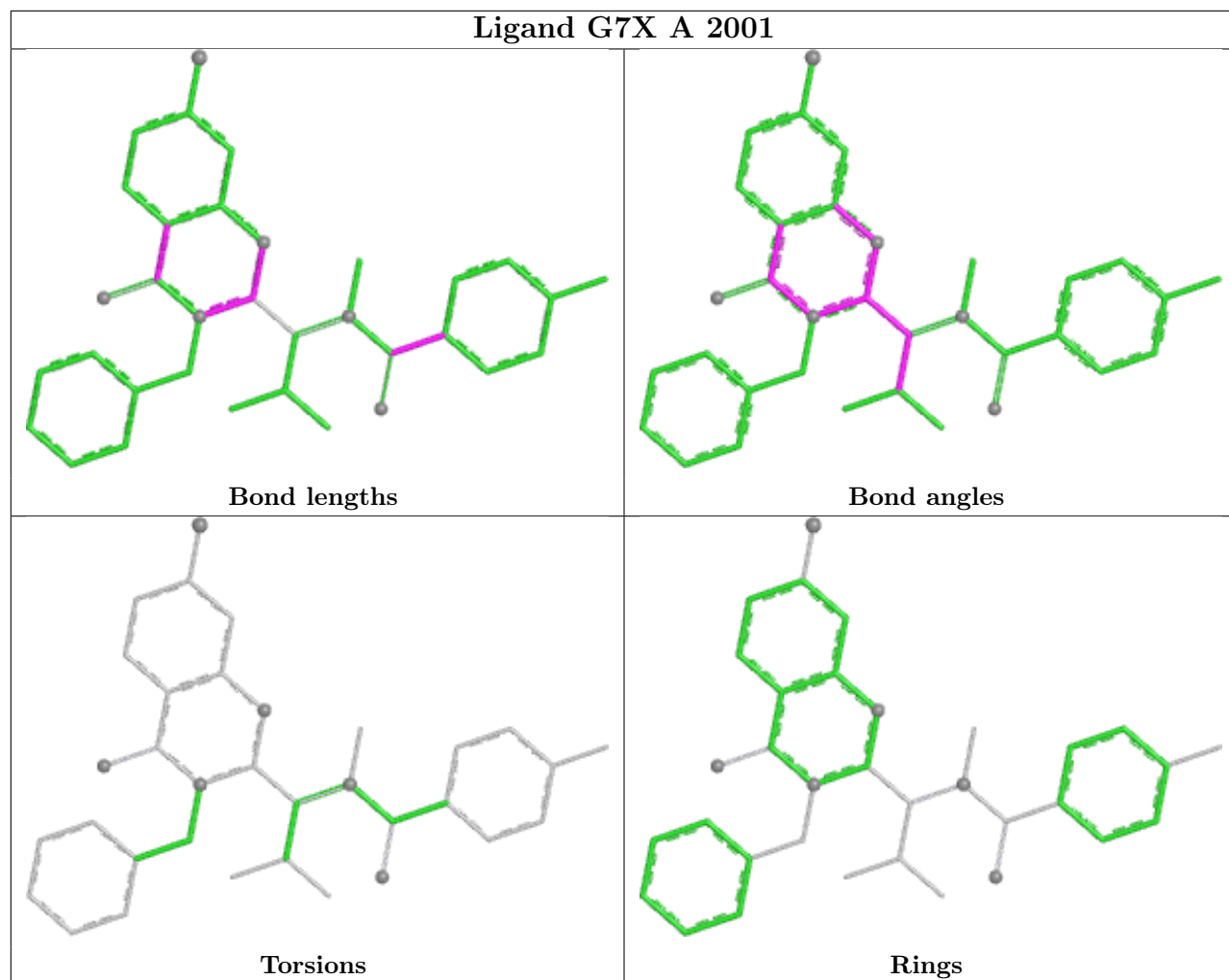
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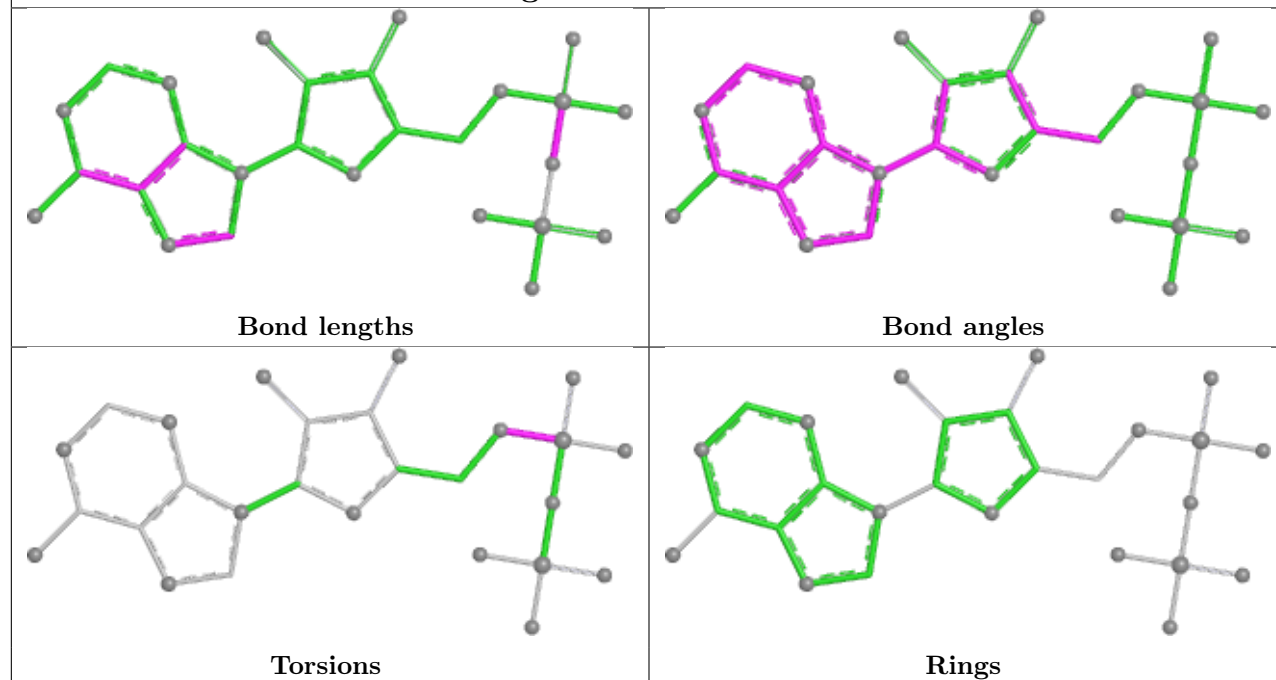
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1003	ADP	2	0
5	B	2001	G7X	14	0

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.

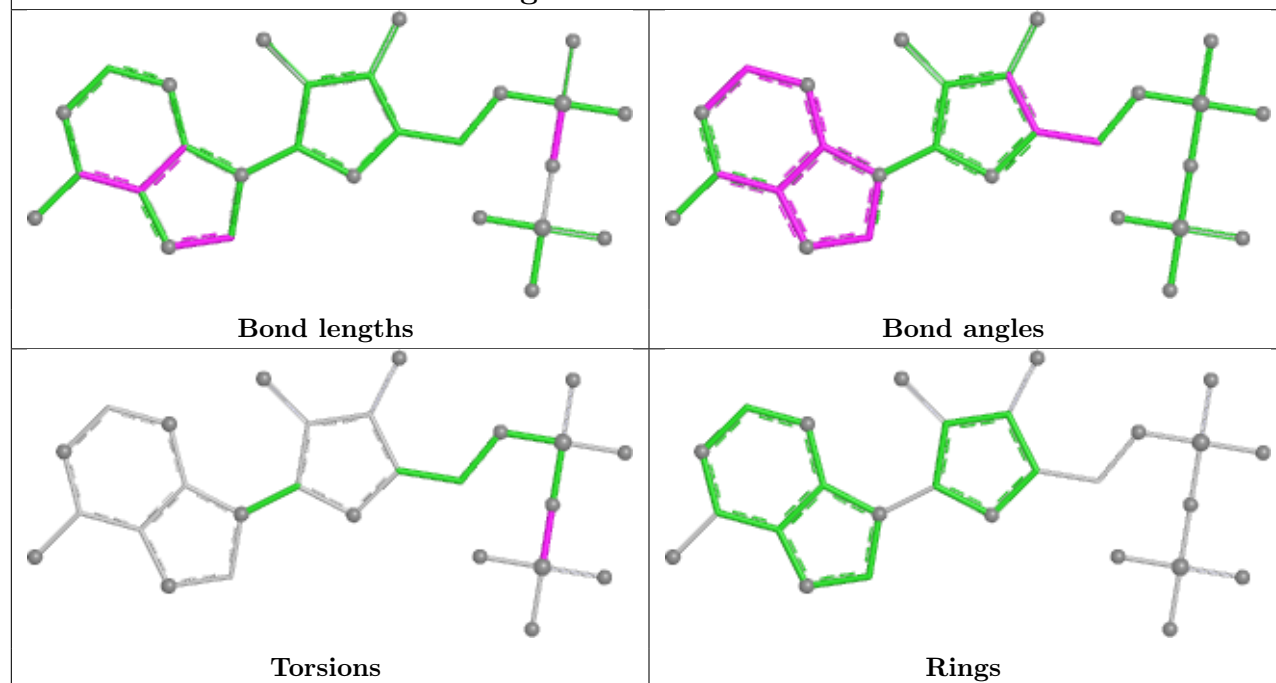


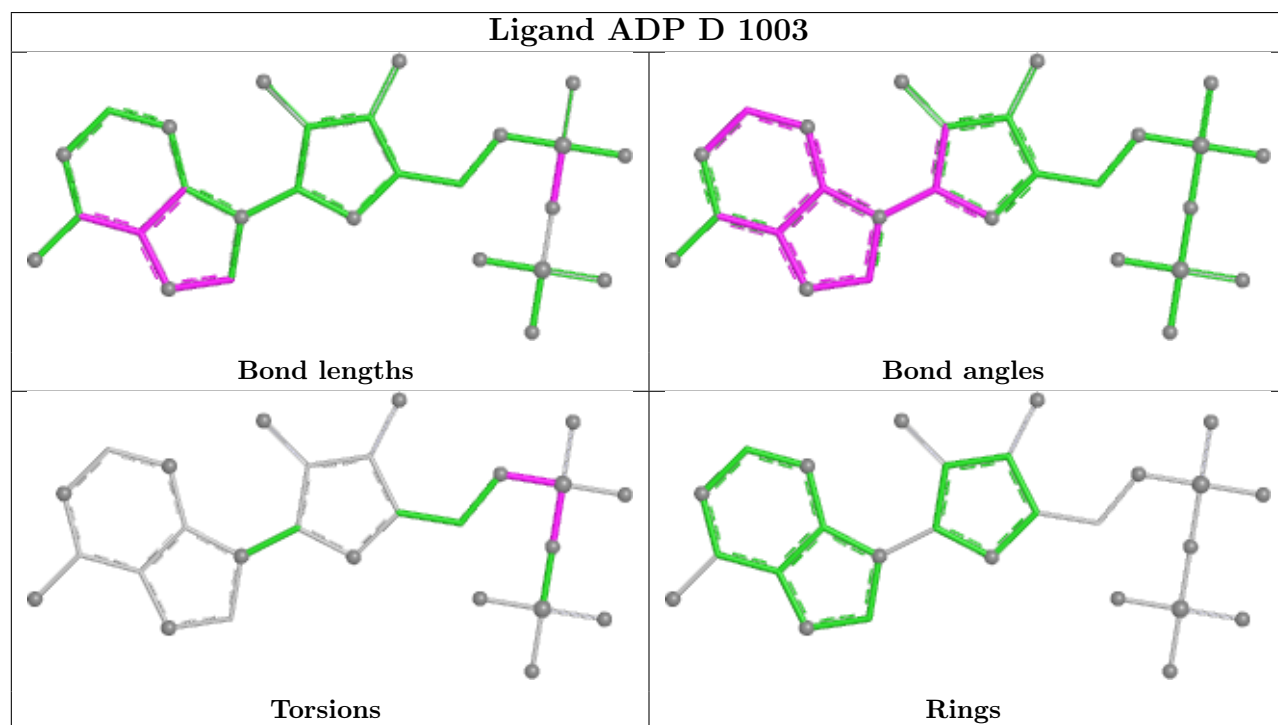
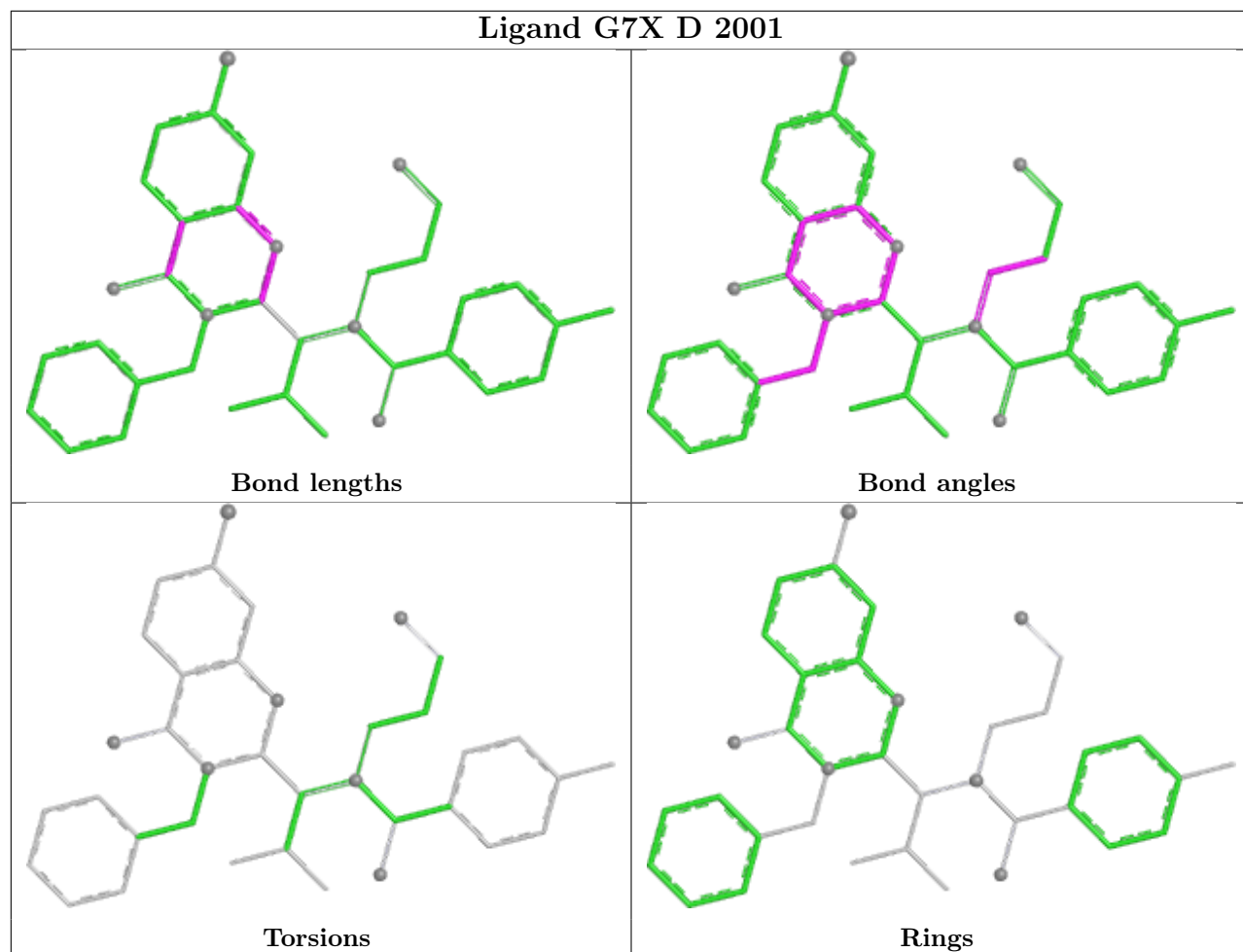


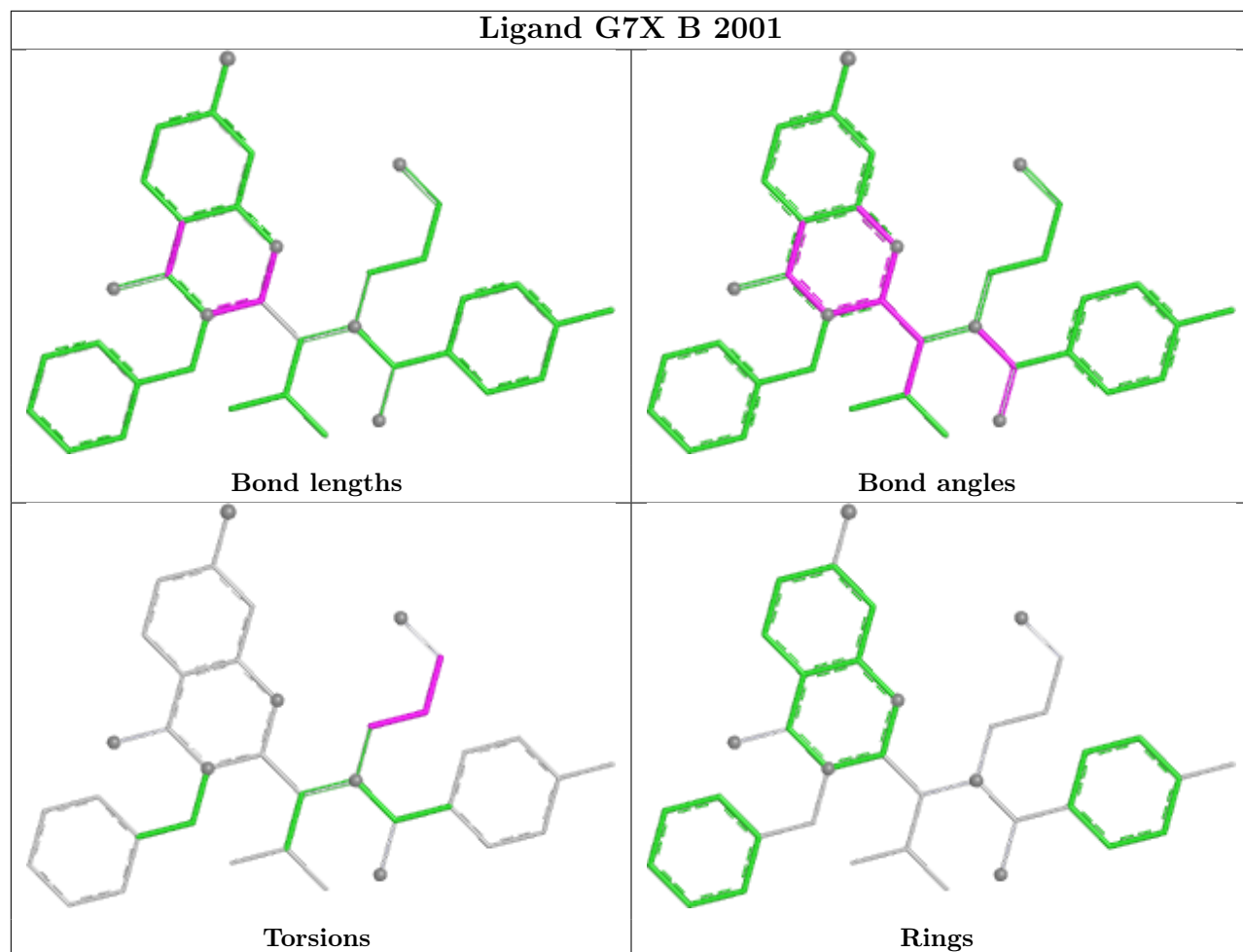
Ligand ADP B 1003



Ligand ADP A 1003







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	325/370 (87%)	-1.00	0 100 100	22, 56, 102, 129	0
1	B	312/370 (84%)	-0.98	0 100 100	28, 58, 105, 137	0
1	C	311/370 (84%)	-1.06	0 100 100	23, 51, 102, 153	0
1	D	309/370 (83%)	-1.09	0 100 100	21, 50, 89, 112	0
All	All	1257/1480 (84%)	-1.03	0 100 100	21, 54, 101, 153	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.

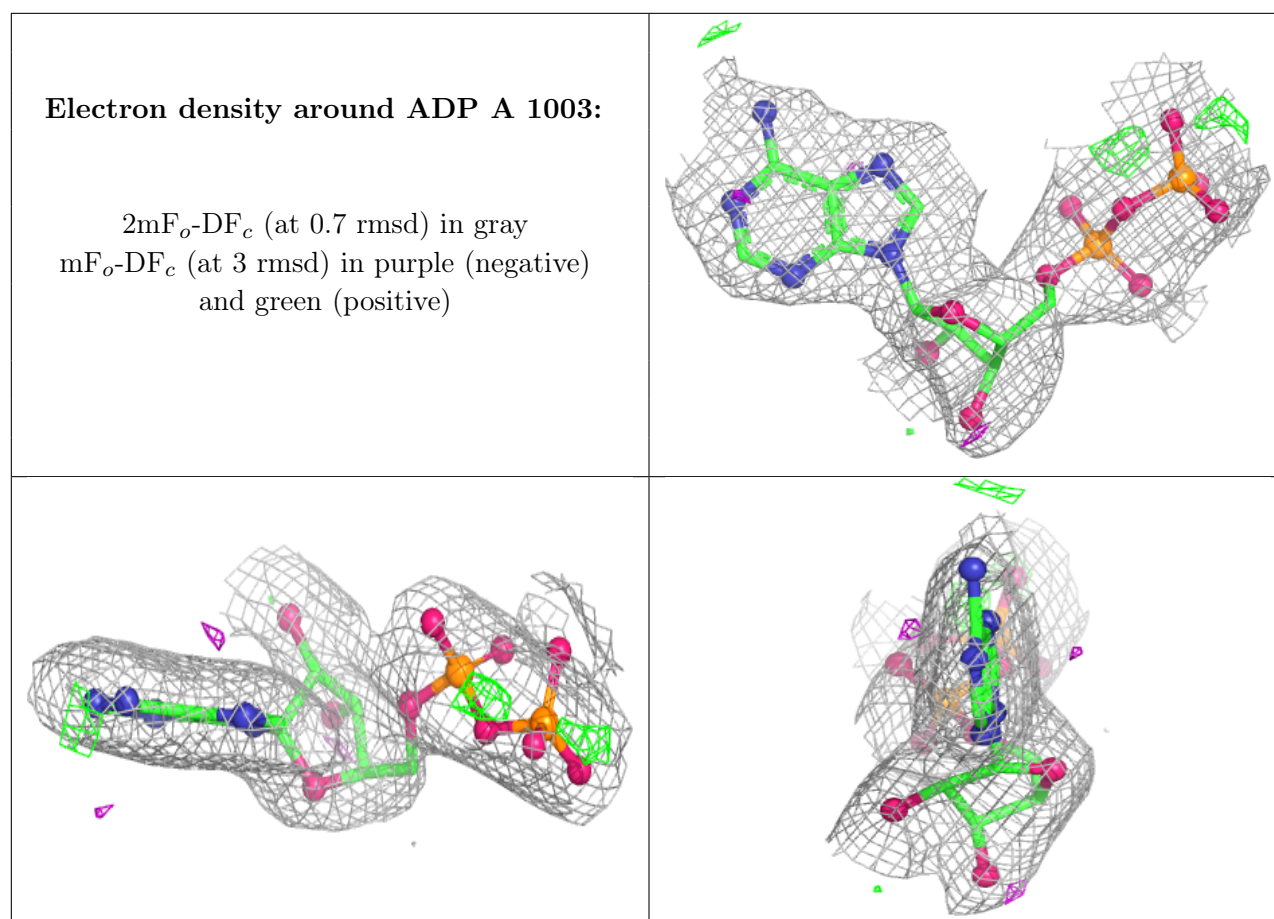
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CL	A	1367	1/1	0.98	0.06	38,38,38,38	0
4	CL	B	1361	1/1	0.98	0.07	60,60,60,60	0
4	CL	B	1362	1/1	0.98	0.05	53,53,53,53	0
4	CL	D	1365	1/1	0.98	0.06	51,51,51,51	0

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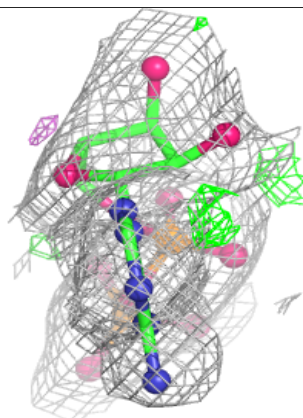
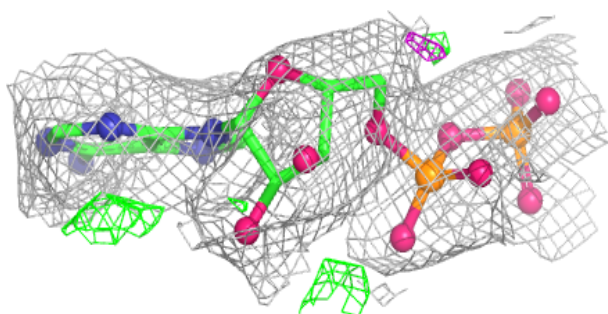
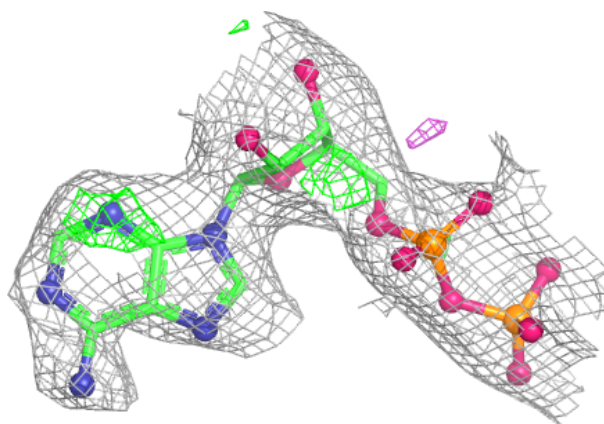
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MG	D	1001	1/1	0.99	0.04	50,50,50,50	0
4	CL	A	1368	1/1	0.99	0.04	65,65,65,65	0
3	ADP	A	1003	27/27	0.99	0.04	15,33,42,45	0
3	ADP	B	1003	27/27	0.99	0.04	18,36,45,54	0
3	ADP	D	1003	27/27	0.99	0.04	15,31,45,55	0
5	G7X	A	2001	34/37	0.99	0.04	12,42,74,80	0
5	G7X	B	2001	37/37	0.99	0.04	26,46,64,69	0
5	G7X	C	2001	37/37	0.99	0.04	18,39,56,58	0
5	G7X	D	2001	37/37	0.99	0.05	25,43,61,69	0
2	MG	B	1001	1/1	1.00	0.03	35,35,35,35	0
2	MG	C	1001	1/1	1.00	0.04	55,55,55,55	0
4	CL	B	1360	1/1	1.00	0.03	59,59,59,59	0
3	ADP	C	1003	27/27	1.00	0.03	15,30,47,50	0
2	MG	A	1001	1/1	1.00	0.01	30,30,30,30	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.



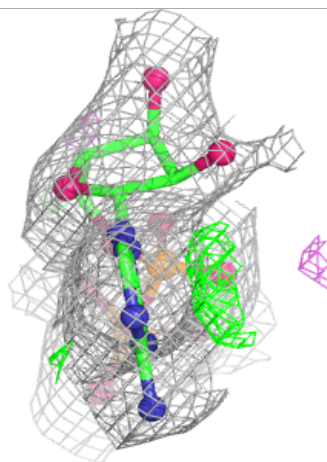
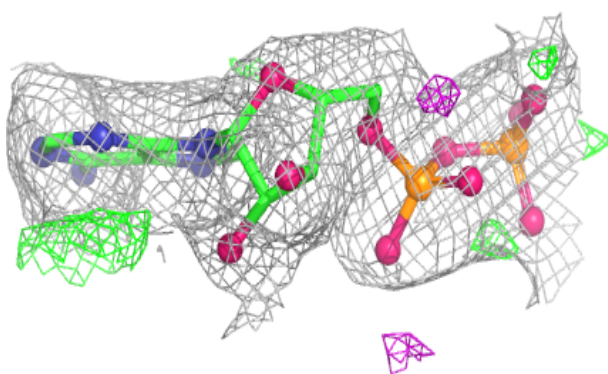
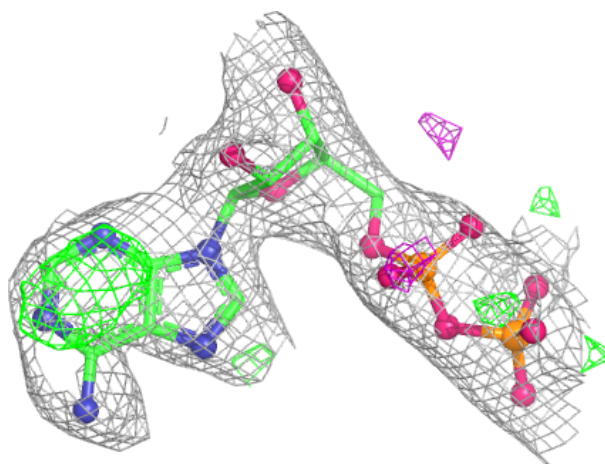
Electron density around ADP B 1003:

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



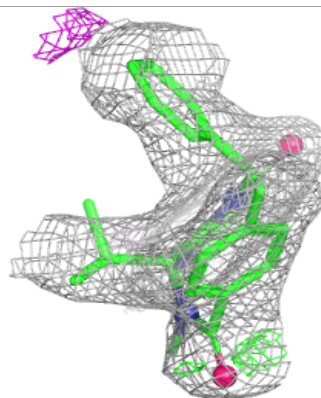
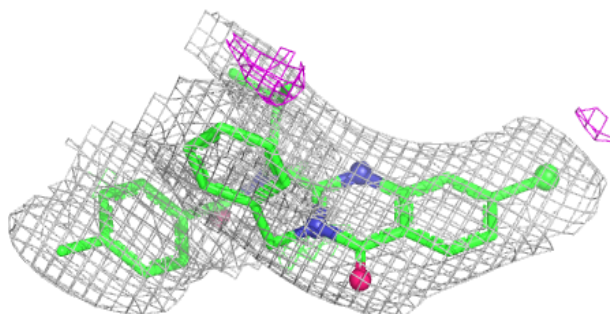
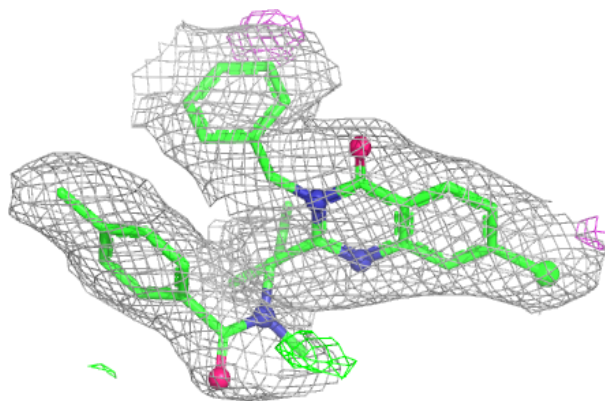
Electron density around ADP D 1003:

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

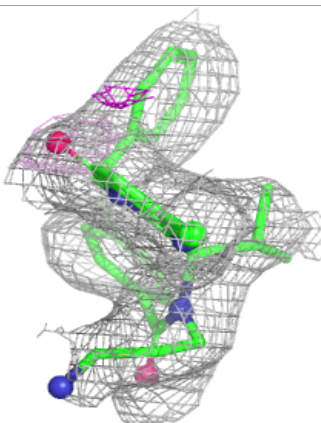
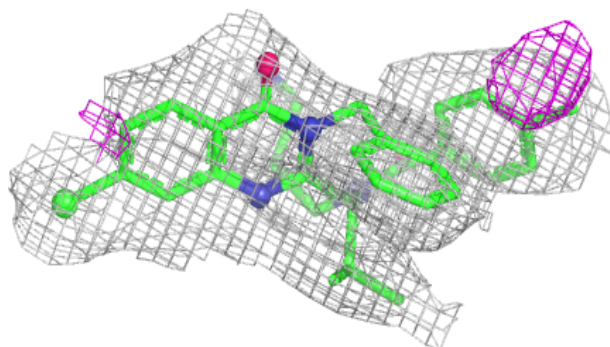
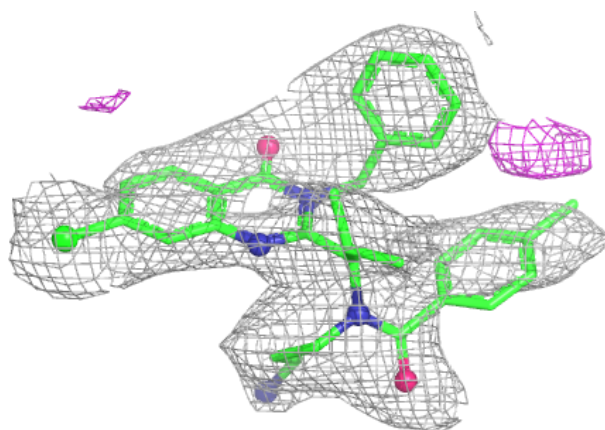


Electron density around G7X A 2001:

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

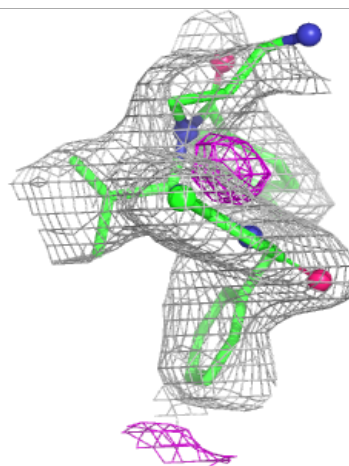
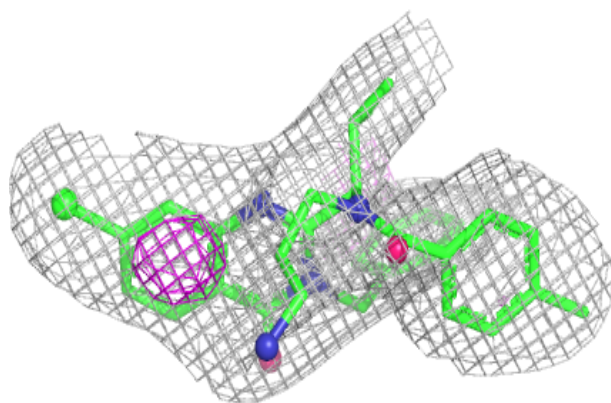
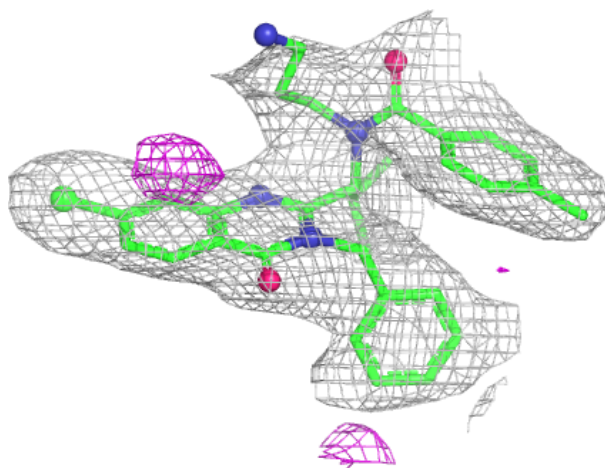
**Electron density around G7X B 2001:**

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



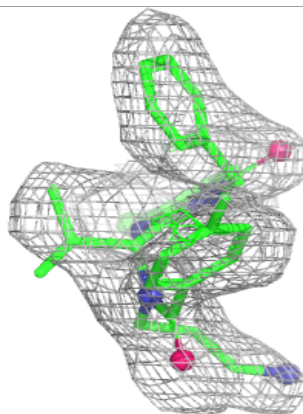
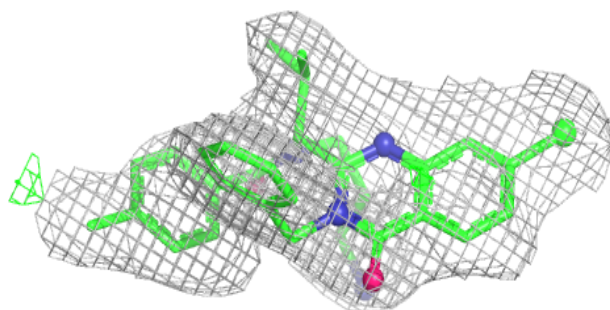
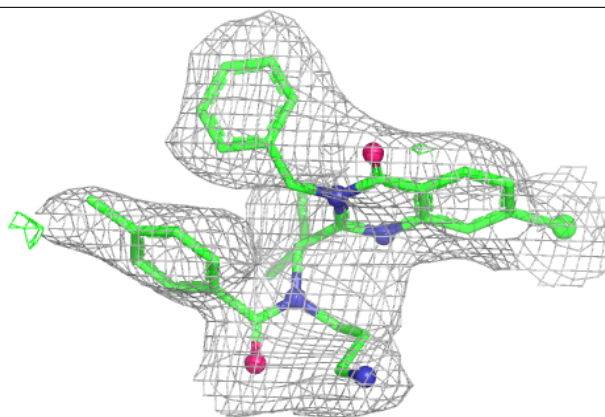
Electron density around G7X C 2001:

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

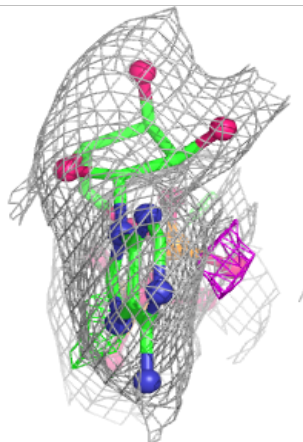
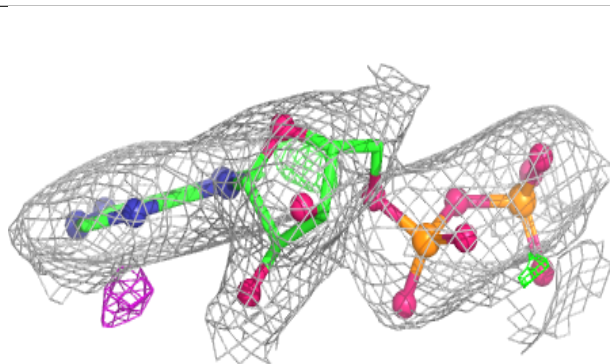
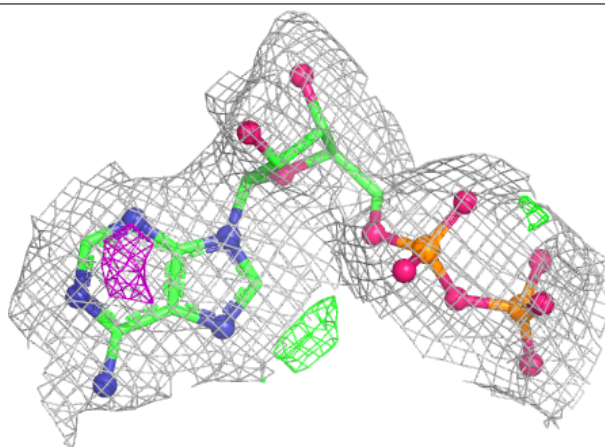


Electron density around G7X D 2001:

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

**Electron density around ADP C 1003:**

$2mF_o-DF_c$ (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.