



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:03 AM UTC

PDB ID : 3IRO / pdb_00003iro
Title : Trypanosoma cruzi Dihydrofolate Reductase-Thymidylate Synthase complexed with NADPH and Q-8 antifolate
Authors : Chitnumsub, P.; Yuvaniyama, J.; Yuthavong, Y.
Deposited on : 2009-08-24
Resolution : 2.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

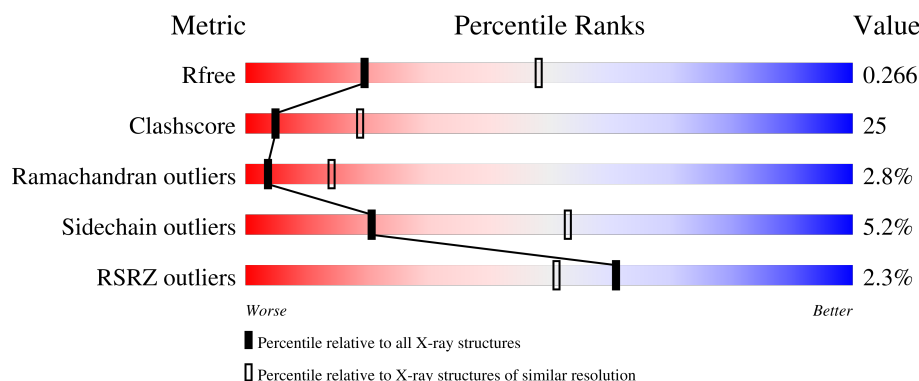
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	521	2% 52% 42% 5%
1	B	521	3% 49% 43% 7%
1	C	521	% 52% 40% 6%
1	D	521	2% 53% 40% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	ACT	A	809	-	-	X	-

2 Entry composition [i](#)

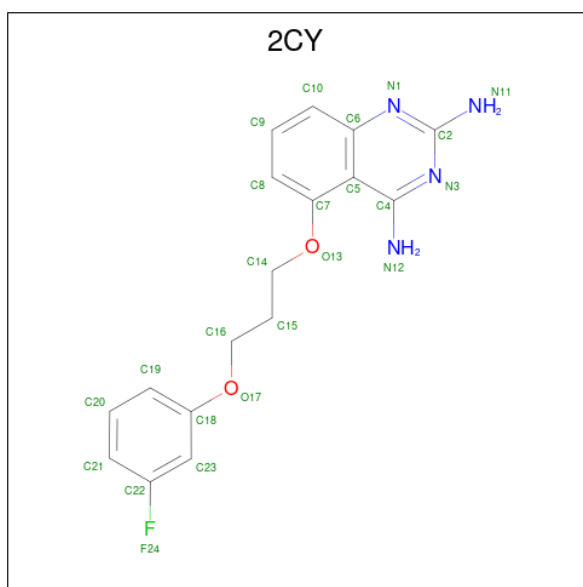
There are 7 unique types of molecules in this entry. The entry contains 16862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	518	Total	C	N	O	S	0	0	0
			4124	2616	729	759	20			
1	B	515	Total	C	N	O	S	0	0	0
			4101	2602	725	755	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 5-[3-(3-fluorophenoxy)propoxy]quinazoline-2,4-diamine (CCD ID: 2CY) (formula: C₁₇H₁₇FN₄O₂).



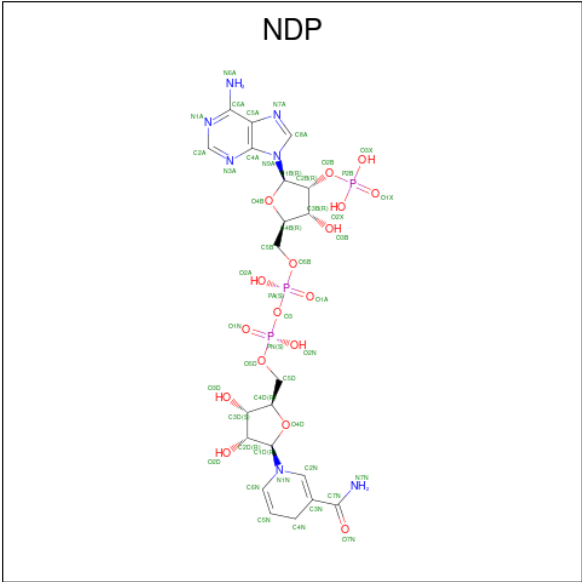
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			24	17	1	4	2		
2	B	1	Total	C	F	N	O	0	0
			24	17	1	4	2		

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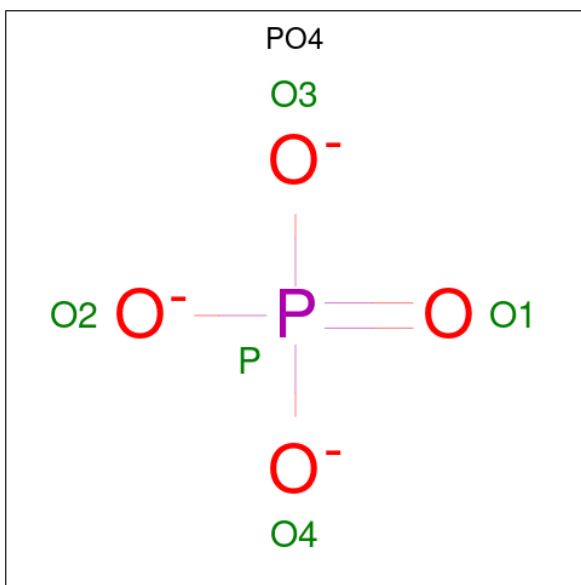
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	F	N	O	0	0
			24	17	1	4	2		
2	D	1	Total	C	F	N	O	0	0
			24	17	1	4	2		

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



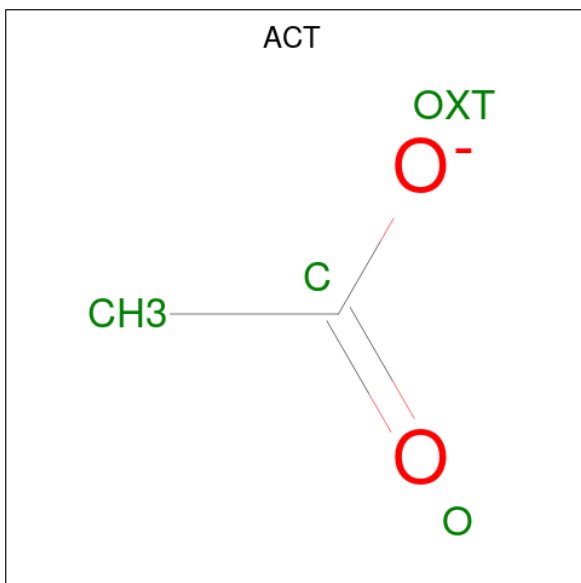
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



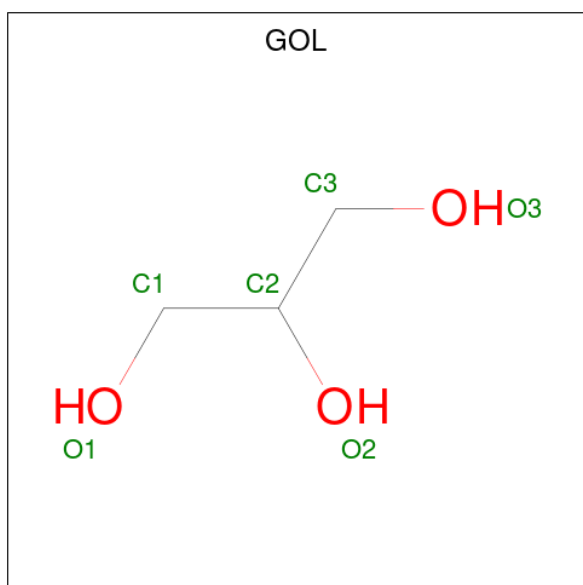
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	B	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	C	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0
5	D	1	Total C O 4 2 2	0	0

- Molecule 6 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

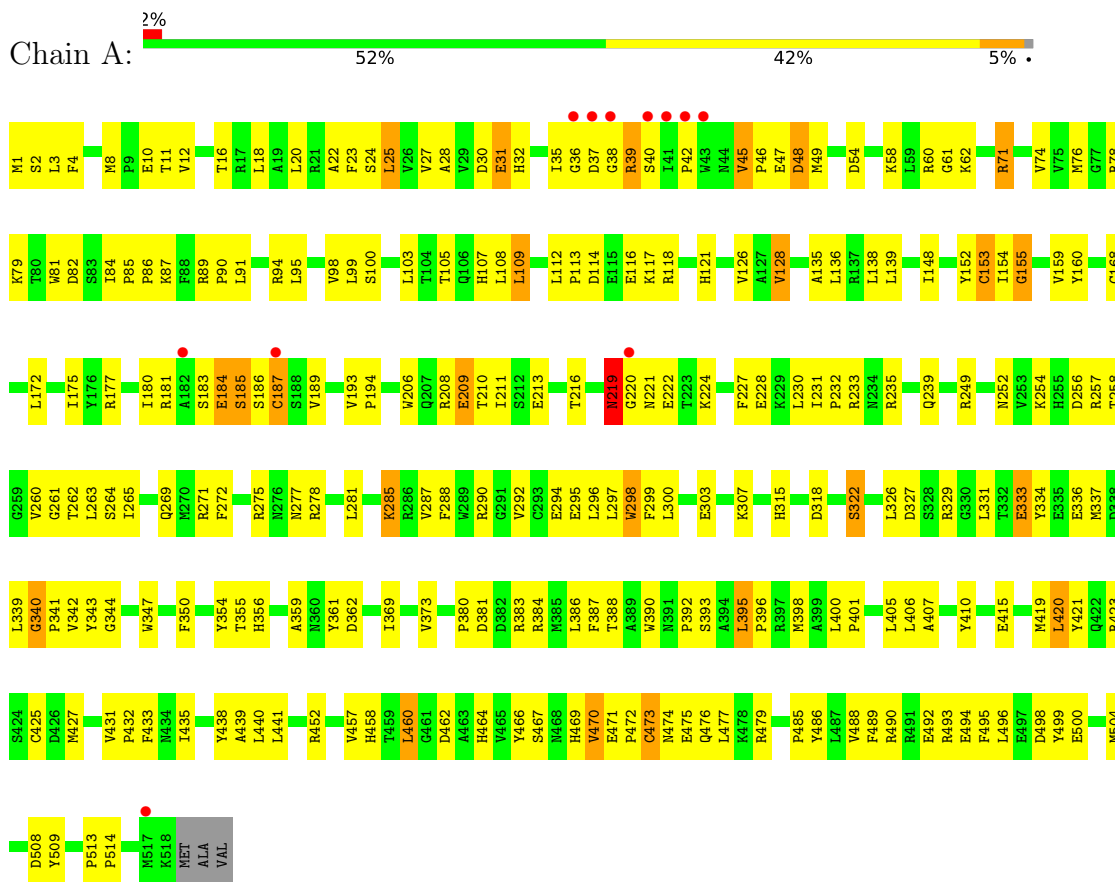
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	23	Total 23	O 23	0	0
7	B	12	Total 12	O 12	0	0
7	C	23	Total 23	O 23	0	0
7	D	25	Total 25	O 25	0	0

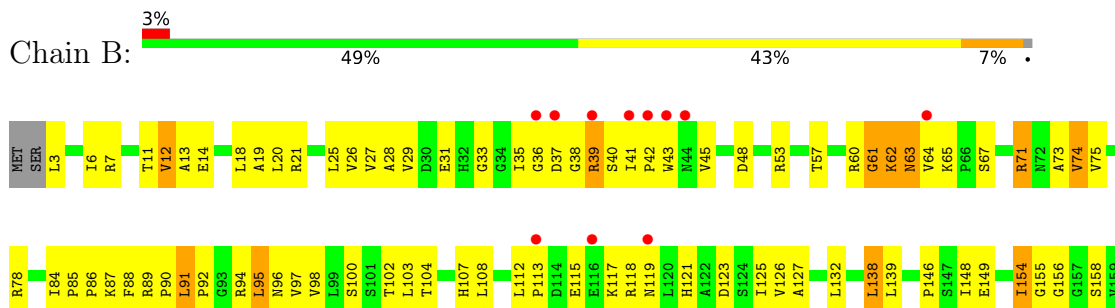
3 Residue-property plots

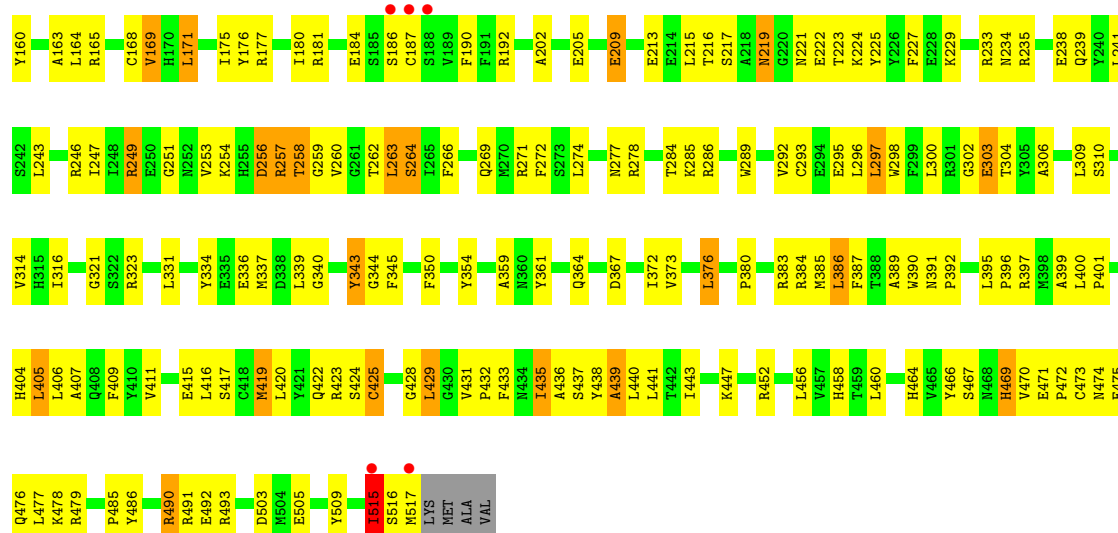
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

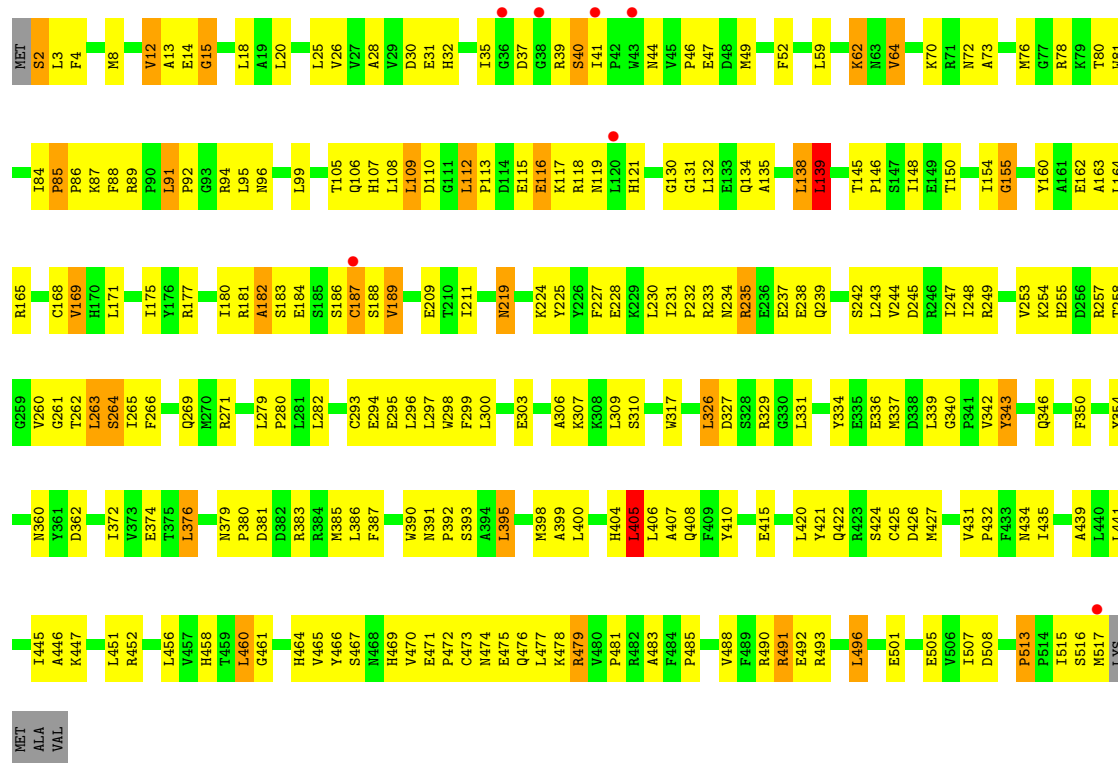


- Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





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VAL	T435	D338	H285	A163	R89
	A436	L339	D256	L164	P90
	S437	G340	R257	R165	L91
	Y438	P341	T258		
	A439	Y342	G259	V169	L95
	L440	Y343		H170	R96
	L441				Y97
		Q346	T263	L171	V98
	A448	W347	S264	L172	L99
		R348	L265		S100
	R452	H349	F266	L175	S101
	P453	F350		R177	T102
	G454	Y354	M270	T178	L103
	L456	T355	R271	T104	T105
		H356	F272	R181	
	L460		S273	E184	Q106
	A463	N360	R275	L107	H107
		Y361	R276	S185	L108
	Y466	D362	M277	S186	L109
		D367	R278	C187	D110
				S188	G111
	H469		T283		L112
	W470	L376	T284	V193	P113
	E471			P194	D114
	P472	N379	F288	E195	D115
	C473				E116
	W474	M385	V292	A201	K117
	E475	L386			R118
	K478	A389	L296	Q207	N119
		W390	L297	R208	L120
	P485	N391	F299	E209	H121
	Y486	P392	L300	T210	A122
			R301		
			G302	A218	G131
	F489	L395	E303	N219	L132
	R490	P396		G220	E133
	R491	R397		R221	Q134
	E492	M398	K307	A135	
	R493	A399	K308	Y225	L136
	F495		L309	R137	L138
	L496	H404	S310	E228	L139
	E497	L405	D311	R229	
	D498	L406	K312	L230	A140
		A407			S141
		Q408		R233	
	M504	F409	H315	N234	Y144
	E505			R235	T145
		E415	D318	E236	P146
	Y509	L416	S322	E237	S147
				L148	E149
	Y512	L420	F325	L241	T150
	P513		L326	S242	V151
	P514	C425	D327	R246	Y152
	SER		S328	T247	C153
	MET	G430		I154	
	LYS	V431	E333	R249	G155
	MET	F432			G156
	ALA	F433	E336	V253	
		N424	W327	V254	

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.54Å 165.94Å 84.72Å 90.00° 113.41° 90.00°	Depositor
Resolution (Å)	45.07 – 2.80 45.07 – 2.80	Depositor EDS
% Data completeness (in resolution range)	95.1 (45.07-2.80) 95.0 (45.07-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 2.81Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.206 , 0.277 0.198 , 0.266	Depositor DCC
R_{free} test set	2478 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.024 for l,-k,h	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16862	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: NDP, ACT, 2CY, PO4, GOL

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	0.47	0/4224	0.99	15/5729 (0.3%)
1	B	0.46	0/4201	1.02	19/5700 (0.3%)
1	C	0.46	0/4207	1.00	19/5708 (0.3%)
1	D	0.47	0/4187	1.01	17/5682 (0.3%)
All	All	0.46	0/16819	1.00	70/22819 (0.3%)

There are no bond length outliers.

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	GLY	N-CA-C	9.92	125.01	110.63
1	D	209	GLU	N-CA-C	-9.24	100.32	111.69
1	D	154	ILE	N-CA-C	8.88	120.60	112.17
1	C	138	LEU	N-CA-C	-8.71	101.47	110.97
1	A	209	GLU	N-CA-C	-8.08	101.54	111.40
1	B	469	HIS	N-CA-C	-7.96	104.04	114.31
1	B	257	ARG	N-CA-C	-7.88	103.67	113.28
1	D	405	LEU	N-CA-C	7.49	121.66	112.23
1	A	155	GLY	N-CA-C	7.36	121.89	111.00
1	D	91	LEU	CA-C-N	7.31	127.74	119.92
1	D	91	LEU	C-N-CA	7.31	127.74	119.92
1	C	379	ASN	CA-C-N	7.18	126.88	119.56
1	C	379	ASN	C-N-CA	7.18	126.88	119.56
1	D	454	GLY	N-CA-C	7.07	116.64	110.21
1	B	154	ILE	N-CA-C	7.00	120.85	112.80
1	B	263	LEU	N-CA-C	-6.69	98.81	109.59
1	B	40	SER	N-CA-C	6.64	118.62	108.52
1	B	439	ALA	N-CA-C	-6.61	103.56	111.69
1	A	470	VAL	N-CA-C	6.48	117.16	110.36
1	C	209	GLU	N-CA-C	-6.41	102.81	112.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	249	ARG	N-CA-C	6.29	117.81	111.07
1	A	439	ALA	N-CA-C	-6.22	103.80	112.45
1	C	439	ALA	N-CA-C	-6.20	104.60	111.36
1	C	513	PRO	CA-C-N	6.19	127.57	119.84
1	C	513	PRO	C-N-CA	6.19	127.57	119.84
1	B	209	GLU	N-CA-C	-6.13	105.93	113.41
1	B	399	ALA	N-CA-C	-6.08	104.72	111.71
1	C	405	LEU	N-CA-C	6.04	120.72	113.23
1	C	263	LEU	N-CA-C	-6.04	99.86	109.76
1	B	435	ILE	N-CA-C	-6.03	104.47	110.62
1	C	479	ARG	N-CA-C	6.03	119.11	110.24
1	D	322	SER	N-CA-C	5.95	118.68	110.35
1	D	221	ASN	N-CA-C	-5.90	104.94	114.09
1	B	249	ARG	N-CA-C	5.88	117.77	111.36
1	C	40	SER	N-CA-C	5.84	117.81	108.41
1	B	405	LEU	N-CA-C	5.83	120.52	113.17
1	D	379	ASN	CA-C-N	5.75	126.69	120.83
1	D	379	ASN	C-N-CA	5.75	126.69	120.83
1	A	213	GLU	N-CA-C	-5.73	103.36	110.41
1	C	168	CYS	N-CA-C	5.70	117.49	111.28
1	B	168	CYS	N-CA-C	5.68	117.15	111.07
1	A	298	TRP	N-CA-C	-5.65	105.04	111.14
1	C	112	LEU	CA-C-N	5.60	126.84	119.84
1	C	112	LEU	C-N-CA	5.60	126.84	119.84
1	A	81	TRP	N-CA-C	-5.59	105.08	111.07
1	A	153	CYS	N-CA-C	-5.51	100.12	108.67
1	B	91	LEU	CA-C-N	5.46	125.38	119.76
1	B	91	LEU	C-N-CA	5.46	125.38	119.76
1	A	45	VAL	CA-C-N	5.44	126.64	119.84
1	A	45	VAL	C-N-CA	5.44	126.64	119.84
1	A	290	ARG	N-CA-C	-5.34	105.46	111.28
1	D	11	THR	N-CA-C	-5.33	106.55	113.16
1	A	475	GLU	N-CA-C	-5.29	105.59	111.36
1	D	389	ALA	N-CA-C	-5.28	106.79	114.12
1	D	116	GLU	N-CA-C	-5.26	105.02	111.75
1	D	119	ASN	N-CA-C	-5.26	108.12	114.75
1	D	85	PRO	CA-C-N	5.22	126.36	119.84
1	D	85	PRO	C-N-CA	5.22	126.36	119.84
1	B	389	ALA	N-CA-C	-5.16	106.94	114.12
1	C	264	SER	N-CA-C	5.16	116.37	108.42
1	A	3	LEU	N-CA-C	-5.16	105.78	111.71
1	A	340	GLY	CA-C-N	5.15	126.28	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	GLY	C-N-CA	5.15	126.28	119.84
1	C	91	LEU	CA-C-N	5.12	125.02	119.85
1	C	91	LEU	C-N-CA	5.12	125.02	119.85
1	B	258	THR	N-CA-C	-5.12	106.63	112.92
1	B	264	SER	N-CA-C	5.12	116.58	108.96
1	B	92	PRO	N-CA-C	5.11	119.11	111.14
1	D	263	LEU	N-CA-C	-5.04	101.47	109.59
1	B	177	ARG	N-CA-C	5.01	116.94	108.02

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	4124	0	4085	191	0
1	B	4101	0	4055	252	0
1	C	4107	0	4060	216	0
1	D	4087	0	4041	203	0
2	A	24	0	17	1	0
2	B	24	0	17	2	0
2	C	24	0	17	1	0
2	D	24	0	17	3	0
3	A	48	0	26	1	0
3	B	48	0	26	5	0
3	C	48	0	26	4	0
3	D	48	0	26	5	0
4	A	5	0	0	0	0
4	B	5	0	0	1	0
4	C	10	0	0	1	0
5	A	12	0	9	2	0
5	B	4	0	3	0	0
5	C	8	0	6	0	0
5	D	16	0	12	1	0
6	B	6	0	8	0	0
6	C	6	0	8	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	23	0	0	1	0
7	B	12	0	0	0	0
7	C	23	0	0	1	0
7	D	25	0	0	0	0
All	All	16862	0	16459	836	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 25.

All (836) 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:37:ASP:HB3	1:C:40:SER:HB3	1.40	1.02
1:C:62:LYS:HE2	1:C:64:VAL:HB	1.41	1.00
1:A:329:ARG:HH12	1:A:400:LEU:HA	1.35	0.90
1:C:116:GLU:HA	1:C:119:ASN:ND2	1.87	0.90
1:C:233:ARG:NH1	1:C:235:ARG:HH12	1.70	0.89
1:B:53:ARG:NH1	1:B:94:ARG:HH22	1.73	0.87
1:C:233:ARG:CZ	1:C:235:ARG:HH12	1.88	0.86
1:C:237:GLU:HG3	1:C:282:LEU:HD22	1.54	0.86
1:D:112:LEU:HD12	1:D:113:PRO:HD2	1.56	0.86
1:B:37:ASP:HB2	1:B:186:SER:O	1.77	0.85
1:D:106:GLN:HA	1:D:109:LEU:HD13	1.61	0.82
1:C:155:GLY:HA3	3:C:703:NDP:H5N	1.61	0.82
1:A:387:PHE:CE1	1:A:407:ALA:HB3	2.15	0.81
1:C:181:ARG:HH21	1:C:224:LYS:HG3	1.45	0.81
1:A:40:SER:O	1:A:42:PRO:HD3	1.81	0.80
1:C:20:LEU:HB2	1:C:171:LEU:CD1	2.14	0.78
1:D:386:LEU:HB2	1:D:407:ALA:O	1.84	0.78
1:C:306:ALA:HB3	1:C:337:MET:HE3	1.66	0.78
1:C:376:LEU:HD13	1:C:385:MET:SD	2.24	0.77
1:D:376:LEU:HD13	1:D:385:MET:SD	2.25	0.77
1:A:8:MET:HE2	1:A:499:TYR:CE1	2.19	0.77
1:B:257:ARG:H	1:B:257:ARG:HD3	1.49	0.77
1:B:490:ARG:HB3	1:B:490:ARG:NH1	2.00	0.77
1:C:425:CYS:SG	1:C:460:LEU:HD12	2.24	0.76
1:A:1:MET:HA	1:A:4:PHE:HD2	1.51	0.76
1:C:35:ILE:HD12	1:C:189:VAL:HG12	1.67	0.76
1:D:131:GLY:H	1:D:134:GLN:CD	1.93	0.76
1:B:289:TRP:CH2	1:B:440:LEU:HD22	2.21	0.76
1:D:397:ARG:HG2	1:D:397:ARG:HH11	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:GLY:HA3	3:A:701:NDP:H5N	1.67	0.75
1:B:491:ARG:HD3	1:B:493:ARG:HH12	1.51	0.75
1:A:1:MET:HA	1:A:4:PHE:CD2	2.23	0.74
1:B:104:THR:HG22	1:B:107:HIS:CG	2.23	0.73
1:C:115:GLU:HG2	1:C:118:ARG:HH12	1.53	0.73
1:C:300:LEU:HD13	1:C:496:LEU:HD11	1.68	0.73
1:D:234:ASN:C	1:D:234:ASN:HD22	1.94	0.73
1:A:256:ASP:HB2	1:A:257:ARG:HH11	1.51	0.73
1:A:281:LEU:HD22	1:A:287:VAL:HB	1.70	0.73
1:B:117:LYS:HB2	1:B:121:HIS:HD2	1.55	0.72
1:B:219:ASN:C	1:B:219:ASN:HD22	1.96	0.72
1:D:270:MET:HE2	1:D:460:LEU:HD21	1.71	0.72
1:B:115:GLU:HG2	1:B:118:ARG:HH11	1.54	0.72
1:D:241:LEU:HD11	1:D:284:THR:HG21	1.72	0.72
1:B:112:LEU:HB3	1:B:117:LYS:HE3	1.72	0.71
1:B:117:LYS:HB2	1:B:121:HIS:CD2	2.24	0.71
1:B:115:GLU:HG2	1:B:118:ARG:NH1	2.05	0.71
1:B:422:GLN:NE2	1:B:425:CYS:HB3	2.06	0.71
1:C:447:LYS:HZ1	1:C:492:GLU:CD	1.97	0.71
1:C:41:ILE:O	1:C:41:ILE:HG23	1.91	0.70
1:B:213:GLU:O	1:B:215:LEU:HD13	1.90	0.70
1:C:350:PHE:CE1	1:D:392:PRO:HD2	2.27	0.70
1:C:20:LEU:HB2	1:C:171:LEU:HD13	1.72	0.70
1:B:376:LEU:HD13	1:B:385:MET:SD	2.32	0.70
1:A:16:THR:HG21	1:A:489:PHE:CD2	2.27	0.69
1:C:350:PHE:CZ	1:D:392:PRO:HD2	2.27	0.69
1:C:386:LEU:HD12	1:C:406:LEU:HD11	1.74	0.69
1:B:233:ARG:CZ	1:B:235:ARG:NH1	2.55	0.69
1:B:296:LEU:CD2	1:B:440:LEU:HG	2.22	0.69
1:C:31:GLU:OE1	1:C:181:ARG:HD3	1.93	0.69
1:A:420:LEU:HD12	1:A:421:TYR:N	2.08	0.69
1:A:219:ASN:N	1:A:219:ASN:HD22	1.91	0.69
1:A:489:PHE:HE1	1:A:504:MET:HE2	1.57	0.69
1:D:81:TRP:CZ2	1:D:89:ARG:HD3	2.28	0.69
1:C:109:LEU:O	1:C:112:LEU:HD13	1.92	0.68
1:D:117:LYS:HE2	1:D:121:HIS:NE2	2.08	0.68
1:C:491:ARG:HD3	1:C:493:ARG:NH1	2.08	0.68
1:B:6:ILE:HD13	1:B:373:VAL:HG21	1.76	0.68
1:B:429:LEU:N	1:B:429:LEU:HD22	2.08	0.68
1:B:89:ARG:HH21	1:B:112:LEU:HD23	1.58	0.68
1:C:116:GLU:HA	1:C:119:ASN:HD22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:PHE:CZ	1:B:392:PRO:HD2	2.30	0.67
1:A:208:ARG:HG2	1:A:230:LEU:CD2	2.25	0.67
1:A:275:ARG:O	1:A:278:ARG:HG3	1.94	0.67
1:C:31:GLU:CD	1:C:181:ARG:HD3	2.20	0.67
1:B:26:VAL:HG12	2:B:602:2CY:N3	2.10	0.66
1:C:331:LEU:HD22	1:C:334:TYR:CE2	2.30	0.66
1:C:427:MET:SD	1:C:431:VAL:HG21	2.35	0.66
1:C:395:LEU:HD12	1:C:398:MET:HE3	1.78	0.66
1:C:427:MET:HB2	1:C:465:VAL:HG22	1.77	0.66
1:A:257:ARG:HD3	1:A:257:ARG:N	2.11	0.66
1:D:175:ILE:HB	1:D:230:LEU:HB2	1.77	0.66
1:A:265:ILE:HD12	1:A:265:ILE:C	2.21	0.66
1:C:146:PRO:HG3	1:C:505:GLU:CD	2.21	0.66
1:D:490:ARG:HB3	1:D:490:ARG:NH1	2.11	0.66
1:C:181:ARG:NH2	1:C:224:LYS:HG3	2.11	0.66
1:D:115:GLU:HG3	1:D:118:ARG:NH1	2.10	0.65
1:B:233:ARG:CZ	1:B:235:ARG:HH12	2.08	0.65
1:C:239:GLN:HE22	1:C:271:ARG:H	1.44	0.65
1:D:12:VAL:HG22	1:D:492:GLU:OE1	1.95	0.65
1:B:29:VAL:HG21	1:B:33:GLY:HA2	1.79	0.65
1:C:360:ASN:HD21	1:C:362:ASP:CG	2.05	0.65
1:D:340:GLY:HA2	1:D:354:TYR:CE2	2.32	0.65
1:A:420:LEU:HD12	1:A:421:TYR:H	1.62	0.65
1:C:8:MET:HE3	1:C:12:VAL:HG23	1.79	0.64
1:C:14:GLU:HG2	1:C:15:GLY:N	2.12	0.64
1:A:16:THR:HG21	1:A:489:PHE:HD2	1.62	0.64
1:A:239:GLN:HE22	1:A:271:ARG:H	1.45	0.64
1:D:425:CYS:SG	1:D:460:LEU:HD12	2.37	0.64
1:B:491:ARG:HD3	1:B:493:ARG:NH1	2.11	0.64
1:D:117:LYS:C	1:D:119:ASN:H	2.06	0.64
1:A:35:ILE:HG13	1:A:36:GLY:N	2.11	0.64
1:B:336:GLU:O	1:B:337:MET:HB2	1.97	0.64
1:D:308:LYS:O	1:D:312:LYS:HG2	1.98	0.64
1:C:115:GLU:HA	1:C:118:ARG:NH2	2.13	0.64
1:B:256:ASP:HB2	1:B:260:VAL:H	1.63	0.63
1:D:489:PHE:CD1	1:D:504:MET:HB3	2.34	0.63
1:D:325:PHE:O	1:D:328:SER:HB3	1.97	0.63
1:B:78:ARG:HD3	3:B:702:NDP:O2X	1.98	0.63
1:C:235:ARG:HH11	1:C:235:ARG:HG3	1.62	0.63
1:C:470:VAL:O	1:C:474:ASN:HB2	1.98	0.63
1:D:272:PHE:CZ	1:D:435:ILE:HD13	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:41:ILE:O	1:B:41:ILE:HG13	1.97	0.63
1:D:310:SER:C	1:D:312:LYS:H	2.05	0.63
1:A:342:VAL:HG12	1:A:398:MET:HB3	1.81	0.63
1:B:115:GLU:HA	1:B:118:ARG:HD3	1.79	0.63
1:D:115:GLU:HA	1:D:118:ARG:HG2	1.80	0.63
1:D:155:GLY:HA2	3:D:704:NDP:H5N	1.81	0.63
1:C:300:LEU:HD13	1:C:496:LEU:CD1	2.29	0.63
1:A:415:GLU:HA	1:A:452:ARG:O	1.99	0.62
1:B:209:GLU:OE1	1:B:229:LYS:NZ	2.25	0.62
1:B:420:LEU:HD22	1:B:438:TYR:CD2	2.34	0.62
1:D:104:THR:O	1:D:108:LEU:HD13	2.00	0.62
1:C:233:ARG:CZ	1:C:235:ARG:NH1	2.62	0.62
1:D:253:VAL:HG22	1:D:263:LEU:CD2	2.30	0.62
1:D:275:ARG:NE	1:D:415:GLU:OE2	2.32	0.62
1:A:4:PHE:CZ	1:A:362:ASP:HB3	2.35	0.62
1:D:288:PHE:O	1:D:292:VAL:HG23	1.99	0.62
1:B:20:LEU:HB2	1:B:171:LEU:HD13	1.82	0.62
1:B:466:TYR:HB2	1:B:469:HIS:CE1	2.35	0.62
1:D:110:ASP:HA	1:D:118:ARG:HD3	1.82	0.62
1:A:288:PHE:O	1:A:292:VAL:HG23	2.00	0.62
1:B:251:GLY:O	1:D:208:ARG:NH2	2.31	0.62
1:D:31:GLU:HG2	1:D:181:ARG:HA	1.82	0.62
1:B:19:ALA:O	1:B:20:LEU:HD23	2.00	0.61
1:B:29:VAL:CG2	1:B:33:GLY:HA2	2.30	0.61
1:A:23:PHE:CE1	1:A:172:LEU:HD13	2.36	0.61
1:C:8:MET:HE3	1:C:12:VAL:CG2	2.30	0.61
1:A:155:GLY:HA2	1:A:160:TYR:CZ	2.35	0.61
1:B:296:LEU:HD11	1:B:441:LEU:HD13	1.81	0.61
1:D:37:ASP:OD2	1:D:42:PRO:HD3	2.00	0.61
1:D:210:THR:HA	5:D:810:ACT:H2	1.81	0.61
1:B:85:PRO:O	1:B:87:LYS:N	2.32	0.61
1:A:300:LEU:HD21	1:A:441:LEU:CD1	2.31	0.61
1:C:258:THR:HB	1:C:260:VAL:HG23	1.82	0.61
1:A:336:GLU:O	1:A:337:MET:HB2	1.99	0.61
1:D:186:SER:C	1:D:188:SER:H	2.05	0.61
1:B:155:GLY:HA2	3:B:702:NDP:H5N	1.83	0.61
1:A:262:THR:HG22	1:A:466:TYR:HA	1.82	0.60
1:A:350:PHE:CE1	1:B:392:PRO:HD2	2.36	0.60
1:B:104:THR:HG22	1:B:107:HIS:CD2	2.36	0.60
1:C:76:MET:HE2	1:C:154:ILE:HD11	1.81	0.60
1:B:12:VAL:HG13	1:B:13:ALA:H	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:30:ASP:HA	1:C:180:ILE:O	2.01	0.60
1:D:471:GLU:N	1:D:472:PRO:HD2	2.16	0.60
1:A:49:MET:SD	2:A:601:2CY:H9	2.41	0.60
1:B:425:CYS:SG	1:B:460:LEU:HB3	2.41	0.60
1:B:492:GLU:O	1:B:493:ARG:HD2	2.00	0.60
1:A:257:ARG:HD3	1:A:257:ARG:H	1.67	0.60
1:B:246:ARG:HA	1:B:249:ARG:NH1	2.17	0.60
1:B:264:SER:HB3	1:B:464:HIS:HB3	1.84	0.60
1:A:25:LEU:C	1:A:25:LEU:HD23	2.26	0.60
1:A:219:ASN:HD22	1:A:219:ASN:H	1.48	0.60
1:B:298:TRP:CD2	1:B:309:LEU:HD21	2.35	0.60
1:C:37:ASP:HB2	1:C:186:SER:HB3	1.83	0.60
1:C:73:ALA:HB2	1:C:148:ILE:HD12	1.84	0.60
1:D:406:LEU:C	1:D:406:LEU:HD12	2.27	0.60
1:A:340:GLY:HA2	1:A:354:TYR:CE2	2.37	0.60
1:C:18:LEU:HD22	1:C:488:VAL:HG11	1.84	0.60
1:C:37:ASP:CG	1:C:186:SER:HB3	2.27	0.60
1:C:165:ARG:C	1:C:169:VAL:HG22	2.27	0.59
1:B:45:VAL:HG13	1:B:217:SER:HB3	1.84	0.59
1:B:467:SER:O	1:B:470:VAL:HG23	2.02	0.59
1:B:65:LYS:HD2	1:B:65:LYS:N	2.16	0.59
1:B:219:ASN:HD21	1:B:221:ASN:HB2	1.66	0.59
1:A:420:LEU:HD22	1:A:438:TYR:CD2	2.37	0.59
1:B:165:ARG:C	1:B:169:VAL:HG22	2.27	0.59
1:C:475:GLU:OE2	1:C:478:LYS:HE2	2.03	0.59
1:D:360:ASN:HD22	1:D:361:TYR:N	2.00	0.59
1:A:322:SER:O	1:A:326:LEU:HB2	2.03	0.59
1:B:298:TRP:CE2	1:B:309:LEU:HD21	2.37	0.59
1:A:489:PHE:CE1	1:A:504:MET:HE2	2.37	0.59
1:D:391:ASN:O	1:D:395:LEU:HG	2.03	0.59
1:C:395:LEU:HA	1:C:398:MET:HE3	1.83	0.59
1:C:491:ARG:HD3	1:C:493:ARG:HH12	1.66	0.59
1:D:246:ARG:HA	1:D:249:ARG:NH1	2.18	0.58
1:A:492:GLU:O	1:A:493:ARG:HD3	2.03	0.58
1:B:176:TYR:CE2	1:B:229:LYS:HG3	2.38	0.58
1:C:132:LEU:HB3	1:C:162:GLU:HG2	1.85	0.58
1:A:233:ARG:CZ	1:A:235:ARG:NH1	2.66	0.58
1:B:323:ARG:NH1	1:B:334:TYR:O	2.35	0.58
1:A:105:THR:HG23	1:A:126:VAL:HA	1.86	0.58
1:A:18:LEU:HD22	1:A:488:VAL:HG11	1.85	0.58
1:B:138:LEU:HD22	1:B:138:LEU:O	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:LEU:HD13	1:A:496:LEU:HD21	1.86	0.58
1:B:485:PRO:HB3	1:B:509:TYR:HA	1.84	0.58
1:C:392:PRO:HD2	1:D:350:PHE:CZ	2.38	0.58
1:B:397:ARG:HG3	1:B:397:ARG:HH11	1.69	0.58
1:C:306:ALA:CB	1:C:337:MET:HE3	2.33	0.58
1:C:181:ARG:O	1:C:182:ALA:HB2	2.03	0.58
1:B:235:ARG:HA	1:B:238:GLU:HG3	1.86	0.57
1:C:41:ILE:O	1:C:41:ILE:CG2	2.50	0.57
1:C:44:ASN:O	1:C:46:PRO:HD3	2.04	0.57
1:B:156:GLY:HA3	3:B:702:NDP:O1A	2.04	0.57
1:D:497:GLU:N	1:D:497:GLU:OE2	2.36	0.57
1:B:234:ASN:O	1:B:238:GLU:HG3	2.05	0.57
1:C:386:LEU:N	1:C:386:LEU:HD23	2.18	0.57
1:D:219:ASN:N	1:D:219:ASN:HD22	2.01	0.57
1:C:184:GLU:HG2	1:C:186:SER:H	1.70	0.57
1:C:340:GLY:HA2	1:C:354:TYR:CE2	2.40	0.57
1:D:336:GLU:CD	1:D:336:GLU:H	2.13	0.57
1:C:469:HIS:O	1:C:473:CYS:HB2	2.05	0.57
1:C:476:GLN:NE2	1:C:517:MET:HE1	2.20	0.57
1:D:139:LEU:HD23	1:D:151:VAL:CG2	2.35	0.57
1:A:46:PRO:HG2	1:A:47:GLU:OE1	2.05	0.56
1:B:259:GLY:HA2	1:D:181:ARG:HH12	1.70	0.56
1:C:135:ALA:O	1:C:139:LEU:HB2	2.05	0.56
1:D:131:GLY:H	1:D:134:GLN:NE2	2.02	0.56
1:B:490:ARG:HB3	1:B:490:ARG:HH11	1.70	0.56
1:C:81:TRP:CH2	1:C:89:ARG:HG2	2.39	0.56
1:B:219:ASN:C	1:B:219:ASN:ND2	2.58	0.56
1:B:395:LEU:HB2	1:B:396:PRO:HD3	1.87	0.56
1:C:62:LYS:O	1:C:64:VAL:HG12	2.04	0.56
1:C:247:ILE:HG23	1:C:264:SER:HA	1.88	0.56
1:C:505:GLU:HA	7:C:1017:HOH:O	2.06	0.56
1:B:29:VAL:HG23	1:B:33:GLY:C	2.31	0.56
1:B:73:ALA:HB2	1:B:148:ILE:HD12	1.88	0.56
1:C:115:GLU:HA	1:C:118:ARG:HH22	1.71	0.56
1:C:471:GLU:HB2	1:C:472:PRO:CD	2.35	0.56
1:D:18:LEU:HA	1:D:277:ASN:ND2	2.19	0.56
1:D:233:ARG:CZ	1:D:235:ARG:NH1	2.69	0.56
1:B:103:LEU:HB3	1:B:108:LEU:HD12	1.88	0.56
1:C:475:GLU:O	1:C:478:LYS:HG3	2.06	0.56
1:B:469:HIS:C	1:B:472:PRO:HD2	2.31	0.56
1:D:78:ARG:HB2	1:D:100:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:219:ASN:CG	1:A:220:GLY:H	2.13	0.55
1:C:110:ASP:HA	1:C:118:ARG:HD3	1.88	0.55
1:C:298:TRP:CD1	1:C:303:GLU:HB2	2.40	0.55
1:B:35:ILE:HG13	1:B:36:GLY:N	2.21	0.55
1:B:115:GLU:HA	1:B:118:ARG:HB2	1.88	0.55
1:C:28:ALA:HB3	3:C:703:NDP:H72N	1.71	0.55
1:A:264:SER:HB3	1:A:464:HIS:HB3	1.88	0.55
1:B:103:LEU:HB3	1:B:108:LEU:CD1	2.37	0.55
1:C:391:ASN:O	1:C:395:LEU:HD13	2.07	0.55
1:C:404:HIS:HB2	1:C:420:LEU:HD11	1.87	0.55
1:D:99:LEU:O	3:D:704:NDP:H1B	2.06	0.55
1:D:234:ASN:HD21	1:D:236:GLU:HB2	1.70	0.55
1:D:360:ASN:ND2	1:D:362:ASP:H	2.04	0.55
1:B:85:PRO:C	1:B:87:LYS:H	2.14	0.55
1:C:310:SER:OG	1:C:337:MET:HE2	2.06	0.55
1:A:472:PRO:C	1:A:474:ASN:H	2.12	0.55
1:D:89:ARG:O	1:D:89:ARG:HG3	2.05	0.55
1:A:135:ALA:O	1:A:139:LEU:HG	2.06	0.55
1:B:74:VAL:HG22	1:B:154:ILE:CG2	2.37	0.55
1:C:20:LEU:HD12	1:C:171:LEU:HD12	1.89	0.55
1:A:35:ILE:HG12	1:A:189:VAL:HB	1.88	0.55
1:C:346:GLN:O	1:C:350:PHE:HB2	2.07	0.54
1:D:492:GLU:O	1:D:493:ARG:HD2	2.06	0.54
1:A:298:TRP:HH2	1:A:339:LEU:HD12	1.72	0.54
1:A:384:ARG:HG2	1:B:423:ARG:NH1	2.22	0.54
1:D:132:LEU:CD2	1:D:163:ALA:HB2	2.37	0.54
1:C:37:ASP:C	1:C:39:ARG:H	2.15	0.54
1:C:386:LEU:HD21	1:D:390:TRP:CH2	2.41	0.54
1:D:452:ARG:CD	1:D:453:PRO:HD2	2.38	0.54
1:A:84:ILE:O	1:A:89:ARG:HD3	2.07	0.54
1:A:84:ILE:CG2	1:A:89:ARG:HG3	2.38	0.54
1:B:85:PRO:C	1:B:87:LYS:N	2.64	0.54
1:B:181:ARG:HH11	1:B:224:LYS:HB2	1.73	0.54
1:D:265:ILE:CD1	1:D:463:ALA:HB3	2.38	0.54
1:B:239:GLN:HE22	1:B:271:ARG:H	1.56	0.53
1:A:37:ASP:O	1:A:39:ARG:N	2.40	0.53
1:C:175:ILE:HB	1:C:230:LEU:HB2	1.88	0.53
1:A:219:ASN:H	1:A:219:ASN:ND2	2.06	0.53
1:B:256:ASP:HB3	1:B:258:THR:H	1.73	0.53
1:B:296:LEU:HD23	1:B:440:LEU:HG	1.89	0.53
1:B:380:PRO:HB2	1:B:411:VAL:HG11	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ALA:O	1:B:443:ILE:HG13	2.08	0.53
1:D:96:ASN:N	1:D:96:ASN:HD22	2.06	0.53
1:D:466:TYR:HB2	1:D:469:HIS:CE1	2.43	0.53
1:B:298:TRP:CD1	1:B:303:GLU:HB3	2.43	0.53
1:C:188:SER:O	1:C:189:VAL:HB	2.08	0.53
1:C:387:PHE:O	1:C:406:LEU:HD12	2.08	0.53
1:D:9:PRO:HD2	1:D:448:ALA:HA	1.91	0.53
1:D:26:VAL:HG12	2:D:604:2CY:N3	2.24	0.53
1:D:234:ASN:C	1:D:234:ASN:ND2	2.62	0.53
1:C:88:PHE:N	1:C:88:PHE:CD2	2.74	0.53
1:C:336:GLU:O	1:C:337:MET:HB2	2.07	0.53
1:A:18:LEU:HD22	1:A:488:VAL:CG1	2.39	0.53
1:B:376:LEU:CD1	1:B:385:MET:SD	2.97	0.53
1:C:395:LEU:HD12	1:C:398:MET:CE	2.37	0.53
1:C:460:LEU:N	1:C:460:LEU:HD22	2.24	0.53
1:D:86:PRO:HA	1:D:89:ARG:HG2	1.90	0.53
1:D:469:HIS:O	1:D:473:CYS:HB2	2.08	0.53
1:B:20:LEU:HB2	1:B:171:LEU:CD1	2.39	0.53
1:B:67:SER:O	1:B:71:ARG:HD2	2.09	0.53
1:D:292:VAL:HA	1:D:433:PHE:CZ	2.44	0.53
1:B:306:ALA:HB2	1:B:339:LEU:HD11	1.90	0.53
1:A:208:ARG:NH2	1:C:263:LEU:HD22	2.24	0.52
1:C:235:ARG:HH11	1:C:235:ARG:CG	2.22	0.52
1:D:395:LEU:HB2	1:D:396:PRO:HD3	1.90	0.52
1:A:45:VAL:CG2	1:A:180:ILE:HD13	2.39	0.52
1:A:209:GLU:HG2	1:A:210:THR:HG23	1.90	0.52
1:B:361:TYR:HA	1:B:364:GLN:HG3	1.91	0.52
1:C:380:PRO:O	1:C:385:MET:HE1	2.09	0.52
1:D:485:PRO:HB3	1:D:509:TYR:HA	1.91	0.52
1:A:85:PRO:O	1:A:87:LYS:N	2.43	0.52
1:A:221:ASN:O	1:A:222:GLU:HB2	2.09	0.52
1:D:115:GLU:HG3	1:D:118:ARG:HH11	1.73	0.52
1:A:257:ARG:H	1:A:257:ARG:CD	2.22	0.52
1:B:241:LEU:HD22	1:B:477:LEU:HD23	1.92	0.52
1:C:329:ARG:NH1	1:C:399:ALA:O	2.42	0.52
5:A:809:ACT:H2	1:C:211:ILE:HG22	1.92	0.52
1:D:20:LEU:HB2	1:D:171:LEU:CD1	2.40	0.52
1:D:105:THR:HG22	1:D:109:LEU:HD11	1.90	0.52
1:D:139:LEU:HD23	1:D:151:VAL:HG21	1.92	0.52
1:D:155:GLY:CA	3:D:704:NDP:H5N	2.38	0.52
1:B:31:GLU:OE1	1:B:181:ARG:CZ	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:HIS:O	1:B:472:PRO:HD2	2.10	0.52
1:C:35:ILE:HD12	1:C:189:VAL:CG1	2.38	0.52
1:A:78:ARG:HB2	1:A:100:SER:HB2	1.91	0.52
1:A:117:LYS:HE2	1:A:121:HIS:NE2	2.25	0.52
1:B:295:GLU:O	1:B:298:TRP:HB3	2.09	0.52
1:B:415:GLU:HA	1:B:452:ARG:O	2.09	0.52
1:D:138:LEU:O	1:D:138:LEU:HD22	2.10	0.52
1:D:256:ASP:C	1:D:258:THR:N	2.65	0.52
1:B:117:LYS:C	1:B:119:ASN:H	2.18	0.51
1:B:314:VAL:HG12	1:B:316:ILE:HG12	1.92	0.51
1:D:247:ILE:HG12	1:D:265:ILE:HG13	1.93	0.51
1:B:321:GLY:O	1:B:337:MET:HE2	2.11	0.51
1:C:296:LEU:HD13	1:C:296:LEU:C	2.35	0.51
1:C:386:LEU:HD23	1:C:386:LEU:H	1.75	0.51
1:D:23:PHE:CE1	1:D:172:LEU:HD13	2.45	0.51
1:A:27:VAL:HG22	1:A:28:ALA:N	2.23	0.51
1:C:473:CYS:O	1:C:477:LEU:HG	2.10	0.51
1:D:85:PRO:O	1:D:87:LYS:N	2.43	0.51
1:A:272:PHE:CZ	1:A:435:ILE:HD13	2.45	0.51
1:B:213:GLU:O	1:B:215:LEU:CD1	2.57	0.51
1:D:246:ARG:HA	1:D:249:ARG:HH12	1.74	0.51
1:D:512:TYR:HB3	1:D:513:PRO:HD2	1.93	0.51
1:A:271:ARG:NH2	1:B:266:PHE:O	2.33	0.51
1:B:256:ASP:HB2	1:B:260:VAL:N	2.24	0.51
1:B:12:VAL:HG13	1:B:13:ALA:N	2.25	0.51
1:B:309:LEU:HB3	1:B:314:VAL:HB	1.93	0.51
1:D:146:PRO:HG3	1:D:505:GLU:OE1	2.11	0.51
1:B:249:ARG:HE	1:D:207:GLN:NE2	2.08	0.51
1:B:491:ARG:CD	1:B:493:ARG:NH1	2.74	0.51
1:A:392:PRO:HD2	1:B:350:PHE:CZ	2.45	0.51
1:A:460:LEU:N	1:A:460:LEU:HD22	2.26	0.51
1:B:485:PRO:HB3	1:B:509:TYR:CA	2.40	0.51
1:C:233:ARG:NH1	1:C:235:ARG:NH1	2.50	0.51
1:D:56:THR:HA	1:D:152:TYR:CE2	2.45	0.51
1:A:383:ARG:C	1:A:384:ARG:HG3	2.36	0.51
1:B:74:VAL:HG22	1:B:154:ILE:HG21	1.92	0.51
1:B:246:ARG:HA	1:B:249:ARG:HH12	1.74	0.51
1:B:466:TYR:HB2	1:B:469:HIS:ND1	2.26	0.51
1:B:473:CYS:O	1:B:477:LEU:HG	2.11	0.51
1:D:114:ASP:HB3	1:D:117:LYS:HB2	1.91	0.51
1:A:4:PHE:CE2	1:A:362:ASP:HB3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:315:HIS:HB3	1:D:318:ASP:OD1	2.10	0.51
1:A:78:ARG:HD2	1:A:78:ARG:C	2.35	0.50
1:B:386:LEU:N	1:B:386:LEU:HD23	2.25	0.50
1:C:331:LEU:HB3	1:C:334:TYR:CD2	2.46	0.50
1:D:110:ASP:O	1:D:112:LEU:N	2.44	0.50
1:A:219:ASN:N	1:A:219:ASN:ND2	2.59	0.50
1:A:254:LYS:O	1:A:261:GLY:HA2	2.11	0.50
1:A:467:SER:HA	1:A:470:VAL:HG23	1.93	0.50
1:C:164:LEU:HA	1:C:169:VAL:CG1	2.41	0.50
1:C:184:GLU:O	1:C:187:CYS:HB2	2.12	0.50
1:C:490:ARG:NH2	1:C:505:GLU:OE1	2.44	0.50
1:D:48:ASP:OD1	1:D:178:THR:HG21	2.11	0.50
1:D:49:MET:SD	2:D:604:2CY:H9	2.51	0.50
1:A:427:MET:SD	1:A:431:VAL:HG21	2.52	0.50
1:A:490:ARG:HB2	1:A:490:ARG:HH11	1.77	0.50
1:C:441:LEU:HD23	1:C:445:ILE:HG12	1.94	0.50
1:D:460:LEU:N	1:D:460:LEU:HD22	2.25	0.50
1:A:112:LEU:HB3	1:A:113:PRO:HD2	1.94	0.50
1:B:91:LEU:HB3	1:B:94:ARG:NH2	2.27	0.50
1:B:278:ARG:CZ	1:B:486:TYR:OH	2.60	0.50
1:C:155:GLY:CA	3:C:703:NDP:H5N	2.37	0.50
1:B:43:TRP:HZ3	1:B:184:GLU:HB3	1.76	0.50
1:D:262:THR:HG22	1:D:466:TYR:HA	1.93	0.50
1:B:98:VAL:HB	1:B:108:LEU:HD21	1.94	0.50
1:C:242:SER:O	1:C:245:ASP:HB3	2.12	0.50
1:A:271:ARG:HG2	1:A:457:VAL:HG22	1.94	0.50
1:C:37:ASP:CB	1:C:186:SER:HB3	2.41	0.50
1:C:49:MET:SD	2:C:603:2CY:H9	2.52	0.50
1:A:90:PRO:O	1:A:91:LEU:C	2.55	0.49
1:A:239:GLN:NE2	1:A:271:ARG:H	2.09	0.49
1:A:473:CYS:O	1:A:477:LEU:HG	2.11	0.49
1:C:162:GLU:HA	1:C:165:ARG:NH1	2.27	0.49
1:D:146:PRO:HG3	1:D:505:GLU:CD	2.36	0.49
1:D:336:GLU:O	1:D:337:MET:HB2	2.12	0.49
1:A:16:THR:O	1:A:277:ASN:ND2	2.39	0.49
1:B:27:VAL:HG22	1:B:28:ALA:N	2.28	0.49
1:B:216:THR:HA	1:B:223:THR:O	2.12	0.49
1:A:295:GLU:O	1:A:298:TRP:HB3	2.12	0.49
1:C:441:LEU:HD23	1:C:441:LEU:O	2.13	0.49
1:B:253:VAL:HG22	1:B:263:LEU:HG	1.94	0.49
1:B:262:THR:HG22	1:B:466:TYR:CD2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ILE:O	1:C:85:PRO:C	2.54	0.49
1:C:467:SER:C	1:C:469:HIS:H	2.21	0.49
1:D:265:ILE:HD12	1:D:265:ILE:C	2.37	0.49
1:D:460:LEU:HD22	1:D:460:LEU:H	1.76	0.49
1:A:425:CYS:SG	1:A:460:LEU:HD12	2.52	0.49
1:A:472:PRO:C	1:A:474:ASN:N	2.70	0.49
1:C:30:ASP:OD1	1:C:32:HIS:HB2	2.11	0.49
1:D:397:ARG:HG2	1:D:397:ARG:NH1	2.24	0.49
1:B:95:LEU:HD12	1:B:148:ILE:HD11	1.94	0.49
1:B:146:PRO:HB3	1:B:505:GLU:HG2	1.93	0.49
1:D:156:GLY:HA3	3:D:704:NDP:O1A	2.13	0.49
1:A:381:ASP:OD1	1:B:254:LYS:HD3	2.12	0.49
1:B:384:ARG:C	1:B:386:LEU:HD23	2.37	0.49
1:C:30:ASP:OD1	1:C:32:HIS:N	2.45	0.49
1:C:99:LEU:HD13	1:C:131:GLY:HA2	1.94	0.49
1:B:296:LEU:HG	1:B:300:LEU:HD23	1.95	0.49
1:B:433:PHE:O	1:B:436:ALA:HB3	2.13	0.49
1:C:47:GLU:CD	1:C:47:GLU:H	2.21	0.49
1:C:387:PHE:CE1	1:C:407:ALA:HB3	2.46	0.49
1:C:410:TYR:HB2	1:D:266:PHE:CE1	2.48	0.49
1:D:85:PRO:C	1:D:87:LYS:H	2.21	0.49
1:D:104:THR:O	1:D:107:HIS:HB2	2.13	0.49
1:A:381:ASP:CG	1:B:254:LYS:HD3	2.38	0.49
1:A:387:PHE:CZ	1:A:407:ALA:HB3	2.48	0.49
1:C:406:LEU:HD21	1:D:405:LEU:HD11	1.95	0.49
1:D:20:LEU:HB2	1:D:171:LEU:HD13	1.95	0.49
1:D:98:VAL:HB	1:D:108:LEU:HD21	1.94	0.49
1:D:114:ASP:HB3	1:D:117:LYS:CB	2.43	0.49
1:A:36:GLY:C	1:A:187:CYS:HB3	2.38	0.48
1:A:299:PHE:HB3	1:A:347:TRP:CZ3	2.48	0.48
1:C:295:GLU:O	1:C:298:TRP:HB3	2.12	0.48
1:D:186:SER:C	1:D:188:SER:N	2.71	0.48
1:B:25:LEU:HD21	1:B:160:TYR:CE1	2.48	0.48
1:B:78:ARG:HB2	1:B:100:SER:HB2	1.95	0.48
1:B:146:PRO:HG3	1:B:505:GLU:HG2	1.95	0.48
1:B:146:PRO:CB	1:B:505:GLU:HG2	2.42	0.48
1:A:485:PRO:HB3	1:A:509:TYR:HA	1.95	0.48
1:B:372:ILE:O	1:B:376:LEU:HB2	2.14	0.48
1:C:327:ASP:C	1:C:329:ARG:H	2.21	0.48
1:D:31:GLU:OE1	1:D:181:ARG:HD3	2.13	0.48
1:A:45:VAL:HG21	1:A:180:ILE:HD13	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:GLY:O	1:B:63:ASN:N	2.41	0.48
1:C:244:VAL:HG22	1:C:427:MET:HB3	1.95	0.48
1:C:406:LEU:CD2	1:D:405:LEU:HD11	2.43	0.48
1:A:31:GLU:HG3	1:A:181:ARG:HA	1.96	0.48
1:B:43:TRP:HH2	1:B:187:CYS:SG	2.37	0.48
1:D:31:GLU:CG	1:D:181:ARG:HA	2.43	0.48
1:D:32:HIS:CD2	1:D:184:GLU:HG2	2.48	0.48
1:D:219:ASN:HD22	1:D:219:ASN:H	1.61	0.48
1:A:493:ARG:HB3	1:A:498:ASP:HB2	1.95	0.48
1:B:390:TRP:HB2	1:B:405:LEU:HB2	1.95	0.48
1:B:515:ILE:O	1:B:517:MET:N	2.46	0.48
1:C:219:ASN:N	1:C:219:ASN:HD22	2.10	0.48
1:C:155:GLY:HA2	1:C:160:TYR:CZ	2.48	0.48
1:C:431:VAL:O	1:C:435:ILE:HG13	2.12	0.48
1:A:219:ASN:CG	1:A:220:GLY:N	2.71	0.48
1:A:462:ASP:OD1	1:B:383:ARG:HG2	2.14	0.48
1:A:494:GLU:HB3	1:A:495:PHE:CD1	2.49	0.48
1:B:431:VAL:O	1:B:435:ILE:HG13	2.14	0.48
1:D:12:VAL:HG13	1:D:13:ALA:N	2.29	0.48
1:D:219:ASN:H	1:D:219:ASN:ND2	2.12	0.48
1:A:419:MET:HG3	1:A:420:LEU:N	2.29	0.48
1:C:262:THR:HG22	1:C:466:TYR:CD2	2.49	0.48
1:B:78:ARG:HG3	1:B:103:LEU:HD12	1.96	0.47
1:C:431:VAL:HB	1:C:432:PRO:HD3	1.95	0.47
1:D:307:LYS:HA	1:D:310:SER:OG	2.13	0.47
1:B:409:PHE:HB3	1:B:416:LEU:HD11	1.96	0.47
1:B:428:GLY:C	1:B:429:LEU:HD22	2.39	0.47
1:C:110:ASP:HA	1:C:118:ARG:CD	2.44	0.47
1:D:109:LEU:HD12	1:D:109:LEU:H	1.79	0.47
1:D:301:ARG:NH1	1:D:303:GLU:HG3	2.29	0.47
1:D:475:GLU:CD	1:D:515:ILE:HG12	2.39	0.47
1:B:192:ARG:HH12	1:C:452:ARG:HH22	1.62	0.47
1:C:255:HIS:HA	1:C:260:VAL:O	2.14	0.47
1:D:116:GLU:O	1:D:120:LEU:N	2.47	0.47
1:B:39:ARG:HD2	1:B:39:ARG:N	2.30	0.47
1:B:309:LEU:H	1:B:309:LEU:HD22	1.79	0.47
1:D:32:HIS:NE2	1:D:184:GLU:HG2	2.30	0.47
1:C:94:ARG:O	1:C:96:ASN:ND2	2.46	0.47
1:C:298:TRP:NE1	1:C:303:GLU:HB2	2.30	0.47
1:A:405:LEU:HD12	1:A:406:LEU:HB2	1.96	0.47
1:B:21:ARG:NH2	1:B:149:GLU:O	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:25:LEU:HD23	1:B:26:VAL:N	2.28	0.47
1:B:340:GLY:HA2	1:B:354:TYR:CE2	2.50	0.47
1:C:181:ARG:O	1:C:182:ALA:CB	2.62	0.47
1:C:479:ARG:NH2	1:C:513:PRO:O	2.48	0.47
1:D:431:VAL:O	1:D:435:ILE:HG13	2.14	0.47
1:D:490:ARG:HB3	1:D:490:ARG:HH11	1.79	0.47
1:D:360:ASN:HD21	1:D:362:ASP:CG	2.22	0.47
1:B:28:ALA:HB3	3:B:702:NDP:O7N	2.15	0.47
1:B:53:ARG:NH1	1:B:94:ARG:NH2	2.54	0.47
1:B:383:ARG:C	1:B:384:ARG:HG3	2.39	0.47
1:C:25:LEU:C	1:C:25:LEU:HD23	2.40	0.47
1:C:44:ASN:OD1	1:C:49:MET:HE3	2.15	0.47
1:B:296:LEU:HD22	1:B:440:LEU:HG	1.98	0.47
1:C:383:ARG:HB2	4:C:804:PO4:O2	2.15	0.47
1:B:57:THR:OG1	1:B:94:ARG:HD3	2.15	0.46
1:D:138:LEU:O	1:D:144:TYR:HD2	1.98	0.46
1:D:299:PHE:HB3	1:D:347:TRP:CZ3	2.50	0.46
1:A:24:SER:HB2	1:A:152:TYR:CD1	2.50	0.46
1:A:114:ASP:OD2	1:A:116:GLU:HB3	2.15	0.46
1:A:401:PRO:HB2	1:A:423:ARG:NH2	2.30	0.46
1:B:405:LEU:HD21	1:B:423:ARG:HB3	1.97	0.46
1:C:253:VAL:HG22	1:C:263:LEU:CD2	2.46	0.46
1:D:415:GLU:HA	1:D:452:ARG:O	2.15	0.46
1:B:104:THR:O	1:B:108:LEU:HD13	2.15	0.46
1:C:254:LYS:O	1:C:261:GLY:HA2	2.16	0.46
1:D:249:ARG:HH11	1:D:249:ARG:HB2	1.79	0.46
1:D:310:SER:C	1:D:312:LYS:N	2.69	0.46
1:A:257:ARG:N	1:A:257:ARG:CD	2.78	0.46
1:B:84:ILE:CG2	1:B:89:ARG:HG2	2.46	0.46
1:C:52:PHE:CD1	1:C:52:PHE:C	2.94	0.46
1:C:219:ASN:H	1:C:219:ASN:ND2	2.13	0.46
1:C:264:SER:HB3	1:C:464:HIS:HB3	1.97	0.46
1:D:42:PRO:HG2	1:D:43:TRP:CD1	2.50	0.46
1:A:405:LEU:HD11	1:B:406:LEU:HD21	1.97	0.46
1:B:95:LEU:C	1:B:95:LEU:CD2	2.89	0.46
1:B:155:GLY:CA	3:B:702:NDP:H5N	2.44	0.46
1:B:293:CYS:O	1:B:297:LEU:HB2	2.16	0.46
1:D:219:ASN:N	1:D:219:ASN:ND2	2.64	0.46
1:D:265:ILE:HD11	1:D:463:ALA:HB3	1.96	0.46
1:D:283:THR:O	1:D:512:TYR:HD1	1.98	0.46
1:D:301:ARG:HH12	1:D:303:GLU:HG3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:452:ARG:HD3	1:D:453:PRO:HD2	1.97	0.46
1:A:285:LYS:HB2	1:A:476:GLN:OE1	2.16	0.46
1:A:386:LEU:HD12	1:A:406:LEU:HD11	1.98	0.46
1:C:160:TYR:OH	3:C:703:NDP:H41N	2.16	0.46
1:C:507:ILE:O	1:C:508:ASP:HB2	2.16	0.46
1:D:471:GLU:N	1:D:472:PRO:CD	2.79	0.46
1:A:265:ILE:C	1:A:265:ILE:CD1	2.89	0.46
1:B:43:TRP:CH2	1:B:187:CYS:SG	3.09	0.46
1:B:298:TRP:NE1	1:B:303:GLU:HB3	2.31	0.46
1:D:249:ARG:NH1	1:D:249:ARG:HB2	2.31	0.46
1:A:175:ILE:HB	1:A:230:LEU:HB2	1.98	0.46
1:A:219:ASN:HD21	1:A:222:GLU:H	1.64	0.46
1:A:269:GLN:HA	1:A:458:HIS:O	2.14	0.46
1:C:257:ARG:HH11	1:C:257:ARG:HG2	1.81	0.46
1:D:115:GLU:C	1:D:117:LYS:N	2.72	0.46
1:D:253:VAL:HG22	1:D:263:LEU:HD21	1.98	0.46
1:D:307:LYS:HA	1:D:310:SER:HG	1.81	0.46
1:A:98:VAL:HB	1:A:108:LEU:HD21	1.97	0.45
1:A:344:GLY:HA2	1:A:347:TRP:HB2	1.96	0.45
1:B:233:ARG:HD3	1:B:235:ARG:CZ	2.47	0.45
1:D:102:THR:OG1	1:D:103:LEU:N	2.49	0.45
1:A:16:THR:HG21	1:A:489:PHE:CE2	2.51	0.45
1:C:265:ILE:C	1:C:265:ILE:HD12	2.41	0.45
1:C:515:ILE:C	1:C:517:MET:H	2.25	0.45
1:B:256:ASP:OD1	1:B:260:VAL:HB	2.17	0.45
1:B:407:ALA:HA	1:B:419:MET:O	2.16	0.45
1:D:73:ALA:HB2	1:D:148:ILE:HD12	1.97	0.45
1:A:76:MET:HE2	1:A:154:ILE:HD11	1.98	0.45
1:B:94:ARG:O	1:B:96:ASN:ND2	2.49	0.45
1:B:258:THR:OG1	1:B:260:VAL:HG23	2.17	0.45
1:B:272:PHE:CZ	1:B:435:ILE:HD13	2.52	0.45
1:B:471:GLU:HB2	1:B:472:PRO:HD3	1.97	0.45
1:C:233:ARG:HD3	1:C:235:ARG:NH1	2.31	0.45
1:B:95:LEU:HD21	1:B:126:VAL:HG12	1.98	0.45
1:B:164:LEU:C	1:B:169:VAL:HG13	2.41	0.45
1:A:71:ARG:NH1	1:A:148:ILE:HD11	2.32	0.45
1:A:386:LEU:N	1:A:386:LEU:HD23	2.32	0.45
1:A:10:GLU:C	1:A:12:VAL:H	2.25	0.45
1:B:321:GLY:C	1:B:337:MET:HE2	2.41	0.45
1:C:134:GLN:CD	1:C:134:GLN:H	2.25	0.45
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:469:HIS:O	1:A:473:CYS:HB2	2.16	0.45
1:C:326:LEU:O	1:C:329:ARG:HB2	2.17	0.45
1:D:430:GLY:O	1:D:434:ASN:ND2	2.50	0.45
1:B:164:LEU:HD21	1:B:175:ILE:HD11	1.99	0.45
1:C:132:LEU:CD2	1:C:163:ALA:HB2	2.46	0.45
1:D:485:PRO:HB3	1:D:509:TYR:CA	2.47	0.45
1:B:3:LEU:HD23	1:B:3:LEU:O	2.17	0.44
1:C:169:VAL:C	1:C:171:LEU:H	2.25	0.44
1:C:415:GLU:HA	1:C:452:ARG:O	2.16	0.44
1:D:16:THR:HA	1:D:452:ARG:NH2	2.32	0.44
1:A:355:THR:OG1	1:A:356:HIS:N	2.50	0.44
1:C:112:LEU:N	1:C:112:LEU:HD12	2.31	0.44
1:D:298:TRP:HH2	1:D:339:LEU:HD12	1.82	0.44
1:A:387:PHE:O	1:A:406:LEU:HD12	2.17	0.44
5:A:809:ACT:CH3	1:C:211:ILE:HG22	2.46	0.44
1:B:11:THR:O	1:B:12:VAL:C	2.60	0.44
1:B:60:ARG:O	1:B:62:LYS:N	2.51	0.44
1:B:102:THR:OG1	1:B:103:LEU:N	2.50	0.44
1:C:72:ASN:OD1	1:C:150:THR:HB	2.17	0.44
1:C:232:PRO:CG	1:C:483:ALA:HB2	2.47	0.44
1:C:225:TYR:HE1	1:C:227:PHE:CE1	2.35	0.44
1:D:234:ASN:ND2	1:D:237:GLU:H	2.15	0.44
1:D:425:CYS:HB3	1:D:431:VAL:HG22	1.97	0.44
1:D:469:HIS:O	1:D:472:PRO:HG2	2.17	0.44
1:A:74:VAL:HG21	1:A:91:LEU:HD12	2.00	0.44
1:A:233:ARG:CZ	1:A:235:ARG:CZ	2.96	0.44
1:A:292:VAL:HG22	1:A:433:PHE:CE1	2.53	0.44
1:A:16:THR:O	1:A:16:THR:HG22	2.17	0.44
1:A:233:ARG:NH2	1:A:235:ARG:NH1	2.66	0.44
1:C:253:VAL:HG22	1:C:263:LEU:HD23	2.00	0.44
1:D:395:LEU:HD23	1:D:398:MET:HE3	1.99	0.44
1:D:434:ASN:O	1:D:437:SER:HB2	2.18	0.44
1:A:103:LEU:HD22	1:A:107:HIS:HB3	1.99	0.44
1:A:216:THR:HG23	1:A:224:LYS:HE2	1.99	0.44
1:D:218:ALA:C	1:D:220:GLY:H	2.26	0.44
1:A:193:VAL:O	1:A:194:PRO:C	2.59	0.44
1:A:471:GLU:N	1:A:472:PRO:HD2	2.32	0.44
1:B:117:LYS:O	1:B:121:HIS:HB2	2.18	0.44
1:B:404:HIS:HB2	1:B:420:LEU:HD11	1.98	0.44
1:B:490:ARG:HB3	1:B:490:ARG:CZ	2.46	0.44
1:C:87:LYS:HD3	1:C:88:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:ARG:HD2	1:C:228:GLU:OE1	2.17	0.44
1:D:104:THR:H	1:D:107:HIS:CG	2.35	0.44
1:D:253:VAL:HG22	1:D:263:LEU:HD23	1.99	0.44
1:D:398:MET:O	1:D:399:ALA:C	2.61	0.44
1:A:22:ALA:HB2	1:A:486:TYR:CE1	2.52	0.44
1:A:184:GLU:O	1:A:186:SER:N	2.48	0.44
1:B:89:ARG:HA	1:B:90:PRO:C	2.43	0.43
1:B:74:VAL:HG12	1:B:74:VAL:O	2.17	0.43
1:B:117:LYS:C	1:B:119:ASN:N	2.75	0.43
1:B:420:LEU:HD13	1:B:438:TYR:CE2	2.53	0.43
1:C:295:GLU:HG2	1:C:299:PHE:CE2	2.53	0.43
1:D:29:VAL:HB	1:D:33:GLY:HA2	1.99	0.43
1:D:47:GLU:HG2	1:D:225:TYR:OH	2.18	0.43
1:D:145:THR:HA	1:D:146:PRO:HA	1.82	0.43
1:A:263:LEU:HD12	1:A:263:LEU:N	2.33	0.43
1:B:286:ARG:HA	1:B:509:TYR:OH	2.18	0.43
1:B:304:THR:CG2	1:B:345:PHE:HB2	2.49	0.43
1:C:235:ARG:NH1	1:C:235:ARG:CG	2.80	0.43
1:C:372:ILE:O	1:C:376:LEU:HD22	2.18	0.43
1:C:376:LEU:O	1:C:380:PRO:HG3	2.17	0.43
1:C:386:LEU:HB3	1:C:408:GLN:HB2	2.01	0.43
1:D:348:ARG:O	1:D:367:ASP:HA	2.18	0.43
1:A:206:TRP:CZ3	1:A:232:PRO:HD3	2.53	0.43
1:A:258:THR:CG2	1:A:260:VAL:HG23	2.49	0.43
1:B:18:LEU:HA	1:B:277:ASN:ND2	2.32	0.43
1:B:192:ARG:NH1	1:C:452:ARG:HH22	2.17	0.43
1:B:405:LEU:HD12	1:B:405:LEU:C	2.43	0.43
1:C:117:LYS:C	1:C:119:ASN:H	2.26	0.43
1:C:422:GLN:HE22	1:C:434:ASN:ND2	2.16	0.43
1:A:79:LYS:O	1:A:82:ASP:HB2	2.19	0.43
1:A:333:GLU:HA	1:A:333:GLU:OE1	2.17	0.43
1:B:84:ILE:O	1:B:89:ARG:HD3	2.19	0.43
1:B:132:LEU:CD2	1:B:163:ALA:HB2	2.47	0.43
1:B:431:VAL:HB	1:B:432:PRO:HD3	2.01	0.43
1:A:294:GLU:OE1	1:A:294:GLU:HA	2.18	0.43
1:A:315:HIS:HB3	1:A:318:ASP:OD1	2.18	0.43
1:B:25:LEU:HD23	1:B:25:LEU:C	2.44	0.43
1:A:490:ARG:NH1	1:A:490:ARG:CB	2.82	0.43
1:B:302:GLY:HA2	1:B:344:GLY:C	2.43	0.43
1:B:425:CYS:HB2	1:B:431:VAL:CG2	2.49	0.43
1:C:269:GLN:HA	1:C:458:HIS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:467:SER:HA	1:C:470:VAL:HG23	2.01	0.43
1:D:495:PHE:HD1	1:D:498:ASP:OD1	2.01	0.43
1:A:249:ARG:HE	1:A:249:ARG:HB2	1.29	0.43
1:A:493:ARG:HH21	1:A:500:GLU:HG3	1.84	0.43
1:D:22:ALA:HA	1:D:171:LEU:HB3	1.99	0.43
1:D:78:ARG:HG3	1:D:103:LEU:HD12	2.00	0.43
1:A:30:ASP:OD2	1:A:30:ASP:C	2.62	0.43
1:B:31:GLU:HG3	1:B:181:ARG:HG2	2.01	0.43
1:B:98:VAL:O	1:B:127:ALA:HA	2.19	0.43
1:C:91:LEU:HA	1:C:92:PRO:HD3	1.83	0.43
1:D:7:ARG:HG3	1:D:7:ARG:HH11	1.83	0.43
1:D:110:ASP:C	1:D:112:LEU:N	2.77	0.43
1:A:307:LYS:HA	1:A:337:MET:HE3	2.01	0.42
1:C:80:THR:O	1:C:80:THR:HG22	2.19	0.42
1:C:234:ASN:O	1:C:238:GLU:HG3	2.19	0.42
1:C:390:TRP:HB2	1:C:405:LEU:HB2	2.00	0.42
1:D:341:PRO:HB2	1:D:346:GLN:NE2	2.33	0.42
1:A:8:MET:HE2	1:A:499:TYR:HE1	1.75	0.42
1:A:233:ARG:NH1	1:A:235:ARG:NH2	2.67	0.42
1:A:256:ASP:CB	1:A:257:ARG:HH11	2.26	0.42
1:A:406:LEU:HB3	1:A:421:TYR:HB3	2.01	0.42
1:B:219:ASN:ND2	1:B:221:ASN:HB2	2.31	0.42
1:B:423:ARG:HG3	1:B:424:SER:N	2.34	0.42
1:C:115:GLU:C	1:C:117:LYS:H	2.27	0.42
1:C:145:THR:HA	1:C:146:PRO:HA	1.84	0.42
1:D:452:ARG:HD3	1:D:453:PRO:CD	2.49	0.42
1:D:490:ARG:CZ	1:D:490:ARG:CB	2.96	0.42
1:A:395:LEU:HA	1:A:395:LEU:HD12	1.81	0.42
1:B:7:ARG:HG3	1:B:7:ARG:HH11	1.84	0.42
1:B:31:GLU:HG3	1:B:181:ARG:HA	2.01	0.42
1:B:289:TRP:O	1:B:292:VAL:HB	2.19	0.42
1:B:367:ASP:OD2	1:B:367:ASP:C	2.63	0.42
1:D:233:ARG:NE	1:D:235:ARG:NH1	2.67	0.42
1:A:60:ARG:HH22	1:A:508:ASP:HA	1.83	0.42
1:A:388:THR:HG21	1:B:390:TRP:HD1	1.85	0.42
1:B:225:TYR:HE1	1:B:227:PHE:CE1	2.37	0.42
1:B:164:LEU:HA	1:B:169:VAL:CG1	2.50	0.42
1:C:2:SER:C	1:C:4:PHE:N	2.74	0.42
1:C:13:ALA:O	1:C:14:GLU:C	2.62	0.42
1:C:78:ARG:HD2	1:C:78:ARG:C	2.45	0.42
1:C:130:GLY:HA3	1:C:134:GLN:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:ILE:HA	1:C:263:LEU:HD13	2.01	0.42
1:B:85:PRO:O	1:B:89:ARG:HG3	2.19	0.42
1:B:233:ARG:NE	1:B:235:ARG:NH1	2.67	0.42
1:B:343:TYR:CE1	1:B:404:HIS:CE1	3.07	0.42
1:B:447:LYS:NZ	1:B:492:GLU:OE2	2.41	0.42
1:D:194:PRO:CB	1:D:201:ALA:HA	2.50	0.42
1:A:8:MET:HE2	1:A:499:TYR:CZ	2.55	0.42
1:A:45:VAL:HA	1:A:46:PRO:HD2	1.77	0.42
1:A:54:ASP:HB3	1:A:58:LYS:HE3	2.00	0.42
1:A:71:ARG:HH11	1:A:148:ILE:HD11	1.84	0.42
1:A:208:ARG:HD3	1:A:228:GLU:OE1	2.19	0.42
1:B:269:GLN:HA	1:B:458:HIS:O	2.19	0.42
1:B:470:VAL:O	1:B:474:ASN:ND2	2.52	0.42
1:C:329:ARG:NH2	1:C:398:MET:O	2.52	0.42
1:A:231:ILE:HB	1:A:232:PRO:HD2	2.02	0.42
1:B:29:VAL:CG2	1:B:33:GLY:CA	2.97	0.42
1:B:243:LEU:O	1:B:247:ILE:HG13	2.20	0.42
1:B:391:ASN:OD1	1:B:391:ASN:C	2.61	0.42
1:D:48:ASP:OD2	2:D:604:2CY:N1	2.53	0.42
1:D:409:PHE:HB3	1:D:416:LEU:HD11	2.02	0.42
1:A:492:GLU:OE2	1:A:499:TYR:OH	2.35	0.42
1:D:36:GLY:HA2	1:D:186:SER:OG	2.19	0.42
1:D:117:LYS:C	1:D:119:ASN:N	2.75	0.42
1:D:333:GLU:O	1:D:356:HIS:HE1	2.03	0.42
1:D:360:ASN:ND2	1:D:360:ASN:C	2.77	0.42
1:A:20:LEU:HD22	1:A:136:LEU:HB2	2.01	0.42
1:A:496:LEU:HD23	1:A:496:LEU:O	2.20	0.42
1:B:85:PRO:O	1:B:88:PHE:N	2.53	0.42
1:B:309:LEU:HD22	1:B:309:LEU:N	2.34	0.42
1:B:424:SER:OG	1:B:464:HIS:HE1	2.03	0.42
1:C:115:GLU:O	1:C:117:LYS:N	2.53	0.42
1:D:80:THR:O	1:D:84:ILE:HG13	2.20	0.42
1:D:420:LEU:HD22	1:D:438:TYR:CD2	2.55	0.42
1:A:401:PRO:HB2	1:A:423:ARG:HH21	1.84	0.41
1:B:36:GLY:C	1:B:187:CYS:HA	2.45	0.41
1:B:479:ARG:HH22	1:B:515:ILE:HA	1.85	0.41
1:C:293:CYS:SG	1:C:501:GLU:HA	2.59	0.41
1:B:11:THR:O	1:B:14:GLU:N	2.52	0.41
1:B:48:ASP:OD2	2:B:602:2CY:H10	2.19	0.41
1:B:238:GLU:O	1:B:239:GLN:C	2.63	0.41
1:C:188:SER:O	1:C:189:VAL:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:406:LEU:HB3	1:C:421:TYR:HB3	2.02	0.41
1:C:424:SER:OG	1:C:464:HIS:HE1	2.04	0.41
1:C:471:GLU:HB2	1:C:472:PRO:HD3	2.00	0.41
1:D:486:TYR:CD1	1:D:486:TYR:N	2.88	0.41
1:A:89:ARG:HA	1:A:90:PRO:HA	1.87	0.41
1:A:211:ILE:HA	1:A:227:PHE:O	2.20	0.41
1:A:228:GLU:HG3	7:A:1033:HOH:O	2.20	0.41
1:A:296:LEU:HD13	1:A:296:LEU:C	2.46	0.41
1:D:193:VAL:O	1:D:194:PRO:C	2.62	0.41
1:D:466:TYR:HB2	1:D:469:HIS:ND1	2.36	0.41
1:A:177:ARG:HH11	1:A:228:GLU:CD	2.27	0.41
1:B:11:THR:O	1:B:13:ALA:N	2.54	0.41
1:B:490:ARG:HD3	1:B:505:GLU:HB2	2.01	0.41
1:C:342:VAL:O	1:C:343:TYR:C	2.63	0.41
1:D:132:LEU:O	1:D:136:LEU:HG	2.20	0.41
1:A:10:GLU:CG	1:A:11:THR:N	2.84	0.41
1:B:74:VAL:HG22	1:B:154:ILE:HG23	2.02	0.41
1:B:156:GLY:C	1:B:158:SER:N	2.75	0.41
1:B:380:PRO:O	1:B:411:VAL:HB	2.21	0.41
1:C:112:LEU:N	1:C:112:LEU:CD1	2.84	0.41
1:C:163:ALA:O	1:C:169:VAL:HG13	2.20	0.41
1:C:234:ASN:HB3	1:C:481:PRO:HB2	2.02	0.41
1:C:329:ARG:HD2	1:C:329:ARG:HA	1.95	0.41
1:D:56:THR:HG22	1:D:152:TYR:CG	2.55	0.41
1:A:153:CYS:SG	1:A:159:VAL:HG12	2.60	0.41
1:A:327:ASP:C	1:A:329:ARG:H	2.28	0.41
1:C:117:LYS:HG2	1:C:121:HIS:CE1	2.56	0.41
1:C:219:ASN:HD22	1:C:219:ASN:C	2.29	0.41
1:C:231:ILE:HB	1:C:232:PRO:HD2	2.03	0.41
1:D:475:GLU:O	1:D:478:LYS:HB2	2.20	0.41
1:C:211:ILE:HG23	1:C:211:ILE:O	2.20	0.41
1:D:208:ARG:NH1	1:D:228:GLU:OE1	2.50	0.41
1:D:489:PHE:CE1	1:D:504:MET:HB3	2.56	0.41
1:A:300:LEU:HD13	1:A:496:LEU:CD2	2.50	0.41
1:B:331:LEU:HD22	1:B:334:TYR:CZ	2.56	0.41
1:B:490:ARG:H	1:B:490:ARG:HG2	1.57	0.41
1:D:109:LEU:O	1:D:110:ASP:C	2.64	0.41
1:D:138:LEU:O	1:D:144:TYR:CD2	2.73	0.41
1:D:176:TYR:CE2	1:D:229:LYS:HG3	2.55	0.41
1:D:296:LEU:HD23	1:D:440:LEU:HD23	2.02	0.41
1:D:297:LEU:HD12	1:D:297:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ASP:OD2	1:A:48:ASP:C	2.64	0.41
1:A:252:ASN:O	1:A:263:LEU:HA	2.21	0.41
1:A:390:TRP:HB2	1:A:405:LEU:HB2	2.03	0.41
1:A:393:SER:O	1:A:396:PRO:HD2	2.21	0.41
1:B:108:LEU:CD1	1:B:108:LEU:H	2.33	0.41
1:B:233:ARG:NH1	1:B:235:ARG:HH12	2.18	0.41
1:B:384:ARG:HH21	4:B:801:PO4:P	2.44	0.41
1:B:405:LEU:HD12	1:B:406:LEU:HB2	2.02	0.41
1:B:490:ARG:HG2	1:B:503:ASP:O	2.21	0.41
1:C:31:GLU:OE2	1:C:181:ARG:HD3	2.21	0.41
1:C:169:VAL:C	1:C:171:LEU:N	2.78	0.41
1:C:294:GLU:OE1	1:C:294:GLU:HA	2.21	0.41
1:C:426:ASP:OD2	1:C:426:ASP:C	2.63	0.41
1:D:360:ASN:ND2	1:D:361:TYR:N	2.67	0.41
1:D:475:GLU:HA	1:D:478:LYS:HE2	2.03	0.41
1:A:136:LEU:HD12	1:A:168:CYS:SG	2.61	0.41
1:A:183:SER:C	1:A:185:SER:H	2.29	0.41
1:A:331:LEU:HD22	1:A:334:TYR:CE2	2.56	0.41
1:B:216:THR:CG2	1:B:222:GLU:HA	2.50	0.41
1:C:279:LEU:HD12	1:C:280:PRO:HD2	2.02	0.41
1:D:195:GLU:O	1:D:201:ALA:HB2	2.20	0.41
1:A:91:LEU:HB3	1:A:94:ARG:NH2	2.36	0.40
1:A:109:LEU:O	1:A:118:ARG:HD3	2.21	0.40
1:B:190:PHE:N	1:B:190:PHE:CD1	2.89	0.40
1:B:285:LYS:HD2	1:B:476:GLN:HE22	1.86	0.40
1:B:380:PRO:HB2	1:B:411:VAL:CG1	2.51	0.40
1:B:400:LEU:HA	1:B:401:PRO:HD3	1.96	0.40
1:B:515:ILE:HG13	1:B:517:MET:HE2	2.03	0.40
1:C:59:LEU:HD13	1:C:70:LYS:HG3	2.03	0.40
1:D:278:ARG:HH11	1:D:278:ARG:HG3	1.86	0.40
1:D:420:LEU:HD13	1:D:438:TYR:CE2	2.57	0.40
1:A:410:TYR:CD1	1:B:266:PHE:HB2	2.56	0.40
1:A:431:VAL:HB	1:A:432:PRO:HD3	2.03	0.40
1:B:132:LEU:HD22	1:B:163:ALA:HB2	2.02	0.40
1:B:241:LEU:HD11	1:B:284:THR:HG21	2.03	0.40
1:B:475:GLU:O	1:B:478:LYS:HB2	2.21	0.40
1:C:105:THR:O	1:C:109:LEU:HB2	2.21	0.40
1:C:391:ASN:OD1	1:C:393:SER:HB2	2.21	0.40
1:C:392:PRO:HD2	1:D:350:PHE:CE1	2.56	0.40
1:D:105:THR:O	1:D:109:LEU:HD12	2.21	0.40
1:D:300:LEU:HD21	1:D:441:LEU:HD13	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:GLU:O	1:A:337:MET:CB	2.69	0.40
1:A:369:ILE:O	1:A:373:VAL:HG23	2.22	0.40
1:B:75:VAL:HA	1:B:97:VAL:HB	2.04	0.40
1:B:90:PRO:HD3	1:B:125:ILE:HD11	2.03	0.40
1:B:104:THR:H	1:B:107:HIS:HB2	1.86	0.40
1:B:235:ARG:CA	1:B:238:GLU:HG3	2.49	0.40
1:C:107:HIS:O	1:C:108:LEU:C	2.62	0.40
1:C:266:PHE:HA	1:C:461:GLY:O	2.21	0.40
1:C:360:ASN:ND2	1:C:362:ASP:H	2.19	0.40
1:D:102:THR:HG23	3:D:704:NDP:O2X	2.21	0.40
1:D:404:HIS:HB2	1:D:420:LEU:HD11	2.03	0.40
1:A:359:ALA:HB3	1:A:361:TYR:CZ	2.57	0.40
1:A:479:ARG:NH2	1:A:513:PRO:O	2.55	0.40
1:B:387:PHE:CE2	1:B:407:ALA:HB3	2.57	0.40
1:C:3:LEU:HD23	1:C:3:LEU:HA	1.91	0.40
1:C:446:ALA:HB1	1:C:451:LEU:O	2.21	0.40
1:D:162:GLU:HG3	1:D:165:ARG:NH1	2.36	0.40
1:D:248:ILE:HA	1:D:263:LEU:HD13	2.03	0.40
1:A:30:ASP:O	1:A:32:HIS:N	2.55	0.40
1:A:99:LEU:HD23	1:A:128:VAL:CG1	2.52	0.40
1:A:315:HIS:HB3	1:A:318:ASP:CG	2.47	0.40
1:B:45:VAL:HG21	1:B:180:ILE:HD12	2.04	0.40
1:B:205:GLU:OE1	1:B:235:ARG:NH2	2.54	0.40
1:B:420:LEU:HD13	1:B:438:TYR:CZ	2.56	0.40
1:C:307:LYS:C	1:C:309:LEU:N	2.79	0.40
1:C:317:TRP:CE3	1:C:339:LEU:HD13	2.56	0.40
1:C:381:ASP:CG	1:D:254:LYS:HD3	2.47	0.40
1:D:233:ARG:NH2	1:D:235:ARG:NH1	2.69	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	516/521 (99%)	463 (90%)	39 (8%)	14 (3%)	4	15
1	B	513/521 (98%)	466 (91%)	33 (6%)	14 (3%)	4	15
1	C	514/521 (99%)	453 (88%)	46 (9%)	15 (3%)	3	13
1	D	511/521 (98%)	448 (88%)	49 (10%)	14 (3%)	4	15
All	All	2054/2084 (99%)	1830 (89%)	167 (8%)	57 (3%)	4	14

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	GLY
1	B	12	VAL
1	B	113	PRO
1	B	516	SER
1	C	182	ALA
1	C	343	TYR
1	D	37	ASP
1	D	113	PRO
1	D	184	GLU
1	D	343	TYR
1	A	31	GLU
1	A	187	CYS
1	A	343	TYR
1	B	38	GLY
1	B	61	GLY
1	B	62	LYS
1	B	202	ALA
1	B	515	ILE
1	C	12	VAL
1	C	62	LYS
1	C	139	LEU
1	D	61	GLY
1	D	86	PRO
1	D	109	LEU
1	D	111	GLY
1	A	62	LYS
1	A	86	PRO
1	A	185	SER
1	A	219	ASN
1	B	256	ASP
1	C	15	GLY
1	C	116	GLU
1	C	183	SER

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Mol	Chain	Res	Type
1	C	187	CYS
1	C	189	VAL
1	C	516	SER
1	D	122	ALA
1	A	184	GLU
1	B	63	ASN
1	B	86	PRO
1	B	343	TYR
1	B	359	ALA
1	D	13	ALA
1	D	14	GLU
1	C	86	PRO
1	D	187	CYS
1	A	2	SER
1	A	322	SER
1	A	380	PRO
1	C	113	PRO
1	A	61	GLY
1	A	341	PRO
1	D	259	GLY
1	B	42	PRO
1	C	85	PRO
1	C	485	PRO
1	D	42	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	444/446 (100%)	426 (96%)	18 (4%)	27	62
1	B	441/446 (99%)	416 (94%)	25 (6%)	18	49
1	C	442/446 (99%)	419 (95%)	23 (5%)	21	53
1	D	439/446 (98%)	413 (94%)	26 (6%)	18	48
All	All	1766/1784 (99%)	1674 (95%)	92 (5%)	21	53

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	39	ARG
1	A	48	ASP
1	A	71	ARG
1	A	95	LEU
1	A	109	LEU
1	A	128	VAL
1	A	138	LEU
1	A	219	ASN
1	A	285	LYS
1	A	297	LEU
1	A	333	GLU
1	A	395	LEU
1	A	420	LEU
1	A	440	LEU
1	A	460	LEU
1	A	473	CYS
1	A	514	PRO
1	B	39	ARG
1	B	64	VAL
1	B	71	ARG
1	B	74	VAL
1	B	95	LEU
1	B	123	ASP
1	B	138	LEU
1	B	139	LEU
1	B	169	VAL
1	B	171	LEU
1	B	219	ASN
1	B	274	LEU
1	B	297	LEU
1	B	303	GLU
1	B	310	SER
1	B	376	LEU
1	B	386	LEU
1	B	417	SER
1	B	419	MET
1	B	425	CYS
1	B	429	LEU
1	B	437	SER
1	B	456	LEU
1	B	490	ARG

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Mol	Chain	Res	Type
1	B	515	ILE
1	C	2	SER
1	C	26	VAL
1	C	64	VAL
1	C	95	LEU
1	C	106	GLN
1	C	109	LEU
1	C	138	LEU
1	C	139	LEU
1	C	169	VAL
1	C	219	ASN
1	C	235	ARG
1	C	243	LEU
1	C	297	LEU
1	C	326	LEU
1	C	374	GLU
1	C	376	LEU
1	C	395	LEU
1	C	400	LEU
1	C	405	LEU
1	C	456	LEU
1	C	460	LEU
1	C	491	ARG
1	C	496	LEU
1	D	43	TRP
1	D	74	VAL
1	D	95	LEU
1	D	96	ASN
1	D	102	THR
1	D	106	GLN
1	D	113	PRO
1	D	138	LEU
1	D	141	SER
1	D	146	PRO
1	D	149	GLU
1	D	169	VAL
1	D	219	ASN
1	D	242	SER
1	D	274	LEU
1	D	297	LEU
1	D	309	LEU
1	D	326	LEU

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Mol	Chain	Res	Type
1	D	355	THR
1	D	376	LEU
1	D	406	LEU
1	D	425	CYS
1	D	452	ARG
1	D	456	LEU
1	D	460	LEU
1	D	473	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	315	HIS
1	A	320	ASN
1	A	434	ASN
1	A	476	GLN
1	B	44	ASN
1	B	106	GLN
1	B	121	HIS
1	B	207	GLN
1	B	219	ASN
1	B	276	ASN
1	B	277	ASN
1	B	356	HIS
1	B	357	HIS
1	B	422	GLN
1	B	434	ASN
1	B	464	HIS
1	B	476	GLN
1	C	106	GLN
1	C	119	ASN
1	C	121	HIS
1	C	170	HIS
1	C	207	GLN
1	C	219	ASN
1	C	239	GLN
1	C	320	ASN
1	C	360	ASN
1	C	368	GLN
1	C	422	GLN
1	C	464	HIS

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Mol	Chain	Res	Type
1	C	469	HIS
1	C	474	ASN
1	C	476	GLN
1	D	63	ASN
1	D	106	GLN
1	D	129	ASN
1	D	143	ASN
1	D	207	GLN
1	D	219	ASN
1	D	234	ASN
1	D	276	ASN
1	D	277	ASN
1	D	315	HIS
1	D	320	ASN
1	D	356	HIS
1	D	360	ASN
1	D	413	ASN
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

24 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	$\# Z > 2$
4	PO4	B	801	-	4,4,4	2.38	1 (25%)	6,6,6	0.95	0
6	GOL	B	806	-	5,5,5	0.52	0	5,5,5	0.22	0
3	NDP	C	703	-	51,52,52	1.71	12 (23%)	71,80,80	1.60	14 (19%)
2	2CY	A	601	-	26,26,26	2.19	10 (38%)	35,35,35	1.79	7 (20%)
6	GOL	C	805	-	5,5,5	0.46	0	5,5,5	0.31	0
5	ACT	D	815	-	3,3,3	0.62	0	3,3,3	1.36	0
3	NDP	A	701	-	51,52,52	1.77	11 (21%)	71,80,80	1.50	13 (18%)
4	PO4	C	804	-	4,4,4	2.68	1 (25%)	6,6,6	0.88	0
2	2CY	C	603	-	26,26,26	2.16	11 (42%)	35,35,35	1.80	8 (22%)
3	NDP	D	704	-	51,52,52	1.75	11 (21%)	71,80,80	1.56	13 (18%)
5	ACT	A	809	-	3,3,3	0.64	0	3,3,3	1.36	0
5	ACT	D	810	-	3,3,3	0.38	0	3,3,3	1.46	0
5	ACT	D	816	-	3,3,3	0.50	0	3,3,3	1.44	0
2	2CY	B	602	-	26,26,26	2.21	11 (42%)	35,35,35	1.76	7 (20%)
5	ACT	A	807	-	3,3,3	0.58	0	3,3,3	1.40	0
5	ACT	B	811	-	3,3,3	0.80	0	3,3,3	1.45	0
5	ACT	C	812	-	3,3,3	0.53	0	3,3,3	1.30	0
5	ACT	D	814	-	3,3,3	0.69	0	3,3,3	1.33	0
4	PO4	A	802	-	4,4,4	2.58	1 (25%)	6,6,6	0.91	0
5	ACT	C	813	-	3,3,3	0.69	0	3,3,3	1.39	0
4	PO4	C	803	-	4,4,4	2.64	1 (25%)	6,6,6	0.90	0
2	2CY	D	604	-	26,26,26	2.20	11 (42%)	35,35,35	1.78	8 (22%)
3	NDP	B	702	-	51,52,52	1.67	11 (21%)	71,80,80	1.60	13 (18%)
5	ACT	A	808	-	3,3,3	0.60	0	3,3,3	1.37	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
6	GOL	B	806	-	-	0/4/4/4	-
2	2CY	C	603	-	-	3/8/8/8	0/3/3/3
3	NDP	C	703	-	-	2/34/77/77	0/5/5/5
2	2CY	B	602	-	-	3/8/8/8	0/3/3/3
3	NDP	D	704	-	-	10/34/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	B	702	-	-	2/34/77/77	0/5/5/5
2	2CY	A	601	-	-	5/8/8/8	0/3/3/3
6	GOL	C	805	-	-	0/4/4/4	-
2	2CY	D	604	-	-	2/8/8/8	0/3/3/3
3	NDP	A	701	-	-	5/34/77/77	0/5/5/5

All (92) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	2CY	O17-C18	-5.11	1.26	1.37
4	C	804	PO4	P-O1	5.09	1.62	1.50
2	D	604	2CY	O17-C18	-5.08	1.26	1.37
4	C	803	PO4	P-O1	5.01	1.62	1.50
3	A	701	NDP	C4N-C3N	-4.92	1.40	1.50
2	C	603	2CY	O17-C18	-4.90	1.26	1.37
4	A	802	PO4	P-O1	4.87	1.61	1.50
3	C	703	NDP	C4N-C3N	-4.84	1.40	1.50
2	B	602	2CY	O17-C18	-4.81	1.26	1.37
3	D	704	NDP	C4N-C3N	-4.63	1.41	1.50
4	B	801	PO4	P-O1	4.53	1.61	1.50
3	B	702	NDP	C4N-C3N	-4.43	1.41	1.50
3	D	704	NDP	C4N-C5N	-4.43	1.37	1.49
3	C	703	NDP	C4N-C5N	-4.42	1.37	1.49
3	A	701	NDP	C4N-C5N	-4.39	1.37	1.49
3	D	704	NDP	C2N-C3N	4.37	1.47	1.35
3	B	702	NDP	C4N-C5N	-4.33	1.37	1.49
3	A	701	NDP	C2N-C3N	4.24	1.46	1.35
3	C	703	NDP	C2N-C3N	3.78	1.45	1.35
2	A	601	2CY	C23-C18	3.74	1.45	1.39
2	B	602	2CY	C23-C18	3.70	1.45	1.39
3	A	701	NDP	C4A-N3A	3.61	1.41	1.34
3	D	704	NDP	P2B-O2B	-3.55	1.53	1.59
3	A	701	NDP	P2B-O2B	-3.48	1.53	1.59
2	C	603	2CY	O13-C7	-3.46	1.26	1.36
2	B	602	2CY	O13-C7	-3.44	1.26	1.36
2	A	601	2CY	O13-C7	-3.42	1.26	1.36
2	C	603	2CY	C23-C22	3.41	1.43	1.37
2	A	601	2CY	C21-C22	3.41	1.43	1.37
2	B	602	2CY	C23-C22	3.41	1.43	1.37
3	B	702	NDP	C2N-C3N	3.39	1.44	1.35
2	B	602	2CY	C8-C7	3.37	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	604	2CY	C23-C22	3.37	1.43	1.37
2	D	604	2CY	C23-C18	3.36	1.44	1.39
2	D	604	2CY	O13-C7	-3.35	1.26	1.36
2	A	601	2CY	C23-C22	3.33	1.43	1.37
2	C	603	2CY	C23-C18	3.32	1.44	1.39
2	D	604	2CY	C21-C22	3.32	1.43	1.37
3	D	704	NDP	C3B-C2B	-3.32	1.45	1.53
2	C	603	2CY	C21-C22	3.18	1.43	1.37
2	D	604	2CY	C8-C7	3.14	1.45	1.38
3	C	703	NDP	P2B-O2B	-3.10	1.54	1.59
3	B	702	NDP	P2B-O2B	-3.07	1.54	1.59
2	D	604	2CY	C19-C18	3.06	1.44	1.38
3	B	702	NDP	C8A-N9A	3.06	1.42	1.37
3	C	703	NDP	C4A-N3A	3.03	1.40	1.34
2	B	602	2CY	C19-C18	3.01	1.44	1.38
3	C	703	NDP	C3B-C2B	-3.01	1.46	1.53
3	D	704	NDP	PN-O3	2.99	1.62	1.59
2	B	602	2CY	C21-C22	2.98	1.43	1.37
2	C	603	2CY	C8-C7	2.93	1.44	1.38
2	A	601	2CY	C8-C7	2.92	1.44	1.38
3	B	702	NDP	C3B-C2B	-2.87	1.46	1.53
3	B	702	NDP	C4A-N3A	2.86	1.39	1.34
2	C	603	2CY	C19-C18	2.84	1.44	1.38
2	B	602	2CY	C9-C10	2.79	1.42	1.36
3	A	701	NDP	C3B-C2B	-2.78	1.46	1.53
2	A	601	2CY	C19-C18	2.72	1.43	1.38
2	C	603	2CY	C9-C10	2.72	1.42	1.36
2	B	602	2CY	C20-C19	2.71	1.43	1.38
2	D	604	2CY	C20-C19	2.68	1.43	1.38
2	A	601	2CY	C20-C21	2.66	1.43	1.38
2	A	601	2CY	C9-C10	2.60	1.42	1.36
2	A	601	2CY	C20-C19	2.58	1.43	1.38
3	A	701	NDP	C3B-C4B	-2.55	1.46	1.53
2	D	604	2CY	C9-C10	2.53	1.42	1.36
3	A	701	NDP	C8A-N9A	2.53	1.41	1.37
2	B	602	2CY	C20-C21	2.51	1.43	1.38
2	C	603	2CY	C20-C19	2.48	1.43	1.38
3	D	704	NDP	C8A-N9A	2.44	1.41	1.37
3	D	704	NDP	C4A-N3A	2.42	1.38	1.34
2	D	604	2CY	C20-C21	2.35	1.42	1.38
3	C	703	NDP	C8A-N9A	2.30	1.41	1.37
3	C	703	NDP	C5D-C4D	2.30	1.58	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	702	NDP	C3B-C4B	-2.29	1.47	1.53
3	B	702	NDP	PA-O1A	-2.19	1.43	1.50
3	A	701	NDP	C2D-C1D	2.19	1.60	1.53
3	D	704	NDP	PA-O1A	-2.18	1.43	1.50
3	B	702	NDP	C6N-N1N	2.18	1.42	1.37
3	C	703	NDP	C3B-C4B	-2.17	1.47	1.53
2	C	603	2CY	C20-C21	2.16	1.42	1.38
3	B	702	NDP	PN-O3	2.16	1.61	1.59
3	D	704	NDP	C6N-N1N	2.14	1.42	1.37
3	C	703	NDP	PA-O1A	-2.11	1.43	1.50
3	D	704	NDP	C3B-C4B	-2.09	1.47	1.53
3	C	703	NDP	C2D-C1D	2.08	1.60	1.53
3	A	701	NDP	C5D-C4D	2.06	1.57	1.51
2	B	602	2CY	C9-C8	2.04	1.42	1.38
3	A	701	NDP	C6N-N1N	2.04	1.42	1.37
2	D	604	2CY	C9-C8	2.02	1.42	1.38
3	C	703	NDP	C6N-N1N	2.01	1.42	1.37
2	C	603	2CY	C4-N3	2.00	1.37	1.33

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	2CY	N1-C2-N3	-5.58	120.12	127.21
2	D	604	2CY	N1-C2-N3	-5.48	120.24	127.21
2	A	601	2CY	N1-C2-N3	-5.41	120.33	127.21
2	B	602	2CY	N1-C2-N3	-5.38	120.36	127.21
3	B	702	NDP	C1D-N1N-C2N	-4.76	113.31	121.14
3	C	703	NDP	C3N-C2N-N1N	-4.72	116.28	123.20
3	D	704	NDP	C3N-C2N-N1N	-4.56	116.51	123.20
3	D	704	NDP	O4B-C1B-N9A	4.52	116.78	108.09
2	C	603	2CY	C16-O17-C18	4.45	129.50	117.93
3	B	702	NDP	C3N-C2N-N1N	-4.40	116.75	123.20
2	D	604	2CY	C16-O17-C18	4.39	129.35	117.93
2	A	601	2CY	C16-O17-C18	4.33	129.18	117.93
3	A	701	NDP	C3N-C2N-N1N	-4.30	116.89	123.20
2	B	602	2CY	C16-O17-C18	4.03	128.41	117.93
3	C	703	NDP	C1D-N1N-C2N	-3.97	114.59	121.14
3	A	701	NDP	O4B-C1B-N9A	3.81	115.41	108.09
3	C	703	NDP	C3B-C2B-C1B	-3.79	95.56	102.81
3	B	702	NDP	C3B-C2B-C1B	-3.77	95.60	102.81
3	D	704	NDP	C3B-C2B-C1B	-3.65	95.82	102.81
3	C	703	NDP	O4B-C1B-N9A	3.65	115.09	108.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	702	NDP	O4B-C1B-N9A	3.56	114.92	108.09
3	D	704	NDP	C1D-N1N-C2N	-3.31	115.68	121.14
3	A	701	NDP	C1D-N1N-C2N	-3.19	115.89	121.14
2	B	602	2CY	C14-O13-C7	3.13	126.94	117.74
2	A	601	2CY	C14-O13-C7	3.11	126.88	117.74
2	C	603	2CY	C14-O13-C7	3.04	126.69	117.74
2	D	604	2CY	C14-O13-C7	2.96	126.44	117.74
3	D	704	NDP	O7N-C7N-N7N	-2.96	116.26	122.89
3	A	701	NDP	C3B-C2B-C1B	-2.96	97.15	102.81
3	B	702	NDP	C6N-N1N-C2N	2.95	122.48	119.32
3	B	702	NDP	C3D-C2D-C1D	-2.91	95.95	101.46
3	C	703	NDP	C6N-N1N-C2N	2.90	122.42	119.32
3	A	701	NDP	O7N-C7N-N7N	-2.77	116.67	122.89
3	C	703	NDP	C3D-C2D-C1D	-2.76	96.24	101.46
3	C	703	NDP	O7N-C7N-N7N	-2.67	116.90	122.89
3	A	701	NDP	O3B-C3B-C4B	2.60	118.55	111.08
3	B	702	NDP	O7N-C7N-N7N	-2.59	117.10	122.89
3	B	702	NDP	C2D-C3D-C4D	2.54	107.52	102.61
3	C	703	NDP	C2D-C3D-C4D	2.54	107.52	102.61
3	D	704	NDP	C4B-O4B-C1B	-2.54	103.86	109.47
3	A	701	NDP	N3A-C2A-N1A	-2.54	124.74	128.58
3	A	701	NDP	O3B-C3B-C2B	2.53	118.26	111.19
3	C	703	NDP	N3A-C2A-N1A	-2.50	124.79	128.58
3	D	704	NDP	O3B-C3B-C4B	2.48	118.21	111.08
3	B	702	NDP	O3B-C3B-C2B	2.44	118.03	111.19
3	C	703	NDP	O3B-C3B-C4B	2.42	118.03	111.08
2	A	601	2CY	C21-C22-C23	-2.41	120.05	123.23
3	B	702	NDP	N3A-C2A-N1A	-2.40	124.95	128.58
2	C	603	2CY	C16-C15-C14	-2.30	106.23	113.67
3	D	704	NDP	N3A-C2A-N1A	-2.30	125.10	128.58
3	D	704	NDP	C6N-N1N-C2N	2.26	121.74	119.32
3	D	704	NDP	C2D-C3D-C4D	2.25	106.96	102.61
3	C	703	NDP	C4B-O4B-C1B	-2.25	104.50	109.47
3	C	703	NDP	O3B-C3B-C2B	2.23	117.43	111.19
2	B	602	2CY	C16-C15-C14	-2.23	106.48	113.67
2	C	603	2CY	O13-C7-C8	-2.22	119.57	124.45
3	B	702	NDP	O3B-C3B-C4B	2.21	117.43	111.08
3	A	701	NDP	C2D-C3D-C4D	2.20	106.85	102.61
3	D	704	NDP	O3B-C3B-C2B	2.19	117.32	111.19
3	A	701	NDP	C5A-N7A-C8A	2.19	106.89	103.45
3	B	702	NDP	C4B-O4B-C1B	-2.16	104.69	109.47
3	C	703	NDP	O2A-PA-O1A	2.13	122.36	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	704	NDP	C5A-N7A-C8A	2.13	106.80	103.45
3	B	702	NDP	O2A-PA-O1A	2.11	122.26	112.44
2	B	602	2CY	C2-N3-C4	2.11	122.73	116.72
2	D	604	2CY	C2-N1-C6	2.09	121.29	116.35
2	C	603	2CY	C2-N3-C4	2.09	122.68	116.72
2	D	604	2CY	C16-C15-C14	-2.09	106.92	113.67
2	A	601	2CY	C18-C23-C22	2.08	120.15	117.55
3	D	704	NDP	N9A-C8A-N7A	-2.08	110.98	113.94
2	D	604	2CY	N11-C2-N3	2.06	120.31	117.22
3	A	701	NDP	N9A-C8A-N7A	-2.06	111.01	113.94
2	C	603	2CY	C2-N1-C6	2.06	121.21	116.35
3	A	701	NDP	C4B-O4B-C1B	-2.05	104.93	109.47
2	D	604	2CY	C2-N3-C4	2.05	122.57	116.72
2	A	601	2CY	C2-N3-C4	2.04	122.55	116.72
2	C	603	2CY	N11-C2-N3	2.04	120.28	117.22
2	A	601	2CY	C2-N1-C6	2.03	121.16	116.35
3	C	703	NDP	C5A-N7A-C8A	2.03	106.63	103.45
2	B	602	2CY	O13-C7-C8	-2.01	120.03	124.45
2	B	602	2CY	C21-C22-C23	-2.00	120.58	123.23
3	A	701	NDP	O2B-C2B-C3B	2.00	118.87	111.68
2	D	604	2CY	O13-C7-C8	-2.00	120.05	124.45

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	704	NDP	C5D-O5D-PN-O1N
2	C	603	2CY	O13-C14-C15-C16
2	D	604	2CY	O13-C14-C15-C16
2	B	602	2CY	O13-C14-C15-C16
2	A	601	2CY	C15-C14-O13-C7
2	B	602	2CY	C15-C14-O13-C7
2	C	603	2CY	C15-C14-O13-C7
3	A	701	NDP	C3B-C2B-O2B-P2B
3	B	702	NDP	O4D-C1D-N1N-C2N
2	D	604	2CY	C15-C14-O13-C7
2	A	601	2CY	C14-C15-C16-O17
3	A	701	NDP	O4D-C1D-N1N-C2N
3	C	703	NDP	O4D-C1D-N1N-C2N
3	D	704	NDP	O4D-C1D-N1N-C2N
2	A	601	2CY	O13-C14-C15-C16
3	D	704	NDP	C5D-O5D-PN-O3

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Mol	Chain	Res	Type	Atoms
3	D	704	NDP	C5D-O5D-PN-O2N
2	C	603	2CY	C15-C16-O17-C18
2	A	601	2CY	C5-C7-O13-C14
3	D	704	NDP	C3B-C4B-C5B-O5B
2	A	601	2CY	C8-C7-O13-C14
3	A	701	NDP	C1B-C2B-O2B-P2B
3	A	701	NDP	C2N-C3N-C7N-N7N
3	B	702	NDP	C2N-C3N-C7N-N7N
3	C	703	NDP	C2N-C3N-C7N-N7N
3	D	704	NDP	C3D-C4D-C5D-O5D
3	D	704	NDP	C2N-C3N-C7N-N7N
3	D	704	NDP	O4D-C4D-C5D-O5D
3	A	701	NDP	C2B-O2B-P2B-O3X
3	D	704	NDP	C2B-O2B-P2B-O1X
2	B	602	2CY	C14-C15-C16-O17
3	D	704	NDP	PN-O3-PA-O2A

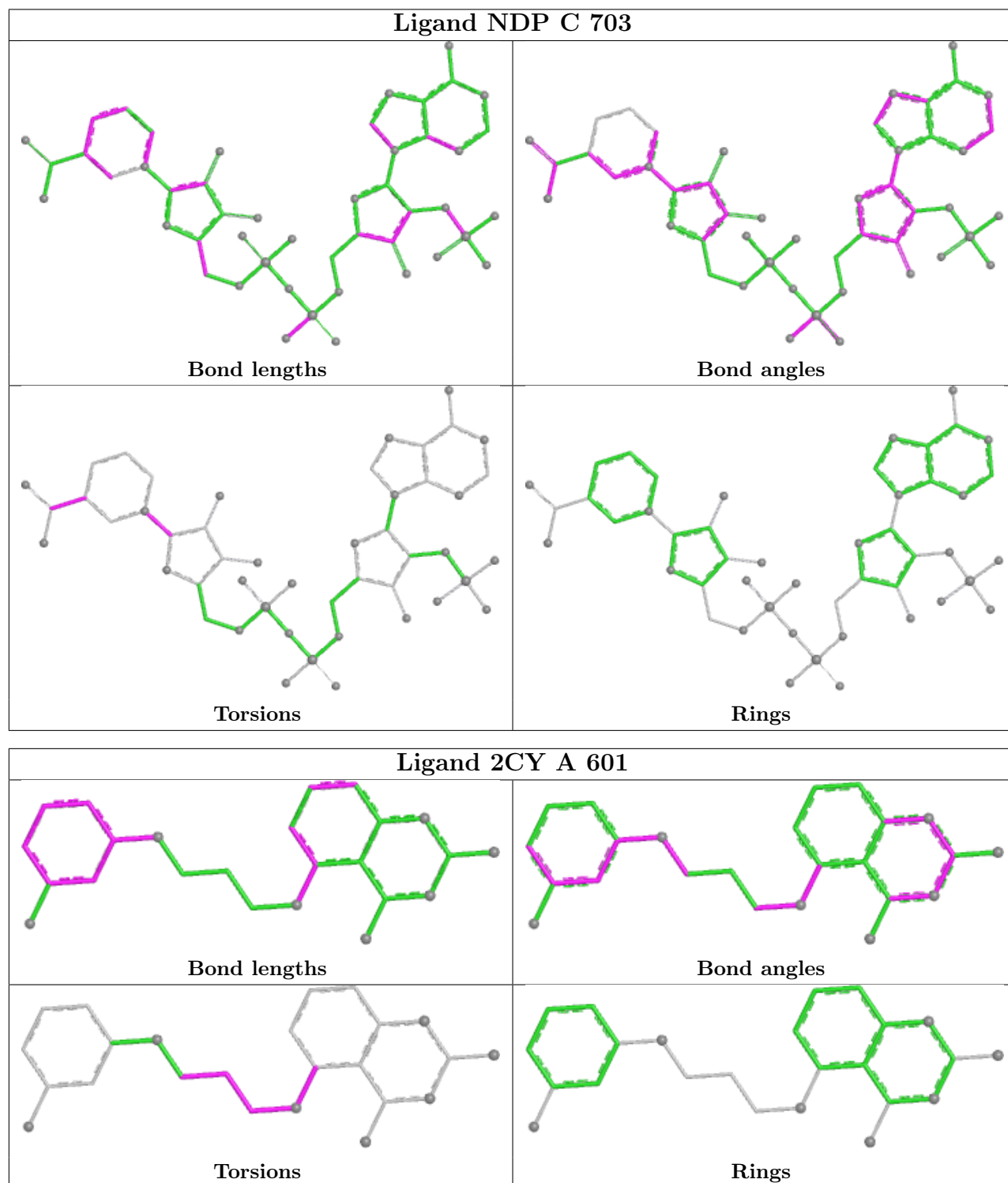
There are no ring outliers.

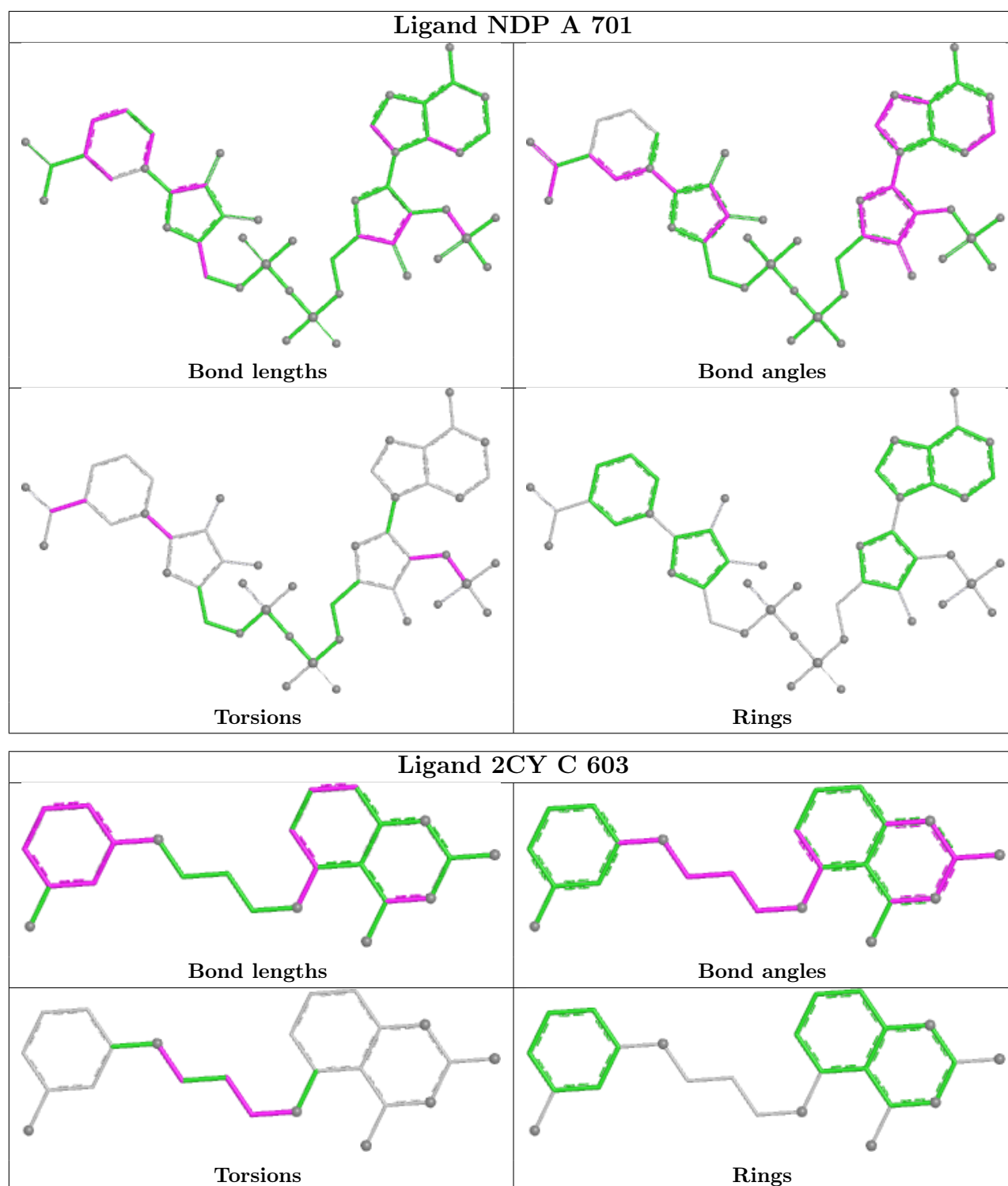
12 monomers are involved in 27 short contacts:

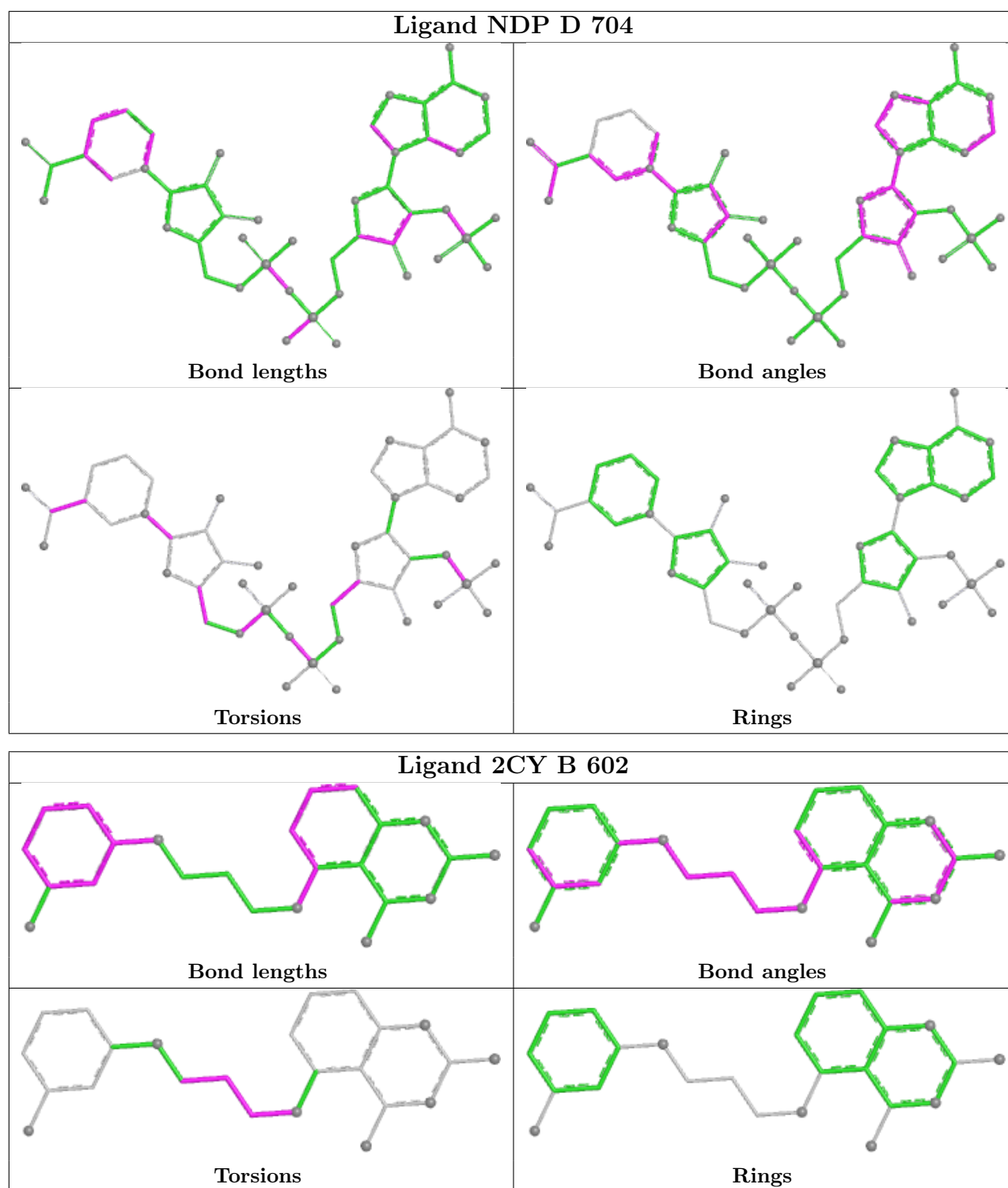
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	801	PO4	1	0
3	C	703	NDP	4	0
2	A	601	2CY	1	0
3	A	701	NDP	1	0
4	C	804	PO4	1	0
2	C	603	2CY	1	0
3	D	704	NDP	5	0
5	A	809	ACT	2	0
5	D	810	ACT	1	0
2	B	602	2CY	2	0
2	D	604	2CY	3	0
3	B	702	NDP	5	0

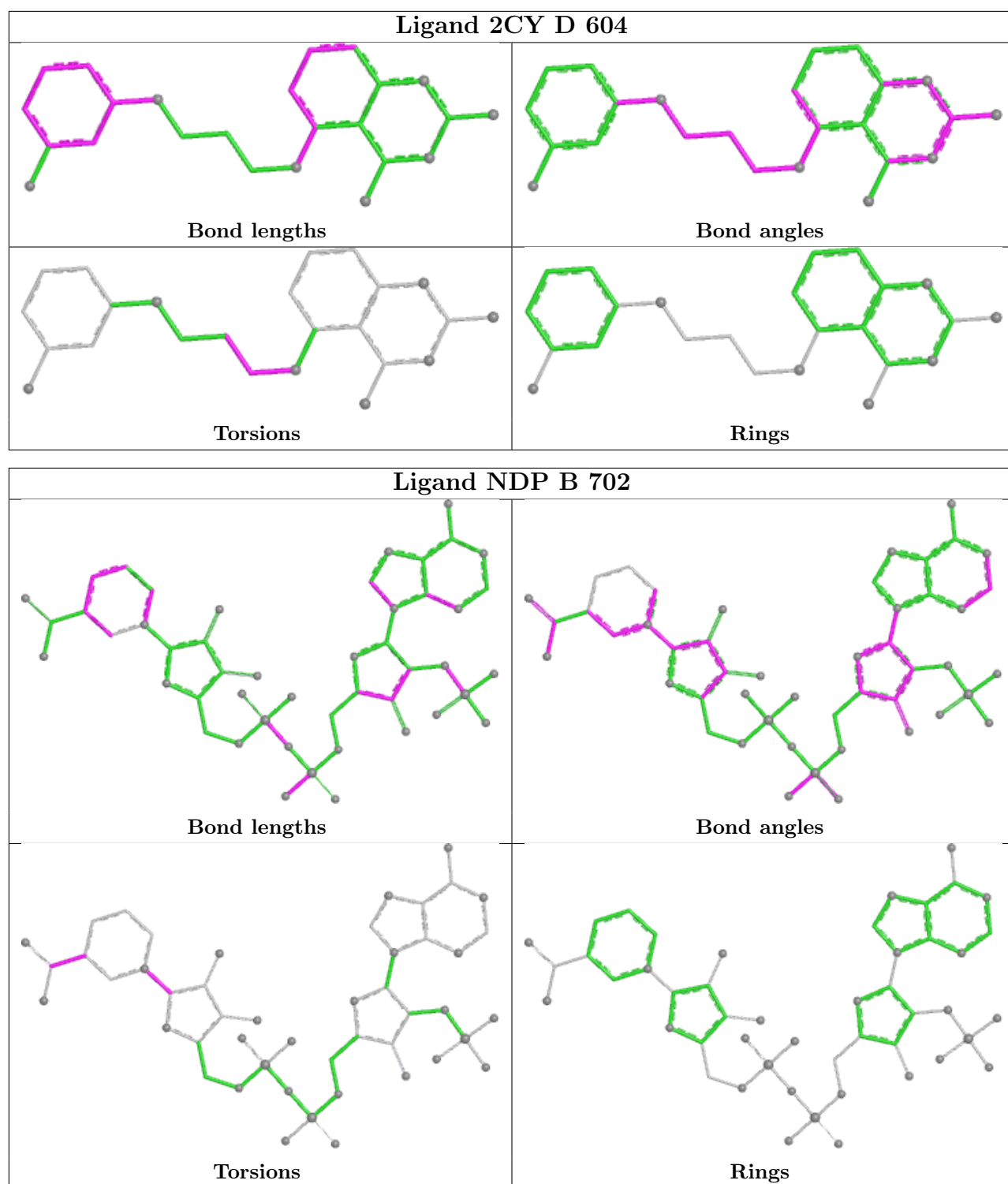
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	518/521 (99%)	-0.21	11 (2%) 63 54	12, 26, 61, 91	0
1	B	515/521 (98%)	-0.07	16 (3%) 51 41	11, 29, 76, 91	0
1	C	516/521 (99%)	-0.26	7 (1%) 73 64	10, 26, 69, 91	0
1	D	513/521 (98%)	-0.15	13 (2%) 58 48	7, 28, 70, 91	0
All	All	2062/2084 (98%)	-0.17	47 (2%) 61 51	7, 27, 69, 91	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	SER	3.8
1	A	38	GLY	3.4
1	D	38	GLY	3.3
1	B	41	ILE	3.2
1	C	41	ILE	3.2
1	A	41	ILE	3.0
1	C	38	GLY	3.0
1	D	36	GLY	2.9
1	D	185	SER	2.9
1	A	517	MET	2.9
1	A	36	GLY	2.9
1	B	43	TRP	2.9
1	D	39	ARG	2.8
1	D	515	ILE	2.8
1	C	43	TRP	2.7
1	B	42	PRO	2.7
1	D	113	PRO	2.7
1	B	64	VAL	2.7
1	D	37	ASP	2.7
1	D	186	SER	2.7
1	A	42	PRO	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	44	ASN	2.6
1	D	42	PRO	2.6
1	D	114	ASP	2.6
1	B	113	PRO	2.6
1	D	41	ILE	2.5
1	A	43	TRP	2.5
1	B	187	CYS	2.4
1	B	119	ASN	2.3
1	C	517	MET	2.3
1	A	40	SER	2.3
1	B	39	ARG	2.3
1	B	517	MET	2.3
1	C	120	LEU	2.3
1	B	515	ILE	2.2
1	C	187	CYS	2.2
1	B	36	GLY	2.2
1	D	111	GLY	2.2
1	A	187	CYS	2.2
1	A	182	ALA	2.1
1	A	37	ASP	2.1
1	A	220	GLY	2.1
1	D	257	ARG	2.1
1	B	116	GLU	2.1
1	C	36	GLY	2.1
1	B	188	SER	2.0
1	B	37	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

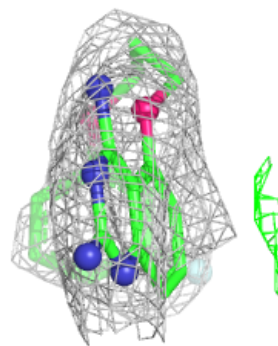
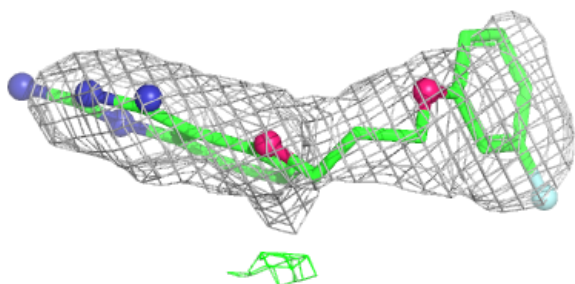
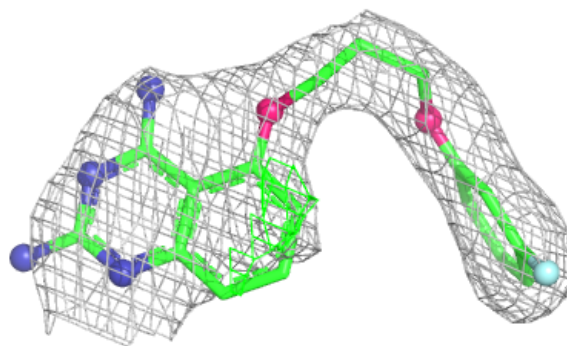
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ACT	B	811	4/4	0.67	0.19	42,45,45,46	0
5	ACT	D	814	4/4	0.73	0.16	31,34,35,37	0
4	PO4	A	802	5/5	0.79	0.14	87,87,88,89	0
4	PO4	C	804	5/5	0.79	0.14	84,84,85,85	0
5	ACT	C	812	4/4	0.80	0.16	32,33,33,35	0
5	ACT	C	813	4/4	0.82	0.19	56,57,57,58	0
4	PO4	C	803	5/5	0.84	0.12	76,76,78,78	0
6	GOL	C	805	6/6	0.84	0.17	42,47,47,48	0
2	2CY	B	602	24/24	0.85	0.16	46,51,55,58	0
5	ACT	D	815	4/4	0.88	0.21	45,45,45,46	0
6	GOL	B	806	6/6	0.88	0.14	40,42,43,44	0
2	2CY	D	604	24/24	0.88	0.16	47,53,58,60	0
2	2CY	A	601	24/24	0.89	0.13	44,49,60,61	0
2	2CY	C	603	24/24	0.90	0.12	44,47,51,52	0
5	ACT	A	808	4/4	0.90	0.11	35,36,36,36	0
3	NDP	B	702	48/48	0.90	0.13	44,52,89,90	0
4	PO4	B	801	5/5	0.91	0.10	64,65,66,67	0
5	ACT	D	816	4/4	0.92	0.12	29,29,30,30	0
5	ACT	A	809	4/4	0.92	0.11	38,39,39,41	0
3	NDP	D	704	48/48	0.92	0.13	41,50,88,90	0
3	NDP	C	703	48/48	0.93	0.11	32,42,80,80	0
3	NDP	A	701	48/48	0.93	0.11	37,45,78,79	0
5	ACT	D	810	4/4	0.93	0.09	32,32,32,33	0
5	ACT	A	807	4/4	0.93	0.14	35,37,37,37	0

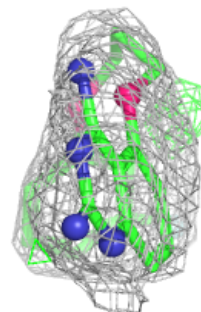
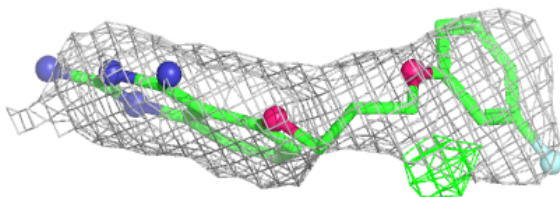
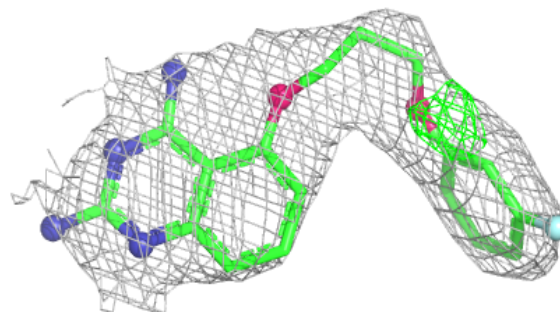
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 2CY 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)

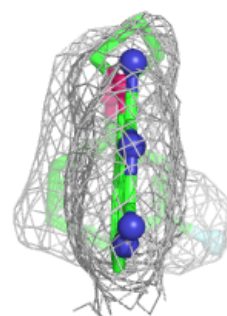
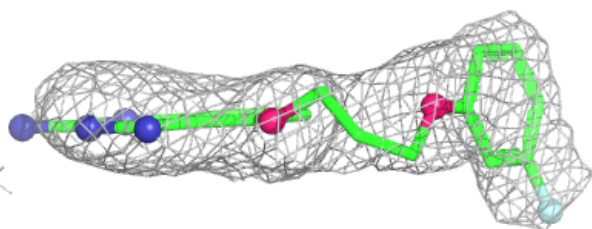
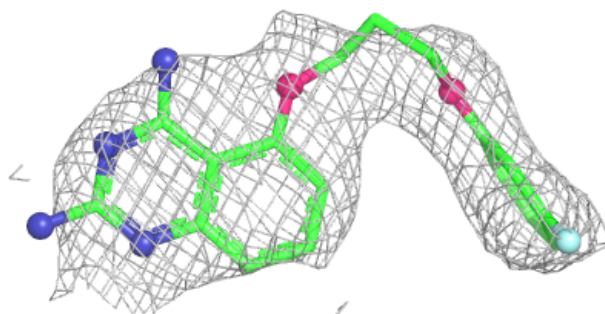
**Electron density around 2CY D 604:**

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

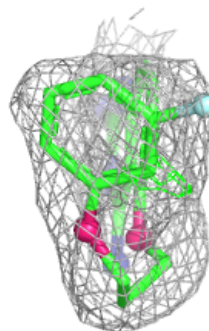
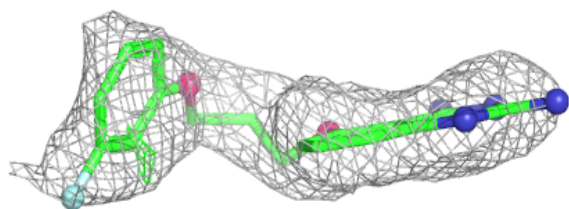
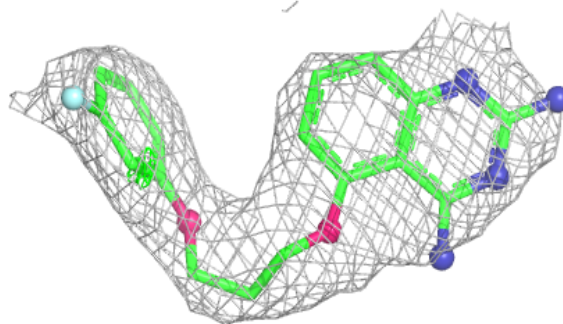


Electron density around 2CY A 601:

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

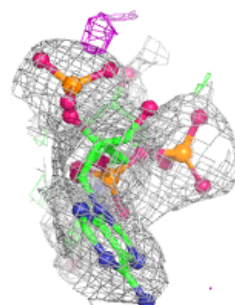
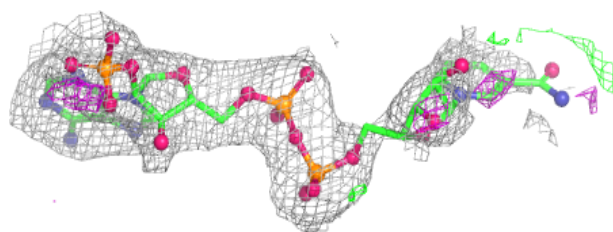
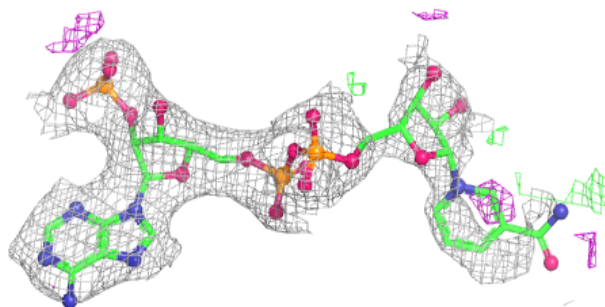
**Electron density around 2CY C 603:**

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

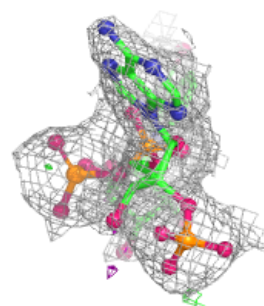
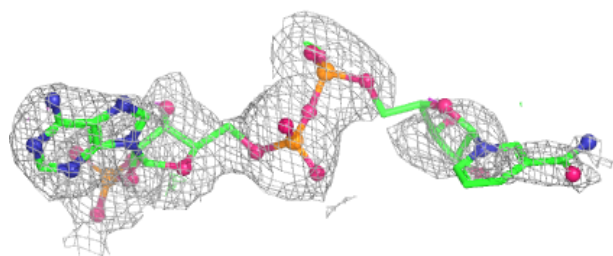
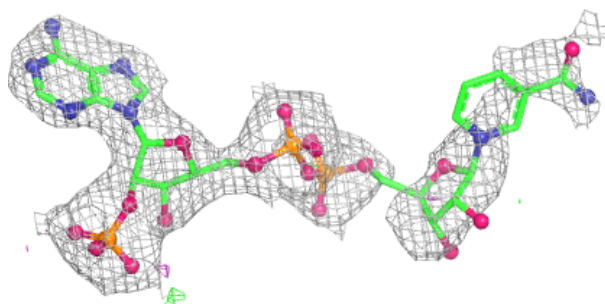


Electron density around NDP B 702:

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

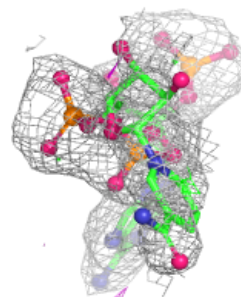
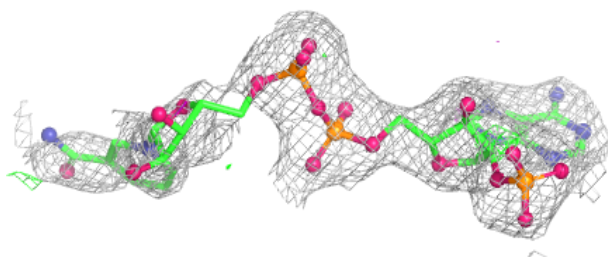
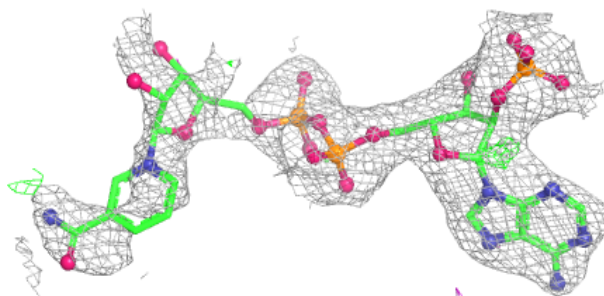
**Electron density around NDP D 704:**

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

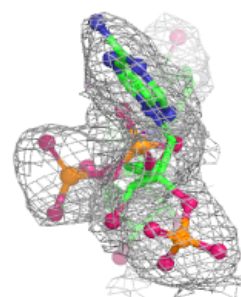
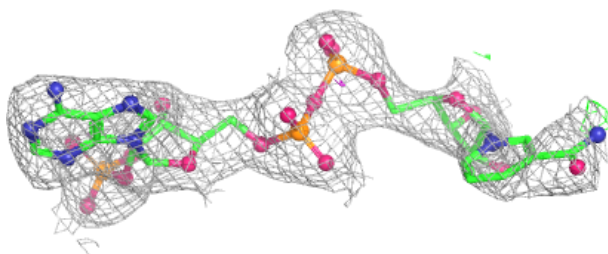
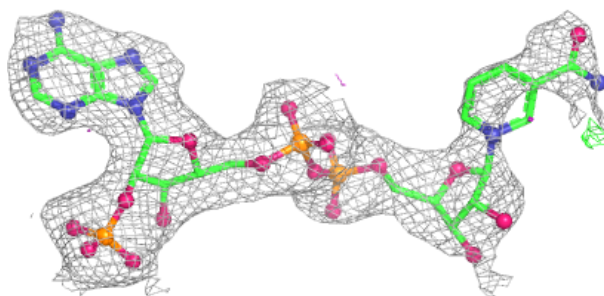


Electron density around NDP C 703:

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

**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)



6.5 Other polymers [i](#)

There are no such residues in this entry.