



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:04 PM UTC

PDB ID : 3IRN / pdb_00003irn
Title : Trypanosoma cruzi Dihydrofolate Reductase-Thymidylate Synthase COM-
PLEXED WITH NADPH AND Cycloguanil
Authors : Chitnumsub, P.; Yuvaniyama, J.; Yuthavong, Y.
Deposited on : 2009-08-24
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

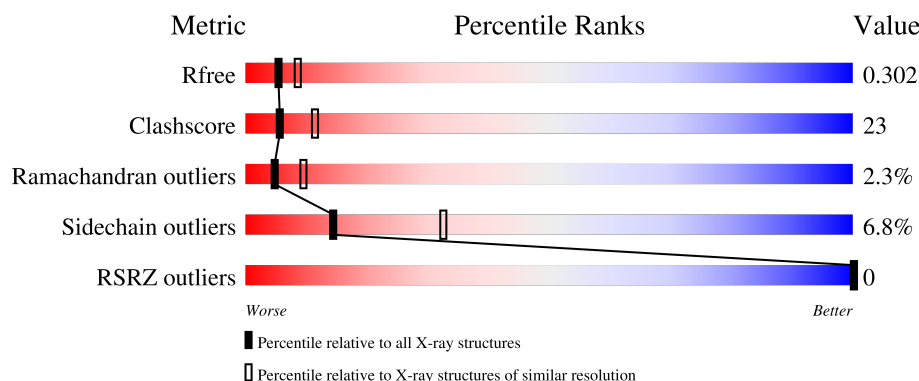
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	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	521	 58% 36% . .
1	B	521	 50% 40% 8% . .
1	C	521	 57% 38% . .
1	D	521	 52% 38% 7% . .

2 Entry composition [i](#)

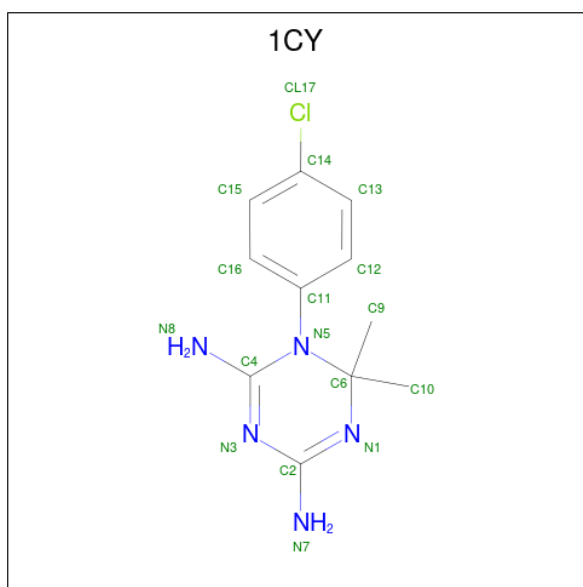
There are 5 unique types of molecules in this entry. The entry contains 16901 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 dihydrofolate reductase-thymidylate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	516	Total	C	N	O	S	0	0	0
			4107	2605	726	757	19			
1	B	516	Total	C	N	O	S	0	0	0
			4110	2608	727	756	19			
1	C	516	Total	C	N	O	S	0	0	0
			4107	2605	726	757	19			
1	D	513	Total	C	N	O	S	0	0	0
			4087	2594	723	752	18			

- Molecule 2 is 1-(4-chlorophenyl)-6,6-dimethyl-1,6-dihydro-1,3,5-triazine-2,4-diamine (CCD ID: 1CY) (formula: C₁₁H₁₄ClN₅).



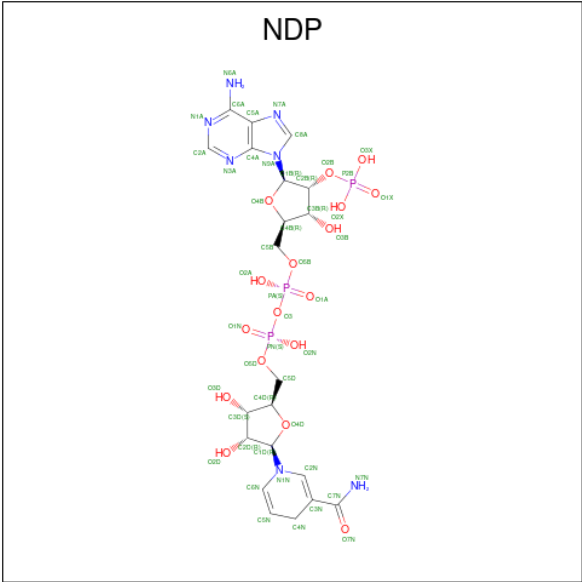
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	0	0
			17	11	1	5		
2	B	1	Total	C	Cl	N	0	0
			17	11	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	Cl	N	0	0
			17	11	1	5		
2	D	1	Total	C	Cl	N	0	0
			17	11	1	5		

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: C₂₁H₃₀N₇O₁₇P₃).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	A	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		

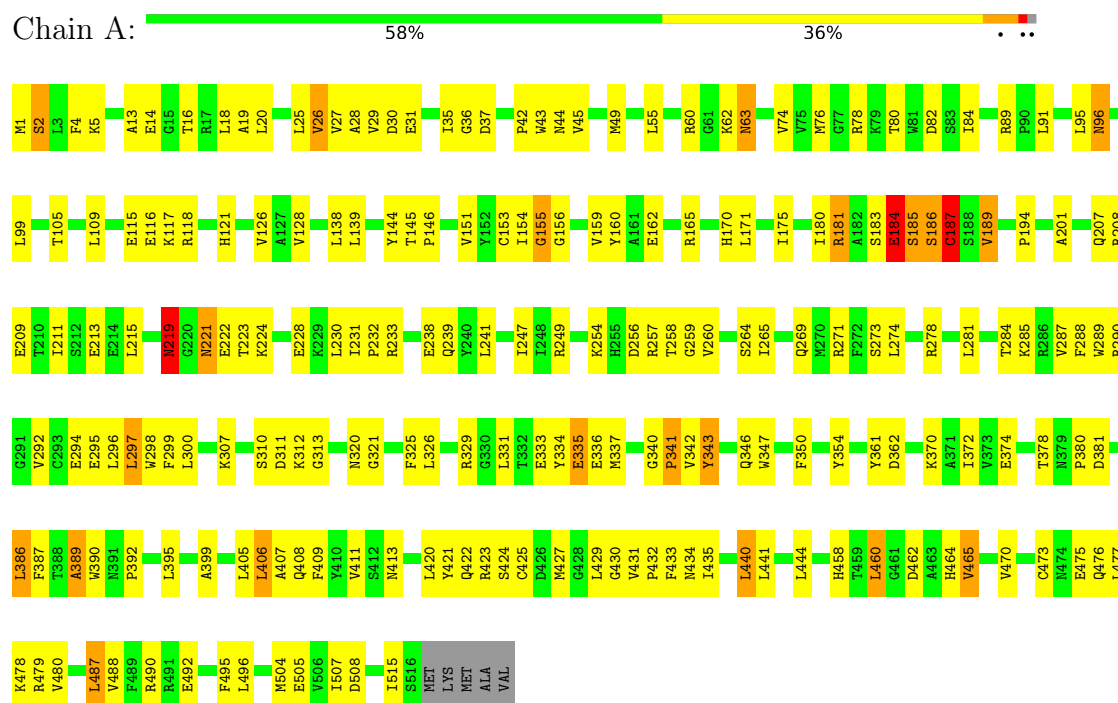
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total	O	0	0
			58	58		
5	B	49	Total	O	0	0
			49	49		
5	C	60	Total	O	0	0
			60	60		
5	D	43	Total	O	0	0
			43	43		

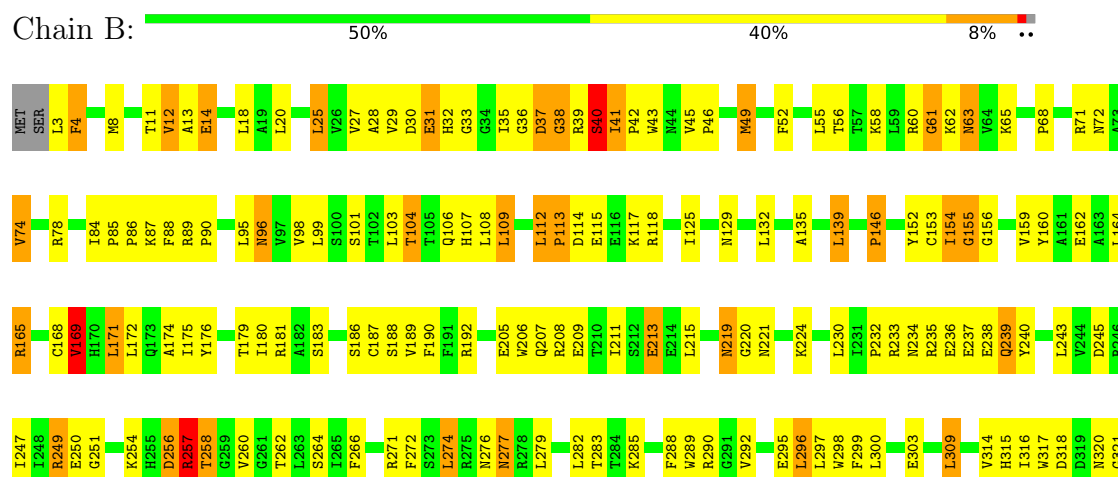
3 Residue-property plots

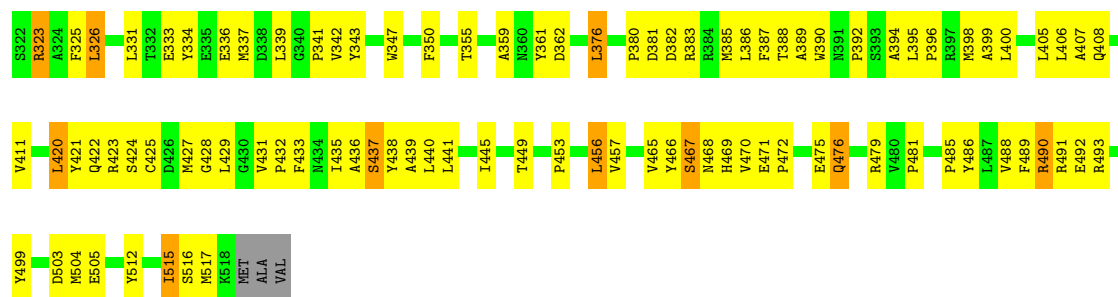
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



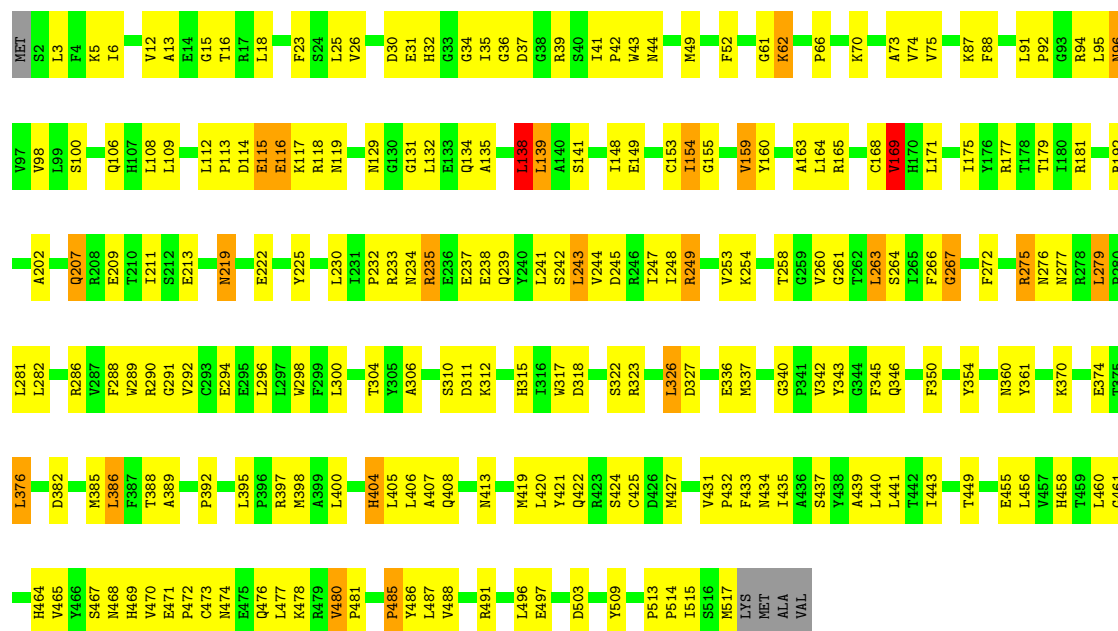
- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





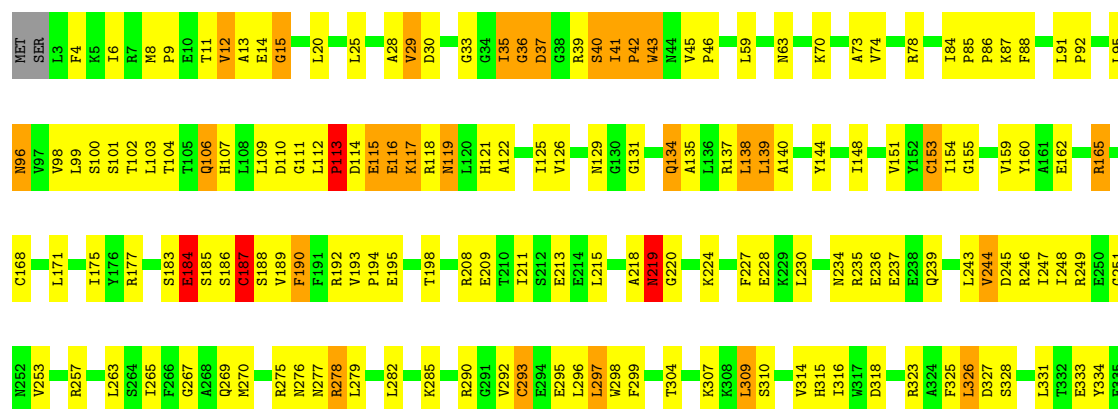
• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain C: 57% 38%



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase

Chain D: 52% 38% 7%



E336	M337	D338	L339	G340	P341	V342	Y343	G344	F345	Q346	W347	F380	G351	Y354	T355	H356	H357	D358	A359	D362	L376	N379	P380	D381	D382	R383	R384	M385	L386	A389	W390	N391	P392	S393	A394	L395	P396	R397	M398	L405	L406	A407	Q408	E415	M419	L420	Y421	Q422	R423	S424
C425	D426	M427	P432	F433	M434	Y438	A439	L440	L441	T442	I443	L444	I445	A446	K447	A448	L456	V457	H458	T459	L460	H464	V465	E471	P472	C473	R474	E475	Q476	P481	P485	Y486	L487	R490	R491	E492	L496	E497	P514	I515	SER	MET	LYS	MET	ALA	VAL				

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.34Å 165.59Å 84.85Å 90.00° 113.36° 90.00°	Depositor
Resolution (Å)	44.48 – 2.60 44.48 – 2.60	Depositor EDS
% Data completeness (in resolution range)	93.9 (44.48-2.60) 94.0 (44.48-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.51 (at 2.61Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.230 , 0.299 0.233 , 0.302	Depositor DCC
R_{free} test set	3003 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	32.4	Xtriage
Anisotropy	0.127	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 9.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.086 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	16901	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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: 1CY, PO4, NDP

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	0.50	0/4207	1.01	14/5708 (0.2%)
1	B	0.48	0/4210	1.03	21/5711 (0.4%)
1	C	0.49	0/4207	1.03	22/5708 (0.4%)
1	D	0.47	0/4187	1.06	31/5682 (0.5%)
All	All	0.48	0/16811	1.03	88/22809 (0.4%)

There are no bond length outliers.

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	36	GLY	N-CA-C	-11.10	101.87	115.08
1	D	405	LEU	N-CA-C	9.82	122.06	111.36
1	C	209	GLU	N-CA-C	-9.64	101.41	113.55
1	A	155	GLY	N-CA-C	9.33	123.64	111.70
1	D	209	GLU	N-CA-C	-8.75	102.52	113.55
1	D	165	ARG	CA-C-N	-8.54	113.52	119.66
1	D	165	ARG	C-N-CA	-8.54	113.52	119.66
1	D	91	LEU	CA-C-N	8.51	128.55	119.78
1	D	91	LEU	C-N-CA	8.51	128.55	119.78
1	B	155	GLY	N-CA-C	8.33	123.32	111.00
1	A	209	GLU	N-CA-C	-8.28	103.12	113.55
1	D	117	LYS	N-CA-C	-8.28	102.34	111.36
1	D	257	ARG	N-CA-C	-7.75	103.63	113.23
1	D	465	VAL	N-CA-C	-7.69	97.40	108.48
1	C	3	LEU	N-CA-C	-7.43	104.19	113.18
1	D	213	GLU	N-CA-C	-7.41	100.74	110.53
1	C	439	ALA	N-CA-C	-7.20	103.43	111.28
1	D	154	ILE	N-CA-C	7.19	119.25	111.77
1	C	41	ILE	N-CA-C	-7.16	102.36	109.02
1	C	138	LEU	N-CA-C	-7.11	103.46	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	168	CYS	N-CA-C	7.06	119.87	111.33
1	C	153	CYS	N-CA-C	-7.03	98.50	109.25
1	C	514	PRO	N-CA-C	6.92	122.11	111.11
1	D	11	THR	N-CA-C	-6.80	105.76	112.97
1	B	209	GLU	N-CA-C	-6.80	103.00	112.45
1	B	11	THR	N-CA-C	-6.80	104.86	113.02
1	C	91	LEU	CA-C-N	6.79	126.81	119.89
1	C	91	LEU	C-N-CA	6.79	126.81	119.89
1	B	439	ALA	N-CA-C	-6.72	103.42	111.69
1	A	259	GLY	N-CA-C	-6.68	105.89	115.64
1	B	257	ARG	N-CA-C	-6.64	105.18	113.28
1	B	239	GLN	N-CA-C	-6.61	104.00	111.14
1	C	513	PRO	CA-C-N	6.59	126.61	119.89
1	C	513	PRO	C-N-CA	6.59	126.61	119.89
1	D	190	PHE	N-CA-C	6.58	121.01	109.96
1	B	264	SER	N-CA-C	6.45	118.88	109.07
1	A	290	ARG	N-CA-C	-6.41	104.21	111.14
1	B	249	ARG	N-CA-C	6.39	117.91	111.07
1	D	439	ALA	N-CA-C	-6.38	104.25	111.14
1	A	389	ALA	N-CA-C	-6.32	104.73	112.88
1	D	379	ASN	CA-C-N	6.28	125.97	119.56
1	D	379	ASN	C-N-CA	6.28	125.97	119.56
1	A	156	GLY	N-CA-C	-6.22	98.45	113.18
1	B	183	SER	N-CA-C	-6.17	105.23	112.89
1	D	168	CYS	N-CA-C	6.12	118.74	111.33
1	B	168	CYS	N-CA-C	6.02	118.63	111.71
1	D	292	VAL	N-CA-C	-5.93	104.55	110.30
1	B	12	VAL	N-CA-C	5.88	116.53	110.36
1	D	293	CYS	N-CA-C	5.86	117.67	111.28
1	B	251	GLY	N-CA-C	5.71	118.61	112.33
1	A	213	GLU	N-CA-C	-5.68	103.03	110.53
1	A	189	VAL	N-CA-C	5.65	116.30	108.84
1	D	389	ALA	N-CA-C	-5.62	106.77	113.97
1	A	470	VAL	N-CA-C	5.60	116.24	110.36
1	A	465	VAL	N-CA-C	-5.58	100.03	108.17
1	B	154	ILE	N-CA-C	5.55	117.51	112.29
1	C	149	GLU	N-CA-C	5.55	117.13	111.14
1	B	437	SER	N-CA-C	5.51	117.73	111.11
1	D	119	ASN	N-CA-C	-5.51	108.34	114.62
1	B	4	PHE	N-CA-C	-5.48	106.95	113.97
1	C	389	ALA	N-CA-C	-5.48	106.60	113.28
1	B	169	VAL	CB-CA-C	-5.47	104.97	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	LEU	N-CA-C	-5.47	105.32	111.28
1	C	275	ARG	N-CA-C	5.47	118.38	110.28
1	D	98	VAL	N-CA-C	5.43	115.68	107.80
1	A	14	GLU	N-CA-C	5.42	117.27	111.36
1	B	323	ARG	N-CA-C	-5.41	105.49	111.71
1	C	169	VAL	CB-CA-C	-5.38	103.82	112.16
1	C	249	ARG	N-CA-C	5.35	117.19	111.36
1	C	213	GLU	N-CA-C	-5.35	103.83	110.41
1	A	399	ALA	N-CA-C	-5.31	105.49	111.28
1	A	335	GLU	N-CA-C	-5.30	103.14	110.35
1	B	165	ARG	CA-C-N	-5.25	114.97	120.38
1	B	165	ARG	C-N-CA	-5.25	114.97	120.38
1	D	239	GLN	N-CA-C	-5.25	105.47	111.14
1	D	102	THR	N-CA-C	-5.24	108.65	114.62
1	D	12	VAL	N-CA-C	5.24	115.45	110.53
1	C	239	GLN	N-CA-C	-5.22	105.49	111.07
1	D	153	CYS	N-CA-C	-5.19	101.31	109.25
1	B	213	GLU	N-CA-C	-5.19	103.84	110.53
1	D	92	PRO	N-CA-C	5.15	119.39	111.21
1	D	327	ASP	N-CA-C	-5.12	105.59	111.07
1	D	244	VAL	N-CA-C	-5.10	105.42	110.62
1	B	389	ALA	N-CA-C	-5.10	107.09	113.72
1	C	154	ILE	N-CA-C	5.06	117.76	112.90
1	D	116	GLU	N-CA-C	-5.02	107.33	113.50
1	C	480	VAL	CA-C-N	5.00	125.28	119.93
1	C	480	VAL	C-N-CA	5.00	125.28	119.93

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	4107	0	4063	176	0
1	B	4110	0	4068	235	0
1	C	4107	0	4060	178	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4087	0	4041	217	0
2	A	17	0	14	1	0
2	B	17	0	14	1	0
2	C	17	0	14	0	0
2	D	17	0	14	0	0
3	A	48	0	26	2	0
3	B	48	0	26	7	0
3	C	48	0	26	3	0
3	D	48	0	26	3	0
4	A	10	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
5	A	58	0	0	0	0
5	B	49	0	0	3	0
5	C	60	0	0	3	0
5	D	43	0	0	3	0
All	All	16901	0	16392	776	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 (776) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ARG:HH11	1:B:490:ARG:HB3	1.24	0.99
1:B:181:ARG:HG3	1:B:224:LYS:HB2	1.42	0.97
1:C:300:LEU:HD13	1:C:496:LEU:HD11	1.48	0.95
1:D:114:ASP:HB3	1:D:117:LYS:HB2	1.48	0.95
1:A:181:ARG:HH11	1:A:181:ARG:HB3	1.33	0.93
1:B:112:LEU:HB3	1:B:117:LYS:HE3	1.52	0.91
1:D:117:LYS:HE2	1:D:121:HIS:NE2	1.86	0.91
1:A:1:MET:HB2	1:A:5:LYS:HG3	1.52	0.91
1:A:146:PRO:HB3	1:A:505:GLU:HG2	1.54	0.90
1:B:257:ARG:H	1:B:257:ARG:HD3	1.37	0.90
1:D:397:ARG:HG2	1:D:397:ARG:HH11	1.35	0.90
1:D:40:SER:C	1:D:42:PRO:HD3	1.97	0.89
1:C:279:LEU:HD23	1:C:281:LEU:HG	1.53	0.88
1:D:114:ASP:HB3	1:D:117:LYS:CB	2.04	0.87
1:B:285:LYS:HD2	1:B:476:GLN:HE21	1.41	0.84
1:B:490:ARG:HB3	1:B:490:ARG:NH1	1.94	0.83
1:D:278:ARG:NH1	5:D:1080:HOH:O	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:ASN:ND2	1:B:221:ASN:H	1.78	0.81
1:D:192:ARG:HE	1:D:193:VAL:H	1.30	0.80
1:A:62:LYS:O	1:A:63:ASN:HB2	1.78	0.80
1:B:155:GLY:HA3	3:B:702:NDP:H5N	1.65	0.79
1:C:254:LYS:HD3	1:D:381:ASP:CG	2.07	0.79
1:B:101:SER:HA	1:B:129:ASN:OD1	1.82	0.79
1:B:386:LEU:HD12	1:B:406:LEU:HD11	1.63	0.79
1:B:285:LYS:HD2	1:B:476:GLN:NE2	1.98	0.78
1:D:20:LEU:HB2	1:D:171:LEU:HD13	1.67	0.77
1:B:285:LYS:HE3	1:B:515:ILE:HD11	1.66	0.76
1:A:281:LEU:HD22	1:A:287:VAL:HB	1.67	0.75
1:D:246:ARG:HA	1:D:249:ARG:HH12	1.50	0.75
1:D:177:ARG:HH12	1:D:192:ARG:NH2	1.84	0.75
1:A:479:ARG:HH12	1:A:515:ILE:HG12	1.52	0.75
1:C:234:ASN:O	1:C:238:GLU:HG3	1.86	0.75
1:C:253:VAL:HG22	1:C:263:LEU:HD22	1.69	0.75
1:D:112:LEU:HD12	1:D:113:PRO:HD2	1.70	0.74
1:B:8:MET:HE3	1:B:12:VAL:HG23	1.70	0.73
1:B:239:GLN:HE22	1:B:271:ARG:H	1.36	0.73
1:C:96:ASN:N	1:C:96:ASN:HD22	1.86	0.73
1:C:471:GLU:HB2	1:C:472:PRO:HD3	1.70	0.73
1:A:1:MET:HB3	1:A:4:PHE:HB2	1.72	0.72
1:D:340:GLY:HA2	1:D:354:TYR:CE2	2.25	0.72
1:B:472:PRO:HG2	1:B:517:MET:HE3	1.72	0.71
1:A:117:LYS:HG3	1:A:121:HIS:HD2	1.54	0.71
1:D:246:ARG:HA	1:D:249:ARG:NH1	2.06	0.71
1:A:257:ARG:H	1:A:257:ARG:HD3	1.54	0.71
1:A:300:LEU:HD21	1:A:441:LEU:CD1	2.21	0.71
1:B:492:GLU:O	1:B:493:ARG:HD2	1.90	0.70
1:B:219:ASN:C	1:B:219:ASN:HD22	1.98	0.70
1:A:254:LYS:HD3	1:B:381:ASP:OD1	1.91	0.70
1:D:192:ARG:HE	1:D:193:VAL:N	1.88	0.70
1:B:85:PRO:HB2	1:B:88:PHE:HD2	1.55	0.70
1:D:234:ASN:C	1:D:234:ASN:HD22	2.00	0.69
1:B:234:ASN:O	1:B:238:GLU:HG3	1.92	0.69
1:B:321:GLY:O	1:B:337:MET:HE2	1.92	0.69
1:C:115:GLU:HG3	1:C:118:ARG:NH1	2.07	0.69
1:D:115:GLU:HA	1:D:118:ARG:NH1	2.07	0.69
1:A:117:LYS:HG3	1:A:121:HIS:CD2	2.28	0.68
1:C:296:LEU:HD13	1:C:296:LEU:C	2.17	0.68
1:A:239:GLN:HE22	1:A:271:ARG:H	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLY:O	1:B:190:PHE:HA	1.92	0.68
1:B:146:PRO:CB	1:B:505:GLU:HG2	2.22	0.68
1:B:104:THR:H	1:B:107:HIS:HB2	1.58	0.68
1:B:109:LEU:HD12	1:B:125:ILE:HD12	1.74	0.68
1:C:237:GLU:HG3	1:C:282:LEU:HD22	1.74	0.68
1:C:247:ILE:HG21	1:C:465:VAL:HG23	1.73	0.68
1:A:171:LEU:HD12	1:A:171:LEU:N	2.08	0.68
1:D:8:MET:HE3	1:D:8:MET:HA	1.76	0.68
1:B:431:VAL:O	1:B:435:ILE:HG13	1.93	0.68
1:A:60:ARG:NH2	1:A:508:ASP:HA	2.09	0.67
1:D:35:ILE:C	1:D:37:ASP:H	1.99	0.67
1:D:355:THR:HG22	1:D:356:HIS:CD2	2.29	0.67
1:C:241:LEU:HD22	1:C:477:LEU:HD23	1.75	0.67
1:D:85:PRO:HG2	1:D:88:PHE:HB2	1.76	0.67
1:D:117:LYS:C	1:D:119:ASN:H	2.03	0.66
1:A:431:VAL:O	1:A:435:ILE:HG13	1.94	0.66
1:D:397:ARG:HH11	1:D:397:ARG:CG	2.08	0.66
1:C:244:VAL:O	1:C:248:ILE:HG13	1.96	0.66
1:B:341:PRO:O	1:B:398:MET:HE2	1.96	0.66
1:C:37:ASP:OD2	1:C:42:PRO:HG3	1.96	0.66
1:A:381:ASP:CG	1:B:254:LYS:HD3	2.21	0.66
1:B:146:PRO:HB3	1:B:505:GLU:HG2	1.78	0.66
1:C:264:SER:HB3	1:C:464:HIS:HB3	1.77	0.66
1:D:8:MET:HE3	1:D:9:PRO:HD2	1.77	0.65
1:A:257:ARG:H	1:A:257:ARG:CD	2.08	0.65
1:A:37:ASP:HB2	1:A:42:PRO:HD3	1.78	0.65
1:C:31:GLU:OE2	1:C:181:ARG:HD2	1.96	0.65
1:D:395:LEU:HB2	1:D:396:PRO:HD3	1.78	0.65
1:B:376:LEU:HD23	1:B:449:THR:HG21	1.79	0.65
1:D:278:ARG:HG3	1:D:278:ARG:HH11	1.61	0.65
1:C:322:SER:O	1:C:326:LEU:HB2	1.96	0.65
1:B:296:LEU:HD11	1:B:441:LEU:HB2	1.78	0.64
1:C:425:CYS:SG	1:C:460:LEU:HD22	2.37	0.64
1:B:213:GLU:O	1:B:215:LEU:HD13	1.97	0.64
1:C:392:PRO:HD2	1:D:350:PHE:CZ	2.31	0.64
1:A:145:THR:HG23	1:A:507:ILE:HG21	1.80	0.64
1:B:285:LYS:HB2	1:B:476:GLN:NE2	2.13	0.64
1:D:110:ASP:HA	1:D:118:ARG:HE	1.62	0.64
1:D:96:ASN:N	1:D:96:ASN:HD22	1.95	0.64
1:C:254:LYS:HD3	1:D:381:ASP:OD2	1.98	0.63
1:C:350:PHE:CE1	1:D:392:PRO:HD2	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:VAL:HG12	1:A:35:ILE:HG22	1.80	0.63
1:D:441:LEU:O	1:D:445:ILE:HG12	1.98	0.63
1:A:181:ARG:HB3	1:A:181:ARG:NH1	2.11	0.63
1:A:479:ARG:NH1	1:A:515:ILE:HG12	2.14	0.63
1:B:84:ILE:HG22	1:B:89:ARG:HG2	1.81	0.63
1:D:298:TRP:CD1	1:D:309:LEU:HD13	2.33	0.63
1:A:31:GLU:OE2	1:A:181:ARG:HD2	1.98	0.63
1:A:254:LYS:HD3	1:B:381:ASP:CG	2.24	0.63
1:D:276:ASN:O	1:D:277:ASN:HB2	1.98	0.62
1:D:351:GLY:HA2	5:D:1157:HOH:O	1.99	0.62
1:B:114:ASP:O	1:B:118:ARG:HG3	1.99	0.62
1:C:135:ALA:O	1:C:139:LEU:HB2	1.97	0.62
1:A:96:ASN:N	1:A:96:ASN:HD22	1.94	0.62
1:A:406:LEU:HB3	1:A:421:TYR:HB3	1.82	0.62
1:B:86:PRO:HA	1:B:89:ARG:HG3	1.81	0.62
1:A:406:LEU:HD23	1:A:421:TYR:HB2	1.82	0.62
1:D:424:SER:OG	1:D:464:HIS:HE1	1.82	0.62
1:C:164:LEU:HA	1:C:169:VAL:HG13	1.81	0.61
1:D:379:ASN:ND2	1:D:382:ASP:HB2	2.15	0.61
1:B:219:ASN:ND2	1:B:219:ASN:C	2.54	0.61
1:A:473:CYS:O	1:A:477:LEU:HG	2.00	0.61
1:D:20:LEU:CD2	1:D:137:ARG:HG3	2.31	0.61
1:A:269:GLN:HA	1:A:458:HIS:O	1.99	0.61
1:D:41:ILE:HD12	1:D:41:ILE:N	2.16	0.61
1:D:195:GLU:HB3	1:D:198:THR:HG21	1.82	0.61
1:B:469:HIS:C	1:B:472:PRO:HD2	2.25	0.61
1:D:386:LEU:HB3	1:D:408:GLN:HA	1.83	0.61
1:D:14:GLU:HG3	1:D:15:GLY:H	1.66	0.60
1:C:12:VAL:HG13	1:C:13:ALA:N	2.16	0.60
1:D:192:ARG:NE	1:D:192:ARG:HA	2.16	0.60
1:C:253:VAL:HG22	1:C:263:LEU:CD2	2.31	0.60
1:C:272:PHE:CZ	1:C:435:ILE:HD13	2.36	0.60
1:A:478:LYS:HD3	1:C:478:LYS:NZ	2.16	0.60
1:A:490:ARG:HB2	1:A:490:ARG:HH11	1.65	0.60
1:B:87:LYS:HE3	1:B:88:PHE:CE2	2.36	0.60
1:A:370:LYS:O	1:A:374:GLU:HG2	2.02	0.60
1:B:471:GLU:HB2	1:B:472:PRO:HD3	1.83	0.60
1:C:424:SER:OG	1:C:464:HIS:HE1	1.84	0.60
1:D:234:ASN:HD21	1:D:236:GLU:HB2	1.67	0.59
1:B:315:HIS:HB3	1:B:318:ASP:OD1	2.03	0.59
1:B:382:ASP:O	1:B:385:MET:HE2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:427:MET:SD	1:B:431:VAL:HG21	2.43	0.59
1:C:155:GLY:HA3	3:C:703:NDP:H5N	1.84	0.59
1:D:20:LEU:HB2	1:D:171:LEU:CD1	2.32	0.59
1:D:420:LEU:HD23	1:D:458:HIS:CD2	2.38	0.59
1:D:39:ARG:HD2	1:D:186:SER:HB2	1.83	0.59
1:A:241:LEU:HD11	1:A:284:THR:HG21	1.85	0.59
1:B:37:ASP:C	1:B:39:ARG:H	2.10	0.59
1:C:61:GLY:O	1:C:62:LYS:O	2.20	0.59
1:C:400:LEU:HD11	1:D:384:ARG:HH22	1.67	0.59
1:D:314:VAL:HG12	1:D:316:ILE:HG12	1.84	0.59
1:D:42:PRO:HB2	1:D:185:SER:OG	2.02	0.58
1:D:135:ALA:O	1:D:139:LEU:HD22	2.03	0.58
1:B:257:ARG:HD3	1:B:257:ARG:N	2.13	0.58
1:A:45:VAL:HG21	1:A:180:ILE:HG12	1.84	0.58
1:B:274:LEU:O	1:B:453:PRO:HB2	2.03	0.58
1:C:192:ARG:HG2	1:C:192:ARG:HH11	1.68	0.58
1:C:247:ILE:HD12	1:C:427:MET:HG3	1.86	0.58
1:D:114:ASP:HB3	1:D:117:LYS:HB3	1.85	0.58
1:D:116:GLU:O	1:D:119:ASN:HB3	2.02	0.58
1:C:207:GLN:NE2	1:C:233:ARG:HD2	2.19	0.58
1:D:299:PHE:HB3	1:D:347:TRP:CZ3	2.37	0.58
1:A:300:LEU:HD21	1:A:441:LEU:HD13	1.85	0.58
1:B:20:LEU:HB2	1:B:171:LEU:HD13	1.85	0.58
1:D:131:GLY:H	1:D:134:GLN:NE2	2.02	0.58
1:A:336:GLU:O	1:A:337:MET:HB2	2.02	0.58
1:A:350:PHE:CZ	1:B:392:PRO:HD2	2.38	0.58
1:A:381:ASP:OD1	1:B:254:LYS:HD3	2.04	0.58
1:A:387:PHE:CE1	1:A:407:ALA:HB3	2.38	0.58
1:B:359:ALA:HB3	1:B:361:TYR:CZ	2.39	0.58
1:A:422:GLN:HB3	1:A:425:CYS:SG	2.43	0.58
1:B:89:ARG:HB2	1:B:112:LEU:HD22	1.85	0.58
1:B:109:LEU:O	1:B:112:LEU:HG	2.03	0.58
1:B:376:LEU:HD13	1:B:385:MET:SD	2.44	0.58
1:A:288:PHE:O	1:A:292:VAL:HG23	2.04	0.58
1:B:296:LEU:CD1	1:B:441:LEU:HB2	2.33	0.58
1:B:336:GLU:O	1:B:337:MET:HB2	2.04	0.57
1:B:420:LEU:HD22	1:B:438:TYR:CD2	2.39	0.57
1:D:115:GLU:HG2	1:D:118:ARG:HH11	1.67	0.57
1:B:85:PRO:HB2	1:B:88:PHE:CD2	2.37	0.57
1:C:247:ILE:CD1	1:C:427:MET:HG3	2.34	0.57
1:A:35:ILE:HG13	1:A:36:GLY:N	2.20	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:THR:HG22	1:B:106:GLN:H	1.69	0.57
1:B:256:ASP:OD2	1:B:260:VAL:HB	2.05	0.57
1:B:431:VAL:HB	1:B:432:PRO:HD3	1.86	0.57
1:D:331:LEU:HD13	1:D:334:TYR:CE2	2.39	0.57
1:A:300:LEU:HD21	1:A:441:LEU:HD11	1.85	0.57
1:B:298:TRP:HH2	1:B:339:LEU:HD12	1.70	0.57
1:C:491:ARG:HD2	1:C:503:ASP:OD2	2.04	0.57
1:A:295:GLU:O	1:A:298:TRP:HB3	2.05	0.57
1:B:115:GLU:HA	1:B:118:ARG:HB2	1.86	0.56
1:C:12:VAL:HG13	1:C:13:ALA:H	1.70	0.56
1:C:323:ARG:HG3	1:C:327:ASP:OD2	2.05	0.56
1:C:336:GLU:O	1:C:337:MET:HB2	2.05	0.56
1:A:208:ARG:NH2	1:C:263:LEU:HD13	2.20	0.56
1:A:247:ILE:HG21	1:A:465:VAL:HG23	1.87	0.56
1:C:279:LEU:HD13	1:C:487:LEU:HB2	1.87	0.56
1:A:31:GLU:HG3	1:A:181:ARG:HA	1.86	0.56
1:A:311:ASP:C	1:A:313:GLY:H	2.14	0.56
1:A:1:MET:HB2	1:A:5:LYS:CG	2.31	0.56
1:A:256:ASP:HB2	1:A:257:ARG:HH11	1.70	0.56
1:B:90:PRO:HB2	1:B:96:ASN:CG	2.30	0.56
1:D:296:LEU:CD2	1:D:440:LEU:HG	2.36	0.56
1:B:4:PHE:CD1	1:B:362:ASP:HB3	2.41	0.56
1:B:489:PHE:CE1	1:B:504:MET:HE2	2.41	0.56
1:B:420:LEU:HD12	1:B:421:TYR:N	2.21	0.56
1:B:192:ARG:HD3	1:C:413:ASN:OD1	2.06	0.56
1:D:331:LEU:HB3	1:D:334:TYR:CD2	2.40	0.56
1:C:35:ILE:O	3:C:703:NDP:N7N	2.39	0.56
1:D:497:GLU:N	1:D:497:GLU:OE2	2.38	0.56
1:D:28:ALA:HB3	3:D:704:NDP:O7N	2.06	0.55
1:A:37:ASP:CB	1:A:42:PRO:HD3	2.35	0.55
1:C:219:ASN:C	1:C:219:ASN:HD22	2.14	0.55
1:D:336:GLU:OE1	1:D:336:GLU:N	2.33	0.55
1:A:1:MET:H3	1:A:5:LYS:HD2	1.71	0.55
1:C:266:PHE:CE2	1:D:419:MET:HB2	2.41	0.55
1:D:376:LEU:HD13	1:D:385:MET:SD	2.45	0.55
1:B:113:PRO:O	1:B:118:ARG:HD2	2.07	0.55
1:D:177:ARG:HH12	1:D:192:ARG:HH22	1.52	0.55
1:A:99:LEU:HD12	1:A:159:VAL:HG22	1.88	0.55
1:B:219:ASN:HD22	1:B:220:GLY:N	2.04	0.55
1:B:276:ASN:C	1:B:277:ASN:HD22	2.15	0.55
1:D:175:ILE:HB	1:D:230:LEU:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:35:ILE:HG13	1:B:36:GLY:N	2.21	0.55
1:B:295:GLU:O	1:B:298:TRP:HB3	2.05	0.55
1:D:41:ILE:O	1:D:43:TRP:N	2.35	0.55
1:D:386:LEU:HB2	1:D:407:ALA:O	2.07	0.55
1:B:245:ASP:O	1:B:249:ARG:HB2	2.06	0.55
1:A:146:PRO:CB	1:A:505:GLU:HG2	2.32	0.54
1:B:491:ARG:HD3	1:B:493:ARG:NH1	2.22	0.54
1:D:397:ARG:HG2	1:D:397:ARG:NH1	2.15	0.54
1:A:31:GLU:OE2	1:A:181:ARG:NH1	2.40	0.54
1:A:420:LEU:HD12	1:A:421:TYR:H	1.73	0.54
1:C:87:LYS:HG3	1:C:88:PHE:CD2	2.42	0.54
1:D:39:ARG:N	1:D:187:CYS:SG	2.81	0.54
1:D:114:ASP:OD1	1:D:116:GLU:HG2	2.08	0.54
1:D:138:LEU:HD22	1:D:144:TYR:CE2	2.42	0.54
1:B:289:TRP:HH2	1:B:440:LEU:HD13	1.71	0.54
1:B:331:LEU:HB3	1:B:334:TYR:CD2	2.43	0.54
1:D:331:LEU:HD13	1:D:334:TYR:HE2	1.73	0.54
1:A:299:PHE:HB3	1:A:347:TRP:CZ3	2.43	0.54
1:C:34:GLY:O	1:C:43:TRP:HH2	1.90	0.54
1:A:18:LEU:HD22	1:A:488:VAL:HG11	1.88	0.54
1:B:181:ARG:HG2	1:B:181:ARG:HH11	1.72	0.54
1:B:467:SER:O	1:B:470:VAL:HG23	2.07	0.54
1:C:164:LEU:HA	1:C:169:VAL:CG1	2.38	0.54
1:C:233:ARG:CZ	1:C:235:ARG:NH1	2.71	0.54
1:B:206:TRP:CH2	1:B:232:PRO:HG3	2.43	0.54
1:D:30:ASP:HB3	1:D:43:TRP:CH2	2.43	0.54
1:B:331:LEU:HD22	1:B:334:TYR:CE2	2.43	0.54
1:B:55:LEU:HD21	1:B:176:TYR:CD1	2.43	0.54
1:B:386:LEU:HB3	1:B:408:GLN:HG3	1.90	0.54
1:B:395:LEU:N	1:B:396:PRO:CD	2.71	0.53
1:B:491:ARG:HD3	1:B:493:ARG:HH12	1.73	0.53
1:D:25:LEU:HD23	1:D:25:LEU:C	2.33	0.53
1:B:236:GLU:O	1:B:239:GLN:HB2	2.09	0.53
1:D:99:LEU:HD12	1:D:159:VAL:HG22	1.91	0.53
1:D:116:GLU:HA	1:D:119:ASN:HB3	1.90	0.53
1:D:285:LYS:HD2	1:D:476:GLN:HE22	1.73	0.53
1:D:407:ALA:HA	1:D:419:MET:O	2.08	0.53
1:B:58:LYS:O	1:B:72:ASN:ND2	2.40	0.53
1:B:45:VAL:HG21	1:B:180:ILE:HD12	1.91	0.53
1:B:146:PRO:HG3	1:B:505:GLU:HG2	1.90	0.53
1:B:428:GLY:O	1:B:429:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:207:GLN:HE21	1:C:233:ARG:HD2	1.72	0.53
1:C:279:LEU:HD23	1:C:281:LEU:CG	2.34	0.53
1:B:235:ARG:HB2	5:B:1152:HOH:O	2.08	0.53
1:A:219:ASN:N	1:A:219:ASN:HD22	2.05	0.53
1:C:392:PRO:HD2	1:D:350:PHE:CE1	2.44	0.53
1:D:12:VAL:HG13	1:D:13:ALA:N	2.24	0.53
1:A:289:TRP:HH2	1:A:440:LEU:HG	1.74	0.53
1:B:405:LEU:HD12	1:B:406:LEU:HB2	1.90	0.53
1:C:296:LEU:HD21	1:C:441:LEU:HB2	1.90	0.53
1:C:473:CYS:O	1:C:477:LEU:HG	2.08	0.53
1:D:341:PRO:O	1:D:398:MET:HE2	2.08	0.53
1:D:425:CYS:SG	1:D:460:LEU:HD13	2.48	0.53
1:A:340:GLY:HA2	1:A:354:TYR:CE2	2.44	0.53
1:B:156:GLY:HA3	3:B:702:NDP:O2A	2.09	0.53
1:B:314:VAL:HA	5:B:1183:HOH:O	2.09	0.53
1:C:282:LEU:HD12	1:C:432:PRO:HG3	1.91	0.53
1:C:406:LEU:HD22	1:D:406:LEU:HD21	1.91	0.53
1:D:234:ASN:C	1:D:234:ASN:ND2	2.67	0.53
1:D:307:LYS:HA	1:D:310:SER:OG	2.09	0.53
1:B:321:GLY:O	1:B:336:GLU:HG3	2.09	0.53
1:C:35:ILE:HG13	1:C:36:GLY:N	2.24	0.53
1:C:376:LEU:CD1	1:C:385:MET:SD	2.97	0.53
1:B:96:ASN:HD22	1:B:96:ASN:N	2.07	0.53
1:C:242:SER:O	1:C:245:ASP:HB3	2.08	0.53
1:C:315:HIS:HB3	1:C:318:ASP:OD1	2.09	0.53
1:C:388:THR:HB	1:C:406:LEU:HD12	1.91	0.53
1:D:357:HIS:O	1:D:359:ALA:N	2.42	0.53
1:C:248:ILE:HA	1:C:263:LEU:HD12	1.91	0.52
1:C:350:PHE:CZ	1:D:392:PRO:HD2	2.44	0.52
1:D:41:ILE:N	1:D:42:PRO:HD3	2.24	0.52
1:C:165:ARG:C	1:C:169:VAL:HG22	2.34	0.52
1:D:8:MET:HE1	1:D:448:ALA:HA	1.90	0.52
1:D:155:GLY:HA2	3:D:704:NDP:H5N	1.91	0.52
1:A:208:ARG:HD3	1:A:228:GLU:OE1	2.09	0.52
1:B:423:ARG:HG3	1:B:424:SER:N	2.24	0.52
1:D:36:GLY:N	1:D:43:TRP:CZ2	2.76	0.52
1:A:289:TRP:CH2	1:A:440:LEU:HG	2.44	0.52
1:B:342:VAL:HG12	1:B:398:MET:HB3	1.91	0.52
1:D:115:GLU:HA	1:D:118:ARG:HH11	1.72	0.52
1:A:43:TRP:CD1	1:A:43:TRP:O	2.63	0.52
1:B:115:GLU:HA	1:B:118:ARG:HD3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:MET:CE	1:D:448:ALA:HA	2.40	0.52
1:D:293:CYS:O	1:D:297:LEU:HD22	2.09	0.52
1:A:60:ARG:HH22	1:A:508:ASP:HA	1.73	0.52
1:A:350:PHE:CE1	1:B:392:PRO:HD2	2.44	0.52
1:B:31:GLU:OE1	1:B:181:ARG:HD3	2.10	0.52
1:C:155:GLY:HA2	1:C:160:TYR:CZ	2.45	0.52
1:C:469:HIS:C	1:C:472:PRO:HD2	2.35	0.52
1:B:299:PHE:HB3	1:B:347:TRP:CZ3	2.45	0.52
1:B:469:HIS:O	1:B:472:PRO:HD2	2.09	0.52
1:B:472:PRO:CG	1:B:517:MET:HE3	2.40	0.52
1:C:376:LEU:HD13	1:C:385:MET:SD	2.49	0.52
1:B:296:LEU:HD22	1:B:440:LEU:HD23	1.92	0.52
1:A:162:GLU:HA	1:A:165:ARG:NH1	2.25	0.51
1:B:296:LEU:O	1:B:300:LEU:HD23	2.10	0.51
1:B:472:PRO:O	1:B:475:GLU:HB2	2.10	0.51
1:D:115:GLU:HA	1:D:118:ARG:HG2	1.92	0.51
1:A:296:LEU:HD13	1:A:296:LEU:C	2.34	0.51
1:A:413:ASN:OD1	1:D:192:ARG:HD3	2.10	0.51
1:A:424:SER:OG	1:B:383:ARG:HD2	2.11	0.51
1:B:169:VAL:C	1:B:171:LEU:N	2.68	0.51
1:B:192:ARG:HD3	1:C:413:ASN:CG	2.35	0.51
1:B:285:LYS:CE	1:B:515:ILE:HD11	2.37	0.51
1:B:380:PRO:HB2	1:B:411:VAL:HG11	1.93	0.51
1:B:490:ARG:HG2	1:B:503:ASP:O	2.10	0.51
1:C:155:GLY:CA	3:C:703:NDP:H5N	2.40	0.51
1:D:59:LEU:HD13	1:D:70:LYS:HG3	1.91	0.51
1:A:16:THR:O	1:A:16:THR:HG22	2.10	0.51
1:B:86:PRO:HG3	1:B:89:ARG:NH1	2.26	0.51
1:B:288:PHE:O	1:B:292:VAL:HG23	2.11	0.51
1:D:20:LEU:HD23	1:D:137:ARG:HG3	1.92	0.51
1:D:63:ASN:C	1:D:63:ASN:HD22	2.19	0.51
1:A:208:ARG:HH21	1:C:263:LEU:HD13	1.75	0.51
1:B:282:LEU:HD12	1:B:432:PRO:HB3	1.92	0.51
1:B:321:GLY:C	1:B:337:MET:HE2	2.35	0.51
1:D:434:ASN:N	1:D:434:ASN:HD22	2.08	0.51
1:A:256:ASP:OD2	1:A:260:VAL:HB	2.09	0.51
1:B:169:VAL:C	1:B:171:LEU:H	2.19	0.51
1:D:106:GLN:HA	1:D:109:LEU:HD23	1.92	0.51
1:D:347:TRP:HE1	1:D:389:ALA:HB2	1.75	0.51
1:B:37:ASP:OD2	1:B:42:PRO:HG2	2.11	0.51
1:B:206:TRP:CZ3	1:B:232:PRO:HG3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:490:ARG:HB3	1:D:490:ARG:NH1	2.25	0.51
1:A:115:GLU:OE2	1:A:118:ARG:NE	2.42	0.51
1:A:374:GLU:O	1:A:378:THR:HG23	2.11	0.50
1:B:98:VAL:HB	1:B:108:LEU:HD21	1.92	0.50
1:A:62:LYS:O	1:A:63:ASN:CB	2.56	0.50
1:A:392:PRO:HD2	1:B:350:PHE:CZ	2.47	0.50
1:C:342:VAL:HG12	1:C:398:MET:HB3	1.92	0.50
1:D:243:LEU:HD23	1:D:427:MET:HE1	1.94	0.50
1:A:19:ALA:O	1:A:20:LEU:HD23	2.11	0.50
1:B:165:ARG:C	1:B:169:VAL:HG22	2.36	0.50
1:D:35:ILE:C	1:D:37:ASP:N	2.68	0.50
1:D:40:SER:OG	1:D:41:ILE:N	2.44	0.50
1:D:336:GLU:O	1:D:337:MET:HB2	2.12	0.50
1:A:84:ILE:O	1:A:89:ARG:HD3	2.10	0.50
1:A:84:ILE:HD13	1:A:91:LEU:HD21	1.92	0.50
1:C:281:LEU:HD21	1:C:289:TRP:HE3	1.77	0.50
1:B:296:LEU:HG	1:B:300:LEU:HD23	1.94	0.50
1:B:386:LEU:HB2	1:B:407:ALA:O	2.11	0.50
1:C:431:VAL:O	1:C:435:ILE:HG13	2.12	0.50
1:D:355:THR:HG22	1:D:356:HIS:HD2	1.74	0.50
1:A:271:ARG:NH2	1:B:266:PHE:O	2.39	0.50
1:B:146:PRO:CG	1:B:505:GLU:HG2	2.41	0.50
1:C:175:ILE:HB	1:C:230:LEU:HB2	1.92	0.50
1:C:407:ALA:HA	1:C:419:MET:O	2.12	0.50
1:C:420:LEU:HD23	1:C:458:HIS:CD2	2.47	0.50
1:A:37:ASP:HB2	1:A:42:PRO:CD	2.42	0.49
1:B:109:LEU:CD1	1:B:125:ILE:HD12	2.41	0.49
1:B:285:LYS:CB	1:B:476:GLN:NE2	2.75	0.49
1:B:292:VAL:HG13	1:B:437:SER:OG	2.12	0.49
1:D:195:GLU:HB3	1:D:198:THR:CG2	2.40	0.49
1:A:180:ILE:HG23	1:A:223:THR:HG21	1.93	0.49
1:B:361:TYR:O	1:B:362:ASP:C	2.55	0.49
1:D:110:ASP:C	1:D:112:LEU:H	2.21	0.49
1:D:193:VAL:O	1:D:194:PRO:C	2.55	0.49
1:D:357:HIS:CG	1:D:358:ASP:H	2.30	0.49
1:A:264:SER:HB3	1:A:464:HIS:HB3	1.94	0.49
1:D:110:ASP:HA	1:D:118:ARG:NE	2.28	0.49
1:C:406:LEU:HB3	1:C:421:TYR:HB3	1.94	0.49
1:B:207:GLN:O	1:B:230:LEU:HA	2.13	0.49
1:B:395:LEU:HB2	1:B:396:PRO:HD3	1.94	0.49
1:C:6:ILE:HD11	1:C:370:LYS:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:101:SER:HA	1:D:129:ASN:ND2	2.27	0.49
1:D:247:ILE:O	1:D:251:GLY:N	2.44	0.49
1:D:279:LEU:HD22	1:D:487:LEU:HB2	1.94	0.49
1:A:183:SER:O	1:A:184:GLU:HB2	2.13	0.49
1:B:132:LEU:HB3	1:B:162:GLU:HG2	1.94	0.49
1:C:52:PHE:CD1	1:C:52:PHE:C	2.91	0.49
1:C:116:GLU:HA	1:C:119:ASN:HD22	1.78	0.49
1:C:92:PRO:O	1:C:94:ARG:NE	2.43	0.49
1:B:84:ILE:CG2	1:B:89:ARG:HG2	2.43	0.48
1:B:104:THR:HB	1:B:107:HIS:ND1	2.28	0.48
1:D:333:GLU:O	1:D:356:HIS:HE1	1.96	0.48
1:A:139:LEU:HD13	1:A:151:VAL:HG22	1.94	0.48
1:C:296:LEU:C	1:C:296:LEU:CD1	2.86	0.48
1:C:304:THR:HB	1:C:340:GLY:O	2.13	0.48
1:C:340:GLY:HA2	1:C:354:TYR:CE2	2.49	0.48
1:C:386:LEU:HB3	1:C:408:GLN:HA	1.94	0.48
1:A:331:LEU:HB3	1:A:334:TYR:CD2	2.48	0.48
1:C:100:SER:O	1:C:129:ASN:HA	2.13	0.48
1:C:397:ARG:HG3	1:C:397:ARG:HH11	1.78	0.48
1:A:372:ILE:HG21	1:A:409:PHE:CD1	2.49	0.48
1:B:233:ARG:NH1	1:D:249:ARG:NH2	2.61	0.48
1:B:515:ILE:O	1:B:517:MET:N	2.42	0.48
1:A:2:SER:H	1:A:5:LYS:HD3	1.77	0.48
1:B:388:THR:HB	1:B:406:LEU:HD13	1.96	0.48
1:A:431:VAL:HB	1:A:432:PRO:HD3	1.96	0.48
1:B:52:PHE:CE1	1:B:56:THR:HG21	2.48	0.48
1:C:219:ASN:C	1:C:219:ASN:ND2	2.71	0.48
1:D:138:LEU:HD22	1:D:144:TYR:HE2	1.77	0.48
1:D:325:PHE:O	1:D:328:SER:HB3	2.14	0.48
1:A:139:LEU:HD13	1:A:151:VAL:CG2	2.43	0.48
1:B:208:ARG:NH2	1:D:251:GLY:O	2.41	0.48
1:C:155:GLY:O	1:C:159:VAL:HG21	2.13	0.48
1:C:296:LEU:HD13	1:C:296:LEU:O	2.14	0.48
1:D:183:SER:O	1:D:184:GLU:C	2.57	0.48
1:D:394:ALA:O	1:D:395:LEU:C	2.56	0.48
1:A:25:LEU:HD11	1:A:160:TYR:HD1	1.79	0.48
1:A:256:ASP:CG	1:A:260:VAL:HB	2.39	0.48
1:B:39:ARG:O	1:B:40:SER:HB2	2.12	0.48
1:C:467:SER:O	1:C:470:VAL:HG23	2.13	0.48
1:A:231:ILE:HB	1:A:232:PRO:HD2	1.96	0.48
1:B:27:VAL:HG22	1:B:28:ALA:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:ASP:CG	1:C:42:PRO:HG3	2.39	0.48
1:C:192:ARG:HG2	1:C:192:ARG:NH1	2.26	0.48
1:D:295:GLU:OE1	1:D:433:PHE:HE2	1.97	0.48
1:D:423:ARG:HG3	1:D:423:ARG:HH11	1.78	0.48
1:B:422:GLN:HG2	1:B:425:CYS:SG	2.54	0.47
1:C:75:VAL:O	1:C:154:ILE:HG12	2.14	0.47
1:B:20:LEU:HB2	1:B:171:LEU:CD1	2.44	0.47
1:D:153:CYS:SG	1:D:159:VAL:HG12	2.54	0.47
1:C:422:GLN:HE22	1:C:434:ASN:ND2	2.10	0.47
1:D:290:ARG:HG2	1:D:290:ARG:HH11	1.79	0.47
1:A:208:ARG:HD2	1:A:211:ILE:HB	1.96	0.47
1:D:29:VAL:HG22	1:D:33:GLY:C	2.39	0.47
1:A:292:VAL:HA	1:A:433:PHE:CZ	2.50	0.47
1:A:413:ASN:CG	1:D:192:ARG:HD3	2.40	0.47
1:C:345:PHE:HE2	1:C:361:TYR:CD2	2.31	0.47
1:C:346:GLN:O	1:C:350:PHE:HB2	2.13	0.47
1:D:186:SER:C	1:D:187:CYS:SG	2.97	0.47
1:A:36:GLY:O	1:A:187:CYS:HB3	2.14	0.47
1:A:76:MET:SD	1:A:154:ILE:HD11	2.54	0.47
1:B:285:LYS:CD	1:B:476:GLN:NE2	2.76	0.47
1:C:441:LEU:C	1:C:441:LEU:HD23	2.39	0.47
1:D:78:ARG:HE	1:D:103:LEU:HD11	1.79	0.47
1:D:338:ASP:OD2	1:D:354:TYR:OH	2.29	0.47
1:D:456:LEU:C	1:D:456:LEU:HD13	2.40	0.47
1:A:128:VAL:HG23	1:A:128:VAL:O	2.14	0.47
1:A:257:ARG:HD3	1:A:257:ARG:N	2.25	0.47
1:A:487:LEU:HD11	1:A:504:MET:HB2	1.96	0.47
1:D:253:VAL:HG22	1:D:263:LEU:CD2	2.43	0.47
1:A:296:LEU:HD21	1:A:441:LEU:HB2	1.96	0.47
1:C:18:LEU:HD22	1:C:488:VAL:HG11	1.96	0.47
1:D:73:ALA:HB2	1:D:148:ILE:HG21	1.97	0.47
1:B:65:LYS:HD2	1:B:65:LYS:N	2.30	0.47
1:B:320:ASN:ND2	1:B:400:LEU:HD22	2.30	0.47
1:A:273:SER:O	1:A:274:LEU:HD23	2.15	0.47
1:A:478:LYS:HD3	1:C:478:LYS:HZ2	1.79	0.47
1:D:342:VAL:O	1:D:343:TYR:C	2.58	0.47
1:A:74:VAL:HB	1:A:154:ILE:CG2	2.44	0.46
1:B:37:ASP:OD2	1:B:42:PRO:CG	2.63	0.46
1:B:257:ARG:H	1:B:257:ARG:CD	2.14	0.46
1:C:386:LEU:HD12	1:C:406:LEU:HD11	1.96	0.46
1:D:485:PRO:C	1:D:486:TYR:CD1	2.93	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:SER:HA	1:A:495:PHE:CE2	2.50	0.46
1:A:109:LEU:O	1:A:118:ARG:HD3	2.15	0.46
1:A:170:HIS:C	1:A:171:LEU:HD12	2.40	0.46
1:B:25:LEU:C	1:B:25:LEU:HD23	2.40	0.46
1:C:164:LEU:C	1:C:169:VAL:HG13	2.40	0.46
1:C:405:LEU:HD12	1:C:406:LEU:HB2	1.96	0.46
1:D:42:PRO:CB	1:D:185:SER:OG	2.62	0.46
1:D:218:ALA:C	1:D:220:GLY:H	2.23	0.46
1:A:422:GLN:HE21	1:A:425:CYS:HA	1.80	0.46
1:C:15:GLY:HA3	5:C:1110:HOH:O	2.15	0.46
1:C:266:PHE:HA	1:C:461:GLY:O	2.15	0.46
1:D:341:PRO:HD3	1:D:354:TYR:CD2	2.50	0.46
1:D:405:LEU:HD12	1:D:406:LEU:HD23	1.97	0.46
1:D:496:LEU:HD12	1:D:496:LEU:O	2.15	0.46
1:A:460:LEU:HD23	1:A:460:LEU:N	2.30	0.46
1:B:12:VAL:HG13	1:B:13:ALA:N	2.29	0.46
1:B:233:ARG:NH1	1:D:249:ARG:HH21	2.13	0.46
1:D:237:GLU:HB3	1:D:481:PRO:HB3	1.98	0.46
1:A:13:ALA:HB2	1:A:492:GLU:HG3	1.96	0.46
1:B:3:LEU:HD23	1:B:3:LEU:O	2.16	0.46
1:B:152:TYR:O	1:B:154:ILE:HG23	2.16	0.46
1:A:361:TYR:O	1:A:362:ASP:C	2.59	0.46
1:B:323:ARG:NH2	1:B:326:LEU:HB3	2.31	0.46
1:C:30:ASP:OD2	1:C:32:HIS:N	2.49	0.46
1:D:183:SER:O	1:D:184:GLU:O	2.34	0.46
1:B:41:ILE:HD11	1:B:43:TRP:O	2.16	0.46
1:B:78:ARG:HG3	1:B:103:LEU:HD12	1.96	0.46
1:B:219:ASN:HD21	1:B:221:ASN:H	1.56	0.46
1:C:74:VAL:HG23	1:C:74:VAL:O	2.14	0.46
1:C:267:GLY:HA2	1:C:460:LEU:O	2.15	0.46
1:C:400:LEU:HD11	1:D:384:ARG:NH2	2.30	0.46
1:D:162:GLU:HG3	1:D:165:ARG:NH1	2.31	0.46
1:D:265:ILE:HD12	1:D:265:ILE:C	2.40	0.46
1:A:341:PRO:HB2	1:A:346:GLN:HE21	1.80	0.46
1:A:490:ARG:NH1	1:A:490:ARG:CB	2.79	0.46
2:B:602:ICY:H16	3:B:702:NDP:H42N	1.97	0.46
1:C:25:LEU:C	1:C:25:LEU:HD23	2.41	0.46
1:C:181:ARG:HB3	1:C:181:ARG:NH1	2.31	0.46
1:B:45:VAL:HG21	1:B:180:ILE:CD1	2.46	0.46
1:B:433:PHE:O	1:B:436:ALA:HB3	2.16	0.46
1:C:211:ILE:HG23	1:C:211:ILE:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:427:MET:SD	1:C:431:VAL:HG21	2.55	0.46
1:D:215:LEU:O	1:D:224:LYS:HA	2.15	0.46
1:D:219:ASN:C	1:D:219:ASN:HD22	2.23	0.46
1:D:490:ARG:HB3	1:D:490:ARG:CZ	2.46	0.46
1:A:427:MET:SD	1:A:431:VAL:HG21	2.56	0.45
1:C:294:GLU:O	1:C:298:TRP:HB2	2.16	0.45
1:C:476:GLN:NE2	1:C:517:MET:HE1	2.31	0.45
1:D:282:LEU:HD12	1:D:432:PRO:HB3	1.98	0.45
1:B:205:GLU:HA	5:B:1041:HOH:O	2.16	0.45
1:D:315:HIS:HB3	1:D:318:ASP:OD1	2.15	0.45
1:A:180:ILE:HG23	1:A:223:THR:CG2	2.46	0.45
1:B:277:ASN:O	1:B:486:TYR:HA	2.16	0.45
1:B:316:ILE:HG13	1:B:317:TRP:CD1	2.52	0.45
1:D:84:ILE:O	1:D:85:PRO:C	2.58	0.45
1:D:298:TRP:HH2	1:D:339:LEU:HD12	1.80	0.45
1:C:163:ALA:O	1:C:169:VAL:HG13	2.17	0.45
1:C:164:LEU:CA	1:C:169:VAL:HG13	2.45	0.45
1:C:281:LEU:O	1:C:282:LEU:C	2.60	0.45
1:A:380:PRO:HB2	1:A:411:VAL:HG11	1.98	0.45
1:B:153:CYS:SG	1:B:159:VAL:HG12	2.56	0.45
1:C:112:LEU:HB2	1:C:118:ARG:HG2	1.98	0.45
1:D:397:ARG:CG	1:D:397:ARG:NH1	2.72	0.45
1:A:476:GLN:HB2	1:A:515:ILE:CD1	2.47	0.45
1:B:68:PRO:HA	1:B:71:ARG:HD3	1.98	0.45
1:D:104:THR:O	1:D:107:HIS:HB2	2.16	0.45
1:D:116:GLU:C	1:D:119:ASN:HB3	2.42	0.45
1:D:285:LYS:HD2	1:D:476:GLN:NE2	2.31	0.45
1:D:386:LEU:CB	1:D:408:GLN:HA	2.45	0.45
1:C:292:VAL:HA	1:C:433:PHE:CZ	2.52	0.45
1:B:164:LEU:C	1:B:169:VAL:HG13	2.42	0.45
1:B:456:LEU:HD22	1:B:457:VAL:N	2.32	0.45
1:C:310:SER:OG	1:C:337:MET:HE2	2.17	0.45
1:B:279:LEU:O	1:B:485:PRO:HD2	2.17	0.45
1:B:296:LEU:HD22	1:B:440:LEU:CG	2.47	0.45
1:C:39:ARG:O	1:C:39:ARG:HG2	2.15	0.45
1:C:179:THR:O	1:C:225:TYR:HA	2.17	0.45
1:C:317:TRP:HB2	5:C:1026:HOH:O	2.17	0.45
1:D:35:ILE:HG12	1:D:189:VAL:O	2.17	0.45
1:D:36:GLY:O	1:D:37:ASP:HB2	2.16	0.45
1:D:208:ARG:NH1	1:D:228:GLU:OE1	2.46	0.45
1:B:78:ARG:HD3	3:B:702:NDP:O2X	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:262:THR:HG22	1:B:466:TYR:CD2	2.51	0.44
1:A:185:SER:O	1:A:186:SER:C	2.60	0.44
1:A:265:ILE:HD12	1:A:265:ILE:C	2.42	0.44
1:C:138:LEU:O	1:C:141:SER:OG	2.31	0.44
1:C:431:VAL:O	1:C:432:PRO:C	2.58	0.44
1:D:325:PHE:HA	1:D:328:SER:HB3	1.99	0.44
1:C:98:VAL:HB	1:C:108:LEU:HD21	1.99	0.44
1:C:266:PHE:CZ	1:D:419:MET:HB2	2.52	0.44
1:C:382:ASP:O	1:C:385:MET:HE2	2.17	0.44
1:D:295:GLU:O	1:D:298:TRP:HB3	2.18	0.44
1:A:320:ASN:HA	1:A:325:PHE:CD2	2.53	0.44
1:A:342:VAL:O	1:A:343:TYR:C	2.60	0.44
1:B:35:ILE:O	3:B:702:NDP:N7N	2.50	0.44
1:B:233:ARG:CZ	1:B:235:ARG:NH1	2.80	0.44
1:C:232:PRO:O	1:C:233:ARG:C	2.59	0.44
1:A:74:VAL:HB	1:A:154:ILE:HG23	1.99	0.44
1:A:78:ARG:NH1	1:A:82:ASP:OD1	2.42	0.44
1:A:175:ILE:HB	1:A:230:LEU:HB2	2.00	0.44
1:B:428:GLY:C	1:B:429:LEU:HD23	2.42	0.44
1:C:115:GLU:C	1:C:117:LYS:H	2.24	0.44
1:C:275:ARG:HH12	1:C:455:GLU:CG	2.31	0.44
1:A:42:PRO:HG2	1:A:43:TRP:CE3	2.53	0.44
1:A:153:CYS:SG	1:A:159:VAL:HG12	2.58	0.44
1:B:30:ASP:O	1:B:32:HIS:N	2.51	0.44
1:C:279:LEU:HD13	1:C:487:LEU:HD22	1.98	0.44
1:C:279:LEU:CD1	1:C:487:LEU:HD22	2.48	0.44
1:D:45:VAL:HA	1:D:46:PRO:HD2	1.88	0.44
1:D:278:ARG:HH11	1:D:278:ARG:CG	2.27	0.44
1:A:341:PRO:HB2	1:A:346:GLN:NE2	2.33	0.44
1:B:441:LEU:O	1:B:445:ILE:HG12	2.17	0.44
1:D:304:THR:HG22	1:D:345:PHE:HB2	2.00	0.44
1:D:391:ASN:OD1	1:D:393:SER:HB2	2.17	0.44
1:D:395:LEU:N	1:D:396:PRO:CD	2.81	0.44
1:A:249:ARG:HE	1:A:249:ARG:HB2	1.62	0.44
1:B:37:ASP:C	1:B:39:ARG:N	2.76	0.44
1:B:296:LEU:O	1:B:299:PHE:HB2	2.18	0.44
1:C:31:GLU:HG3	1:C:181:ARG:HA	1.99	0.44
1:D:29:VAL:CG2	1:D:33:GLY:C	2.91	0.44
1:D:40:SER:C	1:D:41:ILE:HD12	2.43	0.44
1:D:100:SER:O	1:D:129:ASN:HA	2.17	0.44
1:A:115:GLU:O	1:A:116:GLU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:O	1:A:224:LYS:HA	2.17	0.43
1:A:321:GLY:O	1:A:337:MET:N	2.51	0.43
1:B:4:PHE:CE1	1:B:362:ASP:HB3	2.53	0.43
1:B:14:GLU:N	1:B:14:GLU:OE1	2.51	0.43
1:B:296:LEU:HD22	1:B:440:LEU:CD2	2.48	0.43
1:C:386:LEU:N	1:C:386:LEU:HD23	2.33	0.43
1:D:8:MET:HE1	1:D:448:ALA:CA	2.48	0.43
1:D:357:HIS:C	1:D:359:ALA:H	2.26	0.43
1:A:30:ASP:OD2	1:A:30:ASP:C	2.61	0.43
1:B:164:LEU:HD13	1:B:192:ARG:O	2.18	0.43
1:C:254:LYS:O	1:C:261:GLY:HA2	2.18	0.43
1:A:420:LEU:HD12	1:A:421:TYR:N	2.33	0.43
1:B:104:THR:CG2	1:B:106:GLN:H	2.31	0.43
1:B:146:PRO:HG3	1:B:505:GLU:CG	2.47	0.43
1:B:296:LEU:HD22	1:B:440:LEU:HG	2.00	0.43
1:C:288:PHE:CD1	1:C:291:GLY:HA3	2.53	0.43
1:D:36:GLY:HA2	1:D:43:TRP:CZ2	2.53	0.43
1:A:258:THR:HB	1:A:260:VAL:HG23	2.00	0.43
1:B:155:GLY:HA2	1:B:160:TYR:CZ	2.52	0.43
1:B:479:ARG:HD3	1:B:512:TYR:CG	2.54	0.43
1:D:155:GLY:HA2	1:D:160:TYR:CZ	2.53	0.43
1:A:27:VAL:HG22	1:A:28:ALA:N	2.33	0.43
1:B:243:LEU:HD23	1:B:427:MET:HE1	2.01	0.43
1:B:256:ASP:HB3	1:B:258:THR:H	1.83	0.43
1:B:272:PHE:CZ	1:B:435:ILE:HD13	2.54	0.43
1:B:285:LYS:HB2	1:B:476:GLN:CD	2.44	0.43
1:C:5:LYS:HB3	1:C:497:GLU:OE2	2.19	0.43
1:C:404:HIS:H	1:C:404:HIS:CD2	2.35	0.43
1:C:515:ILE:C	1:C:517:MET:H	2.27	0.43
1:D:59:LEU:CD1	1:D:70:LYS:HG3	2.49	0.43
1:B:387:PHE:O	1:B:406:LEU:HD12	2.18	0.43
1:C:310:SER:C	1:C:312:LYS:H	2.26	0.43
1:D:422:GLN:NE2	1:D:425:CYS:HB3	2.33	0.43
1:A:155:GLY:HA2	1:A:160:TYR:CZ	2.54	0.43
1:A:36:GLY:HA3	3:A:701:NDP:H1D	2.01	0.43
1:A:207:GLN:NE2	1:A:480:VAL:HG11	2.34	0.43
1:A:430:GLY:O	1:A:434:ASN:ND2	2.52	0.43
1:B:99:LEU:HD12	1:B:159:VAL:HG22	2.00	0.43
1:B:104:THR:HG22	1:B:106:GLN:N	2.31	0.43
1:B:390:TRP:CE3	1:B:405:LEU:HD22	2.53	0.43
1:C:23:PHE:N	1:C:23:PHE:CD2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:PHE:CE2	1:D:362:ASP:HB3	2.54	0.43
1:D:244:VAL:O	1:D:248:ILE:HG13	2.19	0.43
1:A:232:PRO:O	1:A:233:ARG:C	2.61	0.43
1:B:233:ARG:HD3	1:B:235:ARG:NE	2.34	0.43
1:D:40:SER:O	1:D:42:PRO:HD3	2.18	0.43
1:D:357:HIS:CG	1:D:358:ASP:N	2.87	0.43
1:A:43:TRP:CH2	1:A:187:CYS:SG	3.11	0.42
1:C:243:LEU:O	1:C:247:ILE:HG13	2.19	0.42
1:D:125:ILE:HG22	1:D:126:VAL:N	2.34	0.42
1:A:25:LEU:HD11	1:A:160:TYR:CD1	2.54	0.42
1:A:115:GLU:OE2	1:A:118:ARG:NH1	2.50	0.42
1:A:289:TRP:CZ2	1:A:487:LEU:HD13	2.54	0.42
1:A:386:LEU:HD22	1:A:408:GLN:HG3	2.01	0.42
1:A:423:ARG:HG3	1:A:424:SER:N	2.34	0.42
1:A:440:LEU:HD22	1:A:444:LEU:CD1	2.49	0.42
1:B:43:TRP:HH2	1:B:187:CYS:SG	2.42	0.42
1:B:61:GLY:C	1:B:63:ASN:H	2.25	0.42
1:B:420:LEU:HD12	1:B:421:TYR:H	1.84	0.42
1:C:376:LEU:HB3	1:C:449:THR:HG21	2.00	0.42
1:D:78:ARG:HG2	1:D:103:LEU:HD12	2.00	0.42
1:B:27:VAL:CG2	1:B:28:ALA:N	2.82	0.42
1:B:247:ILE:HG21	1:B:465:VAL:HG23	2.01	0.42
1:B:493:ARG:HB2	1:B:499:TYR:CE1	2.54	0.42
1:C:115:GLU:C	1:C:117:LYS:N	2.74	0.42
1:D:386:LEU:HD12	1:D:406:LEU:HD13	2.01	0.42
1:A:238:GLU:O	1:A:239:GLN:C	2.62	0.42
1:B:29:VAL:O	1:B:179:THR:HA	2.20	0.42
1:B:172:LEU:HD21	1:B:175:ILE:HD11	2.01	0.42
1:D:188:SER:HB2	1:D:190:PHE:CE1	2.54	0.42
1:A:422:GLN:HG2	1:A:424:SER:O	2.19	0.42
1:B:493:ARG:HB2	1:B:499:TYR:CZ	2.55	0.42
1:C:73:ALA:HB2	1:C:148:ILE:HD12	2.00	0.42
1:C:468:ASN:O	1:C:469:HIS:HD2	2.02	0.42
1:A:331:LEU:HD13	1:A:334:TYR:CE2	2.54	0.42
1:B:103:LEU:HB3	1:B:108:LEU:CD1	2.50	0.42
1:B:233:ARG:HE	1:B:235:ARG:HD3	1.84	0.42
1:C:472:PRO:HB2	1:C:517:MET:HG3	2.01	0.42
1:C:485:PRO:C	1:C:486:TYR:CD1	2.97	0.42
1:A:194:PRO:HB2	1:A:201:ALA:HA	2.01	0.42
1:A:490:ARG:HB2	1:A:490:ARG:NH1	2.33	0.42
1:B:35:ILE:HD11	1:B:189:VAL:HB	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:ARG:HG2	1:B:290:ARG:HH11	1.84	0.42
1:C:66:PRO:HA	1:C:70:LYS:O	2.20	0.42
1:D:390:TRP:HB2	1:D:405:LEU:HB2	2.02	0.42
1:A:256:ASP:HB2	1:A:257:ARG:HD3	2.01	0.42
1:A:390:TRP:HD1	1:B:388:THR:HG21	1.85	0.42
1:B:61:GLY:O	1:B:63:ASN:N	2.44	0.42
1:C:219:ASN:ND2	1:C:222:GLU:H	2.17	0.42
1:D:12:VAL:HG22	1:D:492:GLU:OE1	2.20	0.42
2:A:601:1CY:H16	3:A:701:NDP:H42N	2.01	0.42
1:C:114:ASP:OD2	1:C:117:LYS:HB2	2.19	0.42
1:C:258:THR:OG1	1:C:260:VAL:HG23	2.20	0.42
1:C:404:HIS:HB2	1:C:420:LEU:HD11	2.02	0.42
1:C:480:VAL:HA	1:C:481:PRO:HD3	1.84	0.42
1:D:138:LEU:C	1:D:140:ALA:H	2.28	0.42
1:D:475:GLU:OE2	1:D:515:ILE:HG12	2.20	0.42
1:B:74:VAL:O	1:B:74:VAL:HG12	2.20	0.42
1:C:30:ASP:OD2	1:C:30:ASP:C	2.63	0.42
1:C:249:ARG:NH1	1:C:249:ARG:HB2	2.35	0.42
1:C:276:ASN:O	1:C:277:ASN:HB2	2.19	0.42
1:A:139:LEU:O	1:A:144:TYR:HB2	2.19	0.41
1:B:4:PHE:CG	1:B:362:ASP:HB3	2.54	0.41
1:B:211:ILE:HG23	1:B:211:ILE:O	2.18	0.41
1:C:131:GLY:O	1:C:132:LEU:C	2.63	0.41
1:C:310:SER:C	1:C:312:LYS:N	2.78	0.41
1:A:26:VAL:HG13	1:A:55:LEU:HD23	2.03	0.41
1:A:311:ASP:C	1:A:313:GLY:N	2.78	0.41
1:B:237:GLU:HB3	1:B:481:PRO:HB3	2.02	0.41
1:C:87:LYS:CD	1:C:88:PHE:CE2	3.03	0.41
1:D:6:ILE:HD12	1:D:496:LEU:HD23	2.02	0.41
1:D:138:LEU:HD23	1:D:138:LEU:HA	1.90	0.41
1:A:76:MET:HB3	1:A:154:ILE:CG1	2.51	0.41
1:A:99:LEU:HD23	1:A:128:VAL:CG2	2.51	0.41
1:A:307:LYS:HA	1:A:310:SER:OG	2.21	0.41
1:C:279:LEU:HD21	1:C:289:TRP:CZ3	2.56	0.41
1:D:85:PRO:O	1:D:87:LYS:N	2.54	0.41
1:D:355:THR:CG2	1:D:356:HIS:CD2	3.00	0.41
1:B:237:GLU:CD	1:B:283:THR:H	2.29	0.41
1:C:290:ARG:HD2	5:C:1133:HOH:O	2.19	0.41
1:C:485:PRO:HB3	1:C:509:TYR:HA	2.03	0.41
1:D:253:VAL:HG22	1:D:263:LEU:HD22	2.02	0.41
1:D:443:ILE:O	1:D:447:LYS:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ASN:O	1:A:222:GLU:C	2.64	0.41
1:B:60:ARG:O	1:B:62:LYS:N	2.53	0.41
1:A:171:LEU:N	1:A:171:LEU:CD1	2.80	0.41
1:A:390:TRP:HB2	1:A:405:LEU:HD13	2.01	0.41
1:A:475:GLU:HB2	1:A:515:ILE:HG21	2.02	0.41
1:B:325:PHE:HE2	1:B:399:ALA:O	2.04	0.41
1:C:12:VAL:CG1	1:C:13:ALA:N	2.83	0.41
1:C:115:GLU:CG	1:C:118:ARG:NH1	2.81	0.41
1:C:281:LEU:HD21	1:C:289:TRP:CE3	2.55	0.41
1:D:73:ALA:HB3	1:D:151:VAL:HG22	2.01	0.41
1:D:116:GLU:CA	1:D:119:ASN:HB3	2.50	0.41
1:D:270:MET:HE2	1:D:460:LEU:HD21	2.02	0.41
1:D:278:ARG:NH1	1:D:278:ARG:CG	2.84	0.41
1:D:422:GLN:NE2	5:D:1210:HOH:O	2.52	0.41
1:A:346:GLN:HB3	1:A:389:ALA:HA	2.01	0.41
1:B:18:LEU:HD22	1:B:488:VAL:HG11	2.03	0.41
1:C:134:GLN:OE1	1:C:134:GLN:N	2.53	0.41
1:C:437:SER:O	1:C:440:LEU:HB3	2.20	0.41
1:A:329:ARG:HA	1:A:329:ARG:HD2	1.76	0.41
1:B:38:GLY:HA2	3:B:702:NDP:H4D	2.03	0.41
1:B:155:GLY:CA	3:B:702:NDP:H5N	2.43	0.41
1:B:394:ALA:O	1:B:398:MET:HG3	2.21	0.41
1:C:443:ILE:HD12	1:C:487:LEU:HD23	2.03	0.41
1:D:155:GLY:CA	3:D:704:NDP:H5N	2.50	0.41
1:D:211:ILE:HA	1:D:227:PHE:O	2.20	0.41
1:D:323:ARG:HH21	1:D:326:LEU:HB3	1.86	0.41
1:A:208:ARG:HG2	1:A:230:LEU:CD2	2.51	0.41
1:B:43:TRP:CH2	1:B:187:CYS:SG	3.14	0.41
1:B:239:GLN:NE2	1:B:271:ARG:H	2.12	0.41
1:B:298:TRP:CD1	1:B:309:LEU:HD13	2.56	0.41
1:D:78:ARG:HB2	1:D:100:SER:HB2	2.03	0.41
1:D:85:PRO:O	1:D:88:PHE:N	2.51	0.41
1:A:181:ARG:HH11	1:A:181:ARG:CB	2.18	0.40
1:B:240:TYR:CD1	1:B:240:TYR:C	2.99	0.40
1:B:422:GLN:HG2	1:B:424:SER:O	2.21	0.40
1:C:272:PHE:CE2	1:C:435:ILE:HD13	2.56	0.40
1:D:234:ASN:ND2	1:D:236:GLU:HB2	2.35	0.40
1:D:275:ARG:NE	1:D:415:GLU:OE2	2.54	0.40
1:D:425:CYS:SG	1:D:460:LEU:CD1	3.09	0.40
1:A:257:ARG:CD	1:A:257:ARG:N	2.81	0.40
1:B:135:ALA:O	1:B:139:LEU:HD22	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ARG:HG2	1:B:490:ARG:H	1.60	0.40
1:D:115:GLU:CG	1:D:118:ARG:HH11	2.34	0.40
1:D:420:LEU:HD13	1:D:438:TYR:CE1	2.56	0.40
1:A:462:ASP:C	1:A:462:ASP:OD2	2.64	0.40
1:B:49:MET:HE2	1:B:49:MET:HB3	1.81	0.40
1:B:381:ASP:O	1:B:382:ASP:C	2.64	0.40
1:C:386:LEU:HD22	1:C:408:GLN:HG3	2.02	0.40
1:D:245:ASP:O	1:D:249:ARG:HB2	2.21	0.40
1:A:105:THR:HG23	1:A:126:VAL:HA	2.03	0.40
1:B:37:ASP:HA	1:B:187:CYS:HA	2.04	0.40
1:B:172:LEU:HD11	1:B:174:ALA:O	2.21	0.40
1:C:306:ALA:C	1:C:337:MET:HE3	2.46	0.40
1:C:323:ARG:HB2	1:C:336:GLU:OE2	2.21	0.40
1:C:467:SER:C	1:C:469:HIS:H	2.29	0.40
1:D:269:GLN:NE2	1:D:419:MET:HE1	2.36	0.40
1:A:221:ASN:OD1	1:A:221:ASN:N	2.54	0.40
1:A:294:GLU:OE2	1:A:312:LYS:HD3	2.21	0.40
1:B:245:ASP:OD2	1:B:249:ARG:NH1	2.47	0.40
1:C:233:ARG:CZ	1:C:235:ARG:HH12	2.34	0.40
1:C:286:ARG:HA	1:C:509:TYR:OH	2.22	0.40
1:D:309:LEU:HD12	1:D:309:LEU:HA	1.93	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	514/521 (99%)	468 (91%)	37 (7%)	9 (2%)	6	14
1	B	514/521 (99%)	467 (91%)	36 (7%)	11 (2%)	5	11
1	C	514/521 (99%)	467 (91%)	39 (8%)	8 (2%)	7	16
1	D	511/521 (98%)	446 (87%)	45 (9%)	20 (4%)	2	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2053/2084 (98%)	1848 (90%)	157 (8%)	48 (2%)	5 9

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	GLU
1	A	219	ASN
1	A	343	TYR
1	B	113	PRO
1	C	44	ASN
1	C	62	LYS
1	C	343	TYR
1	D	122	ALA
1	D	184	GLU
1	D	343	TYR
1	A	2	SER
1	A	63	ASN
1	A	186	SER
1	B	31	GLU
1	B	186	SER
1	B	188	SER
1	B	343	TYR
1	B	516	SER
1	D	15	GLY
1	D	37	ASP
1	D	43	TRP
1	D	187	CYS
1	D	358	ASP
1	C	113	PRO
1	D	113	PRO
1	A	187	CYS
1	B	63	ASN
1	C	311	ASP
1	D	111	GLY
1	D	219	ASN
1	D	514	PRO
1	C	202	ALA
1	D	40	SER
1	D	235	ARG
1	A	185	SER
1	B	40	SER
1	D	42	PRO

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Mol	Chain	Res	Type
1	D	86	PRO
1	D	485	PRO
1	C	267	GLY
1	A	341	PRO
1	B	46	PRO
1	B	61	GLY
1	C	485	PRO
1	D	267	GLY
1	D	344	GLY
1	B	38	GLY
1	D	35	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	442/446 (99%)	415 (94%)	27 (6%)	17	37
1	B	442/446 (99%)	404 (91%)	38 (9%)	10	22
1	C	442/446 (99%)	412 (93%)	30 (7%)	14	32
1	D	439/446 (98%)	414 (94%)	25 (6%)	18	40
All	All	1765/1784 (99%)	1645 (93%)	120 (7%)	14	32

All (120) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	VAL
1	A	44	ASN
1	A	49	MET
1	A	80	THR
1	A	95	LEU
1	A	96	ASN
1	A	138	LEU
1	A	181	ARG
1	A	184	GLU
1	A	187	CYS

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Mol	Chain	Res	Type
1	A	189	VAL
1	A	219	ASN
1	A	221	ASN
1	A	278	ARG
1	A	285	LYS
1	A	297	LEU
1	A	326	LEU
1	A	333	GLU
1	A	335	GLU
1	A	386	LEU
1	A	395	LEU
1	A	406	LEU
1	A	429	LEU
1	A	440	LEU
1	A	460	LEU
1	A	487	LEU
1	A	496	LEU
1	B	14	GLU
1	B	25	LEU
1	B	37	ASP
1	B	40	SER
1	B	41	ILE
1	B	49	MET
1	B	74	VAL
1	B	95	LEU
1	B	96	ASN
1	B	104	THR
1	B	109	LEU
1	B	112	LEU
1	B	139	LEU
1	B	146	PRO
1	B	169	VAL
1	B	171	LEU
1	B	219	ASN
1	B	250	GLU
1	B	256	ASP
1	B	257	ARG
1	B	258	THR
1	B	274	LEU
1	B	277	ASN
1	B	296	LEU
1	B	297	LEU

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Mol	Chain	Res	Type
1	B	303	GLU
1	B	309	LEU
1	B	326	LEU
1	B	333	GLU
1	B	355	THR
1	B	376	LEU
1	B	420	LEU
1	B	456	LEU
1	B	467	SER
1	B	468	ASN
1	B	476	GLN
1	B	490	ARG
1	B	515	ILE
1	C	16	THR
1	C	26	VAL
1	C	49	MET
1	C	95	LEU
1	C	96	ASN
1	C	106	GLN
1	C	109	LEU
1	C	115	GLU
1	C	116	GLU
1	C	138	LEU
1	C	139	LEU
1	C	159	VAL
1	C	169	VAL
1	C	171	LEU
1	C	177	ARG
1	C	207	GLN
1	C	219	ASN
1	C	235	ARG
1	C	243	LEU
1	C	263	LEU
1	C	279	LEU
1	C	326	LEU
1	C	360	ASN
1	C	374	GLU
1	C	376	LEU
1	C	386	LEU
1	C	395	LEU
1	C	404	HIS
1	C	456	LEU

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Mol	Chain	Res	Type
1	C	474	ASN
1	D	29	VAL
1	D	41	ILE
1	D	74	VAL
1	D	95	LEU
1	D	96	ASN
1	D	106	GLN
1	D	113	PRO
1	D	115	GLU
1	D	134	GLN
1	D	138	LEU
1	D	139	LEU
1	D	184	GLU
1	D	187	CYS
1	D	219	ASN
1	D	278	ARG
1	D	297	LEU
1	D	309	LEU
1	D	326	LEU
1	D	376	LEU
1	D	397	ARG
1	D	405	LEU
1	D	425	CYS
1	D	460	LEU
1	D	471	GLU
1	D	473	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	106	GLN
1	A	121	HIS
1	A	219	ASN
1	A	239	GLN
1	A	320	ASN
1	A	422	GLN
1	B	44	ASN
1	B	207	GLN
1	B	219	ASN
1	B	239	GLN
1	B	276	ASN

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Mol	Chain	Res	Type
1	B	277	ASN
1	B	320	ASN
1	B	346	GLN
1	B	379	ASN
1	B	422	GLN
1	B	434	ASN
1	B	464	HIS
1	B	476	GLN
1	C	119	ASN
1	C	207	GLN
1	C	219	ASN
1	C	239	GLN
1	C	360	ASN
1	C	434	ASN
1	C	469	HIS
1	C	476	GLN
1	D	63	ASN
1	D	134	GLN
1	D	143	ASN
1	D	173	GLN
1	D	207	GLN
1	D	219	ASN
1	D	234	ASN
1	D	239	GLN
1	D	269	GLN
1	D	276	ASN
1	D	356	HIS
1	D	364	GLN
1	D	379	ASN
1	D	458	HIS
1	D	464	HIS
1	D	476	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	1CY	B	602	-	16,18,18	1.68	3 (18%)	18,27,27	1.79	3 (16%)
2	1CY	A	601	-	16,18,18	1.75	3 (18%)	18,27,27	1.74	3 (16%)
3	NDP	D	704	-	51,52,52	1.71	11 (21%)	71,80,80	1.54	15 (21%)
4	PO4	A	801	-	4,4,4	2.58	1 (25%)	6,6,6	0.94	0
4	PO4	A	802	-	4,4,4	2.50	1 (25%)	6,6,6	0.89	0
3	NDP	A	701	-	51,52,52	1.68	11 (21%)	71,80,80	1.60	15 (21%)
2	1CY	C	603	-	16,18,18	1.71	3 (18%)	18,27,27	2.03	2 (11%)
4	PO4	D	803	-	4,4,4	2.59	1 (25%)	6,6,6	0.85	0
3	NDP	B	702	-	51,52,52	1.69	11 (21%)	71,80,80	1.54	11 (15%)
3	NDP	C	703	-	51,52,52	1.63	10 (19%)	71,80,80	1.58	14 (19%)
2	1CY	D	604	-	16,18,18	1.65	3 (18%)	18,27,27	1.82	3 (16%)
4	PO4	C	804	-	4,4,4	2.52	1 (25%)	6,6,6	0.87	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1CY	B	602	-	-	0/4/23/23	0/2/2/2
2	1CY	A	601	-	-	0/4/23/23	0/2/2/2
3	NDP	D	704	-	-	10/34/77/77	0/5/5/5
3	NDP	A	701	-	-	3/34/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	1CY	C	603	-	-	0/4/23/23	0/2/2/2
3	NDP	B	702	-	-	9/34/77/77	0/5/5/5
3	NDP	C	703	-	-	8/34/77/77	0/5/5/5
2	1CY	D	604	-	-	0/4/23/23	0/2/2/2

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	803	PO4	P-O1	4.90	1.62	1.50
4	A	801	PO4	P-O1	4.87	1.61	1.50
4	C	804	PO4	P-O1	4.79	1.61	1.50
4	A	802	PO4	P-O1	4.77	1.61	1.50
3	B	702	NDP	C4N-C3N	-4.60	1.41	1.50
3	A	701	NDP	C4N-C3N	-4.44	1.41	1.50
3	B	702	NDP	C4N-C5N	-4.42	1.37	1.49
3	C	703	NDP	C4N-C5N	-4.33	1.37	1.49
2	A	601	1CY	C2-N3	-4.33	1.27	1.36
3	D	704	NDP	C4N-C5N	-4.28	1.37	1.49
3	D	704	NDP	C4N-C3N	-4.21	1.42	1.50
2	C	603	1CY	C2-N3	-4.19	1.27	1.36
2	B	602	1CY	C2-N3	-4.16	1.27	1.36
3	B	702	NDP	C2N-C3N	4.13	1.46	1.35
3	A	701	NDP	C4N-C5N	-3.97	1.38	1.49
2	C	603	1CY	C4-N3	-3.89	1.27	1.33
2	D	604	1CY	C2-N3	-3.86	1.28	1.36
2	A	601	1CY	C4-N3	-3.84	1.27	1.33
3	C	703	NDP	C2N-C3N	3.84	1.45	1.35
2	D	604	1CY	C4-N3	-3.67	1.28	1.33
3	D	704	NDP	C3B-C2B	-3.65	1.45	1.53
3	C	703	NDP	C4N-C3N	-3.63	1.43	1.50
3	D	704	NDP	C2N-C3N	3.60	1.45	1.35
3	D	704	NDP	P2B-O2B	-3.60	1.53	1.59
2	B	602	1CY	C4-N3	-3.57	1.28	1.33
3	A	701	NDP	C2N-C3N	3.56	1.45	1.35
3	A	701	NDP	P2B-O2B	-3.46	1.53	1.59
3	A	701	NDP	C4A-N3A	3.21	1.40	1.34
3	C	703	NDP	C3B-C2B	-3.16	1.46	1.53
3	D	704	NDP	C4A-N3A	3.01	1.40	1.34
3	D	704	NDP	C5D-C4D	2.95	1.60	1.51
3	B	702	NDP	P2B-O2B	-2.94	1.54	1.59
3	B	702	NDP	C8A-N9A	2.84	1.42	1.37
3	B	702	NDP	PN-O3	2.78	1.62	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	NDP	C8A-N9A	2.78	1.42	1.37
3	A	701	NDP	C8A-N9A	2.77	1.42	1.37
3	B	702	NDP	C3B-C2B	-2.71	1.47	1.53
2	B	602	1CY	C2-N1	-2.66	1.27	1.34
2	D	604	1CY	C2-N1	-2.63	1.27	1.34
3	C	703	NDP	PN-O3	2.58	1.62	1.59
2	A	601	1CY	C2-N1	-2.58	1.27	1.34
2	C	603	1CY	C2-N1	-2.57	1.27	1.34
3	C	703	NDP	P2B-O2B	-2.53	1.55	1.59
3	B	702	NDP	C3B-C4B	-2.50	1.46	1.53
3	A	701	NDP	PA-O3	-2.49	1.56	1.59
3	C	703	NDP	C6N-N1N	2.47	1.43	1.37
3	B	702	NDP	C4A-N3A	2.43	1.39	1.34
3	C	703	NDP	C4A-N3A	2.42	1.38	1.34
3	D	704	NDP	C8A-N9A	2.42	1.41	1.37
3	A	701	NDP	C3B-C2B	-2.42	1.47	1.53
3	D	704	NDP	C6N-N1N	2.37	1.43	1.37
3	B	702	NDP	C6N-N1N	2.36	1.43	1.37
3	D	704	NDP	C3B-C4B	-2.26	1.47	1.53
3	A	701	NDP	PA-O1A	-2.24	1.43	1.50
3	D	704	NDP	PA-O1A	-2.23	1.43	1.50
3	C	703	NDP	C3B-C4B	-2.18	1.47	1.53
3	B	702	NDP	PA-O1A	-2.15	1.43	1.50
3	A	701	NDP	C6N-N1N	2.13	1.42	1.37
3	A	701	NDP	C3B-C4B	-2.08	1.47	1.53

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	1CY	N8-C4-N5	6.56	124.06	118.79
2	B	602	1CY	N8-C4-N5	6.41	123.94	118.79
2	D	604	1CY	N8-C4-N5	6.01	123.62	118.79
2	A	601	1CY	N8-C4-N5	5.95	123.57	118.79
3	B	702	NDP	C3N-C2N-N1N	-4.91	116.00	123.20
3	C	703	NDP	C3N-C2N-N1N	-4.90	116.02	123.20
3	D	704	NDP	C1D-N1N-C2N	-4.51	113.71	121.14
3	A	701	NDP	C3N-C2N-N1N	-4.44	116.68	123.20
3	A	701	NDP	C1D-N1N-C2N	-4.29	114.08	121.14
2	C	603	1CY	C9-C6-N5	4.28	113.44	110.24
3	D	704	NDP	C3N-C2N-N1N	-4.19	117.05	123.20
3	A	701	NDP	O4B-C1B-N9A	4.11	115.98	108.09
3	C	703	NDP	O4B-C1B-N9A	3.92	115.62	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	NDP	C1D-N1N-C2N	-3.82	114.85	121.14
3	D	704	NDP	O4B-C1B-N9A	3.52	114.85	108.09
3	B	702	NDP	O4B-C1B-N9A	3.35	114.53	108.09
3	A	701	NDP	C3B-C2B-C1B	-3.28	96.53	102.81
3	C	703	NDP	C3B-C2B-C1B	-3.21	96.65	102.81
3	B	702	NDP	C1D-N1N-C2N	-3.18	115.90	121.14
3	A	701	NDP	C6N-N1N-C2N	3.10	122.64	119.32
3	D	704	NDP	C3B-C2B-C1B	-3.06	96.95	102.81
3	D	704	NDP	O7N-C7N-N7N	-2.91	116.36	122.89
3	B	702	NDP	O3B-C3B-C2B	2.90	119.31	111.19
3	B	702	NDP	O3B-C3B-C4B	2.82	119.19	111.08
3	B	702	NDP	C3B-C2B-C1B	-2.82	97.41	102.81
3	B	702	NDP	O7N-C7N-N7N	-2.78	116.66	122.89
3	C	703	NDP	C6N-N1N-C2N	2.78	122.29	119.32
3	C	703	NDP	O7N-C7N-N7N	-2.76	116.71	122.89
2	A	601	1CY	C9-C6-N5	2.73	112.28	110.24
3	A	701	NDP	O3B-C3B-C2B	2.70	118.75	111.19
3	A	701	NDP	O7N-C7N-N7N	-2.68	116.88	122.89
3	D	704	NDP	O3B-C3B-C4B	2.67	118.76	111.08
3	C	703	NDP	O3B-C3B-C4B	2.62	118.60	111.08
3	B	702	NDP	C6N-N1N-C2N	2.57	122.07	119.32
3	C	703	NDP	N3A-C2A-N1A	-2.50	124.79	128.58
3	A	701	NDP	O3B-C3B-C4B	2.49	118.24	111.08
3	A	701	NDP	N3A-C2A-N1A	-2.44	124.89	128.58
3	D	704	NDP	C6N-N1N-C2N	2.41	121.89	119.32
3	C	703	NDP	O3B-C3B-C2B	2.41	117.92	111.19
3	D	704	NDP	N3A-C2A-N1A	-2.36	125.02	128.58
2	D	604	1CY	C10-C6-N5	2.34	111.99	110.24
3	B	702	NDP	N3A-C2A-N1A	-2.33	125.05	128.58
2	B	602	1CY	C10-C6-N5	2.32	111.98	110.24
3	A	701	NDP	C3D-C2D-C1D	-2.31	97.09	101.46
2	A	601	1CY	C10-C6-N5	2.28	111.95	110.24
3	B	702	NDP	C2B-C3B-C4B	2.27	106.87	101.99
3	C	703	NDP	O2A-PA-O1A	2.26	122.96	112.44
3	D	704	NDP	C4B-O4B-C1B	-2.25	104.49	109.47
2	D	604	1CY	C9-C6-N5	2.25	111.92	110.24
3	A	701	NDP	O2N-PN-O1N	2.24	122.86	112.44
2	B	602	1CY	C9-C6-N5	2.23	111.91	110.24
3	D	704	NDP	O3B-C3B-C2B	2.21	117.37	111.19
3	C	703	NDP	O2N-PN-O1N	2.20	122.69	112.44
3	C	703	NDP	C2B-C3B-C4B	2.12	106.55	101.99
3	D	704	NDP	O5D-PN-O1N	2.11	117.28	108.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	701	NDP	O2A-PA-O1A	2.10	122.21	112.44
3	D	704	NDP	C3N-C7N-N7N	2.09	121.39	117.67
3	B	702	NDP	O2B-C2B-C3B	2.09	119.18	111.68
3	D	704	NDP	O2A-PA-O1A	2.08	122.13	112.44
3	C	703	NDP	N9A-C8A-N7A	-2.08	110.98	113.94
3	A	701	NDP	C5A-N7A-C8A	2.08	106.72	103.45
3	D	704	NDP	C5A-N7A-C8A	2.06	106.68	103.45
3	A	701	NDP	C4B-O4B-C1B	-2.04	104.96	109.47
3	D	704	NDP	C2D-C3D-C4D	2.02	106.51	102.61
3	C	703	NDP	C4B-O4B-C1B	-2.01	105.03	109.47
3	A	701	NDP	C2D-C3D-C4D	2.00	106.48	102.61

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	703	NDP	C5D-O5D-PN-O3
3	D	704	NDP	C2D-C1D-N1N-C6N
3	D	704	NDP	O4D-C4D-C5D-O5D
3	D	704	NDP	C2D-C1D-N1N-C2N
3	B	702	NDP	C3B-C4B-C5B-O5B
3	D	704	NDP	C3D-C4D-C5D-O5D
3	B	702	NDP	C3D-C4D-C5D-O5D
3	B	702	NDP	O4D-C4D-C5D-O5D
3	B	702	NDP	O4B-C4B-C5B-O5B
3	B	702	NDP	PA-O3-PN-O5D
3	A	701	NDP	O4D-C1D-N1N-C2N
3	C	703	NDP	C2D-C1D-N1N-C2N
3	C	703	NDP	C5D-O5D-PN-O1N
3	D	704	NDP	C5D-O5D-PN-O1N
3	D	704	NDP	O4D-C1D-N1N-C6N
3	D	704	NDP	O4D-C1D-N1N-C2N
3	C	703	NDP	O4D-C1D-N1N-C2N
3	B	702	NDP	C2D-C1D-N1N-C2N
3	A	701	NDP	C2N-C3N-C7N-N7N
3	B	702	NDP	O4D-C1D-N1N-C2N
3	B	702	NDP	C2N-C3N-C7N-N7N
3	C	703	NDP	C2N-C3N-C7N-N7N
3	D	704	NDP	C2N-C3N-C7N-N7N
3	C	703	NDP	C2D-C1D-N1N-C6N
3	C	703	NDP	O4D-C1D-N1N-C6N
3	D	704	NDP	C2B-O2B-P2B-O1X

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Mol	Chain	Res	Type	Atoms
3	B	702	NDP	C2D-C1D-N1N-C6N
3	D	704	NDP	C4D-C5D-O5D-PN
3	A	701	NDP	PN-O3-PA-O2A
3	C	703	NDP	C3D-C4D-C5D-O5D

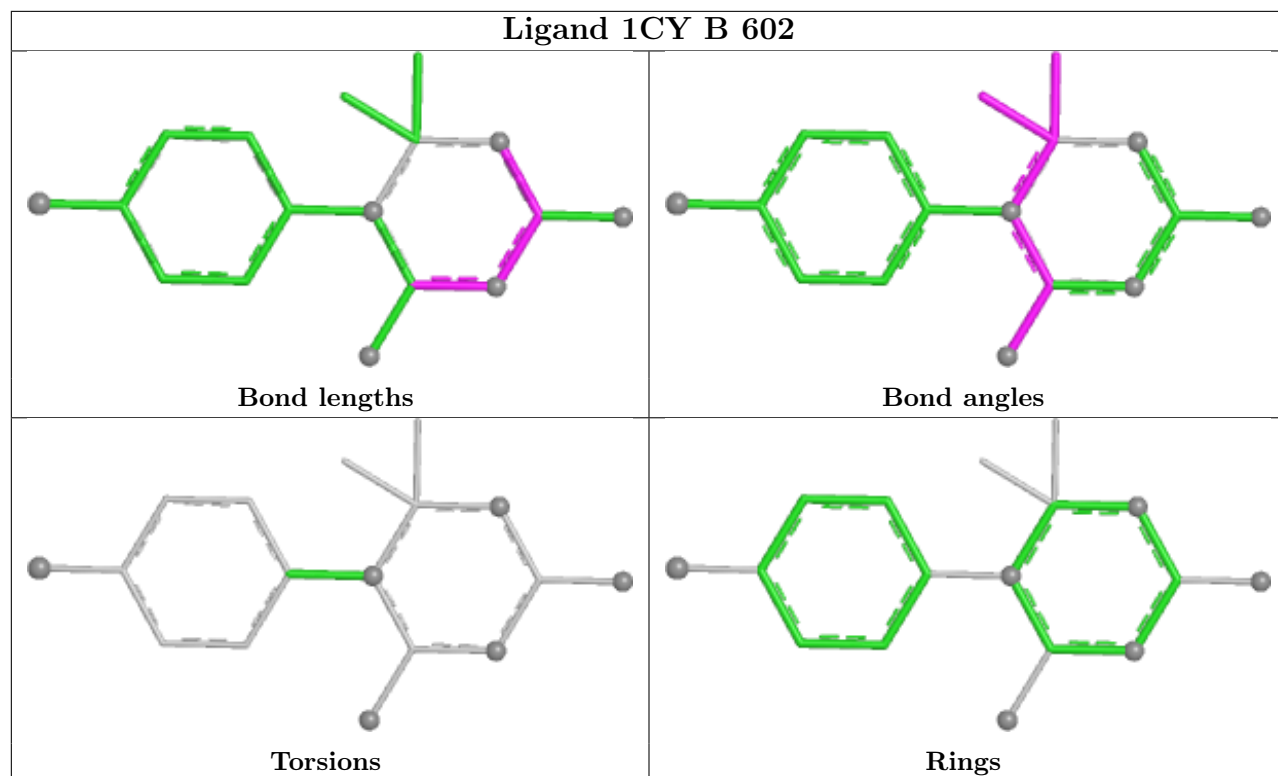
There are no ring outliers.

6 monomers are involved in 15 short contacts:

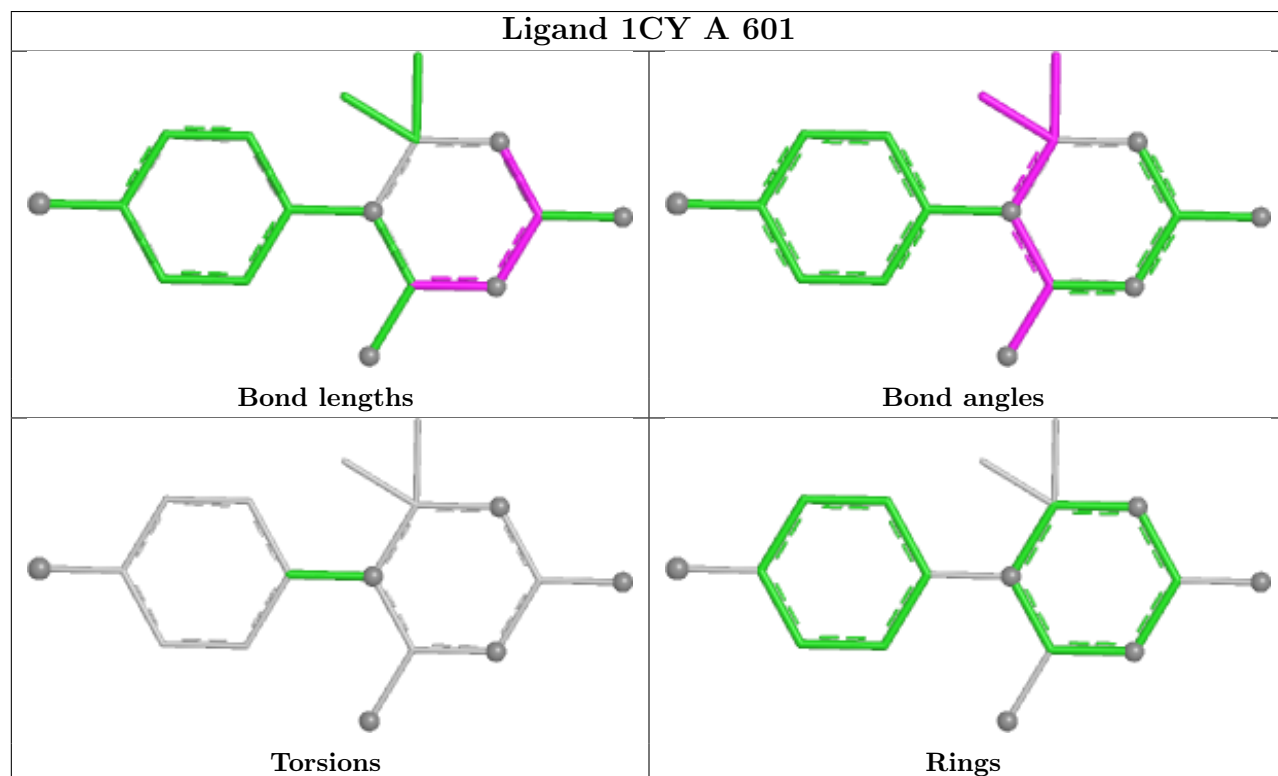
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	602	1CY	1	0
2	A	601	1CY	1	0
3	D	704	NDP	3	0
3	A	701	NDP	2	0
3	B	702	NDP	7	0
3	C	703	NDP	3	0

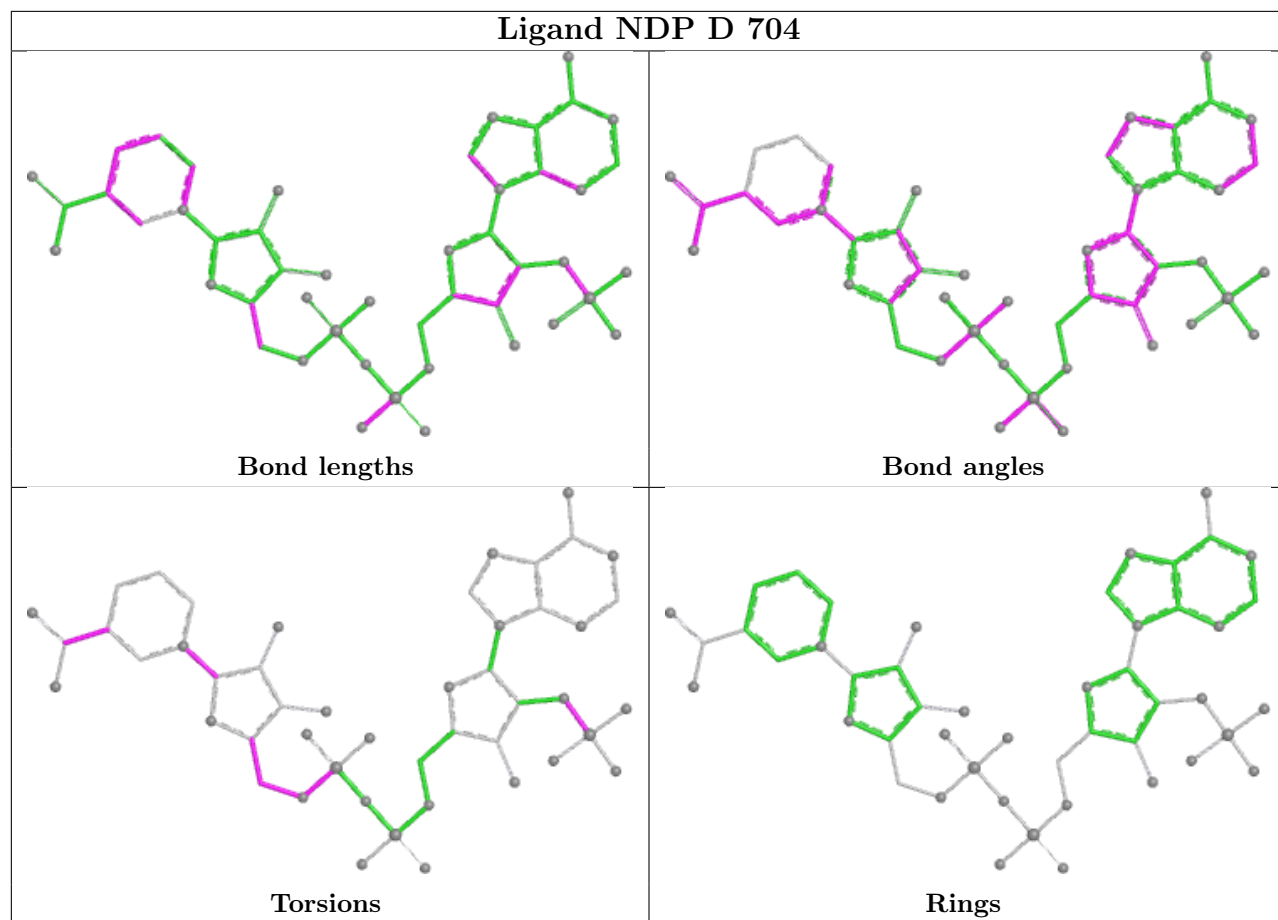
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

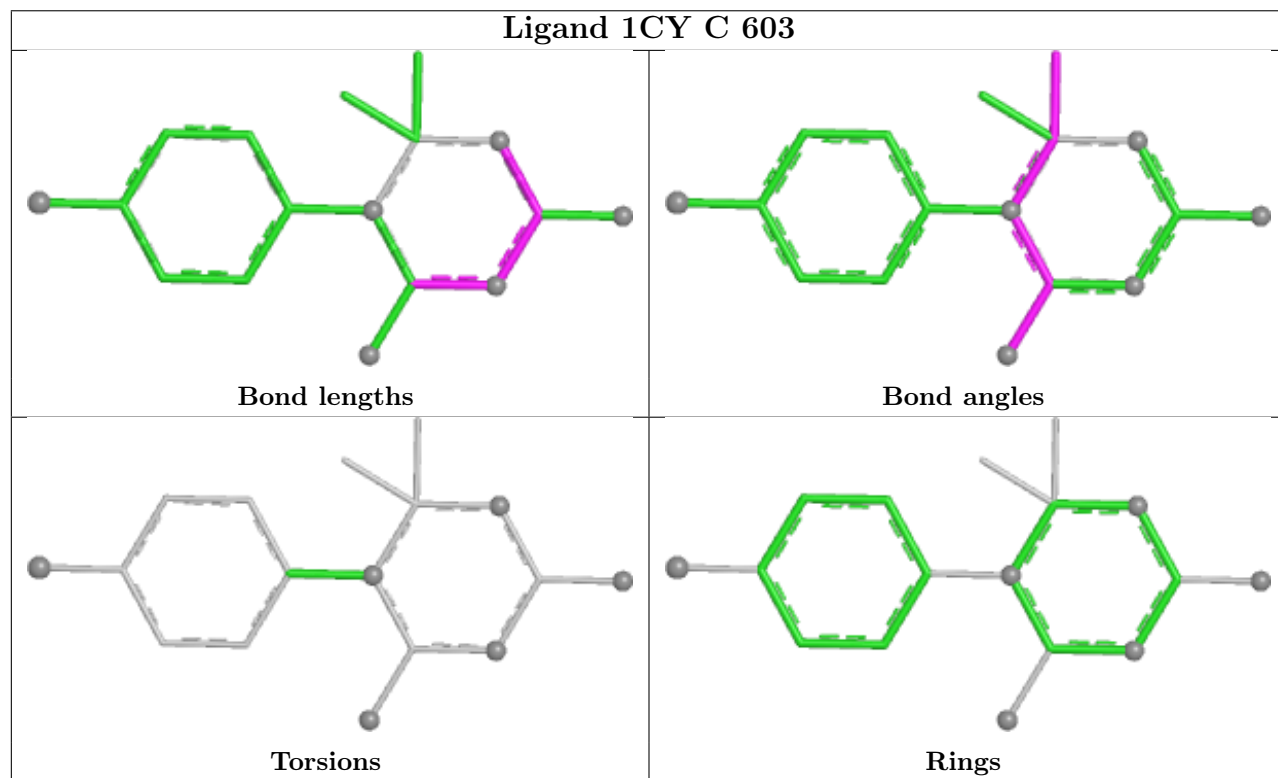
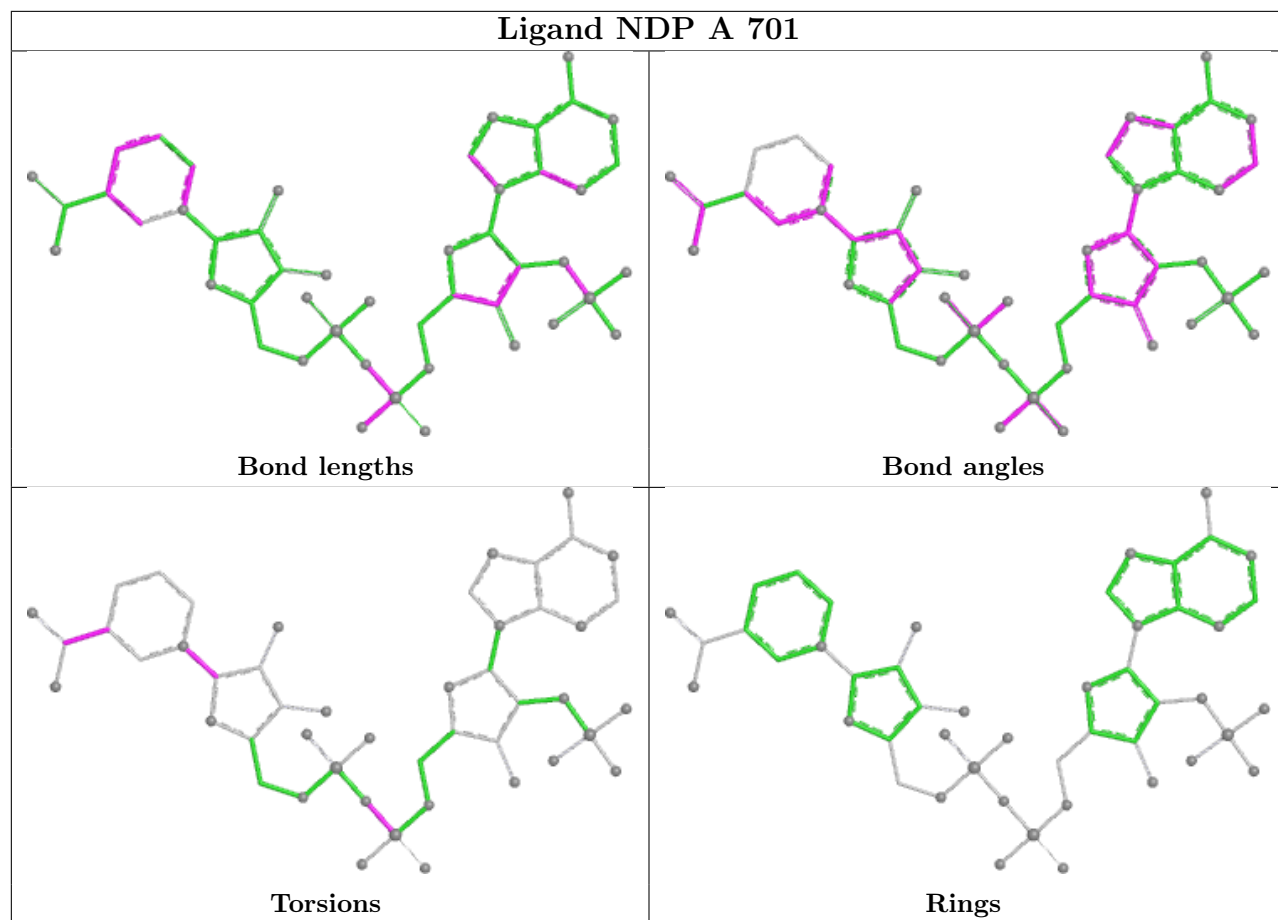
Ligand 1CY B 602

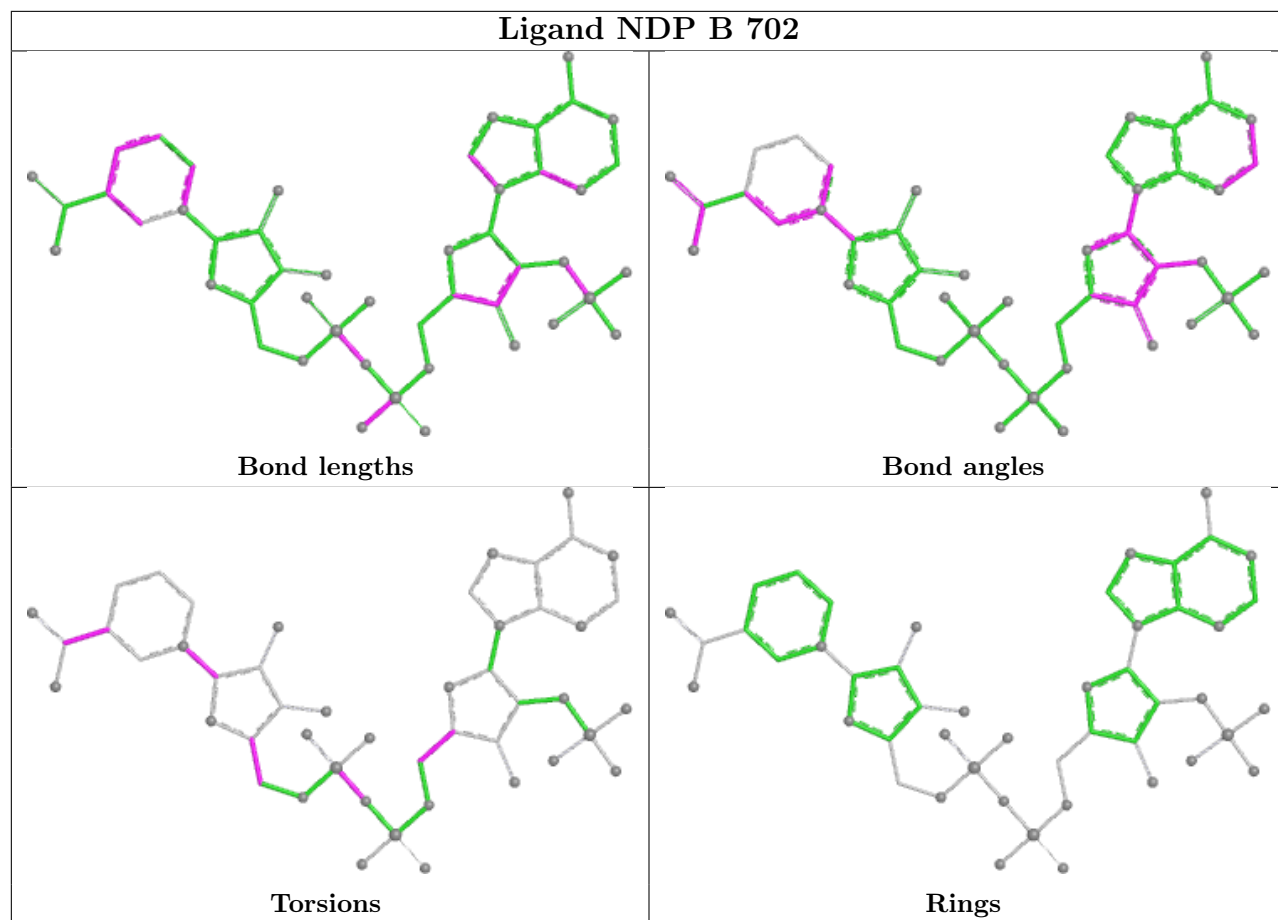


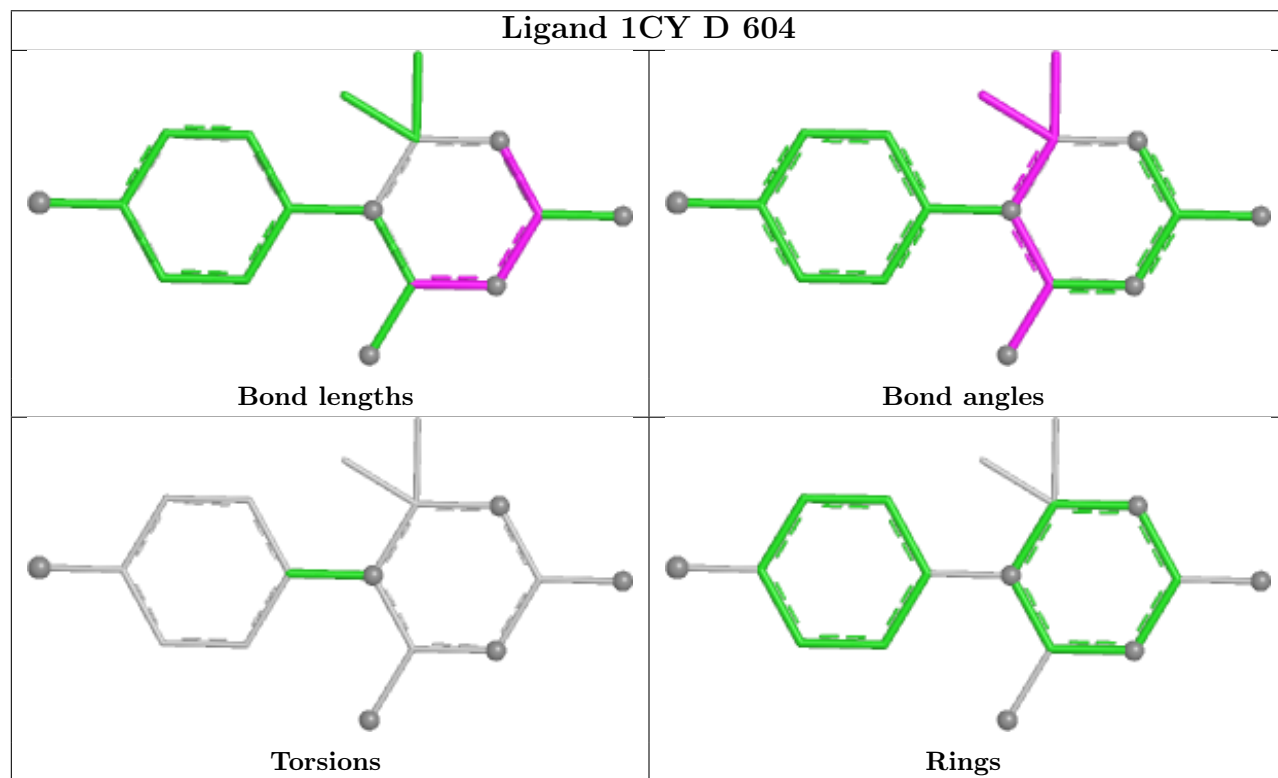
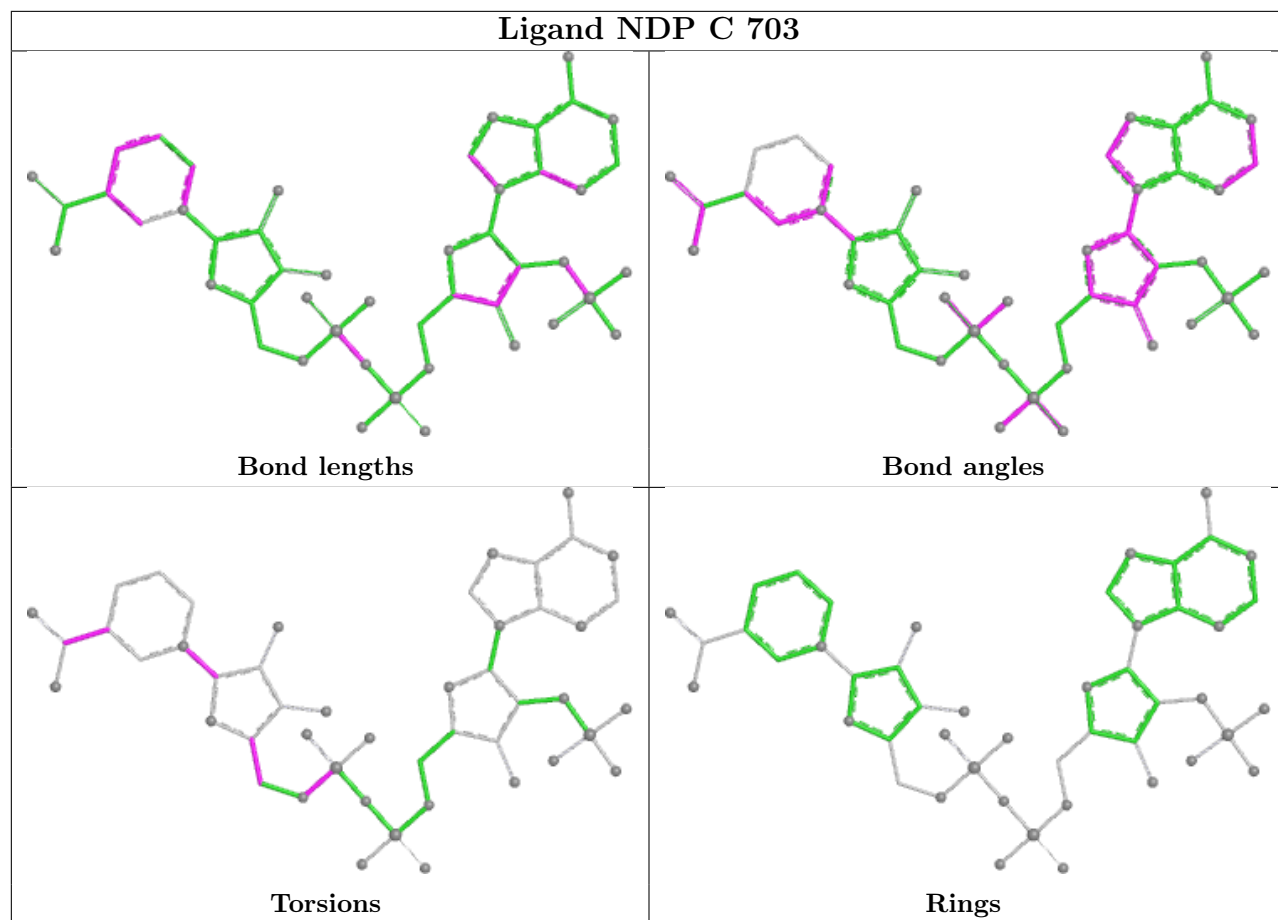
Ligand 1CY A 601











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	516/521 (99%)	-1.63	0 100 100	13, 28, 56, 79	0
1	B	516/521 (99%)	-1.59	0 100 100	12, 31, 70, 91	0
1	C	516/521 (99%)	-1.63	0 100 100	11, 28, 65, 89	0
1	D	513/521 (98%)	-1.59	0 100 100	13, 31, 67, 91	0
All	All	2061/2084 (98%)	-1.61	0 100 100	11, 29, 65, 91	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
2	1CY	A	601	17/17	0.99	0.03	31,34,35,37	0
2	1CY	B	602	17/17	0.99	0.03	40,42,44,46	0
2	1CY	C	603	17/17	0.99	0.03	30,31,33,33	0
2	1CY	D	604	17/17	0.99	0.03	34,36,38,38	0

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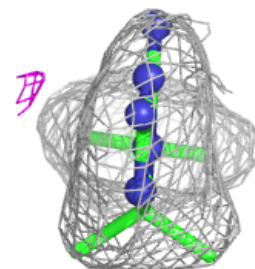
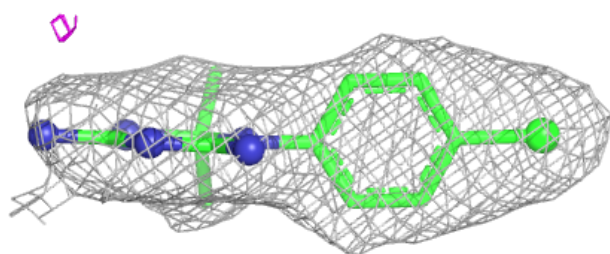
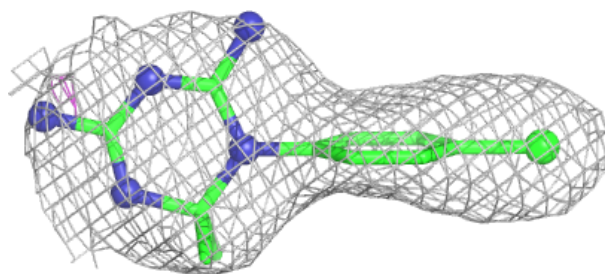
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	NDP	A	701	48/48	0.99	0.03	29,39,66,67	0
3	NDP	B	702	48/48	0.99	0.04	43,55,79,81	0
3	NDP	C	703	48/48	0.99	0.03	30,37,64,67	0
3	NDP	D	704	48/48	0.99	0.03	36,44,64,64	0
4	PO4	A	801	5/5	0.99	0.03	33,33,34,35	0
4	PO4	A	802	5/5	0.99	0.04	57,57,58,58	0
4	PO4	C	804	5/5	0.99	0.04	66,67,68,68	0
4	PO4	D	803	5/5	0.99	0.03	57,59,60,61	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.

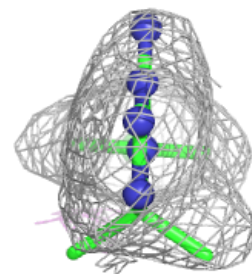
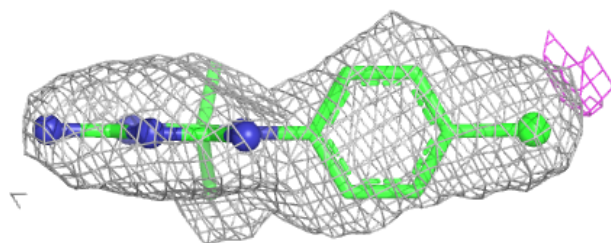
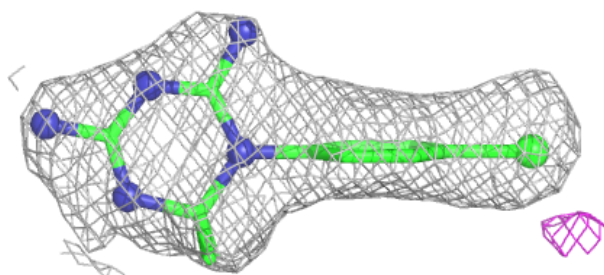
Electron density around 1CY A 601:

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

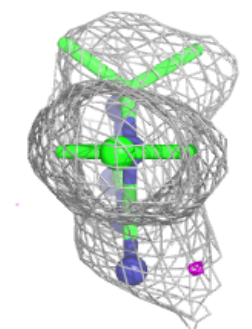
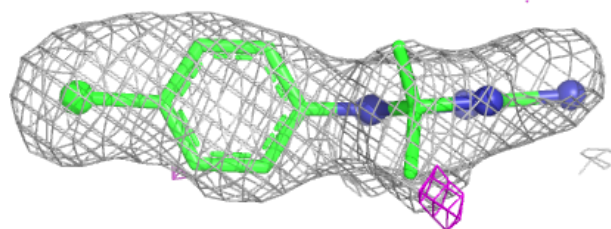
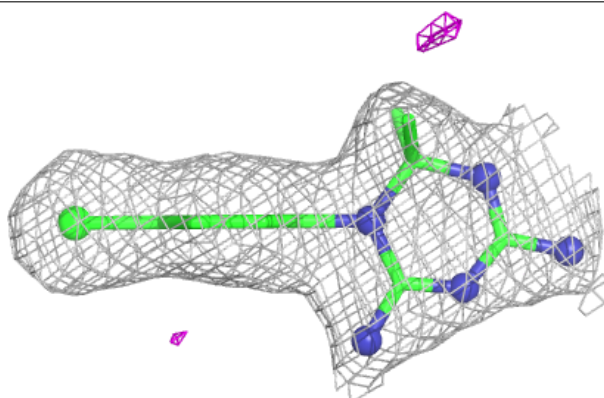


Electron density around 1CY B 602:

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

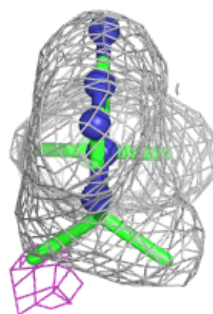
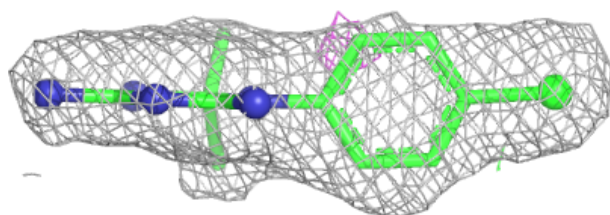
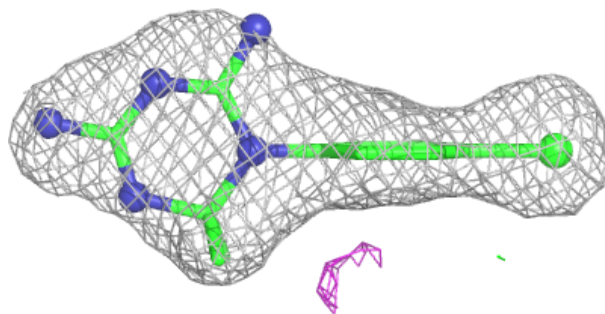
**Electron density around 1CY C 603:**

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

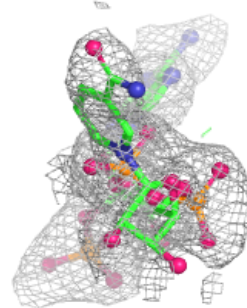
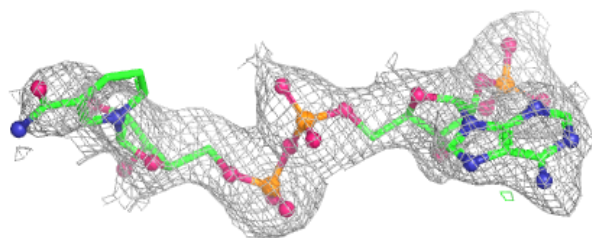
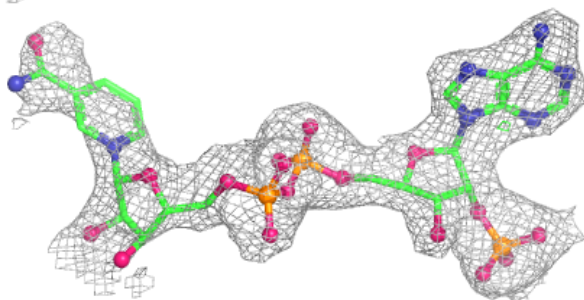


Electron density around 1CY D 604:

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

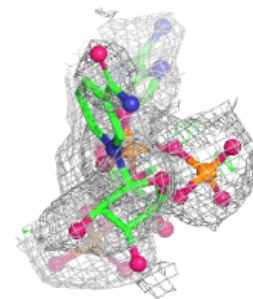
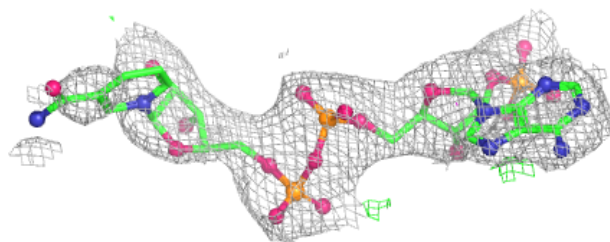
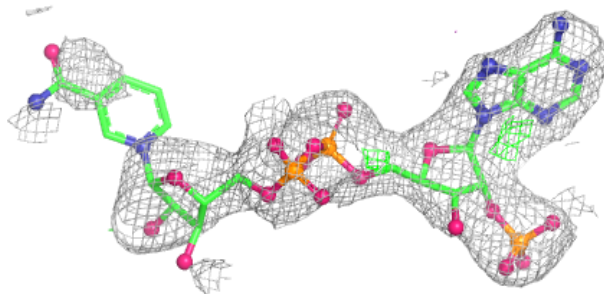
**Electron density around NDP A 701:**

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

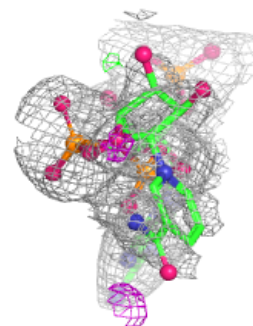
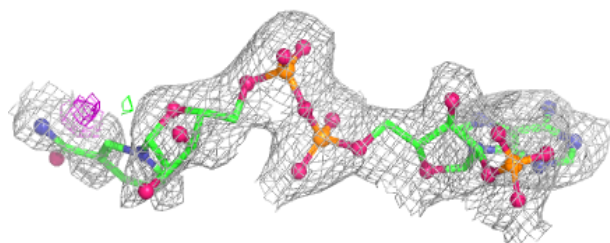
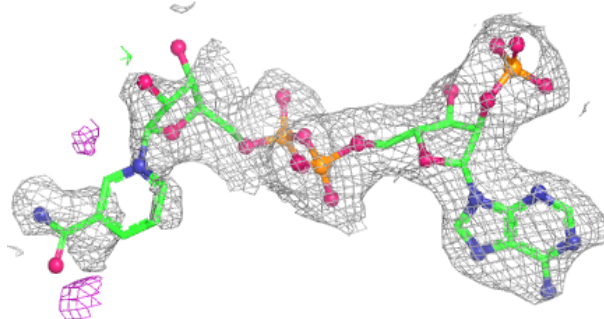


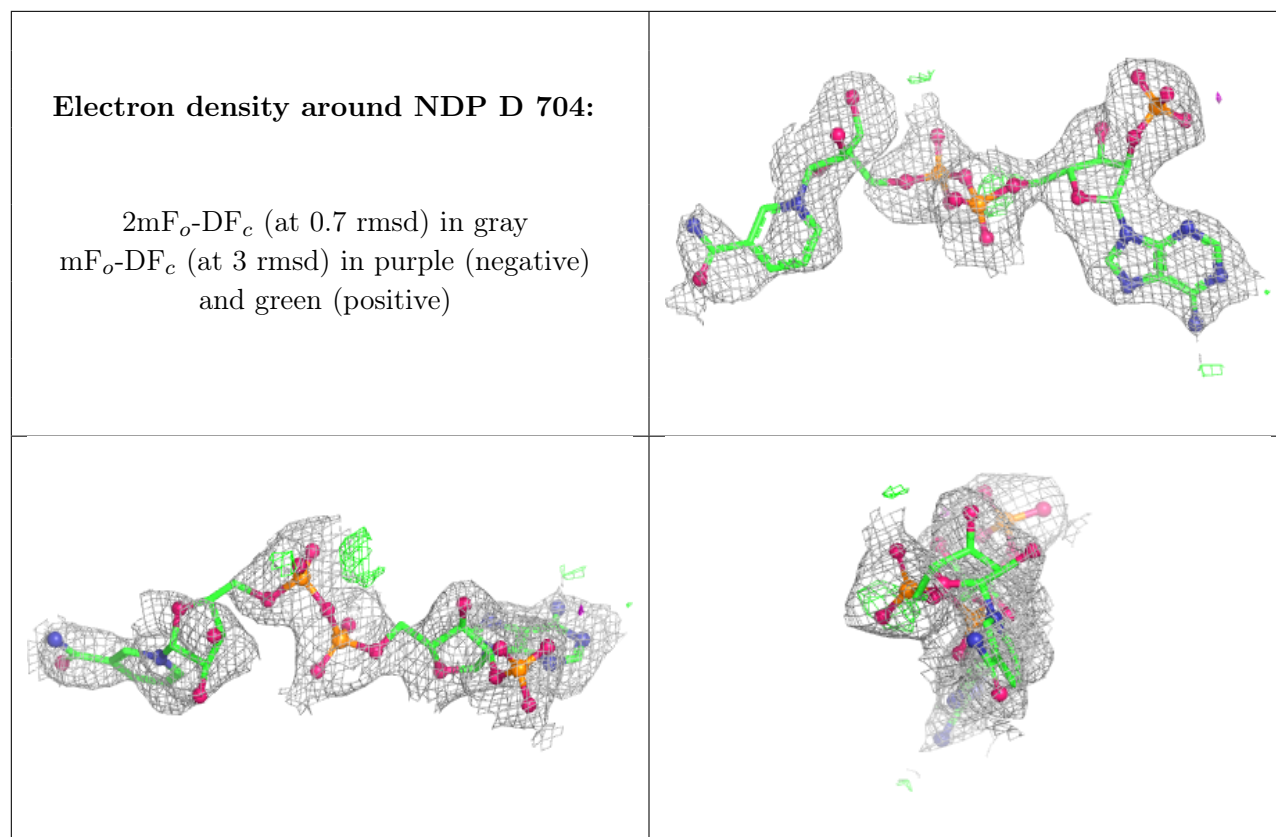
Electron density around NDP B 702:

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

**Electron density around NDP C 703:**

$2mF_o-DF_c$ (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.