Full wwPDB X-ray Structure Validation Report (i)

Mar 3, 2025 – 09:10 am GMT

PDB ID	:	8RVX
Title	:	Cph1 phytochrome PAS-GAF-PHY Y176H mutant
Authors	:	Nagano, S.; Hughes, J.
Deposited on	:	2024-02-02
Resolution	:	3.70 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 (i) 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 (i)) were used in the production of this report:

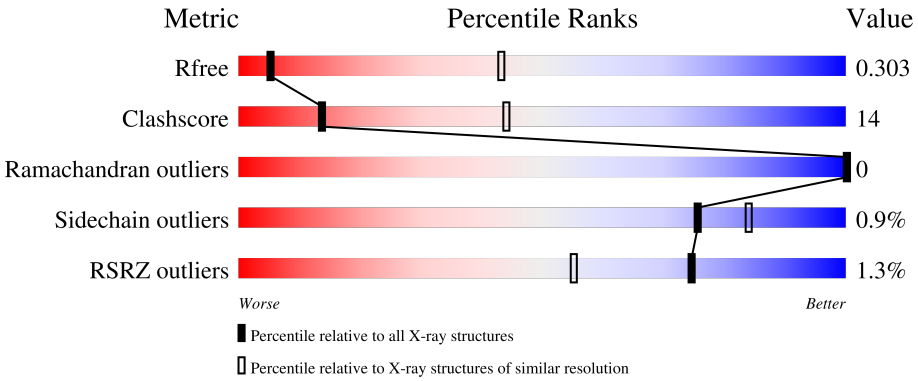
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.70 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}	164625	1017 (3.80-3.60)
Clashscore	180529	1074 (3.80-3.60)
Ramachandran outliers	177936	1055 (3.80-3.60)
Sidechain outliers	177891	1052 (3.80-3.60)
RSRZ outliers	164620	1017 (3.80-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	520	68% 27% 5%
1	B	520	64% 28% 7%
1	C	520	67% 26% 7%
1	D	520	2% 68% 24% 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 15679 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 Phytochrome-like protein Cph1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	495	Total	C	N	O	S	0	0	0
			3935	2509	685	728	13			
1	B	484	Total	C	N	O	S	0	0	0
			3849	2458	669	709	13			
1	C	486	Total	C	N	O	S	0	0	0
			3865	2465	671	716	13			
1	D	484	Total	C	N	O	S	0	0	0
			3854	2463	670	708	13			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ARG	ASN	conflict	UNP Q55168
A	176	HIS	TYR	engineered mutation	UNP Q55168
A	515	HIS	-	expression tag	UNP Q55168
A	516	HIS	-	expression tag	UNP Q55168
A	517	HIS	-	expression tag	UNP Q55168
A	518	HIS	-	expression tag	UNP Q55168
A	519	HIS	-	expression tag	UNP Q55168
A	520	HIS	-	expression tag	UNP Q55168
B	141	ARG	ASN	conflict	UNP Q55168
B	176	HIS	TYR	engineered mutation	UNP Q55168
B	515	HIS	-	expression tag	UNP Q55168
B	516	HIS	-	expression tag	UNP Q55168
B	517	HIS	-	expression tag	UNP Q55168
B	518	HIS	-	expression tag	UNP Q55168
B	519	HIS	-	expression tag	UNP Q55168
B	520	HIS	-	expression tag	UNP Q55168
C	141	ARG	ASN	conflict	UNP Q55168
C	176	HIS	TYR	engineered mutation	UNP Q55168
C	515	HIS	-	expression tag	UNP Q55168
C	516	HIS	-	expression tag	UNP Q55168
C	517	HIS	-	expression tag	UNP Q55168

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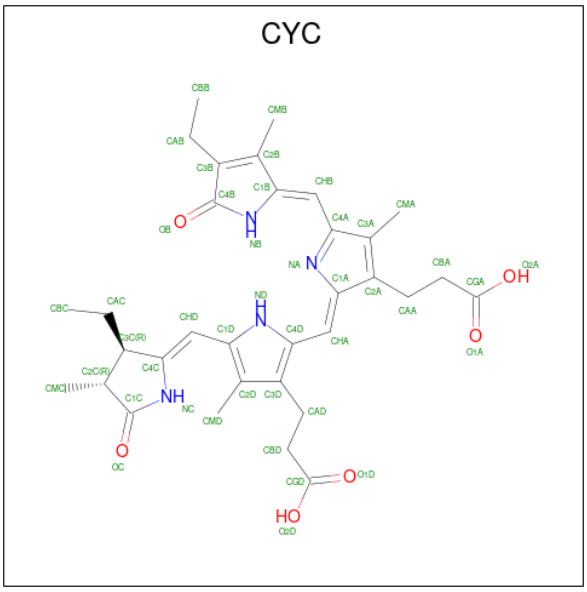
Chain	Residue	Modelled	Actual	Comment	Reference
C	518	HIS	-	expression tag	UNP Q55168
C	519	HIS	-	expression tag	UNP Q55168
C	520	HIS	-	expression tag	UNP Q55168
D	141	ARG	ASN	conflict	UNP Q55168
D	176	HIS	TYR	engineered mutation	UNP Q55168
D	515	HIS	-	expression tag	UNP Q55168
D	516	HIS	-	expression tag	UNP Q55168
D	517	HIS	-	expression tag	UNP Q55168
D	518	HIS	-	expression tag	UNP Q55168
D	519	HIS	-	expression tag	UNP Q55168
D	520	HIS	-	expression tag	UNP Q55168

- Molecule 2 is PHYCOCYANOBILIN (three-letter code: CYC) (formula: $C_{33}H_{40}N_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 43 33 4 6	0	0
2	B	1	Total C N O 43 33 4 6	0	0
2	C	1	Total C N O 43 33 4 6	0	0
2	D	1	Total C N O 43 33 4 6	0	0

- Molecule 3 is water.

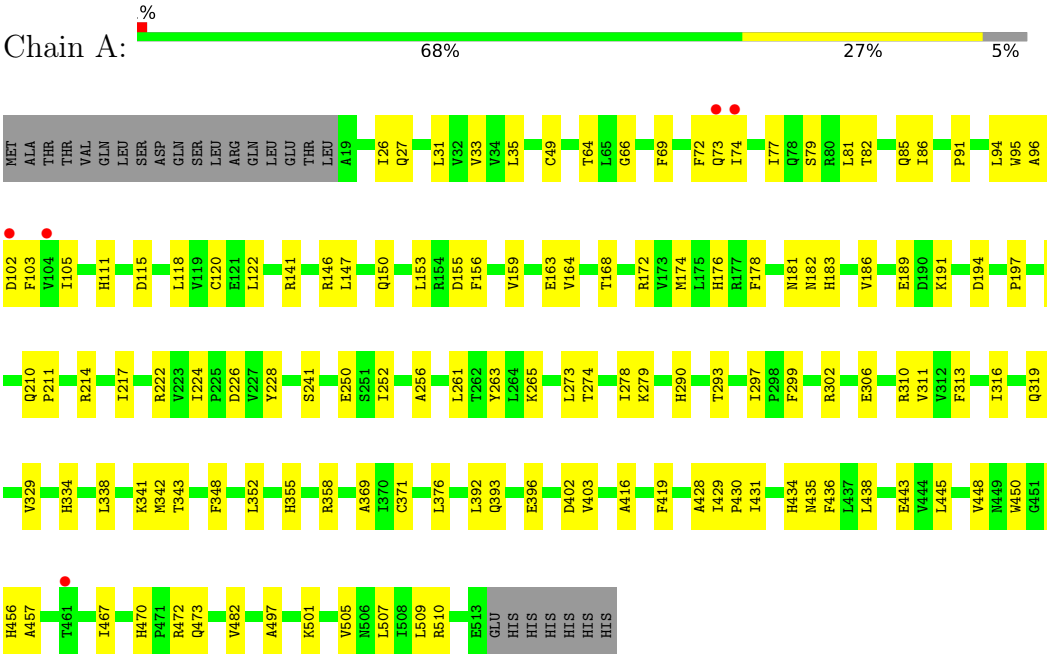
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O 1 1	0	0
3	B	1	Total O 1 1	0	0
3	C	1	Total O 1 1	0	0
3	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

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.

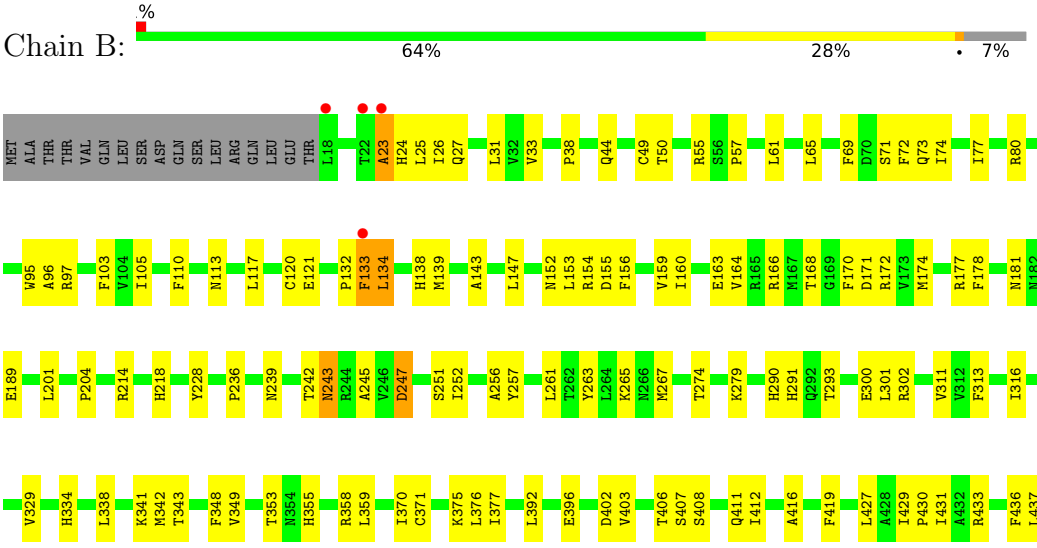
• Molecule 1: Phytochrome-like protein Cph1

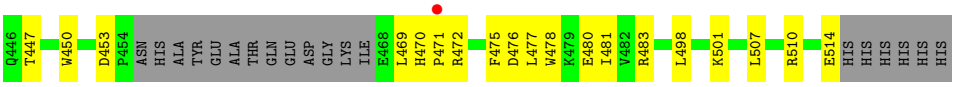
Chain A:



• Molecule 1: Phytochrome-like protein Cph1

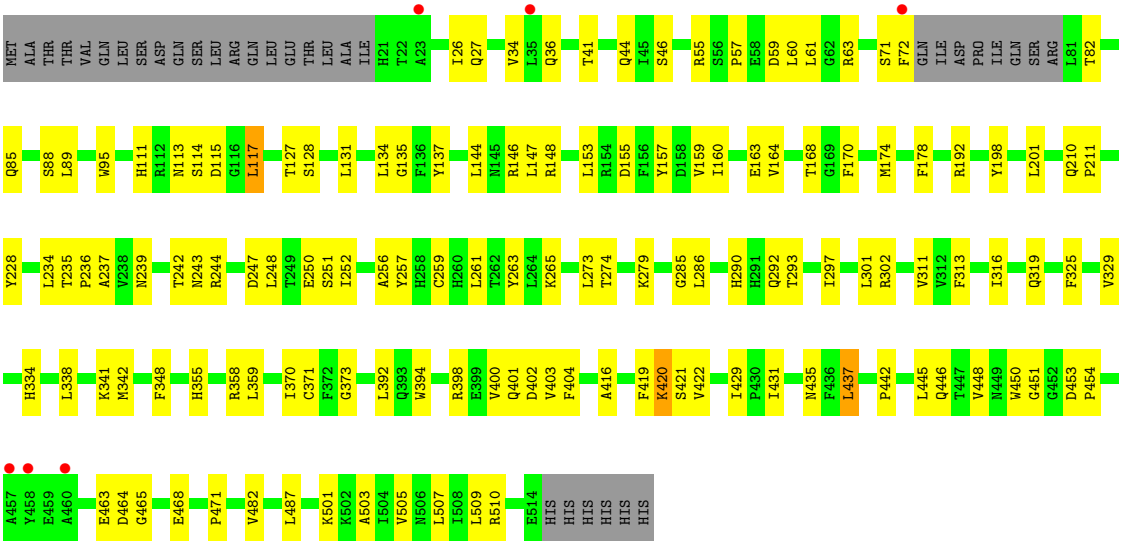
Chain B:





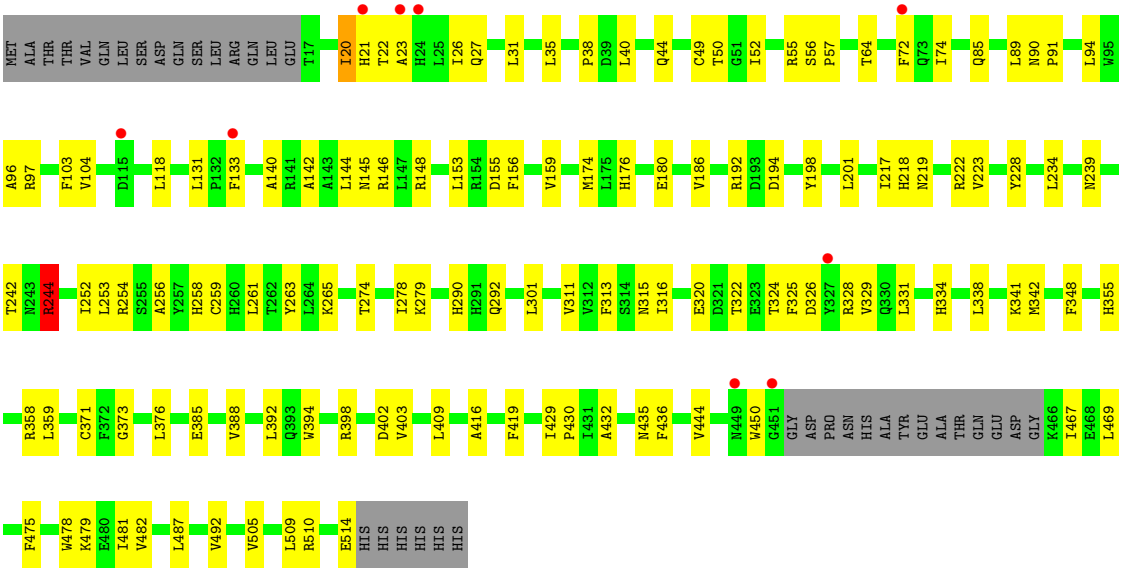
• Molecule 1: Phytochrome-like protein Cph1

Chain C:



• Molecule 1: Phytochrome-like protein Cph1

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	135.87Å 135.87Å 355.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 3.70 47.65 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.1 (47.65-3.70) 99.1 (47.65-3.70)	Depositor EDS
R_{merge}	0.80	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.23 (at 3.67Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.266 , 0.307 0.264 , 0.303	Depositor DCC
R_{free} test set	1768 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å^2)	86.9	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 82.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	15679	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.23% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CYC

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	0/4029	0.69	0/5483
1	B	0.37	0/3940	0.67	0/5361
1	C	0.37	0/3957	0.63	0/5383
1	D	0.38	0/3944	0.67	1/5365 (0.0%)
All	All	0.38	0/15870	0.66	1/21592 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	244	ARG	NE-CZ-NH2	5.16	122.88	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	23	ALA	Peptide

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	3935	0	3881	108	4
1	B	3849	0	3807	131	0
1	C	3865	0	3803	116	1
1	D	3854	0	3824	103	3
2	A	43	0	37	8	0
2	B	43	0	37	6	0
2	C	43	0	37	8	0
2	D	43	0	37	6	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	15679	0	15463	445	4

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 14.

All (445) 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:44:GLN:HA	1:C:236:PRO:HG2	1.30	1.12
1:A:467:ILE:HG22	1:A:473:GLN:HB2	1.54	0.89
1:D:403:VAL:HG22	1:D:429:ILE:HG22	1.56	0.88
1:B:470:HIS:CG	1:B:471:PRO:HD2	2.08	0.87
1:B:164:VAL:O	1:B:168:THR:HG22	1.77	0.85
1:C:44:GLN:OE1	1:C:236:PRO:HB2	1.76	0.85
1:C:134:LEU:HD12	1:C:135:GLY:N	1.92	0.84
1:C:164:VAL:O	1:C:168:THR:HG22	1.76	0.84
1:D:341:LYS:HG2	1:D:355:HIS:CE1	2.13	0.84
1:A:338:LEU:HD21	1:A:352:LEU:CD2	2.09	0.83
1:A:164:VAL:O	1:A:168:THR:HG22	1.78	0.82
1:D:274:THR:HG21	2:D:601:CYC:HBA1	1.59	0.81
1:C:34:VAL:CG2	1:C:44:GLN:HB2	2.11	0.81
1:C:61:LEU:HD21	1:C:236:PRO:HG3	1.62	0.79
1:D:144:LEU:O	1:D:148:ARG:HG2	1.84	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:198:TYR:HA	1:D:450:TRP:HZ2	1.49	0.78
1:D:432:ALA:HB3	1:D:435:ASN:HB2	1.65	0.77
1:B:406:THR:HG21	1:B:412:ILE:HD12	1.66	0.77
1:B:450:TRP:HD1	1:B:475:PHE:CD2	2.03	0.77
1:A:263:TYR:CE2	2:A:601:CYC:HMB3	2.21	0.76
1:D:239:ASN:HB3	1:D:242:THR:HG22	1.69	0.75
1:C:34:VAL:HB	1:C:44:GLN:HB2	1.70	0.74
1:A:470:HIS:HD2	1:A:472:ARG:H	1.35	0.74
1:B:97:ARG:HA	1:B:103:PHE:HA	1.70	0.73
1:D:142:ALA:O	1:D:146:ARG:HG2	1.89	0.72
1:B:470:HIS:CE1	1:B:471:PRO:HD2	2.25	0.72
1:C:137:TYR:HB3	1:D:329:VAL:HG23	1.71	0.71
1:B:470:HIS:ND1	1:B:471:PRO:HD2	2.05	0.71
1:B:69:PHE:HA	1:B:96:ALA:HB2	1.73	0.71
1:D:430:PRO:HA	1:D:436:PHE:HD1	1.56	0.71
1:A:146:ARG:HH21	1:A:163:GLU:HG2	1.56	0.71
1:C:146:ARG:NH1	1:C:163:GLU:OE1	2.24	0.70
1:C:301:LEU:O	1:C:301:LEU:HD23	1.91	0.70
1:C:403:VAL:HG23	1:C:429:ILE:HG12	1.73	0.69
1:B:274:THR:HG21	2:B:601:CYC:HBA1	1.72	0.69
1:B:470:HIS:CD2	1:B:471:PRO:HD2	2.27	0.69
1:D:26:ILE:HD11	1:D:234:LEU:HD21	1.75	0.69
1:A:338:LEU:HD21	1:A:352:LEU:HD22	1.72	0.69
1:D:409:LEU:HD12	1:D:416:ALA:CB	2.23	0.68
1:D:180:GLU:CD	1:D:180:GLU:H	1.98	0.68
1:C:341:LYS:HG2	1:C:355:HIS:CE1	2.30	0.67
1:B:469:LEU:O	1:B:469:LEU:HG	1.94	0.67
1:A:443:GLU:HG2	1:A:445:LEU:HG	1.77	0.67
1:D:409:LEU:CD1	1:D:416:ALA:CB	2.73	0.66
1:B:470:HIS:CG	1:B:471:PRO:CD	2.78	0.65
1:D:97:ARG:HA	1:D:103:PHE:HA	1.76	0.65
1:D:301:LEU:HD23	1:D:301:LEU:O	1.95	0.65
1:D:444:VAL:HG22	1:D:487:LEU:HD23	1.77	0.65
1:B:86:ILE:H	1:B:86:ILE:HD12	1.62	0.65
1:C:34:VAL:CB	1:C:44:GLN:HB2	2.25	0.65
1:A:396:GLU:OE2	1:A:434:HIS:HB3	1.98	0.64
1:A:430:PRO:HA	1:A:436:PHE:CD2	2.33	0.63
1:A:77:ILE:HD12	1:A:77:ILE:H	1.64	0.63
1:A:111:HIS:CE1	1:A:250:GLU:HB2	2.34	0.63
1:B:480:GLU:HA	1:B:483:ARG:HE	1.63	0.62
1:A:74:ILE:H	1:A:74:ILE:HD12	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:THR:HG21	2:C:601:CYC:HBA1	1.82	0.62
1:D:242:THR:HG23	1:D:244:ARG:H	1.63	0.62
1:B:341:LYS:HG2	1:B:355:HIS:CE1	2.34	0.62
1:B:431:ILE:HD13	1:B:501:LYS:HG2	1.81	0.61
1:A:241:SER:O	1:C:422:VAL:HG23	1.99	0.61
1:A:252:ILE:HD13	1:A:302:ARG:NH2	2.15	0.61
1:D:331:LEU:HD12	1:D:492:VAL:HG22	1.82	0.61
1:C:61:LEU:HD21	1:C:236:PRO:CG	2.31	0.60
1:C:46:SER:HA	1:C:234:LEU:HD12	1.83	0.60
1:C:242:THR:HG22	1:C:244:ARG:HB3	1.84	0.60
1:B:338:LEU:HD11	1:B:359:LEU:HA	1.84	0.60
1:C:44:GLN:NE2	1:C:237:ALA:O	2.35	0.60
1:A:81:LEU:HD23	1:A:86:ILE:HG12	1.82	0.59
1:B:183:HIS:HD2	1:B:204:PRO:HA	1.67	0.59
1:D:505:VAL:O	1:D:509:LEU:HG	2.02	0.59
1:B:143:ALA:HB2	1:B:163:GLU:HG2	1.83	0.59
1:C:115:ASP:HB2	1:C:117:LEU:CD2	2.32	0.59
1:A:263:TYR:HE2	2:A:601:CYC:CMB	2.16	0.59
1:A:217:ILE:HG22	1:A:278:ILE:HD12	1.84	0.59
1:B:153:LEU:HD13	1:B:319:GLN:HB3	1.85	0.59
1:B:343:THR:HG22	1:B:507:LEU:HD13	1.85	0.59
1:A:69:PHE:HA	1:A:96:ALA:HB2	1.85	0.58
1:D:239:ASN:HB3	1:D:242:THR:CG2	2.32	0.58
1:B:77:ILE:HD12	1:B:77:ILE:H	1.68	0.58
1:B:23:ALA:HB1	1:B:25:LEU:HD13	1.85	0.58
1:B:71:SER:OG	1:B:73:GLN:HB2	2.04	0.58
1:A:311:VAL:HG11	1:B:325:PHE:HB2	1.85	0.58
1:C:82:THR:HG23	1:C:85:GLN:H	1.67	0.58
1:B:450:TRP:HB3	1:B:475:PHE:CZ	2.39	0.58
1:C:55:ARG:HD2	1:C:60:LEU:HD21	1.85	0.58
1:C:453:ASP:N	1:C:454:PRO:HD2	2.19	0.58
1:B:267:MET:HA	1:B:470:HIS:HE1	1.68	0.58
1:A:306:GLU:O	1:A:310:ARG:HG3	2.04	0.58
1:C:263:TYR:CE2	2:C:601:CYC:HMB3	2.38	0.58
1:C:34:VAL:HG23	1:C:44:GLN:HB2	1.86	0.57
1:B:353:THR:HG21	1:B:377:ILE:HG21	1.85	0.57
1:B:470:HIS:ND1	1:B:471:PRO:CD	2.67	0.57
2:A:601:CYC:HBA2	2:A:601:CYC:HMA2	1.85	0.57
1:D:242:THR:OG1	1:D:244:ARG:NH2	2.37	0.57
1:C:111:HIS:CE1	1:C:250:GLU:HB2	2.40	0.57
1:D:263:TYR:CE2	2:D:601:CYC:HMB3	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:263:TYR:CE2	2:A:601:CYC:CMB	2.89	0.56
1:B:252:ILE:HD13	1:B:302:ARG:NH2	2.21	0.56
1:D:385:GLU:HA	1:D:388:VAL:CG1	2.34	0.56
1:B:143:ALA:CB	1:B:163:GLU:HG2	2.35	0.56
1:B:443:GLU:O	1:B:445:LEU:HG	2.05	0.56
1:C:36:GLN:HE21	1:C:41:THR:HG23	1.70	0.56
1:C:117:LEU:H	1:C:117:LEU:HD23	1.70	0.56
1:C:338:LEU:HD11	1:C:359:LEU:HA	1.86	0.56
1:D:50:THR:HA	1:D:55:ARG:O	2.06	0.56
1:B:396:GLU:HB2	1:B:433:ARG:HH12	1.70	0.56
1:C:319:GLN:HA	1:D:148:ARG:HH12	1.70	0.56
1:A:371:CYS:HB2	1:A:392:LEU:HD21	1.88	0.56
1:C:198:TYR:HA	1:C:450:TRP:HE1	1.70	0.56
1:A:97:ARG:NH2	1:A:101:ASP:OD1	2.39	0.56
1:A:470:HIS:CD2	1:A:472:ARG:H	2.22	0.55
1:A:338:LEU:CD2	1:A:352:LEU:CD2	2.84	0.55
1:C:482:VAL:HG12	1:C:482:VAL:O	2.06	0.55
1:A:72:PHE:CE2	1:A:74:ILE:HA	2.42	0.55
1:A:443:GLU:OE1	1:A:445:LEU:HD12	2.07	0.55
1:B:371:CYS:HB2	1:B:392:LEU:HD21	1.89	0.55
1:C:113:ASN:HD22	1:C:117:LEU:HD21	1.72	0.55
1:A:27:GLN:HE22	1:A:224:ILE:HA	1.71	0.55
1:A:482:VAL:HG12	1:A:482:VAL:O	2.07	0.55
2:B:601:CYC:HBA2	2:B:601:CYC:HMA2	1.89	0.55
1:C:257:TYR:HB3	2:C:601:CYC:HMD2	1.88	0.55
1:B:50:THR:HA	1:B:55:ARG:O	2.07	0.54
1:B:431:ILE:HD11	1:B:437:LEU:HD12	1.89	0.54
1:D:482:VAL:HG12	1:D:482:VAL:O	2.07	0.54
1:C:57:PRO:HB2	1:C:235:THR:HG21	1.90	0.54
1:D:142:ALA:HA	1:D:145:ASN:ND2	2.23	0.54
1:C:155:ASP:O	1:C:159:VAL:HG23	2.08	0.54
1:D:409:LEU:CD1	1:D:416:ALA:HB2	2.38	0.54
1:A:141:ARG:HD2	1:B:326:ASP:OD1	2.06	0.54
1:B:97:ARG:HA	1:B:103:PHE:CA	2.37	0.54
1:C:505:VAL:O	1:C:509:LEU:HG	2.08	0.54
1:A:228:TYR:CZ	1:A:265:LYS:HG2	2.43	0.54
1:B:86:ILE:HG23	1:B:110:PHE:HB2	1.90	0.54
1:C:370:ILE:HG23	1:C:437:LEU:HD21	1.90	0.54
1:A:467:ILE:HG22	1:A:467:ILE:O	2.07	0.54
1:B:95:TRP:HE3	1:B:105:ILE:HG23	1.73	0.53
1:A:82:THR:HG23	1:A:85:GLN:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:PRO:HG2	1:B:133:PHE:CD2	2.43	0.53
1:D:56:SER:HB2	1:D:57:PRO:HD2	1.91	0.53
1:A:376:LEU:HD13	1:A:376:LEU:C	2.29	0.53
1:A:97:ARG:HA	1:A:102:ASP:O	2.09	0.53
1:B:376:LEU:C	1:B:376:LEU:HD13	2.29	0.53
1:B:267:MET:HA	1:B:470:HIS:CE1	2.44	0.53
1:B:403:VAL:HG22	1:B:429:ILE:HG12	1.91	0.53
1:C:325:PHE:HB2	1:D:311:VAL:HG21	1.91	0.53
1:B:334:HIS:CE1	1:B:358:ARG:HH11	2.26	0.53
1:C:311:VAL:HG21	1:D:325:PHE:HB2	1.90	0.53
1:A:155:ASP:O	1:A:159:VAL:HG23	2.09	0.53
1:B:290:HIS:CE1	2:B:601:CYC:OB	2.62	0.53
1:B:174:MET:CE	2:B:601:CYC:HBB2	2.40	0.52
1:C:44:GLN:HB3	1:C:234:LEU:HD23	1.91	0.52
1:D:26:ILE:HG23	1:D:253:LEU:HB3	1.90	0.52
1:D:279:LYS:HB2	1:D:313:PHE:CZ	2.44	0.52
1:C:71:SER:O	1:C:72:PHE:C	2.48	0.52
1:B:168:THR:HG1	1:B:170:PHE:HD2	1.57	0.52
1:C:420:LYS:HG3	1:C:421:SER:N	2.23	0.52
1:A:326:ASP:O	1:A:329:VAL:HG22	2.09	0.52
1:C:26:ILE:HG22	1:C:27:GLN:O	2.09	0.52
1:D:385:GLU:HA	1:D:388:VAL:HG12	1.92	0.52
1:A:98:VAL:HG23	1:A:102:ASP:HB2	1.92	0.52
1:B:239:ASN:HB3	1:B:242:THR:OG1	2.09	0.52
1:B:291:HIS:CE1	1:B:293:THR:OG1	2.62	0.52
1:D:376:LEU:C	1:D:376:LEU:HD13	2.30	0.52
1:C:371:CYS:HB2	1:C:392:LEU:HD21	1.92	0.52
1:C:429:ILE:CG2	1:C:501:LYS:HD2	2.40	0.51
1:D:155:ASP:O	1:D:159:VAL:HG23	2.10	0.51
1:A:274:THR:HG21	2:A:601:CYC:HBA1	1.92	0.51
1:B:263:TYR:CD1	1:B:267:MET:HE3	2.45	0.51
1:C:400:VAL:HG21	1:C:404:PHE:HB2	1.92	0.51
1:D:228:TYR:CZ	1:D:265:LYS:HG2	2.46	0.51
1:B:406:THR:HG21	1:B:412:ILE:CD1	2.38	0.51
1:C:88:SER:OG	1:D:402:ASP:OD2	2.22	0.51
1:B:228:TYR:CZ	1:B:265:LYS:HG2	2.46	0.51
1:B:263:TYR:CE1	1:B:267:MET:HE1	2.46	0.51
1:C:34:VAL:HB	1:C:44:GLN:CB	2.40	0.51
1:D:342:MET:HG3	1:D:348:PHE:HB2	1.92	0.51
1:A:325:PHE:CG	1:B:311:VAL:HG21	2.46	0.50
1:B:113:ASN:HD22	1:B:247:ASP:H	1.59	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:HIS:HB2	1:C:192:ARG:HH22	1.75	0.50
1:D:20:ILE:HG23	1:D:258:HIS:NE2	2.26	0.50
1:B:26:ILE:HG22	1:B:27:GLN:O	2.11	0.50
1:B:450:TRP:CD1	1:B:475:PHE:CD2	2.93	0.50
1:B:263:TYR:HE1	1:B:267:MET:HE1	1.76	0.50
1:A:105:ILE:N	1:A:105:ILE:HD12	2.27	0.50
1:A:290:HIS:CE1	2:A:601:CYC:OB	2.65	0.50
1:B:291:HIS:CE1	1:B:293:THR:HG1	2.30	0.50
1:A:341:LYS:HG2	1:A:355:HIS:CE1	2.47	0.49
1:B:38:PRO:HB3	1:B:80:ARG:HA	1.92	0.49
1:C:168:THR:HG1	1:C:170:PHE:HD2	1.58	0.49
2:C:601:CYC:HMA2	2:C:601:CYC:HBA2	1.94	0.49
1:D:341:LYS:HG2	1:D:355:HIS:NE2	2.27	0.49
1:A:150:GLN:HE21	1:A:155:ASP:HB3	1.75	0.49
1:A:153:LEU:HD13	1:A:319:GLN:HB3	1.94	0.49
1:B:95:TRP:HB3	1:B:105:ILE:HG23	1.94	0.49
1:B:139:MET:CE	1:B:166:ARG:HG2	2.42	0.49
1:B:430:PRO:HB3	1:B:436:PHE:CE2	2.48	0.49
1:C:113:ASN:HD21	1:C:247:ASP:H	1.59	0.49
1:C:285:GLY:O	1:C:286:LEU:HD12	2.12	0.49
1:A:429:ILE:HD11	1:A:497:ALA:HB1	1.94	0.49
1:A:505:VAL:O	1:A:509:LEU:HG	2.12	0.49
1:C:134:LEU:HD12	1:C:134:LEU:C	2.33	0.49
1:C:252:ILE:HD13	1:C:302:ARG:NH2	2.27	0.49
1:C:334:HIS:CE1	1:C:358:ARG:HH11	2.29	0.49
1:D:201:LEU:HB2	1:D:450:TRP:CZ2	2.47	0.49
1:A:91:PRO:HD3	1:A:299:PHE:CE2	2.48	0.49
1:A:429:ILE:HG21	1:A:501:LYS:HB2	1.94	0.49
1:D:242:THR:HG1	1:D:244:ARG:HH21	1.59	0.49
1:A:98:VAL:CG2	1:A:102:ASP:HB2	2.43	0.49
1:A:450:TRP:CZ3	1:A:452:GLY:HA3	2.48	0.49
1:B:252:ILE:HD13	1:B:302:ARG:HH21	1.78	0.49
1:B:408:SER:OG	1:B:411:GLN:HG2	2.12	0.49
1:A:431:ILE:CG2	1:A:435:ASN:HB2	2.42	0.49
1:D:85:GLN:O	1:D:89:LEU:HG	2.13	0.49
1:A:241:SER:O	1:C:421:SER:HB3	2.12	0.49
1:B:447:THR:HG22	1:B:478:TRP:HH2	1.78	0.49
1:C:85:GLN:O	1:C:89:LEU:HG	2.12	0.49
2:D:601:CYC:HMA2	2:D:601:CYC:HBA2	1.94	0.49
1:A:334:HIS:CE1	1:A:358:ARG:HH11	2.30	0.48
1:C:153:LEU:HD11	1:C:157:TYR:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:442:PRO:HB2	1:C:446:GLN:NE2	2.28	0.48
1:D:198:TYR:HA	1:D:450:TRP:CZ2	2.39	0.48
1:C:228:TYR:CZ	1:C:265:LYS:HG2	2.48	0.48
1:B:403:VAL:HG21	1:B:498:LEU:HD11	1.95	0.48
1:D:44:GLN:OE1	1:D:239:ASN:HB2	2.13	0.48
1:D:475:PHE:CE2	1:D:479:LYS:HE3	2.48	0.48
1:B:65:LEU:HD23	1:B:74:ILE:HG12	1.94	0.48
1:A:183:HIS:HD2	1:A:204:PRO:HA	1.79	0.48
1:A:313:PHE:HA	1:A:316:ILE:HD12	1.95	0.48
1:A:428:ALA:HB2	1:A:438:LEU:HD12	1.95	0.48
1:B:83:ALA:C	1:B:85:GLN:H	2.17	0.48
1:C:174:MET:CE	2:C:601:CYC:HBB2	2.43	0.48
1:A:31:LEU:HD21	1:A:49:CYS:HA	1.95	0.48
1:A:470:HIS:HD2	1:A:472:ARG:N	2.07	0.48
1:D:31:LEU:HD21	1:D:52:ILE:HG21	1.95	0.48
1:A:263:TYR:HE2	2:A:601:CYC:C2B	2.27	0.47
1:D:148:ARG:HD3	1:D:315:ASN:ND2	2.29	0.47
1:B:263:TYR:CE1	1:B:267:MET:CE	2.98	0.47
1:B:300:GLU:HB2	1:B:301:LEU:HD12	1.95	0.47
1:A:141:ARG:CD	1:B:326:ASP:OD1	2.63	0.47
1:A:454:PRO:HD2	1:A:457:ALA:HB2	1.95	0.47
1:D:338:LEU:HD11	1:D:359:LEU:HA	1.95	0.47
1:B:134:LEU:HD22	1:B:138:HIS:CE1	2.50	0.47
1:B:139:MET:HE1	1:B:166:ARG:HG2	1.95	0.47
1:B:31:LEU:HD21	1:B:49:CYS:HA	1.97	0.47
1:C:95:TRP:CZ3	1:C:128:SER:HB2	2.50	0.47
1:D:192:ARG:HH12	1:D:292:GLN:CD	2.18	0.47
1:B:218:HIS:CB	1:C:192:ARG:HH22	2.28	0.47
1:B:510:ARG:O	1:B:514:GLU:N	2.42	0.47
1:D:217:ILE:HD13	1:D:278:ILE:HD12	1.96	0.47
1:A:510:ARG:HA	1:A:510:ARG:NE	2.30	0.47
1:D:328:ARG:CG	1:D:328:ARG:HH11	2.28	0.47
1:D:334:HIS:ND1	1:D:358:ARG:HD3	2.30	0.47
1:C:178:PHE:CZ	1:C:286:LEU:HD13	2.51	0.46
1:A:178:PHE:HB3	1:A:182:ASN:HA	1.98	0.46
1:A:214:ARG:O	1:A:217:ILE:HG12	2.15	0.46
1:B:476:ASP:O	1:B:480:GLU:HG2	2.15	0.46
1:C:44:GLN:HB3	1:C:234:LEU:CD2	2.46	0.46
1:C:450:TRP:CG	1:C:451:GLY:N	2.83	0.46
1:B:57:PRO:O	1:B:61:LEU:HB2	2.15	0.46
1:C:59:ASP:OD1	1:C:63:ARG:NH1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:140:ALA:O	1:D:144:LEU:HG	2.16	0.46
1:B:171:ASP:H	1:B:291:HIS:HD2	1.62	0.46
1:C:507:LEU:HD13	1:C:510:ARG:HH11	1.79	0.46
1:D:131:LEU:HA	1:D:133:PHE:CE1	2.51	0.46
1:C:242:THR:CG2	1:C:244:ARG:HB3	2.46	0.46
1:D:222:ARG:HH21	1:D:256:ALA:HB2	1.81	0.46
1:D:467:ILE:HG22	1:D:469:LEU:HD12	1.98	0.46
1:B:444:VAL:HG12	1:B:447:THR:HG23	1.98	0.46
1:C:273:LEU:HD22	1:C:297:ILE:CD1	2.46	0.46
1:C:210:GLN:N	1:C:211:PRO:HD2	2.31	0.46
1:A:210:GLN:N	1:A:211:PRO:HD2	2.30	0.46
1:D:328:ARG:HH11	1:D:328:ARG:HG2	1.81	0.46
1:A:256:ALA:HB3	1:A:261:LEU:CD1	2.46	0.46
1:A:279:LYS:HB2	1:A:313:PHE:CZ	2.50	0.46
1:A:467:ILE:HG23	1:A:470:HIS:HB3	1.98	0.46
1:D:21:HIS:CE1	1:D:22:THR:HG23	2.51	0.46
1:C:285:GLY:C	1:C:286:LEU:HD12	2.37	0.45
1:D:96:ALA:O	1:D:104:VAL:HG22	2.16	0.45
1:A:467:ILE:CG2	1:A:470:HIS:HB3	2.46	0.45
1:B:154:ARG:NH2	1:B:187:ILE:O	2.49	0.45
1:B:155:ASP:O	1:B:159:VAL:HG23	2.17	0.45
1:C:201:LEU:HD11	1:C:471:PRO:HB3	1.99	0.45
1:C:279:LYS:HB2	1:C:313:PHE:CZ	2.51	0.45
1:C:313:PHE:HA	1:C:316:ILE:HD12	1.98	0.45
1:C:401:GLN:HG3	1:C:402:ASP:OD1	2.17	0.45
1:B:33:VAL:HG23	1:B:120:CYS:HB3	1.98	0.45
1:B:480:GLU:HB3	1:B:483:ARG:HH21	1.81	0.45
1:C:370:ILE:HG23	1:C:437:LEU:CD2	2.46	0.45
1:A:26:ILE:HG22	1:A:27:GLN:O	2.15	0.45
1:B:341:LYS:CG	1:B:355:HIS:CE1	2.99	0.45
1:B:431:ILE:HD11	1:B:437:LEU:CD1	2.46	0.45
1:D:256:ALA:HB3	1:D:261:LEU:HD11	1.98	0.45
1:B:86:ILE:HD12	1:B:86:ILE:N	2.30	0.45
1:B:469:LEU:O	1:B:469:LEU:CG	2.62	0.45
1:A:77:ILE:HG22	1:A:79:SER:H	1.81	0.45
1:B:450:TRP:HD1	1:B:475:PHE:CG	2.32	0.45
1:C:259:CYS:SG	2:C:601:CYC:C1C	2.98	0.45
1:B:370:ILE:HG23	1:B:437:LEU:CD2	2.47	0.45
1:B:24:HIS:NE2	1:B:245:ALA:HB1	2.32	0.45
1:D:64:THR:HB	1:D:74:ILE:CD1	2.47	0.45
1:D:192:ARG:NH2	1:D:194:ASP:OD1	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ARG:NH2	1:C:292:GLN:HE21	2.14	0.45
1:D:223:VAL:HG12	1:D:252:ILE:HG22	1.98	0.45
1:D:409:LEU:HD12	1:D:416:ALA:HB1	1.96	0.45
1:A:94:LEU:HD12	1:A:122:LEU:HD22	1.99	0.45
1:A:172:ARG:NH1	1:A:189:GLU:OE2	2.48	0.45
1:C:248:LEU:O	1:C:251:SER:HB3	2.17	0.45
1:D:242:THR:HG23	1:D:244:ARG:O	2.16	0.45
1:A:341:LYS:CG	1:A:355:HIS:CE1	3.00	0.44
1:D:26:ILE:HG22	1:D:27:GLN:O	2.17	0.44
1:D:49:CYS:HA	1:D:52:ILE:HG22	1.99	0.44
1:D:467:ILE:HG22	1:D:469:LEU:CD1	2.48	0.44
1:A:201:LEU:HD23	1:A:450:TRP:CZ3	2.53	0.44
1:A:443:GLU:OE1	1:A:445:LEU:CD1	2.65	0.44
1:B:406:THR:HG22	1:C:464:ASP:O	2.16	0.44
1:B:279:LYS:HB2	1:B:313:PHE:CZ	2.53	0.44
1:B:204:PRO:HG2	1:B:477:LEU:HD23	2.00	0.44
1:B:121:GLU:OE2	1:B:251:SER:OG	2.25	0.44
1:A:95:TRP:CD1	1:A:103:PHE:CZ	3.05	0.44
1:A:371:CYS:HB2	1:A:376:LEU:HD23	1.99	0.44
1:A:431:ILE:HB	1:A:435:ASN:HB2	2.00	0.44
1:B:402:ASP:O	1:B:403:VAL:HG23	2.18	0.44
1:D:38:PRO:O	1:D:40:LEU:HD23	2.18	0.44
1:A:35:LEU:HB2	1:A:118:LEU:HD23	1.99	0.44
1:A:115:ASP:N	1:A:115:ASP:OD1	2.51	0.44
1:B:243:ASN:N	1:B:243:ASN:HD22	2.16	0.44
1:B:477:LEU:O	1:B:481:ILE:HG12	2.16	0.44
1:A:74:ILE:HD12	1:A:74:ILE:N	2.33	0.44
1:B:147:LEU:HG	1:B:156:PHE:CE2	2.53	0.43
1:C:115:ASP:HB2	1:C:117:LEU:HD23	1.99	0.43
1:C:256:ALA:HB3	1:C:261:LEU:CD1	2.48	0.43
1:C:341:LYS:CG	1:C:355:HIS:CE1	2.98	0.43
1:A:467:ILE:HG22	1:A:473:GLN:CB	2.37	0.43
1:C:442:PRO:HB2	1:C:446:GLN:HE22	1.83	0.43
1:A:343:THR:HG22	1:A:507:LEU:HD21	2.00	0.43
1:C:113:ASN:OD1	1:C:247:ASP:HB3	2.18	0.43
1:C:403:VAL:HG23	1:C:429:ILE:CG1	2.45	0.43
1:A:33:VAL:HG23	1:A:120:CYS:HB3	2.01	0.43
1:B:256:ALA:HB3	1:B:261:LEU:HD11	2.00	0.43
1:D:222:ARG:NH2	1:D:254:ARG:O	2.49	0.43
1:B:95:TRP:HB3	1:B:105:ILE:HA	2.01	0.43
1:D:313:PHE:HA	1:D:316:ILE:HD12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:MET:O	1:D:348:PHE:HA	2.18	0.43
1:A:273:LEU:HD22	1:A:297:ILE:CD1	2.48	0.43
1:D:26:ILE:HD11	1:D:234:LEU:CD2	2.45	0.43
1:D:334:HIS:HA	1:D:358:ARG:HD2	2.01	0.43
1:A:64:THR:HB	1:A:73:GLN:HE21	1.83	0.43
1:A:416:ALA:HA	1:A:419:PHE:CZ	2.54	0.43
1:B:44:GLN:OE1	1:B:239:ASN:HB2	2.19	0.43
1:B:407:SER:H	1:C:463:GLU:CD	2.23	0.43
1:A:222:ARG:HD2	1:A:222:ARG:HA	1.90	0.42
1:B:172:ARG:NH1	1:B:189:GLU:OE2	2.50	0.42
1:B:412:ILE:HD13	1:C:465:GLY:HA3	2.01	0.42
1:C:290:HIS:CE1	2:C:601:CYC:OB	2.72	0.42
1:B:325:PHE:O	1:B:329:VAL:HG23	2.19	0.42
1:C:178:PHE:CE2	1:C:286:LEU:HD13	2.54	0.42
1:C:325:PHE:O	1:C:329:VAL:HG23	2.19	0.42
1:A:507:LEU:HD23	1:A:507:LEU:HA	1.92	0.42
1:B:313:PHE:HA	1:B:316:ILE:HD12	2.00	0.42
1:B:341:LYS:HG2	1:B:355:HIS:NE2	2.35	0.42
1:D:259:CYS:SG	1:D:469:LEU:HD21	2.60	0.42
1:A:153:LEU:O	1:A:156:PHE:HB3	2.20	0.42
1:C:394:TRP:CZ2	1:C:398:ARG:HD2	2.54	0.42
1:D:153:LEU:O	1:D:156:PHE:HB3	2.20	0.42
1:D:290:HIS:CE1	2:D:601:CYC:OB	2.72	0.42
1:C:256:ALA:HB3	1:C:261:LEU:HD11	2.02	0.42
1:D:373:GLY:H	1:D:435:ASN:CG	2.23	0.42
1:A:342:MET:O	1:A:348:PHE:HA	2.20	0.42
1:A:431:ILE:N	1:A:431:ILE:HD12	2.35	0.42
1:C:416:ALA:HA	1:C:419:PHE:CZ	2.55	0.42
1:D:35:LEU:HB2	1:D:118:LEU:HD23	2.02	0.42
1:D:90:ASN:HA	1:D:91:PRO:HA	1.82	0.42
1:D:348:PHE:C	1:D:348:PHE:CD1	2.93	0.42
1:A:66:GLY:HA3	1:A:73:GLN:HB2	2.02	0.42
1:A:191:LYS:HE2	1:A:197:PRO:HB3	2.02	0.42
1:A:402:ASP:O	1:A:403:VAL:HG23	2.20	0.42
1:B:72:PHE:O	1:B:73:GLN:C	2.58	0.42
1:C:342:MET:HG3	1:C:348:PHE:HB2	2.01	0.42
1:D:416:ALA:HA	1:D:419:PHE:CZ	2.55	0.42
1:B:152:ASN:OD1	1:B:153:LEU:N	2.53	0.41
1:C:127:THR:HG21	1:C:131:LEU:HD21	2.02	0.41
1:C:342:MET:O	1:C:348:PHE:HA	2.20	0.41
1:B:416:ALA:HA	1:B:419:PHE:CZ	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:SER:CA	1:C:234:LEU:HD12	2.48	0.41
1:D:20:ILE:O	1:D:23:ALA:N	2.28	0.41
1:A:174:MET:CE	2:A:601:CYC:HBB2	2.51	0.41
1:B:201:LEU:CD1	1:B:475:PHE:HB2	2.50	0.41
1:C:373:GLY:H	1:C:435:ASN:CG	2.24	0.41
1:D:274:THR:HG21	2:D:601:CYC:CBA	2.41	0.41
1:D:394:TRP:CZ2	1:D:398:ARG:NE	2.84	0.41
1:B:147:LEU:HD11	1:B:160:ILE:HG13	2.02	0.41
1:B:371:CYS:HB2	1:B:376:LEU:HD23	2.02	0.41
1:C:168:THR:HG23	1:C:170:PHE:H	1.86	0.41
1:D:320:GLU:O	1:D:324:THR:HG23	2.20	0.41
1:D:510:ARG:O	1:D:514:GLU:N	2.49	0.41
1:B:177:ARG:HG2	1:B:178:PHE:N	2.36	0.41
1:B:349:VAL:HG11	1:B:375:LYS:HE3	2.02	0.41
1:C:144:LEU:O	1:C:148:ARG:HG3	2.20	0.41
1:C:311:VAL:HG13	1:D:322:THR:HG22	2.03	0.41
1:C:341:LYS:HG2	1:C:355:HIS:NE2	2.35	0.41
1:A:111:HIS:ND1	1:A:250:GLU:HB2	2.36	0.41
1:B:44:GLN:HB3	1:B:236:PRO:HD2	2.01	0.41
1:B:348:PHE:CD1	1:B:348:PHE:C	2.94	0.41
1:D:31:LEU:HD21	1:D:52:ILE:CG2	2.50	0.41
1:A:147:LEU:HD23	1:A:147:LEU:HA	1.93	0.41
1:A:369:ALA:HB3	1:A:438:LEU:HD23	2.02	0.41
1:B:427:LEU:C	1:B:427:LEU:HD23	2.40	0.41
1:B:453:ASP:O	1:B:472:ARG:HG2	2.21	0.41
1:C:263:TYR:CE2	2:C:601:CYC:CMB	3.03	0.41
1:D:174:MET:CE	2:D:601:CYC:HBB2	2.50	0.41
1:D:432:ALA:HB3	1:D:435:ASN:CB	2.44	0.41
1:C:239:ASN:O	1:C:243:ASN:N	2.52	0.41
1:C:431:ILE:HD11	1:C:437:LEU:HG	2.03	0.41
1:C:445:LEU:HA	1:C:448:VAL:CG1	2.51	0.41
1:D:20:ILE:H	1:D:20:ILE:HG12	1.64	0.41
1:D:201:LEU:CD1	1:D:475:PHE:HB2	2.50	0.41
1:D:326:ASP:HA	1:D:329:VAL:HG12	2.02	0.41
1:A:338:LEU:O	1:A:342:MET:HB2	2.21	0.41
1:B:181:ASN:HB2	1:B:183:HIS:ND1	2.36	0.41
1:C:487:LEU:HD12	1:C:487:LEU:H	1.86	0.41
1:A:403:VAL:HG22	1:A:429:ILE:HG12	2.02	0.40
1:B:342:MET:O	1:B:348:PHE:HA	2.21	0.40
1:C:235:THR:N	1:C:236:PRO:CD	2.83	0.40
1:A:176:HIS:CE1	1:A:186:VAL:HG22	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD13	1:B:239:ASN:ND2	2.36	0.40
1:C:113:ASN:OD1	1:C:114:SER:N	2.55	0.40
1:D:176:HIS:CE1	1:D:186:VAL:HG22	2.56	0.40
1:D:371:CYS:HB2	1:D:392:LEU:HD21	2.03	0.40
1:B:132:PRO:HG2	1:B:133:PHE:CE2	2.56	0.40
1:B:153:LEU:O	1:B:156:PHE:HB3	2.21	0.40
2:B:601:CYC:HMA1	2:B:601:CYC:NB	2.37	0.40
1:C:503:ALA:O	1:C:507:LEU:HD23	2.20	0.40
1:A:202:HIS:CE1	1:A:448:VAL:HG11	2.55	0.40
1:B:171:ASP:OD2	1:B:291:HIS:CD2	2.74	0.40
1:B:257:TYR:HD2	2:B:601:CYC:HMD1	1.86	0.40
1:C:273:LEU:HD13	1:C:297:ILE:HD12	2.04	0.40
1:D:72:PHE:HD1	1:D:94:LEU:HD22	1.87	0.40
1:D:478:TRP:HA	1:D:481:ILE:HD12	2.04	0.40
1:A:146:ARG:CZ	1:A:159:VAL:HG13	2.52	0.40
1:A:181:ASN:HB2	1:A:183:HIS:ND1	2.36	0.40
1:C:147:LEU:HD11	1:C:160:ILE:HG13	2.04	0.40
1:C:482:VAL:O	1:C:482:VAL:CG1	2.69	0.40
1:D:31:LEU:HD21	1:D:49:CYS:HA	2.04	0.40
1:D:242:THR:OG1	1:D:244:ARG:HB3	2.21	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:THR:O	1:D:244:ARG:NH1[3_554]	1.63	0.57
1:A:226:ASP:OD2	1:D:20:ILE:CD1[3_554]	2.03	0.17
1:A:194:ASP:OD1	1:D:218:HIS:NE2[3_554]	2.16	0.04
1:A:456:HIS:NE2	1:C:250:GLU:OE1[3_554]	2.18	0.02

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	493/520 (95%)	466 (94%)	27 (6%)	0	100	100
1	B	480/520 (92%)	458 (95%)	22 (5%)	0	100	100
1	C	482/520 (93%)	467 (97%)	15 (3%)	0	100	100
1	D	480/520 (92%)	462 (96%)	18 (4%)	0	100	100
All	All	1935/2080 (93%)	1853 (96%)	82 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	429/453 (95%)	426 (99%)	3 (1%)	81	88
1	B	421/453 (93%)	417 (99%)	4 (1%)	73	82
1	C	421/453 (93%)	416 (99%)	5 (1%)	67	79
1	D	422/453 (93%)	419 (99%)	3 (1%)	81	88
All	All	1693/1812 (93%)	1678 (99%)	15 (1%)	75	84

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	293	THR
1	A	320	GLU
1	A	393	GLN
1	B	133	PHE
1	B	134	LEU
1	B	243	ASN
1	B	247	ASP
1	C	117	LEU
1	C	293	THR
1	C	420	LYS
1	C	437	LEU
1	C	468	GLU
1	D	20	ILE

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Mol	Chain	Res	Type
1	D	219	ASN
1	D	244	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	27	GLN
1	A	29	HIS
1	A	130	ASN
1	A	149	GLN
1	A	150	GLN
1	A	290	HIS
1	A	389	GLN
1	A	470	HIS
1	A	506	ASN
1	B	78	GLN
1	B	85	GLN
1	B	150	GLN
1	B	176	HIS
1	B	181	ASN
1	B	183	HIS
1	B	243	ASN
1	B	290	HIS
1	B	354	ASN
1	C	36	GLN
1	C	138	HIS
1	C	176	HIS
1	C	290	HIS
1	C	292	GLN
1	C	354	ASN
1	C	470	HIS
1	C	506	ASN
1	D	152	ASN
1	D	176	HIS
1	D	219	ASN
1	D	266	ASN
1	D	290	HIS
1	D	411	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	CYC	B	601	1	42,46,46	2.06	11 (26%)	50,67,67	1.40	10 (20%)
2	CYC	C	601	1	42,46,46	2.24	10 (23%)	50,67,67	1.51	7 (14%)
2	CYC	D	601	1	42,46,46	2.23	13 (30%)	50,67,67	1.51	9 (18%)
2	CYC	A	601	1	42,46,46	2.24	12 (28%)	50,67,67	1.54	13 (26%)

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	CYC	B	601	1	-	9/25/74/74	0/4/4/4
2	CYC	C	601	1	-	9/25/74/74	0/4/4/4
2	CYC	D	601	1	-	9/25/74/74	0/4/4/4
2	CYC	A	601	1	-	9/25/74/74	0/4/4/4

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	CYC	CHA-C1A	8.18	1.42	1.35
2	A	601	CYC	CHA-C1A	7.28	1.41	1.35
2	D	601	CYC	CHA-C1A	7.16	1.41	1.35
2	B	601	CYC	CHA-C1A	6.53	1.40	1.35
2	D	601	CYC	C4B-C3B	-5.46	1.37	1.48
2	A	601	CYC	C4B-C3B	-5.15	1.38	1.48
2	C	601	CYC	C4B-C3B	-5.09	1.38	1.48
2	A	601	CYC	C1A-C2A	-5.06	1.37	1.45
2	D	601	CYC	C1A-C2A	-4.73	1.38	1.45
2	B	601	CYC	C4B-C3B	-4.61	1.39	1.48
2	A	601	CYC	C4A-C3A	-4.52	1.36	1.45
2	B	601	CYC	C1A-C2A	-4.47	1.38	1.45
2	A	601	CYC	C2C-C1C	4.38	1.56	1.52
2	C	601	CYC	C1A-C2A	-4.32	1.38	1.45
2	D	601	CYC	C4A-C3A	-4.11	1.37	1.45
2	C	601	CYC	C1B-C2B	-4.06	1.37	1.45
2	C	601	CYC	C4A-C3A	-4.04	1.37	1.45
2	B	601	CYC	C4A-C3A	-4.03	1.37	1.45
2	D	601	CYC	C1B-C2B	-3.77	1.38	1.45
2	A	601	CYC	C1B-C2B	-3.47	1.38	1.45
2	B	601	CYC	CAD-C3D	3.46	1.57	1.52
2	D	601	CYC	CBD-CGD	3.26	1.58	1.50
2	C	601	CYC	C2C-C1C	3.16	1.54	1.52
2	D	601	CYC	C2C-C1C	3.07	1.54	1.52
2	B	601	CYC	C2C-C1C	3.03	1.54	1.52
2	B	601	CYC	C1B-C2B	-2.95	1.39	1.45
2	A	601	CYC	CBD-CGD	2.74	1.56	1.50
2	D	601	CYC	C3C-C4C	2.65	1.54	1.50
2	C	601	CYC	CBD-CGD	2.54	1.56	1.50
2	D	601	CYC	CMB-C2B	2.52	1.56	1.50
2	C	601	CYC	CMD-C2D	2.49	1.56	1.51
2	A	601	CYC	CMB-C2B	2.47	1.56	1.50
2	D	601	CYC	CAD-C3D	2.41	1.55	1.52
2	A	601	CYC	CMD-C2D	2.40	1.56	1.51
2	D	601	CYC	CBA-CAA	2.36	1.59	1.52
2	A	601	CYC	O1A-CGA	2.35	1.30	1.22
2	B	601	CYC	CBD-CGD	2.27	1.55	1.50
2	C	601	CYC	C3C-C4C	2.20	1.54	1.50
2	B	601	CYC	CMA-C3A	2.13	1.55	1.50
2	B	601	CYC	CMB-C2B	2.13	1.55	1.50
2	D	601	CYC	CAB-C3B	2.10	1.56	1.51
2	D	601	CYC	CMA-C3A	2.07	1.55	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	CYC	C3C-C4C	2.02	1.53	1.50
2	A	601	CYC	CMA-C3A	2.01	1.55	1.50
2	B	601	CYC	CBA-CAA	2.01	1.58	1.52
2	C	601	CYC	CAB-C3B	2.00	1.56	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	CYC	CBC-CAC-C3C	5.44	125.58	113.47
2	D	601	CYC	CBC-CAC-C3C	4.59	123.68	113.47
2	D	601	CYC	O1A-CGA-CBA	-3.68	111.27	123.08
2	B	601	CYC	O1A-CGA-CBA	-3.22	112.73	123.08
2	A	601	CYC	C4A-C3A-C2A	3.21	110.20	106.51
2	A	601	CYC	O1A-CGA-CBA	-3.12	113.06	123.08
2	A	601	CYC	CBC-CAC-C3C	3.11	120.39	113.47
2	B	601	CYC	CBC-CAC-C3C	3.07	120.31	113.47
2	C	601	CYC	O1A-CGA-CBA	-2.96	113.57	123.08
2	C	601	CYC	C4A-C3A-C2A	2.90	109.84	106.51
2	C	601	CYC	CHB-C4A-C3A	2.87	132.29	124.90
2	A	601	CYC	C2A-C1A-NA	-2.87	105.87	110.05
2	A	601	CYC	O2A-CGA-O1A	2.73	130.11	123.30
2	B	601	CYC	C4A-C3A-C2A	2.71	109.62	106.51
2	A	601	CYC	CHB-C4A-C3A	2.67	131.77	124.90
2	B	601	CYC	C4D-CHA-C1A	2.63	131.96	128.81
2	D	601	CYC	C4A-C3A-C2A	2.59	109.48	106.51
2	B	601	CYC	O2A-CGA-O1A	2.52	129.57	123.30
2	A	601	CYC	OB-C4B-C3B	2.50	130.76	128.04
2	A	601	CYC	O1D-CGD-CBD	-2.50	115.06	123.08
2	B	601	CYC	CHB-C4A-C3A	2.46	131.24	124.90
2	D	601	CYC	CAB-C3B-C4B	2.45	125.25	121.38
2	D	601	CYC	CHB-C4A-C3A	2.45	131.19	124.90
2	B	601	CYC	CAB-C3B-C4B	2.42	125.20	121.38
2	A	601	CYC	C1A-NA-C4A	2.38	111.00	106.51
2	C	601	CYC	C2A-C1A-NA	-2.38	106.58	110.05
2	A	601	CYC	C3A-C4A-NA	-2.37	105.46	110.53
2	B	601	CYC	CHD-C4C-NC	2.36	128.01	125.20
2	D	601	CYC	CAD-CBD-CGD	-2.33	107.22	113.76
2	A	601	CYC	OC-C1C-C2C	2.29	127.99	126.17
2	A	601	CYC	CAC-C3C-C2C	-2.22	108.72	114.26
2	D	601	CYC	O2A-CGA-O1A	2.17	128.71	123.30
2	A	601	CYC	CAB-C3B-C4B	2.17	124.80	121.38
2	B	601	CYC	C3A-C4A-NA	-2.07	106.10	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	601	CYC	C3A-C4A-NA	-2.07	106.11	110.53
2	C	601	CYC	C1A-NA-C4A	2.04	110.36	106.51
2	B	601	CYC	C1A-NA-C4A	2.02	110.32	106.51
2	D	601	CYC	C2A-C1A-NA	-2.02	107.11	110.05
2	D	601	CYC	C1A-NA-C4A	2.00	110.29	106.51

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	CYC	NA-C4A-CHB-C1B
2	A	601	CYC	C3A-C4A-CHB-C1B
2	A	601	CYC	ND-C1D-CHD-C4C
2	B	601	CYC	C1A-C2A-CAA-CBA
2	B	601	CYC	NA-C4A-CHB-C1B
2	B	601	CYC	C3A-C4A-CHB-C1B
2	B	601	CYC	ND-C1D-CHD-C4C
2	C	601	CYC	NA-C4A-CHB-C1B
2	C	601	CYC	C3A-C4A-CHB-C1B
2	C	601	CYC	ND-C1D-CHD-C4C
2	D	601	CYC	NA-C4A-CHB-C1B
2	D	601	CYC	C3A-C4A-CHB-C1B
2	D	601	CYC	ND-C1D-CHD-C4C
2	D	601	CYC	C1A-C2A-CAA-CBA
2	B	601	CYC	C3A-C2A-CAA-CBA
2	A	601	CYC	C1A-C2A-CAA-CBA
2	C	601	CYC	C1A-C2A-CAA-CBA
2	D	601	CYC	C3A-C2A-CAA-CBA
2	A	601	CYC	C3A-C2A-CAA-CBA
2	C	601	CYC	C3A-C2A-CAA-CBA
2	A	601	CYC	CAD-CBD-CGD-O2D
2	B	601	CYC	CAD-CBD-CGD-O2D
2	C	601	CYC	CAD-CBD-CGD-O2D
2	D	601	CYC	CAD-CBD-CGD-O2D
2	A	601	CYC	CAA-CBA-CGA-O1A
2	B	601	CYC	CAA-CBA-CGA-O1A
2	C	601	CYC	CAA-CBA-CGA-O1A
2	D	601	CYC	CAA-CBA-CGA-O1A
2	A	601	CYC	CAD-CBD-CGD-O1D
2	D	601	CYC	CAD-CBD-CGD-O1D
2	C	601	CYC	CAD-CBD-CGD-O1D
2	B	601	CYC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
2	B	601	CYC	CAA-CBA-CGA-O2A
2	D	601	CYC	CAA-CBA-CGA-O2A
2	A	601	CYC	CAA-CBA-CGA-O2A
2	C	601	CYC	CAA-CBA-CGA-O2A

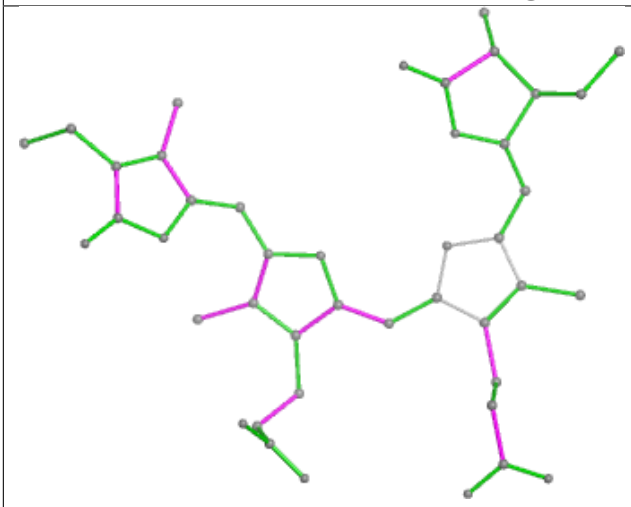
There are no ring outliers.

4 monomers are involved in 28 short contacts:

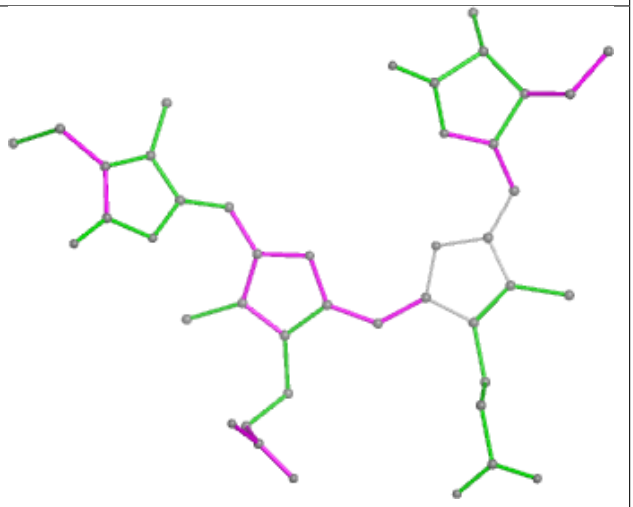
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	CYC	6	0
2	C	601	CYC	8	0
2	D	601	CYC	6	0
2	A	601	CYC	8	0

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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

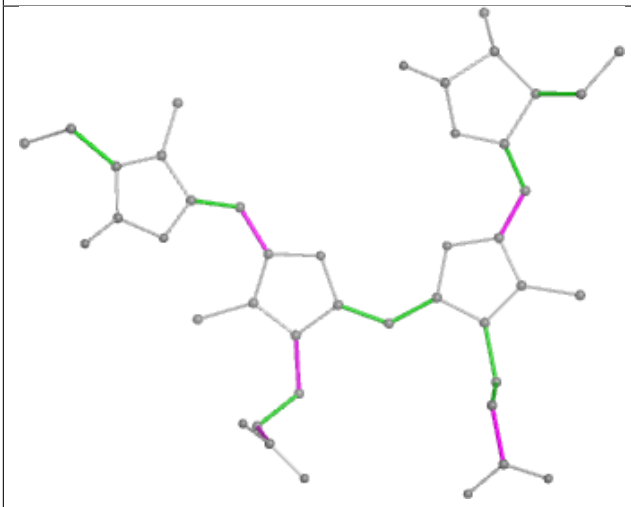
Ligand CYC B 601



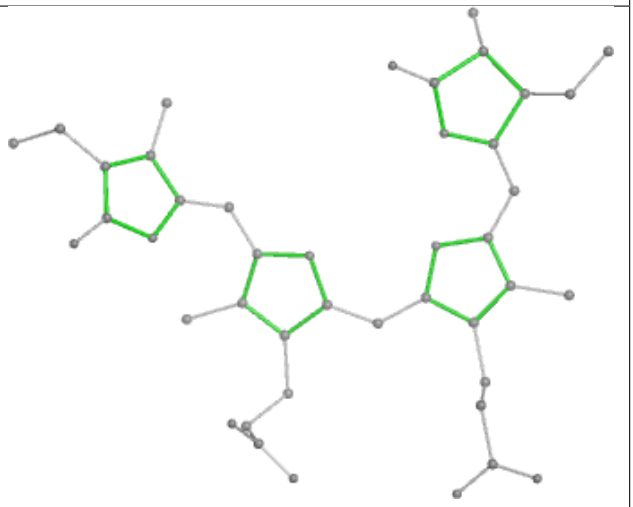
Bond lengths



Bond angles

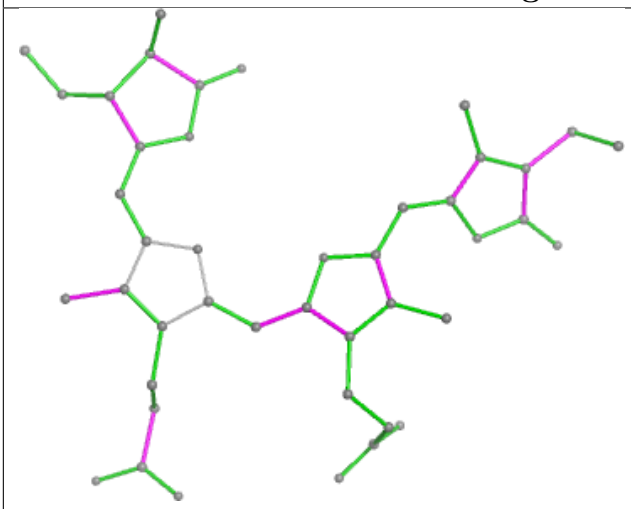


Torsions

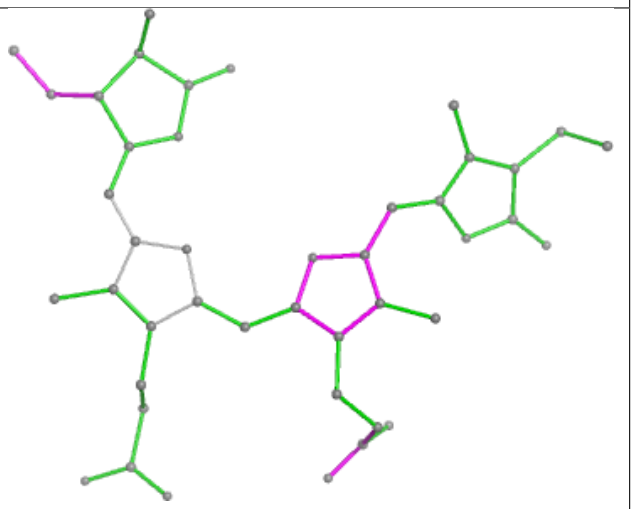


Rings

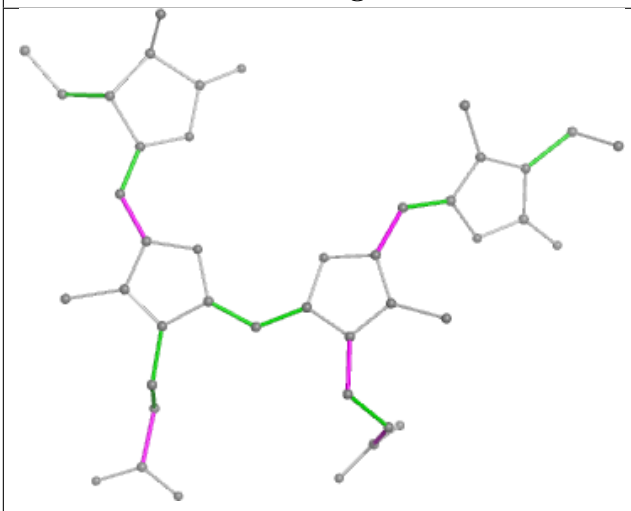
Ligand CYC C 601



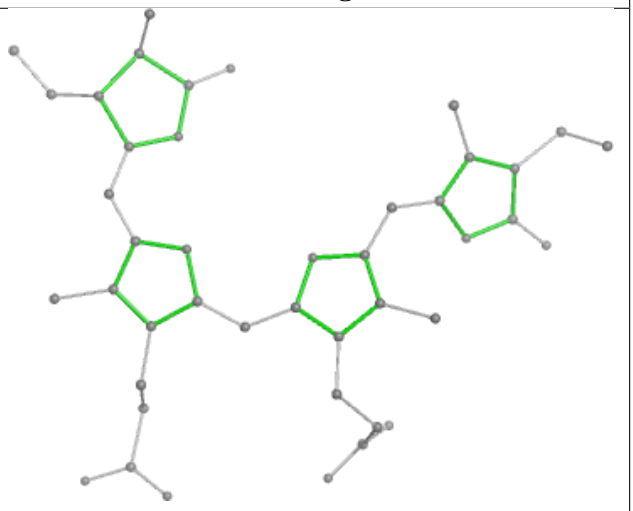
Bond lengths



Bond angles

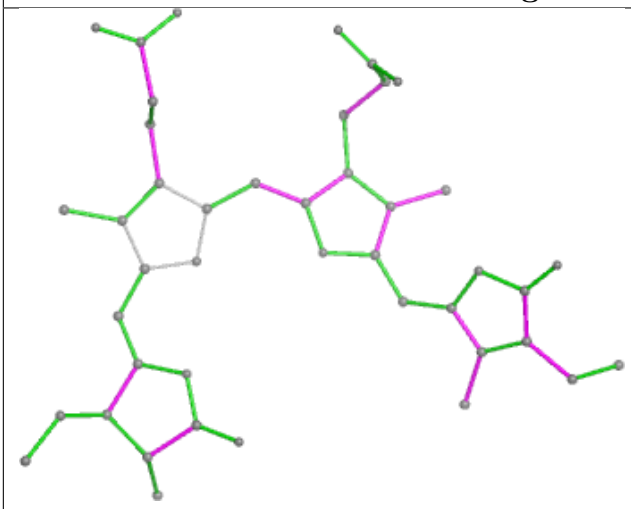


Torsions

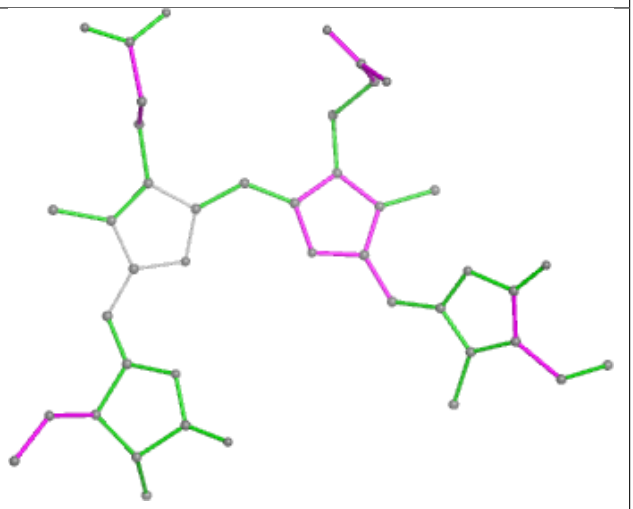


Rings

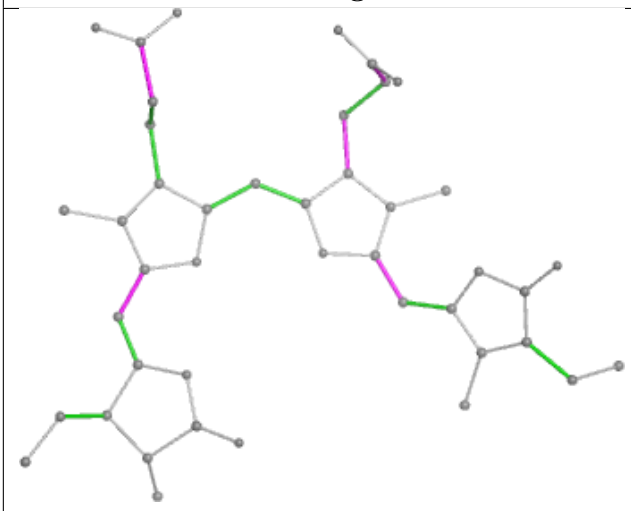
Ligand CYC D 601



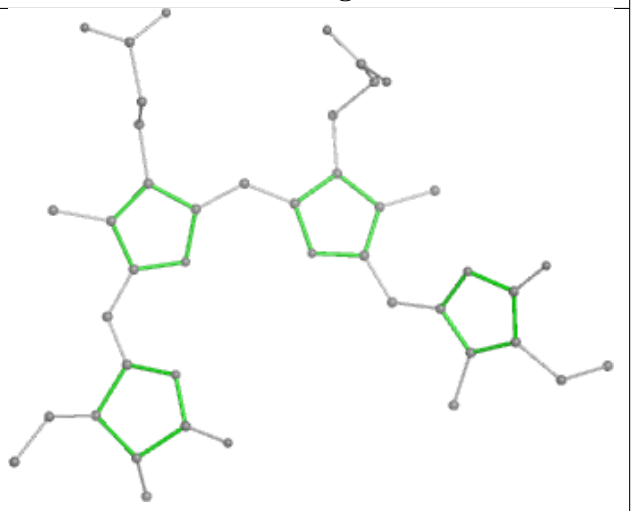
Bond lengths



Bond angles

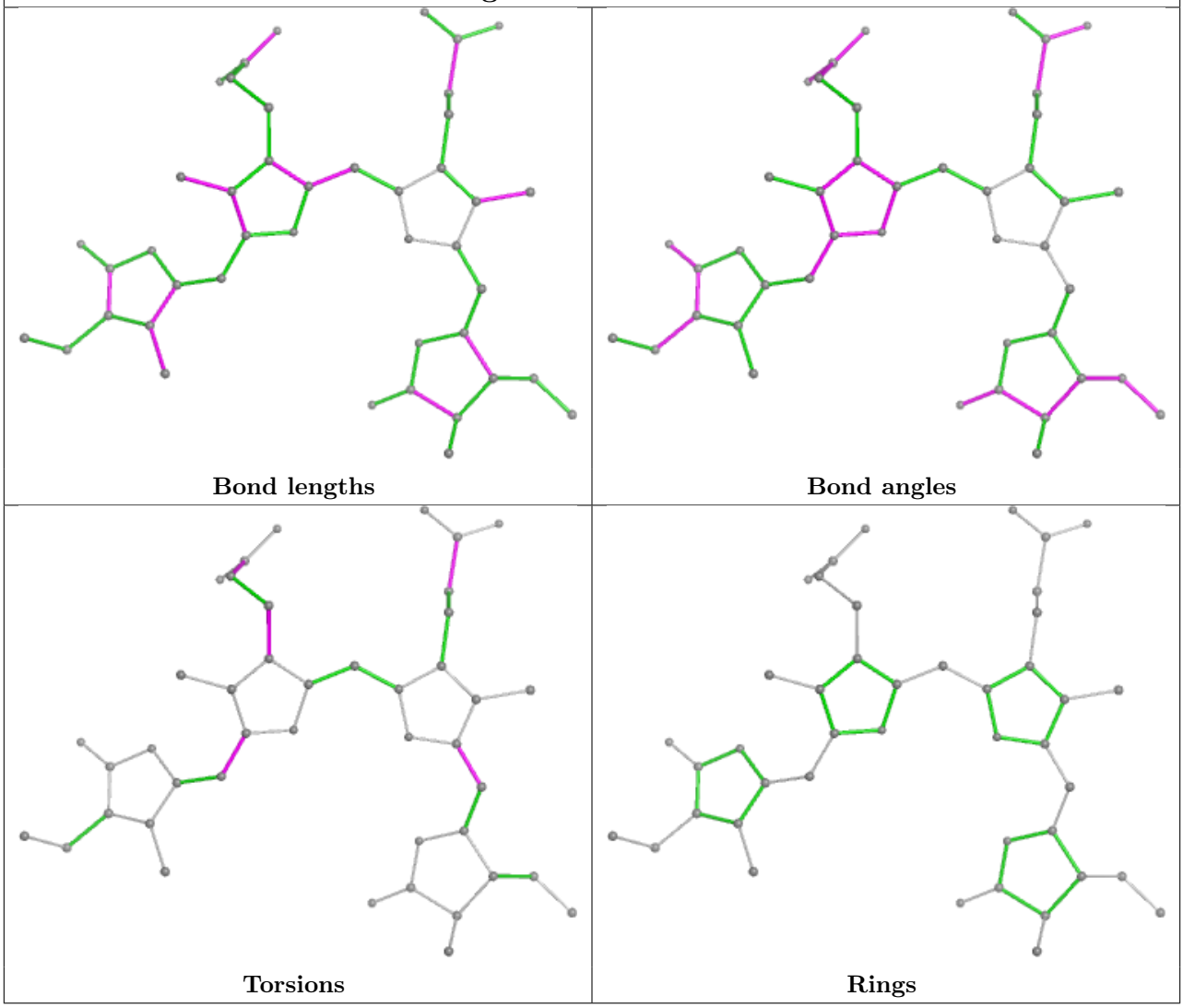


Torsions



Rings

Ligand CYC A 601



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, 95^{th} 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	495/520 (95%)	0.24	5 (1%)	79	61	83, 103, 184, 262	0
1	B	484/520 (93%)	0.20	6 (1%)	76	57	91, 100, 164, 237	0
1	C	486/520 (93%)	0.16	6 (1%)	76	57	93, 108, 170, 256	0
1	D	484/520 (93%)	0.18	9 (1%)	66	47	77, 108, 180, 290	0
All	All	1949/2080 (93%)	0.20	26 (1%)	74	55	77, 105, 179, 290	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	104	VAL	3.5
1	D	115	ASP	3.4
1	D	23	ALA	3.3
1	B	18	LEU	3.2
1	D	449	ASN	3.1
1	C	460	ALA	3.0
1	C	23	ALA	3.0
1	D	451	GLY	2.9
1	B	133	PHE	2.9
1	A	102	ASP	2.8
1	D	21	HIS	2.8
1	C	72	PHE	2.6
1	C	457	ALA	2.4
1	A	74	ILE	2.3
1	D	24	HIS	2.3
1	D	327	TYR	2.3
1	B	444	VAL	2.3
1	C	458	TYR	2.2
1	B	22	THR	2.2
1	B	23	ALA	2.1
1	D	72	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	73	GLN	2.1
1	B	471	PRO	2.1
1	D	133	PHE	2.0
1	A	461	THR	2.0
1	C	35	LEU	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)

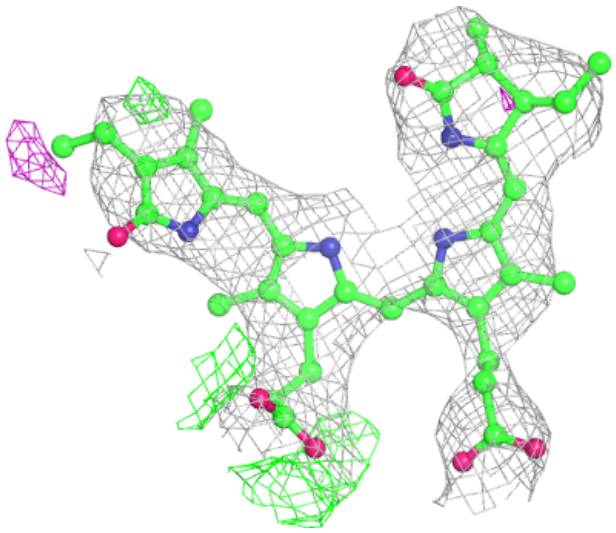
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

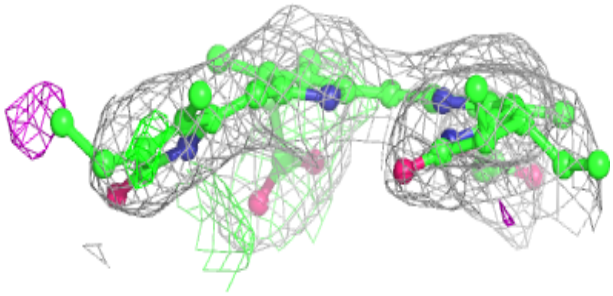
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	CYC	B	601	43/43	0.89	0.17	92,93,94,95	0
2	CYC	C	601	43/43	0.90	0.19	94,97,101,104	0
2	CYC	D	601	43/43	0.92	0.16	77,78,80,81	0
2	CYC	A	601	43/43	0.94	0.14	83,86,91,92	0

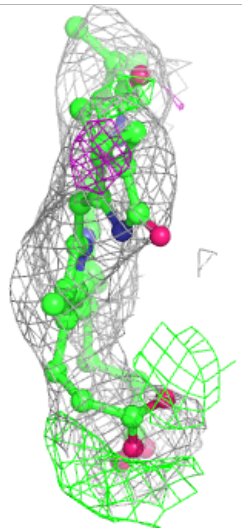
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around CYC B 601:

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

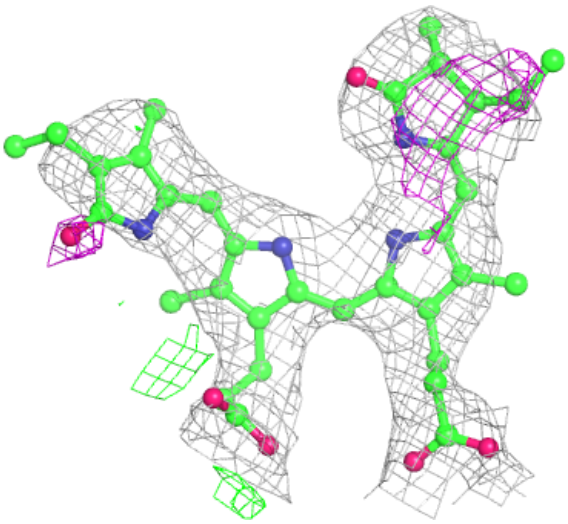


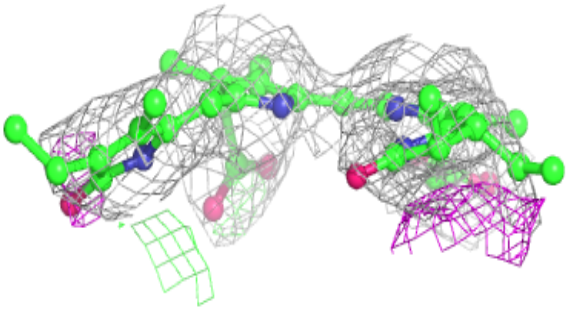


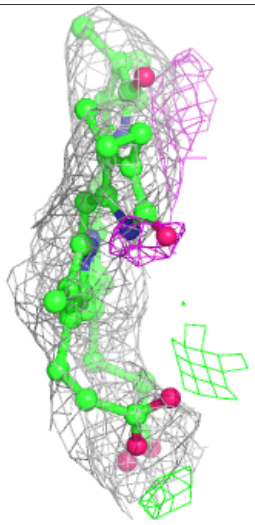


Electron density around CYC C 601:

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

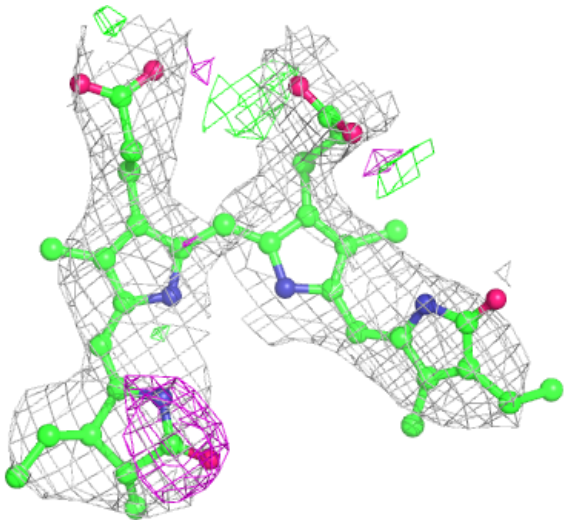


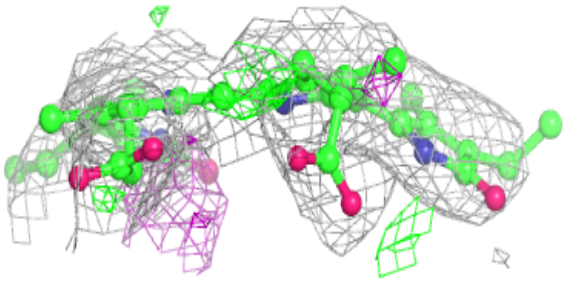


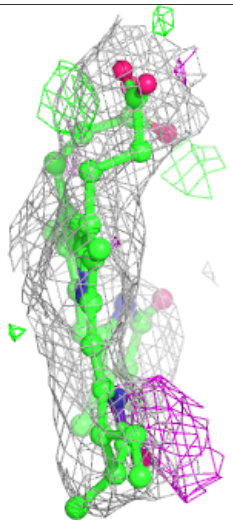


Electron density around CYC D 601:

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

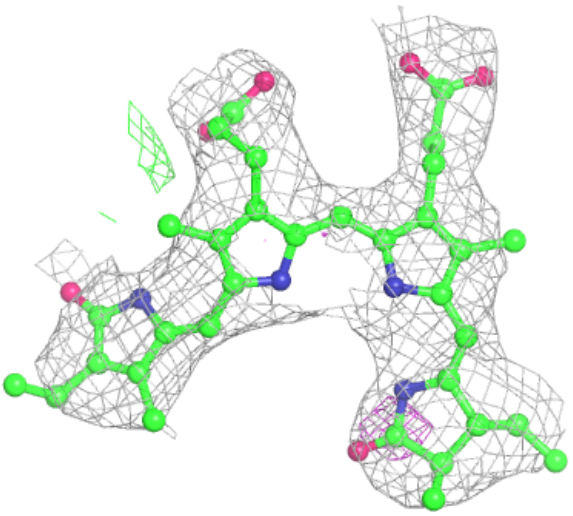


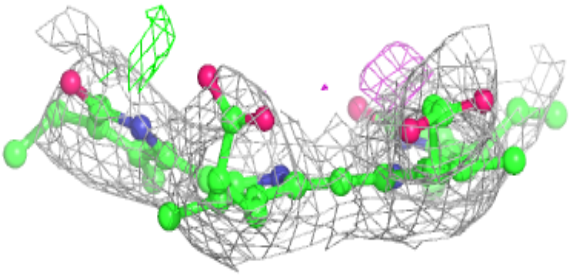


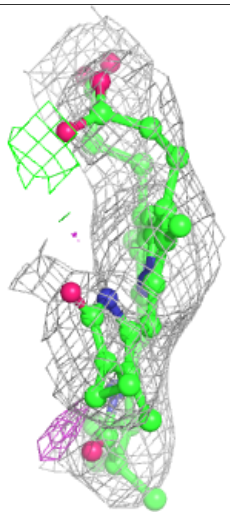


Electron density around CYC A 601:

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







6.5 Other polymers

There are no such residues in this entry.