Full wwPDB X-ray Structure Validation Report ⓘ

Aug 21, 2020 – 09:12 AM BST

PDB ID	:	3VSL
Title	:	Crystal structure of penicillin-binding protein 3 (PBP3) from methicilin-resistant Staphylococcus aureus in the cefotaxime bound form.
Authors	:	Yoshida, H.; Tame, J.R.; Park, S.Y.
Deposited on	:	2012-04-25
Resolution	:	2.40 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:

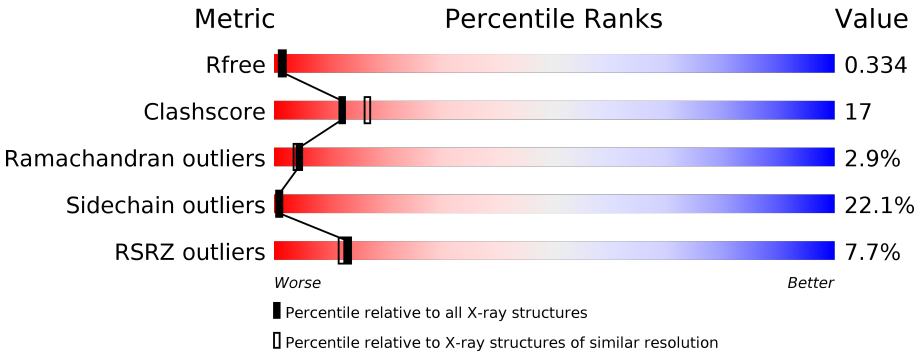
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 <=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	646	5% 56% 32% 8%
1	B	646	10% 51% 36% 10%

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
2	CEF	A	701	X	-	-	-
2	CEF	B	701	X	-	-	-

2 Entry composition

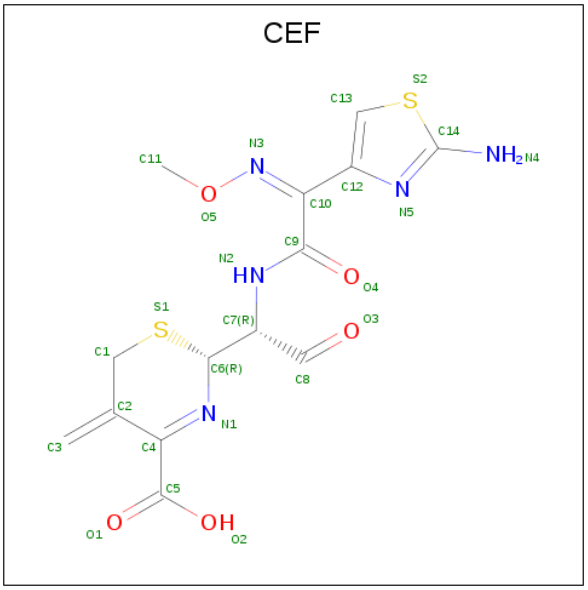
There are 3 unique types of molecules in this entry. The entry contains 10198 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Penicillin-binding protein 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	631	Total	C	N	O	S	0	0	0
			4943	3105	852	967	19			
1	B	631	Total	C	N	O	S	0	0	0
			4947	3107	853	968	19			

- Molecule 2 is CEFOTAXIME, C3' cleaved, open, bound form (three-letter code: CEF) (formula: $C_{14}H_{15}N_5O_5S_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	5	5	2		
2	B	1	Total	C	N	O	S	0	0
			26	14	5	5	2		

- Molecule 3 is water.

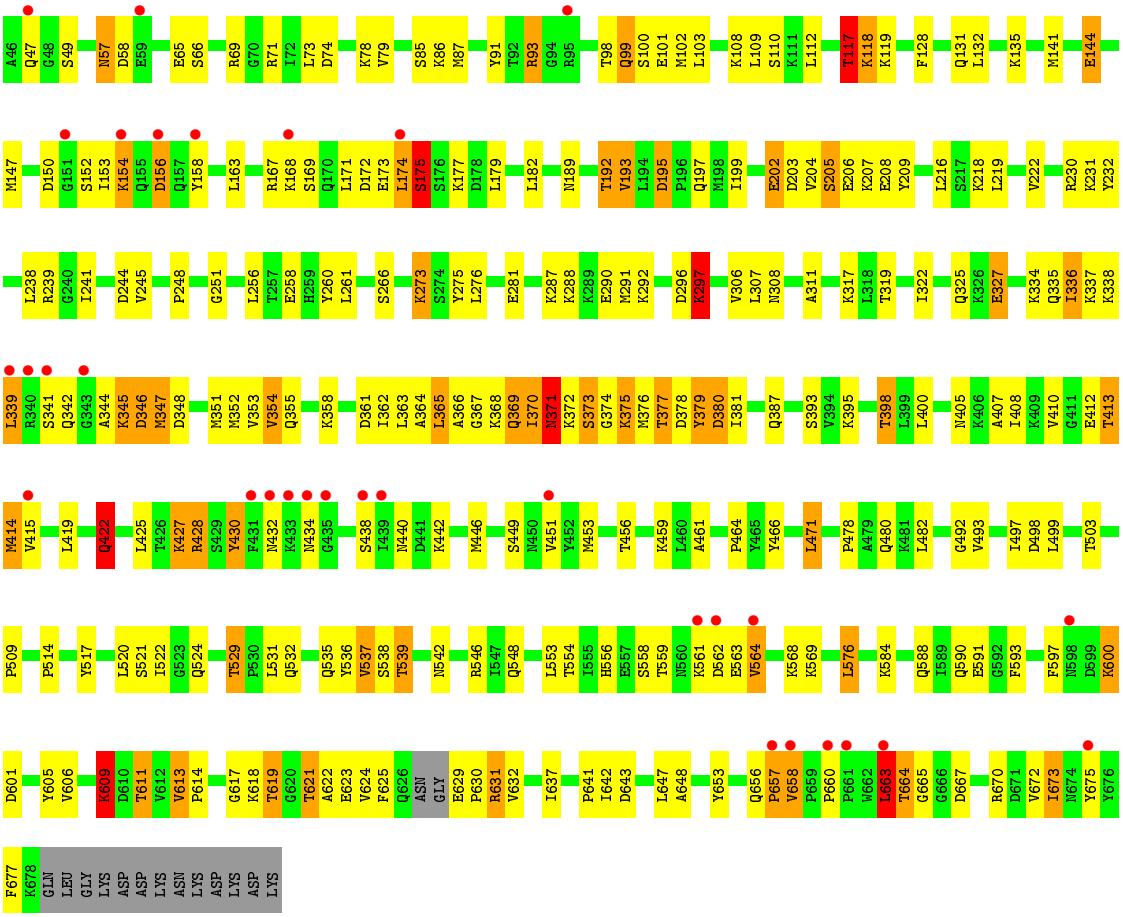
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	140	Total 140	O 140	0	0
3	B	116	Total 116	O 116	0	0

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.

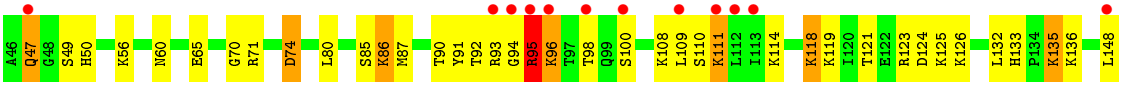
- Molecule 1: Penicillin-binding protein 3

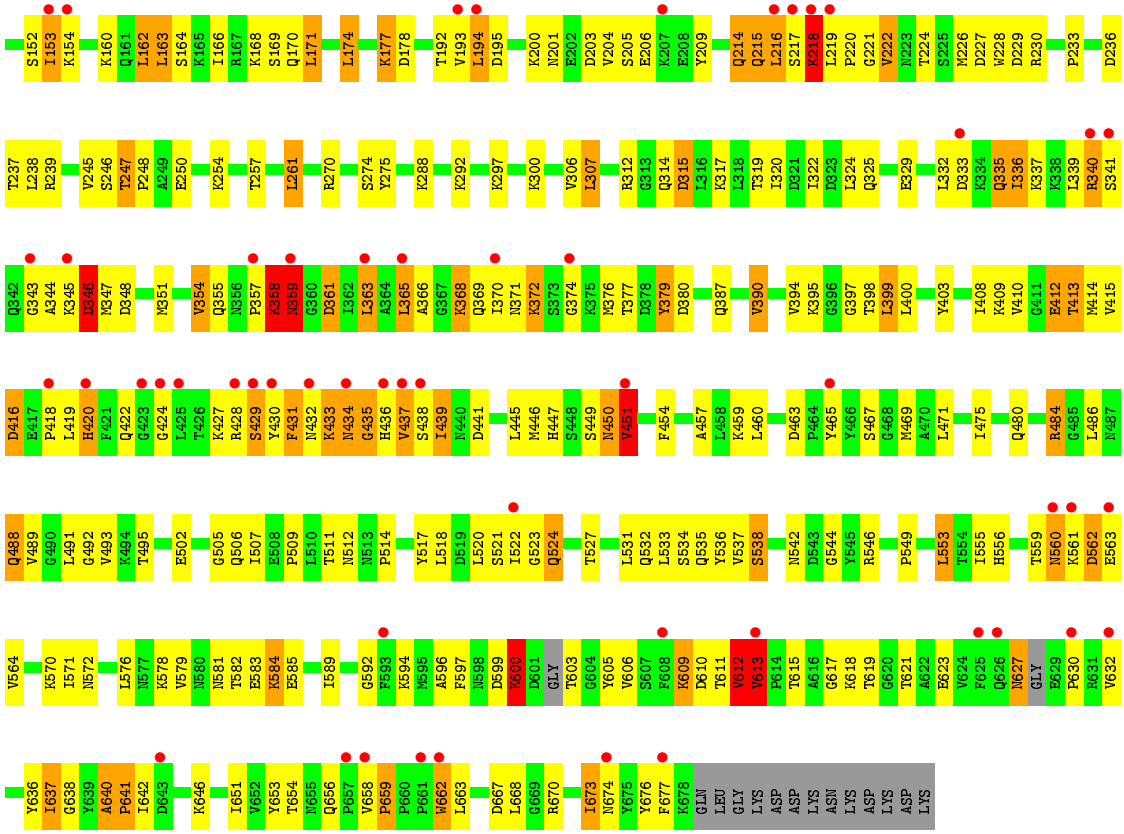
Chain A:



- Molecule 1: Penicillin-binding protein 3

Chain B:




S152 I153 K154 K160 Q161 L162 L163 S164 K165 I166 R167 K168 S169 Q170 L171 L174 K177 D178 T192 V193 L194 D195 K200 N201 E202 D203 V204 S205 E206 K207 E208 Y209 Q214 Q215 L216 S217 K218 L219 P220 G221 V222 N223 T224 S225 M226 D227 W228 D229 R230 P233 D236
T237 L238 R239 V245 S246 T247 P248 A249 E250 K254 T257 L261 R270 S274 Y275 K288 K292 K297 K300 V306 L307 R312 G313 Q314 D315 L316 K317 L318 T319 I320 D321 I322 D323 L324 Q325 E329 L332 D333 K334 Q335 I336 K337 K338 L339 R340 S341
Q342 G343 A344 K345 D346 M347 D348 M351 V354 Q355 N356 P357 K358 N359 G360 D361 I362 L363 A364 L365 A366 G367 K368 Q369 I370 N371 K372 S373 G374 K375 M376 T377 D378 Y379 D380 Q387 V390 V394 K395 G396 G397 T398 L399 L400 Y403 I408 K409 V410 G411 E412 T413 M414 V415
D416 E417 P418 L419 H420 F421 Q422 G423 G424 L425 T426 K427 R428 S429 Y430 F431 N432 K433 N434 G435 H436 V437 S438 I439 N440 D441 L445 M446 H447 S448 S449 N450 V451 F454 A457 L458 K459 L460 D463 P464 Y465 Y466 S467 G468 M469 A470 L471 I475 Q480 R484 G485 L486 N487
Q488 V489 G490 L491 G492 V493 K494 T495 E502 G505 Q506 I507 E508 P509 L510 T511 N512 N513 P514 Y517 L518 D519 L520 S521 I522 G523 Q524 T527 L531 Q532 L533 S534 Q535 Y536 V537 S538 N542 D543 G544 Y545 R546 P549 L553 T554 I555 H556 T559 N560 K561 D562 E563
V564 K570 I571 N572 L576 N577 K578 V579 N580 N581 T582 E583 K584 E585 I589 G592 F593 K594 N595 A596 F597 N598 D599 K600 D601 G603 T603 G604 Y605 V606 S607 F608 K609 D610 T611 V612 V613 P614 T615 A616 G617 K618 T619 S620 T621 A622 E623 V624 F625 Q626 N627 G629 P630 R631 V632
Y636 I637 G638 Y639 A640 P641 I642 D643 K646 I651 V652 Y653 T654 N655 Q656 P657 V658 P659 P660 P661 W662 L663 D667 L668 G669 R670 I673 N674 Y675 Y676 F677 K678 GLN LEU GLY LYS ASP ASP LYS ASN LYS ASP LYS ASP LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	143.03Å 143.03Å 189.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.86 – 2.40 48.86 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (48.86-2.40) 98.2 (48.86-2.40)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.55 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.247 , 0.316 0.273 , 0.334	Depositor DCC
R_{free} test set	3800 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	33.3	Xtriage
Anisotropy	0.046	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 67.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	10198	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.81% 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: CEF

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	0.46	0/5025	0.67	1/6769 (0.0%)
1	B	0.46	0/5029	0.70	0/6775
All	All	0.46	0/10054	0.69	1/13544 (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	A	0	8
1	B	0	11
All	All	0	19

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	A	230	ARG	NE-CZ-NH2	-5.40	117.60	120.30

There are no chirality outliers.

All (19) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	174	LEU	Peptide
1	A	251	GLY	Peptide
1	A	296	ASP	Peptide
1	A	371	ASN	Peptide
1	A	430	TYR	Peptide

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Mol	Chain	Res	Type	Group
1	A	657	PRO	Peptide
1	A	658	VAL	Peptide
1	A	660	PRO	Peptide
1	B	218	LYS	Peptide
1	B	346	ASP	Peptide
1	B	358	LYS	Peptide
1	B	359	ASN	Peptide
1	B	428	ARG	Peptide
1	B	429	SER	Peptide
1	B	560	ASN	Peptide
1	B	600	LYS	Peptide
1	B	612	VAL	Peptide
1	B	613	VAL	Peptide
1	B	640	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	4943	0	4991	166	0
1	B	4947	0	4994	180	0
2	A	26	0	1	6	0
2	B	26	0	1	6	0
3	A	140	0	0	4	0
3	B	116	0	0	5	0
All	All	10198	0	9987	341	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 17.

All (341) 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)
2:A:701:CEF:N5	2:A:701:CEF:C14	1.72	1.45
2:B:701:CEF:C14	2:B:701:CEF:N5	1.73	1.43
2:A:701:CEF:HN2	2:A:701:CEF:C14	1.54	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:529:THR:HG22	1:A:532:GLN:H	1.27	0.95
1:A:600:LYS:H	1:A:600:LYS:HE3	1.35	0.89
2:B:701:CEF:C14	2:B:701:CEF:HN2	1.79	0.88
1:A:367:GLY:HA2	1:A:379:TYR:H	1.37	0.87
1:A:408:ILE:HG21	1:A:456:THR:HG22	1.62	0.80
1:A:354:VAL:H	1:A:364:ALA:HB2	1.46	0.79
1:A:99:GLN:HG2	1:A:131:GLN:HE22	1.50	0.77
1:B:94:GLY:HA3	1:B:193:VAL:HG13	1.68	0.75
1:B:329:GLU:HA	1:B:365:LEU:HD22	1.68	0.75
1:B:416:ASP:OD1	1:B:416:ASP:N	2.21	0.73
1:B:365:LEU:HG	1:B:366:ALA:N	2.05	0.71
1:A:205:SER:HB3	1:A:208:GLU:HG3	1.72	0.71
1:A:535:GLN:O	1:A:539:THR:HG22	1.91	0.70
1:A:147:MET:HA	1:A:150:ASP:HB2	1.74	0.70
1:B:446:MET:HA	1:B:596:ALA:HB2	1.74	0.70
1:A:482:LEU:HD23	1:A:520:LEU:HD23	1.74	0.69
1:A:623:GLU:OE1	2:A:701:CEF:N5	2.25	0.69
1:A:537:VAL:HG13	1:A:637:ILE:HD12	1.75	0.69
1:A:336:ILE:HD13	1:A:337:LYS:HG2	1.76	0.68
1:A:71:ARG:HH22	1:A:563:GLU:HA	1.59	0.68
1:A:427:LYS:HD3	1:A:432:ASN:HB3	1.77	0.67
1:B:354:VAL:HG13	1:B:363:LEU:HB3	1.77	0.67
1:A:410:VAL:HG23	1:A:588:GLN:HG3	1.78	0.66
1:B:49:SER:HB2	1:B:65:GLU:HB3	1.78	0.66
1:B:641:PRO:HD3	1:B:677:PHE:CZ	2.31	0.65
1:A:614:PRO:HB2	1:A:642:ILE:HD13	1.79	0.64
1:A:276:LEU:HD13	1:A:499:LEU:HD21	1.79	0.64
1:B:495:THR:HG21	1:B:531:LEU:HG	1.79	0.64
1:A:144:GLU:HA	1:A:147:MET:HG2	1.79	0.64
1:B:319:THR:HA	1:B:553:LEU:HD12	1.79	0.64
1:A:150:ASP:HB3	1:A:152:SER:H	1.63	0.63
1:A:631:ARG:HG3	1:A:657:PRO:HA	1.80	0.63
1:A:337:LYS:HA	1:A:339:LEU:HG	1.80	0.62
1:A:524:GLN:HE22	1:A:622:ALA:HA	1.64	0.61
1:A:365:LEU:HD11	1:A:380:ASP:HB3	1.81	0.61
1:B:86:LYS:HD3	1:B:201:ASN:CG	2.21	0.61
1:B:332:LEU:O	1:B:336:ILE:HG23	2.01	0.60
1:B:95:ARG:H	1:B:193:VAL:HG13	1.67	0.60
1:A:428:ARG:HH21	1:A:451:VAL:HB	1.66	0.60
1:B:340:ARG:HG2	1:B:372:LYS:HE2	1.83	0.60
1:A:529:THR:HG23	1:A:531:LEU:H	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:387:GLN:HE21	1:A:503:THR:HB	1.67	0.60
1:B:214:GLN:O	1:B:216:LEU:N	2.35	0.60
1:B:390:VAL:HG21	1:B:533:LEU:HD21	1.84	0.59
1:A:387:GLN:H	1:B:506:GLN:HE22	1.49	0.59
1:A:371:ASN:HA	1:A:374:GLY:H	1.67	0.59
1:A:509:PRO:HG2	1:B:368:LYS:HG2	1.83	0.59
1:B:80:LEU:O	1:B:233:PRO:HD2	2.02	0.59
1:A:352:MET:H	1:A:366:ALA:HB2	1.67	0.59
1:A:625:PHE:HD2	1:B:627:ASN:HA	1.67	0.59
1:A:658:VAL:HG11	1:A:663:LEU:HG	1.83	0.58
1:B:465:TYR:HA	1:B:469:MET:SD	2.43	0.58
1:A:442:LYS:HE2	1:A:591:GLU:HB3	1.83	0.58
1:B:95:ARG:N	1:B:193:VAL:HG13	2.18	0.58
1:B:312:ARG:NH1	1:B:562:ASP:OD1	2.36	0.58
1:B:399:LEU:HD11	1:B:441:ASP:HB2	1.86	0.58
1:A:91:TYR:HB2	1:A:199:ILE:HD11	1.86	0.58
1:A:353:VAL:HA	1:A:364:ALA:HB1	1.84	0.58
1:B:419:LEU:HB2	1:B:465:TYR:CZ	2.38	0.58
1:B:228:TRP:O	1:B:270:ARG:NH1	2.34	0.58
1:A:428:ARG:HB3	1:A:451:VAL:HG23	1.86	0.58
1:A:657:PRO:HD2	1:A:658:VAL:HG13	1.86	0.58
1:B:214:GLN:OE1	1:B:218:LYS:NZ	2.35	0.57
1:A:354:VAL:H	1:A:364:ALA:CB	2.17	0.57
1:A:631:ARG:NH2	1:A:657:PRO:HB3	2.20	0.57
1:A:625:PHE:CD2	1:B:627:ASN:HA	2.40	0.57
1:B:91:TYR:CZ	1:B:93:ARG:HB2	2.41	0.56
1:A:117:THR:O	1:A:119:LYS:N	2.33	0.56
1:B:450:ASN:HB2	3:B:899:HOH:O	2.04	0.56
1:A:248:PRO:HA	3:A:854:HOH:O	2.05	0.56
1:B:612:VAL:H	1:B:613:VAL:HG22	1.71	0.56
1:A:641:PRO:HD3	1:A:677:PHE:CE2	2.41	0.55
1:B:454:PHE:CE1	1:B:518:LEU:HB3	2.42	0.55
1:A:141:MET:HB3	1:A:144:GLU:HG3	1.88	0.55
1:B:623:GLU:OE1	2:B:701:CEF:N5	2.40	0.55
1:A:348:ASP:N	1:A:348:ASP:OD1	2.39	0.54
1:B:446:MET:HB3	1:B:600:LYS:CB	2.38	0.54
1:B:319:THR:HG22	1:B:553:LEU:HG	1.90	0.54
1:B:641:PRO:HD2	1:B:646:LYS:H	1.72	0.54
1:A:351:MET:HA	1:A:366:ALA:HB1	1.88	0.54
1:A:368:LYS:HE3	1:A:370:ILE:HG23	1.89	0.54
1:A:546:ARG:NH1	1:A:576:LEU:HD23	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:TYR:O	1:A:197:GLN:N	2.40	0.54
1:B:445:LEU:HD12	1:B:592:GLY:HA3	1.89	0.54
1:A:346:ASP:OD1	1:A:346:ASP:N	2.40	0.54
1:A:339:LEU:HD12	1:A:341:SER:HA	1.89	0.54
1:A:461:ALA:HA	1:A:478:PRO:HG3	1.90	0.54
1:B:457:ALA:HB1	1:B:517:TYR:CE2	2.43	0.53
1:A:308:ASN:HB2	3:A:933:HOH:O	2.08	0.53
1:B:335:GLN:HG3	1:B:668:LEU:HB2	1.89	0.53
1:A:464:PRO:O	1:B:123:ARG:NH2	2.40	0.53
1:A:471:LEU:HG	1:A:514:PRO:HB2	1.91	0.53
1:B:372:LYS:C	1:B:374:GLY:H	2.11	0.53
1:A:258:GLU:HB2	1:B:576:LEU:HA	1.91	0.53
2:A:701:CEF:N5	2:A:701:CEF:N4	2.45	0.53
1:B:86:LYS:NZ	1:B:227:ASP:HB2	2.22	0.53
1:B:340:ARG:CA	1:B:372:LYS:HZ1	2.21	0.53
1:B:366:ALA:HB3	1:B:379:TYR:O	2.09	0.53
1:B:365:LEU:HD12	1:B:380:ASP:OD1	2.09	0.53
1:A:232:TYR:CD1	1:A:239:ARG:HD3	2.43	0.53
1:B:615:THR:HG21	1:B:673:ILE:HD12	1.89	0.53
1:B:50:HIS:NE2	1:B:85:SER:OG	2.34	0.53
1:B:514:PRO:HA	1:B:517:TYR:HB3	1.90	0.52
1:A:87:MET:HG3	1:A:209:TYR:CE1	2.44	0.52
1:B:292:LYS:HB2	1:B:307:LEU:HD11	1.90	0.52
1:B:70:GLY:HA3	1:B:314:GLN:O	2.09	0.52
1:B:201:ASN:ND2	1:B:229:ASP:OD2	2.43	0.52
1:B:492:GLY:H	1:B:532:GLN:NE2	2.08	0.52
1:B:343:GLY:O	1:B:345:LYS:N	2.43	0.52
1:B:94:GLY:O	1:B:96:LYS:N	2.42	0.52
1:B:133:HIS:HB3	1:B:136:LYS:HB2	1.91	0.51
1:B:403:TYR:CD2	1:B:585:GLU:HB3	2.45	0.51
1:B:324:LEU:HD11	1:B:676:TYR:HD1	1.75	0.51
1:A:337:LYS:C	1:A:339:LEU:H	2.14	0.51
1:A:434:ASN:N	1:A:434:ASN:OD1	2.42	0.51
1:A:408:ILE:CG2	1:A:456:THR:HG22	2.38	0.51
1:B:636:TYR:HB2	1:B:651:ILE:HB	1.91	0.51
1:B:465:TYR:CZ	1:B:467:SER:HA	2.46	0.51
1:A:345:LYS:O	1:A:371:ASN:HB3	2.10	0.51
1:B:325:GLN:HA	1:B:363:LEU:HD21	1.92	0.51
1:B:410:VAL:HG11	1:B:584:LYS:HG3	1.93	0.51
1:A:453:MET:HB2	1:A:522:ILE:HD13	1.93	0.51
1:B:518:LEU:O	1:B:521:SER:OG	2.27	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:MET:CE	1:A:672:VAL:HG11	2.41	0.50
1:A:337:LYS:HE2	1:A:344:ALA:O	2.11	0.50
1:A:339:LEU:HB2	1:A:342:GLN:H	1.76	0.50
1:A:355:GLN:HG3	1:A:362:ILE:HD13	1.94	0.50
1:A:371:ASN:HA	1:A:374:GLY:N	2.26	0.50
2:B:701:CEF:N4	2:B:701:CEF:N5	2.47	0.50
1:B:662:TRP:HD1	1:B:663:LEU:N	2.09	0.50
1:A:348:ASP:HA	1:A:369:GLN:O	2.12	0.50
1:B:522:ILE:HD12	1:B:524:GLN:HB2	1.94	0.50
1:A:219:LEU:HB2	1:A:222:VAL:HG21	1.92	0.50
1:B:320:ILE:HD13	1:B:361:ASP:O	2.11	0.50
1:A:297:LYS:HE3	1:A:297:LYS:H	1.77	0.49
1:A:290:GLU:HB2	1:A:307:LEU:HB2	1.93	0.49
1:B:370:ILE:HB	1:B:371:ASN:HD22	1.76	0.49
1:A:428:ARG:HE	1:A:451:VAL:HB	1.77	0.49
1:B:125:LYS:HB3	1:B:171:LEU:HG	1.93	0.49
1:B:118:LYS:HG3	1:B:119:LYS:HG2	1.94	0.49
1:B:597:PHE:CZ	1:B:617:GLY:HA3	2.47	0.49
1:A:370:ILE:HD11	1:B:512:ASN:OD1	2.12	0.49
1:B:433:LYS:O	1:B:435:GLY:N	2.46	0.49
1:B:340:ARG:HA	1:B:372:LYS:NZ	2.28	0.49
1:A:86:LYS:HG2	1:A:202:GLU:C	2.33	0.49
1:B:71:ARG:NE	1:B:315:ASP:OD2	2.45	0.49
1:B:332:LEU:HD13	1:B:365:LEU:HD23	1.93	0.49
1:A:238:LEU:HD23	1:A:365:LEU:HG	1.93	0.49
1:B:162:LEU:HD22	1:B:166:ILE:HD11	1.95	0.49
1:B:336:ILE:HD13	1:B:369:GLN:NE2	2.28	0.49
1:A:273:LYS:CE	1:B:484:ARG:HH12	2.26	0.49
1:B:555:ILE:HD11	1:B:571:ILE:HD11	1.95	0.49
1:A:241:ILE:O	1:A:276:LEU:HB2	2.13	0.48
1:A:514:PRO:O	1:A:517:TYR:HB3	2.12	0.48
1:B:329:GLU:CD	1:B:365:LEU:HD13	2.33	0.48
1:A:554:THR:OG1	1:A:556:HIS:NE2	2.38	0.48
1:A:466:TYR:CD2	1:B:163:LEU:HD23	2.48	0.48
1:B:562:ASP:N	1:B:562:ASP:OD1	2.46	0.48
1:A:171:LEU:C	1:A:173:GLU:H	2.17	0.48
1:B:446:MET:HE3	1:B:600:LYS:HB2	1.95	0.48
1:A:128:PHE:CG	1:A:182:LEU:HD13	2.49	0.48
1:A:71:ARG:HH12	1:A:563:GLU:HG3	1.78	0.48
1:B:87:MET:HB2	1:B:204:VAL:HG12	1.96	0.48
1:B:247:THR:HG22	1:B:248:PRO:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:MET:HE2	1:B:600:LYS:HG3	1.94	0.48
1:A:365:LEU:HD13	1:A:366:ALA:H	1.79	0.48
1:A:631:ARG:HH21	1:A:657:PRO:HB3	1.79	0.48
1:A:653:TYR:CE2	1:A:665:GLY:HA3	2.49	0.47
1:A:605:TYR:O	1:A:609:LYS:HD2	2.14	0.47
1:B:90:THR:O	1:B:222:VAL:HA	2.14	0.47
1:A:351:MET:HA	1:A:366:ALA:CB	2.44	0.47
1:A:529:THR:HG22	1:A:532:GLN:N	2.11	0.47
1:B:578:LYS:HG2	1:B:579:VAL:O	2.15	0.47
1:B:340:ARG:HA	1:B:372:LYS:HZ1	1.79	0.47
1:B:450:ASN:N	1:B:450:ASN:OD1	2.44	0.47
1:A:144:GLU:HB2	1:A:158:TYR:CD1	2.49	0.47
1:B:506:GLN:HG2	3:B:847:HOH:O	2.14	0.47
1:B:582:THR:OG1	1:B:583:GLU:OE1	2.32	0.47
1:A:395:LYS:HG2	1:A:453:MET:HG3	1.97	0.47
1:A:600:LYS:HE3	1:A:600:LYS:N	2.17	0.47
1:B:121:THR:O	1:B:124:ASP:HB2	2.15	0.46
1:B:247:THR:OG1	1:B:250:GLU:OE1	2.32	0.46
1:A:175:SER:O	1:A:175:SER:OG	2.33	0.46
1:A:548:GLN:HB2	1:A:576:LEU:HD11	1.96	0.46
1:A:352:MET:HE2	1:A:672:VAL:HG11	1.98	0.46
1:A:590:GLN:HA	1:A:593:PHE:HB2	1.96	0.46
1:A:629:GLU:HA	1:A:630:PRO:HD3	1.79	0.46
1:A:93:ARG:HB3	1:A:93:ARG:HE	1.61	0.46
1:B:493:VAL:O	1:B:532:GLN:NE2	2.48	0.46
1:B:618:LYS:HD3	1:B:619:THR:N	2.31	0.46
1:A:664:THR:HB	1:A:667:ASP:OD2	2.16	0.46
1:A:73:LEU:HD23	1:A:79:VAL:HA	1.97	0.46
1:B:336:ILE:HD13	1:B:369:GLN:HE21	1.80	0.46
1:A:65:GLU:O	1:A:288:LYS:HB2	2.16	0.46
1:B:219:LEU:HB2	1:B:222:VAL:CG2	2.46	0.46
1:B:359:ASN:HB2	3:B:825:HOH:O	2.15	0.46
1:B:570:LYS:HD3	1:B:572:ASN:OD1	2.16	0.46
1:A:414:MET:SD	1:A:415:VAL:HG22	2.56	0.46
1:A:192:THR:HB	1:A:195:ASP:HB2	1.98	0.46
1:A:322:ILE:O	1:A:325:GLN:HB3	2.15	0.45
1:A:377:THR:HG21	1:B:511:THR:HG21	1.98	0.45
1:B:358:LYS:NZ	1:B:359:ASN:HD21	2.14	0.45
1:B:246:SER:HB2	1:B:250:GLU:HG3	1.98	0.45
1:B:394:VAL:HG13	1:B:491:LEU:HD13	1.99	0.45
1:B:641:PRO:HD3	1:B:677:PHE:CE2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:ASN:HB3	1:A:58:ASP:H	1.59	0.45
1:A:670:ARG:O	1:A:673:ILE:HG22	2.16	0.45
1:B:346:ASP:OD1	1:B:371:ASN:N	2.47	0.45
1:B:347:MET:HE1	1:B:653:TYR:HB3	1.98	0.45
1:A:398:THR:HG21	1:A:521:SER:O	2.16	0.45
1:B:148:LEU:HD23	1:B:153:ILE:O	2.16	0.45
1:A:144:GLU:H	1:A:144:GLU:HG2	1.25	0.45
1:A:412:GLU:OE2	1:A:459:LYS:NZ	2.43	0.45
1:B:523:GLY:HA2	3:B:858:HOH:O	2.16	0.45
1:B:348:ASP:OD1	1:B:348:ASP:N	2.39	0.45
1:A:379:TYR:CZ	1:B:509:PRO:HD3	2.52	0.45
1:A:428:ARG:NH1	1:A:430:TYR:HE1	2.15	0.45
1:B:257:THR:HG22	1:B:261:LEU:HD22	1.99	0.45
1:B:524:GLN:HB2	1:B:524:GLN:HE21	1.59	0.45
1:A:369:GLN:HB2	1:A:369:GLN:HE21	1.54	0.45
1:A:611:THR:O	1:A:613:VAL:N	2.49	0.45
1:A:49:SER:OG	1:A:65:GLU:OE2	2.22	0.45
2:A:701:CEF:N2	2:A:701:CEF:O5	2.50	0.45
1:B:488:GLN:O	1:B:546:ARG:HD3	2.17	0.44
1:B:618:LYS:HD3	1:B:619:THR:H	1.82	0.44
1:B:594:LYS:HD3	1:B:642:ILE:HG21	1.98	0.44
1:A:154:LYS:HD2	1:A:156:ASP:HB2	1.99	0.44
1:A:522:ILE:HD12	1:A:522:ILE:HA	1.82	0.44
1:B:325:GLN:O	1:B:329:GLU:HG3	2.16	0.44
1:A:153:ILE:HD12	1:A:158:TYR:HB2	1.98	0.44
1:A:336:ILE:HG13	1:A:369:GLN:OE1	2.18	0.44
1:B:372:LYS:HD2	1:B:372:LYS:HA	1.60	0.44
1:B:412:GLU:HG3	1:B:413:THR:N	2.32	0.44
1:A:273:LYS:CD	1:B:484:ARG:HH12	2.30	0.44
1:A:291:MET:SD	1:A:306:VAL:HG22	2.57	0.44
1:B:430:TYR:OH	1:B:447:HIS:NE2	2.49	0.44
1:B:673:ILE:HG22	1:B:677:PHE:CE1	2.53	0.44
1:A:498:ASP:OD1	1:A:498:ASP:N	2.50	0.44
1:B:74:ASP:HB2	1:B:320:ILE:O	2.17	0.44
1:B:314:GLN:HB3	1:B:556:HIS:O	2.17	0.44
1:A:492:GLY:H	1:A:532:GLN:NE2	2.16	0.44
1:A:667:ASP:HB3	1:A:670:ARG:NH1	2.33	0.44
1:A:548:GLN:HB2	1:A:576:LEU:CD1	2.48	0.43
1:B:489:VAL:O	1:B:536:TYR:HA	2.18	0.43
1:B:86:LYS:HB3	1:B:86:LYS:HE2	1.70	0.43
1:A:618:LYS:HD2	1:A:619:THR:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:415:VAL:HB	1:B:437:VAL:HA	1.99	0.43
1:B:431:PHE:CD1	1:B:434:ASN:HB2	2.53	0.43
1:B:512:ASN:OD1	1:B:512:ASN:N	2.52	0.43
1:A:372:LYS:HA	1:A:372:LYS:HD2	1.84	0.43
1:B:400:LEU:HB3	1:B:581:ASN:CG	2.39	0.43
1:B:621:THR:OG1	2:B:701:CEF:O1	2.28	0.43
1:A:260:TYR:HE1	1:A:281:GLU:HG2	1.83	0.43
1:A:369:GLN:HG3	1:A:376:MET:HG2	2.00	0.43
1:B:193:VAL:HG12	1:B:194:LEU:HD22	2.00	0.43
1:B:397:GLY:HA2	1:B:400:LEU:HD12	1.99	0.43
1:A:414:MET:N	3:A:902:HOH:O	2.51	0.43
1:A:597:PHE:CE2	1:A:617:GLY:HA3	2.54	0.43
1:B:216:LEU:HD21	1:B:224:THR:H	1.83	0.43
1:B:617:GLY:HA2	1:B:638:GLY:HA2	2.00	0.43
1:B:585:GLU:O	1:B:589:ILE:HD13	2.19	0.43
1:A:204:VAL:HG22	1:A:205:SER:O	2.18	0.43
1:A:422:GLN:OE1	1:A:422:GLN:N	2.52	0.43
1:A:337:LYS:NZ	1:A:371:ASN:OD1	2.52	0.42
1:A:405:ASN:O	1:A:407:ALA:N	2.51	0.42
1:B:582:THR:OG1	1:B:583:GLU:N	2.51	0.42
1:A:621:THR:HB	2:A:701:CEF:O4	2.18	0.42
1:B:171:LEU:HA	1:B:171:LEU:HD12	1.85	0.42
1:B:420:HIS:HB3	1:B:427:LYS:HB3	2.01	0.42
1:B:537:VAL:HB	1:B:637:ILE:HD12	1.99	0.42
1:B:347:MET:CE	1:B:653:TYR:HB3	2.49	0.42
1:A:287:LYS:HB2	1:A:311:ALA:HB3	2.02	0.42
1:A:375:LYS:HA	1:A:375:LYS:HD2	1.90	0.42
1:B:395:LYS:HA	1:B:398:THR:OG1	2.19	0.42
1:B:416:ASP:HB3	1:B:451:VAL:HG11	2.02	0.42
1:B:434:ASN:O	1:B:436:HIS:N	2.53	0.42
1:B:439:ILE:HG13	1:B:439:ILE:H	1.65	0.42
1:B:636:TYR:O	1:B:651:ILE:N	2.49	0.42
1:A:69:ARG:HG2	3:A:925:HOH:O	2.19	0.42
1:B:108:LYS:O	1:B:111:LYS:HG2	2.20	0.42
1:B:505:GLY:O	1:B:507:ILE:HG13	2.20	0.42
1:A:373:SER:OG	1:A:374:GLY:N	2.52	0.42
1:B:133:HIS:ND1	1:B:135:LYS:HE2	2.35	0.42
1:B:177:LYS:HG2	1:B:178:ASP:N	2.35	0.42
1:B:605:TYR:O	1:B:609:LYS:HB2	2.20	0.42
1:A:336:ILE:HG13	1:A:369:GLN:CD	2.40	0.42
1:A:335:GLN:HA	1:A:338:LYS:HB2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:339:LEU:HA	1:A:342:GLN:NE2	2.35	0.42
1:B:214:GLN:OE1	1:B:215:GLN:N	2.53	0.42
1:B:659:PRO:HB3	2:B:701:CEF:N4	2.35	0.42
1:A:319:THR:HB	1:A:361:ASP:HB3	2.00	0.42
1:A:327:GLU:HG3	1:A:675:TYR:CE2	2.55	0.42
1:A:87:MET:HG3	1:A:209:TYR:CD1	2.55	0.42
1:B:247:THR:HG1	1:B:250:GLU:HG2	1.84	0.42
1:B:347:MET:HE3	1:B:656:GLN:HG2	2.02	0.42
1:B:358:LYS:HG3	1:B:359:ASN:H	1.85	0.42
1:B:400:LEU:HB3	1:B:581:ASN:OD1	2.19	0.42
1:A:546:ARG:CZ	1:A:576:LEU:HD23	2.50	0.42
1:A:347:MET:CE	1:A:656:GLN:HE21	2.33	0.42
1:A:261:LEU:HD12	1:A:261:LEU:HA	1.83	0.41
1:A:367:GLY:HA2	1:A:379:TYR:N	2.19	0.41
1:A:647:LEU:HD23	1:A:648:ALA:N	2.35	0.41
1:B:337:LYS:HA	1:B:337:LYS:HD3	2.00	0.41
1:B:92:THR:HG23	1:B:195:ASP:C	2.40	0.41
1:B:93:ARG:HG2	1:B:221:GLY:CA	2.50	0.41
1:A:147:MET:O	1:A:153:ILE:HG12	2.20	0.41
1:B:126:LYS:HG3	1:B:171:LEU:HD11	2.03	0.41
1:A:219:LEU:HB2	1:A:222:VAL:CG2	2.51	0.41
1:B:209:TYR:CE2	1:B:226:MET:HG2	2.56	0.41
1:B:354:VAL:HG22	1:B:363:LEU:HB2	2.03	0.41
1:B:534:SER:O	1:B:538:SER:HB2	2.20	0.41
1:A:336:ILE:HG21	1:A:376:MET:CE	2.50	0.41
1:A:171:LEU:HD12	1:A:174:LEU:HD22	2.02	0.41
1:A:370:ILE:O	1:A:373:SER:OG	2.37	0.41
1:B:236:ASP:HA	1:B:239:ARG:CG	2.51	0.41
1:B:432:ASN:O	1:B:433:LYS:HB2	2.21	0.41
1:B:433:LYS:HB2	1:B:433:LYS:HE2	1.93	0.41
1:B:47:GLN:NE2	1:B:560:ASN:OD1	2.53	0.41
1:B:612:VAL:HG21	1:B:674:ASN:HA	2.02	0.41
1:B:98:THR:C	1:B:100:SER:H	2.24	0.41
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.86	0.41
1:A:427:LYS:NZ	1:A:432:ASN:O	2.50	0.41
1:A:173:GLU:C	1:A:175:SER:N	2.74	0.41
1:B:527:THR:HG21	3:B:895:HOH:O	2.21	0.41
1:B:95:ARG:H	1:B:193:VAL:CG1	2.33	0.41
1:A:87:MET:HG3	1:A:209:TYR:HE1	1.86	0.41
1:B:337:LYS:HZ3	1:B:340:ARG:HH11	1.68	0.41
1:B:430:TYR:CZ	1:B:431:PHE:CE2	3.09	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LYS:HD3	1:A:556:HIS:NE2	2.36	0.40
1:A:413:THR:HG23	1:A:440:ASN:HB3	2.03	0.40
1:B:174:LEU:HD12	1:B:174:LEU:HA	1.79	0.40
1:B:329:GLU:CG	1:B:365:LEU:HD13	2.51	0.40
1:B:86:LYS:HD3	1:B:201:ASN:ND2	2.36	0.40
1:A:337:LYS:HD3	1:A:339:LEU:HD11	2.03	0.40
1:B:544:GLY:O	1:B:578:LYS:HA	2.22	0.40
1:B:535:GLN:HE21	1:B:549:PRO:HD3	1.87	0.40
1:A:605:TYR:CD1	1:A:609:LYS:HA	2.56	0.40
1:B:163:LEU:HD12	1:B:163:LEU:HA	1.94	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	627/646 (97%)	554 (88%)	60 (10%)	13 (2%)	7	8
1	B	627/646 (97%)	544 (87%)	60 (10%)	23 (4%)	3	2
All	All	1254/1292 (97%)	1098 (88%)	120 (10%)	36 (3%)	4	4

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	LYS
1	A	373	SER
1	B	95	ARG
1	B	215	GLN
1	B	344	ALA
1	B	434	ASN
1	B	561	LYS
1	B	562	ASP

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Mol	Chain	Res	Type
1	A	172	ASP
1	A	175	SER
1	A	297	LYS
1	A	609	LYS
1	B	275	TYR
1	B	359	ASN
1	B	433	LYS
1	B	435	GLY
1	B	609	LYS
1	A	422	GLN
1	A	663	LEU
1	B	203	ASP
1	B	220	PRO
1	B	357	PRO
1	B	599	ASP
1	B	630	PRO
1	A	117	THR
1	A	167	ARG
1	B	358	LYS
1	B	424	GLY
1	B	451	VAL
1	B	640	ALA
1	A	275	TYR
1	B	659	PRO
1	A	193	VAL
1	B	641	PRO
1	A	564	VAL
1	B	418	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	546/559 (98%)	429 (79%)	117 (21%)	1 1
1	B	547/559 (98%)	422 (77%)	125 (23%)	1 1
All	All	1093/1118 (98%)	851 (78%)	242 (22%)	1 1

All (242) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	57	ASN
1	A	66	SER
1	A	74	ASP
1	A	78	LYS
1	A	85	SER
1	A	93	ARG
1	A	98	THR
1	A	99	GLN
1	A	100	SER
1	A	101	GLU
1	A	102	MET
1	A	103	LEU
1	A	108	LYS
1	A	109	LEU
1	A	110	SER
1	A	112	LEU
1	A	117	THR
1	A	118	LYS
1	A	132	LEU
1	A	135	LYS
1	A	144	GLU
1	A	154	LYS
1	A	156	ASP
1	A	163	LEU
1	A	168	LYS
1	A	169	SER
1	A	175	SER
1	A	177	LYS
1	A	179	LEU
1	A	189	ASN
1	A	192	THR
1	A	193	VAL
1	A	195	ASP
1	A	202	GLU
1	A	203	ASP
1	A	205	SER
1	A	206	GLU
1	A	207	LYS
1	A	216	LEU
1	A	218	LYS
1	A	231	LYS

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Mol	Chain	Res	Type
1	A	244	ASP
1	A	245	VAL
1	A	256	LEU
1	A	266	SER
1	A	273	LYS
1	A	292	LYS
1	A	297	LYS
1	A	327	GLU
1	A	334	LYS
1	A	336	ILE
1	A	339	LEU
1	A	345	LYS
1	A	346	ASP
1	A	347	MET
1	A	354	VAL
1	A	358	LYS
1	A	363	LEU
1	A	365	LEU
1	A	369	GLN
1	A	370	ILE
1	A	371	ASN
1	A	375	LYS
1	A	377	THR
1	A	378	ASP
1	A	379	TYR
1	A	380	ASP
1	A	381	ILE
1	A	393	SER
1	A	398	THR
1	A	400	LEU
1	A	413	THR
1	A	414	MET
1	A	419	LEU
1	A	422	GLN
1	A	425	LEU
1	A	427	LYS
1	A	428	ARG
1	A	438	SER
1	A	446	MET
1	A	449	SER
1	A	471	LEU
1	A	480	GLN

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Mol	Chain	Res	Type
1	A	493	VAL
1	A	497	ILE
1	A	529	THR
1	A	536	TYR
1	A	537	VAL
1	A	538	SER
1	A	539	THR
1	A	542	ASN
1	A	553	LEU
1	A	558	SER
1	A	559	THR
1	A	561	LYS
1	A	562	ASP
1	A	564	VAL
1	A	568	LYS
1	A	569	LYS
1	A	576	LEU
1	A	584	LYS
1	A	600	LYS
1	A	601	ASP
1	A	606	VAL
1	A	609	LYS
1	A	611	THR
1	A	613	VAL
1	A	619	THR
1	A	621	THR
1	A	624	VAL
1	A	631	ARG
1	A	632	VAL
1	A	643	ASP
1	A	663	LEU
1	A	664	THR
1	A	673	ILE
1	B	47	GLN
1	B	56	LYS
1	B	60	ASN
1	B	74	ASP
1	B	86	LYS
1	B	95	ARG
1	B	96	LYS
1	B	109	LEU
1	B	110	SER

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Mol	Chain	Res	Type
1	B	111	LYS
1	B	114	LYS
1	B	118	LYS
1	B	132	LEU
1	B	135	LYS
1	B	152	SER
1	B	153	ILE
1	B	154	LYS
1	B	160	LYS
1	B	162	LEU
1	B	163	LEU
1	B	164	SER
1	B	168	LYS
1	B	169	SER
1	B	170	GLN
1	B	171	LEU
1	B	174	LEU
1	B	177	LYS
1	B	192	THR
1	B	194	LEU
1	B	200	LYS
1	B	205	SER
1	B	206	GLU
1	B	214	GLN
1	B	216	LEU
1	B	217	SER
1	B	218	LYS
1	B	222	VAL
1	B	230	ARG
1	B	237	THR
1	B	238	LEU
1	B	245	VAL
1	B	247	THR
1	B	254	LYS
1	B	261	LEU
1	B	274	SER
1	B	288	LYS
1	B	297	LYS
1	B	300	LYS
1	B	306	VAL
1	B	307	LEU
1	B	315	ASP

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Mol	Chain	Res	Type
1	B	317	LYS
1	B	322	ILE
1	B	333	ASP
1	B	335	GLN
1	B	336	ILE
1	B	339	LEU
1	B	340	ARG
1	B	341	SER
1	B	346	ASP
1	B	351	MET
1	B	354	VAL
1	B	355	GLN
1	B	361	ASP
1	B	363	LEU
1	B	365	LEU
1	B	368	LYS
1	B	372	LYS
1	B	376	MET
1	B	377	THR
1	B	379	TYR
1	B	387	GLN
1	B	390	VAL
1	B	399	LEU
1	B	408	ILE
1	B	409	LYS
1	B	412	GLU
1	B	413	THR
1	B	414	MET
1	B	416	ASP
1	B	420	HIS
1	B	422	GLN
1	B	429	SER
1	B	431	PHE
1	B	437	VAL
1	B	438	SER
1	B	439	ILE
1	B	449	SER
1	B	450	ASN
1	B	451	VAL
1	B	459	LYS
1	B	460	LEU
1	B	463	ASP

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Mol	Chain	Res	Type
1	B	471	LEU
1	B	475	ILE
1	B	480	GLN
1	B	484	ARG
1	B	486	LEU
1	B	488	GLN
1	B	502	GLU
1	B	520	LEU
1	B	524	GLN
1	B	538	SER
1	B	542	ASN
1	B	553	LEU
1	B	559	THR
1	B	563	GLU
1	B	564	VAL
1	B	584	LYS
1	B	600	LYS
1	B	603	THR
1	B	606	VAL
1	B	610	ASP
1	B	611	THR
1	B	612	VAL
1	B	613	VAL
1	B	627	ASN
1	B	632	VAL
1	B	637	ILE
1	B	654	THR
1	B	658	VAL
1	B	662	TRP
1	B	667	ASP
1	B	670	ARG
1	B	673	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	145	GLN
1	A	387	GLN
1	A	590	GLN
1	A	656	GLN
1	B	47	GLN

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Mol	Chain	Res	Type
1	B	201	ASN
1	B	335	GLN
1	B	359	ASN
1	B	371	ASN
1	B	387	GLN
1	B	432	ASN
1	B	436	HIS
1	B	480	GLN
1	B	488	GLN
1	B	524	GLN
1	B	542	ASN
1	B	560	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

2 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	CEF	A	701	1	17,27,27	9.14	12 (70%)	11,37,37	6.62	7 (63%)
2	CEF	B	701	1	17,27,27	9.20	12 (70%)	11,37,37	5.04	7 (63%)

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	CEF	A	701	1	1/1/7/9	4/11/38/38	0/1/2/2
2	CEF	B	701	1	1/1/7/9	5/11/38/38	0/1/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	CEF	C4-N1	28.79	1.60	1.28
2	B	701	CEF	C4-N1	28.75	1.60	1.28
2	B	701	CEF	C10-N3	12.90	1.50	1.29
2	A	701	CEF	C10-N3	11.93	1.48	1.29
2	A	701	CEF	C12-C10	-11.61	1.30	1.48
2	B	701	CEF	C12-C10	-10.97	1.31	1.48
2	B	701	CEF	C1-S1	-9.43	1.60	1.82
2	A	701	CEF	C1-S1	-9.20	1.61	1.82
2	B	701	CEF	C5-C4	-8.45	1.39	1.52
2	A	701	CEF	C5-C4	-8.04	1.39	1.52
2	B	701	CEF	C3-C2	6.86	1.47	1.32
2	A	701	CEF	C3-C2	6.83	1.47	1.32
2	B	701	CEF	C9-N2	6.23	1.46	1.34
2	A	701	CEF	C9-N2	6.07	1.46	1.34
2	B	701	CEF	C4-C2	5.10	1.63	1.46
2	A	701	CEF	C12-N5	4.93	1.52	1.37
2	A	701	CEF	C4-C2	4.80	1.62	1.46
2	B	701	CEF	C12-N5	4.76	1.52	1.37
2	A	701	CEF	O5-N3	-3.80	1.31	1.40
2	B	701	CEF	O5-N3	-3.24	1.33	1.40
2	A	701	CEF	C14-N4	-2.81	1.26	1.35
2	B	701	CEF	C14-N4	-2.78	1.26	1.35
2	B	701	CEF	C10-C9	2.39	1.55	1.50
2	A	701	CEF	C13-S2	-2.16	1.67	1.70

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	CEF	C12-C13-S2	-11.91	97.16	111.79
2	A	701	CEF	N4-C14-N5	-10.91	109.06	123.19
2	B	701	CEF	C11-O5-N3	10.08	120.11	108.40
2	B	701	CEF	N4-C14-N5	-9.82	110.47	123.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	701	CEF	C1-S1-C6	9.35	112.81	94.47
2	A	701	CEF	C11-O5-N3	8.19	117.92	108.40
2	B	701	CEF	C1-S1-C6	6.05	106.34	94.47
2	A	701	CEF	C10-C9-N2	5.15	122.93	114.38
2	A	701	CEF	C7-N2-C9	-5.04	114.40	122.26
2	B	701	CEF	C12-C13-S2	-4.75	105.96	111.79
2	A	701	CEF	O4-C9-N2	-3.18	117.50	123.08
2	B	701	CEF	C10-C9-N2	2.34	118.27	114.38
2	B	701	CEF	O4-C9-N2	-2.19	119.24	123.08
2	B	701	CEF	O3-C8-C7	-2.07	119.05	124.83

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	701	CEF	C7
2	B	701	CEF	C6

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	CEF	C9-C10-N3-O5
2	B	701	CEF	C12-C10-C9-N2
2	B	701	CEF	C12-C10-C9-O4
2	B	701	CEF	C12-C10-N3-O5
2	A	701	CEF	C12-C10-N3-O5
2	A	701	CEF	N3-C10-C9-O4
2	B	701	CEF	N3-C10-C9-O4
2	A	701	CEF	C12-C10-C9-O4
2	B	701	CEF	C8-C7-N2-C9

There are no ring outliers.

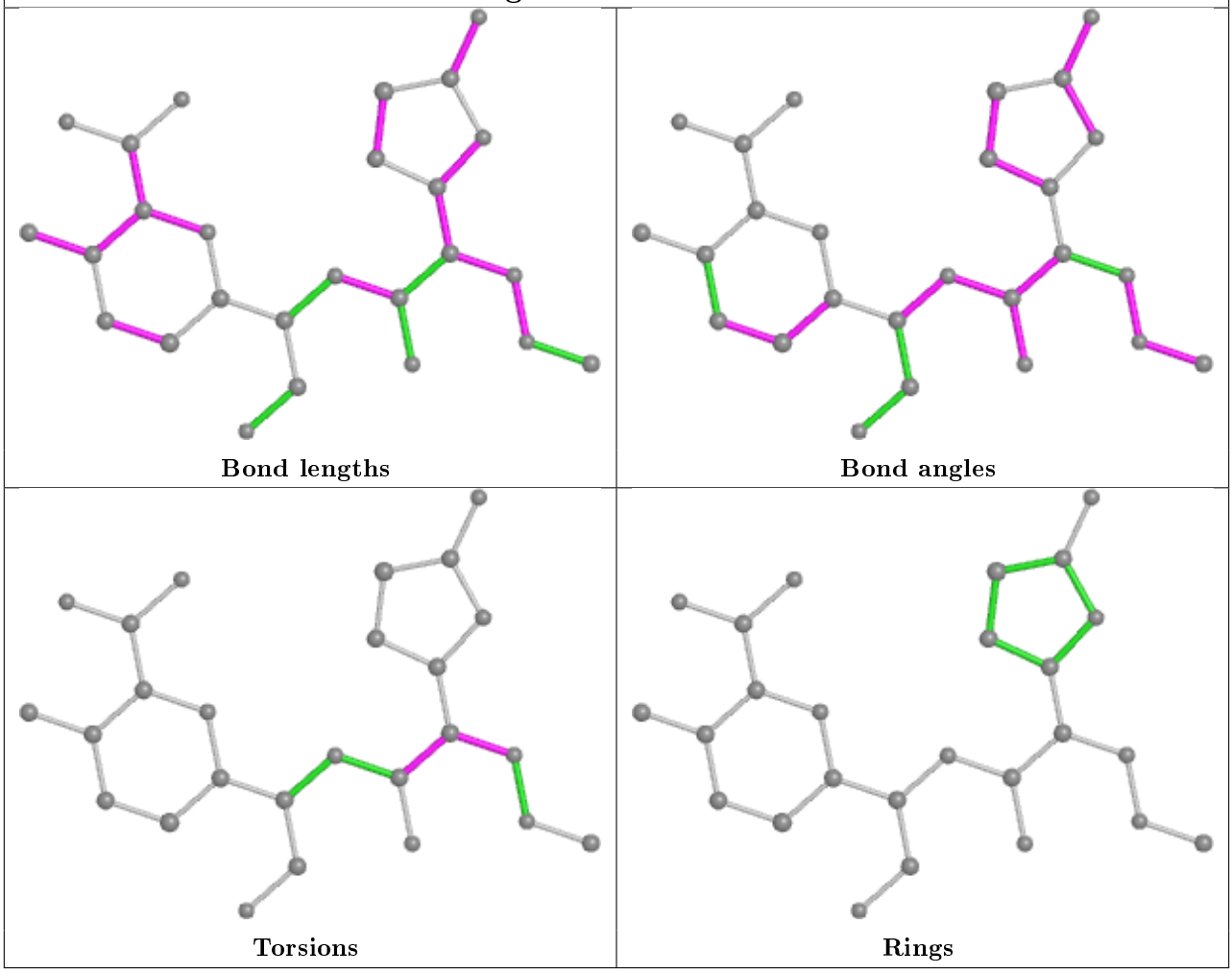
2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	CEF	6	0
2	B	701	CEF	6	0

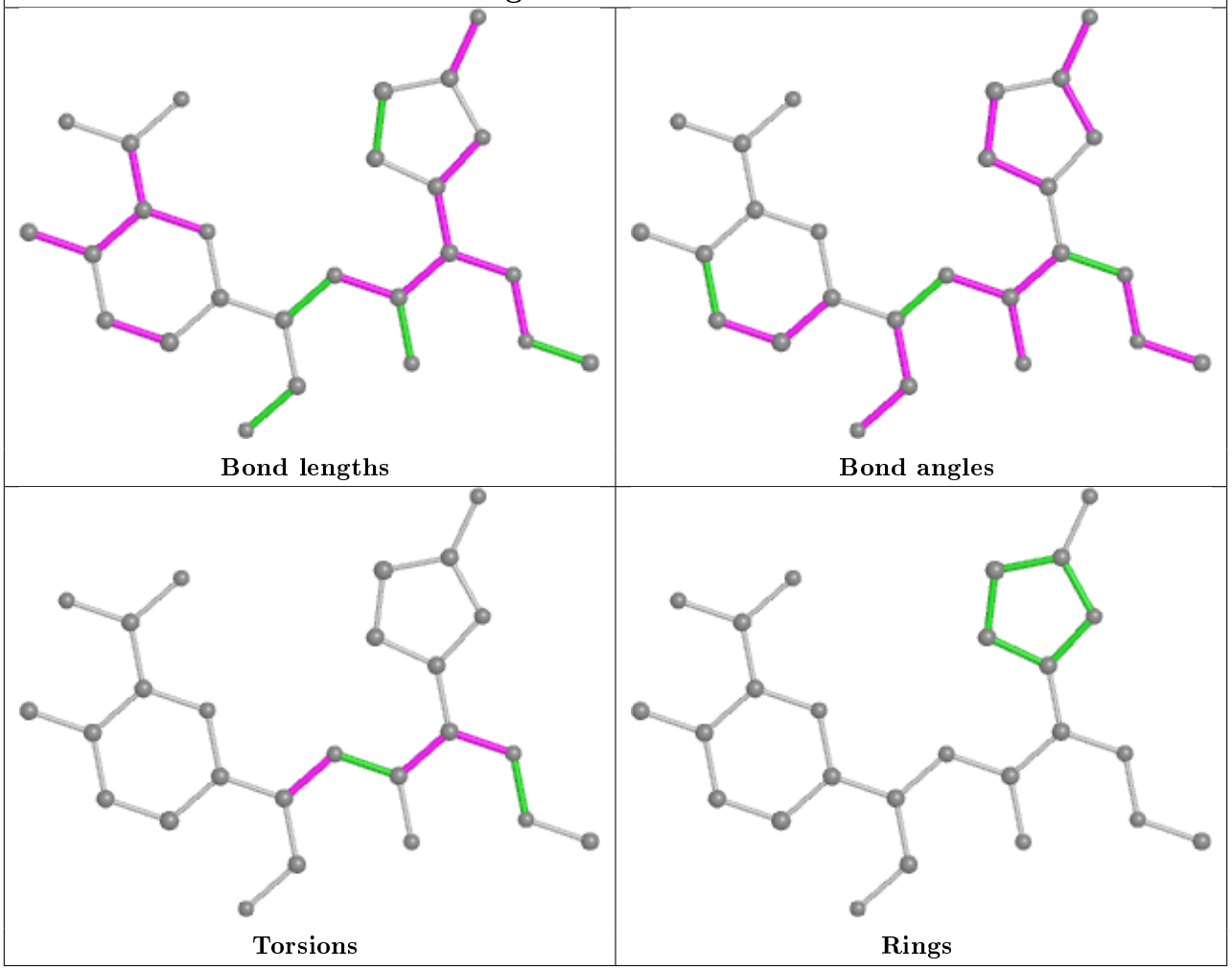
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 CEF A 701



Ligand CEF B 701



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	631/646 (97%)	0.38	32 (5%) 28 26	27, 61, 117, 146	0
1	B	631/646 (97%)	0.61	65 (10%) 6 6	29, 70, 124, 161	0
All	All	1262/1292 (97%)	0.50	97 (7%) 13 12	27, 66, 121, 161	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	217	SER	11.2
1	B	425	LEU	10.0
1	A	174	LEU	9.3
1	B	218	LYS	9.1
1	A	562	ASP	7.1
1	B	432	ASN	6.5
1	B	424	GLY	6.4
1	B	658	VAL	5.7
1	B	216	LEU	5.5
1	B	436	HIS	5.5
1	B	94	GLY	5.2
1	A	340	ARG	5.2
1	B	194	LEU	5.0
1	B	429	SER	5.0
1	B	423	GLY	4.9
1	B	98	THR	4.8
1	B	418	PRO	4.7
1	A	661	PRO	4.7
1	B	657	PRO	4.7
1	B	625	PHE	4.6
1	A	435	GLY	4.6
1	B	111	LYS	4.5
1	B	154	LYS	4.4
1	B	661	PRO	4.3

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Mol	Chain	Res	Type	RSRZ
1	B	437	VAL	4.2
1	A	658	VAL	4.2
1	B	438	SER	4.1
1	B	374	GLY	4.1
1	B	47	GLN	4.0
1	B	343	GLY	4.0
1	B	451	VAL	3.9
1	A	343	GLY	3.9
1	B	113	ILE	3.9
1	A	439	ILE	3.9
1	B	643	ASP	3.7
1	B	561	LYS	3.7
1	B	428	ARG	3.5
1	B	674	ASN	3.5
1	B	96	LYS	3.5
1	A	47	GLN	3.4
1	A	341	SER	3.4
1	B	93	ARG	3.3
1	A	657	PRO	3.2
1	B	465	TYR	3.2
1	B	677	PHE	3.2
1	B	626	GLN	3.1
1	B	345	LYS	3.0
1	B	363	LEU	3.0
1	A	451	VAL	3.0
1	B	193	VAL	2.9
1	B	109	LEU	2.9
1	B	434	ASN	2.9
1	A	95	ARG	2.9
1	A	433	LYS	2.9
1	B	593	PHE	2.8
1	A	660	PRO	2.7
1	B	630	PRO	2.7
1	A	415	VAL	2.7
1	A	59	GLU	2.6
1	A	438	SER	2.6
1	A	432	ASN	2.6
1	B	207	LYS	2.6
1	A	434	ASN	2.6
1	B	522	ILE	2.6
1	B	219	LEU	2.5
1	B	153	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	95	ARG	2.5
1	B	365	LEU	2.5
1	A	154	LYS	2.4
1	A	158	TYR	2.4
1	A	663	LEU	2.4
1	A	598	ASN	2.3
1	B	560	ASN	2.3
1	A	561	LYS	2.3
1	A	675	TYR	2.3
1	B	662	TRP	2.2
1	B	370	ILE	2.2
1	B	359	ASN	2.2
1	A	156	ASP	2.2
1	B	341	SER	2.2
1	A	564	VAL	2.2
1	A	431	PHE	2.2
1	B	112	LEU	2.2
1	B	148	LEU	2.2
1	B	340	ARG	2.1
1	B	430	TYR	2.1
1	A	339	LEU	2.1
1	B	563	GLU	2.1
1	B	632	VAL	2.1
1	B	420	HIS	2.1
1	B	613	VAL	2.1
1	B	608	PHE	2.1
1	B	333	ASP	2.0
1	B	100	SER	2.0
1	A	151	GLY	2.0
1	B	357	PRO	2.0
1	A	168	LYS	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

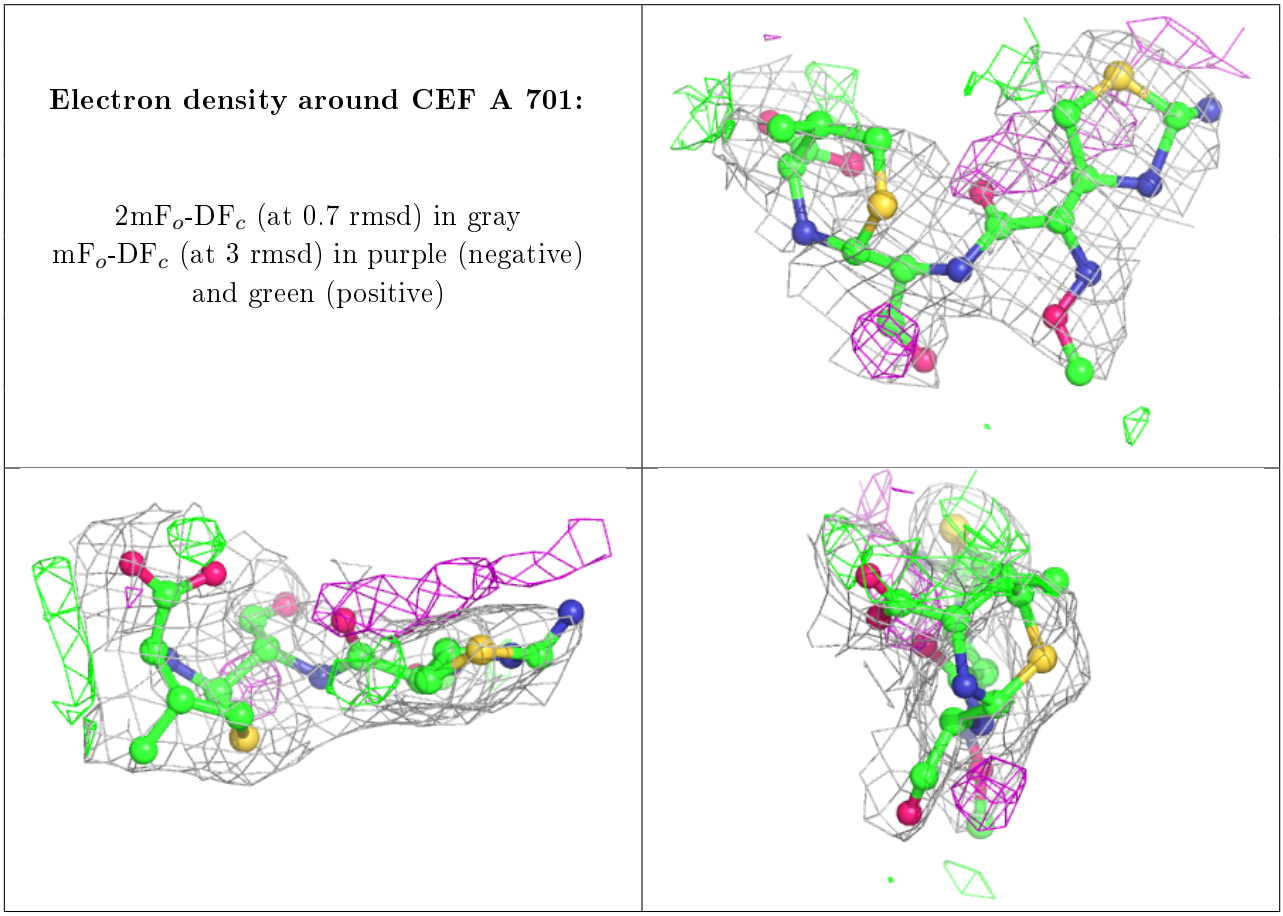
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	CEF	A	701	26/26	0.80	0.21	68,89,111,143	0
2	CEF	B	701	26/26	0.85	0.19	77,99,154,157	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.

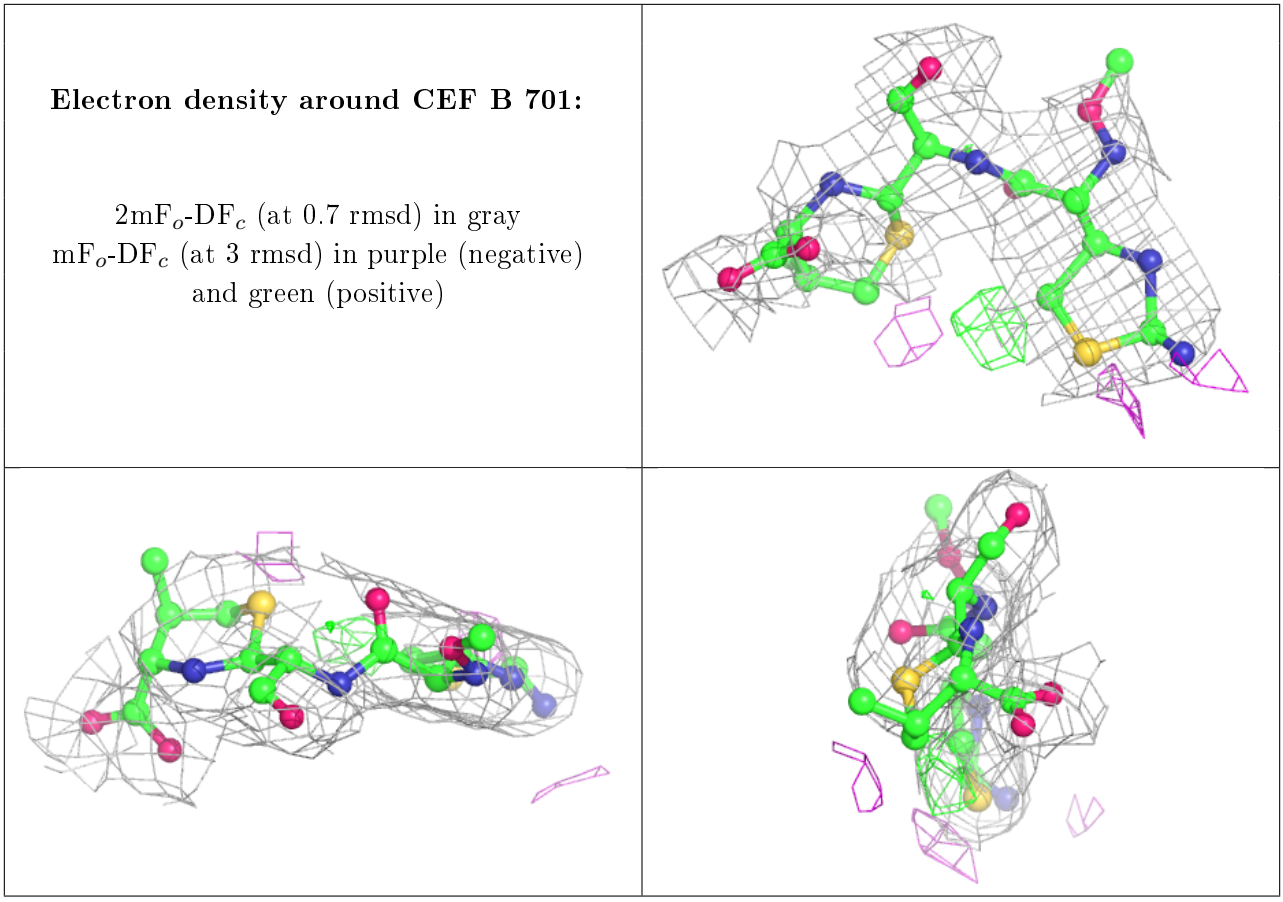
Electron density around CEF A 701:

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



Electron density around CEF B 701:

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



6.5 Other polymers

There are no such residues in this entry.