



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 05:44 AM EDT

PDB ID : 3IRO
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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

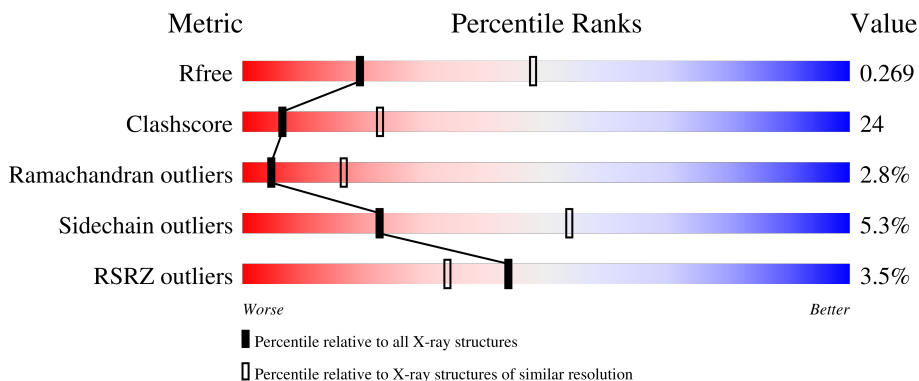
1 Overall quality at a glance

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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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	 3% 55% 42% ..
1	B	521	 4% 51% 43% ..
1	C	521	 3% 56% 38% ..
1	D	521	 4% 56% 37% 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](#)

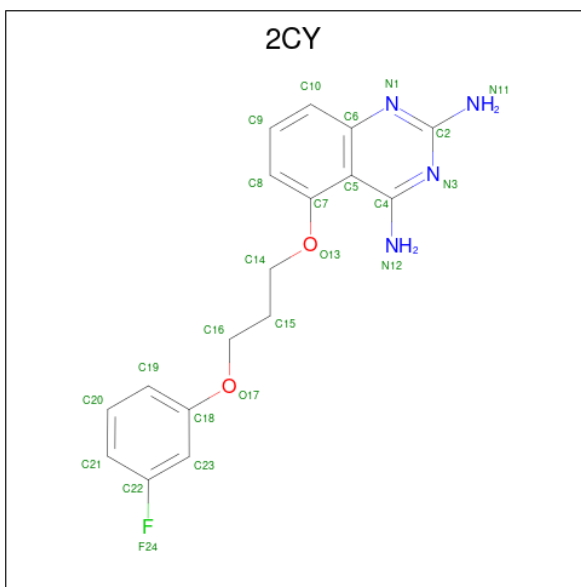
There are 7 unique types of molecules in this entry. The entry contains 16862 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	518	Total 4124	C 2616	N 729	O 759	S 20	0	0	0
1	B	515	Total 4101	C 2602	N 725	O 755	S 19	0	0	0
1	C	516	Total 4107	C 2605	N 726	O 757	S 19	0	0	0
1	D	513	Total 4087	C 2594	N 723	O 752	S 18	0	0	0

- Molecule 2 is 5-[3-(3-fluorophenoxy)propoxy]quinazoline-2,4-diamine (three-letter code: 2CY) (formula: C₁₇H₁₇FN₄O₂).



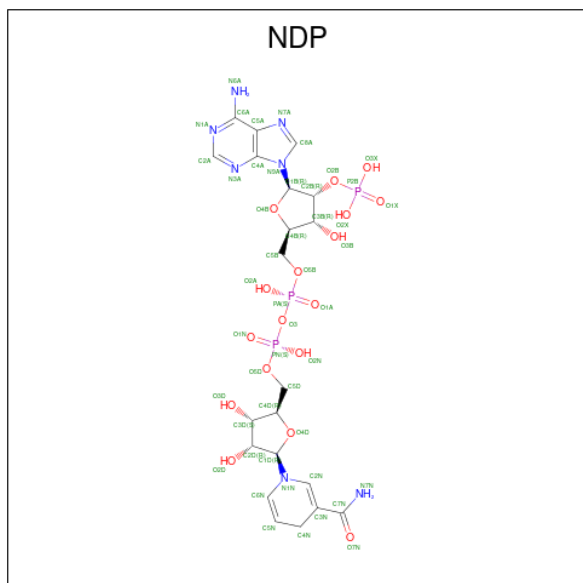
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
			Total	C	F	N			O
2	A	1	Total 24	C 17	F 1	N 4	O 2	0	0
2	B	1	Total 24	C 17	F 1	N 4	O 2	0	0

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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 (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$).



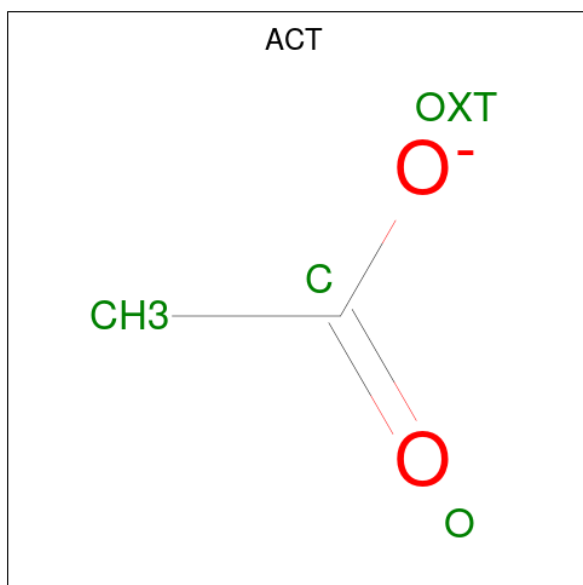
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
3	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	C	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
3	D	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

- Molecule 4 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



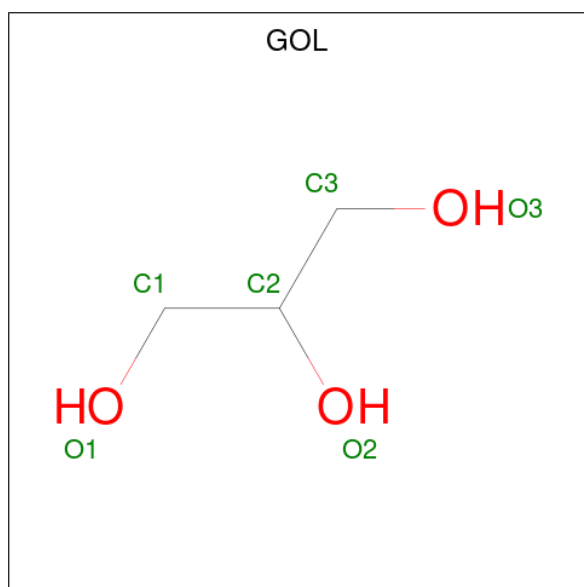
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O P 5 4 1	0	0
4	B	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0
4	C	1	Total O P 5 4 1	0	0

- Molecule 5 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



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

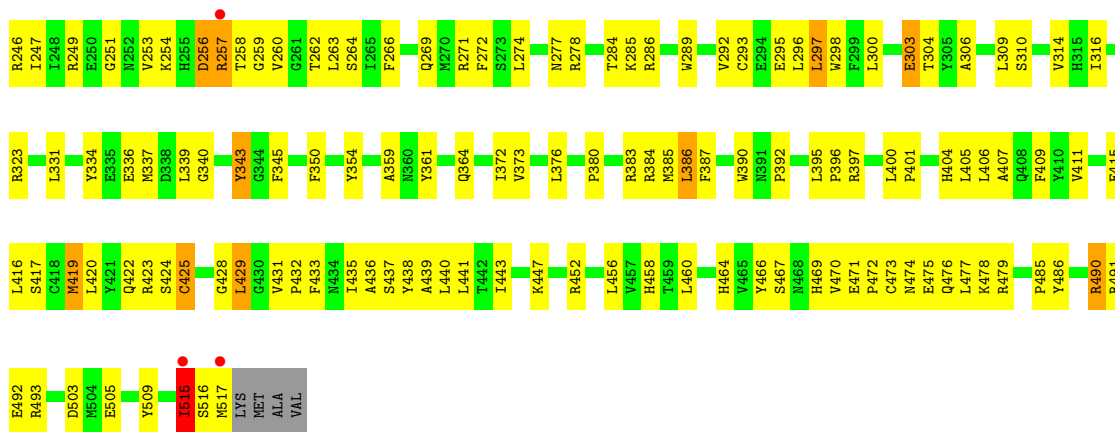
- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



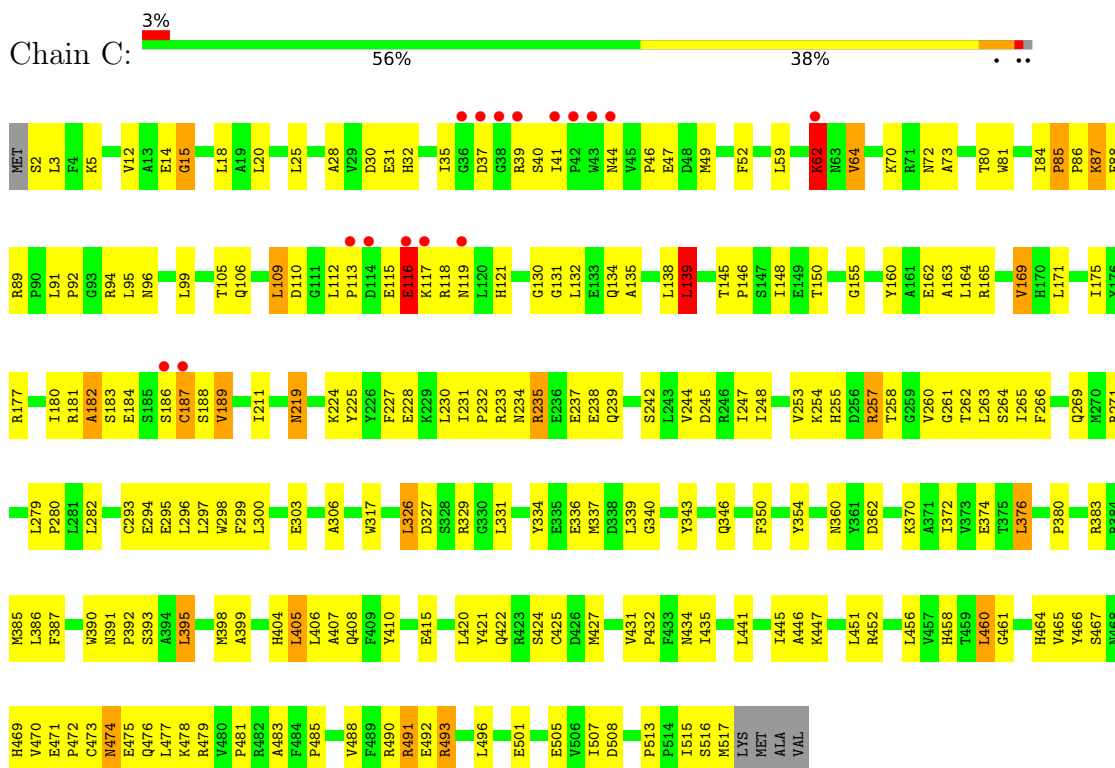
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	C	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

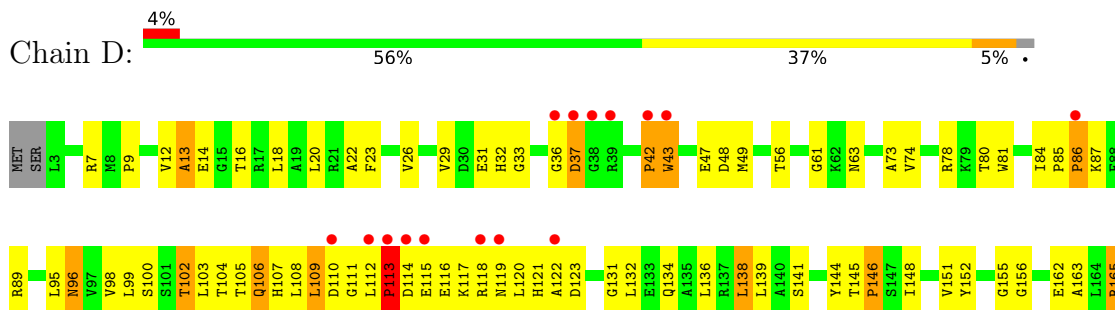
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	23	Total 23	O 23	0	0
7	B	12	Total 12	O 12	0	0
7	C	23	Total 23	O 23	0	0
7	D	25	Total 25	O 25	0	0

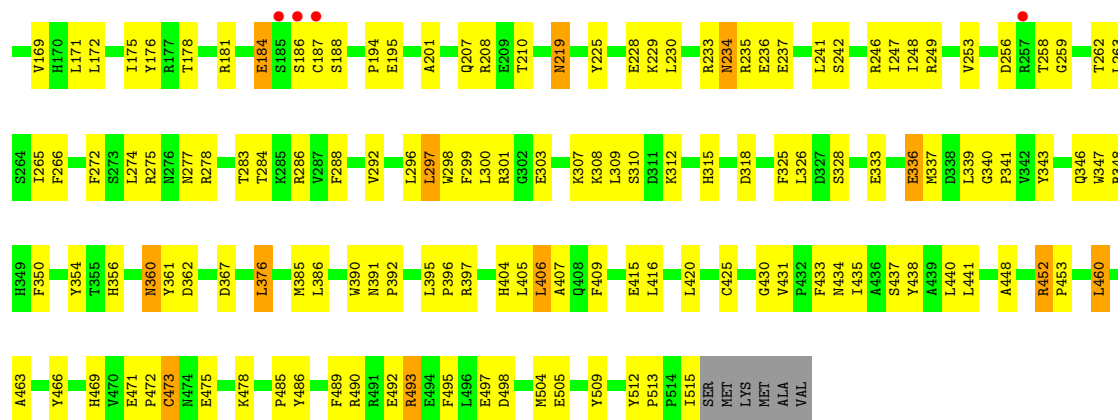


• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase



• Molecule 1: Bifunctional dihydrofolate reductase-thymidylate synthase





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) 95.1 (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)	Xtrriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.206 , 0.277 0.199 , 0.269	Depositor DCC
R_{free} test set	2478 reflections (5.13%)	wwPDB-VP
Wilson B-factor (Å ²)	32.9	Xtrriage
Anisotropy	0.033	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.024 for l,-k,h	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	16862	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtrriage'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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2CY, PO4, NDP, ACT, 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	0.38	0/4224	0.65	0/5729
1	B	0.37	0/4201	0.67	0/5700
1	C	0.37	0/4207	0.66	0/5708
1	D	0.38	0/4187	0.67	0/5682
All	All	0.37	0/16819	0.66	0/22819

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	175	0
1	B	4101	0	4055	241	0
1	C	4107	0	4060	203	0
1	D	4087	0	4041	192	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	786	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 24.

All (786) 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:C:306:ALA:HB3	1:C:337:MET:HE3	1.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:386:LEU:HB2	1:D:407:ALA:O	1.84	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: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: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
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: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: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:D:131:GLY:H	1:D:134:GLN:CD	1.93	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: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:D:234:ASN:C	1:D:234:ASN:HD22	1.94	0.69
1:D:81:TRP:CZ2	1:D:89:ARG:HD3	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:219:ASN:C	1:B:219:ASN:HD22	1.96	0.67
1:C:116:GLU:HA	1:C:119:ASN:HD22	1.59	0.67
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: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: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: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:A:35:ILE:HG13	1:A:36:GLY:N	2.11	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: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: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:C:306:ALA:CB	1:C:337:MET:HE3	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:B:41:ILE:O	1:B:41:ILE:HG13	1.97	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: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:C:31:GLU:CD	1:C:181:ARG:HD3	2.20	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: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:A:265:ILE:HD12	1:A:265:ILE:C	2.21	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: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:B:12:VAL:HG13	1:B:13:ALA:H	1.65	0.60
1:C:30:ASP:HA	1:C:180:ILE:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:146:PRO:HG3	1:C:505:GLU:CD	2.21	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:C:360:ASN:HD21	1:C:362:ASP:CG	2.05	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: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: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:D:310:SER:C	1:D:312:LYS:H	2.05	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: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:D:391:ASN:O	1:D:395:LEU:HG	2.03	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:D:117:LYS:C	1:D:119:ASN:H	2.06	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:219:ASN:C	1:B:219:ASN:ND2	2.58	0.57
1:C:340:GLY:HA2	1:C:354:TYR:CE2	2.40	0.57
1:C:469:HIS:O	1:C:473:CYS:HB2	2.05	0.57
1:D:139:LEU:HD23	1:D:151:VAL:CG2	2.35	0.57
1:D:186:SER:C	1:D:188:SER:H	2.05	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: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: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:D:78:ARG:HB2	1:D:100:SER:HB2	1.87	0.56
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:25:LEU:C	1:A:25:LEU:HD23	2.26	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:406:LEU:C	1:D:406:LEU:HD12	2.27	0.55
1:C:37:ASP:CG	1:C:186:SER:HB3	2.27	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:165:ARG:C	1:B:169:VAL:HG22	2.27	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:C:165:ARG:C	1:C:169:VAL:HG22	2.27	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: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: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:A:27:VAL:HG22	1:A:28:ALA:N	2.23	0.53
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:C:395:LEU:HA	1:C:398:MET:HE3	1.90	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:26:VAL:HG12	2:D:604:2CY:N3	2.24	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:234:ASN:C	1:D:234:ASN:ND2	2.62	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:D:485:PRO:HB3	1:D:509:TYR:HA	1.91	0.52
1:A:472:PRO:C	1:A:474:ASN:H	2.12	0.52
1:D:336:GLU:CD	1:D:336:GLU:H	2.13	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:B:447:LYS:NZ	1:B:492:GLU:OE2	2.41	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
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:C:447:LYS:HZ1	1:C:492:GLU:CD	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:29:VAL:HG23	1:B:33:GLY:C	2.31	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: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:85:PRO:C	1:B:87:LYS:N	2.64	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:A:219:ASN:CG	1:A:220:GLY:H	2.13	0.51
1:B:249:ARG:HE	1:D:207:GLN:NE2	2.08	0.51
1:B:469:HIS:C	1:B:472:PRO:HD2	2.31	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:B:74:VAL:HG22	1:B:154:ILE:HG21	1.92	0.51
1:B:209:GLU:OE1	1:B:229:LYS:NZ	2.25	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
1:D:315:HIS:HB3	1:D:318:ASP:OD1	2.10	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:85:PRO:C	1:B:87:LYS:H	2.14	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:37:ASP:C	1:C:39:ARG:H	2.15	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: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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:104:THR:O	1:D:107:HIS:HB2	2.13	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: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: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:B:515:ILE:HG13	1:B:517:MET:HE2	1.95	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:VAL:O	1:B:435:ILE:HG13	2.14	0.48
1:C:296:LEU:HD13	1:C:296:LEU:C	2.35	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:256:ASP:C	1:D:258:THR:N	2.65	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: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: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
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: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:117:LYS:C	1:B:119:ASN:H	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:383:ARG:C	1:A:384:ARG:HG3	2.36	0.46
1:A:405:LEU:HD11	1:B:406:LEU:HD21	1.97	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
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:44:ASN:HA	1:C:49:MET:HE1	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:78:ARG:HD2	1:A:78:ARG:C	2.35	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:253:VAL:HG22	1:D:263:LEU:HD21	1.98	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:B:256:ASP:OD1	1:B:260:VAL:HB	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:395:LEU:HD12	1:C:398:MET:HE1	1.97	0.45
1:A:71:ARG:NH1	1:A:148:ILE:HD11	2.32	0.45
1:A:90:PRO:O	1:A:91:LEU:C	2.55	0.45
1:A:386:LEU:N	1:A:386:LEU:HD23	2.32	0.45
1:D:146:PRO:HG3	1:D:505:GLU:CD	2.36	0.45
1:B:74:VAL:HG12	1:B:74:VAL:O	2.17	0.45
1:A:303:GLU:OE1	1:A:303:GLU:HA	2.16	0.45
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:A:16:THR:O	1:A:16:THR:HG22	2.17	0.45
1:B:164:LEU:HD21	1:B:175:ILE:HD11	1.99	0.45
1:C:84:ILE:O	1:C:85:PRO:C	2.54	0.45
1:C:132:LEU:CD2	1:C:163:ALA:HB2	2.46	0.45
1:C:467:SER:C	1:C:469:HIS:H	2.21	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: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:D:265:ILE:HD12	1:D:265:ILE:C	2.37	0.44
1:A:355:THR:OG1	1:A:356:HIS:N	2.50	0.44
1:A:472:PRO:C	1:A:474:ASN:N	2.70	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: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:B:384:ARG:C	1:B:386:LEU:HD23	2.37	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:85:PRO:C	1:D:87:LYS:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:333:GLU:HA	1:A:333:GLU:OE1	2.17	0.44
1:C:47:GLU:CD	1:C:47:GLU:H	2.21	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: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:186:SER:C	1:D:188:SER:N	2.71	0.44
1:A:36:GLY:C	1:A:187:CYS:HB3	2.38	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
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: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:C:327:ASP:C	1:C:329:ARG:H	2.21	0.43
1:C:473:CYS:SG	1:C:517:MET:HE1	2.58	0.43
1:A:381:ASP:CG	1:B:254:LYS:HD3	2.38	0.43
1:B:420:LEU:HD13	1:B:438:TYR:CE2	2.53	0.43
1:C:219:ASN:N	1:C:219:ASN:ND2	2.66	0.43
1:C:295:GLU:HG2	1:C:299:PHE:CE2	2.53	0.43
1:C:476:GLN:NE2	1:C:517:MET:HE1	2.34	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:D:310:SER:C	1:D:312:LYS:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:A:490:ARG:NH1	1:A:490:ARG:CB	2.82	0.43
1:A:219:ASN:CG	1:A:220:GLY:N	2.71	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
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:B:428:GLY:C	1:B:429:LEU:HD22	2.39	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:D:475:GLU:CD	1:D:515:ILE:HG12	2.39	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: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:C:395:LEU:HD12	1:C:398:MET:HE3	2.01	0.42
1:D:341:PRO:HB2	1:D:346:GLN:NE2	2.33	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:383:ARG:C	1:B:384:ARG:HG3	2.39	0.42
1:B:423:ARG:HG3	1:B:424:SER:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:THR:HA	1:C:146:PRO:HA	1.84	0.42
1:D:360:ASN:HD21	1:D:362:ASP:CG	2.22	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:D:233:ARG:NE	1:D:235:ARG:NH1	2.67	0.42
1:A:8:MET:HE1	1:A:499:TYR:CE1	2.54	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:8:MET:HE3	1:B:12:VAL:HG23	2.02	0.42
1:B:164:LEU:HA	1:B:169:VAL:CG1	2.50	0.42
1:C:130:GLY:HA3	1:C:134:GLN:HG2	2.00	0.42
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:D:194:PRO:CB	1:D:201:ALA:HA	2.50	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:C:25:LEU:C	1:C:25:LEU:HD23	2.40	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:D:36:GLY:HA2	1:D:186:SER:OG	2.19	0.42
1:D:333:GLU:O	1:D:356:HIS:HE1	2.03	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:188:SER:O	1:C:189:VAL:CB	2.68	0.41
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:B:95:LEU:C	1:B:95:LEU:CD2	2.89	0.41
1:C:52:PHE:CD1	1:C:52:PHE:C	2.94	0.41
1:D:466:TYR:HB2	1:D:469:HIS:ND1	2.36	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: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:A:193:VAL:O	1:A:194:PRO:C	2.59	0.41
1:B:74:VAL:HG22	1:B:154:ILE:HG23	2.02	0.41
1:B:380:PRO:O	1:B:411:VAL:HB	2.21	0.41
1:C:5:LYS:O	1:C:370:LYS:NZ	2.53	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:C:117:LYS:HG2	1:C:121:HIS:CE1	2.56	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:ARG:H	1:B:490:ARG:HG2	1.57	0.41
1:C:447:LYS:NZ	1:C:492:GLU:OE2	2.49	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
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:265:ILE:C	1:C:265:ILE:HD12	2.41	0.41
1:C:294:GLU:OE1	1:C:294:GLU:HA	2.21	0.41
1:D:115:GLU:C	1:D:117:LYS:N	2.72	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: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:C:515:ILE:C	1:C:517:MET:H	2.25	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: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:164:LEU:C	1:B:169:VAL:HG13	2.41	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:156:GLY:C	1:B:158:SER:N	2.75	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: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:134:GLN:H	1:C:134:GLN:CD	2.25	0.40
1:C:317:TRP:CE3	1:C:339:LEU:HD13	2.56	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

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	516/521 (99%)	463 (90%)	39 (8%)	14 (3%)	5	17
1	B	513/521 (98%)	466 (91%)	33 (6%)	14 (3%)	5	17
1	C	514/521 (99%)	453 (88%)	46 (9%)	15 (3%)	4	15
1	D	511/521 (98%)	448 (88%)	49 (10%)	14 (3%)	5	17
All	All	2054/2084 (99%)	1830 (89%)	167 (8%)	57 (3%)	5	17

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

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Mol	Chain	Res	Type
1	C	15	GLY
1	C	116	GLU
1	C	183	SER
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 [i](#)

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%)	429 (97%)	15 (3%)	37 71
1	B	441/446 (99%)	418 (95%)	23 (5%)	23 55
1	C	442/446 (99%)	417 (94%)	25 (6%)	20 50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	439/446 (98%)	409 (93%)	30 (7%)	16	42
All	All	1766/1784 (99%)	1673 (95%)	93 (5%)	22	54

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	39	ARG
1	A	43	TRP
1	A	48	ASP
1	A	95	LEU
1	A	109	LEU
1	A	128	VAL
1	A	138	LEU
1	A	219	ASN
1	A	257	ARG
1	A	297	LEU
1	A	333	GLU
1	A	440	LEU
1	A	460	LEU
1	A	473	CYS
1	B	39	ARG
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	219	ASN
1	B	257	ARG
1	B	274	LEU
1	B	297	LEU
1	B	303	GLU
1	B	310	SER
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

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Mol	Chain	Res	Type
1	B	490	ARG
1	B	515	ILE
1	C	2	SER
1	C	62	LYS
1	C	64	VAL
1	C	87	LYS
1	C	95	LEU
1	C	106	GLN
1	C	109	LEU
1	C	116	GLU
1	C	138	LEU
1	C	139	LEU
1	C	169	VAL
1	C	219	ASN
1	C	235	ARG
1	C	257	ARG
1	C	297	LEU
1	C	326	LEU
1	C	374	GLU
1	C	376	LEU
1	C	395	LEU
1	C	405	LEU
1	C	456	LEU
1	C	460	LEU
1	C	474	ASN
1	C	491	ARG
1	C	493	ARG
1	D	43	TRP
1	D	63	ASN
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	123	ASP
1	D	138	LEU
1	D	141	SER
1	D	146	PRO
1	D	165	ARG
1	D	169	VAL
1	D	219	ASN

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Mol	Chain	Res	Type
1	D	234	ASN
1	D	242	SER
1	D	274	LEU
1	D	286	ARG
1	D	297	LEU
1	D	309	LEU
1	D	326	LEU
1	D	336	GLU
1	D	360	ASN
1	D	376	LEU
1	D	406	LEU
1	D	452	ARG
1	D	460	LEU
1	D	473	CYS
1	D	493	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	219	ASN
1	A	239	GLN
1	A	320	ASN
1	A	434	ASN
1	A	476	GLN
1	B	121	HIS
1	B	219	ASN
1	B	239	GLN
1	B	276	ASN
1	B	277	ASN
1	B	356	HIS
1	B	464	HIS
1	B	474	ASN
1	B	476	GLN
1	C	106	GLN
1	C	119	ASN
1	C	121	HIS
1	C	173	GLN
1	C	207	GLN
1	C	219	ASN
1	C	239	GLN
1	C	320	ASN
1	C	360	ASN

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Mol	Chain	Res	Type
1	C	434	ASN
1	C	464	HIS
1	C	469	HIS
1	C	476	GLN
1	D	63	ASN
1	D	106	GLN
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	356	HIS
1	D	360	ASN
1	D	464	HIS
1	D	476	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
5	ACT	B	811	-	3,3,3	0.76	0	3,3,3	1.47	0
2	2CY	C	603	-	26,26,26	2.07	10 (38%)	35,35,35	1.88	7 (20%)
5	ACT	A	809	-	3,3,3	0.60	0	3,3,3	1.38	0
3	NDP	C	703	-	45,52,52	1.81	12 (26%)	53,80,80	1.58	10 (18%)
5	ACT	A	808	-	3,3,3	0.57	0	3,3,3	1.39	0
3	NDP	A	701	-	45,52,52	1.87	10 (22%)	53,80,80	1.49	9 (16%)
4	PO4	C	804	-	4,4,4	2.59	1 (25%)	6,6,6	0.83	0
5	ACT	D	815	-	3,3,3	0.59	0	3,3,3	1.37	0
3	NDP	B	702	-	45,52,52	1.73	10 (22%)	53,80,80	1.62	11 (20%)
6	GOL	C	805	-	5,5,5	0.44	0	5,5,5	0.28	0
5	ACT	D	814	-	3,3,3	0.66	0	3,3,3	1.34	0
2	2CY	B	602	-	26,26,26	2.11	10 (38%)	35,35,35	1.88	8 (22%)
5	ACT	A	807	-	3,3,3	0.55	0	3,3,3	1.42	0
2	2CY	A	601	-	26,26,26	2.10	10 (38%)	35,35,35	1.92	6 (17%)
2	2CY	D	604	-	26,26,26	2.11	9 (34%)	35,35,35	1.90	9 (25%)
5	ACT	D	810	-	3,3,3	0.36	0	3,3,3	1.48	0
5	ACT	C	813	-	3,3,3	0.66	0	3,3,3	1.41	0
4	PO4	C	803	-	4,4,4	2.56	1 (25%)	6,6,6	0.85	0
3	NDP	D	704	-	45,52,52	1.79	10 (22%)	53,80,80	1.51	9 (16%)
4	PO4	A	802	-	4,4,4	2.50	1 (25%)	6,6,6	0.87	0
5	ACT	C	812	-	3,3,3	0.50	0	3,3,3	1.31	0
4	PO4	B	801	-	4,4,4	2.30	1 (25%)	6,6,6	0.90	0
5	ACT	D	816	-	3,3,3	0.47	0	3,3,3	1.46	0
6	GOL	B	806	-	5,5,5	0.49	0	5,5,5	0.19	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	2CY	A	601	-	-	5/8/8/8	0/3/3/3
2	2CY	D	604	-	-	2/8/8/8	0/3/3/3
2	2CY	C	603	-	-	3/8/8/8	0/3/3/3
3	NDP	A	701	-	-	4/30/77/77	0/5/5/5
3	NDP	C	703	-	-	2/30/77/77	0/5/5/5
6	GOL	B	806	-	-	0/4/4/4	-
3	NDP	B	702	-	-	2/30/77/77	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDP	D	704	-	-	9/30/77/77	0/5/5/5
6	GOL	C	805	-	-	0/4/4/4	-
2	2CY	B	602	-	-	2/8/8/8	0/3/3/3

All (85) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	2CY	O17-C18	-5.02	1.26	1.37
2	D	604	2CY	O17-C18	-4.99	1.26	1.37
4	C	804	PO4	P-O1	4.92	1.62	1.50
4	C	803	PO4	P-O1	4.84	1.62	1.50
2	C	603	2CY	O17-C18	-4.81	1.26	1.37
2	B	602	2CY	O17-C18	-4.72	1.26	1.37
4	A	802	PO4	P-O1	4.71	1.61	1.50
3	A	701	NDP	C4N-C3N	-4.70	1.40	1.49
3	C	703	NDP	C4N-C3N	-4.62	1.40	1.49
3	D	704	NDP	C4N-C3N	-4.41	1.41	1.49
3	D	704	NDP	C2N-C3N	4.38	1.47	1.34
4	B	801	PO4	P-O1	4.37	1.61	1.50
3	D	704	NDP	C4N-C5N	-4.35	1.37	1.48
3	C	703	NDP	C4N-C5N	-4.35	1.37	1.48
3	A	701	NDP	C4N-C5N	-4.31	1.37	1.48
3	A	701	NDP	C2N-C3N	4.26	1.46	1.34
3	B	702	NDP	C4N-C5N	-4.25	1.37	1.48
3	B	702	NDP	C4N-C3N	-4.23	1.41	1.49
3	A	701	NDP	C4A-N3A	4.00	1.41	1.35
3	C	703	NDP	C2N-C3N	3.81	1.45	1.34
2	A	601	2CY	C23-C18	3.56	1.45	1.38
2	B	602	2CY	C23-C18	3.52	1.45	1.38
2	C	603	2CY	O13-C7	-3.50	1.26	1.36
2	B	602	2CY	O13-C7	-3.49	1.26	1.36
2	A	601	2CY	O13-C7	-3.46	1.26	1.36
2	A	601	2CY	C21-C22	3.44	1.43	1.37
3	B	702	NDP	C2N-C3N	3.42	1.44	1.34
2	D	604	2CY	O13-C7	-3.40	1.26	1.36
2	C	603	2CY	C23-C22	3.38	1.43	1.37
2	B	602	2CY	C23-C22	3.38	1.43	1.37
2	D	604	2CY	C21-C22	3.35	1.43	1.37
2	D	604	2CY	C23-C22	3.34	1.43	1.37
2	B	602	2CY	C8-C7	3.31	1.45	1.38
2	A	601	2CY	C23-C22	3.30	1.43	1.37
3	D	704	NDP	C3B-C2B	-3.23	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	701	NDP	C6N-C5N	3.22	1.39	1.33
3	C	703	NDP	C4A-N3A	3.21	1.40	1.35
2	C	603	2CY	C21-C22	3.21	1.43	1.37
2	D	604	2CY	C23-C18	3.19	1.44	1.38
3	D	704	NDP	P2B-O2B	-3.18	1.53	1.59
3	D	704	NDP	C6N-C5N	3.18	1.39	1.33
3	B	702	NDP	C6N-C5N	3.17	1.39	1.33
2	C	603	2CY	C23-C18	3.16	1.44	1.38
3	A	701	NDP	P2B-O2B	-3.12	1.53	1.59
2	D	604	2CY	C8-C7	3.09	1.45	1.38
2	B	602	2CY	C21-C22	3.01	1.43	1.37
3	B	702	NDP	C4A-N3A	2.98	1.39	1.35
3	C	703	NDP	C3B-C2B	-2.93	1.46	1.52
2	D	604	2CY	C19-C18	2.91	1.44	1.38
2	C	603	2CY	C8-C7	2.88	1.44	1.38
2	B	602	2CY	C19-C18	2.87	1.44	1.38
2	A	601	2CY	C8-C7	2.87	1.44	1.38
3	B	702	NDP	C3B-C2B	-2.79	1.46	1.52
3	C	703	NDP	P2B-O2B	-2.76	1.54	1.59
3	B	702	NDP	P2B-O2B	-2.73	1.54	1.59
3	A	701	NDP	C3B-C2B	-2.71	1.46	1.52
2	C	603	2CY	C19-C18	2.71	1.44	1.38
3	C	703	NDP	C6N-C5N	2.70	1.38	1.33
2	A	601	2CY	C19-C18	2.60	1.43	1.38
2	B	602	2CY	C9-C10	2.59	1.42	1.36
3	A	701	NDP	C3B-C4B	-2.53	1.46	1.53
2	C	603	2CY	C9-C10	2.53	1.42	1.36
2	A	601	2CY	C9-C10	2.43	1.42	1.36
3	D	704	NDP	C4A-N3A	2.39	1.38	1.35
2	D	604	2CY	C9-C10	2.36	1.42	1.36
3	B	702	NDP	C3B-C4B	-2.28	1.47	1.53
3	C	703	NDP	C5D-C4D	2.21	1.58	1.51
2	B	602	2CY	C20-C19	2.19	1.43	1.38
2	D	604	2CY	C20-C19	2.17	1.43	1.38
3	C	703	NDP	C2A-N3A	2.17	1.35	1.32
3	B	702	NDP	PA-O1A	-2.17	1.43	1.50
3	D	704	NDP	PA-O1A	-2.16	1.43	1.50
3	C	703	NDP	C3B-C4B	-2.16	1.47	1.53
2	A	601	2CY	C20-C21	2.15	1.43	1.38
3	A	701	NDP	C2D-C1D	2.15	1.60	1.53
3	B	702	NDP	C6N-N1N	2.11	1.42	1.37
3	A	701	NDP	O4B-C1B	2.10	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	703	NDP	PA-O1A	-2.09	1.43	1.50
2	A	601	2CY	C20-C19	2.09	1.43	1.38
3	D	704	NDP	C3B-C4B	-2.07	1.47	1.53
3	D	704	NDP	C6N-N1N	2.07	1.42	1.37
3	C	703	NDP	C2D-C1D	2.05	1.60	1.53
2	C	603	2CY	C4-N3	2.03	1.37	1.33
2	B	602	2CY	C20-C21	2.03	1.43	1.38
2	C	603	2CY	C20-C19	2.01	1.43	1.38

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	603	2CY	N1-C2-N3	-5.32	120.12	127.22
2	D	604	2CY	N1-C2-N3	-5.23	120.24	127.22
2	A	601	2CY	N1-C2-N3	-5.17	120.33	127.22
2	B	602	2CY	N1-C2-N3	-5.14	120.36	127.22
2	A	601	2CY	C7-C5-C4	-4.88	124.88	127.36
3	C	703	NDP	C3N-C2N-N1N	-4.78	116.28	123.10
3	B	702	NDP	C1D-N1N-C2N	-4.69	113.31	121.11
2	D	604	2CY	C7-C5-C4	-4.65	124.99	127.36
2	B	602	2CY	C7-C5-C4	-4.65	125.00	127.36
3	D	704	NDP	C3N-C2N-N1N	-4.62	116.51	123.10
3	B	702	NDP	C3N-C2N-N1N	-4.45	116.75	123.10
2	C	603	2CY	C16-O17-C18	4.43	129.50	117.93
2	D	604	2CY	C16-O17-C18	4.37	129.35	117.93
3	A	701	NDP	C3N-C2N-N1N	-4.35	116.89	123.10
2	A	601	2CY	C16-O17-C18	4.30	129.18	117.93
2	C	603	2CY	C7-C5-C4	-4.04	125.30	127.36
2	B	602	2CY	C16-O17-C18	4.01	128.41	117.93
3	C	703	NDP	C1D-N1N-C2N	-3.92	114.59	121.11
3	C	703	NDP	C3B-C2B-C1B	-3.90	95.56	102.89
3	B	702	NDP	C3B-C2B-C1B	-3.88	95.60	102.89
3	D	704	NDP	C3B-C2B-C1B	-3.76	95.82	102.89
3	D	704	NDP	C1D-N1N-C2N	-3.26	115.68	121.11
3	A	701	NDP	C1D-N1N-C2N	-3.14	115.89	121.11
2	B	602	2CY	C14-O13-C7	3.08	126.94	117.74
2	A	601	2CY	C14-O13-C7	3.06	126.88	117.74
3	A	701	NDP	C3B-C2B-C1B	-3.05	97.15	102.89
2	C	603	2CY	C14-O13-C7	3.00	126.69	117.74
2	D	604	2CY	C14-O13-C7	2.91	126.44	117.74
3	B	702	NDP	C3D-C2D-C1D	-2.88	95.95	101.43
3	D	704	NDP	O7N-C7N-N7N	-2.83	116.26	122.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	703	NDP	C3D-C2D-C1D	-2.73	96.24	101.43
3	A	701	NDP	O7N-C7N-N7N	-2.65	116.67	122.88
3	A	701	NDP	O3B-C3B-C4B	2.60	118.55	111.05
3	C	703	NDP	O7N-C7N-N7N	-2.56	116.90	122.88
3	A	701	NDP	N3A-C2A-N1A	-2.52	124.74	128.68
3	B	702	NDP	C2D-C3D-C4D	2.51	107.52	102.64
3	C	703	NDP	C2D-C3D-C4D	2.51	107.52	102.64
3	A	701	NDP	O3B-C3B-C2B	2.50	118.26	111.17
2	A	601	2CY	C21-C22-C23	-2.49	120.05	123.29
3	C	703	NDP	N3A-C2A-N1A	-2.49	124.79	128.68
3	D	704	NDP	O3B-C3B-C4B	2.48	118.21	111.05
3	B	702	NDP	O7N-C7N-N7N	-2.47	117.10	122.88
3	B	702	NDP	O3B-C3B-C2B	2.42	118.03	111.17
3	C	703	NDP	O3B-C3B-C4B	2.41	118.03	111.05
3	B	702	NDP	N3A-C2A-N1A	-2.38	124.95	128.68
3	B	702	NDP	PN-O3-PA	2.34	140.84	132.83
3	A	701	NDP	PN-O3-PA	2.30	140.71	132.83
3	D	704	NDP	PN-O3-PA	2.30	140.70	132.83
3	D	704	NDP	N3A-C2A-N1A	-2.29	125.10	128.68
2	C	603	2CY	C16-C15-C14	-2.25	106.23	113.70
3	D	704	NDP	C2D-C3D-C4D	2.22	106.96	102.64
2	C	603	2CY	O13-C7-C8	-2.22	119.57	124.46
3	B	702	NDP	O3B-C3B-C4B	2.21	117.43	111.05
3	C	703	NDP	O3B-C3B-C2B	2.21	117.43	111.17
2	B	602	2CY	C16-C15-C14	-2.17	106.48	113.70
3	D	704	NDP	O3B-C3B-C2B	2.17	117.32	111.17
3	A	701	NDP	C2D-C3D-C4D	2.17	106.85	102.64
2	B	602	2CY	C2-N3-C4	2.11	122.73	116.72
2	C	603	2CY	C2-N3-C4	2.09	122.68	116.72
2	B	602	2CY	C21-C22-C23	-2.08	120.58	123.29
2	D	604	2CY	C2-N3-C4	2.05	122.57	116.72
2	D	604	2CY	C21-C22-C23	-2.05	120.63	123.29
3	C	703	NDP	O2A-PA-O1A	2.05	122.36	112.24
2	A	601	2CY	C2-N3-C4	2.04	122.55	116.72
2	D	604	2CY	C16-C15-C14	-2.04	106.92	113.70
3	B	702	NDP	O2A-PA-O1A	2.03	122.26	112.24
2	B	602	2CY	O13-C7-C8	-2.01	120.03	124.46
2	D	604	2CY	C2-N1-C6	2.01	121.29	116.33
2	D	604	2CY	O13-C7-C8	-2.00	120.05	124.46

There are no chirality outliers.

All (29) 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
3	A	701	NDP	C3B-C2B-O2B-P2B
2	C	603	2CY	C15-C14-O13-C7
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	D	704	NDP	C5D-O5D-PN-O3
3	A	701	NDP	O4D-C1D-N1N-C2N
3	C	703	NDP	O4D-C1D-N1N-C2N
3	D	704	NDP	O4D-C1D-N1N-C2N
3	D	704	NDP	C5D-O5D-PN-O2N
2	A	601	2CY	O13-C14-C15-C16
2	C	603	2CY	C15-C16-O17-C18
2	A	601	2CY	C5-C7-O13-C14
2	A	601	2CY	C8-C7-O13-C14
3	D	704	NDP	C3B-C4B-C5B-O5B
3	A	701	NDP	C1B-C2B-O2B-P2B
3	D	704	NDP	O4D-C4D-C5D-O5D
3	D	704	NDP	C3D-C4D-C5D-O5D
3	D	704	NDP	C2B-O2B-P2B-O2X
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	C2N-C3N-C7N-N7N

There are no ring outliers.

12 monomers are involved in 27 short contacts:

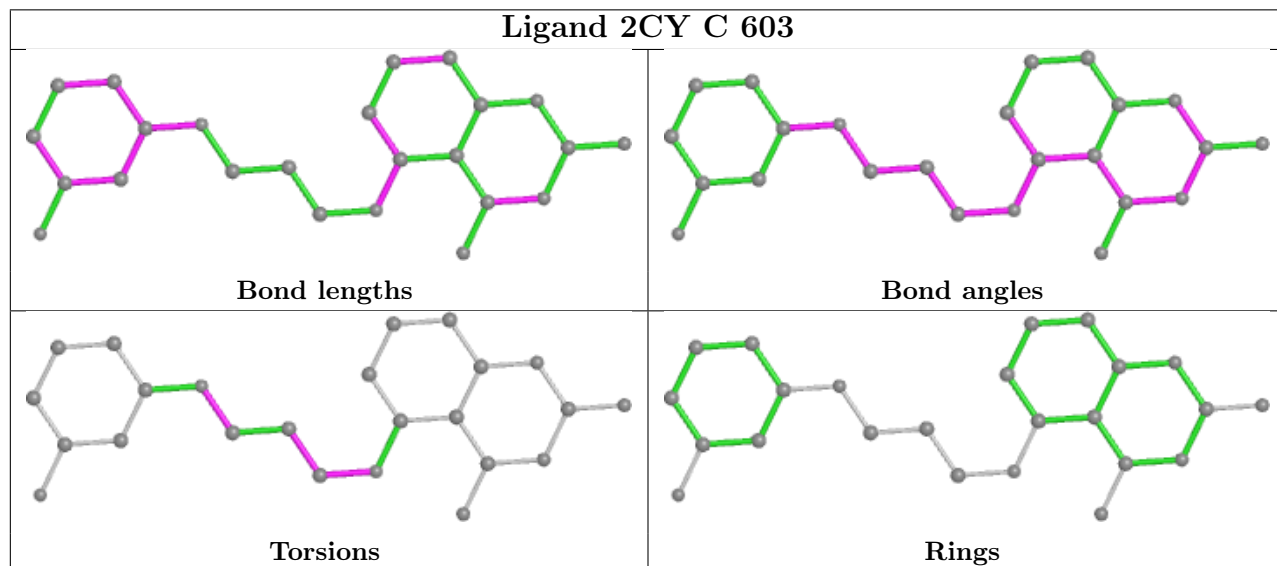
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	603	2CY	1	0
5	A	809	ACT	2	0
3	C	703	NDP	4	0
3	A	701	NDP	1	0
4	C	804	PO4	1	0
3	B	702	NDP	5	0
2	B	602	2CY	2	0
2	A	601	2CY	1	0
2	D	604	2CY	3	0

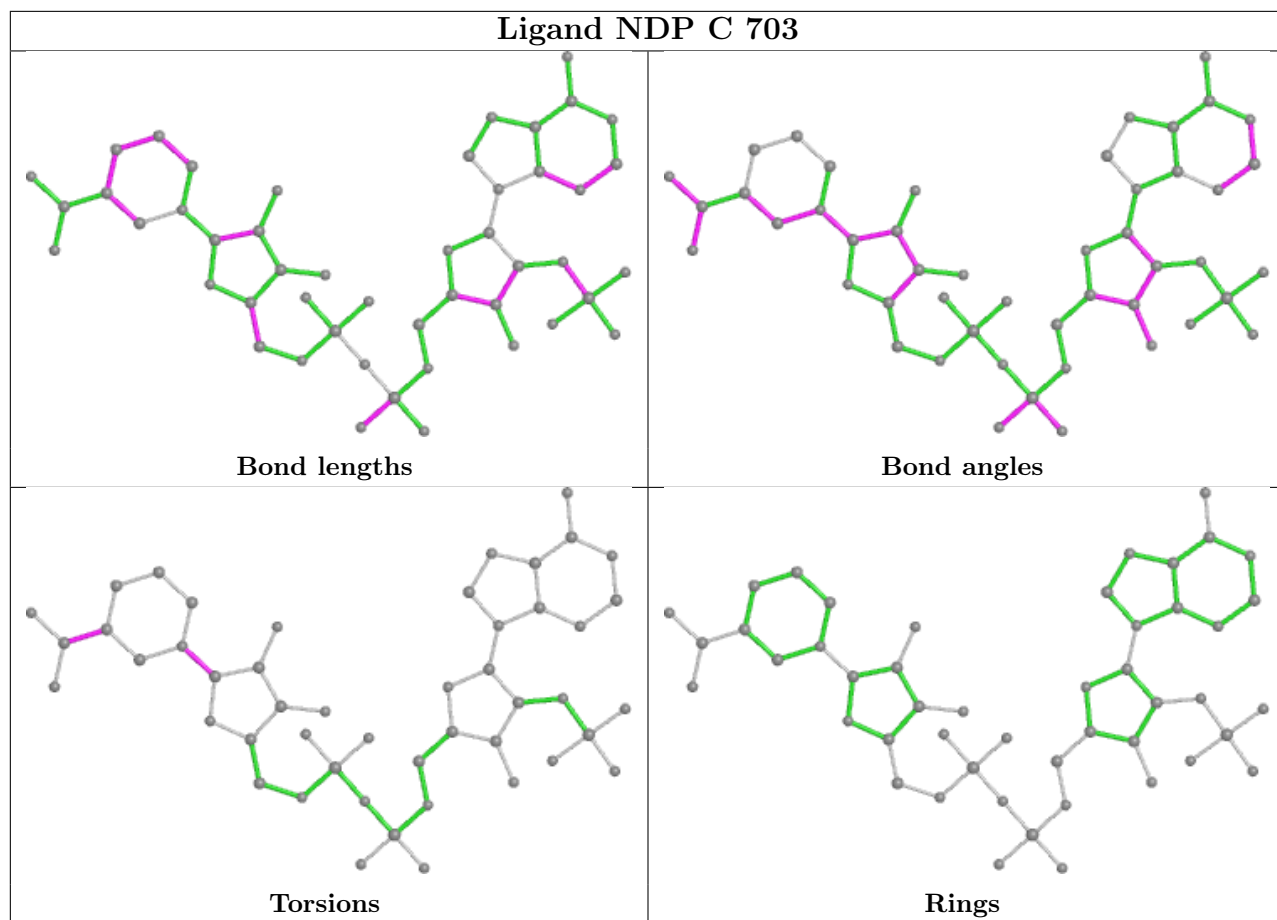
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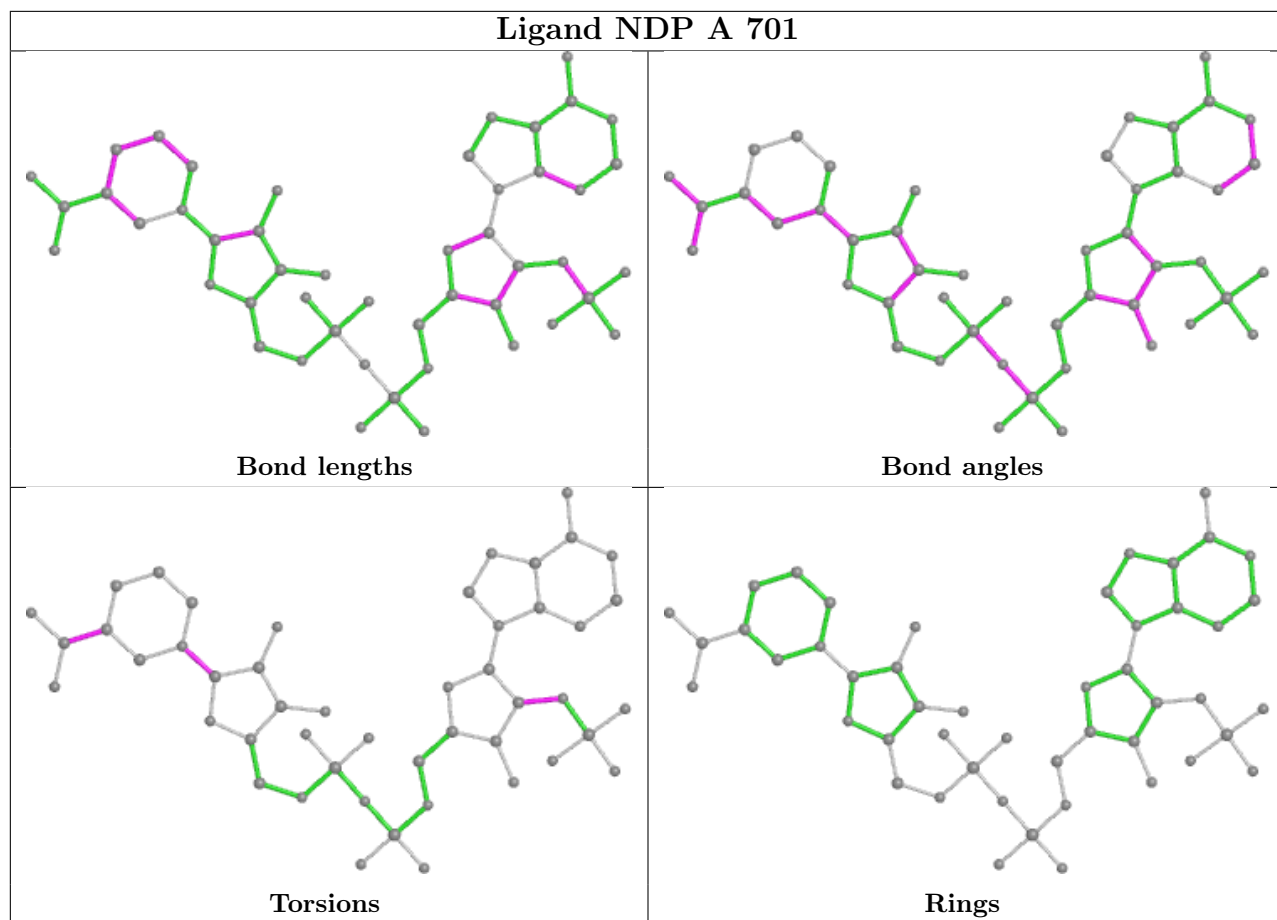
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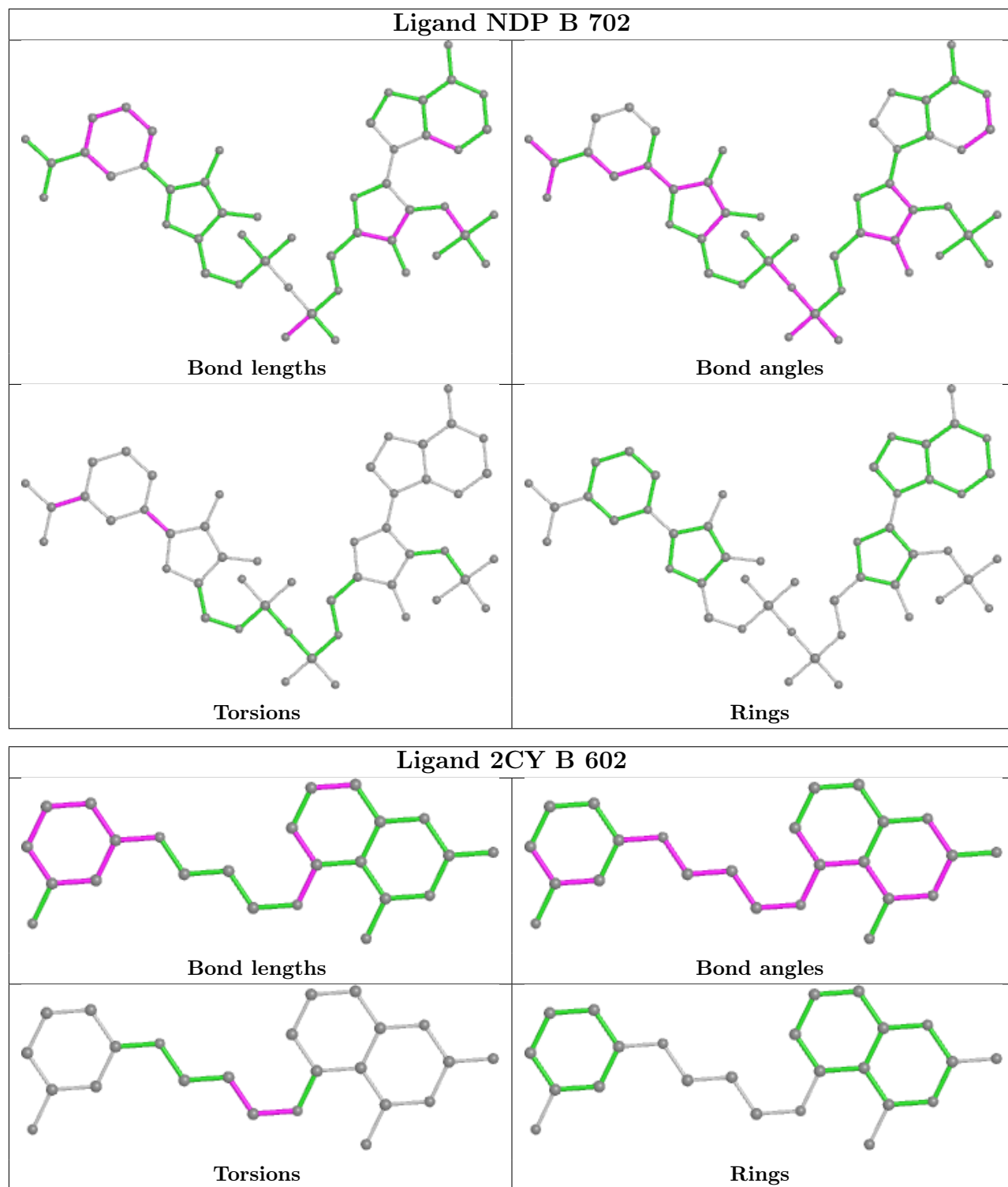
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	810	ACT	1	0
3	D	704	NDP	5	0
4	B	801	PO4	1	0

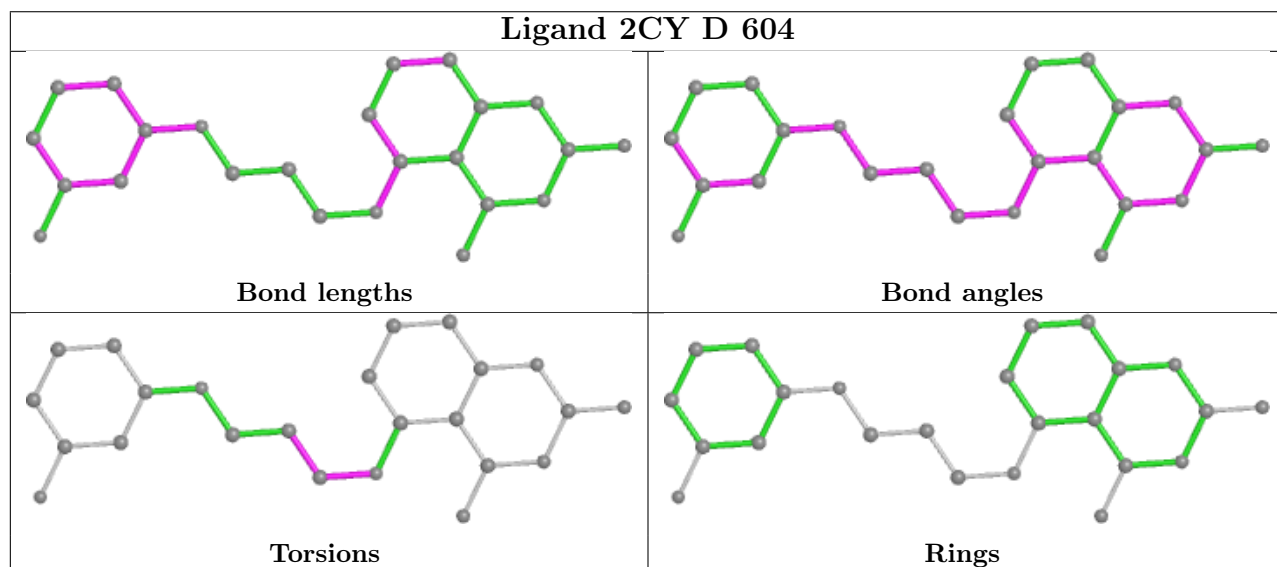
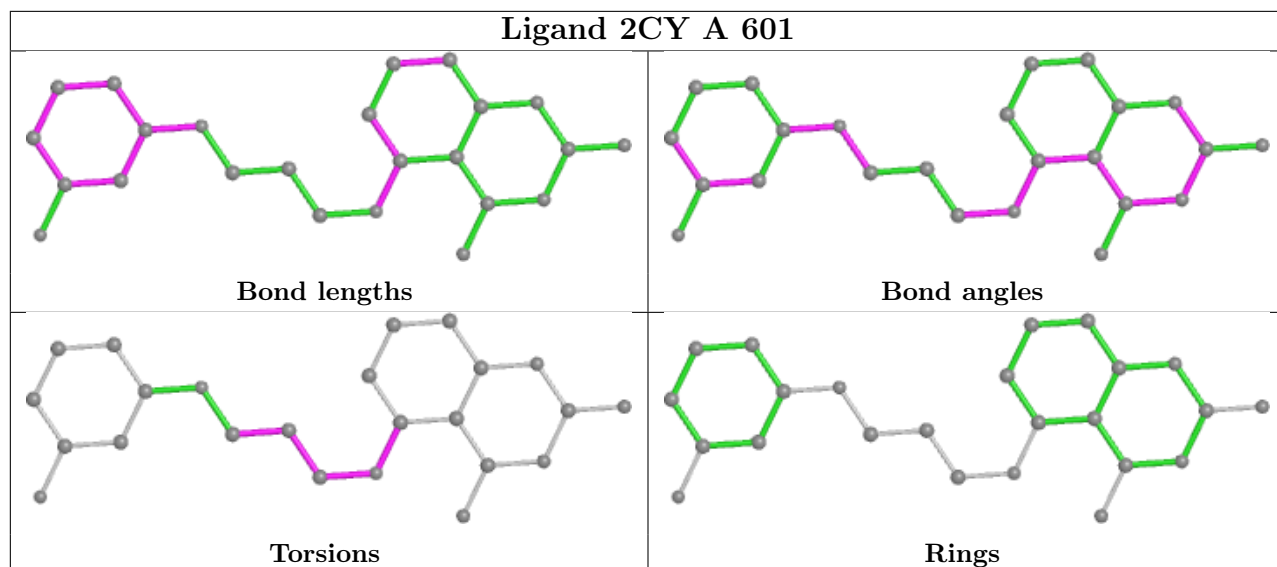
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

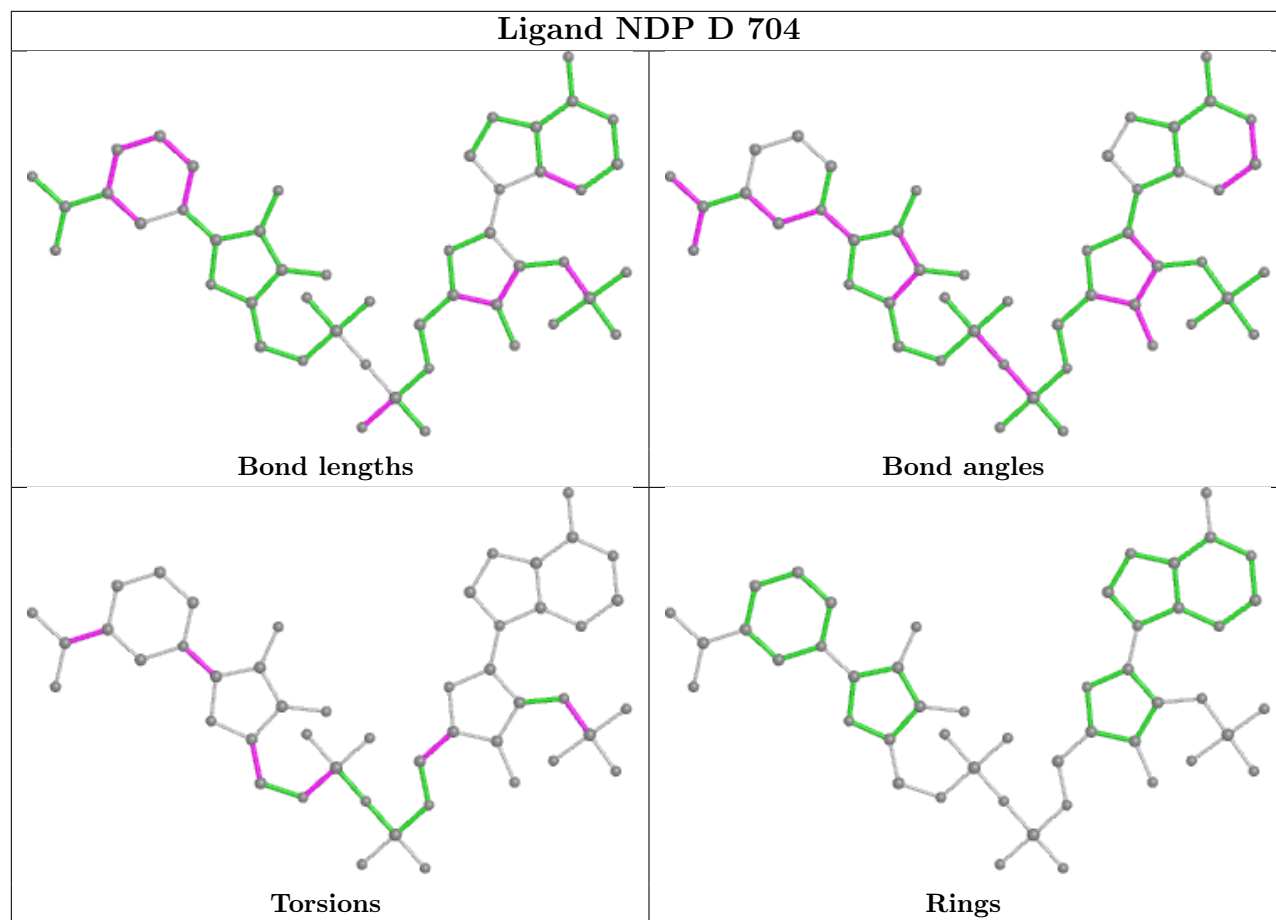












5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.29	16 (3%) 49 39	12, 26, 61, 91	0
1	B	515/521 (98%)	-0.17	21 (4%) 37 27	11, 29, 76, 91	0
1	C	516/521 (99%)	-0.35	16 (3%) 49 39	10, 26, 69, 91	0
1	D	513/521 (98%)	-0.26	19 (3%) 41 31	7, 28, 70, 91	0
All	All	2062/2084 (98%)	-0.27	72 (3%) 44 34	7, 27, 69, 91	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	38	GLY	7.9
1	B	186	SER	7.7
1	A	38	GLY	5.9
1	D	39	ARG	5.3
1	B	39	ARG	5.1
1	A	517	MET	4.7
1	A	184	GLU	4.7
1	A	37	ASP	4.6
1	C	38	GLY	4.4
1	B	37	ASP	4.3
1	C	42	PRO	4.3
1	A	43	TRP	4.1
1	B	43	TRP	4.1
1	C	37	ASP	4.1
1	C	44	ASN	4.0
1	B	42	PRO	4.0
1	B	187	CYS	3.8
1	A	183	SER	3.7
1	A	39	ARG	3.6
1	B	40	SER	3.6
1	A	186	SER	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	36	GLY	3.3
1	D	118	ARG	3.1
1	D	187	CYS	3.1
1	D	119	ASN	3.1
1	A	187	CYS	3.1
1	D	114	ASP	3.0
1	B	36	GLY	3.0
1	D	113	PRO	3.0
1	C	43	TRP	2.9
1	D	86	PRO	2.9
1	C	117	LYS	2.8
1	B	64	VAL	2.7
1	C	41	ILE	2.7
1	C	39	ARG	2.7
1	D	122	ALA	2.7
1	B	515	ILE	2.6
1	C	36	GLY	2.6
1	D	42	PRO	2.6
1	B	44	ASN	2.6
1	D	257	ARG	2.6
1	A	42	PRO	2.6
1	A	1	MET	2.5
1	B	185	SER	2.5
1	C	116	GLU	2.5
1	C	187	CYS	2.5
1	B	41	ILE	2.5
1	D	37	ASP	2.5
1	D	112	LEU	2.5
1	B	184	GLU	2.5
1	D	43	TRP	2.4
1	B	121	HIS	2.3
1	C	114	ASP	2.3
1	A	41	ILE	2.3
1	B	63	ASN	2.3
1	B	517	MET	2.3
1	D	185	SER	2.3
1	A	516	SER	2.2
1	C	62	LYS	2.2
1	D	36	GLY	2.2
1	D	110	ASP	2.2
1	B	120	LEU	2.2
1	B	257	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	180	ILE	2.1
1	C	119	ASN	2.1
1	A	185	SER	2.1
1	B	38	GLY	2.1
1	D	186	SER	2.1
1	A	63	ASN	2.1
1	D	115	GLU	2.0
1	C	186	SER	2.0
1	C	113	PRO	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 monosaccharides 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.

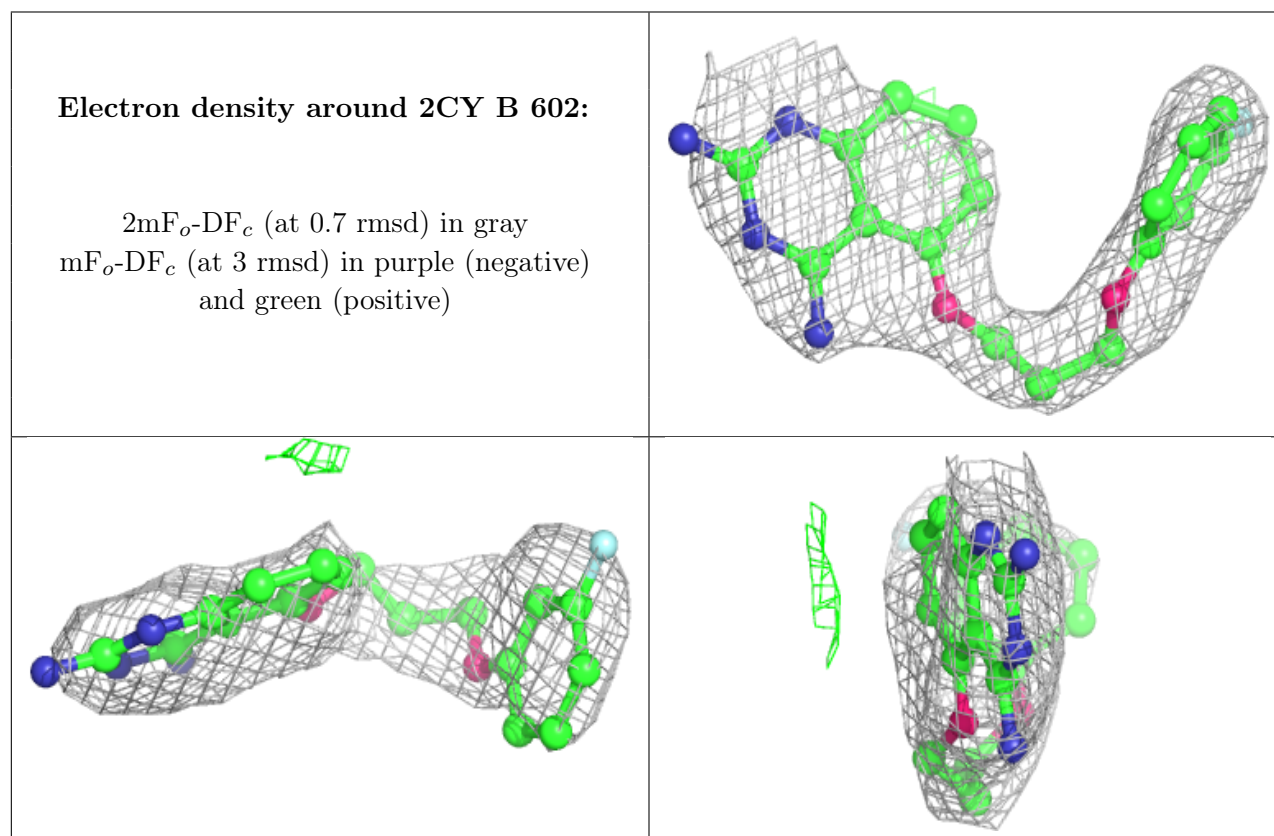
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	ACT	B	811	4/4	0.72	0.34	42,45,45,46	0
5	ACT	C	812	4/4	0.81	0.27	32,33,33,35	0
4	PO4	A	802	5/5	0.85	0.22	87,87,88,89	0
6	GOL	C	805	6/6	0.87	0.26	42,47,47,48	0
2	2CY	B	602	24/24	0.88	0.31	46,51,55,58	0
4	PO4	C	803	5/5	0.88	0.22	76,76,78,78	0
5	ACT	C	813	4/4	0.88	0.26	56,57,57,58	0
4	PO4	C	804	5/5	0.88	0.19	84,84,85,85	0
5	ACT	D	814	4/4	0.89	0.26	31,34,35,37	0
5	ACT	A	808	4/4	0.89	0.23	35,36,36,36	0
6	GOL	B	806	6/6	0.90	0.23	40,42,43,44	0
2	2CY	D	604	24/24	0.92	0.28	47,53,58,60	0
3	NDP	B	702	48/48	0.92	0.19	44,52,89,90	0
2	2CY	A	601	24/24	0.92	0.26	44,49,60,61	0

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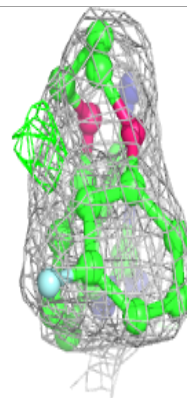
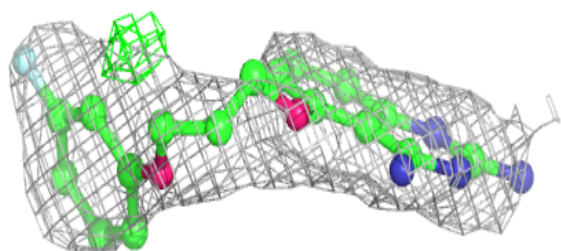
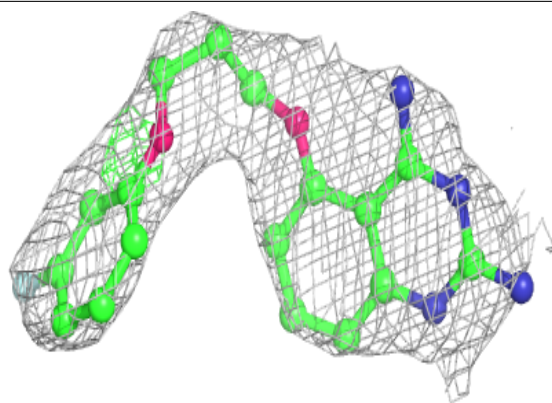
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	2CY	C	603	24/24	0.92	0.25	44,47,51,52	0
3	NDP	D	704	48/48	0.93	0.22	41,50,88,90	0
5	ACT	A	809	4/4	0.93	0.26	38,39,39,41	0
3	NDP	C	703	48/48	0.94	0.22	32,42,80,80	0
5	ACT	D	816	4/4	0.94	0.21	29,29,30,30	0
3	NDP	A	701	48/48	0.94	0.20	37,45,78,79	0
5	ACT	D	810	4/4	0.94	0.18	32,32,32,33	0
5	ACT	A	807	4/4	0.95	0.20	35,37,37,37	0
5	ACT	D	815	4/4	0.96	0.16	45,45,45,46	0
4	PO4	B	801	5/5	0.96	0.17	64,65,66,67	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.

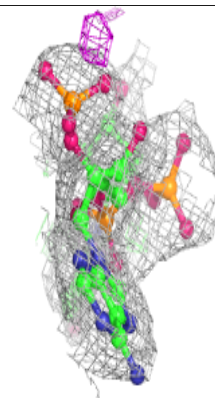
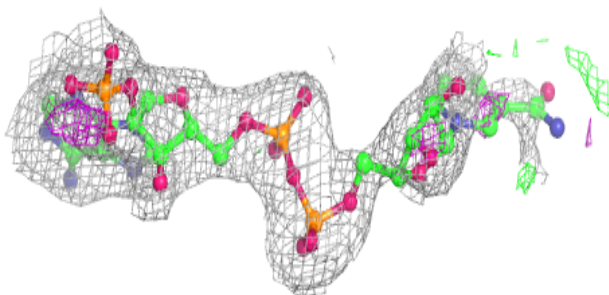
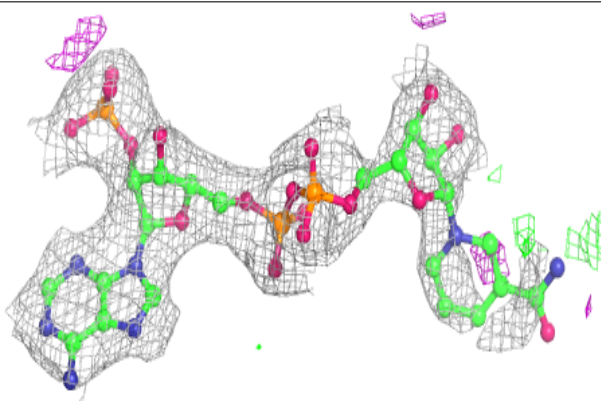


Electron density around 2CY D 604:

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

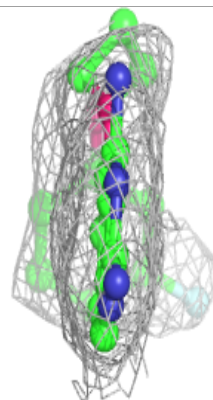
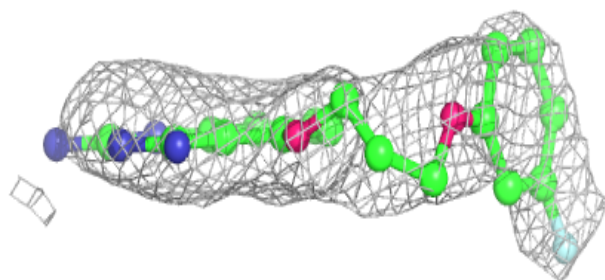
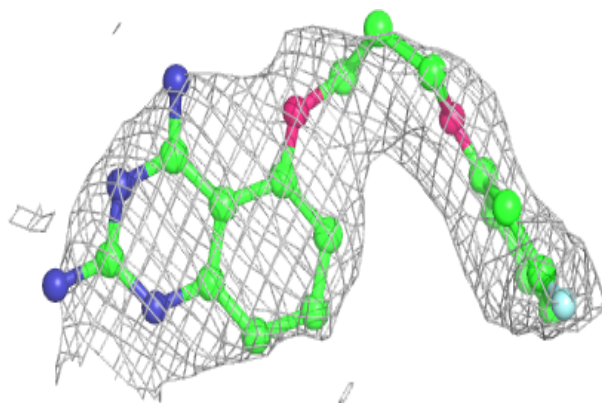
**Electron density around NDP B 702:**

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

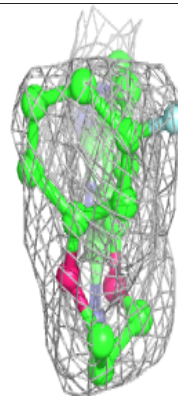
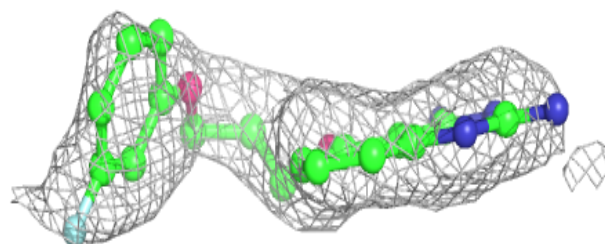
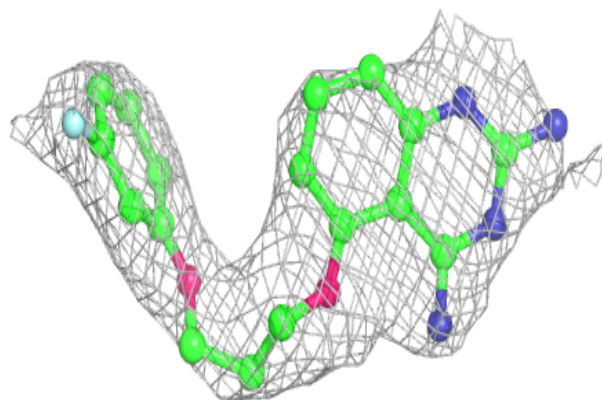


Electron density around 2CY A 601:

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

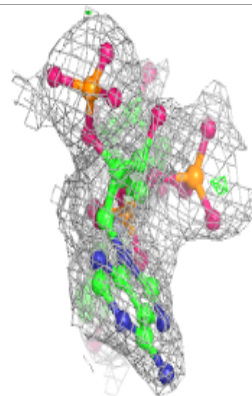
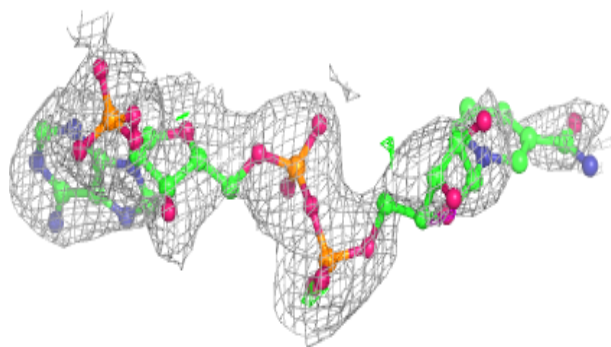
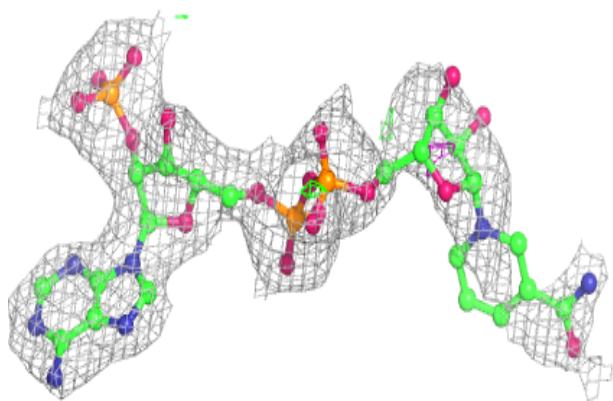
**Electron density around 2CY C 603:**

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

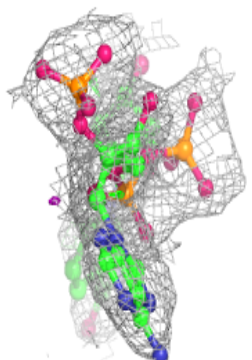
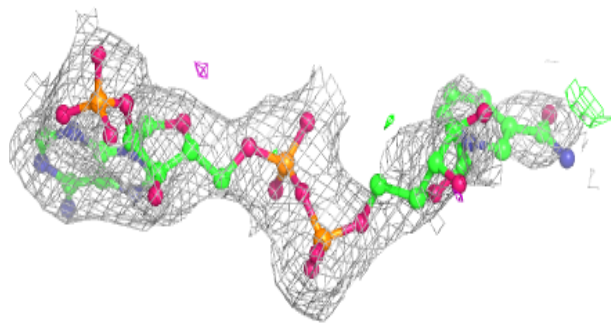
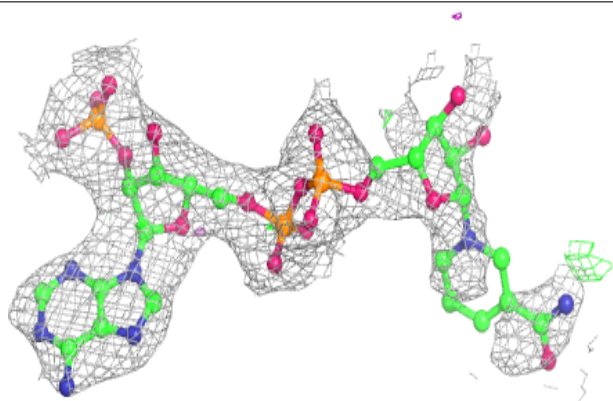


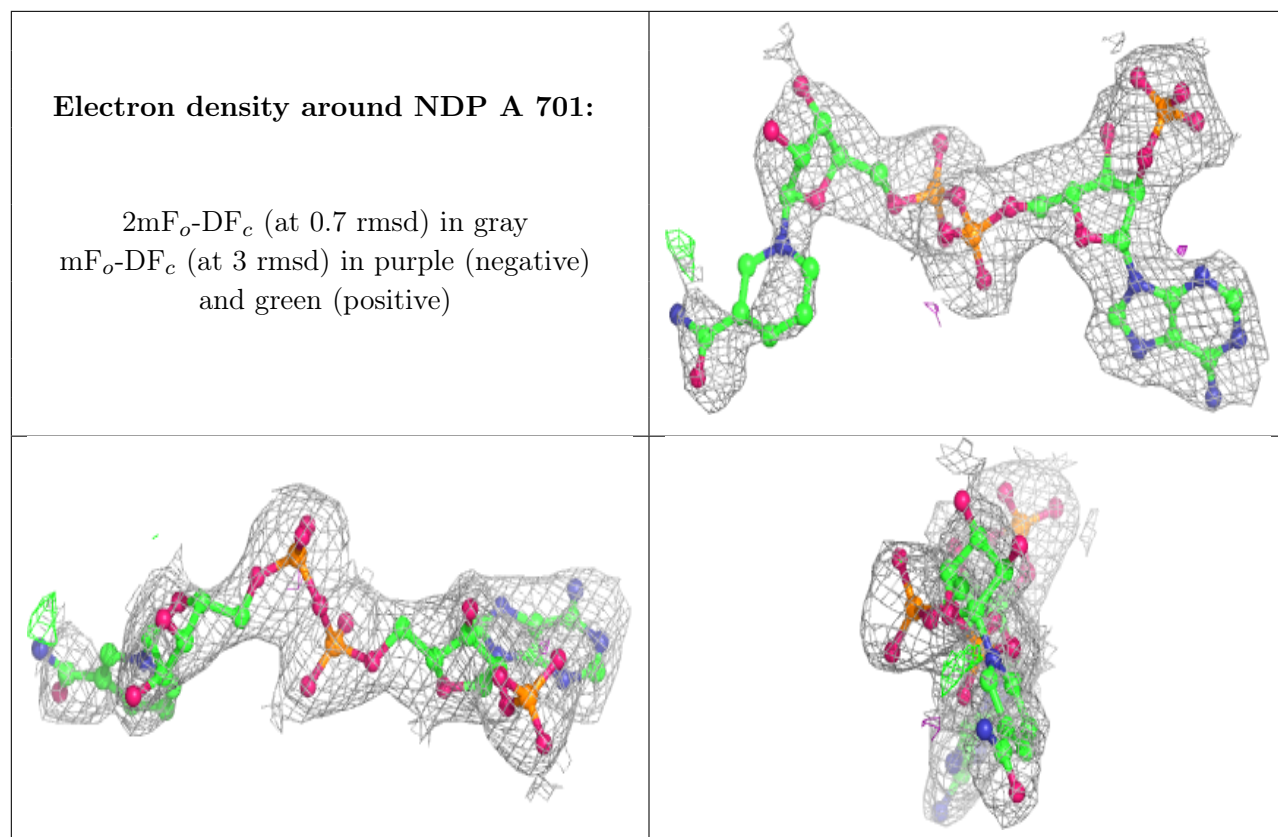
Electron density around NDP D 704:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.