WORLDWIDE PDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 03:52 PM GMT

PDB ID : 2A1T
Title : Structure of the human MCAD:ETF E165betaA complex
Authors : Toogood, H.S.; Van Thiel, A.; Scrutton, N.S.; Leys, D.
Deposited on : 2005-06-21
Resolution : 2.80 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.200
Clashscore		9
Ramachandran outliers		0.9%
Sidechain outliers		11.0%
RSRZ outliers		3.4%

Worse *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
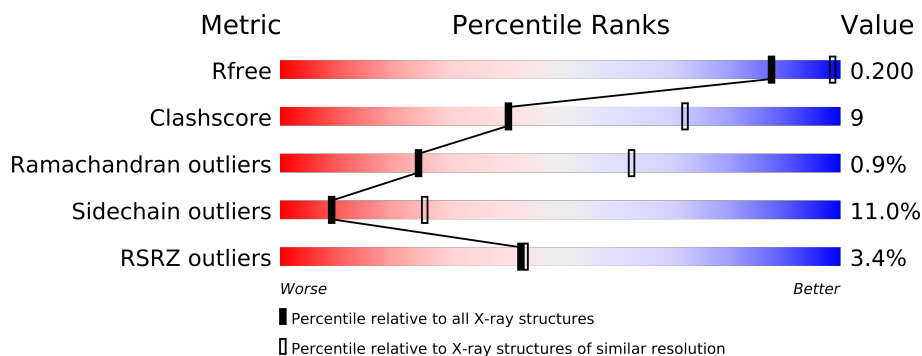
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1799 (2.80-2.80)
Clashscore	79885	2295 (2.80-2.80)
Ramachandran outliers	78287	2252 (2.80-2.80)
Sidechain outliers	78261	2254 (2.80-2.80)
RSRZ outliers	66119	1802 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	421	
1	B	421	
1	C	421	
1	D	421	
2	R	333	
3	S	255	

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 16189 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	386	Total	C	N	O	S	0	0	0
			2933	1862	496	557	18			
1	B	387	Total	C	N	O	S	0	0	0
			2949	1869	501	561	18			
1	C	388	Total	C	N	O	S	0	0	0
			2961	1875	508	560	18			
1	D	387	Total	C	N	O	S	0	0	0
			2972	1880	508	566	18			

- Molecule 2 is a protein called Electron transfer flavoprotein alpha-subunit, mitochondrial precursor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	313	Total	C	N	O	S	0	0	0
			2264	1441	377	437	9			

- Molecule 3 is a protein called Electron transfer flavoprotein beta-subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	S	239	Total	C	N	O	S	0	0	0
			1758	1119	294	337	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	165	ALA	GLU	ENGINEERED	UNP P38117

- Molecule 4 is ADENOSINE MONOPHOSPHATE (three-letter code: AMP) (formula: $C_{10}H_{14}N_5O_7P$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	S	1	Total	C	N	O	P	0	0
			23	10	5	7	1		

- Molecule 5 is FLAVIN-ADENINE DINUCLEOTIDE (three-letter code: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).
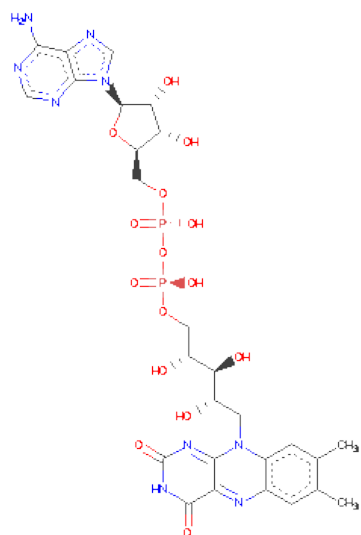
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			53	27	9	15	2		
5	B	1	Total	C	N	O	P	0	0
			53	27	9	15	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	D	1	Total 53	C 27	N 9	O 15	P 2	0	0
5	R	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	13	Total 13	O 13	0	0
6	B	9	Total 9	O 9	0	0
6	C	17	Total 17	O 17	0	0
6	D	12	Total 12	O 12	0	0
6	R	3	Total 3	O 3	0	0
6	S	10	Total 10	O 10	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.
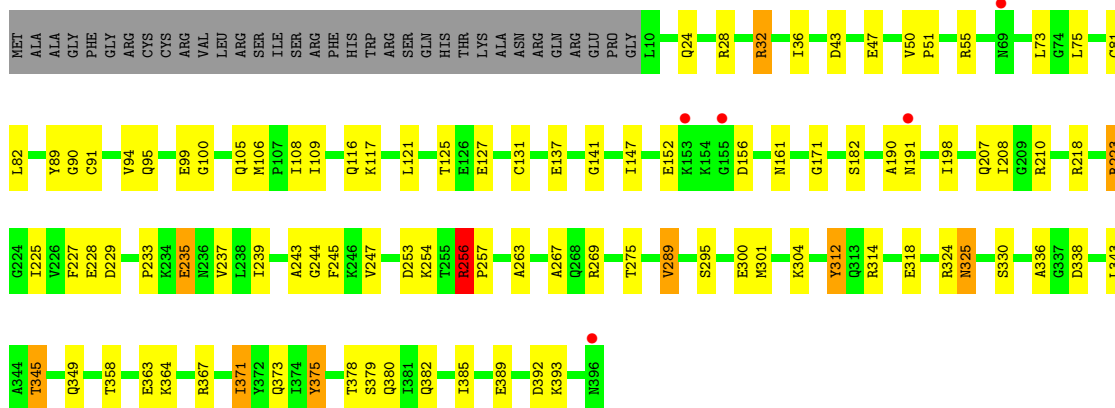
- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor
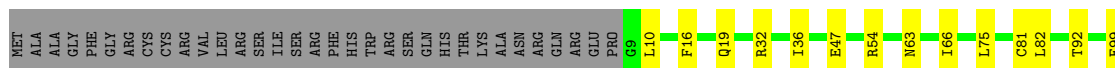
Chain A:
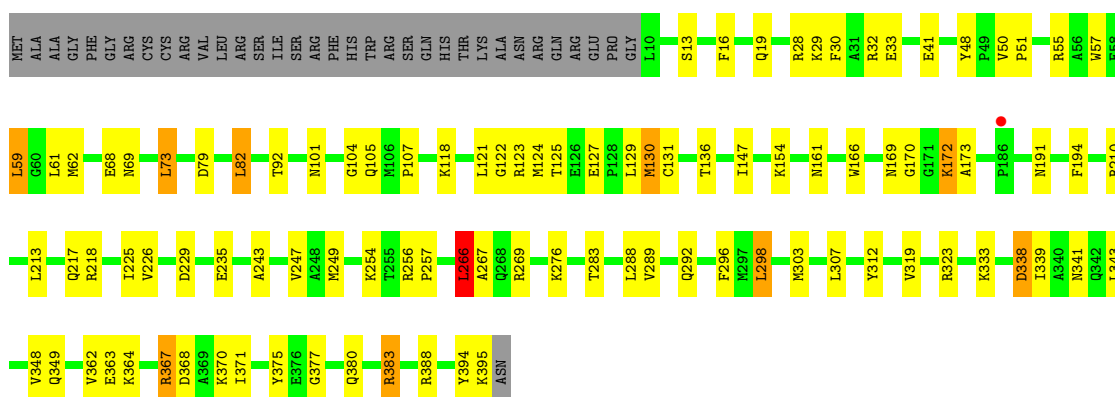
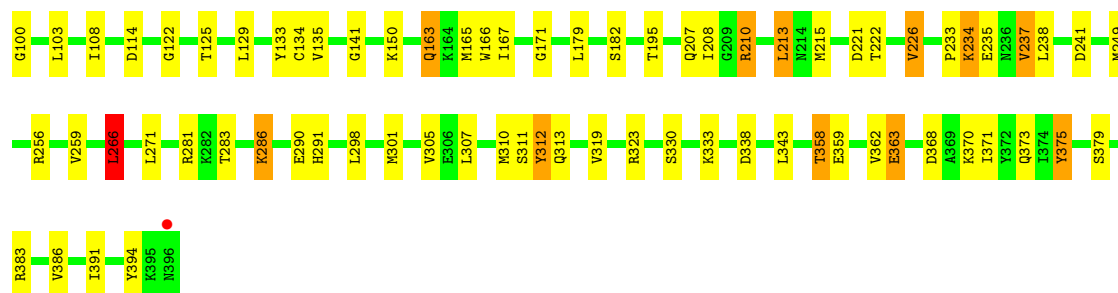- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor

Chain B:

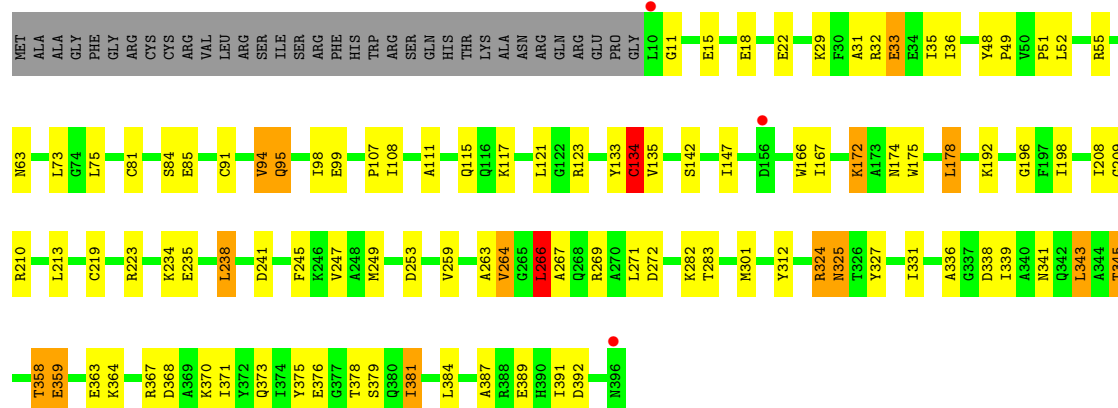- Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor
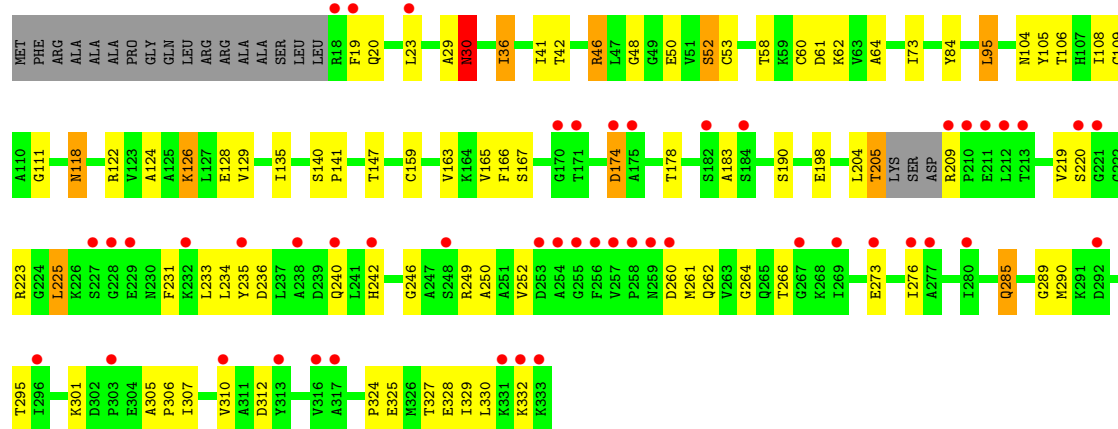
Chain C:

G100 L103 I108 D114 G122 T125 L129 Y133 C134 V135 G141 K150 Q163 K164 M165 W166 I167 G171 L179 S182 T195 Q207 I208 G209 R210 L213 N214 M215 D221 T222 V226 P233 K234 E235 N236 V237 L238 D241 M249

R256 V259 I264 L271 R281 K282 T283 K286 E290 H291 L298 M301 V305 E306 L307 M310 S311 Y312 Q313 V319 R323 S330 K333 D338 L343 T358 E359 V362 E363 D368 A369 K370 I371 Y372 Q373 I374 Y375 S379

R383 V386 I391 Y394 K395 N396

• Molecule 1: Acyl-CoA dehydrogenase, medium-chain specific, mitochondrial precursor

Chain D:

MET ALA ALA GLY PHE GLY ARG CYS CYS ARG VAL LEU ARG SER ILE SER ARG PHE HIS TRP ARG SER GLN HIS THR LYS ALA ASN ARG GLN ARG GLU PRO GLY L10 G11 E15 E18 E22 K29 F30 A31 R32 E33 E34 I35 I36 Y48 P49 V50 P51 L52 R55

N63 L73 G74 L75 C81 S84 E85 C91 V94 Q95 I98 E99 P107 I108 A111 Q115 Q116 K117 L121 G122 R123 Y133 C134 V135 S142 I147 D156 W166 I167 K172 A173 N174 W175 L178 K192 G196 F197 I198 I208 G209

R210 L213 C219 R223 K234 E235 L238 D241 F245 K246 V247 A248 M249 D253 V259 A263 V264 G265 L266 A267 Q268 R269 A270 L271 D272 K282 T283 M301 Y312 R324 N325 T326 Y327 I331 A336 G337 D338 I339 A340 N341 Q342 L343 A344 T345

T358 E359 E363 K364 R367 D368 A369 K370 I371 Y372 Q373 I374 Y375 E376 G377 T378 S379 Q380 I381 L384 A387 R388 E389 H390 I391 D392 N396

• Molecule 2: Electron transfer flavoprotein alpha-subunit, mitochondrial precursor

Chain R:

MET PHE ARG ALA ALA ALA PRO GLY GLN LEU ARG ARG ALA ALA SER LEU LEU R18 F19 Q20 L23 A29 N30 I36 I41 T42 R46 L47 G48 G49 E50 V51 S52 C53 T58 K59 C60 D61 K62 V63 A64 I73 Y84 L95 N104 Y105 T106 H107 I108 C109

A110 G111 N118 R122 V123 A124 A125 K126 L127 E128 V129 I135 S140 P141 T147 C159 V163 K164 V165 F166 S167 G170 T171 D174 A175 T178 S182 A183 S184 S190 E198 L204 T205 LYS SER ASP R209 P210 E211 L212 T213 V219 S220 G221 G222

R223 G224 L225 K226 S227 G228 E229 N230 F231 K232 L233 L234 Y235 D236 L237 A238 D239 Q240 L241 H242 G246 A247 S248 R249 A250 A251 V252 D253 A254 G255 F256 V257 P258 N259 D260 M261 Q262 V263 G264 Q265 T266 G267 K268 I269 E273 I276 A277 I280 Q285 G289 M290 K291 D292

T295 I296 K301 D302 P303 E304 A305 P306 I307 V310 A311 D312 Y313 V316 A317 P324 E325 M326 T327 E328 I329 L330 K331 K332 K333

• Molecule 3: Electron transfer flavoprotein beta-subunit

Chain S:

MET ALA E3 L4 L7 I14 D15 Y16 A17 V18 K19 I20 R21 V22 K23 P24 D25 G28 G33 S37 M38 N39 P40 F41 C42 E43 I44 A45 V46 K53 E60 V61 I62 A63 V64 S65 C66 Q70 I75 R76 L79 D84 R85 A94 A109 K110 L111

L122 G123 K124 I127 C131 N132 G140 F141 L142 D143 W144 P145 Q146 G147 T148 F149 T154 L155 K159 R164 K176 L177 L185 N188 Y192 A193 T194 L195 P196 M199 D217 L218 T219 S220 S226 V227 P230 P231 GLN ARG THR ALA GLY VAL LYS

VAL GLU T241 T242 E243 D244 L245 V246 A247 K248 L249 K250 GLU ILE GLY ARG ILE

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	94.18Å 100.66Å 244.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.98 – 2.80 19.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.98-2.80) 93.0 (19.98-2.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.74 (at 2.79Å)	Xtriage
Refinement program	REFMAC 5.2.0011	Depositor
R, R_{free}	0.199 , 0.269 0.205 , 0.200	Depositor DCC
R_{free} test set	2734 reflections (5.35%)	DCC
Wilson B-factor (Å^2)	46.7	Xtriage
Anisotropy	0.310	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 23.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Outliers	0 of 53814 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	16189	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5   Model quality ⓘ

5.1   Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AMP, 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	0.74	1/2988 (0.0%)	0.83	6/4040 (0.1%)
1	B	0.76	0/3004	0.80	1/4062 (0.0%)
1	C	0.73	0/3016	0.83	3/4074 (0.1%)
1	D	0.72	1/3027 (0.0%)	0.81	1/4085 (0.0%)
2	R	0.63	0/2298	0.73	1/3129 (0.0%)
3	S	0.68	2/1778 (0.1%)	0.77	1/2417 (0.0%)
All	All	0.72	4/16111 (0.0%)	0.80	13/21807 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
3	S	0	2
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	S	66	CYS	CB-SG	-5.89	1.72	1.81
3	S	131	CYS	CB-SG	-5.59	1.72	1.81
1	D	134	CYS	CB-SG	-5.39	1.73	1.81
1	A	41	GLU	CG-CD	5.04	1.59	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	269	ARG	NE-CZ-NH1	7.56	124.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	383	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	A	388	ARG	NE-CZ-NH2	-6.49	117.06	120.30
1	A	388	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	B	256	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	266	LEU	CA-CB-CG	6.01	129.13	115.30
1	A	266	LEU	CA-CB-CG	5.94	128.96	115.30
1	A	338	ASP	CB-CG-OD1	5.52	123.27	118.30
2	R	46	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	266	LEU	CA-CB-CG	5.46	127.87	115.30
1	A	367	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	C	383	ARG	NE-CZ-NH2	-5.18	117.71	120.30
3	S	177	LEU	C-N-CD	5.17	139.25	128.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	325	ASN	Peptide
3	S	176	LYS	Peptide
3	S	177	LEU	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2933	0	2855	57	0
1	B	2949	0	2862	60	0
1	C	2961	0	2903	50	0
1	D	2972	0	2916	63	0
2	R	2264	0	2268	50	0
3	S	1758	0	1795	42	0
4	S	23	0	12	1	0
5	A	53	0	31	7	0
5	B	53	0	31	3	0
5	C	53	0	31	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	D	53	0	31	4	0
5	R	53	0	31	4	0
6	A	13	0	0	3	0
6	B	9	0	0	0	0
6	C	17	0	0	2	0
6	D	12	0	0	3	0
6	R	3	0	0	1	0
6	S	10	0	0	0	0
All	All	16189	0	15766	298	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 9.

All (298) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:378:THR:HG21	5:B:1399:FAD:O2B	1.51	1.07
2:R:84:TYR:OH	2:R:95:LEU:HD23	1.71	0.91
1:A:341:ASN:HD21	1:A:370:LYS:HA	1.40	0.85
1:B:116:GLN:NE2	1:B:237:VAL:O	2.09	0.84
6:D:3411:HOH:O	2:R:266:THR:HG21	1.78	0.84
3:S:39:ASN:ND2	3:S:127:ILE:HG12	1.92	0.84
1:C:213:LEU:O	1:D:358:THR:HB	1.79	0.82
3:S:39:ASN:HD22	3:S:127:ILE:HG12	1.43	0.81
6:A:411:HOH:O	1:B:345:THR:HG21	1.90	0.72
1:D:259:VAL:HG21	1:D:376:GLU:HG3	1.69	0.71
3:S:28:GLY:HA2	3:S:227:VAL:HG21	1.70	0.71
1:D:325:ASN:HD22	1:D:325:ASN:H	1.36	0.71
2:R:61:ASP:HA	2:R:64:ALA:HB3	1.73	0.70
1:A:380:GLN:NE2	5:A:399:FAD:O2B	2.25	0.70
1:C:234:LYS:O	1:C:237:VAL:HG12	1.94	0.68
1:B:253:ASP:O	1:B:325:ASN:ND2	2.27	0.67
3:S:177:LEU:O	3:S:177:LEU:HD23	1.94	0.67
3:S:124:LYS:O	3:S:132:ASN:ND2	2.27	0.67
2:R:122:ARG:HH11	3:S:146:GLN:HE21	1.42	0.67
1:D:387:ALA:O	1:D:391:ILE:HG12	1.95	0.66
1:D:108:ILE:HD12	1:D:175:TRP:CH2	2.32	0.65
1:C:171:GLY:HA2	1:C:208:ILE:HD13	1.77	0.64
1:A:364:LYS:HA	1:A:367:ARG:NH1	2.13	0.64
1:C:358:THR:HB	1:D:213:LEU:O	1.96	0.64
1:D:208:ILE:CG2	1:D:223:ARG:HD2	2.29	0.62
2:R:23:LEU:HA	2:R:52:SER:O	1.99	0.61
1:B:256:ARG:CG	1:B:256:ARG:HH11	2.13	0.60

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:137:GLU:OE2	1:B:147:ILE:HB	2.01	0.60
1:C:108:ILE:N	1:C:108:ILE:HD12	2.16	0.60
2:R:46:ARG:HG2	2:R:46:ARG:HH11	1.67	0.59
1:C:207:GLN:HB2	1:C:226:VAL:HG13	1.84	0.59
1:C:338:ASP:HA	1:C:373:GLN:HE21	1.68	0.59
1:A:333:LYS:NZ	1:A:377:GLY:O	2.36	0.59
1:C:333:LYS:NZ	1:C:375:TYR:O	2.28	0.59
1:A:123:ARG:HG3	1:A:124:MET:HE2	1.84	0.59
2:R:122:ARG:HH11	3:S:146:GLN:NE2	2.01	0.58
1:A:131:CYS:HA	1:A:173:ALA:HB1	1.85	0.58
1:B:314:ARG:NH1	1:B:318:GLU:OE2	2.36	0.58
1:A:371:ILE:CD1	5:A:399:FAD:HM83	2.34	0.58
1:D:18:GLU:O	1:D:22:GLU:HG3	2.03	0.58
1:B:28:ARG:O	1:B:32:ARG:HG2	2.04	0.58
1:B:363:GLU:OE2	1:B:367:ARG:NE	2.36	0.57
2:R:329:ILE:HD12	3:S:242:THR:HG23	1.87	0.57
2:R:220:SER:HA	2:R:246:GLY:O	2.05	0.57
1:D:378:THR:HG23	6:D:3402:HOH:O	2.04	0.57
3:S:159:LYS:C	3:S:177:LEU:HD12	2.25	0.56
1:D:271:LEU:HD13	1:D:301:MET:HB3	1.86	0.56
2:R:36:ILE:HG12	2:R:111:GLY:HA3	1.87	0.56
1:A:394:TYR:OH	1:D:272:ASP:OD1	2.18	0.56
1:C:133:TYR:CE2	1:C:135:VAL:HG21	2.40	0.56
1:A:371:ILE:HD11	5:A:399:FAD:HM83	1.88	0.56
1:A:101:ASN:HD21	1:A:130:MET:HA	1.71	0.56
2:R:124:ALA:O	2:R:128:GLU:N	2.39	0.56
1:C:310:MET:HA	1:C:313:GLN:HE21	1.71	0.55
1:D:81:CYS:HB3	1:D:312:TYR:CE1	2.42	0.55
3:S:177:LEU:O	3:S:177:LEU:CD2	2.55	0.55
3:S:60:GLU:OE2	3:S:85:ARG:HD3	2.06	0.55
1:B:233:PRO:CB	1:B:235:GLU:HG2	2.36	0.55
1:A:16:PHE:CE2	1:A:82:LEU:HD21	2.41	0.55
1:D:266:LEU:C	1:D:266:LEU:HD12	2.27	0.55
1:C:166:TRP:O	5:C:2399:FAD:C4X	2.54	0.55
2:R:262:GLN:NE2	2:R:266:THR:OG1	2.39	0.55
1:B:267:ALA:HB1	1:B:343:LEU:HD22	1.89	0.55
2:R:126:LYS:NZ	3:S:140:GLY:O	2.35	0.55
1:B:89:TYR:CE2	1:B:269:ARG:HA	2.42	0.55
1:D:133:TYR:CZ	1:D:135:VAL:HG21	2.42	0.55
1:D:29:LYS:O	1:D:33:GLU:HB2	2.07	0.55
2:R:73:ILE:O	2:R:183:ALA:HB2	2.07	0.55
1:B:338:ASP:HA	1:B:373:GLN:HE21	1.71	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:79:ASP:HA	1:A:82:LEU:HD12	1.88	0.54
1:B:190:ALA:HB1	1:B:245:PHE:CD1	2.42	0.54
1:D:135:VAL:HG13	1:D:147:ILE:HD11	1.88	0.54
3:S:195:LEU:O	3:S:199:MET:HE3	2.06	0.54
3:S:53:LYS:NZ	3:S:84:ASP:OD2	2.32	0.54
1:C:32:ARG:HA	1:C:36:ILE:HD12	1.90	0.54
1:A:73:LEU:HD12	1:A:73:LEU:H	1.71	0.54
1:B:161:ASN:ND2	1:B:229:ASP:H	2.05	0.54
1:B:32:ARG:NH1	1:B:89:TYR:CE1	2.76	0.53
1:B:378:THR:CG2	1:B:380:GLN:HE21	2.21	0.53
1:A:341:ASN:HB3	6:A:411:HOH:O	2.06	0.53
1:B:233:PRO:HB3	1:B:235:GLU:HG2	1.89	0.53
1:D:209:GLY:O	1:D:223:ARG:HD3	2.08	0.53
1:C:371:ILE:CD1	5:C:2399:FAD:HM83	2.38	0.53
1:C:283:THR:HG22	6:C:2415:HOH:O	2.09	0.53
1:A:123:ARG:HG3	1:A:124:MET:CE	2.38	0.53
1:D:371:ILE:CD1	5:D:3399:FAD:HM83	2.39	0.53
1:B:208:ILE:HG12	1:B:225:ILE:HD12	1.91	0.53
1:D:245:PHE:O	1:D:249:MET:HG2	2.09	0.53
1:D:49:PRO:HB2	1:D:52:LEU:HD12	1.90	0.53
1:A:213:LEU:O	1:B:358:THR:HB	2.09	0.53
3:S:194:THR:HG23	3:S:196:PRO:HD2	1.91	0.52
2:R:305:ALA:O	2:R:307:ILE:N	2.42	0.52
1:D:117:LYS:O	1:D:121:LEU:HB2	2.09	0.52
3:S:44:ILE:HG23	3:S:188:ASN:ND2	2.24	0.52
1:A:28:ARG:O	1:A:32:ARG:HG3	2.09	0.52
1:B:73:LEU:HB3	1:B:75:LEU:HD13	1.91	0.52
1:C:266:LEU:C	1:C:266:LEU:HD12	2.30	0.51
1:A:267:ALA:HB1	1:A:343:LEU:HD22	1.92	0.51
1:D:253:ASP:HA	1:D:325:ASN:HD21	1.76	0.51
1:A:370:LYS:NZ	1:B:349:GLN:HE21	2.06	0.51
1:B:300:GLU:O	1:B:304:LYS:HG3	2.09	0.51
1:C:368:ASP:O	1:C:371:ILE:HG22	2.10	0.51
1:D:32:ARG:HA	1:D:36:ILE:HD12	1.92	0.51
1:A:29:LYS:O	1:A:33:GLU:HB2	2.10	0.51
2:R:325:GLU:O	2:R:329:ILE:HG13	2.10	0.51
3:S:7:LEU:HD12	3:S:62:ILE:HB	1.93	0.51
2:R:231:PHE:CD2	2:R:234:LEU:HD12	2.45	0.51
1:C:371:ILE:HD13	5:C:2399:FAD:HM83	1.92	0.50
1:B:256:ARG:HG3	1:B:256:ARG:HH11	1.76	0.50
2:R:41:ILE:HG21	2:R:73:ILE:HD11	1.93	0.50
2:R:260:ASP:OD1	2:R:260:ASP:N	2.44	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:13:SER:HB3	1:D:11:GLY:O	2.11	0.50
1:A:349:GLN:HE22	1:B:373:GLN:HB3	1.76	0.50
1:C:210:ARG:NE	2:R:249:ARG:HH21	2.09	0.50
1:C:234:LYS:O	1:C:237:VAL:CG1	2.58	0.50
1:B:378:THR:HG21	1:B:380:GLN:HE21	1.77	0.50
2:R:124:ALA:HB1	2:R:129:VAL:O	2.11	0.50
3:S:14:ILE:HD12	3:S:14:ILE:N	2.27	0.50
2:R:285:GLN:NE2	5:R:599:FAD:O2'	2.45	0.50
1:B:301:MET:HG2	1:B:343:LEU:HG	1.94	0.50
3:S:40:PRO:HA	3:S:43:GLU:HG3	1.93	0.50
1:A:256:ARG:N	1:A:257:PRO:CD	2.75	0.50
1:B:81:CYS:HB3	1:B:312:TYR:CE1	2.48	0.49
1:A:338:ASP:OD2	1:A:383:ARG:NH2	2.42	0.49
2:R:73:ILE:O	2:R:183:ALA:CB	2.60	0.49
2:R:41:ILE:CG2	2:R:73:ILE:HD11	2.41	0.49
1:A:296:PHE:HE1	1:D:384:LEU:HD21	1.77	0.49
2:R:140:SER:HB2	2:R:141:PRO:CD	2.42	0.49
3:S:44:ILE:HA	3:S:188:ASN:HD21	1.76	0.49
2:R:109:CYS:HB2	2:R:166:PHE:O	2.11	0.49
1:B:378:THR:HG21	5:B:1399:FAD:HO2A	1.70	0.49
1:D:31:ALA:HA	1:D:35:ILE:HD12	1.94	0.49
1:C:233:PRO:O	1:C:235:GLU:N	2.46	0.49
1:B:289:VAL:HG22	1:C:391:ILE:CD1	2.43	0.48
1:A:368:ASP:O	1:A:371:ILE:HG22	2.13	0.48
1:B:371:ILE:CG2	5:B:1399:FAD:HM83	2.43	0.48
1:A:105:GLN:HG2	1:A:121:LEU:HD22	1.95	0.48
3:S:7:LEU:HD11	3:S:64:VAL:HG11	1.95	0.48
1:A:348:VAL:HG22	1:A:362:VAL:HG23	1.95	0.48
1:C:81:CYS:HB3	1:C:312:TYR:CE1	2.49	0.48
1:C:108:ILE:N	1:C:108:ILE:CD1	2.77	0.48
3:S:188:ASN:C	3:S:188:ASN:HD22	2.17	0.48
2:R:204:LEU:C	2:R:205:THR:HG23	2.34	0.48
2:R:301:LYS:HG2	5:R:599:FAD:C4A	2.44	0.47
1:A:92:THR:HB	1:A:217:GLN:OE1	2.14	0.47
1:B:24:GLN:HB2	1:B:82:LEU:HD13	1.96	0.47
1:D:107:PRO:O	1:D:111:ALA:N	2.47	0.47
1:A:30:PHE:HE1	1:A:55:ARG:HG2	1.79	0.47
1:C:63:ASN:HB3	1:C:66:ILE:HD12	1.96	0.47
1:C:16:PHE:CZ	1:C:82:LEU:HD21	2.50	0.47
1:B:378:THR:O	1:B:382:GLN:HG2	2.14	0.47
2:R:61:ASP:OD1	2:R:62:LYS:N	2.48	0.47
5:A:399:FAD:H2'	5:A:399:FAD:H9	1.97	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:161:ASN:HD21	1:B:229:ASP:H	1.61	0.47
1:D:91:CYS:HB3	1:D:94:VAL:HG13	1.97	0.47
1:A:48:TYR:CE2	1:A:172:LYS:HG2	2.50	0.47
1:C:134:CYS:HA	1:C:167:ILE:HD12	1.95	0.47
3:S:39:ASN:ND2	3:S:127:ILE:H	2.13	0.47
1:C:281:ARG:NH1	5:D:3399:FAD:O2A	2.47	0.47
1:C:312:TYR:C	1:C:312:TYR:CD1	2.88	0.46
1:C:163:GLN:HG2	6:R:602:HOH:O	2.15	0.46
2:R:42:THR:OG1	2:R:174:ASP:O	2.27	0.46
1:A:50:VAL:N	1:A:51:PRO:CD	2.79	0.46
3:S:4:LEU:HD11	3:S:155:LEU:HD21	1.96	0.46
3:S:4:LEU:HD23	3:S:4:LEU:N	2.30	0.46
1:D:51:PRO:O	1:D:55:ARG:HG2	2.15	0.46
1:D:359:GLU:OE1	6:D:3411:HOH:O	2.20	0.46
3:S:70:GLN:N	3:S:70:GLN:NE2	2.63	0.46
1:C:215:MET:HB2	1:D:363:GLU:HG3	1.97	0.46
1:A:370:LYS:HZ1	1:B:349:GLN:NE2	2.13	0.46
1:D:108:ILE:HD11	1:D:198:ILE:HG12	1.97	0.46
1:B:106:MET:HE3	1:B:109:ILE:HB	1.96	0.46
1:D:327:TYR:O	1:D:331:ILE:HG13	2.15	0.46
1:D:84:SER:HB2	1:D:95:GLN:OE1	2.16	0.46
1:A:57:TRP:CZ2	1:A:127:GLU:HA	2.51	0.46
1:B:378:THR:CG2	1:B:380:GLN:NE2	2.78	0.46
1:A:292:GLN:NE2	5:D:3399:FAD:N1A	2.63	0.46
1:B:378:THR:HG22	1:B:380:GLN:N	2.31	0.45
1:B:43:ASP:HB2	1:B:364:LYS:HE2	1.99	0.45
1:D:263:ALA:HB3	1:D:336:ALA:HB1	1.98	0.45
2:R:233:LEU:HD22	2:R:324:PRO:HG3	1.99	0.45
1:A:161:ASN:HD21	1:A:229:ASP:H	1.64	0.45
2:R:252:VAL:HG21	2:R:262:GLN:HB2	1.99	0.45
3:S:75:ILE:O	3:S:79:LEU:HG	2.15	0.45
1:A:50:VAL:N	1:A:51:PRO:HD2	2.31	0.45
1:D:338:ASP:HA	1:D:373:GLN:HE21	1.82	0.45
2:R:135:ILE:HG12	2:R:167:SER:O	2.17	0.45
2:R:108:ILE:O	2:R:165:VAL:HA	2.17	0.45
2:R:29:ALA:O	2:R:30:ASN:C	2.56	0.45
1:D:238:LEU:HA	1:D:238:LEU:HD12	1.82	0.44
1:D:238:LEU:HD23	1:D:247:VAL:HG11	1.98	0.44
5:A:399:FAD:H2'	5:A:399:FAD:C9	2.48	0.44
1:D:48:TYR:CE2	1:D:172:LYS:HG2	2.52	0.44
1:D:301:MET:HG2	1:D:343:LEU:HG	1.99	0.44
2:R:266:THR:HG23	5:R:599:FAD:N5	2.32	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:312:TYR:CD1	1:C:313:GLN:N	2.86	0.44
1:A:303:MET:HG2	1:D:331:ILE:HG23	1.99	0.44
1:C:286:LYS:HB3	1:C:290:GLU:OE1	2.18	0.44
1:B:243:ALA:O	1:B:247:VAL:HG13	2.18	0.44
1:B:161:ASN:HA	1:B:227:PHE:O	2.18	0.44
1:C:271:LEU:HD13	1:C:301:MET:HB3	2.00	0.44
1:B:375:TYR:C	1:B:375:TYR:CD1	2.92	0.44
3:S:28:GLY:HA2	3:S:227:VAL:CG2	2.45	0.44
1:C:210:ARG:HE	2:R:249:ARG:HH21	1.64	0.43
1:A:57:TRP:HB2	1:A:62:MET:HE3	2.00	0.43
2:R:324:PRO:O	2:R:328:GLU:HG2	2.18	0.43
1:A:123:ARG:HG3	1:A:129:LEU:HD12	1.99	0.43
1:C:16:PHE:CZ	1:C:82:LEU:CD2	3.01	0.43
1:D:253:ASP:CB	1:D:325:ASN:HD21	2.31	0.43
1:A:136:THR:OG1	5:A:399:FAD:H1'1	2.18	0.43
1:A:266:LEU:HD12	1:A:266:LEU:C	2.37	0.43
1:C:122:GLY:O	1:C:125:THR:HB	2.19	0.43
1:D:135:VAL:CG1	1:D:147:ILE:HD11	2.49	0.43
2:R:118:ASN:ND2	3:S:146:GLN:OE1	2.51	0.43
1:B:235:GLU:CD	1:B:235:GLU:H	2.22	0.43
3:S:42:CYS:O	3:S:46:VAL:HG23	2.18	0.43
1:A:283:THR:HG23	1:A:288:LEU:HD21	2.00	0.43
3:S:149:PHE:N	3:S:149:PHE:CD1	2.86	0.43
1:D:99:GLU:OE1	1:D:99:GLU:HA	2.19	0.43
1:A:166:TRP:O	5:A:399:FAD:C4X	2.66	0.43
1:D:301:MET:HA	1:D:343:LEU:HD11	2.01	0.43
1:A:147:ILE:HD11	1:A:194:PHE:CD1	2.54	0.43
1:B:233:PRO:HB2	1:B:235:GLU:HG2	2.01	0.43
1:C:362:VAL:O	1:C:363:GLU:C	2.56	0.43
2:R:23:LEU:HD22	2:R:105:TYR:CE2	2.54	0.43
3:S:41:PHE:HB3	3:S:123:GLY:HA3	2.01	0.43
1:D:73:LEU:HG	3:S:199:MET:HE1	2.01	0.42
1:D:324:ARG:NH2	1:D:389:GLU:OE1	2.52	0.42
1:B:50:VAL:N	1:B:51:PRO:CD	2.81	0.42
1:D:368:ASP:O	1:D:371:ILE:HG22	2.19	0.42
1:D:142:SER:HB3	1:D:381:ILE:HG21	2.01	0.42
3:S:109:ALA:HA	3:S:142:LEU:HD21	2.01	0.42
1:D:364:LYS:HA	1:D:367:ARG:NH2	2.34	0.42
1:B:105:GLN:HG3	1:B:131:CYS:SG	2.59	0.42
2:R:19:PHE:CG	2:R:19:PHE:O	2.72	0.42
1:A:254:LYS:HG2	1:A:319:VAL:HG21	2.01	0.42
1:A:104:GLY:O	1:A:107:PRO:HD2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:55:ARG:O	1:A:59:LEU:HD22	2.20	0.42
1:C:319:VAL:HA	1:C:323:ARG:O	2.20	0.42
1:A:123:ARG:CG	1:A:124:MET:CE	2.98	0.42
3:S:14:ILE:HD12	3:S:14:ILE:H	1.83	0.42
2:R:30:ASN:HA	2:R:30:ASN:HD22	1.70	0.42
2:R:235:TYR:O	2:R:236:ASP:C	2.58	0.42
1:A:169:ASN:O	1:A:170:GLY:C	2.58	0.42
1:B:256:ARG:N	1:B:257:PRO:CD	2.83	0.42
3:S:144:TRP:HB3	3:S:145:PRO:HD2	2.00	0.42
1:B:263:ALA:HB3	1:B:336:ALA:HB1	2.02	0.42
1:C:226:VAL:HG11	2:R:223:ARG:CZ	2.50	0.42
1:A:243:ALA:O	1:A:247:VAL:HG23	2.19	0.42
1:C:99:GLU:O	1:C:100:GLY:C	2.56	0.42
1:A:28:ARG:HB2	1:A:28:ARG:HE	1.69	0.41
1:C:133:TYR:CE2	1:C:135:VAL:CG2	3.03	0.41
1:C:310:MET:HA	1:C:313:GLN:NE2	2.34	0.41
1:C:286:LYS:HD3	1:C:291:HIS:CE1	2.55	0.41
1:C:330:SER:HB3	1:C:386:VAL:HG23	2.01	0.41
2:R:240:GLN:HG3	2:R:327:THR:HG23	2.02	0.41
1:D:29:LYS:HG2	3:S:192:TYR:CE1	2.55	0.41
1:B:171:GLY:HA3	1:B:223:ARG:HD3	2.02	0.41
1:C:370:LYS:HD3	1:D:345:THR:HG22	2.01	0.41
1:D:134:CYS:HA	1:D:167:ILE:HD12	2.02	0.41
1:B:324:ARG:NH2	1:B:389:GLU:OE1	2.53	0.41
1:A:123:ARG:CG	1:A:124:MET:HE3	2.51	0.41
2:R:225:LEU:CD1	2:R:234:LEU:HD11	2.50	0.41
1:B:99:GLU:O	1:B:100:GLY:C	2.59	0.41
1:D:166:TRP:O	5:D:3399:FAD:C4X	2.69	0.41
2:R:301:LYS:HG2	5:R:599:FAD:N3A	2.36	0.41
1:B:275:THR:HG21	1:C:394:TYR:CD1	2.55	0.41
1:D:341:ASN:OD1	1:D:370:LYS:HA	2.21	0.41
1:A:122:GLY:O	1:A:125:THR:HB	2.20	0.41
3:S:148:THR:OG1	3:S:164:ARG:NH2	2.53	0.41
1:D:267:ALA:HB1	1:D:343:LEU:HD22	2.03	0.41
1:B:289:VAL:HG22	1:C:391:ILE:HD13	2.03	0.41
1:A:363:GLU:OE2	1:A:367:ARG:NH1	2.52	0.41
1:B:256:ARG:CG	1:B:256:ARG:NH1	2.81	0.41
3:S:122:LEU:HD23	4:S:600:AMP:H1'	2.02	0.41
1:B:330:SER:OG	1:B:385:ILE:HG21	2.21	0.41
1:D:253:ASP:CA	1:D:325:ASN:HD21	2.33	0.41
1:A:377:GLY:HA2	6:A:412:HOH:O	2.20	0.41
1:C:166:TRP:O	5:C:2399:FAD:N5	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:178:LEU:O	1:D:196:GLY:HA2	2.21	0.41
1:B:36:ILE:HG13	1:B:90:GLY:HA2	2.03	0.41
2:R:219:VAL:HG22	2:R:276:ILE:HD12	2.03	0.41
1:C:195:THR:HG23	6:C:2412:HOH:O	2.20	0.41
5:C:2399:FAD:H8A	1:D:283:THR:HG21	2.03	0.40
3:S:14:ILE:O	3:S:15:ASP:C	2.59	0.40
1:B:106:MET:HE2	1:B:254:LYS:HD3	2.03	0.40
1:B:244:GLY:O	1:B:247:VAL:HG22	2.21	0.40
1:C:305:VAL:HG23	1:C:343:LEU:HD21	2.02	0.40
1:D:123:ARG:HD3	1:D:174:ASN:HD21	1.86	0.40
1:D:259:VAL:HG21	1:D:376:GLU:CG	2.44	0.40
1:A:298:LEU:HD23	1:D:391:ILE:HD11	2.03	0.40
2:R:223:ARG:NH2	2:R:250:ALA:HB1	2.36	0.40
2:R:264:GLY:HA2	2:R:289:GLY:HA3	2.04	0.40
1:B:108:ILE:HD11	1:B:198:ILE:HG12	2.04	0.40
3:S:38:MET:O	3:S:39:ASN:C	2.59	0.40
3:S:15:ASP:HB3	3:S:18:VAL:HG23	2.04	0.40
1:D:85:GLU:HG3	1:D:264:VAL:HG22	2.02	0.40
1:B:91:CYS:SG	1:B:94:VAL:HG13	2.62	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	384/421 (91%)	361 (94%)	22 (6%)	1 (0%)	50	84
1	B	385/421 (91%)	368 (96%)	15 (4%)	2 (0%)	38	76
1	C	386/421 (92%)	372 (96%)	12 (3%)	2 (0%)	38	76
1	D	385/421 (91%)	365 (95%)	20 (5%)	0	100	100
2	R	309/333 (93%)	270 (87%)	31 (10%)	8 (3%)	8	26
3	S	235/255 (92%)	205 (87%)	25 (11%)	5 (2%)	11	33
All	All	2084/2272 (92%)	1941 (93%)	125 (6%)	18 (1%)	25	63

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	C	234	LYS
3	S	218	LEU
2	R	30	ASN
2	R	50	GLU
2	R	242	HIS
3	S	217	ASP
2	R	306	PRO
3	S	94	ALA
1	B	191	ASN
2	R	48	GLY
2	R	60	CYS
3	S	25	ASP
2	R	290	MET
1	B	141	GLY
2	R	36	ILE
3	S	177	LEU
1	C	141	GLY

5.3.2 Protein sidechains ⓘ

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	287/332 (86%)	259 (90%)	28 (10%)	12	32
1	B	288/332 (87%)	260 (90%)	28 (10%)	12	32
1	C	293/332 (88%)	257 (88%)	36 (12%)	7	20
1	D	296/332 (89%)	263 (89%)	33 (11%)	9	25
2	R	232/262 (88%)	204 (88%)	28 (12%)	7	21
3	S	183/213 (86%)	163 (89%)	20 (11%)	9	26
All	All	1579/1803 (88%)	1406 (89%)	173 (11%)	9	26

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	GLN

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Mol	Chain	Res	Type
1	A	59	LEU
1	A	61	LEU
1	A	68	GLU
1	A	73	LEU
1	A	82	LEU
1	A	118	LYS
1	A	130	MET
1	A	154	LYS
1	A	172	LYS
1	A	191	ASN
1	A	210	ARG
1	A	218	ARG
1	A	225	ILE
1	A	226	VAL
1	A	235	GLU
1	A	249	MET
1	A	266	LEU
1	A	276	LYS
1	A	289	VAL
1	A	298	LEU
1	A	307	LEU
1	A	312	TYR
1	A	323	ARG
1	A	339	ILE
1	A	375	TYR
1	A	383	ARG
1	A	395	LYS
1	B	32	ARG
1	B	47	GLU
1	B	55	ARG
1	B	95	GLN
1	B	117	LYS
1	B	121	LEU
1	B	125	THR
1	B	127	GLU
1	B	152	GLU
1	B	156	ASP
1	B	182	SER
1	B	207	GLN
1	B	210	ARG
1	B	218	ARG
1	B	223	ARG

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Mol	Chain	Res	Type
1	B	228	GLU
1	B	235	GLU
1	B	239	ILE
1	B	256	ARG
1	B	289	VAL
1	B	295	SER
1	B	312	TYR
1	B	345	THR
1	B	371	ILE
1	B	375	TYR
1	B	379	SER
1	B	392	ASP
1	B	393	LYS
1	C	10	LEU
1	C	19	GLN
1	C	47	GLU
1	C	54	ARG
1	C	75	LEU
1	C	92	THR
1	C	103	LEU
1	C	114	ASP
1	C	129	LEU
1	C	150	LYS
1	C	163	GLN
1	C	165	MET
1	C	179	LEU
1	C	182	SER
1	C	210	ARG
1	C	213	LEU
1	C	221	ASP
1	C	222	THR
1	C	226	VAL
1	C	237	VAL
1	C	238	LEU
1	C	241	ASP
1	C	249	MET
1	C	256	ARG
1	C	259	VAL
1	C	266	LEU
1	C	286	LYS
1	C	298	LEU
1	C	307	LEU

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Mol	Chain	Res	Type
1	C	311	SER
1	C	312	TYR
1	C	358	THR
1	C	359	GLU
1	C	363	GLU
1	C	375	TYR
1	C	379	SER
1	D	15	GLU
1	D	33	GLU
1	D	63	ASN
1	D	75	LEU
1	D	94	VAL
1	D	95	GLN
1	D	98	ILE
1	D	115	GLN
1	D	134	CYS
1	D	172	LYS
1	D	178	LEU
1	D	192	LYS
1	D	210	ARG
1	D	219	CYS
1	D	234	LYS
1	D	235	GLU
1	D	238	LEU
1	D	241	ASP
1	D	264	VAL
1	D	266	LEU
1	D	269	ARG
1	D	282	LYS
1	D	324	ARG
1	D	325	ASN
1	D	339	ILE
1	D	343	LEU
1	D	345	THR
1	D	358	THR
1	D	359	GLU
1	D	375	TYR
1	D	379	SER
1	D	381	ILE
1	D	392	ASP
2	R	20	GLN
2	R	30	ASN

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Mol	Chain	Res	Type
2	R	52	SER
2	R	53	CYS
2	R	58	THR
2	R	95	LEU
2	R	104	ASN
2	R	106	THR
2	R	118	ASN
2	R	126	LYS
2	R	147	THR
2	R	159	CYS
2	R	163	VAL
2	R	174	ASP
2	R	178	THR
2	R	190	SER
2	R	198	GLU
2	R	205	THR
2	R	209	ARG
2	R	225	LEU
2	R	261	MET
2	R	273	GLU
2	R	285	GLN
2	R	295	THR
2	R	310	VAL
2	R	312	ASP
2	R	330	LEU
2	R	332	LYS
3	S	20	ILE
3	S	22	VAL
3	S	37	SER
3	S	70	GLN
3	S	76	ARG
3	S	85	ARG
3	S	111	LEU
3	S	149	PHE
3	S	154	THR
3	S	155	LEU
3	S	164	ARG
3	S	177	LEU
3	S	185	LEU
3	S	188	ASN
3	S	194	THR
3	S	219	THR

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Mol	Chain	Res	Type
3	S	226	SER
3	S	241	THR
3	S	242	THR
3	S	244	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (41) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	ASN
1	A	101	ASN
1	A	105	GLN
1	A	161	ASN
1	A	169	ASN
1	A	191	ASN
1	A	341	ASN
1	A	349	GLN
1	A	373	GLN
1	A	380	GLN
1	B	65	HIS
1	B	95	GLN
1	B	161	ASN
1	B	163	GLN
1	B	349	GLN
1	B	380	GLN
1	B	382	GLN
1	C	161	ASN
1	C	313	GLN
1	C	349	GLN
1	C	373	GLN
1	C	382	GLN
1	D	19	GLN
1	D	69	ASN
1	D	115	GLN
1	D	163	GLN
1	D	174	ASN
1	D	236	ASN
1	D	325	ASN
1	D	354	ASN
1	D	373	GLN
2	R	30	ASN
2	R	39	ASN
2	R	118	ASN

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Mol	Chain	Res	Type
2	R	262	GLN
2	R	285	GLN
3	S	39	ASN
3	S	70	GLN
3	S	146	GLN
3	S	188	ASN
3	S	197	ASN

5.3.3　RNA ⓘ

There are no RNA chains 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 carbohydrates in this entry.

5.6　Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z|>2$	Counts	RMSZ	#$|Z|>2$
5	FAD	A	399	-	58,58,58	1.13	5 (8%)	85,89,89	1.99	17 (20%)
5	FAD	B	1399	-	58,58,58	1.09	5 (8%)	85,89,89	2.00	17 (20%)
5	FAD	C	2399	-	58,58,58	1.21	4 (6%)	85,89,89	1.68	12 (14%)
5	FAD	D	3399	-	58,58,58	1.14	4 (6%)	85,89,89	1.81	14 (16%)
5	FAD	R	599	-	58,58,58	1.00	4 (6%)	85,89,89	2.04	17 (20%)
4	AMP	S	600	-	25,25,25	1.16	2 (8%)	38,38,38	1.89	10 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	FAD	A	399	-	-	0/34/50/50	0/1/6/6
5	FAD	B	1399	-	-	0/34/50/50	0/1/6/6
5	FAD	C	2399	-	-	0/34/50/50	0/1/6/6
5	FAD	D	3399	-	-	0/34/50/50	0/1/6/6
5	FAD	R	599	-	-	0/34/50/50	0/1/6/6
4	AMP	S	600	-	-	0/10/26/26	0/1/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	399	FAD	C1'-C2'	4.09	1.55	1.51
4	S	600	AMP	C4-N9	-3.58	1.32	1.37
5	D	3399	FAD	C1'-C2'	3.49	1.54	1.51
5	C	2399	FAD	C1'-N10	3.35	1.52	1.48
5	R	599	FAD	C2A-N3A	3.31	1.38	1.32
5	A	399	FAD	C2A-N3A	3.27	1.38	1.32
5	B	1399	FAD	C1'-N10	3.19	1.51	1.48
5	C	2399	FAD	C1'-C2'	3.12	1.54	1.51
5	B	1399	FAD	C2A-N3A	3.07	1.38	1.32
5	D	3399	FAD	C1'-N10	3.03	1.51	1.48
5	D	3399	FAD	C2A-N3A	2.81	1.37	1.32
5	R	599	FAD	C2A-N1A	2.79	1.39	1.33
4	S	600	AMP	C5-C4	2.66	1.46	1.40
5	A	399	FAD	C1'-N10	2.64	1.51	1.48
5	C	2399	FAD	C2A-N1A	2.63	1.39	1.33
5	D	3399	FAD	C2A-N1A	2.61	1.39	1.33
5	B	1399	FAD	C5X-N5	2.50	1.39	1.35
5	C	2399	FAD	C2A-N3A	2.50	1.37	1.32
5	A	399	FAD	C5X-N5	2.45	1.39	1.35
5	B	1399	FAD	C6-C5X	-2.31	1.39	1.41
5	A	399	FAD	C2A-N1A	2.27	1.38	1.33
5	R	599	FAD	C5X-N5	2.15	1.38	1.35
5	B	1399	FAD	C2A-N1A	2.11	1.38	1.33
5	R	599	FAD	C10-N1	2.11	1.39	1.35

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	R	599	FAD	N3A-C2A-N1A	-11.89	118.77	128.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	399	FAD	N3A-C2A-N1A	-11.21	119.34	128.71
5	B	1399	FAD	N3A-C2A-N1A	-10.54	119.90	128.71
5	D	3399	FAD	N3A-C2A-N1A	-10.35	120.06	128.71
5	C	2399	FAD	N3A-C2A-N1A	-9.44	120.81	128.71
5	R	599	FAD	C2-N1-C10	6.20	121.23	114.98
4	S	600	AMP	N3-C2-N1	-5.90	123.78	128.71
5	B	1399	FAD	C2-N1-C10	5.82	120.85	114.98
5	B	1399	FAD	O4B-C1B-N9A	5.27	113.34	108.44
5	C	2399	FAD	C2-N1-C10	4.91	119.92	114.98
5	A	399	FAD	C5X-C9A-N10	4.64	121.37	116.80
5	D	3399	FAD	C2-N1-C10	4.48	119.49	114.98
5	R	599	FAD	C4X-N5-C5X	4.34	121.57	116.69
5	A	399	FAD	C2-N1-C10	4.34	119.35	114.98
5	B	1399	FAD	N3A-C4A-N9A	4.28	133.16	125.43
4	S	600	AMP	N3-C4-N9	4.16	132.94	125.43
5	D	3399	FAD	C5X-C9A-N10	4.08	120.82	116.80
5	A	399	FAD	C4X-C10-N1	-3.93	118.80	122.73
4	S	600	AMP	C4-C5-N7	-3.87	106.21	109.52
5	B	1399	FAD	C1'-N10-C9A	3.78	122.55	118.87
5	R	599	FAD	C4X-C10-N1	-3.76	118.98	122.73
5	R	599	FAD	N3A-C4A-N9A	3.74	132.18	125.43
5	A	399	FAD	N3A-C4A-N9A	3.70	132.12	125.43
5	A	399	FAD	C9A-N10-C10	-3.68	118.16	121.77
5	D	3399	FAD	P-O3P-PA	-3.44	121.59	131.68
5	B	1399	FAD	C9A-N10-C10	-3.43	118.40	121.77
5	A	399	FAD	C4X-N5-C5X	3.38	120.49	116.69
5	D	3399	FAD	C4X-N5-C5X	3.27	120.37	116.69
5	C	2399	FAD	P-O3P-PA	-3.24	122.17	131.68
5	A	399	FAD	C5A-C6A-N6A	-3.22	113.44	120.72
5	C	2399	FAD	C5X-C9A-N10	3.14	119.89	116.80
5	B	1399	FAD	C5X-C9A-N10	3.08	119.84	116.80
5	D	3399	FAD	N3A-C4A-N9A	3.08	130.99	125.43
5	C	2399	FAD	N3A-C4A-N9A	3.07	130.98	125.43
5	R	599	FAD	P-O3P-PA	-3.05	122.75	131.68
5	R	599	FAD	C1'-N10-C9A	3.03	121.82	118.87
5	B	1399	FAD	P-O3P-PA	-2.95	123.04	131.68
5	B	1399	FAD	C4X-C10-N1	-2.95	119.79	122.73
5	B	1399	FAD	C4X-N5-C5X	2.94	120.00	116.69
4	S	600	AMP	O2P-P-O5'	-2.92	98.58	106.65
5	R	599	FAD	O4'-C4'-C3'	2.88	116.22	109.05
5	A	399	FAD	C4-N3-C2	-2.81	119.61	125.39
5	B	1399	FAD	C4X-C10-N10	2.80	121.91	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	399	FAD	C8M-C8-C9	-2.68	113.92	120.38
5	B	1399	FAD	C5A-C4A-N3A	-2.65	119.94	125.70
5	A	399	FAD	C4-C4X-C10	2.64	121.21	116.95
5	R	599	FAD	C4-N3-C2	-2.60	120.05	125.39
5	A	399	FAD	C1'-N10-C9A	2.59	121.39	118.87
5	D	3399	FAD	C4X-C10-N1	-2.56	120.17	122.73
5	C	2399	FAD	C1'-N10-C9A	2.55	121.35	118.87
4	S	600	AMP	C5-C4-N3	-2.51	120.23	125.70
5	D	3399	FAD	C1B-N9A-C4A	-2.50	122.31	126.64
5	D	3399	FAD	C4-C4X-C10	2.47	120.94	116.95
5	R	599	FAD	C4A-C5A-N7A	-2.46	107.42	109.52
5	B	1399	FAD	C4-N3-C2	-2.42	120.42	125.39
5	D	3399	FAD	C8A-N9A-C4A	2.42	108.74	106.90
4	S	600	AMP	C2-N1-C6	2.42	123.13	118.77
4	S	600	AMP	C8-N9-C4	2.39	108.72	106.90
5	B	1399	FAD	C2A-N3A-C4A	2.38	120.79	114.01
5	D	3399	FAD	N7A-C8A-N9A	-2.38	107.63	114.36
5	C	2399	FAD	C4X-N5-C5X	2.31	119.28	116.69
5	B	1399	FAD	N7A-C8A-N9A	-2.30	107.85	114.36
4	S	600	AMP	O3P-P-O2P	2.26	116.42	107.61
5	R	599	FAD	N7A-C8A-N9A	-2.25	108.00	114.36
5	R	599	FAD	C2A-N1A-C6A	2.25	122.83	118.77
5	A	399	FAD	P-O3P-PA	-2.24	125.13	131.68
5	B	1399	FAD	C4A-C5A-N7A	-2.22	107.62	109.52
5	D	3399	FAD	C9A-N10-C10	-2.21	119.59	121.77
5	R	599	FAD	O4'-C4'-C5'	-2.19	105.62	110.12
5	C	2399	FAD	C4X-C10-N1	-2.19	120.54	122.73
5	R	599	FAD	C2A-N3A-C4A	2.16	120.17	114.01
5	C	2399	FAD	C4-N3-C2	-2.15	120.98	125.39
5	A	399	FAD	O2A-PA-O3P	2.12	115.22	105.14
5	C	2399	FAD	C4-C4X-C10	2.11	120.36	116.95
5	A	399	FAD	C2A-N3A-C4A	2.11	120.01	114.01
4	S	600	AMP	O4'-C1'-N9	-2.10	106.48	108.44
5	R	599	FAD	C5A-C4A-N3A	-2.08	121.18	125.70
5	B	1399	FAD	O2A-PA-O3P	2.07	114.94	105.14
5	A	399	FAD	C9A-C5X-N5	-2.06	119.21	122.37
5	D	3399	FAD	C8M-C8-C9	-2.06	115.41	120.38
5	R	599	FAD	C5X-C9A-N10	2.06	118.83	116.80
5	D	3399	FAD	C2'-C1'-N10	-2.04	109.74	112.45
5	A	399	FAD	C5A-C4A-N3A	-2.04	121.25	125.70
5	C	2399	FAD	C9A-N10-C10	-2.03	119.78	121.77
5	R	599	FAD	C8A-N9A-C4A	2.02	108.44	106.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	S	600	AMP	C4'-O4'-C1'	-2.00	107.58	109.75
5	C	2399	FAD	O5'-P-O1P	-2.00	101.54	109.37

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	386/421 (91%)	-0.51	1 (0%)	91	93	26, 37, 49, 57	0
1	B	387/421 (91%)	-0.42	5 (1%)	74	75	26, 40, 53, 62	0
1	C	388/421 (92%)	-0.54	1 (0%)	91	93	24, 37, 49, 60	0
1	D	387/421 (91%)	-0.50	3 (0%)	83	83	24, 37, 51, 60	0
2	R	313/333 (93%)	0.67	49 (15%)	3	2	43, 63, 91, 104	0
3	S	239/255 (93%)	0.10	13 (5%)	25	25	36, 53, 77, 111	0
All	All	2100/2272 (92%)	-0.25	72 (3%)	43	44	24, 41, 82, 111	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	R	333	LYS	7.0
2	R	213	THR	5.8
2	R	220	SER	5.2
2	R	242	HIS	5.2
2	R	209	ARG	4.8
2	R	303	PRO	4.8
3	S	247	ALA	4.2
2	R	332	LYS	4.2
2	R	18	ARG	4.1
2	R	221	GLY	4.0
2	R	19	PHE	3.9
3	S	241	THR	3.8
2	R	253	ASP	3.8
1	C	396	ASN	3.5
3	S	246	VAL	3.3
2	R	292	ASP	3.3
1	B	396	ASN	3.2
2	R	210	PRO	3.2
3	S	24	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
2	R	232	LYS	3.2
2	R	277	ALA	3.2
2	R	227	SER	3.1
2	R	276	ILE	3.1
2	R	248	SER	3.0
2	R	316	VAL	3.0
1	D	156	ASP	2.9
2	R	255	GLY	2.9
2	R	254	ALA	2.9
3	S	33	GLY	2.9
3	S	250	LYS	2.9
1	D	10	LEU	2.8
2	R	175	ALA	2.8
2	R	182	SER	2.8
2	R	296	ILE	2.7
2	R	174	ASP	2.7
2	R	310	VAL	2.7
2	R	240	GLN	2.7
2	R	317	ALA	2.7
2	R	269	ILE	2.6
2	R	257	VAL	2.6
2	R	211	GLU	2.6
2	R	260	ASP	2.6
2	R	331	LYS	2.5
1	D	396	ASN	2.5
2	R	313	TYR	2.5
2	R	256	PHE	2.5
3	S	248	LYS	2.5
3	S	243	GLU	2.4
1	A	186	PRO	2.4
2	R	23	LEU	2.4
3	S	25	ASP	2.3
2	R	267	GLY	2.3
2	R	212	LEU	2.3
2	R	171	THR	2.2
2	R	273	GLU	2.2
2	R	229	GLU	2.2
2	R	258	PRO	2.1
2	R	170	GLY	2.1
3	S	231	PRO	2.1
1	B	155	GLY	2.1
1	B	69	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
3	S	230	PRO	2.1
3	S	16	TYR	2.1
3	S	220	SER	2.1
1	B	153	LYS	2.1
2	R	280	ILE	2.1
2	R	184	SER	2.1
1	B	191	ASN	2.0
2	R	228	GLY	2.0
2	R	235	TYR	2.0
2	R	259	ASN	2.0
2	R	238	ALA	2.0

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å^2)	Q<0.9
5	FAD	B	1399	53/53	0.14	-0.26	29,35,41,42	0
5	FAD	C	2399	53/53	0.12	-0.42	29,33,36,37	0
5	FAD	D	3399	53/53	0.12	-0.69	28,32,37,37	0
5	FAD	R	599	53/53	0.17	-0.71	61,65,71,71	0
5	FAD	A	399	53/53	0.12	-0.99	27,33,35,36	0
4	AMP	S	600	23/23	0.12	-1.27	41,45,46,46	0

6.5 Other polymers ⓘ

There are no such residues in this entry.