



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 6, 2020 – 11:50 pm BST

PDB ID : 3KCF
Title : Crystal structure of TGFbRI complexed with a pyrazolone inhibitor
Authors : Boriack-Sjodin, P.A.
Deposited on : 2009-10-21
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 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 : 2.11
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) : 2.11

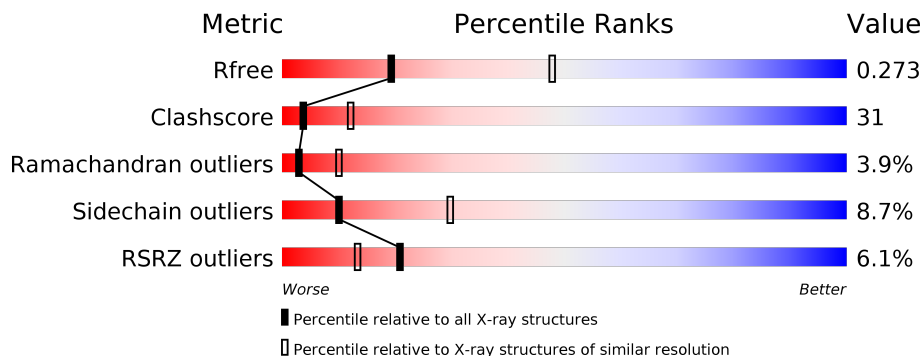
1 Overall quality at a glance

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 on 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	342	
1	B	342	
1	C	342	
1	D	342	
1	E	342	

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
3	PO4	B	11	-	-	X	-
3	PO4	D	15	-	-	X	-
3	PO4	E	2	-	-	X	-
3	PO4	E	3	-	-	X	-

2 Entry composition i

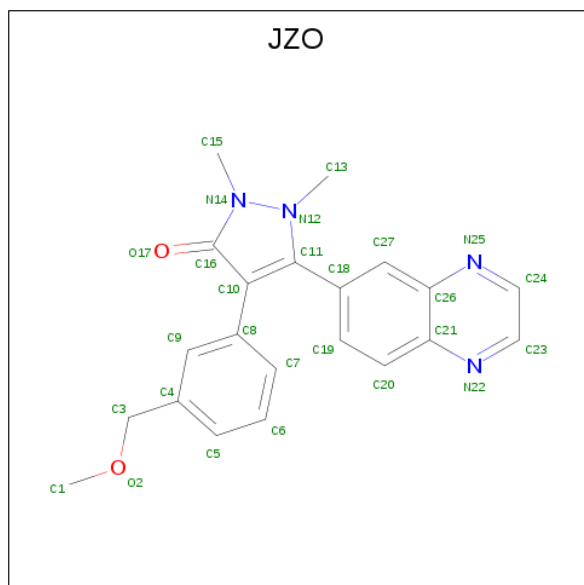
There are 4 unique types of molecules in this entry. The entry contains 13297 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 TGF-beta receptor type-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	328	Total 2617	C 1650	N 469	O 482	S 16	0	0	0
1	B	324	Total 2590	C 1636	N 463	O 475	S 16	0	0	0
1	C	330	Total 2629	C 1658	N 471	O 484	S 16	0	0	0
1	D	330	Total 2629	C 1658	N 471	O 484	S 16	0	0	0
1	E	330	Total 2629	C 1658	N 471	O 484	S 16	0	0	0

- Molecule 2 is 4-[3-(methoxymethyl)phenyl]-1,2-dimethyl-5-quinoxalin-6-yl-1,2-dihydro-3H-pyrazol-3-one (three-letter code: JZO) (formula: C₂₁H₂₀N₄O₂).



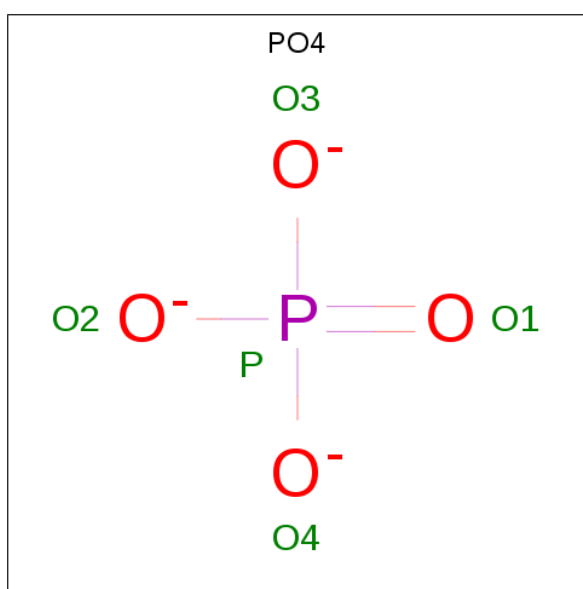
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total 27	C 21	N 4	O 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			27	21	4	2		
2	C	1	Total	C	N	O	0	0
			27	21	4	2		
2	D	1	Total	C	N	O	0	0
			27	21	4	2		
2	E	1	Total	C	N	O	0	0
			27	21	4	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	D	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		
3	E	1	Total	O	P	0	0
			5	4	1		

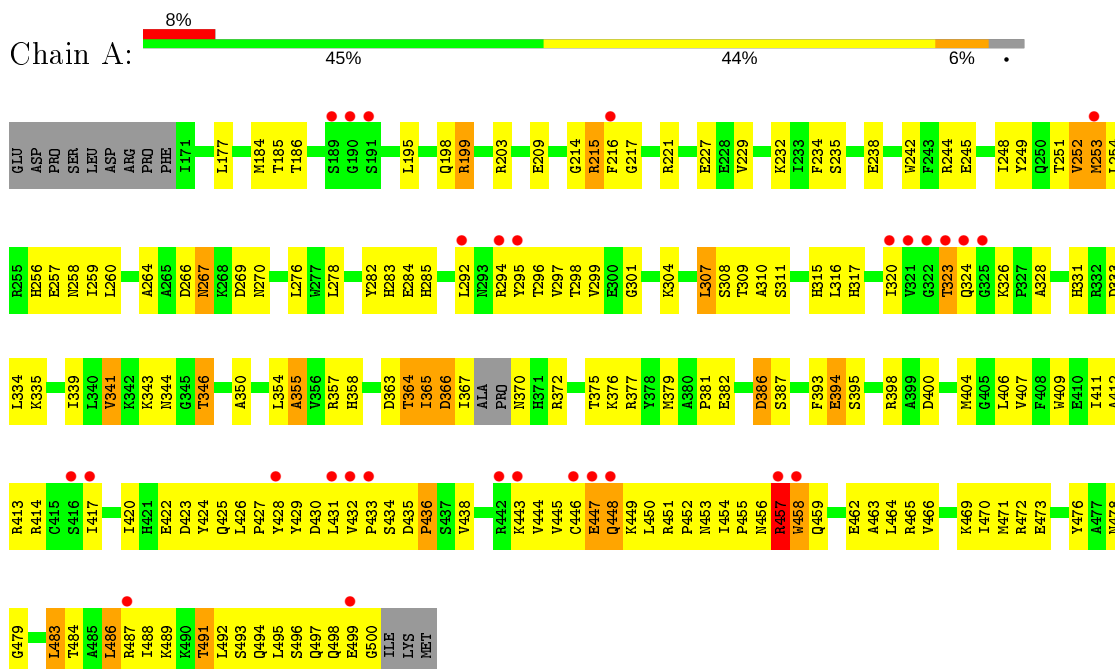
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	E	1	Total	O	0	0
			1	1		

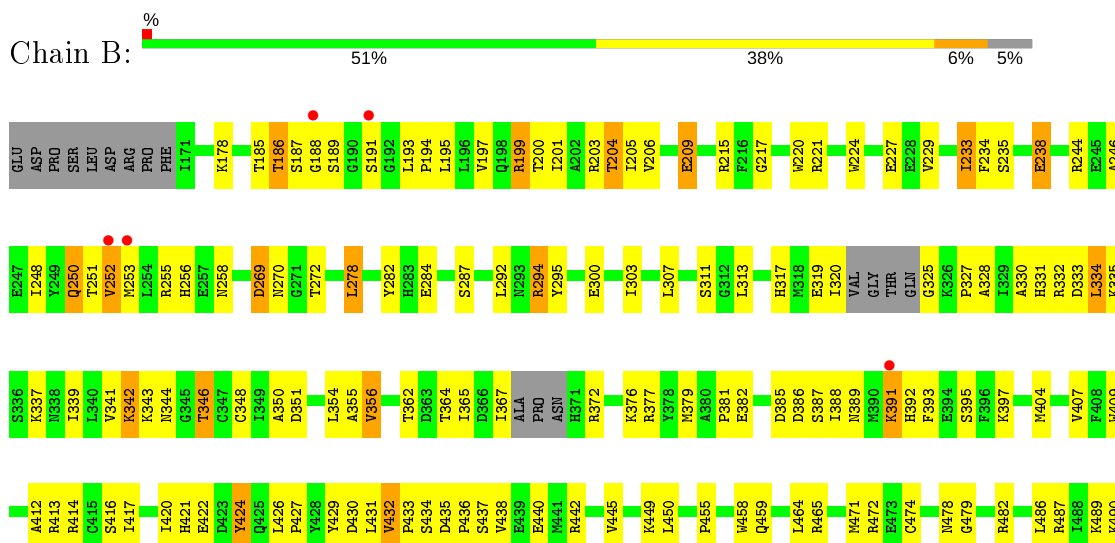
3 Residue-property plots

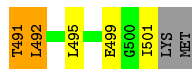
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: TGF-beta receptor type-1

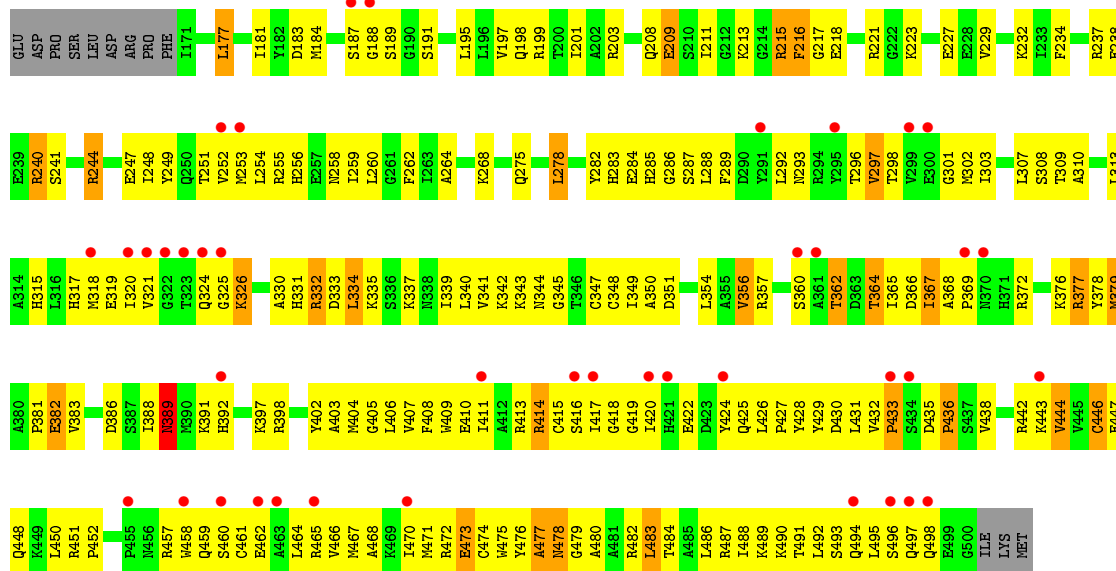


- Molecule 1: TGF-beta receptor type-1

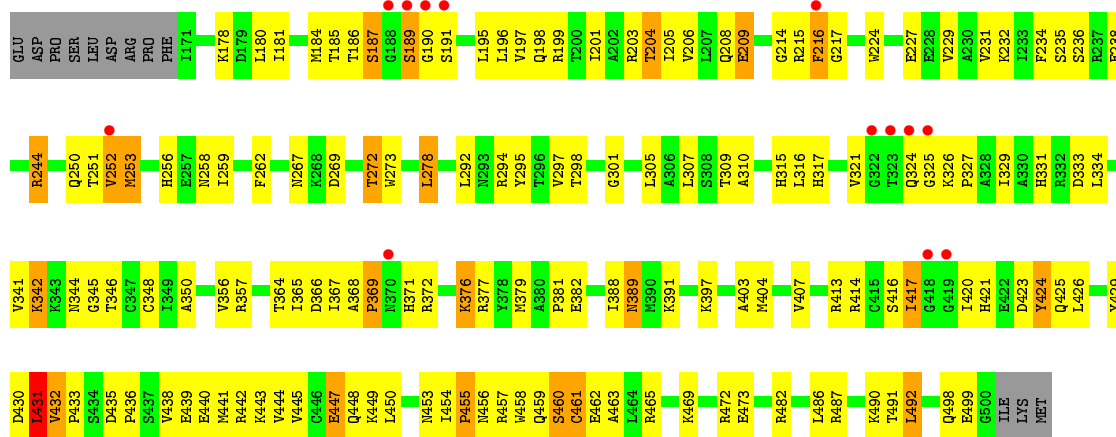




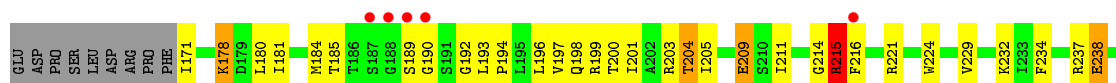
- Molecule 1: TGF-beta receptor type-1

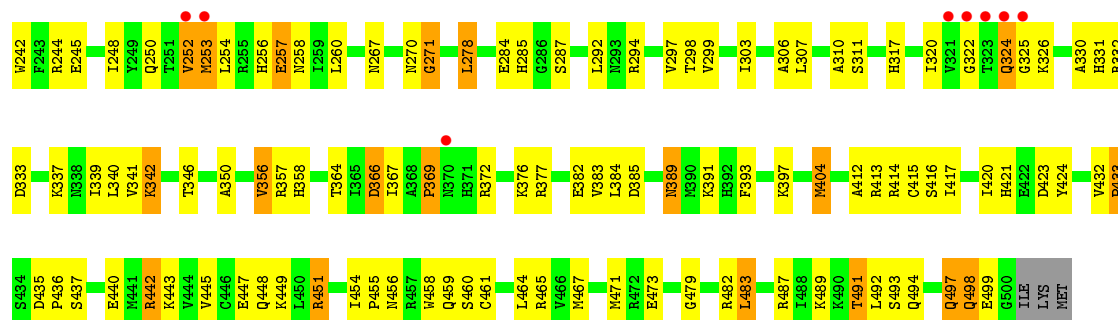


- Molecule 1: TGF-beta receptor type-1



- Molecule 1: TGF-beta receptor type-1





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	174.03Å 249.08Å 138.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.86 – 2.80 49.59 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (34.86-2.80) 99.7 (49.59-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 2.81Å)	Xtrriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.235 , 0.278 0.232 , 0.273	Depositor DCC
R_{free} test set	3747 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtrriage
Anisotropy	0.249	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 65.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	13297	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.45% 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: JZO, PO4

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	0.36	1/2668 (0.0%)	0.58	0/3600
1	B	0.40	0/2640	0.65	0/3560
1	C	0.34	0/2682	0.61	0/3622
1	D	0.39	0/2682	0.69	0/3622
1	E	0.41	0/2682	0.67	0/3622
All	All	0.38	1/13354 (0.0%)	0.64	0/18026

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
1	D	0	1
1	E	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	GLU	N-CA	5.55	1.57	1.46

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	424	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	424	TYR	Sidechain
1	E	424	TYR	Sidechain

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	2617	0	2618	170	0
1	B	2590	0	2595	119	0
1	C	2629	0	2631	251	0
1	D	2629	0	2631	151	0
1	E	2629	0	2631	132	0
2	A	27	0	20	1	0
2	B	27	0	20	0	0
2	C	27	0	20	3	0
2	D	27	0	20	3	0
2	E	27	0	20	1	0
3	A	15	0	0	0	0
3	B	15	0	0	4	0
3	C	5	0	0	1	0
3	D	15	0	0	2	0
3	E	15	0	0	4	0
4	A	1	0	0	1	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
All	All	13297	0	13206	823	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 31.

All (823) 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:E:216:PHE:HB3	1:E:238:GLU:HG2	1.22	1.10
1:A:443:LYS:HG2	1:A:448:GLN:HE21	1.19	1.08
1:C:461:CYS:HB2	1:C:464:LEU:HD23	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:367:ILE:HG13	1:D:369:PRO:HD3	1.40	1.04
1:E:253:MET:HB2	1:E:326:LYS:HB3	1.41	1.01
1:E:367:ILE:HG13	1:E:369:PRO:HD3	1.40	1.01
1:C:253:MET:HB3	1:C:326:LYS:HB3	1.49	0.95
1:E:256:HIS:HD2	1:E:258:ASN:H	1.11	0.94
1:C:244:ARG:HH11	1:C:367:ILE:HG12	1.33	0.93
1:B:331:HIS:HD2	1:B:333:ASP:H	1.17	0.92
1:C:215:ARG:HH11	1:C:215:ARG:HB3	1.33	0.91
1:D:417:ILE:HG13	1:D:420:ILE:HG13	1.49	0.91
1:A:372:ARG:HH11	1:A:438:VAL:HG11	1.33	0.91
1:B:317:HIS:HB3	1:B:397:LYS:HE3	1.53	0.88
1:C:376:LYS:HA	1:C:379:MET:HG3	1.56	0.87
1:C:417:ILE:HB	1:C:420:ILE:HD11	1.57	0.86
1:A:443:LYS:HG2	1:A:448:GLN:NE2	1.88	0.86
1:C:406:LEU:HD12	1:C:427:PRO:HB3	1.58	0.86
1:E:487:ARG:O	1:E:491:THR:HG22	1.76	0.86
1:E:216:PHE:HB3	1:E:238:GLU:CG	2.06	0.86
1:A:267:ASN:H	1:A:267:ASN:HD22	1.20	0.86
1:A:372:ARG:HH21	1:A:386:ASP:HB2	1.39	0.85
1:A:267:ASN:N	1:A:267:ASN:HD22	1.74	0.84
1:D:487:ARG:NH2	1:D:490:LYS:HD2	1.92	0.84
1:C:215:ARG:HG3	1:C:216:PHE:H	1.41	0.83
1:A:498:GLN:HG3	1:A:499:GLU:H	1.44	0.81
1:D:253:MET:HE2	1:D:324:GLN:O	1.80	0.81
1:E:204:THR:HG22	1:E:224:TRP:NE1	1.96	0.80
1:B:244:ARG:HH11	1:B:244:ARG:HG2	1.46	0.80
1:D:251:THR:O	1:D:252:VAL:HG22	1.81	0.80
1:D:389:ASN:ND2	1:D:391:LYS:H	1.79	0.79
1:C:244:ARG:NH1	1:C:367:ILE:HG12	1.97	0.78
1:A:309:THR:HG22	1:A:404:MET:HE2	1.64	0.78
1:A:259:ILE:HD11	1:A:316:LEU:HG	1.66	0.78
1:C:199:ARG:HD2	1:C:203:ARG:CZ	2.14	0.78
1:A:372:ARG:NH2	1:A:386:ASP:HB2	1.97	0.78
1:A:457:ARG:HH11	1:A:457:ARG:HB2	1.49	0.78
1:E:256:HIS:CD2	1:E:258:ASN:H	1.98	0.77
1:D:469:LYS:O	1:D:473:GLU:HG3	1.85	0.77
1:D:487:ARG:HH22	1:D:490:LYS:HD2	1.48	0.76
1:A:417:ILE:HG13	1:A:420:ILE:HD11	1.66	0.76
1:D:252:VAL:HG21	1:D:327:PRO:HD2	1.66	0.75
1:E:204:THR:HG22	1:E:224:TRP:HE1	1.47	0.75
1:A:301:GLY:HA2	1:A:304:LYS:NZ	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:376:LYS:HA	1:A:379:MET:SD	2.27	0.74
1:D:389:ASN:HD21	1:D:391:LYS:HB3	1.51	0.74
1:C:479:GLY:HA2	1:C:482:ARG:HD2	1.69	0.74
1:D:317:HIS:HB3	1:D:397:LYS:HE3	1.70	0.74
1:E:357:ARG:HB2	1:E:366:ASP:HB2	1.68	0.74
1:A:455:PRO:O	1:A:458:TRP:HB2	1.87	0.74
1:C:297:VAL:HG22	1:C:298:THR:H	1.50	0.74
1:E:199:ARG:HD2	1:E:203:ARG:CZ	2.19	0.73
1:B:256:HIS:CD2	1:B:258:ASN:H	2.05	0.73
1:B:344:ASN:OD1	1:B:346:THR:HB	1.88	0.73
1:D:331:HIS:HD2	1:D:333:ASP:H	1.36	0.73
1:C:432:VAL:HG21	1:C:436:PRO:HB3	1.71	0.73
1:C:320:ILE:HG22	1:C:321:VAL:H	1.55	0.72
1:D:198:GLN:HE22	1:D:250:GLN:HE21	1.38	0.72
1:A:249:TYR:HA	1:A:254:LEU:HD23	1.71	0.72
1:C:249:TYR:HA	1:C:254:LEU:HD23	1.72	0.72
1:A:284:GLU:HB3	1:A:343:LYS:HE2	1.73	0.71
1:D:435:ASP:HA	3:D:15:PO4:O3	1.90	0.71
1:E:256:HIS:HD2	1:E:258:ASN:N	1.89	0.71
1:E:417:ILE:O	1:E:420:ILE:HG12	1.91	0.71
1:C:473:GLU:HB3	1:C:483:LEU:HG	1.73	0.71
1:C:406:LEU:HD12	1:C:427:PRO:CB	2.21	0.70
1:C:199:ARG:HD2	1:C:203:ARG:NH2	2.07	0.70
1:D:199:ARG:HD2	1:D:203:ARG:CZ	2.21	0.70
1:D:256:HIS:CD2	1:D:258:ASN:H	2.09	0.70
1:D:414:ARG:HH21	1:D:423:ASP:HA	1.55	0.70
1:A:498:GLN:HG3	1:A:499:GLU:N	2.06	0.70
1:A:307:LEU:HD23	1:A:492:LEU:HB3	1.74	0.69
1:C:461:CYS:CB	1:C:464:LEU:HD23	2.17	0.69
1:C:483:LEU:HD13	1:C:488:ILE:HD11	1.74	0.69
1:E:356:VAL:HG22	1:E:393:PHE:HE1	1.57	0.69
1:C:240:ARG:HB2	1:C:240:ARG:HH11	1.57	0.69
1:C:444:VAL:HG13	1:C:450:LEU:HD12	1.74	0.69
1:C:253:MET:HB3	1:C:326:LYS:CB	2.20	0.69
1:D:357:ARG:HB2	1:D:366:ASP:HB2	1.74	0.69
1:C:320:ILE:HG22	1:C:321:VAL:N	2.07	0.69
1:C:414:ARG:HB3	1:C:414:ARG:HH11	1.57	0.69
1:C:376:LYS:HA	1:C:379:MET:CG	2.20	0.69
1:B:252:VAL:HG12	1:B:253:MET:HG3	1.75	0.69
1:A:309:THR:HG22	1:A:404:MET:CE	2.23	0.68
1:D:389:ASN:HD22	1:D:389:ASN:C	1.97	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:252:VAL:HG12	1:E:253:MET:H	1.58	0.68
1:E:467:MET:O	1:E:471:MET:HG3	1.93	0.68
1:A:469:LYS:O	1:A:473:GLU:HG3	1.94	0.68
1:E:253:MET:HG3	1:E:326:LYS:N	2.09	0.68
1:C:459:GLN:NE2	1:C:465:ARG:HG3	2.09	0.68
1:C:381:PRO:HD2	1:C:482:ARG:HH22	1.58	0.68
1:C:470:ILE:HD13	1:C:488:ILE:HG23	1.76	0.67
1:A:367:ILE:O	1:A:370:ASN:HB2	1.94	0.67
1:B:376:LYS:HA	1:B:379:MET:CE	2.24	0.67
1:E:331:HIS:HD2	1:E:333:ASP:H	1.42	0.67
1:A:267:ASN:ND2	1:A:267:ASN:N	2.42	0.67
1:A:443:LYS:HE2	1:A:448:GLN:NE2	2.11	0.66
1:C:414:ARG:HH11	1:C:414:ARG:CB	2.09	0.66
1:C:215:ARG:HG3	1:C:216:PHE:N	2.11	0.66
1:D:178:LYS:N	1:D:178:LYS:HD3	2.08	0.66
1:C:215:ARG:HH11	1:C:215:ARG:CB	2.07	0.66
1:A:235:SER:HB2	1:A:238:GLU:HG2	1.78	0.66
1:B:431:LEU:O	1:B:432:VAL:HG23	1.96	0.66
1:A:372:ARG:NH1	1:A:438:VAL:HG11	2.10	0.66
1:B:385:ASP:HA	1:B:442:ARG:CZ	2.26	0.66
1:B:376:LYS:HA	1:B:379:MET:HE3	1.78	0.66
1:E:189:SER:O	1:E:252:VAL:HG13	1.96	0.65
1:E:260:LEU:HD13	1:E:340:LEU:HD13	1.78	0.65
1:A:284:GLU:OE2	1:A:343:LYS:HE2	1.96	0.65
1:C:414:ARG:HB3	1:C:414:ARG:NH1	2.11	0.65
1:D:389:ASN:HD22	1:D:391:LYS:H	1.43	0.65
1:E:258:ASN:ND2	1:E:311:SER:HB2	2.12	0.65
1:A:458:TRP:O	1:A:464:LEU:HD12	1.97	0.65
1:C:357:ARG:NE	1:C:366:ASP:OD1	2.28	0.65
1:C:430:ASP:OD1	1:C:431:LEU:HG	1.95	0.65
1:C:372:ARG:NH1	1:C:438:VAL:HG11	2.11	0.65
1:A:394:GLU:O	1:A:398:ARG:HG2	1.97	0.65
1:D:251:THR:HG22	1:D:252:VAL:HG13	1.79	0.65
1:E:297:VAL:HG12	1:E:298:THR:O	1.97	0.64
1:D:443:LYS:HA	1:D:447:GLU:CG	2.27	0.64
1:D:235:SER:O	1:D:238:GLU:HG2	1.97	0.64
1:E:204:THR:CG2	1:E:224:TRP:HE1	2.09	0.64
1:A:217:GLY:N	1:A:238:GLU:OE2	2.31	0.64
1:A:298:THR:HG22	1:A:299:VAL:N	2.11	0.64
1:A:463:ALA:HB1	1:A:495:LEU:HD21	1.79	0.64
1:D:262:PHE:HD1	2:D:4:JZO:H1	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:253:MET:HB2	1:E:326:LYS:CB	2.25	0.64
1:C:331:HIS:HD2	1:C:333:ASP:H	1.44	0.64
1:E:244:ARG:NH2	1:E:366:ASP:OD2	2.30	0.64
1:E:322:GLY:HA3	1:E:324:GLN:NE2	2.13	0.64
1:B:244:ARG:HG2	1:B:244:ARG:NH1	2.11	0.64
1:C:490:LYS:O	1:C:494:GLN:HB2	1.98	0.64
1:A:445:VAL:O	1:A:449:LYS:HA	1.98	0.64
1:C:237:ARG:HD3	1:C:238:GLU:OE2	1.98	0.63
1:C:467:MET:O	1:C:471:MET:HG3	1.99	0.63
1:C:309:THR:HG22	1:C:404:MET:HE2	1.80	0.63
1:D:367:ILE:CG1	1:D:369:PRO:HD3	2.23	0.63
1:B:381:PRO:HG3	1:B:445:VAL:CG1	2.28	0.63
1:C:418:GLY:O	1:C:420:ILE:N	2.31	0.63
1:B:204:THR:CG2	1:B:224:TRP:HE1	2.12	0.63
1:E:357:ARG:H	1:E:366:ASP:HB3	1.63	0.63
1:C:368:ALA:N	1:C:369:PRO:HD2	2.14	0.62
1:C:418:GLY:O	1:C:420:ILE:HG23	1.99	0.62
1:E:445:VAL:HG13	1:E:451:ARG:NH1	2.14	0.62
1:A:454:ILE:HG23	1:A:458:TRP:CE3	2.34	0.62
1:B:215:ARG:HD2	1:B:351:ASP:OD2	2.00	0.62
1:A:301:GLY:HA2	1:A:304:LYS:HZ2	1.64	0.62
1:E:199:ARG:HD2	1:E:203:ARG:NH2	2.15	0.62
1:A:298:THR:HG22	1:A:299:VAL:H	1.63	0.62
1:C:459:GLN:HA	1:C:459:GLN:HE21	1.63	0.62
1:C:285:HIS:HB2	1:C:341:VAL:HG13	1.81	0.62
1:D:244:ARG:NH2	1:D:367:ILE:HG22	2.14	0.62
1:C:297:VAL:HG12	1:C:415:CYS:HA	1.81	0.62
1:E:184:MET:HB3	1:E:193:LEU:HD23	1.82	0.62
1:D:416:SER:HA	1:D:421:HIS:HB3	1.81	0.61
1:C:382:GLU:HB2	1:C:388:ILE:HB	1.82	0.61
1:E:432:VAL:HG22	1:E:433:PRO:HD2	1.82	0.61
1:E:331:HIS:CD2	1:E:333:ASP:H	2.19	0.61
1:D:178:LYS:HG2	1:D:227:GLU:OE2	2.01	0.61
1:A:284:GLU:HB3	1:A:343:LYS:CE	2.30	0.61
1:C:420:ILE:HG13	1:C:420:ILE:O	2.00	0.61
1:D:198:GLN:HE22	1:D:250:GLN:NE2	1.98	0.61
1:C:443:LYS:HG3	1:C:447:GLU:OE1	2.01	0.61
1:C:458:TRP:HZ3	1:C:471:MET:SD	2.23	0.61
1:B:377:ARG:NH1	3:B:11:PO4:O1	2.33	0.61
1:D:216:PHE:HA	1:D:238:GLU:OE2	2.01	0.60
1:E:357:ARG:HB2	1:E:366:ASP:CB	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:466:VAL:O	1:C:470:ILE:HG13	2.01	0.60
1:D:310:ALA:HA	1:D:404:MET:CE	2.31	0.60
1:C:302:MET:HG3	1:C:411:ILE:HG22	1.82	0.60
1:B:432:VAL:HG11	1:B:436:PRO:HG3	1.84	0.60
1:C:377:ARG:HG3	1:C:436:PRO:HG2	1.83	0.60
1:A:381:PRO:HG3	1:A:445:VAL:CG1	2.31	0.60
1:C:425:GLN:HE21	1:C:425:GLN:HA	1.67	0.60
1:C:284:GLU:HB3	1:C:343:LYS:HZ2	1.65	0.59
1:D:459:GLN:NE2	1:D:465:ARG:HG3	2.17	0.59
1:A:464:LEU:O	1:A:464:LEU:HD13	2.01	0.59
1:D:331:HIS:HE1	1:D:350:ALA:O	1.85	0.59
1:C:287:SER:HA	1:C:339:ILE:O	2.02	0.59
1:A:331:HIS:HD2	1:A:333:ASP:H	1.49	0.59
1:A:413:ARG:HH12	1:A:422:GLU:HB3	1.67	0.59
1:D:294:ARG:HH11	1:D:294:ARG:HG2	1.68	0.59
1:E:331:HIS:HD2	1:E:333:ASP:N	1.99	0.59
1:A:377:ARG:NH1	1:A:426:LEU:HD13	2.18	0.59
1:B:432:VAL:CG1	1:B:436:PRO:HG3	2.32	0.59
1:C:459:GLN:HA	1:C:459:GLN:NE2	2.16	0.59
1:E:498:GLN:O	1:E:499:GLU:HG3	2.03	0.59
1:C:478:ASN:C	1:C:478:ASN:HD22	2.06	0.59
1:D:256:HIS:HD2	1:D:258:ASN:H	1.51	0.59
1:C:285:HIS:CB	1:C:341:VAL:HG13	2.33	0.58
1:D:204:THR:CG2	1:D:224:TRP:HE1	2.15	0.58
1:A:398:ARG:HD2	1:A:479:GLY:O	2.03	0.58
1:C:248:ILE:O	1:C:251:THR:HG23	2.03	0.58
1:A:443:LYS:HE2	1:A:448:GLN:HE22	1.68	0.58
1:D:294:ARG:HD3	1:D:295:TYR:CE2	2.38	0.58
1:E:322:GLY:HA3	1:E:324:GLN:HE22	1.68	0.58
1:E:389:ASN:HD21	1:E:391:LYS:HB3	1.68	0.58
1:C:215:ARG:CG	1:C:216:PHE:H	2.15	0.58
1:C:493:SER:O	1:C:497:GLN:HG3	2.02	0.58
1:A:221:ARG:HD2	1:A:282:TYR:OH	2.03	0.58
1:A:413:ARG:HH11	1:A:413:ARG:HG2	1.68	0.58
1:B:362:THR:O	1:B:364:THR:HG23	2.03	0.58
1:C:442:ARG:HA	1:C:446:CYS:SG	2.43	0.58
1:C:487:ARG:NH1	1:C:490:LYS:HD3	2.18	0.58
1:D:178:LYS:HE2	1:D:227:GLU:OE2	2.04	0.58
1:D:262:PHE:CD1	2:D:4:JZO:H1	2.38	0.58
1:D:185:THR:C	1:D:187:SER:H	2.07	0.58
1:D:377:ARG:HE	1:D:426:LEU:HB3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:LEU:HD22	1:C:334:LEU:CD1	2.34	0.58
1:E:330:ALA:HB3	1:E:356:VAL:HG13	1.86	0.58
1:A:459:GLN:HB3	1:A:465:ARG:HD3	1.86	0.58
1:C:260:LEU:HD13	1:C:340:LEU:CD1	2.34	0.58
1:D:315:HIS:O	1:D:326:LYS:HE3	2.05	0.57
1:C:409:TRP:HA	1:C:471:MET:HE3	1.86	0.57
1:B:331:HIS:CD2	1:B:333:ASP:H	2.09	0.57
1:C:313:LEU:HD22	1:C:334:LEU:HD12	1.85	0.57
1:B:365:ILE:HD11	1:B:367:ILE:HD13	1.86	0.57
1:C:183:ASP:O	1:C:187:SER:HB2	2.04	0.57
1:C:451:ARG:HE	1:C:475:TRP:HB3	1.69	0.57
1:D:487:ARG:NE	1:D:487:ARG:HA	2.19	0.57
1:A:364:THR:O	1:A:365:ILE:HG23	2.04	0.57
1:B:437:SER:OG	1:B:440:GLU:HG3	2.03	0.57
1:C:232:LYS:HE3	1:C:234:PHE:CZ	2.39	0.57
1:E:204:THR:CG2	1:E:224:TRP:NE1	2.65	0.57
1:A:466:VAL:O	1:A:470:ILE:HG13	2.04	0.57
1:C:244:ARG:NH2	1:C:366:ASP:OD1	2.38	0.57
1:B:458:TRP:HZ3	1:B:471:MET:HE1	1.70	0.57
1:B:215:ARG:HB3	1:B:215:ARG:NH1	2.19	0.57
1:C:313:LEU:HB3	1:C:404:MET:HE1	1.87	0.57
1:D:368:ALA:HB2	1:E:178:LYS:HD3	1.87	0.56
1:A:463:ALA:HB2	1:A:495:LEU:HD11	1.86	0.56
1:C:331:HIS:CD2	1:C:333:ASP:H	2.23	0.56
1:D:215:ARG:HG2	1:D:215:ARG:HH11	1.69	0.56
1:C:494:GLN:HA	1:C:497:GLN:NE2	2.20	0.56
1:D:342:LYS:HD3	1:D:346:THR:HG23	1.86	0.56
1:A:297:VAL:HG22	1:A:298:THR:N	2.20	0.56
1:E:209:GLU:OE2	1:E:221:ARG:HD3	2.06	0.56
1:E:310:ALA:HA	1:E:404:MET:HE3	1.86	0.56
1:E:317:HIS:HB3	1:E:397:LYS:HE3	1.87	0.56
1:C:256:HIS:CD2	1:C:258:ASN:H	2.24	0.56
1:C:426:LEU:O	1:C:429:TYR:HB3	2.06	0.56
1:E:245:GLU:HB3	1:E:278:LEU:HD21	1.86	0.56
1:A:487:ARG:HE	1:A:491:THR:HG22	1.70	0.56
1:A:195:LEU:HD12	1:A:195:LEU:H	1.70	0.56
1:B:217:GLY:N	1:B:238:GLU:OE2	2.39	0.56
1:D:425:GLN:HB3	1:D:429:TYR:CD2	2.41	0.56
1:B:199:ARG:HH11	1:B:203:ARG:NH2	2.04	0.55
1:C:232:LYS:HE3	1:C:234:PHE:HZ	1.71	0.55
1:D:344:ASN:OD1	1:D:346:THR:HG22	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:432:VAL:CG1	1:D:436:PRO:HG3	2.37	0.55
1:E:435:ASP:N	1:E:436:PRO:HD3	2.21	0.55
1:D:309:THR:HG22	1:D:404:MET:HE2	1.87	0.55
1:E:214:GLY:O	1:E:215:ARG:C	2.44	0.55
1:E:389:ASN:ND2	1:E:391:LYS:HB3	2.21	0.55
1:C:283:HIS:ND1	3:C:10:PO4:O4	2.39	0.55
1:C:313:LEU:HD11	1:C:317:HIS:NE2	2.21	0.55
1:D:189:SER:O	1:D:191:SER:N	2.39	0.55
1:E:256:HIS:CD2	1:E:257:GLU:N	2.74	0.55
1:B:331:HIS:HD2	1:B:333:ASP:N	1.97	0.55
1:C:487:ARG:HH21	1:C:491:THR:HG22	1.71	0.55
1:D:272:THR:HG22	1:D:273:TRP:CD1	2.42	0.55
1:D:217:GLY:N	1:D:238:GLU:OE1	2.40	0.55
1:C:478:ASN:HD21	1:C:480:ALA:HB3	1.72	0.55
1:D:459:GLN:HE22	1:D:465:ARG:HG3	1.72	0.55
1:D:234:PHE:HA	1:D:238:GLU:OE1	2.06	0.55
1:A:177:LEU:N	1:A:227:GLU:OE2	2.40	0.55
1:A:301:GLY:HA2	1:A:304:LYS:HZ3	1.71	0.54
1:E:244:ARG:O	1:E:248:ILE:HG12	2.08	0.54
1:A:447:GLU:O	1:A:449:LYS:N	2.40	0.54
1:C:362:THR:HG22	1:C:364:THR:HG23	1.87	0.54
1:C:458:TRP:HE3	1:C:468:ALA:HB2	1.73	0.54
1:D:376:LYS:HD2	1:D:379:MET:HE1	1.89	0.54
1:C:258:ASN:O	1:C:348:CYS:HA	2.08	0.54
1:A:457:ARG:HH11	1:A:457:ARG:CB	2.20	0.54
1:B:434:SER:O	1:B:435:ASP:HB3	2.07	0.54
1:C:438:VAL:O	1:C:442:ARG:HB2	2.07	0.54
1:C:435:ASP:N	1:C:436:PRO:HD3	2.21	0.54
1:D:417:ILE:O	1:D:420:ILE:HG12	2.08	0.54
1:E:331:HIS:O	1:E:332:ARG:HB2	2.07	0.54
1:C:240:ARG:HH11	1:C:240:ARG:CB	2.20	0.54
1:B:197:VAL:O	1:B:201:ILE:HG12	2.08	0.54
1:C:417:ILE:HG12	1:C:461:CYS:SG	2.47	0.54
1:C:293:ASN:HD22	1:C:424:TYR:HD2	1.55	0.54
1:C:487:ARG:O	1:C:491:THR:HG23	2.08	0.54
1:D:432:VAL:HG13	1:D:436:PRO:HG3	1.90	0.54
1:E:331:HIS:HE1	1:E:350:ALA:O	1.90	0.54
1:E:473:GLU:HB3	1:E:483:LEU:HG	1.90	0.53
1:A:251:THR:O	1:A:252:VAL:HG22	2.08	0.53
1:E:389:ASN:HD21	1:E:391:LYS:CB	2.21	0.53
1:C:356:VAL:HG23	1:C:365:ILE:HG23	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:ILE:HD11	1:D:457:ARG:HH11	1.74	0.53
1:B:409:TRP:HD1	1:B:471:MET:CE	2.22	0.53
1:D:372:ARG:NH1	1:D:438:VAL:HG11	2.24	0.53
1:E:372:ARG:NH1	1:E:383:VAL:O	2.42	0.53
1:A:486:LEU:O	1:A:489:LYS:HB3	2.09	0.53
1:B:246:ALA:O	1:B:250:GLN:HG3	2.08	0.53
1:B:331:HIS:HE1	1:B:350:ALA:O	1.92	0.53
1:E:184:MET:HB3	1:E:193:LEU:CD2	2.39	0.53
1:A:498:GLN:CG	1:A:499:GLU:H	2.17	0.53
1:B:333:ASP:HB2	1:B:354:LEU:HD12	1.91	0.53
1:B:413:ARG:NH1	1:B:422:GLU:HB3	2.24	0.53
1:D:251:THR:O	1:D:252:VAL:CG2	2.54	0.53
1:D:294:ARG:HG2	1:D:294:ARG:O	2.08	0.53
1:E:252:VAL:HG12	1:E:253:MET:N	2.21	0.53
1:C:232:LYS:HG2	1:C:234:PHE:CE1	2.43	0.53
1:D:331:HIS:CD2	1:D:333:ASP:H	2.22	0.53
1:C:256:HIS:HD2	1:C:258:ASN:HB2	1.74	0.52
1:C:372:ARG:HH12	1:C:438:VAL:HG11	1.73	0.52
1:B:430:ASP:O	1:B:431:LEU:HD23	2.08	0.52
1:C:288:LEU:HD12	1:C:292:LEU:HD13	1.92	0.52
1:C:483:LEU:H	1:C:483:LEU:HD12	1.73	0.52
1:E:198:GLN:HE22	1:E:250:GLN:NE2	2.07	0.52
1:D:259:ILE:CD1	1:D:316:LEU:HD13	2.39	0.52
1:C:253:MET:HB3	1:C:326:LYS:CG	2.38	0.52
1:C:403:ALA:O	1:C:407:VAL:HG23	2.09	0.52
1:C:408:PHE:O	1:C:411:ILE:HB	2.09	0.52
1:E:204:THR:HG22	1:E:224:TRP:CD1	2.45	0.52
1:A:214:GLY:O	1:A:215:ARG:C	2.48	0.52
1:A:459:GLN:O	1:A:465:ARG:NH1	2.43	0.52
1:C:472:ARG:C	1:C:474:CYS:H	2.12	0.52
1:A:487:ARG:HH21	1:A:491:THR:N	2.08	0.52
1:B:248:ILE:HD12	1:B:355:ALA:HB3	1.92	0.52
1:C:244:ARG:HH12	1:C:366:ASP:HB3	1.74	0.52
1:D:469:LYS:HE2	1:D:473:GLU:OE2	2.10	0.52
1:C:221:ARG:HD2	1:C:282:TYR:OH	2.09	0.52
1:C:278:LEU:HG	2:C:3:JZO:H1B	1.92	0.52
1:C:317:HIS:HB3	1:C:397:LYS:HE2	1.92	0.52
1:D:389:ASN:ND2	1:D:389:ASN:C	2.59	0.52
1:D:456:ASN:C	1:D:458:TRP:N	2.63	0.52
1:E:200:THR:O	1:E:204:THR:HB	2.09	0.52
1:E:377:ARG:NH1	3:E:3:PO4:O3	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:253:MET:HG2	1:A:324:GLN:O	2.10	0.52
1:A:296:THR:HG22	1:A:414:ARG:HH11	1.73	0.52
1:D:244:ARG:HH21	1:D:367:ILE:CG2	2.22	0.52
1:C:459:GLN:HE22	1:C:465:ARG:HG3	1.72	0.52
1:D:456:ASN:C	1:D:458:TRP:H	2.12	0.52
1:C:372:ARG:CZ	1:C:438:VAL:HG11	2.40	0.51
1:C:425:GLN:NE2	1:C:425:GLN:HA	2.25	0.51
1:A:216:PHE:HA	1:A:238:GLU:OE1	2.10	0.51
1:A:260:LEU:HD23	4:A:504:HOH:O	2.11	0.51
1:A:488:ILE:O	1:A:492:LEU:HB2	2.11	0.51
1:B:471:MET:O	1:B:474:CYS:HB2	2.10	0.51
1:C:209:GLU:OE1	1:C:221:ARG:NH1	2.43	0.51
1:A:462:GLU:O	1:A:466:VAL:HG23	2.09	0.51
1:E:417:ILE:HD11	1:E:464:LEU:HD21	1.91	0.51
1:B:248:ILE:CD1	1:B:355:ALA:HB3	2.40	0.51
1:C:284:GLU:HB3	1:C:343:LYS:NZ	2.26	0.51
1:C:479:GLY:HA2	1:C:482:ARG:CD	2.40	0.51
1:C:483:LEU:N	1:C:483:LEU:HD12	2.25	0.51
1:D:448:GLN:O	1:D:450:LEU:N	2.43	0.51
1:C:332:ARG:NH2	1:C:367:ILE:HG21	2.26	0.51
1:A:195:LEU:CD1	1:A:195:LEU:H	2.24	0.51
1:A:344:ASN:OD1	1:A:346:THR:OG1	2.28	0.51
1:D:178:LYS:HE2	1:D:227:GLU:CD	2.31	0.51
1:D:433:PRO:HG2	1:D:440:GLU:OE1	2.11	0.51
1:B:220:TRP:NE1	1:B:233:ILE:HD11	2.26	0.51
1:B:313:LEU:HD11	1:B:317:HIS:NE2	2.25	0.51
1:C:462:GLU:O	1:C:466:VAL:HG23	2.11	0.51
1:A:177:LEU:H	1:A:227:GLU:CD	2.15	0.50
1:A:407:VAL:O	1:A:411:ILE:HG13	2.11	0.50
1:A:413:ARG:NH1	1:A:422:GLU:HB3	2.26	0.50
1:A:456:ASN:C	1:A:458:TRP:H	2.15	0.50
1:C:181:ILE:HA	1:C:184:MET:CE	2.41	0.50
1:A:417:ILE:HG13	1:A:420:ILE:CD1	2.38	0.50
1:A:417:ILE:CG1	1:A:420:ILE:HD11	2.38	0.50
1:C:376:LYS:O	1:C:378:TYR:N	2.44	0.50
1:C:381:PRO:HD2	1:C:482:ARG:NH2	2.25	0.50
1:D:267:ASN:N	1:D:267:ASN:OD1	2.45	0.50
1:A:372:ARG:HD3	1:A:379:MET:HE1	1.93	0.50
1:B:253:MET:HE3	1:B:325:GLY:O	2.11	0.50
1:E:297:VAL:N	1:E:414:ARG:O	2.44	0.50
1:C:256:HIS:HB2	1:C:315:HIS:ND1	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:342:LYS:HD3	1:D:346:THR:CG2	2.42	0.50
1:A:420:ILE:O	1:A:420:ILE:HG13	2.10	0.50
1:C:368:ALA:H	1:C:369:PRO:HD2	1.75	0.50
1:E:190:GLY:C	1:E:192:GLY:H	2.15	0.50
1:D:244:ARG:HH11	1:D:244:ARG:HG2	1.77	0.50
1:A:431:LEU:HD13	1:A:444:VAL:CG1	2.41	0.50
1:B:377:ARG:HD3	1:B:427:PRO:HD2	1.92	0.50
1:C:288:LEU:HB3	1:C:339:ILE:HB	1.93	0.50
1:C:335:LYS:HG2	1:C:337:LYS:H	1.77	0.50
1:D:417:ILE:HD11	1:D:457:ARG:NH1	2.26	0.50
1:D:205:ILE:CG2	1:D:206:VAL:N	2.75	0.50
1:B:311:SER:HA	1:B:489:LYS:HG3	1.94	0.49
1:C:468:ALA:HA	1:C:471:MET:SD	2.52	0.49
1:A:366:ASP:O	1:A:367:ILE:HB	2.10	0.49
1:A:328:ALA:HB1	1:A:393:PHE:CE2	2.47	0.49
1:C:198:GLN:HB3	1:C:264:ALA:HB1	1.93	0.49
1:D:199:ARG:HD2	1:D:203:ARG:NH2	2.28	0.49
1:D:443:LYS:O	1:D:447:GLU:HB2	2.12	0.49
1:A:215:ARG:HG2	1:A:215:ARG:HH11	1.78	0.49
1:A:470:ILE:HG23	1:A:483:LEU:CD1	2.42	0.49
1:B:385:ASP:HA	1:B:442:ARG:NH2	2.27	0.49
1:C:177:LEU:HB2	1:C:227:GLU:OE1	2.12	0.49
1:C:288:LEU:O	1:C:288:LEU:HD12	2.12	0.49
1:C:406:LEU:H	1:C:406:LEU:HD22	1.78	0.49
1:C:409:TRP:HD1	1:C:471:MET:CE	2.25	0.49
1:D:205:ILE:HG22	1:D:206:VAL:N	2.26	0.49
1:A:375:THR:O	1:A:379:MET:HG3	2.13	0.49
1:B:317:HIS:HB3	1:B:397:LYS:CE	2.36	0.49
1:C:448:GLN:HB2	1:C:450:LEU:HG	1.94	0.49
1:C:476:TYR:O	1:C:478:ASN:N	2.45	0.49
1:D:381:PRO:HG3	1:D:445:VAL:CG1	2.42	0.49
1:E:320:ILE:HD13	1:E:326:LYS:HG2	1.95	0.49
1:A:304:LYS:HB2	1:A:304:LYS:HZ3	1.77	0.49
1:B:433:PRO:HG2	1:B:440:GLU:OE2	2.11	0.49
1:D:368:ALA:HB2	1:E:178:LYS:HG2	1.94	0.49
1:B:195:LEU:CD1	1:B:195:LEU:H	2.25	0.49
1:B:199:ARG:HD3	1:B:203:ARG:CZ	2.42	0.49
1:D:459:GLN:O	1:D:465:ARG:NH1	2.46	0.49
1:B:337:LYS:HD2	3:B:12:PO4:O2	2.12	0.49
1:C:260:LEU:HD13	1:C:340:LEU:HD13	1.94	0.49
1:C:402:TYR:CE1	1:C:406:LEU:HD21	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:LEU:O	1:D:429:TYR:HB3	2.13	0.49
1:D:448:GLN:HB2	1:D:450:LEU:HD12	1.94	0.49
1:E:253:MET:HG3	1:E:326:LYS:H	1.76	0.49
1:E:385:ASP:HA	1:E:442:ARG:HD2	1.95	0.49
1:C:258:ASN:OD1	1:C:308:SER:HB2	2.13	0.49
1:C:406:LEU:N	1:C:406:LEU:HD22	2.28	0.49
1:C:417:ILE:H	1:C:420:ILE:CG1	2.26	0.49
1:D:259:ILE:HD13	1:D:316:LEU:HD13	1.94	0.49
1:E:432:VAL:HG22	1:E:433:PRO:CD	2.43	0.49
1:A:251:THR:OG1	1:A:251:THR:O	2.30	0.48
1:C:197:VAL:O	1:C:201:ILE:HG13	2.12	0.48
1:D:441:MET:O	1:D:442:ARG:C	2.51	0.48
1:E:242:TRP:CD1	1:E:278:LEU:HD13	2.47	0.48
1:C:334:LEU:HD23	1:C:335:LYS:H	1.78	0.48
1:B:282:TYR:HE2	1:B:284:GLU:HG2	1.78	0.48
1:B:287:SER:HA	1:B:339:ILE:O	2.13	0.48
1:D:417:ILE:HG13	1:D:420:ILE:CG1	2.34	0.48
1:B:372:ARG:NH2	1:B:438:VAL:HG11	2.29	0.48
1:B:392:HIS:O	1:B:395:SER:HB3	2.12	0.48
1:C:303:ILE:HG21	1:C:496:SER:HB2	1.95	0.48
1:E:237:ARG:HG2	1:E:237:ARG:O	2.13	0.48
1:A:242:TRP:CD1	1:A:276:LEU:HB3	2.48	0.48
1:A:447:GLU:C	1:A:449:LYS:H	2.17	0.48
1:C:199:ARG:HD2	1:C:203:ARG:NE	2.29	0.48
1:C:320:ILE:CG2	1:C:321:VAL:N	2.76	0.48
1:C:413:ARG:HG3	1:C:422:GLU:HB2	1.95	0.48
1:A:195:LEU:N	1:A:195:LEU:HD12	2.28	0.48
1:A:328:ALA:HB1	1:A:393:PHE:HE2	1.77	0.48
1:C:253:MET:HE2	1:C:325:GLY:HA2	1.96	0.48
1:C:302:MET:CE	1:C:467:MET:HG3	2.44	0.48
1:C:307:LEU:HD22	1:C:493:SER:HA	1.95	0.48
1:B:186:THR:O	1:B:186:THR:HG22	2.13	0.48
1:B:258:ASN:O	1:B:348:CYS:HA	2.13	0.48
1:C:414:ARG:HH11	1:C:414:ARG:CA	2.27	0.48
1:E:447:GLU:O	1:E:449:LYS:HG3	2.13	0.48
1:B:191:SER:HB2	1:B:250:GLN:HA	1.96	0.48
1:B:376:LYS:HD2	1:B:379:MET:HE3	1.95	0.48
1:C:406:LEU:CD2	1:C:406:LEU:H	2.27	0.48
1:B:253:MET:CE	1:B:325:GLY:N	2.77	0.48
1:C:183:ASP:O	1:C:187:SER:CB	2.62	0.48
1:D:459:GLN:HA	1:D:459:GLN:NE2	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:215:ARG:HG3	1:E:215:ARG:NH1	2.29	0.48
1:A:459:GLN:HA	1:A:465:ARG:CG	2.43	0.48
1:C:382:GLU:H	1:C:382:GLU:CD	2.16	0.48
1:D:454:ILE:HG23	1:D:458:TRP:CE3	2.49	0.48
1:D:342:LYS:HE3	1:D:348:CYS:HB3	1.96	0.47
1:D:431:LEU:CD1	1:D:450:LEU:HD13	2.44	0.47
1:A:315:HIS:HE1	1:A:326:LYS:HD2	1.79	0.47
1:A:232:LYS:HE3	1:A:234:PHE:CZ	2.49	0.47
1:A:252:VAL:HG23	1:A:253:MET:N	2.29	0.47
1:A:393:PHE:O	1:A:395:SER:N	2.47	0.47
1:C:211:ILE:HD12	2:C:3:JZO:C24	2.44	0.47
1:C:256:HIS:CD2	1:C:258:ASN:HB2	2.49	0.47
1:D:244:ARG:HH21	1:D:367:ILE:HG22	1.78	0.47
1:B:376:LYS:HD2	1:B:379:MET:CE	2.44	0.47
1:B:317:HIS:CB	1:B:397:LYS:HE3	2.36	0.47
1:C:365:ILE:CG2	1:C:366:ASP:N	2.77	0.47
1:D:216:PHE:CA	1:D:238:GLU:OE2	2.62	0.47
1:E:181:ILE:HA	1:E:184:MET:CE	2.45	0.47
1:E:310:ALA:CA	1:E:404:MET:HE3	2.44	0.47
1:E:285:HIS:HB2	1:E:341:VAL:HG22	1.97	0.47
1:C:464:LEU:H	1:C:464:LEU:HD22	1.79	0.47
1:A:434:SER:O	1:A:435:ASP:HB3	2.14	0.47
1:A:459:GLN:C	1:A:465:ARG:HH11	2.18	0.47
1:B:187:SER:O	1:B:189:SER:N	2.47	0.47
1:C:343:LYS:C	1:C:345:GLY:H	2.18	0.47
1:C:452:PRO:HD2	1:C:475:TRP:CZ3	2.49	0.47
1:A:248:ILE:CD1	1:A:355:ALA:HB3	2.44	0.47
1:A:331:HIS:HD2	1:A:333:ASP:N	2.12	0.47
1:C:415:CYS:SG	1:C:416:SER:N	2.88	0.47
1:E:181:ILE:O	1:E:184:MET:HG2	2.15	0.47
1:A:358:HIS:HB2	1:A:393:PHE:CD1	2.50	0.47
1:D:297:VAL:HG22	1:D:298:THR:O	2.15	0.47
1:D:424:TYR:OH	1:D:426:LEU:HD23	2.15	0.47
1:E:253:MET:CE	1:E:320:ILE:HG21	2.45	0.47
1:E:310:ALA:HB2	1:E:404:MET:HE1	1.97	0.47
1:A:294:ARG:HH11	1:A:294:ARG:HG2	1.78	0.47
1:B:215:ARG:HB3	1:B:215:ARG:CZ	2.44	0.47
1:C:365:ILE:HG22	1:C:366:ASP:N	2.30	0.47
1:C:381:PRO:HD3	1:C:402:TYR:CE2	2.50	0.47
1:C:189:SER:C	1:C:191:SER:H	2.17	0.47
1:C:268:LYS:HG3	1:C:275:GLN:HB2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ARG:NH1	1:D:244:ARG:HG2	2.30	0.47
1:E:460:SER:O	1:E:465:ARG:NH1	2.48	0.47
1:A:406:LEU:HD22	1:A:427:PRO:HB3	1.97	0.46
1:A:409:TRP:HA	1:A:471:MET:HE1	1.97	0.46
1:B:303:ILE:CD1	1:B:499:GLU:HG3	2.45	0.46
1:C:287:SER:C	1:C:289:PHE:N	2.69	0.46
1:E:199:ARG:O	1:E:203:ARG:HG3	2.14	0.46
1:E:232:LYS:HG2	1:E:234:PHE:CE1	2.50	0.46
3:E:2:PO4:O1	3:E:3:PO4:O1	2.34	0.46
1:A:450:LEU:O	1:A:451:ARG:HD2	2.14	0.46
1:C:320:ILE:CG2	1:C:321:VAL:H	2.24	0.46
1:C:457:ARG:HG3	1:C:458:TRP:HD1	1.80	0.46
1:D:403:ALA:O	1:D:407:VAL:HG23	2.16	0.46
1:D:460:SER:OG	1:D:461:CYS:N	2.49	0.46
1:A:459:GLN:OE1	1:A:465:ARG:HG2	2.16	0.46
1:B:251:THR:HG21	1:B:327:PRO:HD2	1.97	0.46
1:C:244:ARG:NH1	1:C:366:ASP:HB3	2.31	0.46
1:E:258:ASN:HD22	1:E:311:SER:HB2	1.79	0.46
1:E:287:SER:HA	1:E:339:ILE:O	2.16	0.46
1:E:294:ARG:HG2	1:E:294:ARG:HH11	1.80	0.46
1:E:432:VAL:CG2	1:E:433:PRO:HD2	2.46	0.46
1:A:184:MET:C	1:A:186:THR:H	2.18	0.46
1:A:199:ARG:O	1:A:203:ARG:HG2	2.16	0.46
1:A:412:ALA:C	1:A:414:ARG:H	2.18	0.46
3:D:15:PO4:O1	3:D:14:PO4:O4	2.34	0.46
1:D:389:ASN:HD21	1:D:391:LYS:CB	2.23	0.46
1:B:432:VAL:HG13	1:B:433:PRO:HD2	1.97	0.46
1:B:449:LYS:HB2	1:B:449:LYS:NZ	2.31	0.46
1:C:302:MET:HE1	1:C:467:MET:HG3	1.97	0.46
1:B:195:LEU:N	1:B:195:LEU:HD12	2.31	0.46
1:B:334:LEU:O	1:B:335:LYS:HB3	2.16	0.46
1:D:429:TYR:CZ	1:D:430:ASP:OD2	2.69	0.46
1:D:185:THR:O	1:D:187:SER:N	2.49	0.46
1:A:365:ILE:O	1:A:367:ILE:N	2.49	0.46
1:C:409:TRP:CD1	1:C:471:MET:HE3	2.51	0.46
1:C:428:TYR:O	1:C:432:VAL:HG12	2.16	0.46
1:C:478:ASN:C	1:C:478:ASN:ND2	2.69	0.46
1:D:431:LEU:HD13	1:D:450:LEU:HD13	1.98	0.46
1:A:417:ILE:O	1:A:420:ILE:HG12	2.17	0.46
1:B:365:ILE:O	1:B:365:ILE:HG13	2.13	0.46
1:C:213:LYS:HG2	1:C:218:GLU:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:431:LEU:HD11	1:D:450:LEU:HD22	1.97	0.46
1:E:443:LYS:HG2	1:E:448:GLN:HE21	1.80	0.46
1:D:295:TYR:O	1:D:414:ARG:NH1	2.49	0.45
1:E:454:ILE:HG23	1:E:458:TRP:CE3	2.51	0.45
1:A:320:ILE:HB	1:A:326:LYS:H	1.80	0.45
1:A:413:ARG:NH1	1:A:423:ASP:O	2.49	0.45
1:A:455:PRO:HB2	1:A:458:TRP:CD1	2.51	0.45
1:C:406:LEU:O	1:C:410:GLU:HG3	2.16	0.45
1:E:385:ASP:C	1:E:385:ASP:OD2	2.54	0.45
1:A:409:TRP:HA	1:A:471:MET:CE	2.46	0.45
1:E:237:ARG:O	1:E:237:ARG:CG	2.64	0.45
1:E:342:LYS:HG2	1:E:346:THR:O	2.16	0.45
1:C:324:GLN:HG3	1:C:325:GLY:N	2.32	0.45
1:C:302:MET:HG3	1:C:411:ILE:CG2	2.45	0.45
1:D:435:ASP:N	1:D:436:PRO:HD3	2.31	0.45
1:E:285:HIS:CB	1:E:341:VAL:HG22	2.47	0.45
1:E:413:ARG:NH1	1:E:423:ASP:O	2.48	0.45
1:E:494:GLN:O	1:E:497:GLN:HB3	2.16	0.45
1:A:426:LEU:O	1:A:429:TYR:HB3	2.17	0.45
1:A:432:VAL:HG21	1:A:436:PRO:HB3	1.98	0.45
1:B:472:ARG:C	1:B:474:CYS:H	2.20	0.45
1:B:479:GLY:HA2	1:B:482:ARG:HD2	1.99	0.45
1:D:310:ALA:HA	1:D:404:MET:HE2	1.98	0.45
1:D:443:LYS:HA	1:D:447:GLU:HG3	1.98	0.45
1:A:294:ARG:NH1	1:A:294:ARG:HG2	2.32	0.45
1:B:200:THR:O	1:B:204:THR:HB	2.17	0.45
1:B:492:LEU:HD12	1:B:492:LEU:HA	1.65	0.45
1:C:278:LEU:HD12	1:C:278:LEU:HA	1.81	0.45
1:C:418:GLY:C	1:C:420:ILE:H	2.20	0.45
1:C:310:ALA:HA	1:C:404:MET:CE	2.46	0.45
1:A:331:HIS:CD2	1:A:333:ASP:H	2.33	0.45
1:B:342:LYS:HD3	1:B:346:THR:HG22	1.99	0.45
1:B:412:ALA:O	1:B:414:ARG:N	2.50	0.45
1:C:340:LEU:O	1:C:347:CYS:HA	2.17	0.45
1:C:407:VAL:O	1:C:408:PHE:C	2.54	0.45
1:E:459:GLN:NE2	1:E:459:GLN:HA	2.32	0.45
1:E:461:CYS:HB3	1:E:464:LEU:HD23	1.98	0.45
1:A:251:THR:HG21	1:A:357:ARG:HD3	1.98	0.45
1:A:215:ARG:HH21	1:A:354:LEU:HD11	1.82	0.45
1:D:372:ARG:HH11	1:D:438:VAL:HG21	1.81	0.45
1:A:458:TRP:CG	1:A:464:LEU:HD11	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:MET:O	1:B:407:VAL:HB	2.17	0.45
1:C:332:ARG:HG3	1:C:356:VAL:HG12	1.98	0.45
1:E:244:ARG:HH21	1:E:248:ILE:HD11	1.82	0.45
1:E:299:VAL:O	1:E:303:ILE:HG13	2.16	0.45
1:A:292:LEU:HD21	1:A:411:ILE:HA	1.98	0.44
1:A:294:ARG:O	1:A:295:TYR:CG	2.70	0.44
1:B:204:THR:CG2	1:B:224:TRP:NE1	2.78	0.44
1:B:431:LEU:HD13	1:B:450:LEU:HD13	1.99	0.44
1:B:432:VAL:HG13	1:B:433:PRO:CD	2.47	0.44
1:C:268:LYS:CG	1:C:275:GLN:HB2	2.46	0.44
1:C:486:LEU:O	1:C:489:LYS:HB3	2.18	0.44
1:D:310:ALA:HA	1:D:404:MET:HE1	2.00	0.44
1:D:329:ILE:HA	1:D:356:VAL:O	2.17	0.44
1:D:413:ARG:NH1	1:D:423:ASP:O	2.50	0.44
1:D:469:LYS:HD2	1:D:472:ARG:HH21	1.83	0.44
1:E:198:GLN:HE22	1:E:250:GLN:HE22	1.64	0.44
1:A:430:ASP:OD1	1:A:431:LEU:HG	2.18	0.44
1:A:432:VAL:CG2	1:A:433:PRO:HD2	2.47	0.44
1:A:435:ASP:N	1:A:436:PRO:HD3	2.32	0.44
1:B:377:ARG:HH12	3:B:11:PO4:P	2.40	0.44
1:E:310:ALA:HA	1:E:404:MET:CE	2.47	0.44
1:E:412:ALA:C	1:E:414:ARG:H	2.21	0.44
1:A:484:THR:O	1:A:488:ILE:HG13	2.17	0.44
1:C:389:ASN:HD21	1:C:391:LYS:HB3	1.81	0.44
1:E:358:HIS:HB2	1:E:393:PHE:CD1	2.52	0.44
1:A:393:PHE:O	1:A:394:GLU:C	2.56	0.44
1:B:412:ALA:C	1:B:414:ARG:N	2.71	0.44
1:B:487:ARG:O	1:B:491:THR:HG23	2.18	0.44
1:C:342:LYS:HB2	1:C:344:ASN:OD1	2.17	0.44
1:D:294:ARG:HD3	1:D:295:TYR:CZ	2.52	0.44
1:B:178:LYS:HD3	1:B:227:GLU:OE2	2.17	0.44
1:B:204:THR:HG22	1:B:224:TRP:HE1	1.81	0.44
1:B:416:SER:HA	1:B:421:HIS:HB3	1.98	0.44
1:E:237:ARG:NH1	1:E:238:GLU:OE2	2.51	0.44
1:A:298:THR:CG2	1:A:299:VAL:N	2.80	0.44
1:B:376:LYS:HA	1:B:379:MET:HE2	1.95	0.44
1:C:319:GLU:OE2	1:C:360:SER:HB3	2.17	0.44
1:D:217:GLY:CA	1:D:238:GLU:OE1	2.66	0.44
1:C:319:GLU:HG2	1:C:320:ILE:N	2.31	0.44
1:C:405:GLY:HA3	1:C:475:TRP:HE1	1.83	0.44
1:E:489:LYS:O	1:E:493:SER:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:THR:OG1	1:A:324:GLN:N	2.51	0.43
1:B:432:VAL:HG11	1:B:436:PRO:CG	2.48	0.43
1:C:368:ALA:N	1:C:369:PRO:CD	2.80	0.43
1:C:409:TRP:HD1	1:C:471:MET:HE3	1.82	0.43
1:C:483:LEU:CD1	1:C:488:ILE:HD11	2.46	0.43
1:E:184:MET:HG3	1:E:185:THR:N	2.33	0.43
1:E:211:ILE:HD12	2:E:5:JZO:C24	2.49	0.43
1:A:331:HIS:HE1	1:A:350:ALA:O	2.01	0.43
1:A:412:ALA:C	1:A:414:ARG:N	2.70	0.43
1:B:385:ASP:O	1:B:387:SER:N	2.51	0.43
1:D:232:LYS:HG2	1:D:234:PHE:CE1	2.54	0.43
1:D:424:TYR:O	1:D:425:GLN:NE2	2.51	0.43
1:A:381:PRO:HG3	1:A:445:VAL:HG12	1.99	0.43
1:A:425:GLN:HB3	1:A:429:TYR:CD2	2.52	0.43
1:C:417:ILE:H	1:C:420:ILE:HG13	1.83	0.43
1:C:425:GLN:CA	1:C:425:GLN:HE21	2.28	0.43
1:C:476:TYR:C	1:C:478:ASN:N	2.72	0.43
1:C:478:ASN:ND2	1:C:480:ALA:H	2.16	0.43
1:D:309:THR:HG22	1:D:404:MET:CE	2.47	0.43
1:C:422:GLU:OE1	1:C:422:GLU:N	2.51	0.43
1:B:209:GLU:OE2	1:B:221:ARG:NH1	2.51	0.43
1:C:313:LEU:N	1:C:349:ILE:HD11	2.34	0.43
1:C:334:LEU:HD23	1:C:335:LYS:N	2.34	0.43
1:C:406:LEU:HB3	1:C:427:PRO:HG2	1.99	0.43
1:C:496:SER:C	1:C:498:GLN:H	2.21	0.43
1:A:358:HIS:HB2	1:A:393:PHE:CE1	2.53	0.43
1:C:199:ARG:O	1:C:203:ARG:HG3	2.18	0.43
1:C:217:GLY:HA3	1:C:234:PHE:HA	2.01	0.43
1:C:262:PHE:CD1	2:C:3:JZO:H1	2.54	0.43
1:C:297:VAL:HG13	1:C:298:THR:N	2.32	0.43
1:C:476:TYR:O	1:C:477:ALA:C	2.56	0.43
1:B:269:ASP:HB3	1:B:270:ASN:H	1.63	0.43
1:B:385:ASP:HB2	1:B:442:ARG:HH21	1.83	0.43
1:E:306:ALA:HB1	1:E:492:LEU:HD21	2.00	0.43
1:E:461:CYS:SG	1:E:464:LEU:HD23	2.59	0.43
1:B:300:GLU:HG3	1:B:501:ILE:HD13	2.01	0.43
1:C:234:PHE:CE1	1:C:278:LEU:HD22	2.54	0.43
1:D:234:PHE:CE1	1:D:278:LEU:HD22	2.53	0.43
1:D:438:VAL:HG12	1:D:439:GLU:N	2.33	0.43
1:E:297:VAL:O	1:E:415:CYS:HA	2.19	0.43
1:E:492:LEU:HD12	1:E:492:LEU:HA	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:499:GLU:HG3	1:A:500:GLY:H	1.84	0.43
1:B:319:GLU:HB2	1:B:328:ALA:HB2	2.01	0.43
1:C:181:ILE:HA	1:C:184:MET:HE2	2.00	0.43
1:D:331:HIS:HD2	1:D:333:ASP:N	2.12	0.43
1:D:371:HIS:N	1:D:371:HIS:ND1	2.66	0.43
1:E:416:SER:HA	1:E:421:HIS:HB3	2.00	0.43
1:B:495:LEU:O	1:B:499:GLU:HG2	2.18	0.43
1:C:414:ARG:HH11	1:C:414:ARG:HA	1.84	0.43
1:C:484:THR:O	1:C:488:ILE:HG13	2.19	0.43
1:B:343:LYS:HG3	3:B:6:PO4:P	2.59	0.42
1:C:372:ARG:NH2	1:C:438:VAL:HG11	2.34	0.42
1:C:488:ILE:HG22	1:C:488:ILE:O	2.18	0.42
1:E:254:LEU:HA	1:E:254:LEU:HD12	1.80	0.42
1:A:215:ARG:NH2	1:A:354:LEU:HD11	2.33	0.42
1:A:409:TRP:CE2	1:A:452:PRO:HB3	2.54	0.42
1:B:389:ASN:HD21	1:B:391:LYS:HB2	1.84	0.42
1:C:432:VAL:HA	1:C:433:PRO:HD3	1.81	0.42
1:C:483:LEU:HD13	1:C:488:ILE:CD1	2.48	0.42
1:D:181:ILE:HG12	1:D:184:MET:HE2	2.01	0.42
1:A:315:HIS:CE1	1:A:326:LYS:CD	3.02	0.42
1:B:412:ALA:C	1:B:414:ARG:H	2.23	0.42
1:C:297:VAL:CG1	1:C:415:CYS:HA	2.49	0.42
1:C:492:LEU:HD12	1:C:495:LEU:HD23	2.01	0.42
1:D:197:VAL:O	1:D:201:ILE:HG13	2.19	0.42
1:D:262:PHE:HD1	2:D:4:JZO:C1	2.31	0.42
1:D:429:TYR:CE1	1:D:430:ASP:HB3	2.53	0.42
1:E:180:LEU:HD13	1:E:201:ILE:HD11	2.02	0.42
1:E:199:ARG:HD2	1:E:203:ARG:NE	2.34	0.42
1:E:479:GLY:HA2	1:E:482:ARG:CZ	2.49	0.42
1:A:335:LYS:O	1:A:339:ILE:HG13	2.19	0.42
1:C:237:ARG:CD	1:C:238:GLU:OE2	2.66	0.42
1:D:234:PHE:HB3	1:D:238:GLU:HG3	2.01	0.42
1:A:198:GLN:HB3	1:A:264:ALA:HB1	2.02	0.42
1:A:447:GLU:C	1:A:449:LYS:N	2.73	0.42
1:A:456:ASN:O	1:A:458:TRP:N	2.52	0.42
1:B:319:GLU:C	1:B:320:ILE:HG13	2.39	0.42
1:B:388:ILE:HG13	1:B:395:SER:OG	2.19	0.42
1:C:298:THR:O	1:C:301:GLY:N	2.52	0.42
1:C:402:TYR:C	1:C:402:TYR:CD1	2.93	0.42
1:C:410:GLU:O	1:C:414:ARG:HG2	2.19	0.42
1:E:377:ARG:NH1	3:E:3:PO4:O4	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:O	1:A:186:THR:N	2.52	0.42
1:B:342:LYS:HB2	1:B:346:THR:HG22	2.02	0.42
1:B:478:ASN:OD1	1:B:478:ASN:C	2.58	0.42
1:C:367:ILE:HG22	1:C:367:ILE:O	2.19	0.42
1:C:464:LEU:CD2	1:C:464:LEU:H	2.32	0.42
1:D:208:GLN:C	1:D:209:GLU:HG3	2.40	0.42
1:D:443:LYS:HA	1:D:447:GLU:HG2	1.99	0.42
1:D:444:VAL:O	1:D:450:LEU:HB2	2.20	0.42
1:E:310:ALA:N	1:E:404:MET:HE3	2.34	0.42
1:E:389:ASN:ND2	1:E:391:LYS:CB	2.82	0.42
1:C:379:MET:CE	1:C:383:VAL:HG11	2.49	0.42
1:C:418:GLY:C	1:C:420:ILE:N	2.73	0.42
1:D:473:GLU:O	1:D:482:ARG:HA	2.19	0.42
1:E:270:ASN:O	1:E:271:GLY:C	2.57	0.42
1:B:409:TRP:CD1	1:B:471:MET:CE	3.03	0.42
1:C:216:PHE:HA	1:C:238:GLU:HG3	2.02	0.42
1:C:259:ILE:O	1:C:260:LEU:C	2.57	0.42
1:C:470:ILE:HG21	1:C:488:ILE:HG23	2.01	0.42
1:D:364:THR:C	1:D:365:ILE:HD12	2.39	0.42
1:A:315:HIS:ND1	1:A:315:HIS:O	2.52	0.42
1:A:317:HIS:HE1	1:A:400:ASP:HB2	1.84	0.42
1:A:454:ILE:O	1:A:455:PRO:C	2.58	0.42
1:A:493:SER:O	1:A:496:SER:HB3	2.19	0.42
1:B:205:ILE:CG2	1:B:206:VAL:N	2.83	0.42
1:B:294:ARG:O	1:B:294:ARG:HD3	2.20	0.42
1:C:215:ARG:HH11	1:C:215:ARG:CG	2.32	0.42
1:C:287:SER:C	1:C:289:PHE:H	2.23	0.42
1:C:307:LEU:HD12	1:C:307:LEU:O	2.19	0.42
1:C:334:LEU:HD21	1:C:339:ILE:HD11	2.02	0.42
1:E:180:LEU:O	1:E:181:ILE:C	2.58	0.42
1:A:199:ARG:HD2	1:A:266:ASP:OD2	2.20	0.42
1:C:177:LEU:HA	1:C:177:LEU:HD23	1.85	0.42
1:A:257:GLU:O	1:A:257:GLU:HG2	2.19	0.41
1:B:331:HIS:O	1:B:332:ARG:HB2	2.20	0.41
1:C:253:MET:HG3	1:C:253:MET:O	2.20	0.41
1:C:333:ASP:HB2	1:C:354:LEU:HD12	2.02	0.41
1:C:486:LEU:HD13	1:C:486:LEU:O	2.20	0.41
1:A:308:SER:HB3	1:A:346:THR:HG22	2.02	0.41
1:A:413:ARG:HH11	1:A:413:ARG:CG	2.32	0.41
1:A:424:TYR:OH	1:A:426:LEU:HD23	2.21	0.41
1:B:294:ARG:HD2	1:B:295:TYR:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:490:LYS:HB2	1:B:490:LYS:HE3	1.86	0.41
1:C:254:LEU:HD12	1:C:254:LEU:HA	1.88	0.41
1:C:414:ARG:HD2	1:C:414:ARG:HA	1.78	0.41
1:D:391:LYS:HG2	1:D:391:LYS:O	2.20	0.41
1:A:297:VAL:CG2	1:A:298:THR:N	2.83	0.41
1:A:310:ALA:HA	1:A:404:MET:HE1	2.01	0.41
1:B:195:LEU:H	1:B:195:LEU:HD12	1.85	0.41
1:B:234:PHE:CE1	1:B:278:LEU:HD22	2.55	0.41
1:B:393:PHE:O	1:B:395:SER:N	2.53	0.41
1:B:459:GLN:O	1:B:465:ARG:HD3	2.20	0.41
1:C:443:LYS:O	1:C:448:GLN:NE2	2.54	0.41
1:D:344:ASN:OD1	1:D:346:THR:CG2	2.68	0.41
1:E:455:PRO:HD2	1:E:458:TRP:CE2	2.55	0.41
1:B:193:LEU:HB3	1:B:194:PRO:CD	2.50	0.41
1:C:471:MET:HE1	1:C:475:TRP:HH2	1.84	0.41
1:D:214:GLY:O	1:D:215:ARG:C	2.59	0.41
1:D:278:LEU:HD12	1:D:278:LEU:HA	1.91	0.41
1:E:201:ILE:O	1:E:205:ILE:HG13	2.21	0.41
1:A:429:TYR:CG	1:A:430:ASP:N	2.88	0.41
1:B:426:LEU:O	1:B:429:TYR:HB3	2.20	0.41
1:D:185:THR:C	1:D:187:SER:N	2.73	0.41
1:B:330:ALA:HB3	1:B:356:VAL:HG22	2.02	0.41
1:C:208:GLN:NE2	1:C:223:LYS:HD2	2.35	0.41
1:C:416:SER:C	1:C:417:ILE:HD12	2.41	0.41
1:D:180:LEU:HD13	1:D:201:ILE:HD11	2.03	0.41
1:E:194:PRO:O	1:E:197:VAL:N	2.54	0.41
1:E:253:MET:CE	1:E:325:GLY:HA2	2.50	0.41
1:A:244:ARG:HD2	1:A:244:ARG:HA	1.85	0.41
1:A:285:HIS:HB3	1:A:341:VAL:HG22	2.03	0.41
1:A:494:GLN:O	1:A:497:GLN:N	2.50	0.41
1:C:240:ARG:CG	1:C:240:ARG:HH11	2.33	0.41
1:D:455:PRO:HD2	1:D:458:TRP:CE3	2.56	0.41
1:D:462:GLU:O	1:D:463:ALA:C	2.59	0.41
1:D:498:GLN:O	1:D:499:GLU:CG	2.69	0.41
1:E:185:THR:O	1:E:185:THR:HG22	2.21	0.41
1:E:337:LYS:NZ	3:E:2:PO4:O1	2.49	0.41
1:A:317:HIS:NE2	1:A:400:ASP:OD2	2.53	0.41
1:D:331:HIS:CE1	1:D:350:ALA:O	2.69	0.41
1:A:256:HIS:CD2	1:A:258:ASN:H	2.38	0.41
1:A:258:ASN:OD1	1:A:311:SER:HB2	2.21	0.41
1:B:393:PHE:C	1:B:395:SER:N	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:LEU:CD1	1:B:450:LEU:HD13	2.51	0.41
1:C:330:ALA:HB3	1:C:356:VAL:HG13	2.02	0.41
1:C:458:TRP:HB3	1:C:464:LEU:HB3	2.02	0.41
1:C:398:ARG:HD3	1:C:479:GLY:C	2.42	0.41
1:C:496:SER:C	1:C:498:GLN:N	2.75	0.41
1:D:215:ARG:HG2	1:D:215:ARG:NH1	2.35	0.41
1:D:305:LEU:HD23	1:D:345:GLY:O	2.21	0.41
1:E:215:ARG:HG3	1:E:215:ARG:HH11	1.84	0.41
1:B:417:ILE:O	1:B:420:ILE:HG12	2.20	0.41
1:B:455:PRO:HD2	1:B:458:TRP:CD2	2.56	0.41
1:C:310:ALA:HA	1:C:404:MET:HE1	2.02	0.41
1:A:328:ALA:HB3	1:A:358:HIS:HB3	2.03	0.41
1:A:476:TYR:C	1:A:478:ASN:H	2.24	0.41
1:C:331:HIS:CD2	1:C:333:ASP:C	2.94	0.41
1:E:384:LEU:O	1:E:442:ARG:HG3	2.21	0.41
1:A:278:LEU:HA	1:A:278:LEU:HD23	1.95	0.40
1:C:216:PHE:HB3	1:C:238:GLU:HB3	2.03	0.40
1:C:478:ASN:ND2	1:C:480:ALA:HB3	2.37	0.40
1:D:492:LEU:HA	1:D:492:LEU:HD12	1.76	0.40
1:E:196:LEU:HA	1:E:196:LEU:HD12	1.93	0.40
1:E:437:SER:OG	1:E:440:GLU:HG3	2.22	0.40
1:E:459:GLN:NE2	1:E:465:ARG:HD2	2.35	0.40
1:A:283:HIS:H	2:A:1:JZO:C23	2.35	0.40
1:C:417:ILE:N	1:C:417:ILE:HD12	2.36	0.40
1:D:453:ASN:O	1:D:455:PRO:HD3	2.20	0.40
1:D:490:LYS:HE3	1:D:490:LYS:HB2	1.84	0.40
1:E:181:ILE:HA	1:E:184:MET:HE2	2.04	0.40
1:A:428:TYR:CE2	1:A:452:PRO:HD3	2.56	0.40
1:B:234:PHE:CD1	1:B:234:PHE:N	2.89	0.40
1:C:286:GLY:O	1:C:340:LEU:HA	2.22	0.40
1:D:235:SER:O	1:D:236:SER:C	2.60	0.40
1:B:424:TYR:C	1:B:424:TYR:CD2	2.95	0.40
1:C:181:ILE:HA	1:C:184:MET:HE3	2.03	0.40
1:C:376:LYS:C	1:C:378:TYR:N	2.73	0.40
1:D:297:VAL:CG2	1:D:301:GLY:HA3	2.51	0.40
1:E:497:GLN:C	1:E:499:GLU:H	2.24	0.40
1:A:398:ARG:HG3	1:A:398:ARG:NH1	2.36	0.40
1:A:453:ASN:O	1:A:455:PRO:HD3	2.21	0.40
1:C:350:ALA:O	1:C:351:ASP:HB3	2.22	0.40
1:C:494:GLN:HG3	1:C:497:GLN:NE2	2.36	0.40
1:D:441:MET:HE3	1:D:441:MET:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	324/342 (95%)	262 (81%)	44 (14%)	18 (6%)	2	5
1	B	318/342 (93%)	281 (88%)	31 (10%)	6 (2%)	8	26
1	C	328/342 (96%)	251 (76%)	61 (19%)	16 (5%)	2	7
1	D	328/342 (96%)	276 (84%)	38 (12%)	14 (4%)	2	8
1	E	328/342 (96%)	291 (89%)	28 (8%)	9 (3%)	5	17
All	All	1626/1710 (95%)	1361 (84%)	202 (12%)	63 (4%)	3	10

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	ARG
1	A	252	VAL
1	A	366	ASP
1	A	447	GLU
1	B	235	SER
1	B	386	ASP
1	D	252	VAL
1	D	253	MET
1	D	449	LYS
1	E	215	ARG
1	E	366	ASP
1	A	185	THR
1	A	253	MET
1	A	323	THR
1	A	363	ASP
1	A	365	ILE
1	A	386	ASP
1	A	436	PRO

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Mol	Chain	Res	Type
1	A	448	GLN
1	A	457	ARG
1	A	483	LEU
1	B	185	THR
1	B	188	GLY
1	C	252	VAL
1	C	318	MET
1	C	362	THR
1	C	377	ARG
1	C	419	GLY
1	D	186	THR
1	D	187	SER
1	D	190	GLY
1	E	271	GLY
1	E	498	GLN
1	A	387	SER
1	A	394	GLU
1	B	186	THR
1	C	386	ASP
1	C	389	ASN
1	C	460	SER
1	C	477	ALA
1	D	189	SER
1	D	369	PRO
1	E	483	LEU
1	A	355	ALA
1	B	252	VAL
1	C	367	ILE
1	D	325	GLY
1	D	431	LEU
1	D	455	PRO
1	D	460	SER
1	E	252	VAL
1	C	433	PRO
1	C	473	GLU
1	E	253	MET
1	A	446	CYS
1	C	332	ARG
1	D	447	GLU
1	E	369	PRO
1	C	436	PRO
1	E	433	PRO

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Mol	Chain	Res	Type
1	C	444	VAL
1	D	388	ILE
1	C	188	GLY

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	281/294 (96%)	264 (94%)	17 (6%)	19	48
1	B	278/294 (95%)	252 (91%)	26 (9%)	8	26
1	C	282/294 (96%)	256 (91%)	26 (9%)	9	27
1	D	282/294 (96%)	255 (90%)	27 (10%)	8	24
1	E	282/294 (96%)	256 (91%)	26 (9%)	9	27
All	All	1405/1470 (96%)	1283 (91%)	122 (9%)	10	30

All (122) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	199	ARG
1	A	209	GLU
1	A	229	VAL
1	A	267	ASN
1	A	269	ASP
1	A	270	ASN
1	A	307	LEU
1	A	334	LEU
1	A	341	VAL
1	A	346	THR
1	A	364	THR
1	A	382	GLU
1	A	457	ARG
1	A	458	TRP
1	A	472	ARG
1	A	486	LEU

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Mol	Chain	Res	Type
1	A	491	THR
1	B	199	ARG
1	B	204	THR
1	B	209	GLU
1	B	229	VAL
1	B	233	ILE
1	B	238	GLU
1	B	250	GLN
1	B	255	ARG
1	B	269	ASP
1	B	272	THR
1	B	278	LEU
1	B	292	LEU
1	B	294	ARG
1	B	307	LEU
1	B	334	LEU
1	B	341	VAL
1	B	342	LYS
1	B	346	THR
1	B	356	VAL
1	B	382	GLU
1	B	391	LYS
1	B	432	VAL
1	B	464	LEU
1	B	486	LEU
1	B	491	THR
1	B	492	LEU
1	C	177	LEU
1	C	195	LEU
1	C	209	GLU
1	C	215	ARG
1	C	216	PHE
1	C	229	VAL
1	C	240	ARG
1	C	241	SER
1	C	244	ARG
1	C	247	GLU
1	C	255	ARG
1	C	278	LEU
1	C	296	THR
1	C	297	VAL
1	C	326	LYS

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Mol	Chain	Res	Type
1	C	334	LEU
1	C	356	VAL
1	C	364	THR
1	C	379	MET
1	C	382	GLU
1	C	389	ASN
1	C	392	HIS
1	C	414	ARG
1	C	446	CYS
1	C	478	ASN
1	C	483	LEU
1	D	195	LEU
1	D	196	LEU
1	D	204	THR
1	D	209	GLU
1	D	216	PHE
1	D	229	VAL
1	D	231	VAL
1	D	244	ARG
1	D	269	ASP
1	D	272	THR
1	D	278	LEU
1	D	292	LEU
1	D	307	LEU
1	D	321	VAL
1	D	334	LEU
1	D	341	VAL
1	D	342	LYS
1	D	376	LYS
1	D	382	GLU
1	D	389	ASN
1	D	417	ILE
1	D	431	LEU
1	D	432	VAL
1	D	461	CYS
1	D	486	LEU
1	D	491	THR
1	D	492	LEU
1	E	171	ILE
1	E	178	LYS
1	E	204	THR
1	E	209	GLU

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Mol	Chain	Res	Type
1	E	215	ARG
1	E	229	VAL
1	E	238	GLU
1	E	257	GLU
1	E	267	ASN
1	E	278	LEU
1	E	284	GLU
1	E	292	LEU
1	E	307	LEU
1	E	324	GLN
1	E	342	LYS
1	E	356	VAL
1	E	364	THR
1	E	376	LYS
1	E	382	GLU
1	E	389	ASN
1	E	404	MET
1	E	442	ARG
1	E	451	ARG
1	E	456	ASN
1	E	491	THR
1	E	497	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	250	GLN
1	A	267	ASN
1	A	270	ASN
1	A	331	HIS
1	A	448	GLN
1	B	250	GLN
1	B	256	HIS
1	B	258	ASN
1	B	315	HIS
1	B	331	HIS
1	B	389	ASN
1	B	421	HIS
1	B	459	GLN
1	C	208	GLN
1	C	250	GLN
1	C	256	HIS

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Mol	Chain	Res	Type
1	C	258	ASN
1	C	331	HIS
1	C	370	ASN
1	C	389	ASN
1	C	425	GLN
1	C	453	ASN
1	C	459	GLN
1	C	478	ASN
1	C	497	GLN
1	D	250	GLN
1	D	256	HIS
1	D	258	ASN
1	D	293	ASN
1	D	315	HIS
1	D	324	GLN
1	D	331	HIS
1	D	370	ASN
1	D	389	ASN
1	D	392	HIS
1	D	425	GLN
1	D	459	GLN
1	D	497	GLN
1	E	250	GLN
1	E	256	HIS
1	E	258	ASN
1	E	315	HIS
1	E	324	GLN
1	E	331	HIS
1	E	370	ASN
1	E	389	ASN
1	E	448	GLN
1	E	459	GLN
1	E	478	ASN
1	E	497	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 carbohydrates in this entry.

5.6 Ligand geometry i

18 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
3	PO4	E	2	-	4,4,4	1.73	1 (25%)	6,6,6	0.43	0
3	PO4	A	22	-	4,4,4	1.67	0	6,6,6	0.45	0
3	PO4	E	1	-	4,4,4	1.66	1 (25%)	6,6,6	0.44	0
2	JZO	E	5	-	26,30,30	1.51	5 (19%)	37,43,43	1.63	8 (21%)
3	PO4	B	12	-	4,4,4	1.74	0	6,6,6	0.43	0
3	PO4	A	21	-	4,4,4	1.62	0	6,6,6	0.44	0
2	JZO	A	1	-	26,30,30	1.53	5 (19%)	37,43,43	1.56	8 (21%)
3	PO4	C	10	-	4,4,4	1.59	0	6,6,6	0.46	0
3	PO4	D	15	-	4,4,4	1.84	2 (50%)	6,6,6	0.39	0
2	JZO	B	2	-	26,30,30	1.50	6 (23%)	37,43,43	1.52	7 (18%)
3	PO4	D	14	-	4,4,4	1.76	1 (25%)	6,6,6	0.42	0
3	PO4	E	3	-	4,4,4	1.78	1 (25%)	6,6,6	0.46	0
3	PO4	B	11	-	4,4,4	1.66	0	6,6,6	0.41	0
2	JZO	C	3	-	26,30,30	1.46	6 (23%)	37,43,43	1.61	7 (18%)
3	PO4	D	13	-	4,4,4	1.66	0	6,6,6	0.44	0
3	PO4	A	9	-	4,4,4	1.70	0	6,6,6	0.43	0
3	PO4	B	6	-	4,4,4	1.51	0	6,6,6	0.45	0
2	JZO	D	4	-	26,30,30	1.61	7 (26%)	37,43,43	1.54	8 (21%)

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	JZO	E	5	-	-	0/11/11/11	0/4/4/4
2	JZO	A	1	-	-	0/11/11/11	0/4/4/4
2	JZO	C	3	-	-	0/11/11/11	0/4/4/4
2	JZO	B	2	-	-	0/11/11/11	0/4/4/4
2	JZO	D	4	-	-	0/11/11/11	0/4/4/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4	JZO	C20-C19	3.33	1.43	1.36
2	A	1	JZO	C20-C19	3.10	1.43	1.36
2	E	5	JZO	C20-C19	3.00	1.42	1.36
2	B	2	JZO	C20-C19	2.97	1.42	1.36
2	C	3	JZO	C20-C19	2.94	1.42	1.36
2	D	4	JZO	C11-N12	2.83	1.41	1.36
2	E	5	JZO	C23-N22	2.71	1.38	1.32
2	D	4	JZO	C23-N22	2.47	1.37	1.32
2	C	3	JZO	C23-N22	2.38	1.37	1.32
2	B	2	JZO	C23-N22	2.37	1.37	1.32
2	D	4	JZO	C7-C8	2.37	1.44	1.39
2	A	1	JZO	C11-N12	2.27	1.40	1.36
2	B	2	JZO	C7-C8	2.26	1.44	1.39
2	A	1	JZO	C23-N22	2.23	1.37	1.32
2	E	5	JZO	C7-C8	2.23	1.44	1.39
3	D	15	PO4	P-O3	-2.23	1.47	1.54
2	C	3	JZO	C11-N12	2.19	1.40	1.36
2	D	4	JZO	C6-C7	2.18	1.43	1.38
2	A	1	JZO	C5-C4	2.17	1.43	1.38
2	A	1	JZO	C7-C8	2.17	1.44	1.39
3	E	3	PO4	P-O2	-2.17	1.48	1.54
2	D	4	JZO	C27-C18	2.16	1.43	1.38
2	D	4	JZO	C5-C4	2.13	1.43	1.38
3	D	14	PO4	P-O4	-2.11	1.48	1.54
2	E	5	JZO	C19-C18	2.09	1.43	1.39
2	B	2	JZO	C11-N12	2.09	1.40	1.36
2	B	2	JZO	C6-C7	2.08	1.43	1.38
2	E	5	JZO	C27-C18	2.08	1.43	1.38
2	C	3	JZO	C19-C18	2.06	1.43	1.39
2	C	3	JZO	C24-N25	2.05	1.36	1.32
3	D	15	PO4	P-O4	-2.04	1.48	1.54
2	B	2	JZO	C19-C18	2.04	1.43	1.39
3	E	1	PO4	P-O3	-2.04	1.48	1.54
2	C	3	JZO	C27-C18	2.03	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	PO4	P-O3	-2.01	1.48	1.54

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	5	JZO	C15-N14-C16	-4.28	124.52	129.46
2	C	3	JZO	C15-N14-C16	-4.17	124.65	129.46
2	A	1	JZO	C15-N14-C16	-3.99	124.86	129.46
2	B	2	JZO	C15-N14-C16	-3.92	124.94	129.46
2	C	3	JZO	C23-N22-C21	3.59	122.50	116.93
2	D	4	JZO	C23-N22-C21	3.52	122.38	116.93
2	E	5	JZO	C23-N22-C21	3.45	122.28	116.93
2	A	1	JZO	C23-N22-C21	3.45	122.27	116.93
2	E	5	JZO	C24-N25-C26	3.32	122.07	116.93
2	D	4	JZO	C15-N14-C16	-3.30	125.65	129.46
2	B	2	JZO	C23-N22-C21	3.26	121.98	116.93
2	D	4	JZO	C24-N25-C26	3.18	121.85	116.93
2	B	2	JZO	C24-N25-C26	3.09	121.72	116.93
2	A	1	JZO	C24-N25-C26	3.04	121.64	116.93
2	C	3	JZO	C24-N25-C26	2.89	121.41	116.93
2	E	5	JZO	C26-C21-N22	-2.80	118.33	121.00
2	A	1	JZO	C26-C21-N22	-2.70	118.42	121.00
2	C	3	JZO	C26-C21-N22	-2.64	118.48	121.00
2	D	4	JZO	C26-C21-N22	-2.61	118.50	121.00
2	D	4	JZO	C24-C23-N22	-2.61	118.56	122.77
2	C	3	JZO	C27-C26-N25	2.60	120.93	117.97
2	B	2	JZO	C26-C21-N22	-2.59	118.52	121.00
2	D	4	JZO	C27-C26-N25	2.58	120.91	117.97
2	E	5	JZO	C24-C23-N22	-2.51	118.72	122.77
2	E	5	JZO	C27-C26-N25	2.51	120.83	117.97
2	C	3	JZO	C24-C23-N22	-2.50	118.73	122.77
2	E	5	JZO	C15-N14-N12	2.45	125.85	121.93
2	C	3	JZO	C15-N14-N12	2.41	125.79	121.93
2	A	1	JZO	C24-C23-N22	-2.41	118.88	122.77
2	A	1	JZO	C27-C26-N25	2.39	120.69	117.97
2	B	2	JZO	C27-C26-N25	2.35	120.65	117.97
2	B	2	JZO	C24-C23-N22	-2.34	118.99	122.77
2	A	1	JZO	C15-N14-N12	2.22	125.48	121.93
2	B	2	JZO	C15-N14-N12	2.19	125.44	121.93
2	E	5	JZO	C23-C24-N25	-2.08	119.41	122.77
2	A	1	JZO	C23-C24-N25	-2.04	119.48	122.77
2	D	4	JZO	C8-C10-C11	2.04	130.92	126.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	4	JZO	C23-C24-N25	-2.00	119.54	122.77

There are no chirality outliers.

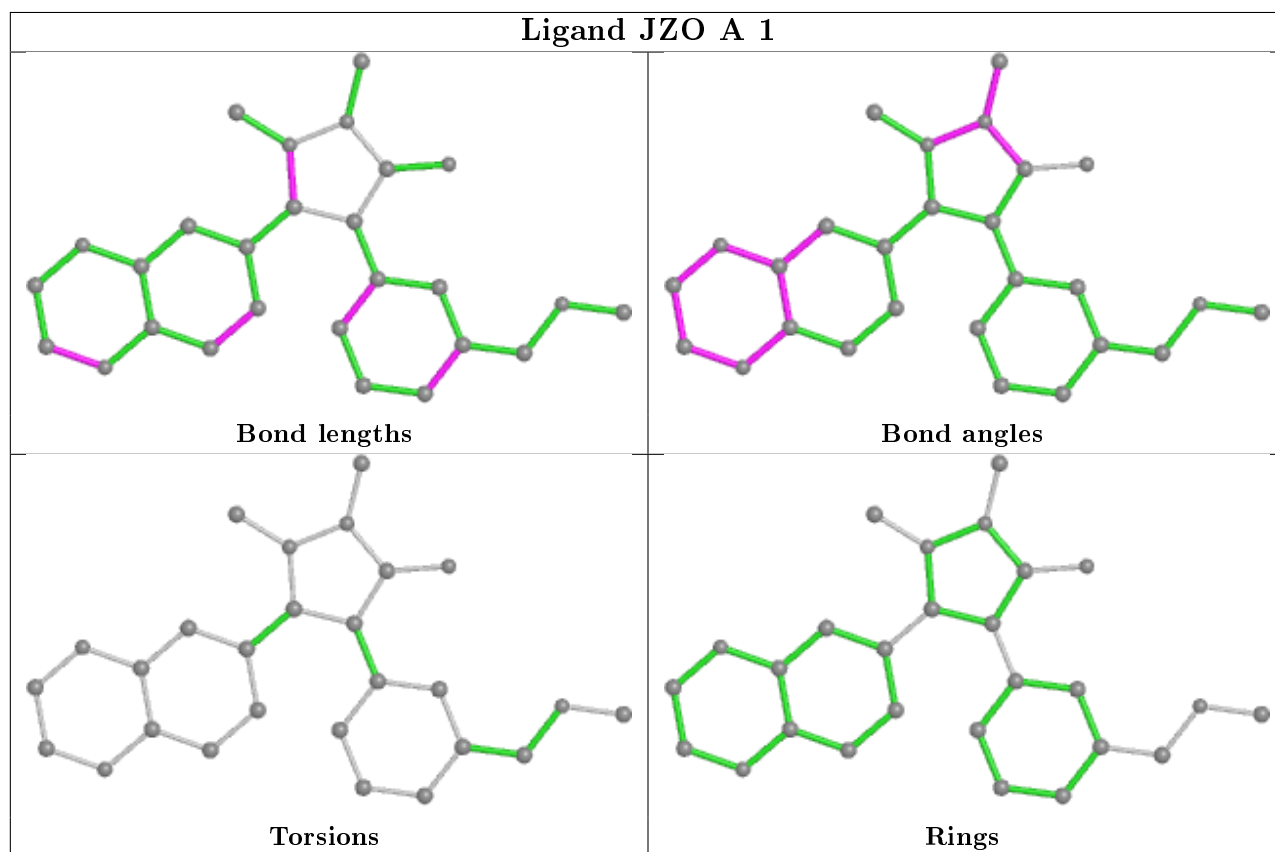
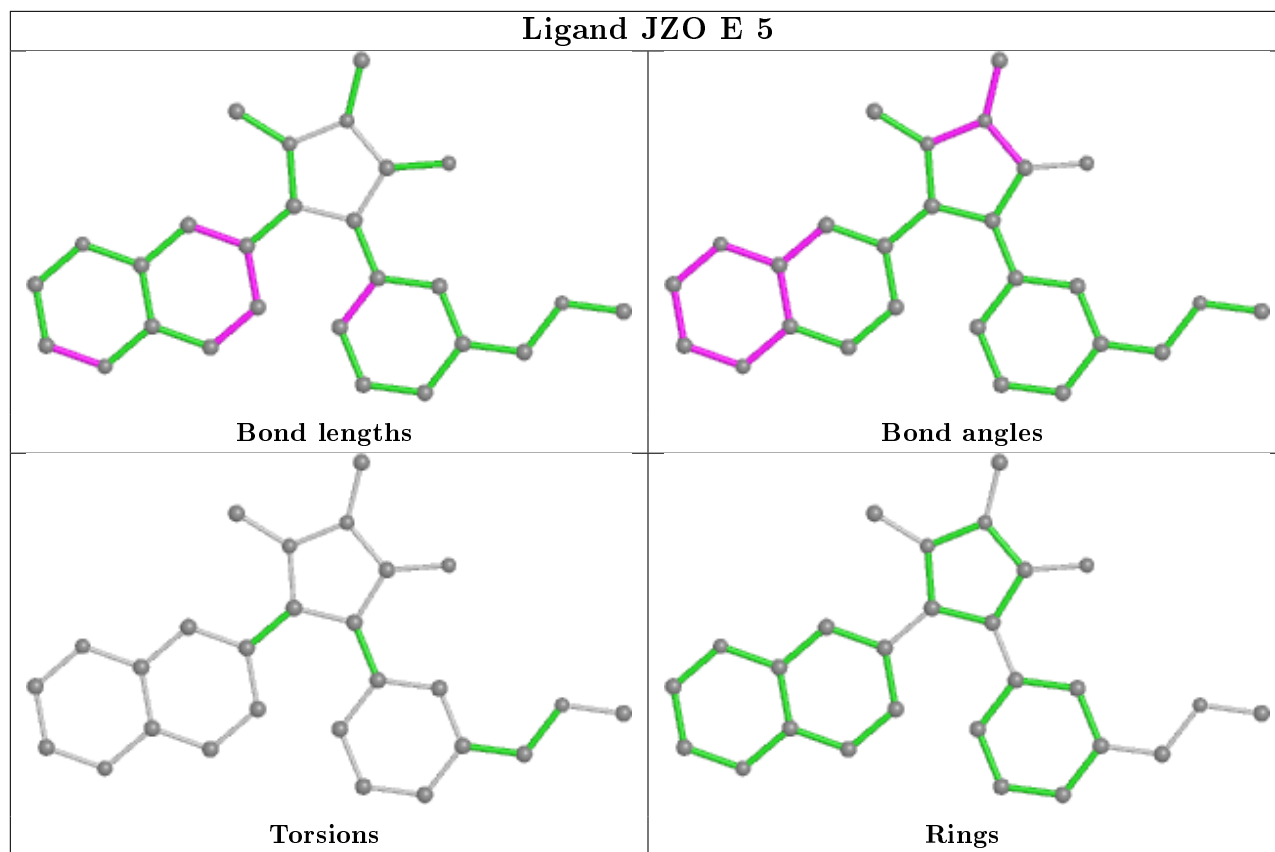
There are no torsion outliers.

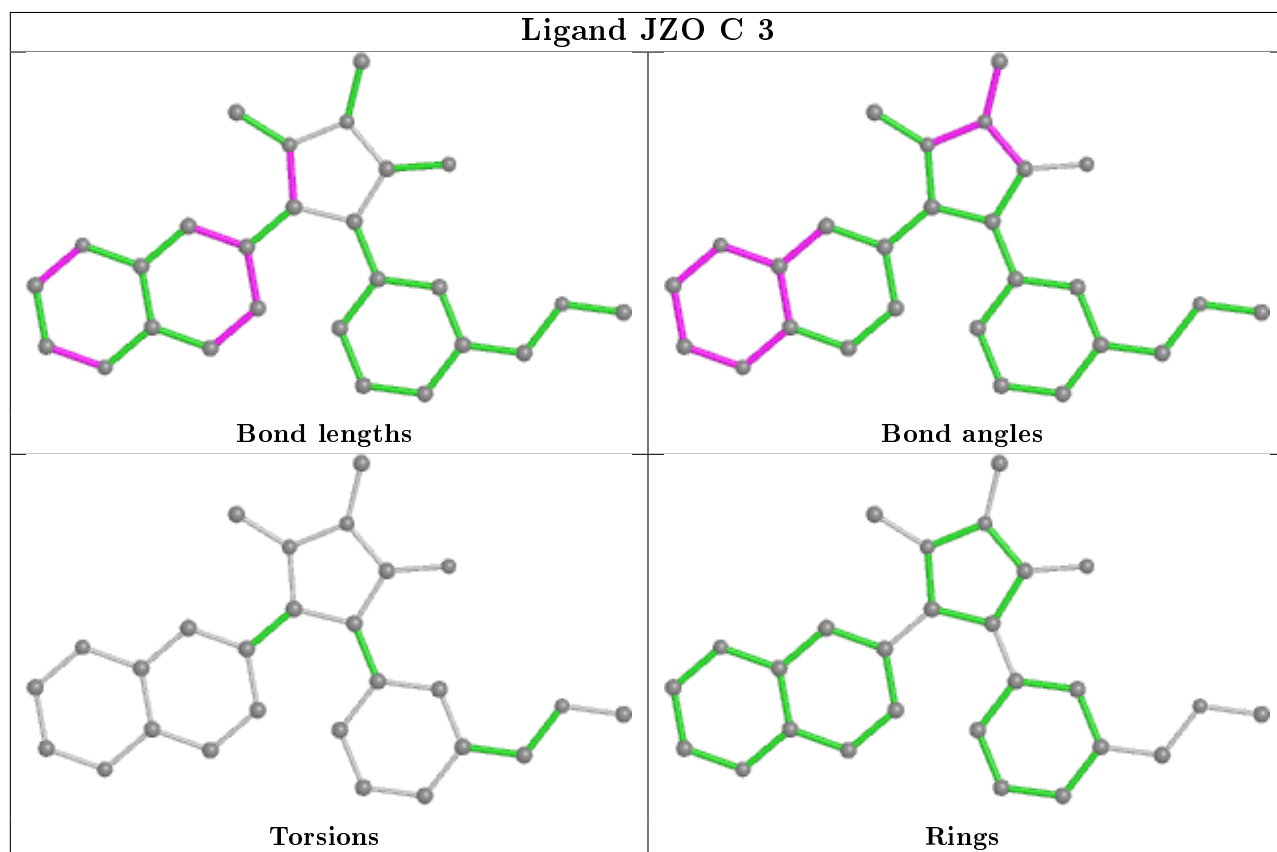
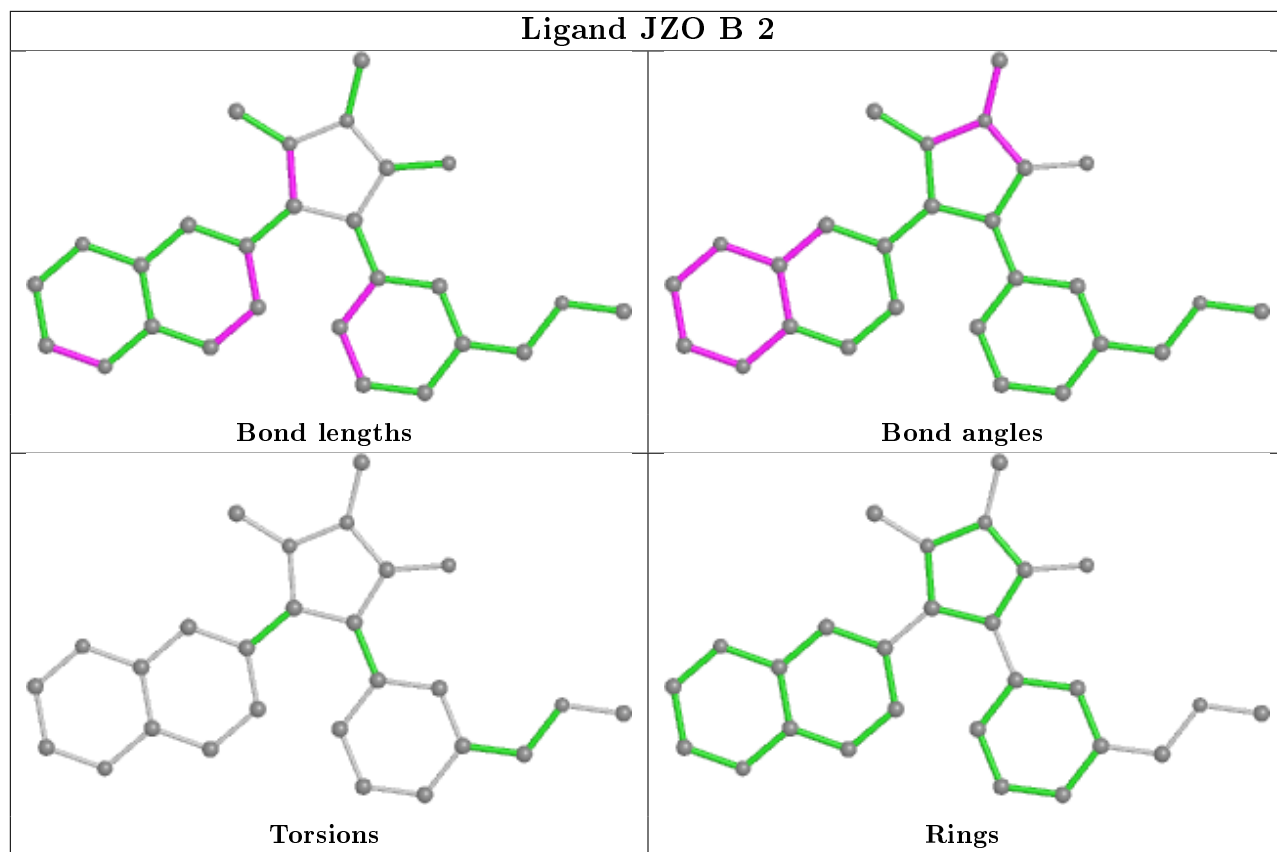
There are no ring outliers.

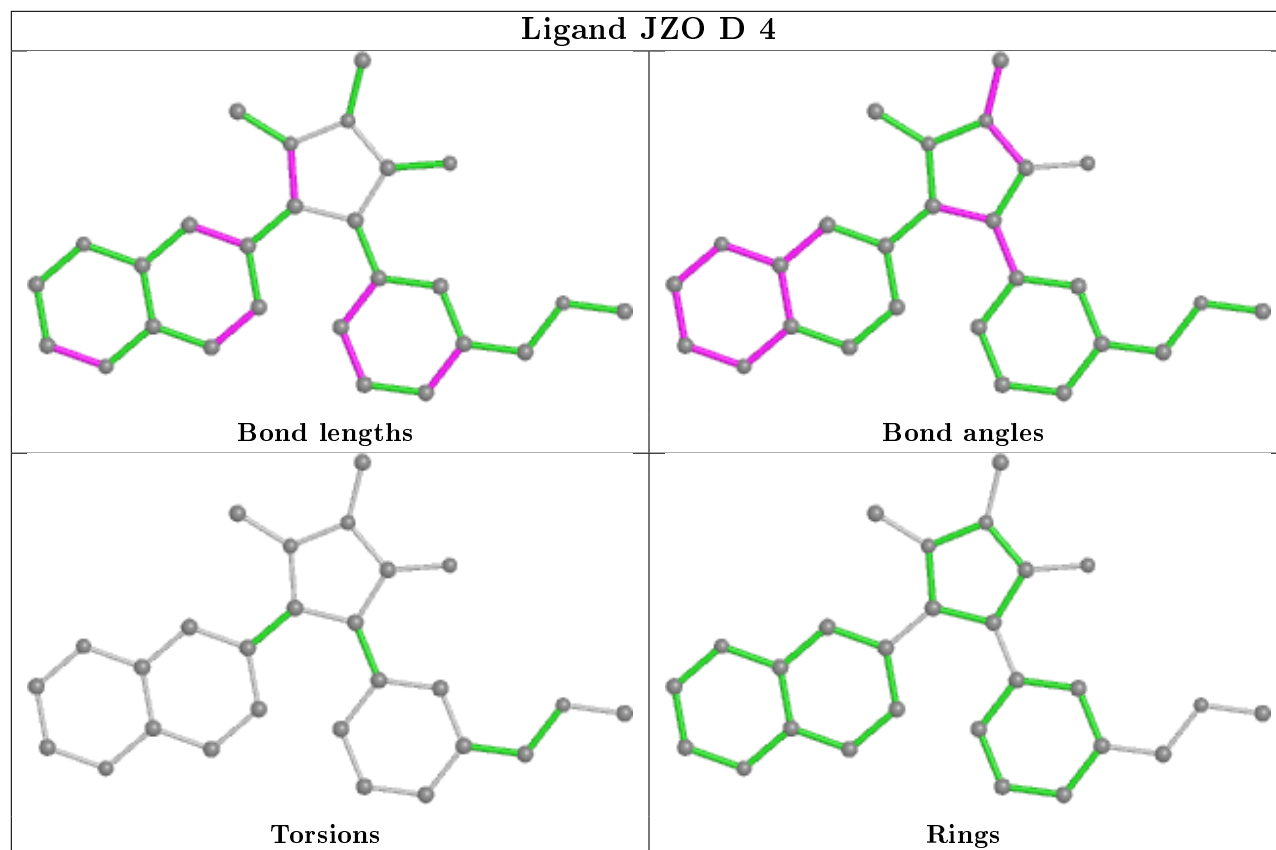
12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	2	PO4	2	0
2	E	5	JZO	1	0
3	B	12	PO4	1	0
2	A	1	JZO	1	0
3	C	10	PO4	1	0
3	D	15	PO4	2	0
3	D	14	PO4	1	0
3	E	3	PO4	3	0
3	B	11	PO4	2	0
2	C	3	JZO	3	0
3	B	6	PO4	1	0
2	D	4	JZO	3	0

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







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	328/342 (95%)	0.46	29 (8%) 10 5	23, 67, 105, 113	0
1	B	324/342 (94%)	-0.05	5 (1%) 73 68	17, 38, 68, 98	0
1	C	330/342 (96%)	0.62	40 (12%) 4 2	21, 71, 100, 110	0
1	D	330/342 (96%)	0.08	13 (3%) 39 29	20, 43, 82, 93	0
1	E	330/342 (96%)	-0.00	13 (3%) 39 29	18, 37, 76, 93	0
All	All	1642/1710 (96%)	0.22	100 (6%) 21 13	17, 47, 96, 113	0

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	252	VAL	5.8
1	A	324	GLN	5.8
1	C	497	GLN	5.3
1	D	323	THR	5.3
1	B	191	SER	4.8
1	E	370	ASN	4.7
1	B	252	VAL	4.7
1	A	323	THR	4.6
1	C	322	GLY	4.6
1	D	190	GLY	4.6
1	C	369	PRO	4.4
1	A	325	GLY	4.4
1	C	323	THR	4.4
1	E	325	GLY	4.3
1	E	323	THR	4.3
1	C	187	SER	4.2
1	A	416	SER	4.1
1	D	325	GLY	4.0
1	A	322	GLY	3.9
1	A	190	GLY	3.9

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Mol	Chain	Res	Type	RSRZ
1	D	189	SER	3.9
1	C	462	GLU	3.9
1	A	253	MET	3.9
1	C	496	SER	3.8
1	A	432	VAL	3.8
1	C	455	PRO	3.7
1	E	188	GLY	3.6
1	A	417	ILE	3.6
1	D	419	GLY	3.5
1	C	443	LYS	3.5
1	D	322	GLY	3.5
1	A	189	SER	3.4
1	E	189	SER	3.4
1	B	188	GLY	3.4
1	A	191	SER	3.3
1	A	446	CYS	3.3
1	E	324	GLN	3.3
1	C	291	TYR	3.3
1	C	321	VAL	3.3
1	D	370	ASN	3.2
1	A	431	LEU	3.1
1	C	361	ALA	3.1
1	C	325	GLY	3.1
1	C	416	SER	3.0
1	A	499	GLU	3.0
1	A	321	VAL	3.0
1	D	324	GLN	2.9
1	C	253	MET	2.9
1	A	443	LYS	2.9
1	A	457	ARG	2.8
1	C	370	ASN	2.8
1	C	411	ILE	2.8
1	C	465	ARG	2.8
1	C	417	ILE	2.7
1	C	324	GLN	2.7
1	E	321	VAL	2.7
1	E	253	MET	2.7
1	E	187	SER	2.7
1	D	188	GLY	2.7
1	D	191	SER	2.7
1	C	360	SER	2.6
1	E	322	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	C	434	SER	2.6
1	A	428	TYR	2.6
1	A	216	PHE	2.5
1	C	320	ILE	2.5
1	A	458	TRP	2.5
1	A	433	PRO	2.5
1	C	424	TYR	2.5
1	C	460	SER	2.5
1	A	295	TYR	2.4
1	E	252	VAL	2.4
1	C	318	MET	2.4
1	C	188	GLY	2.4
1	D	252	VAL	2.4
1	C	421	HIS	2.4
1	C	392	HIS	2.3
1	C	420	ILE	2.3
1	C	300	GLU	2.3
1	C	498	GLN	2.3
1	C	299	VAL	2.2
1	E	216	PHE	2.2
1	C	463	ALA	2.2
1	A	447	GLU	2.2
1	A	294	ARG	2.2
1	E	190	GLY	2.1
1	C	458	TRP	2.1
1	D	216	PHE	2.1
1	C	295	TYR	2.1
1	B	253	MET	2.1
1	A	442	ARG	2.1
1	A	292	LEU	2.1
1	C	494	GLN	2.1
1	A	487	ARG	2.1
1	C	433	PRO	2.1
1	D	418	GLY	2.1
1	A	320	ILE	2.0
1	A	448	GLN	2.0
1	C	470	ILE	2.0
1	B	391	LYS	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

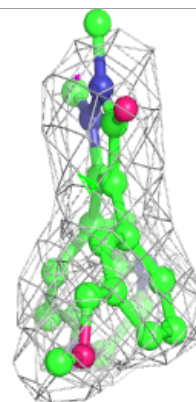
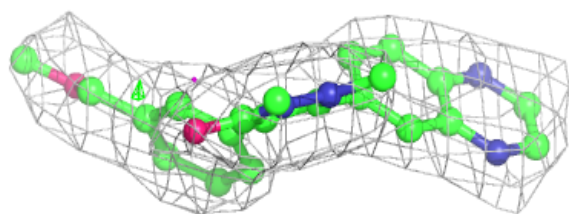
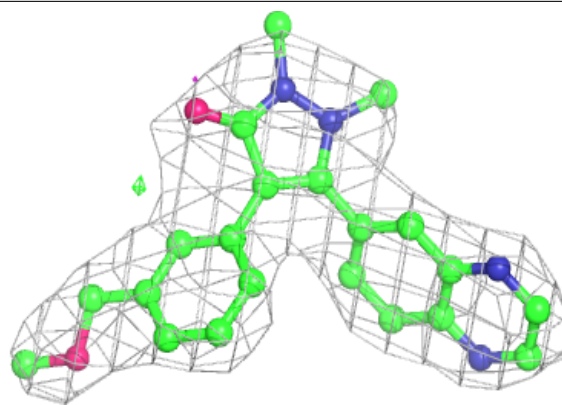
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PO4	C	10	5/5	0.89	0.18	61,61,63,63	0
3	PO4	A	22	5/5	0.93	0.23	19,20,22,23	5
3	PO4	A	21	5/5	0.94	0.22	35,36,36,37	5
3	PO4	D	15	5/5	0.94	0.34	2,7,8,8	5
3	PO4	A	9	5/5	0.94	0.16	69,70,70,71	0
3	PO4	D	14	5/5	0.95	0.32	21,21,21,22	5
3	PO4	B	6	5/5	0.95	0.15	37,37,38,40	0
2	JZO	C	3	27/27	0.96	0.21	41,47,49,50	0
3	PO4	E	1	5/5	0.97	0.15	44,44,46,46	0
3	PO4	D	13	5/5	0.97	0.14	54,54,55,56	0
2	JZO	E	5	27/27	0.97	0.19	25,28,32,32	0
3	PO4	B	11	5/5	0.97	0.24	1,2,6,6	5
2	JZO	D	4	27/27	0.97	0.20	25,28,35,39	0
3	PO4	E	2	5/5	0.98	0.23	7,8,10,11	5
2	JZO	B	2	27/27	0.98	0.17	17,22,26,30	0
2	JZO	A	1	27/27	0.98	0.21	26,30,34,39	0
3	PO4	E	3	5/5	0.98	0.25	1,1,2,3	5
3	PO4	B	12	5/5	0.98	0.20	15,16,16,18	5

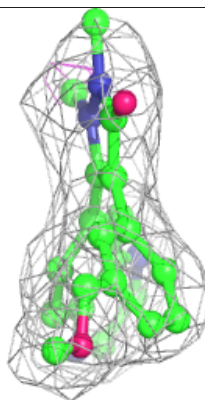
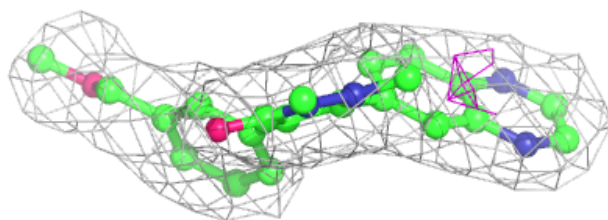
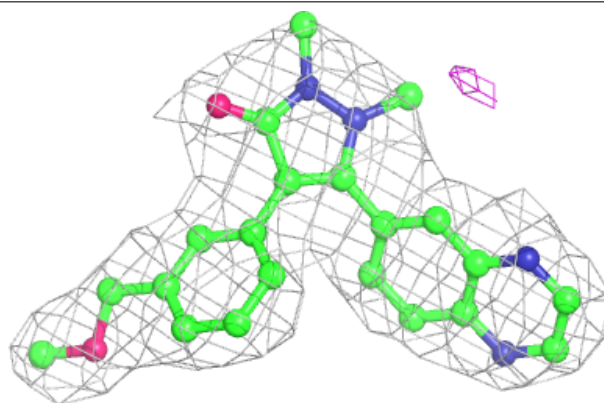
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around JZO C 3:

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

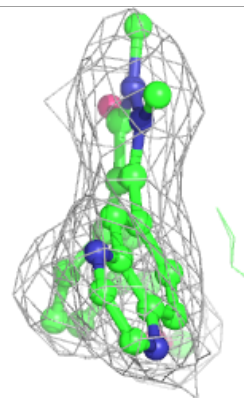
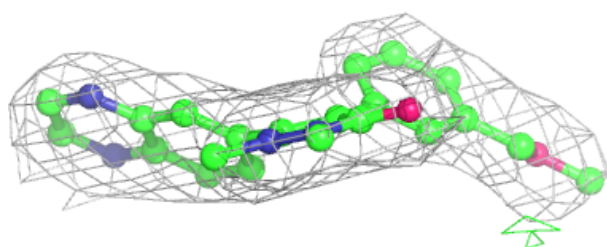
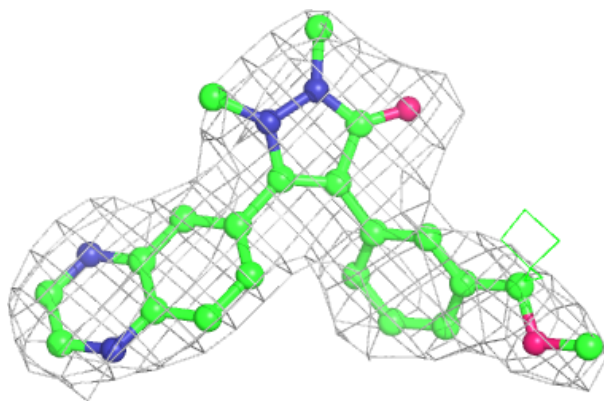
**Electron density around JZO E 5:**

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

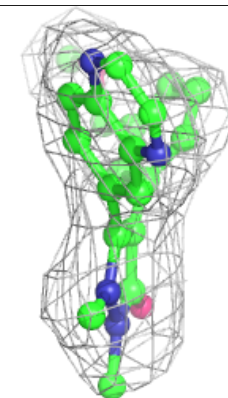
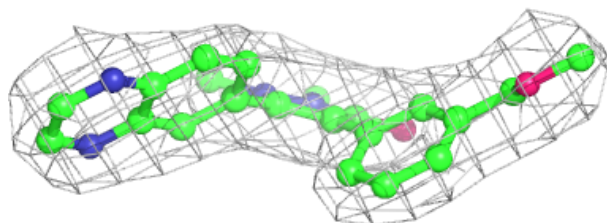
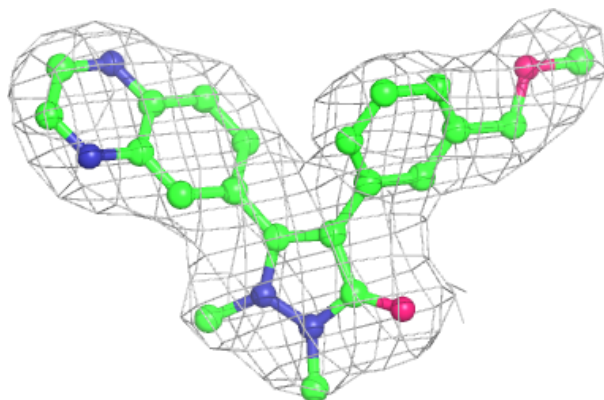


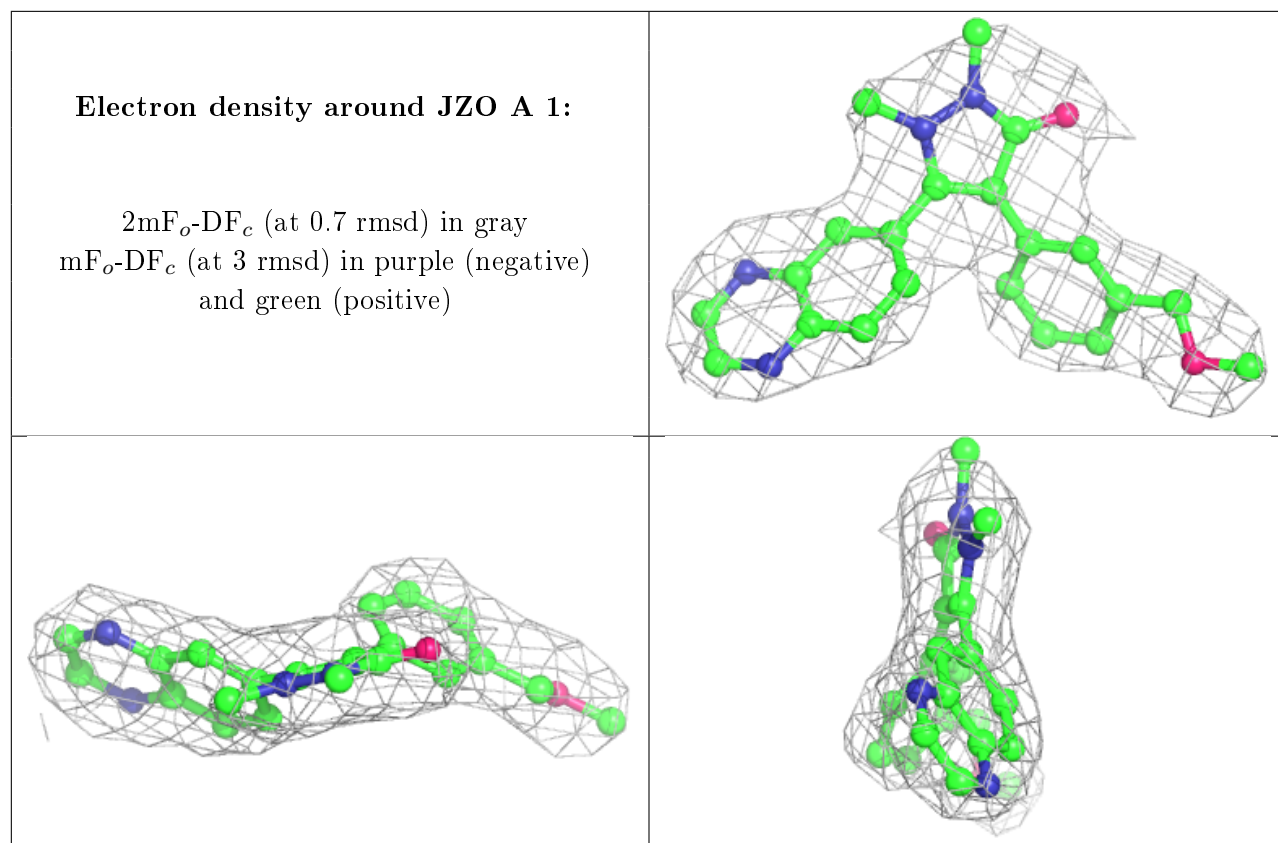
Electron density around JZO D 4:

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

**Electron density around JZO B 2:**

$2mF_o-DF_c$ (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.