Full wwPDB X-ray Structure Validation Report (i)

Mar 5, 2024 – 11:53 AM EST

PDB ID	:	2ZXH
Title	:	Structure of Aquifex aeolicus GidA in the form I crystal
Authors	:	Numata, T.; Osawa, T.
Deposited on	:	2008-12-24
Resolution	:	3.20 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

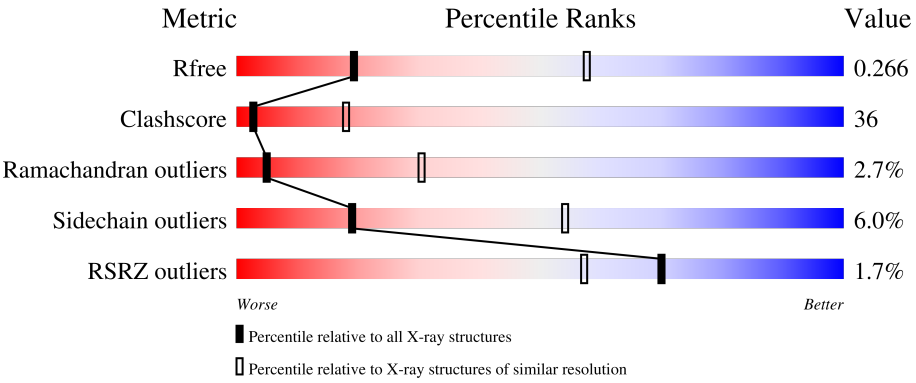
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

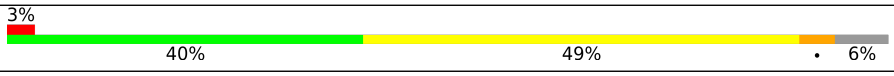
The reported resolution of this entry is 3.20 Å.

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	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	637	
1	B	637	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9714 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 tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	603	Total	C	N	O	S	0	0	0
			4804	3080	816	893	15			
1	B	601	Total	C	N	O	S	0	0	0
			4789	3070	813	891	15			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP O66962
A	-18	GLY	-	expression tag	UNP O66962
A	-17	SER	-	expression tag	UNP O66962
A	-16	SER	-	expression tag	UNP O66962
A	-15	HIS	-	expression tag	UNP O66962
A	-14	HIS	-	expression tag	UNP O66962
A	-13	HIS	-	expression tag	UNP O66962
A	-12	HIS	-	expression tag	UNP O66962
A	-11	HIS	-	expression tag	UNP O66962
A	-10	HIS	-	expression tag	UNP O66962
A	-9	SER	-	expression tag	UNP O66962
A	-8	SER	-	expression tag	UNP O66962
A	-7	GLY	-	expression tag	UNP O66962
A	-6	LEU	-	expression tag	UNP O66962
A	-5	VAL	-	expression tag	UNP O66962
A	-4	PRO	-	expression tag	UNP O66962
A	-3	ALA	-	expression tag	UNP O66962
A	-2	GLY	-	expression tag	UNP O66962
A	-1	SER	-	expression tag	UNP O66962
A	0	HIS	-	expression tag	UNP O66962
B	-19	MET	-	expression tag	UNP O66962
B	-18	GLY	-	expression tag	UNP O66962
B	-17	SER	-	expression tag	UNP O66962
B	-16	SER	-	expression tag	UNP O66962

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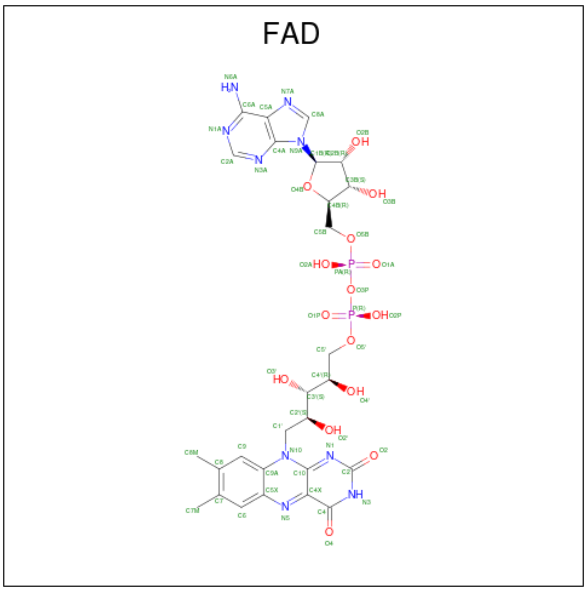
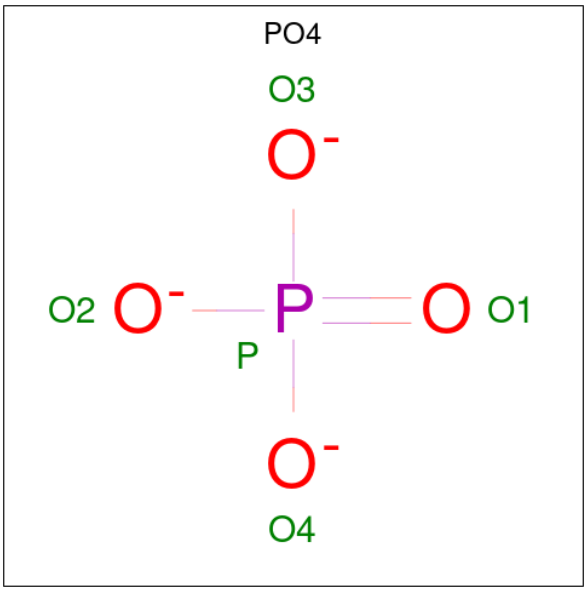
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	expression tag	UNP O66962
B	-14	HIS	-	expression tag	UNP O66962
B	-13	HIS	-	expression tag	UNP O66962
B	-12	HIS	-	expression tag	UNP O66962
B	-11	HIS	-	expression tag	UNP O66962
B	-10	HIS	-	expression tag	UNP O66962
B	-9	SER	-	expression tag	UNP O66962
B	-8	SER	-	expression tag	UNP O66962
B	-7	GLY	-	expression tag	UNP O66962
B	-6	LEU	-	expression tag	UNP O66962
B	-5	VAL	-	expression tag	UNP O66962
B	-4	PRO	-	expression tag	UNP O66962
B	-3	ALA	-	expression tag	UNP O66962
B	-2	GLY	-	expression tag	UNP O66962
B	-1	SER	-	expression tag	UNP O66962
B	0	HIS	-	expression tag	UNP O66962

- Molecule 2 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
2	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



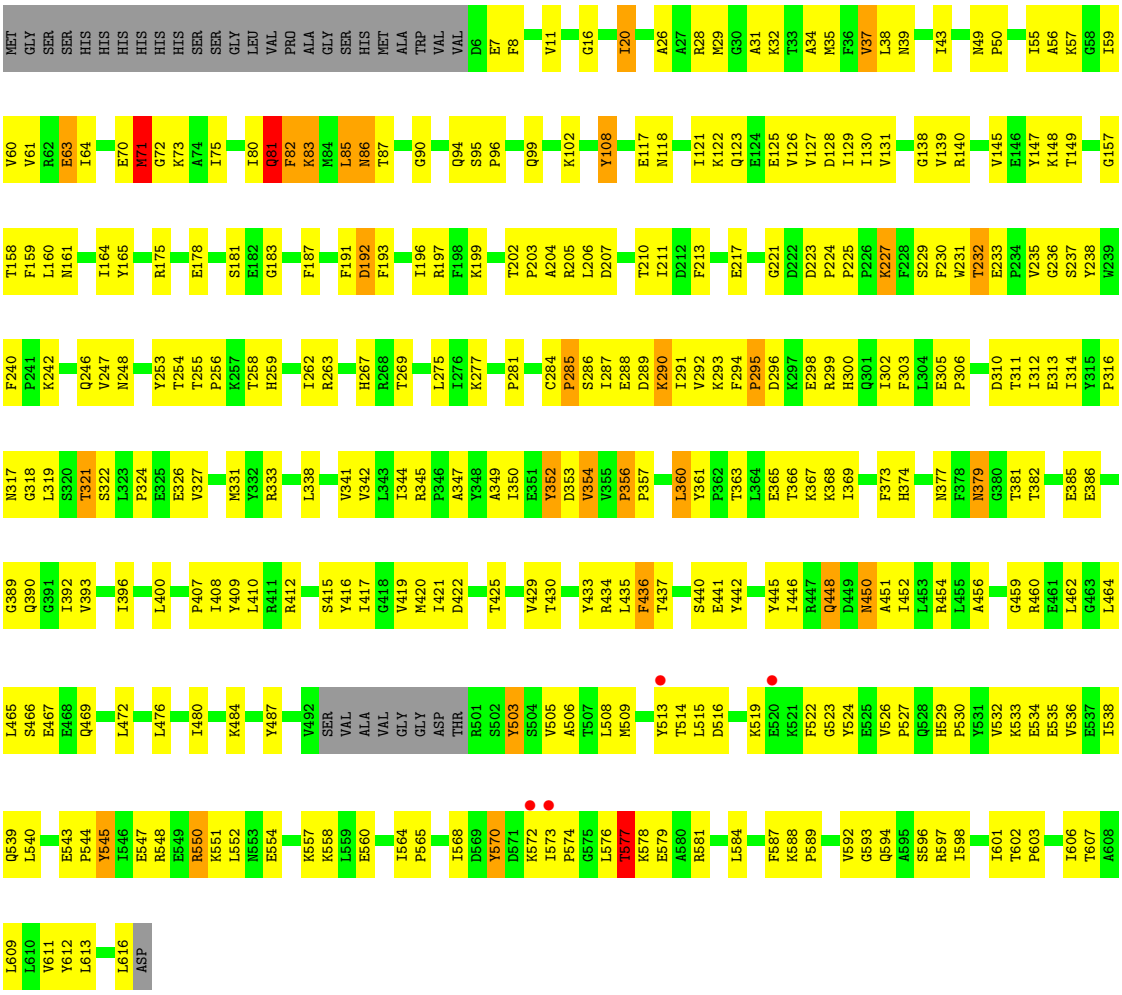
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

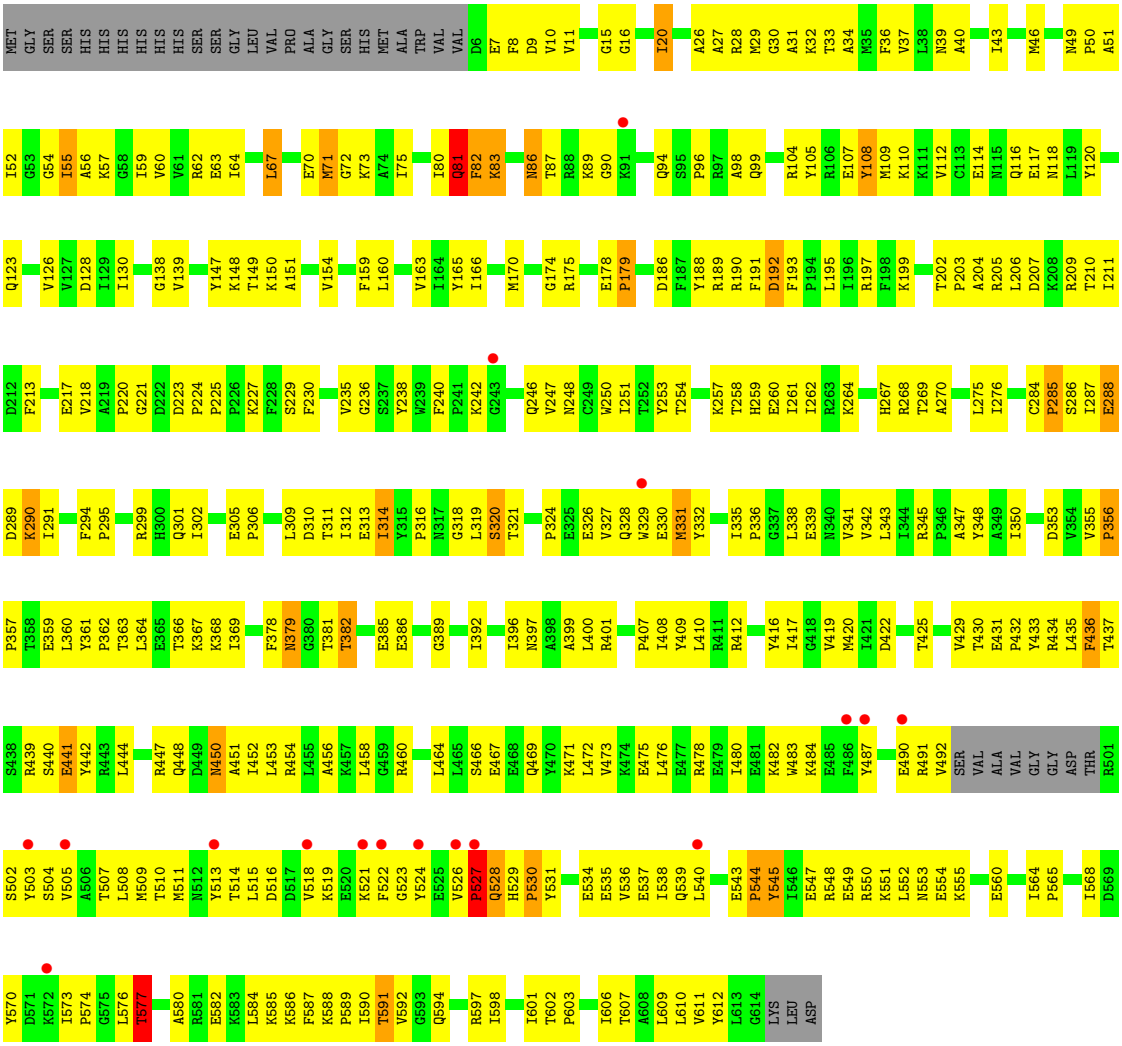
• Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG

Chain A:



• Molecule 1: tRNA uridine 5-carboxymethylaminomethyl modification enzyme mnmG

Chain B:


MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ALA GLY SER HIS MET ALA TRP VAL VAL D6 E7 F8 D9 V10 V11 G15 G16 I20 A26 A27 R28 M29 G30 A31 K32 T33 A34 M35 F36 V37 L38 N39 A40 I43 M46 N49 P50 A51
I52 G53 G54 I55 A56 K57 G58 I59 V60 V61 R62 E63 I64 L67 E70 M71 G72 K73 A74 I75 I80 Q81 F82 K83 N86 T87 R88 K89 G90 K91 Q94 S95 P96 R97 A98 Q99 R104 Y105 R106 E107 Y108 M109 K110 K111 V112 C113 E114 N115 Q116 E117 N118 L119 Y120
Q123 V126 V127 D128 I129 I130 G138 V139 Y147 K148 T149 K150 A151 V154 F159 L160 V163 I164 Y165 I166 M170 G174 R175 E178 P179 D186 F187 Y188 R189 R190 F191 D192 F193 P194 L195 I196 R197 F198 K199 T202 P203 A204 R205 L206 D207 K208 R209 T210 I211
D212 F213 E217 V218 A219 P220 G221 D222 D223 P224 P225 P226 K227 F228 S229 F230 V235 G236 S237 Y238 W239 F240 P241 K242 G243 Q246 V247 N248 C249 W250 I251 T252 Y253 T254 K257 T258 H259 E260 I261 I262 R263 K264 H267 R268 T269 A270 L275 I276 C284 P285 S286 I287 E288
D289 K290 I291 F294 P295 R299 H300 Q301 I302 E305 P306 L309 D310 T311 I312 E313 I314 Y315 P316 N317 G318 L319 S320 T321 P324 E325 E326 V327 Q328 W329 E330 M331 Y332 I335 P336 G337 L338 E339 N340 V341 V342 L343 I344 R345 P346 A347 Y348 A349 I350 D353 V354 V355 P356
P357 T358 E359 L360 Y361 P362 T363 L364 E365 T366 K367 K368 I369 F378 N379 G380 T381 T382 E385 E386 G389 I392 I396 N397 A398 A399 L400 R401 P407 I408 Y409 L410 R411 R412 Y416 I417 G418 V419 M420 I421 D422 T425 V429 T430 E431 P432 Y433 R434 L435 F436 T437
S438 R439 S440 E441 Y442 R443 L444 R447 Q448 P449 N450 A451 I452 L453 R454 L455 A456 K457 L458 G459 R460 L464 L465 S466 E467 E468 Q469 Y470 K471 L472 V473 K474 E475 L476 E477 R478 E479 I480 E481 K482 W483 K484 E485 F486 Y487 E490 R491 V492 SER VAL ALA VAL GLY GLY ASP THR R501
S502 Y503 S504 V505 A506 T507 L508 M509 T510 M511 N512 Y513 T514 L515 D516 D517 V518 K519 E520 K521 F522 G523 Y524 E525 V526 P527 Q528 H529 P530 Y531 E534 E535 V536 E537 I538 Q539 L540 E543 P544 Y545 I546 E547 R548 E549 R550 K551 L552 N553 E554 K555 E560 I564 P565 I568 D569
Y570 D571 K572 I573 P574 G575 L576 T577 A580 R581 E582 K583 L584 K585 K586 F587 K588 P589 I590 T591 V592 G593 Q594 R597 I598 I601 T602 P603 I606 T607 A608 L609 L610 V611 Y612 L613 G614 LYS LEU ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	101.64Å 213.27Å 231.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.97 – 3.20 40.70 – 3.20	Depositor EDS
% Data completeness (in resolution range)	98.0 (19.97-3.20) 99.5 (40.70-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.65 (at 3.18Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.242 , 0.271 0.234 , 0.266	Depositor DCC
R_{free} test set	3801 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å^2)	56.1	Xtriage
Anisotropy	0.666	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 44.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9714	wwPDB-VP
Average B, all atoms (Å^2)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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: PO4, FAD

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	0.43	0/4904	0.66	0/6624
1	B	0.43	0/4889	0.65	0/6605
All	All	0.43	0/9793	0.65	0/13229

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	4804	0	4871	321	0
1	B	4789	0	4854	381	1
2	A	53	0	31	4	0
2	B	53	0	31	2	0
3	A	10	0	0	0	0
3	B	5	0	0	0	0
All	All	9714	0	9787	696	1

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 36.

All (696) 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:B:20:ILE:HG21	1:B:109:MET:HE3	1.35	1.08
1:B:466:SER:HB3	1:B:469:GLN:HG3	1.32	1.06
1:B:480:ILE:HD13	1:B:535:GLU:HG2	1.44	1.00
1:A:311:THR:HG22	1:A:313:GLU:H	1.26	0.97
1:B:311:THR:HG22	1:B:313:GLU:H	1.30	0.94
1:B:7:GLU:HG2	1:B:148:LYS:HB2	1.52	0.91
1:B:87:THR:HA	1:B:94:GLN:HE21	1.36	0.90
1:B:254:THR:HG23	1:B:302:ILE:HD11	1.53	0.90
1:A:254:THR:HG23	1:A:302:ILE:HD11	1.55	0.88
1:B:211:ILE:HB	1:B:213:PHE:CE1	2.09	0.88
1:A:29:MET:HE1	1:A:396:ILE:HA	1.53	0.88
1:B:478:ARG:HH12	1:B:482:LYS:HE2	1.40	0.85
1:B:362:PRO:HG2	1:B:594:GLN:HE22	1.42	0.84
1:A:127:VAL:HG13	1:A:183:GLY:HA3	1.58	0.83
1:B:210:THR:HG21	1:B:342:VAL:HG23	1.59	0.83
1:A:225:PRO:HG2	1:A:240:PHE:HB2	1.60	0.82
1:A:87:THR:HA	1:A:94:GLN:HE21	1.45	0.81
1:B:257:LYS:O	1:B:260:GLU:HG2	1.80	0.81
1:B:508:LEU:HA	1:B:511:MET:HE3	1.64	0.80
1:A:302:ILE:HD13	1:A:319:LEU:HD11	1.65	0.79
1:B:10:VAL:HG23	1:B:33:THR:HG23	1.64	0.78
1:B:466:SER:H	1:B:469:GLN:HE21	1.31	0.78
1:B:8:PHE:CE2	1:B:34:ALA:HB2	2.19	0.78
1:B:483:TRP:HE1	1:B:528:GLN:HE21	1.32	0.77
1:B:20:ILE:HG21	1:B:109:MET:CE	2.13	0.77
1:B:29:MET:HE1	1:B:396:ILE:HG12	1.66	0.77
1:B:412:ARG:HD2	1:B:597:ARG:NH1	2.00	0.77
1:A:122:LYS:HZ3	1:A:147:TYR:HE2	1.33	0.77
1:A:357:PRO:O	1:A:360:LEU:HD12	1.86	0.76
1:A:392:ILE:O	1:A:396:ILE:HG13	1.84	0.76
1:A:287:ILE:HD12	1:A:290:LYS:HD2	1.69	0.75
1:A:7:GLU:HG2	1:A:148:LYS:HB2	1.68	0.75
1:B:362:PRO:CG	1:B:594:GLN:HE22	1.98	0.75
1:B:505:VAL:HA	1:B:508:LEU:HG	1.69	0.75
1:B:224:PRO:HD3	1:B:242:LYS:HE2	1.68	0.75
1:B:476:LEU:O	1:B:480:ILE:HG13	1.87	0.74
1:A:210:THR:HG21	1:A:342:VAL:HG23	1.68	0.74
1:A:71:MET:HE1	1:A:385:GLU:HG3	1.68	0.74
1:B:221:GLY:HA3	1:B:246:GLN:OE1	1.88	0.73
1:A:122:LYS:NZ	1:A:147:TYR:HE2	1.87	0.73
1:B:329:TRP:CD1	1:B:343:LEU:HD12	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:57:LYS:HZ3	1:B:436:PHE:HE1	1.35	0.73
1:A:29:MET:HE1	1:A:396:ILE:HG12	1.71	0.73
1:A:161:ASN:O	1:A:197:ARG:NH2	2.21	0.73
1:B:565:PRO:HB2	1:B:568:ILE:HG23	1.69	0.73
1:A:360:LEU:HD21	1:A:374:HIS:HB2	1.71	0.73
1:B:8:PHE:CD2	1:B:34:ALA:HB2	2.23	0.73
1:A:324:PRO:HB2	1:A:327:VAL:HG23	1.71	0.72
1:B:10:VAL:HG12	1:B:151:ALA:HB3	1.71	0.72
1:B:545:TYR:HD1	1:B:545:TYR:H	1.36	0.72
1:B:573:ILE:HA	1:B:612:TYR:HD1	1.54	0.72
1:A:311:THR:HG22	1:A:313:GLU:N	2.03	0.72
1:A:476:LEU:O	1:A:480:ILE:HG13	1.90	0.72
1:A:505:VAL:HA	1:A:508:LEU:HD12	1.71	0.71
1:B:329:TRP:HD1	1:B:343:LEU:HD12	1.55	0.71
1:B:483:TRP:CZ2	1:B:527:PRO:HA	2.24	0.71
1:A:386:GLU:HG3	1:A:435:LEU:HG	1.72	0.71
1:A:211:ILE:HB	1:A:213:PHE:CE1	2.25	0.71
1:B:594:GLN:HA	1:B:597:ARG:NH2	2.06	0.71
1:B:32:LYS:HZ1	1:B:120:TYR:HE1	1.38	0.70
1:A:275:LEU:HD11	1:B:441:GLU:HG3	1.72	0.70
1:A:160:LEU:HB3	1:A:353:ASP:HB2	1.72	0.70
1:A:363:THR:HG22	1:A:408:ILE:O	1.89	0.70
1:B:37:VAL:HG12	1:B:39:ASN:H	1.57	0.70
1:A:505:VAL:O	1:A:508:LEU:HB2	1.91	0.69
1:B:55:ILE:HG22	1:B:56:ALA:N	2.07	0.69
1:B:472:LEU:O	1:B:476:LEU:HG	1.92	0.69
1:B:476:LEU:HD22	1:B:529:HIS:NE2	2.07	0.69
1:A:420:MET:HG3	1:A:433:TYR:HE1	1.57	0.69
1:B:412:ARG:HD2	1:B:597:ARG:HH11	1.55	0.69
1:A:565:PRO:HB2	1:A:568:ILE:HG23	1.75	0.69
1:A:476:LEU:HD21	1:A:529:HIS:CE1	2.27	0.68
1:A:85:LEU:HD23	1:A:86:ASN:H	1.58	0.68
1:B:70:GLU:O	1:B:72:GLY:N	2.26	0.68
1:B:207:ASP:OD1	1:B:312:ILE:HD12	1.94	0.68
1:B:138:GLY:HA2	1:B:149:THR:HG22	1.75	0.68
1:B:466:SER:H	1:B:469:GLN:NE2	1.91	0.68
1:B:478:ARG:NH1	1:B:482:LYS:HE2	2.09	0.68
1:A:313:GLU:HG2	1:A:344:ILE:HD12	1.75	0.68
1:A:589:PRO:HG3	1:A:598:ILE:HD11	1.76	0.68
1:B:521:LYS:C	1:B:522:PHE:HD2	1.96	0.67
1:A:603:PRO:O	1:A:606:ILE:HG22	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:PRO:HA	1:B:339:GLU:OE2	1.94	0.67
1:B:204:ALA:N	1:B:347:ALA:HB2	2.08	0.67
1:A:480:ILE:HD13	1:A:535:GLU:HG2	1.75	0.66
1:B:382:THR:OG1	1:B:432:PRO:HB3	1.95	0.66
1:B:480:ILE:HG23	1:B:536:VAL:HG23	1.77	0.66
1:B:450:ASN:HD22	1:B:451:ALA:N	1.93	0.66
1:A:381:THR:HG21	1:A:390:GLN:NE2	2.10	0.66
1:B:225:PRO:HG2	1:B:240:PHE:HB2	1.77	0.66
1:A:545:TYR:HD1	1:A:545:TYR:H	1.43	0.66
1:B:211:ILE:HB	1:B:213:PHE:HE1	1.59	0.66
1:A:70:GLU:O	1:A:72:GLY:N	2.28	0.65
1:A:420:MET:HG3	1:A:433:TYR:CE1	2.29	0.65
1:A:37:VAL:O	1:A:123:GLN:HA	1.96	0.65
1:B:37:VAL:HG12	1:B:39:ASN:N	2.12	0.65
1:A:247:VAL:HG12	1:A:248:ASN:N	2.12	0.65
1:B:60:VAL:HG21	1:B:435:LEU:CD1	2.27	0.65
1:A:367:LYS:NZ	1:A:587:PHE:HA	2.11	0.65
1:B:29:MET:HE1	1:B:396:ILE:HA	1.79	0.64
1:B:206:LEU:HD23	1:B:343:LEU:HD23	1.78	0.64
1:A:294:PHE:N	1:A:295:PRO:HD3	2.13	0.64
1:A:357:PRO:HG3	1:A:379:ASN:O	1.97	0.64
1:A:71:MET:HE1	1:A:385:GLU:HA	1.80	0.64
1:B:87:THR:HG22	1:B:94:GLN:NE2	2.13	0.64
1:A:568:ILE:HD11	1:A:570:TYR:CE1	2.33	0.64
1:B:362:PRO:HG2	1:B:594:GLN:NE2	2.12	0.64
1:B:573:ILE:HG12	1:B:612:TYR:CD1	2.33	0.64
1:A:204:ALA:N	1:A:347:ALA:HB2	2.12	0.64
1:B:191:PHE:O	1:B:192:ASP:HB2	1.98	0.64
1:B:452:ILE:O	1:B:456:ALA:HB2	1.98	0.64
1:B:90:GLY:O	1:B:94:GLN:HG3	1.98	0.64
1:B:328:GLN:O	1:B:332:TYR:HD2	1.81	0.63
1:A:130:ILE:N	1:A:130:ILE:HD12	2.13	0.63
1:B:59:ILE:HG12	1:B:448:GLN:HB3	1.81	0.63
1:B:67:LEU:HD21	1:B:458:LEU:HD23	1.81	0.63
1:A:434:ARG:HG2	1:A:434:ARG:HH11	1.63	0.63
1:A:448:GLN:NE2	1:A:448:GLN:O	2.31	0.63
1:B:52:ILE:HD12	1:B:71:MET:CE	2.28	0.63
1:A:8:PHE:O	1:A:149:THR:HA	1.99	0.63
1:A:60:VAL:HG21	1:A:435:LEU:CD1	2.28	0.63
1:B:360:LEU:O	1:B:367:LYS:HE3	1.99	0.63
1:B:37:VAL:O	1:B:123:GLN:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:452:ILE:HD11	1:B:473:VAL:HG21	1.80	0.62
1:B:466:SER:HB3	1:B:469:GLN:CG	2.19	0.62
1:A:57:LYS:HB3	1:A:385:GLU:HG2	1.82	0.62
1:B:311:THR:HG22	1:B:313:GLU:N	2.09	0.62
1:B:492:VAL:HG12	1:B:492:VAL:O	1.97	0.62
1:A:60:VAL:O	1:A:64:ILE:HG13	2.00	0.62
1:B:247:VAL:HG12	1:B:248:ASN:N	2.14	0.62
1:B:108:TYR:C	1:B:108:TYR:HD2	2.03	0.62
1:B:275:LEU:N	1:B:275:LEU:HD22	2.14	0.62
1:A:460:ARG:CZ	1:A:467:GLU:HG2	2.29	0.62
1:B:29:MET:HE2	1:B:464:LEU:HD21	1.82	0.62
1:B:9:ASP:OD1	1:B:150:LYS:HE3	2.00	0.62
1:B:225:PRO:HB3	1:B:246:GLN:HE22	1.64	0.62
1:B:260:GLU:O	1:B:264:LYS:HG3	2.00	0.61
1:B:529:HIS:CE1	1:B:531:TYR:HB3	2.34	0.61
1:A:231:TRP:CZ3	1:A:469:GLN:HG2	2.35	0.61
1:A:366:THR:HG22	1:A:368:LYS:N	2.15	0.61
1:A:138:GLY:HA2	1:A:149:THR:HG22	1.82	0.61
1:A:284:CYS:SG	1:A:293:LYS:HD2	2.41	0.61
1:B:594:GLN:N	1:B:597:ARG:HH21	1.98	0.61
1:A:29:MET:CE	1:A:396:ILE:HG12	2.30	0.61
1:A:129:ILE:HB	1:A:187:PHE:CE1	2.35	0.61
1:B:570:TYR:CD2	1:B:584:LEU:HB3	2.36	0.61
1:A:434:ARG:HG2	1:A:434:ARG:NH1	2.17	0.60
1:B:357:PRO:HG3	1:B:379:ASN:O	2.01	0.60
1:B:57:LYS:NZ	1:B:436:PHE:HE1	1.98	0.60
1:B:108:TYR:C	1:B:108:TYR:CD2	2.75	0.60
1:A:573:ILE:HG21	1:A:576:LEU:HD22	1.83	0.60
1:A:554:GLU:O	1:A:558:LYS:HG3	2.02	0.60
1:A:287:ILE:HD13	1:A:318:GLY:O	2.01	0.60
1:B:8:PHE:HE1	1:B:147:TYR:HD2	1.50	0.60
1:B:159:PHE:CD2	1:B:174:GLY:HA3	2.36	0.60
1:B:363:THR:HG22	1:B:408:ILE:O	2.02	0.60
1:B:381:THR:CG2	1:B:382:THR:N	2.65	0.60
1:B:589:PRO:HA	1:B:594:GLN:OE1	2.00	0.60
1:A:196:ILE:HG13	1:A:354:VAL:HG12	1.83	0.59
1:A:551:LYS:HA	1:A:554:GLU:HG3	1.83	0.59
1:B:564:ILE:HD11	1:B:592:VAL:HA	1.84	0.59
1:B:366:THR:HG22	1:B:368:LYS:N	2.17	0.59
1:B:251:ILE:N	1:B:251:ILE:HD12	2.16	0.59
1:A:204:ALA:O	1:A:205:ARG:HD2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:ASN:N	1:A:450:ASN:HD22	1.99	0.59
1:B:11:VAL:HG23	1:B:149:THR:OG1	2.01	0.59
1:B:612:TYR:CD2	1:B:612:TYR:C	2.75	0.59
1:A:574:PRO:HD3	1:A:612:TYR:HD1	1.66	0.59
1:B:227:LYS:NZ	1:B:229:SER:O	2.36	0.59
1:A:480:ILE:HG23	1:A:536:VAL:HG23	1.84	0.59
1:B:250:TRP:C	1:B:251:ILE:HD12	2.22	0.59
1:B:267:HIS:CD2	1:B:267:HIS:H	2.19	0.59
1:A:82:PHE:CD1	1:A:82:PHE:N	2.70	0.59
1:A:286:SER:HB2	1:A:288:GLU:OE1	2.03	0.59
1:B:8:PHE:O	1:B:149:THR:HA	2.03	0.59
1:A:28:ARG:HH12	1:A:70:GLU:HG2	1.68	0.59
1:A:196:ILE:CG1	1:A:354:VAL:HG12	2.33	0.58
1:B:450:ASN:O	1:B:454:ARG:HG3	2.02	0.58
1:B:29:MET:CE	1:B:464:LEU:HD21	2.32	0.58
1:A:8:PHE:CD2	1:A:34:ALA:HB2	2.38	0.58
1:A:247:VAL:HG12	1:A:248:ASN:H	1.68	0.58
1:B:29:MET:CE	1:B:396:ILE:HG12	2.33	0.58
1:A:81:GLN:HB3	1:A:99:GLN:HB2	1.84	0.58
1:A:435:LEU:C	1:A:437:THR:H	2.06	0.58
1:B:589:PRO:HG3	1:B:598:ILE:HD11	1.86	0.58
1:B:396:ILE:O	1:B:400:LEU:HG	2.04	0.58
1:B:62:ARG:NH1	1:B:238:TYR:CD1	2.72	0.58
1:B:362:PRO:CG	1:B:594:GLN:NE2	2.67	0.58
1:B:573:ILE:HA	1:B:612:TYR:CD1	2.37	0.58
1:A:8:PHE:CE2	1:A:34:ALA:HB2	2.39	0.58
1:A:514:THR:C	1:A:516:ASP:H	2.05	0.58
1:A:160:LEU:HD23	1:A:353:ASP:CB	2.34	0.58
1:B:210:THR:HB	1:B:341:VAL:HA	1.86	0.58
1:B:420:MET:HG3	1:B:433:TYR:CE1	2.38	0.58
1:A:224:PRO:HD3	1:A:242:LYS:HE2	1.84	0.57
1:A:452:ILE:O	1:A:456:ALA:HB2	2.03	0.57
1:B:225:PRO:HB3	1:B:246:GLN:NE2	2.19	0.57
1:B:442:TYR:HA	1:B:549:GLU:OE2	2.04	0.57
1:B:359:GLU:OE1	1:B:368:LYS:HE3	2.04	0.57
1:B:381:THR:HG22	1:B:382:THR:N	2.19	0.57
1:A:206:LEU:HB2	1:A:314:ILE:HB	1.86	0.57
1:B:262:ILE:HB	1:B:291:ILE:HD13	1.84	0.57
1:B:430:THR:HG23	1:B:431:GLU:HG2	1.87	0.57
1:B:191:PHE:CD2	1:B:369:ILE:HD11	2.39	0.57
1:B:329:TRP:HD1	1:B:343:LEU:CD1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:THR:C	1:B:516:ASP:H	2.07	0.57
1:B:63:GLU:O	1:B:67:LEU:HD12	2.05	0.57
1:A:60:VAL:HA	1:A:63:GLU:HG3	1.85	0.57
1:A:160:LEU:HA	1:A:181:SER:OG	2.04	0.57
1:B:453:LEU:HD11	1:B:535:GLU:OE2	2.05	0.57
1:A:589:PRO:HA	1:A:594:GLN:OE1	2.04	0.57
1:A:81:GLN:HG3	1:A:247:VAL:O	2.04	0.57
1:A:365:GLU:HG3	1:A:373:PHE:CE2	2.40	0.57
1:A:584:LEU:HG	1:A:601:ILE:HD11	1.87	0.56
1:A:450:ASN:HD22	1:A:451:ALA:N	2.03	0.56
1:B:81:GLN:HG3	1:B:247:VAL:O	2.05	0.56
1:B:594:GLN:CA	1:B:597:ARG:NH2	2.69	0.56
1:B:285:PRO:HG3	1:B:434:ARG:NH2	2.21	0.56
1:A:560:GLU:OE1	1:A:597:ARG:NH2	2.38	0.56
1:B:319:LEU:HD11	1:B:335:ILE:CD1	2.36	0.56
1:B:82:PHE:O	1:B:83:LYS:HB3	2.06	0.56
1:B:392:ILE:O	1:B:396:ILE:HG13	2.06	0.56
1:B:545:TYR:N	1:B:545:TYR:CD1	2.74	0.56
1:A:389:GLY:O	1:A:392:ILE:HG22	2.05	0.56
1:A:367:LYS:HZ1	1:A:587:PHE:HA	1.71	0.56
1:A:534:GLU:O	1:A:538:ILE:HG13	2.05	0.56
1:B:450:ASN:ND2	1:B:454:ARG:HE	2.03	0.56
1:A:221:GLY:HA3	1:A:246:GLN:OE1	2.06	0.55
1:A:230:PHE:HZ	1:A:476:LEU:HD13	1.71	0.55
1:A:90:GLY:O	1:A:94:GLN:HG3	2.07	0.55
1:A:275:LEU:HD23	1:A:292:VAL:HG13	1.87	0.55
1:B:480:ILE:HD13	1:B:535:GLU:CG	2.28	0.55
1:A:210:THR:HG21	1:A:342:VAL:CG2	2.35	0.55
1:A:290:LYS:HB3	1:A:300:HIS:CE1	2.41	0.55
1:B:199:LYS:HA	1:B:350:ILE:O	2.07	0.55
1:B:275:LEU:HD22	1:B:275:LEU:H	1.72	0.55
1:B:483:TRP:CE3	1:B:527:PRO:HG3	2.41	0.55
1:B:509:MET:CE	1:B:515:LEU:HG	2.37	0.55
1:A:229:SER:HB3	1:A:232:THR:OG1	2.06	0.55
1:A:360:LEU:HD11	1:A:379:ASN:HD21	1.70	0.55
1:A:63:GLU:OE2	1:A:454:ARG:NH2	2.38	0.55
1:A:71:MET:CE	1:A:385:GLU:HA	2.37	0.55
1:A:85:LEU:HD23	1:A:86:ASN:N	2.20	0.55
1:A:573:ILE:HA	1:A:612:TYR:CD1	2.41	0.55
1:B:224:PRO:HB3	1:B:242:LYS:HG2	1.88	0.55
1:B:247:VAL:HG12	1:B:248:ASN:H	1.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:NZ	1:A:205:ARG:HH21	2.04	0.55
1:A:233:GLU:OE1	1:A:235:VAL:HG23	2.06	0.55
1:A:570:TYR:CE2	1:A:584:LEU:HB3	2.42	0.55
1:A:275:LEU:CD1	1:B:441:GLU:HG3	2.37	0.55
1:A:545:TYR:N	1:A:545:TYR:CD1	2.76	0.55
1:A:547:GLU:HA	1:A:547:GLU:OE1	2.07	0.55
1:B:117:GLU:HG2	1:B:118:ASN:OD1	2.07	0.54
1:B:519:LYS:HD2	1:B:526:VAL:CG2	2.37	0.54
1:B:262:ILE:HD13	1:B:287:ILE:HG23	1.89	0.54
1:B:10:VAL:HG21	1:B:26:ALA:HB1	1.90	0.54
1:B:160:LEU:HD23	1:B:353:ASP:CB	2.38	0.54
1:A:386:GLU:CG	1:A:435:LEU:HG	2.36	0.54
1:B:259:HIS:N	1:B:259:HIS:CD2	2.74	0.54
1:B:508:LEU:O	1:B:513:TYR:HB2	2.07	0.54
1:B:435:LEU:C	1:B:437:THR:H	2.10	0.54
1:B:480:ILE:HG23	1:B:536:VAL:CG2	2.37	0.54
1:A:29:MET:HE3	1:A:464:LEU:HD21	1.88	0.54
1:A:199:LYS:HA	1:A:350:ILE:O	2.08	0.54
1:B:514:THR:HG22	1:B:537:GLU:OE2	2.07	0.54
1:A:204:ALA:HB1	1:A:345:ARG:O	2.07	0.54
1:A:547:GLU:OE1	1:A:550:ARG:HD3	2.07	0.53
1:B:548:ARG:O	1:B:552:LEU:HG	2.08	0.53
1:A:108:TYR:C	1:A:108:TYR:CD2	2.81	0.53
1:B:32:LYS:NZ	1:B:120:TYR:HE1	2.05	0.53
1:A:396:ILE:O	1:A:400:LEU:HG	2.09	0.53
1:B:28:ARG:HH12	1:B:70:GLU:HG2	1.73	0.53
1:A:341:VAL:HG22	1:A:342:VAL:N	2.24	0.53
1:B:484:LYS:HE3	1:B:540:LEU:HD23	1.91	0.53
1:A:225:PRO:HG2	1:A:240:PHE:CB	2.35	0.53
1:A:366:THR:HG22	1:A:368:LYS:H	1.74	0.53
1:A:574:PRO:CD	1:A:612:TYR:HD1	2.21	0.53
1:B:204:ALA:HB1	1:B:345:ARG:O	2.08	0.53
1:B:366:THR:HG22	1:B:368:LYS:H	1.73	0.53
1:B:397:ASN:OD1	1:B:408:ILE:N	2.36	0.53
1:A:352:TYR:CD1	1:A:352:TYR:N	2.77	0.53
1:B:409:TYR:CE2	1:B:590:ILE:HD12	2.44	0.53
1:A:82:PHE:O	1:A:83:LYS:HB3	2.07	0.53
1:B:160:LEU:HD23	1:B:353:ASP:HB3	1.91	0.53
1:B:258:THR:HB	1:B:259:HIS:HD2	1.73	0.53
1:B:46:MET:SD	1:B:105:TYR:CD2	3.02	0.53
1:A:396:ILE:HD13	1:A:462:LEU:HD13	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:SER:HB2	1:B:288:GLU:HG2	1.91	0.52
1:B:505:VAL:CA	1:B:508:LEU:HG	2.39	0.52
1:B:335:ILE:HB	1:B:338:LEU:HD12	1.91	0.52
1:B:460:ARG:HD3	1:B:467:GLU:HA	1.91	0.52
1:B:510:THR:HG22	1:B:510:THR:O	2.07	0.52
1:A:20:ILE:HA	1:A:35:MET:HE3	1.91	0.52
1:A:128:ASP:OD1	1:A:129:ILE:N	2.42	0.52
1:B:492:VAL:C	1:B:502:SER:HA	2.30	0.52
1:A:259:HIS:N	1:A:259:HIS:CD2	2.78	0.52
1:A:526:VAL:HG11	1:A:533:LYS:HE3	1.91	0.52
1:B:60:VAL:HG21	1:B:435:LEU:HD13	1.91	0.52
1:B:81:GLN:HB3	1:B:99:GLN:HB2	1.91	0.52
1:B:507:THR:HG22	1:B:511:MET:HE2	1.91	0.52
1:B:534:GLU:O	1:B:538:ILE:HG13	2.08	0.52
1:A:460:ARG:NH2	1:A:467:GLU:HG2	2.25	0.52
1:A:56:ALA:HB3	1:A:435:LEU:HB3	1.91	0.52
1:A:293:LYS:C	1:A:295:PRO:HD3	2.31	0.52
1:A:381:THR:HG21	1:A:390:GLN:HE22	1.73	0.52
1:B:484:LYS:HE3	1:B:540:LEU:CD2	2.40	0.52
1:A:71:MET:CE	1:A:385:GLU:HG3	2.39	0.51
1:A:275:LEU:HD23	1:A:292:VAL:CG1	2.40	0.51
1:B:218:VAL:CG1	1:B:248:ASN:HD22	2.23	0.51
1:B:166:ILE:HD11	1:B:348:TYR:HB3	1.91	0.51
1:A:288:GLU:O	1:A:292:VAL:HG23	2.10	0.51
1:B:82:PHE:CD1	1:B:82:PHE:N	2.79	0.51
1:B:410:LEU:HD12	1:B:417:ILE:CG2	2.40	0.51
1:B:286:SER:CB	1:B:288:GLU:HG2	2.41	0.51
1:A:108:TYR:C	1:A:108:TYR:HD2	2.14	0.51
1:B:361:TYR:O	1:B:425:THR:HG21	2.10	0.51
1:B:126:VAL:HG13	1:B:139:VAL:CG1	2.41	0.51
1:B:416:TYR:O	1:B:419:VAL:HB	2.10	0.51
1:A:160:LEU:HD23	1:A:353:ASP:HB3	1.92	0.51
1:B:8:PHE:CE1	1:B:147:TYR:HD2	2.29	0.51
1:B:154:VAL:HG21	1:B:188:TYR:OH	2.11	0.51
1:A:361:TYR:OH	1:A:588:LYS:HD2	2.10	0.51
1:A:393:VAL:HG21	1:A:421:ILE:HD11	1.93	0.51
1:A:466:SER:HB3	1:A:469:GLN:HB2	1.92	0.51
1:A:60:VAL:HG21	1:A:435:LEU:HD13	1.92	0.50
1:B:440:SER:C	1:B:442:TYR:H	2.14	0.50
1:A:357:PRO:HA	1:A:360:LEU:HD12	1.94	0.50
1:A:126:VAL:HG13	1:A:139:VAL:CG1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:268:ARG:O	1:B:324:PRO:HD3	2.10	0.50
1:A:450:ASN:N	1:A:450:ASN:ND2	2.58	0.50
1:B:460:ARG:NH1	1:B:467:GLU:N	2.59	0.50
1:A:38:LEU:HD21	1:A:125:GLU:HG3	1.94	0.50
1:B:487:TYR:CE2	1:B:515:LEU:HD11	2.47	0.50
1:A:39:ASN:HA	1:A:123:GLN:OE1	2.12	0.50
1:A:255:THR:HB	1:A:256:PRO:HD2	1.93	0.50
1:A:440:SER:C	1:A:442:TYR:H	2.15	0.50
1:B:28:ARG:NH2	1:B:70:GLU:OE2	2.44	0.50
1:B:518:VAL:O	1:B:524:TYR:HB2	2.12	0.50
1:A:381:THR:CG2	1:A:390:GLN:HE22	2.24	0.50
1:A:506:ALA:HB1	1:A:540:LEU:HD22	1.92	0.50
1:B:360:LEU:HD23	1:B:366:THR:HA	1.94	0.50
1:B:434:ARG:HD3	1:B:436:PHE:CE2	2.46	0.50
1:A:202:THR:HG22	2:A:618:FAD:HM72	1.94	0.49
1:B:560:GLU:HA	1:B:591:THR:HG21	1.94	0.49
1:B:509:MET:CE	1:B:537:GLU:HG3	2.42	0.49
1:B:551:LYS:HA	1:B:554:GLU:HG3	1.94	0.49
1:A:290:LYS:O	1:A:300:HIS:CE1	2.66	0.49
1:A:412:ARG:HD2	1:A:597:ARG:NH1	2.26	0.49
1:A:480:ILE:HD13	1:A:535:GLU:CG	2.41	0.49
1:B:324:PRO:O	1:B:328:GLN:HG3	2.12	0.49
1:B:480:ILE:HG21	1:B:535:GLU:HG3	1.93	0.49
1:B:483:TRP:CH2	1:B:527:PRO:HA	2.46	0.49
1:A:94:GLN:O	1:A:448:GLN:HG2	2.11	0.49
1:A:230:PHE:CE1	1:A:236:GLY:O	2.65	0.49
1:B:7:GLU:O	1:B:32:LYS:HD3	2.13	0.49
1:A:365:GLU:HG3	1:A:373:PHE:CZ	2.47	0.49
1:A:539:GLN:O	1:A:543:GLU:HB2	2.11	0.49
1:B:16:GLY:O	1:B:20:ILE:HG13	2.11	0.49
1:B:363:THR:O	1:B:364:LEU:HB2	2.13	0.49
1:A:159:PHE:CE1	1:A:175:ARG:HG3	2.48	0.49
1:A:366:THR:HG22	1:A:369:ILE:H	1.78	0.49
1:A:350:ILE:O	1:A:350:ILE:HG23	2.13	0.49
1:B:203:PRO:O	1:B:205:ARG:NH1	2.46	0.49
1:A:484:LYS:NZ	1:A:539:GLN:HB3	2.27	0.49
1:B:492:VAL:O	1:B:492:VAL:CG1	2.60	0.49
1:B:209:ARG:HD3	1:B:312:ILE:HD12	1.95	0.49
1:B:570:TYR:CE2	1:B:584:LEU:HB3	2.47	0.49
1:A:159:PHE:HE1	1:A:175:ARG:HG3	1.78	0.48
1:A:230:PHE:CE2	1:A:452:ILE:HG12	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ALA:O	1:B:31:ALA:HB3	2.13	0.48
1:B:130:ILE:HD12	1:B:130:ILE:H	1.78	0.48
1:A:294:PHE:C	1:A:296:ASP:H	2.15	0.48
1:B:108:TYR:HE2	1:B:112:VAL:CG2	2.26	0.48
1:B:547:GLU:OE1	1:B:550:ARG:HD3	2.13	0.48
1:B:9:ASP:OD2	1:B:32:LYS:N	2.34	0.48
1:B:286:SER:OG	1:B:288:GLU:HG2	2.13	0.48
1:B:326:GLU:HA	1:B:329:TRP:CE3	2.49	0.48
1:B:412:ARG:CD	1:B:597:ARG:NH1	2.74	0.48
1:B:519:LYS:O	1:B:523:GLY:HA2	2.13	0.48
1:A:213:PHE:CD1	1:A:213:PHE:N	2.81	0.48
1:A:460:ARG:NH1	1:A:467:GLU:HG2	2.28	0.48
1:B:539:GLN:O	1:B:543:GLU:HB2	2.13	0.48
1:B:544:PRO:HB2	1:B:545:TYR:HD1	1.79	0.48
1:A:338:LEU:O	1:A:341:VAL:HG12	2.13	0.48
1:B:52:ILE:HD12	1:B:71:MET:HE2	1.94	0.48
1:A:550:ARG:O	1:A:550:ARG:HG2	2.13	0.48
1:B:29:MET:HE1	1:B:396:ILE:CG1	2.39	0.48
1:B:452:ILE:HG23	1:B:453:LEU:HD23	1.95	0.48
1:A:191:PHE:O	1:A:192:ASP:HB2	2.12	0.48
1:A:363:THR:HG21	1:A:407:PRO:HB2	1.94	0.48
1:A:390:GLN:HG3	1:A:420:MET:HE3	1.96	0.48
1:A:564:ILE:HD11	1:A:592:VAL:HA	1.95	0.48
1:B:130:ILE:HD12	1:B:130:ILE:N	2.29	0.48
1:B:519:LYS:HG3	1:B:524:TYR:O	2.13	0.48
1:B:253:TYR:CE2	1:B:301:GLN:HG3	2.49	0.48
1:A:175:ARG:NE	1:A:178:GLU:OE2	2.42	0.48
1:A:230:PHE:CD2	1:A:452:ILE:HG12	2.48	0.48
1:B:29:MET:HG3	1:B:464:LEU:HD21	1.96	0.48
1:B:230:PHE:HZ	1:B:476:LEU:HD12	1.77	0.48
1:B:389:GLY:O	1:B:392:ILE:HG22	2.14	0.48
1:B:519:LYS:HD2	1:B:526:VAL:HG23	1.96	0.48
1:B:545:TYR:HD1	1:B:545:TYR:N	2.07	0.48
1:A:460:ARG:HD3	1:A:467:GLU:HA	1.96	0.48
1:B:507:THR:O	1:B:511:MET:HE3	2.13	0.48
1:B:594:GLN:CA	1:B:597:ARG:HH21	2.26	0.48
1:A:80:ILE:O	1:A:81:GLN:HB2	2.13	0.47
1:A:140:ARG:HG2	1:A:145:VAL:O	2.13	0.47
1:B:51:ALA:HB1	1:B:98:ALA:O	2.14	0.47
1:B:318:GLY:O	1:B:319:LEU:HD23	2.14	0.47
1:B:509:MET:HE3	1:B:537:GLU:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ILE:HG23	1:A:536:VAL:CG2	2.44	0.47
1:A:514:THR:C	1:A:516:ASP:N	2.67	0.47
1:B:476:LEU:HD22	1:B:529:HIS:CD2	2.48	0.47
1:A:574:PRO:HD3	1:A:612:TYR:CD1	2.46	0.47
1:B:186:ASP:O	1:B:190:ARG:HB2	2.14	0.47
1:B:224:PRO:HB3	1:B:242:LYS:CG	2.45	0.47
1:B:294:PHE:N	1:B:295:PRO:HD3	2.29	0.47
1:A:357:PRO:HA	1:A:360:LEU:CD1	2.45	0.47
1:A:422:ASP:OD2	1:A:597:ARG:NH1	2.48	0.47
1:A:607:THR:O	1:A:611:VAL:HG23	2.13	0.47
1:B:543:GLU:N	1:B:544:PRO:CD	2.78	0.47
1:B:28:ARG:HH22	1:B:70:GLU:CG	2.28	0.47
1:B:218:VAL:HG12	1:B:220:PRO:HD3	1.95	0.47
1:A:11:VAL:HG11	1:A:139:VAL:HG21	1.96	0.47
1:A:289:ASP:O	1:A:291:ILE:N	2.48	0.47
1:B:11:VAL:HG13	1:B:36:PHE:CE1	2.50	0.47
1:B:193:PHE:CZ	1:B:366:THR:HG21	2.50	0.47
1:A:161:ASN:HB3	1:A:197:ARG:NH2	2.30	0.47
1:B:80:ILE:O	1:B:81:GLN:HB2	2.15	0.47
1:B:396:ILE:HG12	1:B:464:LEU:HD11	1.97	0.47
1:B:509:MET:HE1	1:B:515:LEU:N	2.29	0.47
1:B:62:ARG:NH1	1:B:238:TYR:CG	2.82	0.47
1:B:72:GLY:O	1:B:75:ILE:HG22	2.14	0.47
1:B:210:THR:CB	1:B:341:VAL:HA	2.44	0.47
1:B:420:MET:HG3	1:B:433:TYR:HE1	1.79	0.47
1:A:613:LEU:HA	1:A:616:LEU:CD1	2.45	0.47
1:B:165:TYR:CE1	1:B:170:MET:HG2	2.50	0.47
1:B:223:ASP:OD1	1:B:242:LYS:HA	2.15	0.47
1:A:290:LYS:O	1:A:300:HIS:HE1	1.98	0.46
1:A:509:MET:SD	1:A:515:LEU:HD23	2.55	0.46
1:B:178:GLU:HB3	1:B:179:PRO:HD2	1.97	0.46
1:A:361:TYR:O	1:A:425:THR:HG21	2.15	0.46
1:A:472:LEU:HD12	1:A:472:LEU:O	2.15	0.46
1:B:471:LYS:O	1:B:475:GLU:HB2	2.15	0.46
1:B:522:PHE:N	1:B:522:PHE:CD2	2.83	0.46
1:A:294:PHE:O	1:A:296:ASP:N	2.48	0.46
1:A:356:PRO:HA	1:A:357:PRO:HD3	1.77	0.46
1:B:29:MET:CE	1:B:396:ILE:HA	2.43	0.46
1:B:505:VAL:HA	1:B:508:LEU:CG	2.41	0.46
1:B:582:GLU:HG3	1:B:586:LYS:HE3	1.98	0.46
1:B:11:VAL:HG23	1:B:149:THR:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:578:LYS:HG3	1:A:579:GLU:OE2	2.16	0.46
1:A:87:THR:HA	1:A:94:GLN:NE2	2.21	0.46
1:A:293:LYS:HB2	1:A:294:PHE:CD2	2.51	0.46
1:A:446:ILE:O	1:A:446:ILE:HG22	2.16	0.46
1:B:514:THR:C	1:B:516:ASP:N	2.69	0.46
1:A:247:VAL:CG1	1:A:248:ASN:N	2.78	0.46
1:A:303:PHE:HB2	1:A:317:ASN:HB3	1.97	0.46
1:A:437:THR:CG2	1:B:276:ILE:HG23	2.46	0.46
1:B:287:ILE:CD1	1:B:290:LYS:HD2	2.45	0.46
1:B:381:THR:CG2	1:B:386:GLU:HB2	2.46	0.46
1:B:522:PHE:HD2	1:B:522:PHE:N	2.13	0.46
1:A:203:PRO:HB3	1:A:316:PRO:HG2	1.98	0.46
1:A:480:ILE:HG12	1:A:532:VAL:HG13	1.98	0.46
1:A:602:THR:HG21	1:B:165:TYR:CZ	2.51	0.46
1:B:40:ALA:O	1:B:43:ILE:HG13	2.15	0.46
1:B:361:TYR:OH	1:B:588:LYS:HD2	2.15	0.46
1:B:386:GLU:O	1:B:420:MET:HE1	2.15	0.46
1:A:60:VAL:HG21	1:A:435:LEU:HD11	1.97	0.46
1:A:71:MET:HE1	1:A:385:GLU:CA	2.45	0.46
1:A:415:SER:HA	1:A:454:ARG:HH21	1.80	0.46
1:B:483:TRP:O	1:B:487:TYR:CD2	2.69	0.46
1:A:60:VAL:HG12	1:A:64:ILE:HD11	1.98	0.45
1:A:333:ARG:HG2	1:A:338:LEU:O	2.16	0.45
1:A:460:ARG:NH1	1:A:467:GLU:N	2.64	0.45
1:A:526:VAL:HG13	1:A:527:PRO:HD2	1.98	0.45
1:A:551:LYS:O	1:A:554:GLU:HG3	2.16	0.45
1:B:480:ILE:O	1:B:536:VAL:HG22	2.15	0.45
1:A:277:LYS:HG2	1:B:439:ARG:NH1	2.31	0.45
1:B:289:ASP:C	1:B:291:ILE:H	2.19	0.45
1:A:157:GLY:HA2	1:A:377:ASN:HB2	1.98	0.45
1:A:588:LYS:N	1:A:589:PRO:HD3	2.31	0.45
1:B:160:LEU:HB3	1:B:353:ASP:HB2	1.98	0.45
1:B:570:TYR:HB2	1:B:585:LYS:HE2	1.98	0.45
1:A:503:TYR:N	1:A:503:TYR:CD2	2.85	0.45
1:B:28:ARG:HH22	1:B:70:GLU:CD	2.18	0.45
1:B:447:ARG:NH2	1:B:450:ASN:HB3	2.32	0.45
1:B:366:THR:HG22	1:B:369:ILE:H	1.80	0.45
1:B:508:LEU:C	1:B:513:TYR:HB2	2.37	0.45
1:B:612:TYR:C	1:B:612:TYR:HD2	2.20	0.45
1:B:191:PHE:CE2	1:B:369:ILE:HD11	2.51	0.45
1:B:230:PHE:CE1	1:B:236:GLY:O	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ARG:HD2	1:B:502:SER:O	2.17	0.45
1:A:26:ALA:O	1:A:31:ALA:HB3	2.16	0.45
1:B:71:MET:O	1:B:75:ILE:HG22	2.16	0.45
1:B:287:ILE:HD12	1:B:287:ILE:HA	1.80	0.45
1:B:287:ILE:HD12	1:B:290:LYS:HD2	1.98	0.45
1:B:324:PRO:HB2	1:B:327:VAL:HG23	1.99	0.45
1:B:487:TYR:CE1	1:B:515:LEU:HD21	2.51	0.45
1:B:607:THR:O	1:B:611:VAL:HG23	2.17	0.45
1:A:117:GLU:O	1:A:118:ASN:HB2	2.17	0.45
1:B:86:ASN:ND2	1:B:89:LYS:HD2	2.31	0.45
1:B:319:LEU:HD13	1:B:331:MET:CE	2.47	0.45
1:B:573:ILE:HA	1:B:574:PRO:HD3	1.74	0.45
1:A:505:VAL:HA	1:A:508:LEU:CD1	2.42	0.45
1:A:519:LYS:O	1:A:523:GLY:HA2	2.16	0.45
1:A:593:GLY:O	1:A:596:SER:OG	2.28	0.45
1:B:49:ASN:HA	1:B:50:PRO:HD3	1.74	0.45
1:B:259:HIS:CD2	1:B:259:HIS:H	2.35	0.45
1:B:267:HIS:H	1:B:267:HIS:HD2	1.62	0.45
1:B:487:TYR:OH	1:B:527:PRO:HD3	2.17	0.45
1:A:29:MET:CE	1:A:464:LEU:HD21	2.47	0.44
1:A:366:THR:CG2	1:A:369:ILE:H	2.30	0.44
1:A:386:GLU:O	1:A:420:MET:HE1	2.17	0.44
1:A:442:TYR:OH	1:A:557:LYS:HE3	2.17	0.44
1:B:94:GLN:O	1:B:448:GLN:HG2	2.17	0.44
1:A:82:PHE:N	1:A:82:PHE:HD1	2.14	0.44
1:A:158:THR:HB	1:A:350:ILE:HG12	1.99	0.44
1:A:609:LEU:HD12	1:A:609:LEU:O	2.17	0.44
1:A:159:PHE:HB2	2:A:618:FAD:H8A	2.00	0.44
1:A:262:ILE:HD13	1:A:287:ILE:HG23	1.99	0.44
1:A:503:TYR:N	1:A:503:TYR:HD2	2.16	0.44
1:A:589:PRO:CG	1:A:598:ILE:HD11	2.45	0.44
1:A:159:PHE:CE2	2:A:618:FAD:H2B	2.53	0.44
1:A:253:TYR:CD1	1:A:253:TYR:N	2.85	0.44
1:A:400:LEU:CD1	1:A:408:ILE:HG23	2.47	0.44
1:A:519:LYS:HB2	1:A:526:VAL:HG21	1.99	0.44
1:A:547:GLU:OE1	1:A:550:ARG:CD	2.66	0.44
1:B:261:ILE:HD13	1:B:330:GLU:HG2	2.00	0.44
1:B:305:GLU:HA	1:B:306:PRO:HD3	1.75	0.44
1:B:452:ILE:HD11	1:B:473:VAL:CG2	2.46	0.44
1:A:410:LEU:HD12	1:A:417:ILE:CG2	2.48	0.44
1:A:577:THR:O	1:A:581:ARG:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:87:THR:HA	1:B:94:GLN:NE2	2.18	0.44
1:A:59:ILE:HG12	1:A:448:GLN:HB3	2.00	0.44
1:B:507:THR:HG22	1:B:507:THR:O	2.16	0.44
1:A:262:ILE:HB	1:A:291:ILE:HD13	1.99	0.44
1:A:480:ILE:O	1:A:484:LYS:HG3	2.18	0.44
1:A:573:ILE:HA	1:A:574:PRO:HD3	1.75	0.44
1:B:70:GLU:O	1:B:71:MET:C	2.56	0.44
1:B:587:PHE:O	1:B:588:LYS:C	2.55	0.44
1:B:289:ASP:C	1:B:291:ILE:N	2.71	0.44
1:B:314:ILE:HD13	1:B:314:ILE:HA	1.78	0.44
1:A:165:TYR:CZ	1:B:602:THR:HG21	2.54	0.43
1:A:305:GLU:HA	1:A:306:PRO:HD3	1.81	0.43
1:A:568:ILE:HD12	1:A:568:ILE:O	2.18	0.43
1:B:8:PHE:HE1	1:B:147:TYR:CD2	2.32	0.43
1:B:29:MET:HE2	1:B:464:LEU:HD11	2.00	0.43
1:B:350:ILE:HG22	2:B:618:FAD:HM73	1.98	0.43
1:A:49:ASN:HA	1:A:50:PRO:HD3	1.82	0.43
1:A:86:ASN:HD22	1:A:86:ASN:HA	1.61	0.43
1:A:259:HIS:CD2	1:A:259:HIS:H	2.34	0.43
1:A:460:ARG:HA	1:A:460:ARG:HD2	1.91	0.43
1:B:511:MET:O	1:B:513:TYR:HD1	2.01	0.43
1:B:573:ILE:HD13	1:B:609:LEU:HD12	1.99	0.43
1:A:275:LEU:CD2	1:A:292:VAL:HG13	2.49	0.43
1:B:483:TRP:CE2	1:B:527:PRO:HA	2.53	0.43
1:A:587:PHE:O	1:A:588:LYS:C	2.56	0.43
1:B:56:ALA:CB	1:B:435:LEU:HB3	2.49	0.43
1:B:422:ASP:OD2	1:B:597:ARG:NH1	2.52	0.43
1:A:39:ASN:OD1	1:A:39:ASN:C	2.57	0.43
1:A:61:VAL:HA	1:A:64:ILE:HD12	2.01	0.43
1:A:164:ILE:N	1:A:164:ILE:HD12	2.32	0.43
1:B:130:ILE:HD13	1:B:138:GLY:C	2.39	0.43
1:B:197:ARG:NH1	1:B:353:ASP:OD1	2.50	0.43
1:B:230:PHE:CD2	1:B:452:ILE:HG12	2.54	0.43
1:B:235:VAL:HG12	1:B:236:GLY:N	2.33	0.43
1:B:110:LYS:HE2	1:B:114:GLU:OE2	2.19	0.43
1:A:548:ARG:O	1:A:552:LEU:HG	2.19	0.43
1:B:287:ILE:O	1:B:291:ILE:HG23	2.18	0.43
1:B:341:VAL:HG22	1:B:342:VAL:N	2.33	0.43
1:B:519:LYS:HB2	1:B:526:VAL:HG23	2.00	0.43
1:B:568:ILE:O	1:B:568:ILE:HG13	2.19	0.43
1:A:85:LEU:CD2	1:A:86:ASN:N	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:LYS:HZ3	1:A:587:PHE:HA	1.84	0.43
1:A:526:VAL:CG1	1:A:527:PRO:HD2	2.49	0.43
1:B:72:GLY:O	1:B:73:LYS:C	2.57	0.43
1:B:128:ASP:CG	1:B:190:ARG:HH22	2.22	0.43
1:B:163:VAL:O	1:B:350:ILE:HD12	2.18	0.43
1:B:223:ASP:OD1	1:B:224:PRO:HA	2.19	0.43
1:A:572:LYS:O	1:A:612:TYR:HE1	2.01	0.43
1:B:610:LEU:HD23	1:B:610:LEU:HA	1.73	0.43
1:A:408:ILE:HG13	1:A:409:TYR:N	2.31	0.42
1:B:108:TYR:HE2	1:B:112:VAL:HG21	1.84	0.42
1:A:16:GLY:O	1:A:20:ILE:HG13	2.19	0.42
1:A:258:THR:HB	1:A:259:HIS:HD2	1.84	0.42
1:B:381:THR:HG23	1:B:386:GLU:HB2	2.00	0.42
1:A:459:GLY:HA3	1:A:465:LEU:HD12	2.01	0.42
1:B:56:ALA:HB3	1:B:435:LEU:HB3	2.00	0.42
1:B:175:ARG:NE	1:B:178:GLU:OE2	2.52	0.42
1:B:594:GLN:HA	1:B:597:ARG:CZ	2.49	0.42
1:A:193:PHE:CZ	1:A:366:THR:HG21	2.55	0.42
1:B:108:TYR:CE2	1:B:112:VAL:CG2	3.02	0.42
1:B:509:MET:HE2	1:B:515:LEU:HG	2.00	0.42
1:B:588:LYS:N	1:B:589:PRO:HD3	2.35	0.42
1:A:293:LYS:HB2	1:A:294:PHE:CE2	2.54	0.42
1:A:445:TYR:O	1:A:445:TYR:CG	2.73	0.42
1:B:396:ILE:O	1:B:399:ALA:HB3	2.19	0.42
1:A:7:GLU:O	1:A:32:LYS:HE3	2.20	0.42
1:A:43:ILE:HD11	1:A:121:ILE:HD13	2.00	0.42
1:A:287:ILE:HG12	1:A:319:LEU:HD23	2.01	0.42
1:B:450:ASN:ND2	1:B:450:ASN:N	2.67	0.42
1:A:203:PRO:CB	1:A:316:PRO:HG2	2.49	0.42
1:A:532:VAL:O	1:A:536:VAL:HG23	2.19	0.42
1:B:57:LYS:HD3	1:B:385:GLU:CD	2.40	0.42
1:B:203:PRO:HB2	1:B:316:PRO:HG2	2.02	0.42
1:B:204:ALA:H	1:B:347:ALA:HB2	1.82	0.42
1:B:275:LEU:N	1:B:275:LEU:CD2	2.83	0.42
1:B:509:MET:SD	1:B:513:TYR:O	2.78	0.42
1:B:580:ALA:HB1	1:B:601:ILE:CD1	2.49	0.42
1:A:159:PHE:CD2	2:A:618:FAD:H2B	2.55	0.42
1:B:60:VAL:O	1:B:64:ILE:HG13	2.19	0.42
1:A:299:ARG:O	1:A:299:ARG:HG3	2.18	0.42
1:A:377:ASN:HD21	1:A:382:THR:HA	1.84	0.42
1:A:613:LEU:HA	1:A:616:LEU:HG	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:491:ARG:HA	1:B:503:TYR:O	2.20	0.42
1:B:603:PRO:O	1:B:606:ILE:HG22	2.20	0.42
1:A:95:SER:HA	1:A:96:PRO:HD2	1.93	0.41
1:A:255:THR:HB	1:A:256:PRO:CD	2.50	0.41
1:A:522:PHE:HB3	1:A:524:TYR:CE1	2.55	0.41
1:B:54:GLY:O	1:B:55:ILE:C	2.59	0.41
1:B:444:LEU:HD12	1:B:549:GLU:OE1	2.20	0.41
1:B:576:LEU:O	1:B:577:THR:C	2.57	0.41
1:A:70:GLU:O	1:A:71:MET:C	2.58	0.41
1:A:321:THR:OG1	1:A:322:SER:N	2.53	0.41
1:A:415:SER:HA	1:A:454:ARG:NH2	2.35	0.41
1:A:602:THR:HB	1:A:603:PRO:HD2	2.02	0.41
1:A:613:LEU:HD23	1:A:616:LEU:HD11	2.00	0.41
1:B:319:LEU:HD11	1:B:335:ILE:HD11	2.00	0.41
1:B:490:GLU:HB2	1:B:505:VAL:HG23	2.00	0.41
1:B:504:SER:O	1:B:508:LEU:HG	2.20	0.41
1:A:247:VAL:CG1	1:A:248:ASN:H	2.32	0.41
1:B:367:LYS:NZ	1:B:587:PHE:HA	2.36	0.41
1:B:435:LEU:C	1:B:437:THR:N	2.74	0.41
1:B:602:THR:HB	1:B:603:PRO:HD2	2.01	0.41
1:A:7:GLU:O	1:A:32:LYS:CE	2.68	0.41
1:A:29:MET:HE1	1:A:396:ILE:CA	2.36	0.41
1:A:71:MET:O	1:A:75:ILE:HG22	2.21	0.41
1:A:416:TYR:O	1:A:419:VAL:HB	2.21	0.41
1:A:576:LEU:O	1:A:577:THR:C	2.58	0.41
1:B:202:THR:CA	1:B:320:SER:HB3	2.50	0.41
1:B:410:LEU:HD12	1:B:417:ILE:HG21	2.00	0.41
1:B:487:TYR:CZ	1:B:515:LEU:HD21	2.56	0.41
1:B:560:GLU:OE1	1:B:597:ARG:NH2	2.53	0.41
1:A:435:LEU:C	1:A:437:THR:N	2.73	0.41
1:B:284:CYS:HA	1:B:285:PRO:HD3	1.87	0.41
1:B:291:ILE:O	1:B:291:ILE:HG13	2.18	0.41
1:A:416:TYR:O	1:A:416:TYR:HD1	2.03	0.41
1:A:509:MET:HA	1:A:513:TYR:O	2.21	0.41
1:B:82:PHE:N	1:B:82:PHE:HD1	2.18	0.41
1:B:213:PHE:CD1	1:B:213:PHE:N	2.89	0.41
1:A:434:ARG:HD3	1:A:436:PHE:CZ	2.54	0.41
1:A:487:TYR:HD1	1:A:505:VAL:HG11	1.84	0.41
1:B:355:VAL:HG23	1:B:378:PHE:CZ	2.56	0.41
1:A:267:HIS:NE2	1:B:555:LYS:HD2	2.36	0.41
1:B:62:ARG:HE	1:B:96:PRO:HG3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:492:VAL:HG11	1:B:522:PHE:HE1	1.85	0.41
1:A:72:GLY:O	1:A:73:LYS:C	2.59	0.41
1:A:281:PRO:HG3	1:A:294:PHE:CD1	2.55	0.41
1:A:284:CYS:HA	1:A:285:PRO:HD3	1.80	0.41
1:A:312:ILE:O	1:A:312:ILE:HG13	2.19	0.41
1:A:527:PRO:HB2	1:A:533:LYS:HB2	2.02	0.41
1:A:529:HIS:CD2	1:A:529:HIS:C	2.94	0.41
1:B:289:ASP:O	1:B:291:ILE:N	2.54	0.41
1:B:356:PRO:HA	1:B:357:PRO:HD3	1.86	0.41
1:B:363:THR:HG21	1:B:407:PRO:HB2	2.02	0.41
1:B:450:ASN:HD22	1:B:450:ASN:N	2.17	0.41
1:B:591:THR:HB	1:B:594:GLN:H	1.86	0.41
1:A:123:GLN:O	1:A:123:GLN:HG2	2.21	0.41
1:A:57:LYS:HD3	1:A:385:GLU:OE1	2.21	0.40
1:A:130:ILE:N	1:A:130:ILE:CD1	2.80	0.40
1:A:508:LEU:O	1:A:513:TYR:HB2	2.21	0.40
1:A:602:THR:HB	1:A:603:PRO:CD	2.51	0.40
1:B:11:VAL:HG13	1:B:36:PHE:HE1	1.86	0.40
1:B:82:PHE:HB2	1:B:225:PRO:HB2	2.03	0.40
1:B:15:GLY:HA3	1:B:37:VAL:HG22	2.03	0.40
1:B:338:LEU:O	1:B:341:VAL:HG12	2.21	0.40
1:B:553:ASN:O	1:B:554:GLU:C	2.59	0.40
1:A:56:ALA:CB	1:A:435:LEU:HB3	2.51	0.40
1:A:450:ASN:ND2	1:A:454:ARG:HH11	2.18	0.40
1:B:27:ALA:O	1:B:30:GLY:N	2.43	0.40
1:B:189:ARG:CG	1:B:195:LEU:HD12	2.50	0.40
1:B:207:ASP:HB3	1:B:210:THR:OG1	2.21	0.40
1:B:509:MET:HA	1:B:513:TYR:O	2.22	0.40
1:A:207:ASP:HB3	1:A:210:THR:OG1	2.22	0.40
1:A:227:LYS:HE3	1:A:229:SER:O	2.21	0.40
1:A:235:VAL:HG12	1:A:236:GLY:N	2.36	0.40
1:A:322:SER:HB3	1:A:349:ALA:HB2	2.04	0.40
1:A:570:TYR:CD2	1:A:584:LEU:HB3	2.55	0.40
1:B:505:VAL:O	1:B:508:LEU:HB2	2.20	0.40
1:B:529:HIS:CE1	1:B:531:TYR:CB	3.03	0.40
2:B:618:FAD:O1A	2:B:618:FAD:H4'	2.21	0.40
1:A:237:SER:OG	1:A:238:TYR:N	2.53	0.40
1:A:450:ASN:HD21	1:A:454:ARG:HH11	1.69	0.40
1:B:7:GLU:HG2	1:B:148:LYS:CB	2.35	0.40
1:B:203:PRO:CB	1:B:316:PRO:HG2	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:107:GLU:OE1	1:B:107:GLU:OE1[8_565]	1.59	0.61

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	599/637 (94%)	500 (84%)	84 (14%)	15 (2%)	5	32
1	B	597/637 (94%)	497 (83%)	83 (14%)	17 (3%)	5	29
All	All	1196/1274 (94%)	997 (83%)	167 (14%)	32 (3%)	5	30

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	71	MET
1	A	285	PRO
1	B	55	ILE
1	B	71	MET
1	B	285	PRO
1	B	527	PRO
1	A	55	ILE
1	A	81	GLN
1	A	290	LYS
1	A	577	THR
1	B	81	GLN
1	B	577	THR
1	A	295	PRO
1	B	436	PHE
1	B	528	GLN
1	A	436	PHE
1	B	270	ALA
1	B	544	PRO

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Mol	Chain	Res	Type
1	A	83	LYS
1	A	530	PRO
1	A	544	PRO
1	A	570	TYR
1	B	83	LYS
1	B	290	LYS
1	A	217	GLU
1	B	217	GLU
1	A	20	ILE
1	B	20	ILE
1	A	356	PRO
1	B	179	PRO
1	B	356	PRO
1	B	530	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	511/540 (95%)	478 (94%)	33 (6%)	17 51
1	B	510/540 (94%)	482 (94%)	28 (6%)	21 57
All	All	1021/1080 (94%)	960 (94%)	61 (6%)	19 54

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	VAL
1	A	63	GLU
1	A	71	MET
1	A	81	GLN
1	A	82	PHE
1	A	85	LEU
1	A	86	ASN
1	A	108	TYR
1	A	131	VAL

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Mol	Chain	Res	Type
1	A	192	ASP
1	A	223	ASP
1	A	227	LYS
1	A	232	THR
1	A	263	ARG
1	A	269	THR
1	A	298	GLU
1	A	310	ASP
1	A	321	THR
1	A	326	GLU
1	A	331	MET
1	A	352	TYR
1	A	354	VAL
1	A	360	LEU
1	A	379	ASN
1	A	429	VAL
1	A	430	THR
1	A	441	GLU
1	A	448	GLN
1	A	450	ASN
1	A	503	TYR
1	A	545	TYR
1	A	550	ARG
1	A	577	THR
1	B	67	LEU
1	B	81	GLN
1	B	82	PHE
1	B	86	ASN
1	B	104	ARG
1	B	108	TYR
1	B	116	GLN
1	B	192	ASP
1	B	269	THR
1	B	288	GLU
1	B	299	ARG
1	B	309	LEU
1	B	310	ASP
1	B	314	ILE
1	B	320	SER
1	B	321	THR
1	B	331	MET
1	B	379	ASN

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Mol	Chain	Res	Type
1	B	382	THR
1	B	401	ARG
1	B	429	VAL
1	B	441	GLU
1	B	450	ASN
1	B	527	PRO
1	B	530	PRO
1	B	545	TYR
1	B	577	THR
1	B	591	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	ASN
1	A	94	GLN
1	A	115	ASN
1	A	259	HIS
1	A	265	ASN
1	A	300	HIS
1	A	340	ASN
1	A	377	ASN
1	A	379	ASN
1	A	450	ASN
1	A	529	HIS
1	B	86	ASN
1	B	94	GLN
1	B	115	ASN
1	B	161	ASN
1	B	248	ASN
1	B	259	HIS
1	B	267	HIS
1	B	340	ASN
1	B	377	ASN
1	B	390	GLN
1	B	448	GLN
1	B	450	ASN
1	B	469	GLN
1	B	528	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

5 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	A	619	-	4,4,4	1.58	0	6,6,6	0.43	0
3	PO4	A	620	-	4,4,4	1.60	0	6,6,6	0.44	0
2	FAD	A	618	-	53,58,58	1.78	16 (30%)	68,89,89	1.83	18 (26%)
2	FAD	B	618	-	53,58,58	1.90	17 (32%)	68,89,89	1.81	19 (27%)
3	PO4	B	619	-	4,4,4	1.26	1 (25%)	6,6,6	0.43	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	FAD	B	618	-	-	9/30/50/50	0/6/6/6
2	FAD	A	618	-	-	6/30/50/50	0/6/6/6

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	618	FAD	C4X-N5	4.98	1.40	1.30
2	A	618	FAD	C4X-N5	4.81	1.40	1.30
2	B	618	FAD	C6-C7	4.08	1.45	1.39
2	B	618	FAD	C10-N10	3.45	1.44	1.37
2	A	618	FAD	C6-C7	3.26	1.44	1.39
2	B	618	FAD	O4-C4	-3.20	1.17	1.23
2	B	618	FAD	C6-C5X	3.09	1.44	1.40
2	B	618	FAD	C9-C9A	3.02	1.44	1.39
2	A	618	FAD	C9-C9A	2.94	1.44	1.39
2	A	618	FAD	O4-C4	-2.90	1.18	1.23
2	B	618	FAD	P-O2P	-2.90	1.41	1.55
2	B	618	FAD	O4B-C4B	-2.79	1.38	1.45
2	A	618	FAD	C6-C5X	2.78	1.44	1.40
2	A	618	FAD	O4B-C4B	-2.77	1.38	1.45
2	A	618	FAD	C10-N10	2.72	1.43	1.37
2	A	618	FAD	P-O2P	-2.71	1.42	1.55
2	B	618	FAD	C1'-C2'	2.69	1.56	1.52
2	B	618	FAD	PA-O2A	-2.68	1.42	1.55
2	B	618	FAD	C10-N1	2.68	1.38	1.33
2	A	618	FAD	C10-N1	2.56	1.38	1.33
2	A	618	FAD	C8A-N7A	-2.48	1.30	1.34
2	A	618	FAD	PA-O2A	-2.45	1.43	1.55
3	B	619	PO4	P-O1	2.35	1.56	1.50
2	B	618	FAD	C8A-N7A	-2.35	1.30	1.34
2	A	618	FAD	O3'-C3'	-2.34	1.37	1.43
2	B	618	FAD	C2'-C3'	2.33	1.57	1.53
2	A	618	FAD	PA-O1A	-2.31	1.42	1.50
2	B	618	FAD	PA-O1A	-2.23	1.43	1.50
2	B	618	FAD	O3'-C3'	-2.21	1.37	1.43
2	B	618	FAD	C9A-C5X	2.19	1.44	1.41
2	A	618	FAD	C2'-C3'	2.17	1.57	1.53
2	A	618	FAD	P-O1P	-2.09	1.43	1.50
2	A	618	FAD	C2B-C1B	-2.07	1.50	1.53
2	B	618	FAD	P-O1P	-2.02	1.43	1.50

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	618	FAD	N3A-C2A-N1A	-4.54	121.58	128.68
2	B	618	FAD	N3A-C2A-N1A	-4.48	121.67	128.68
2	A	618	FAD	C4-N3-C2	-4.20	117.88	125.64
2	B	618	FAD	C4-N3-C2	-4.18	117.92	125.64
2	A	618	FAD	C4'-C3'-C2'	4.16	122.00	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	618	FAD	C1B-N9A-C4A	-4.09	119.45	126.64
2	B	618	FAD	C10-C4X-N5	-3.68	117.04	124.86
2	B	618	FAD	C4X-C10-N1	-3.60	116.37	124.73
2	B	618	FAD	C4-C4X-N5	3.44	123.13	118.23
2	A	618	FAD	C4X-C4-N3	3.42	121.87	113.19
2	A	618	FAD	C10-C4X-N5	-3.40	117.64	124.86
2	B	618	FAD	C4X-C4-N3	3.35	121.70	113.19
2	A	618	FAD	C4X-C10-N1	-3.27	117.14	124.73
2	B	618	FAD	C4X-C10-N10	3.25	121.23	116.48
2	B	618	FAD	C1B-N9A-C4A	-3.22	120.98	126.64
2	B	618	FAD	C5X-N5-C4X	3.22	123.43	118.07
2	A	618	FAD	C5X-N5-C4X	3.18	123.36	118.07
2	A	618	FAD	C4-C4X-N5	3.09	122.63	118.23
2	B	618	FAD	C10-N1-C2	3.05	123.00	116.90
2	A	618	FAD	C4X-C10-N10	3.03	120.91	116.48
2	A	618	FAD	C10-N1-C2	3.02	122.93	116.90
2	B	618	FAD	C4'-C3'-C2'	2.98	119.56	113.36
2	B	618	FAD	O4-C4-N3	-2.80	114.75	120.12
2	B	618	FAD	C9A-C9-C8	2.67	124.67	119.30
2	A	618	FAD	C9A-C9-C8	2.65	124.64	119.30
2	B	618	FAD	C4A-C5A-N7A	-2.51	106.78	109.40
2	A	618	FAD	C9A-C5X-N5	-2.45	119.77	122.43
2	A	618	FAD	O2'-C2'-C3'	2.38	114.89	109.10
2	B	618	FAD	C3B-C2B-C1B	2.37	104.54	100.98
2	A	618	FAD	O4-C4-N3	-2.31	115.69	120.12
2	A	618	FAD	C3B-C2B-C1B	2.21	104.31	100.98
2	A	618	FAD	O3'-C3'-C2'	-2.18	103.56	108.81
2	B	618	FAD	O2-C2-N1	-2.12	118.31	121.83
2	B	618	FAD	O5'-C5'-C4'	2.08	114.92	109.36
2	B	618	FAD	C9A-C5X-N5	-2.07	120.18	122.43
2	A	618	FAD	C4A-C5A-N7A	-2.04	107.28	109.40
2	B	618	FAD	O2'-C2'-C3'	2.02	114.00	109.10

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	618	FAD	C3'-C4'-C5'-O5'
2	A	618	FAD	O4'-C4'-C5'-O5'
2	B	618	FAD	C3'-C4'-C5'-O5'
2	B	618	FAD	O4'-C4'-C5'-O5'
2	B	618	FAD	PA-O3P-P-O5'

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Mol	Chain	Res	Type	Atoms
2	B	618	FAD	C2'-C3'-C4'-O4'
2	B	618	FAD	C4'-C5'-O5'-P
2	B	618	FAD	O3'-C3'-C4'-C5'
2	B	618	FAD	C2'-C3'-C4'-C5'
2	B	618	FAD	O3'-C3'-C4'-O4'
2	A	618	FAD	C4'-C5'-O5'-P
2	A	618	FAD	PA-O3P-P-O5'
2	A	618	FAD	O4B-C4B-C5B-O5B
2	A	618	FAD	P-O3P-PA-O1A
2	B	618	FAD	O4B-C4B-C5B-O5B

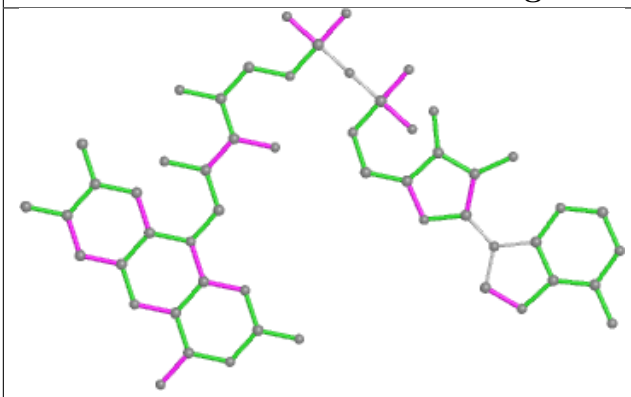
There are no ring outliers.

2 monomers are involved in 6 short contacts:

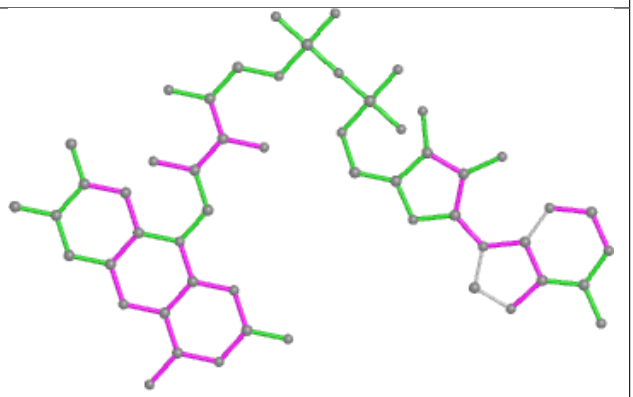
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	618	FAD	4	0
2	B	618	FAD	2	0

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.

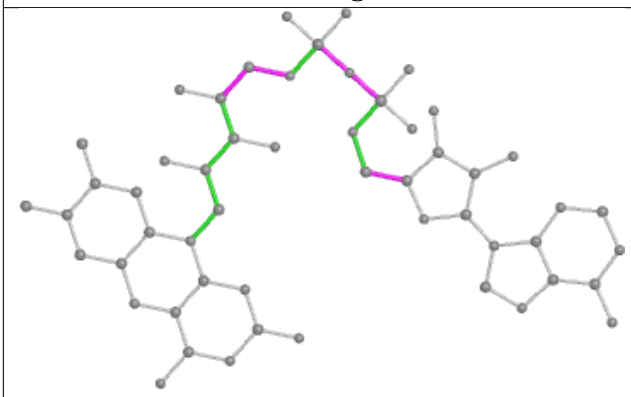
Ligand FAD A 618



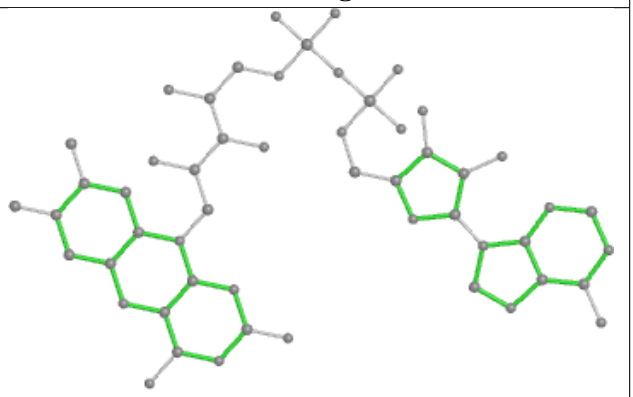
Bond lengths



Bond angles

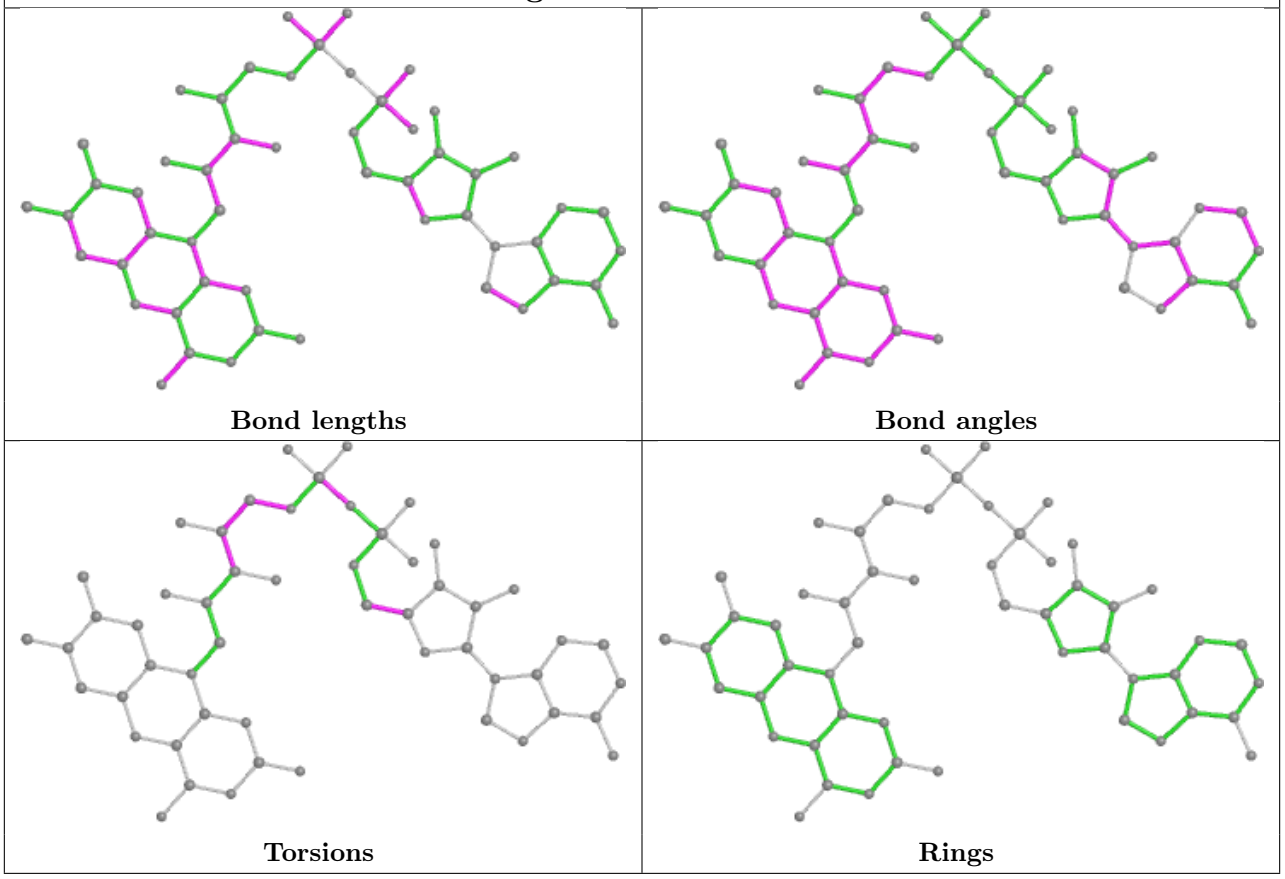


Torsions



Rings

Ligand FAD B 618



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	603/637 (94%)	-0.22	4 (0%) 87 81	31, 60, 99, 118	0
1	B	601/637 (94%)	-0.03	17 (2%) 53 37	32, 72, 123, 147	0
All	All	1204/1274 (94%)	-0.13	21 (1%) 70 57	31, 67, 112, 147	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	513	TYR	4.9
1	B	503	TYR	4.2
1	B	527	PRO	3.9
1	B	486	PHE	3.7
1	B	522	PHE	3.5
1	B	487	TYR	2.9
1	B	572	LYS	2.9
1	B	329	TRP	2.8
1	B	505	VAL	2.7
1	B	526	VAL	2.6
1	B	243	GLY	2.4
1	B	518	VAL	2.3
1	B	91	LYS	2.3
1	A	573	ILE	2.3
1	B	521	LYS	2.2
1	A	513	TYR	2.2
1	A	572	LYS	2.2
1	A	520	GLU	2.2
1	B	524	TYR	2.2
1	B	540	LEU	2.1
1	B	490	GLU	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

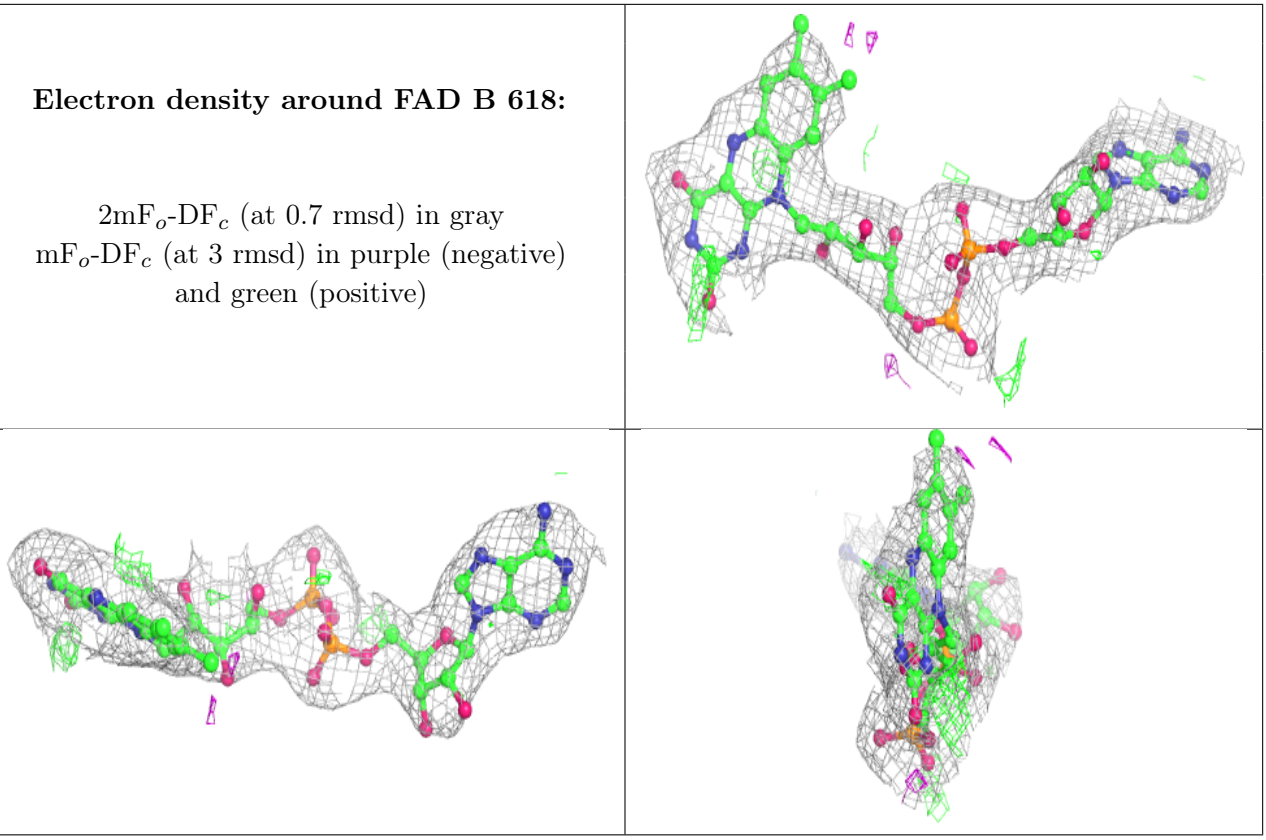
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	PO4	A	619	5/5	0.82	0.23	118,119,123,127	0
3	PO4	A	620	5/5	0.87	0.21	120,122,126,127	0
3	PO4	B	619	5/5	0.93	0.17	123,124,128,130	0
2	FAD	B	618	53/53	0.95	0.26	39,65,78,78	0
2	FAD	A	618	53/53	0.96	0.22	23,47,66,73	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.

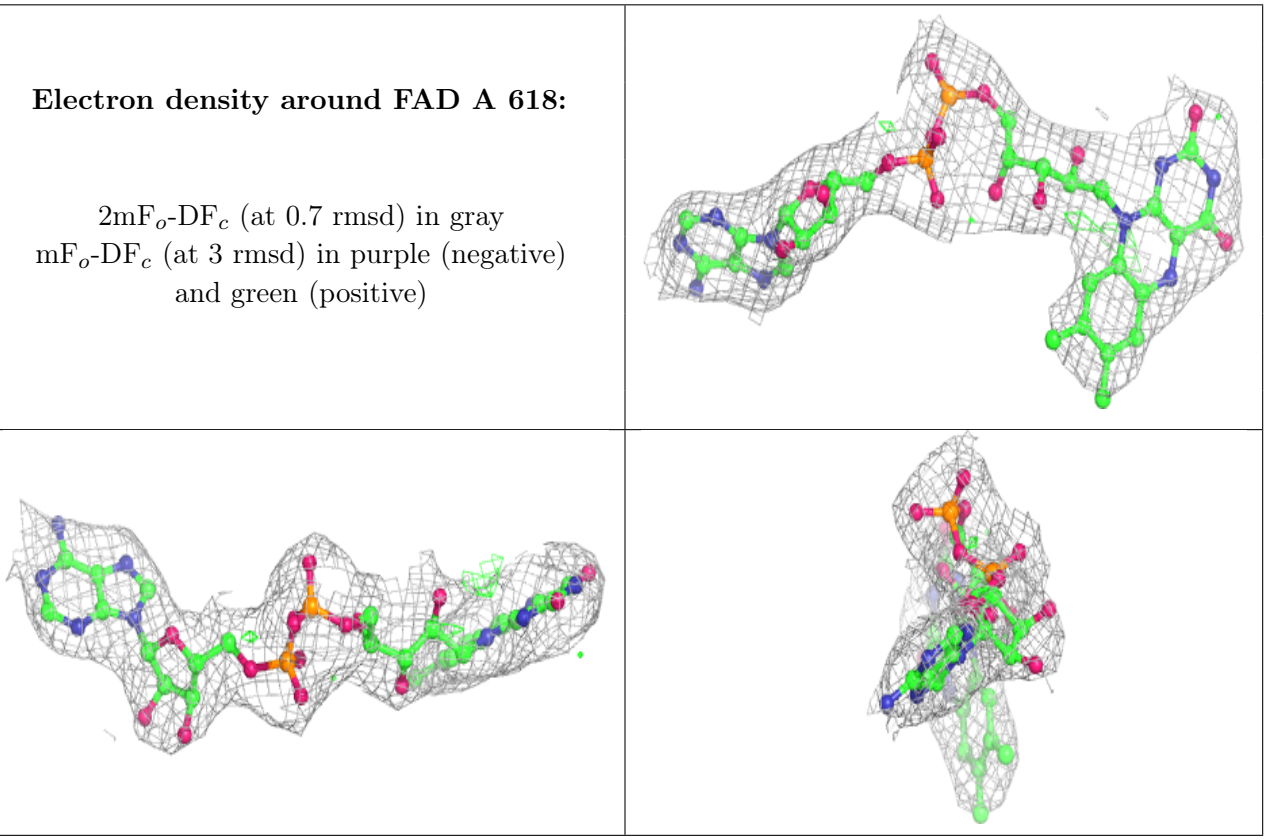
Electron density around FAD B 618:

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



Electron density around FAD A 618:

$2mF_o$-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.