Full wwPDB X-ray Structure Validation Report (i)

Sep 22, 2026 – 12:11 PM JST

PDB ID	:	9M82 / pdb_00009m82
Title	:	Crystal Structure of Human IDH1 in Complex with Kinsenoside
Authors	:	Ouyang, S.; Zhao, Y.
Deposited on	:	2025-03-11
Resolution	:	3.08 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:

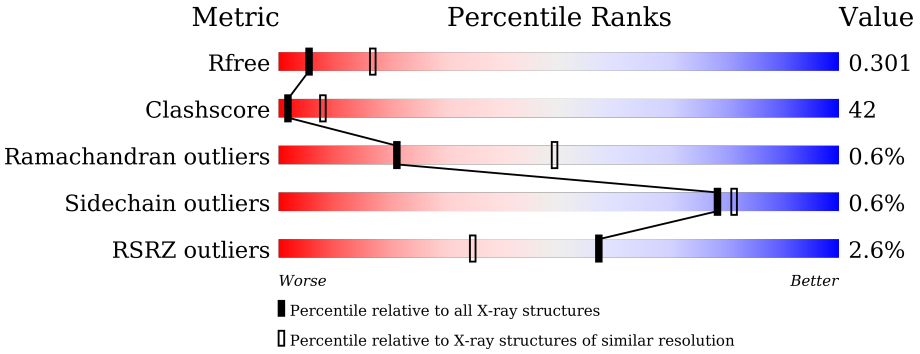
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.08 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}	180053	2010 (3.10-3.06)
Clashscore	190562	2102 (3.10-3.06)
Ramachandran outliers	187476	1982 (3.10-3.06)
Sidechain outliers	187428	1981 (3.10-3.06)
RSRZ outliers	180081	2010 (3.10-3.06)

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	443	3% 39% 53% • 7%
1	B	443	2% 40% 52% • 7%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 6582 atoms, of which 32 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 Isocitrate dehydrogenase [NADP] cytoplasmic.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	411	3257	2071	552	616	18	0	0	0
1	B	411	3257	2071	552	616	18	0	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	HIS	-	expression tag	UNP O75874
A	-27	HIS	-	expression tag	UNP O75874
A	-26	HIS	-	expression tag	UNP O75874
A	-25	HIS	-	expression tag	UNP O75874
A	-24	HIS	-	expression tag	UNP O75874
A	-23	HIS	-	expression tag	UNP O75874
A	-22	SER	-	expression tag	UNP O75874
A	-21	SER	-	expression tag	UNP O75874
A	-20	GLY	-	expression tag	UNP O75874
A	-19	LEU	-	expression tag	UNP O75874
A	-18	VAL	-	expression tag	UNP O75874
A	-17	PRO	-	expression tag	UNP O75874
A	-16	ARG	-	expression tag	UNP O75874
A	-15	GLY	-	expression tag	UNP O75874
A	-14	SER	-	expression tag	UNP O75874
A	-13	HIS	-	expression tag	UNP O75874
A	-12	MET	-	expression tag	UNP O75874
A	-11	ALA	-	expression tag	UNP O75874
A	-10	SER	-	expression tag	UNP O75874
A	-9	MET	-	expression tag	UNP O75874
A	-8	THR	-	expression tag	UNP O75874
A	-7	GLY	-	expression tag	UNP O75874
A	-6	GLY	-	expression tag	UNP O75874
A	-5	GLN	-	expression tag	UNP O75874
A	-4	GLN	-	expression tag	UNP O75874

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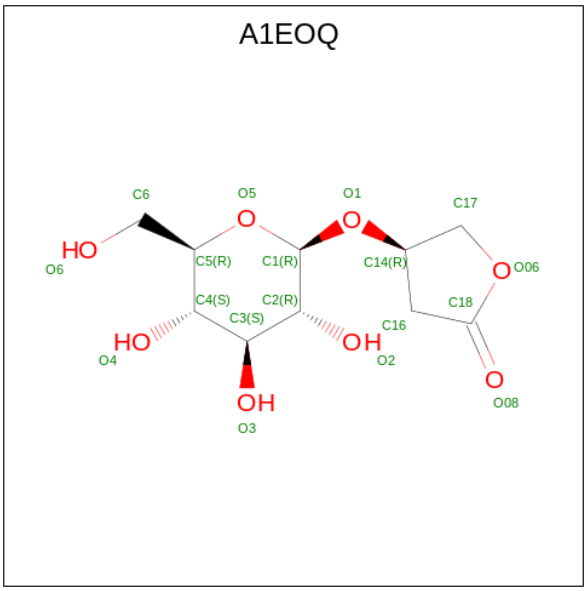
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	expression tag	UNP O75874
A	-2	GLY	-	expression tag	UNP O75874
A	-1	ARG	-	expression tag	UNP O75874
A	0	GLY	-	expression tag	UNP O75874
B	-28	HIS	-	expression tag	UNP O75874
B	-27	HIS	-	expression tag	UNP O75874
B	-26	HIS	-	expression tag	UNP O75874
B	-25	HIS	-	expression tag	UNP O75874
B	-24	HIS	-	expression tag	UNP O75874
B	-23	HIS	-	expression tag	UNP O75874
B	-22	SER	-	expression tag	UNP O75874
B	-21	SER	-	expression tag	UNP O75874
B	-20	GLY	-	expression tag	UNP O75874
B	-19	LEU	-	expression tag	UNP O75874
B	-18	VAL	-	expression tag	UNP O75874
B	-17	PRO	-	expression tag	UNP O75874
B	-16	ARG	-	expression tag	UNP O75874
B	-15	GLY	-	expression tag	UNP O75874
B	-14	SER	-	expression tag	UNP O75874
B	-13	HIS	-	expression tag	UNP O75874
B	-12	MET	-	expression tag	UNP O75874
B	-11	ALA	-	expression tag	UNP O75874
B	-10	SER	-	expression tag	UNP O75874
B	-9	MET	-	expression tag	UNP O75874
B	-8	THR	-	expression tag	UNP O75874
B	-7	GLY	-	expression tag	UNP O75874
B	-6	GLY	-	expression tag	UNP O75874
B	-5	GLN	-	expression tag	UNP O75874
B	-4	GLN	-	expression tag	UNP O75874
B	-3	MET	-	expression tag	UNP O75874
B	-2	GLY	-	expression tag	UNP O75874
B	-1	ARG	-	expression tag	UNP O75874
B	0	GLY	-	expression tag	UNP O75874

- Molecule 2 is Kinsenoside (CCD ID: A1EOQ) (formula: $C_{10}H_{16}O_8$) (labeled as "Ligand of Interest" by depositor).



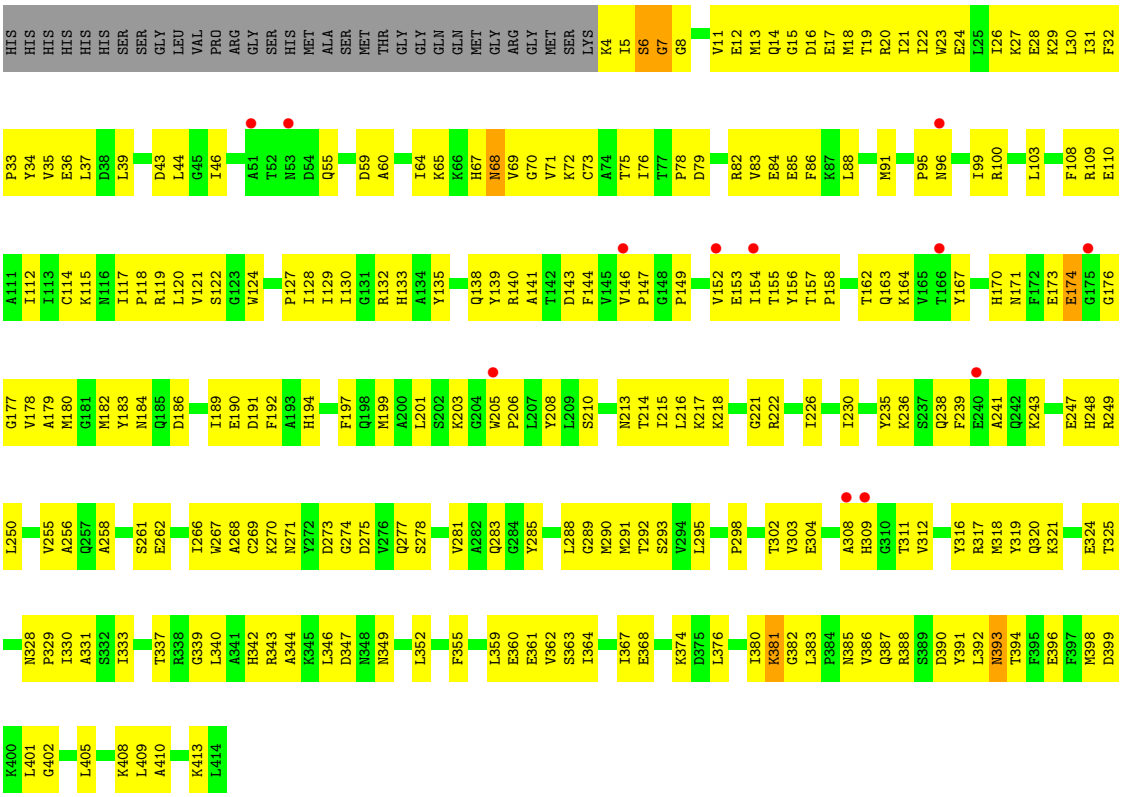
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	H	O		
2	A	1	34	10	16	8	0	0
			Total	C	H	O		
2	B	1	34	10	16	8	0	0

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.

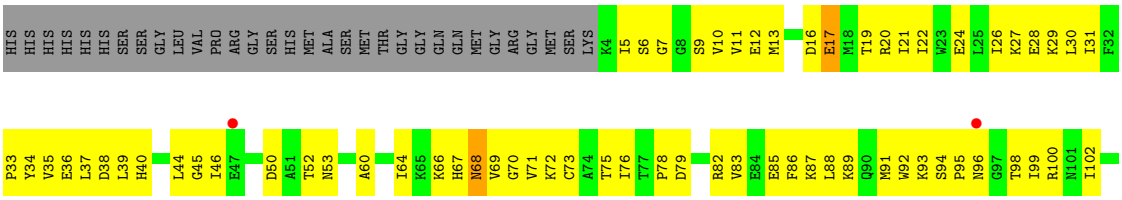
• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

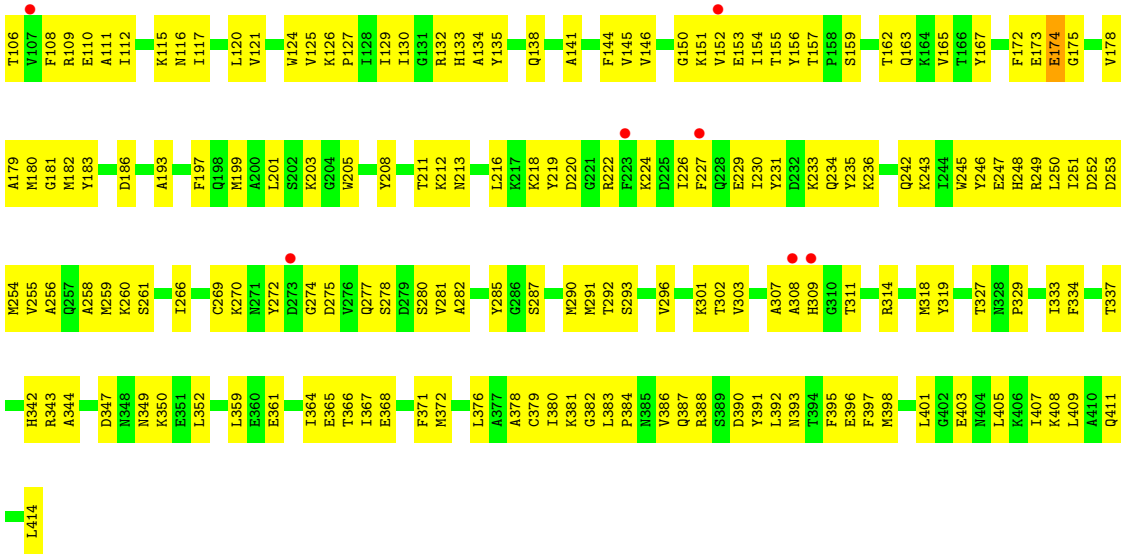
Chain A:



• Molecule 1: Isocitrate dehydrogenase [NADP] cytoplasmic

Chain B:




T106 V107 F108 R109 E110 A111 I112 K115 N116 I117 L120 V121 W124 V125 K126 P127 I128 I129 I130 G131 R132 H133 A134 Y135 Q138 A141 F144 V145 V146 G150 K151 V152 E153 I154 T155 Y156 T157 P158 S159 T162 Q163 K164 V165 T166 Y167 F172 E173 E174 G175 V178
A179 M180 G181 M182 Y183 D186 A193 F197 Q198 M199 A200 L201 S202 K203 G204 W205 Y208 T211 K212 N213 L216 K217 K218 Y219 D220 G221 R222 F223 K224 D225 I226 F227 Q228 E229 I230 Y231 D232 K233 Q234 Y235 K236 Q242 K243 I244 W245 Y246 E247 H248 R249 L250 I251 D252 D253
M254 V255 A256 Q257 A258 M259 K260 S261 I266 C269 K270 M271 Y272 D273 G274 D275 V276 Q277 S278 D279 S280 V281 A282 Y285 G286 S287 M290 M291 T292 S293 V296 K301 T302 V303 A307 A308 H309 G310 T311 R314 M318 Y319 T327 N328 P329 I333 F334 T337
H342 R343 A344 D347 N348 N349 K350 E351 L352 L359 E360 E361 I364 E365 T366 I367 E368 F371 M372 L376 A377 A378 C379 I380 K381 G382 L383 P384 N385 V386 Q387 R388 S389 D390 Y391 L392 N393 T394 F395 E396 F397 M398 L401 G402 E403 N404 L405 K406 I407 K408 L409 A410 Q411
L414

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	94.90Å 112.38Å 97.77Å 90.00° 91.88° 90.00°	Depositor
Resolution (Å)	56.19 – 3.08 56.19 – 3.08	Depositor EDS
% Data completeness (in resolution range)	92.4 (56.19-3.08) 92.0 (56.19-3.08)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.58 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.19.2_4158: ???)	Depositor
R, R_{free}	0.251 , 0.301 0.249 , 0.301	Depositor DCC
R_{free} test set	1910 reflections (10.01%)	wwPDB-VP
Wilson B-factor (Å^2)	62.0	Xtriage
Anisotropy	0.387	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.53$, $< L^2 > = 0.37$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	6582	wwPDB-VP
Average B, all atoms (Å^2)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.26% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: A1EOQ

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	0.22	0/3325	0.50	1/4484 (0.0%)
1	B	0.21	0/3325	0.49	1/4484 (0.0%)
All	All	0.21	0/6650	0.49	2/8968 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	17	GLU	CB-CA-C	-5.70	109.01	115.79
1	A	7	GLY	N-CA-C	-5.05	109.05	115.31

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3257	0	3226	286	0
1	B	3257	0	3226	284	0
2	A	18	16	0	0	0
2	B	18	16	0	2	0
All	All	6550	32	6452	541	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including

hydrogen atoms). The all-atom clashscore for this structure is 42.

All (541) 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:A:393:ASN:OD1	1:A:396:GLU:HG3	1.55	1.07
1:A:156:TYR:HE1	1:B:150:GLY:HA3	1.24	1.02
1:B:208:TYR:HB3	1:B:254:MET:HE1	1.45	0.99
1:A:337:THR:HG22	1:A:359:LEU:HD23	1.45	0.96
1:B:227:PHE:HD2	1:B:246:TYR:CZ	1.84	0.96
1:A:138:GLN:HG3	1:A:182:MET:HE1	1.48	0.95
1:B:361:GLU:O	1:B:365:GLU:HG3	1.67	0.95
1:A:22:ILE:HD11	1:A:394:THR:HG23	1.50	0.94
1:B:22:ILE:O	1:B:26:ILE:HD12	1.69	0.92
1:B:5:ILE:HB	1:B:35:VAL:HG12	1.52	0.90
1:B:249:ARG:HB2	1:B:254:MET:HE2	1.52	0.89
1:A:162:THR:HG22	1:A:163:GLN:H	1.38	0.89
1:B:111:ALA:HA	1:B:291:MET:HG3	1.53	0.88
1:A:388:ARG:HH21	1:A:393:ASN:HD21	1.21	0.88
1:B:392:LEU:HB3	1:B:396:GLU:HB2	1.57	0.86
1:A:180:MET:HE3	1:A:182:MET:HE3	1.58	0.85
1:A:118:PRO:HD3	1:A:380:ILE:HG22	1.57	0.85
1:B:109:ARG:HE	1:B:293:SER:HB2	1.40	0.85
1:A:13:MET:HG2	1:A:44:LEU:HD12	1.60	0.83
1:A:138:GLN:HG3	1:A:182:MET:CE	2.09	0.83
1:B:211:THR:HG1	1:B:248:HIS:HE2	1.23	0.82
1:B:227:PHE:CD2	1:B:246:TYR:CZ	2.68	0.82
1:A:109:ARG:HH21	1:A:308:ALA:HB1	1.44	0.81
1:B:66:LYS:HD2	1:B:67:HIS:CE1	2.15	0.81
1:B:258:ALA:HA	1:B:261:SER:HB3	1.62	0.81
1:B:60:ALA:O	1:B:64:ILE:HG13	1.79	0.81
1:B:115:LYS:HG3	1:B:368:GLU:OE2	1.80	0.80
1:A:28:GLU:O	1:A:33:PRO:HD3	1.82	0.80
1:A:333:ILE:O	1:A:337:THR:HG23	1.81	0.80
1:B:88:LEU:HD22	1:B:92:TRP:HZ3	1.46	0.80
1:B:208:TYR:HB3	1:B:254:MET:CE	2.11	0.80
1:A:83:VAL:HG23	1:A:88:LEU:CD1	2.12	0.79
1:A:381:LYS:HD2	1:A:385:ASN:O	1.83	0.79
1:B:333:ILE:HD11	1:B:398:MET:HE1	1.63	0.79
1:A:156:TYR:CE1	1:B:150:GLY:HA3	2.15	0.78
1:A:383:LEU:O	1:A:386:VAL:HG22	1.83	0.78
1:A:135:TYR:HH	1:A:183:TYR:HE2	1.28	0.78
1:A:4:LYS:NZ	1:A:36:GLU:HG3	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:5:ILE:HB	1:A:35:VAL:HG12	1.65	0.77
1:A:173:GLU:O	1:A:174:GLU:HB2	1.85	0.76
1:B:22:ILE:HG22	1:B:26:ILE:HD11	1.67	0.76
1:B:22:ILE:HD11	1:B:327:THR:CG2	2.15	0.75
1:B:162:THR:HG22	1:B:163:GLN:H	1.50	0.75
1:A:22:ILE:O	1:A:26:ILE:HG13	1.86	0.75
1:A:343:ARG:NH1	1:A:346:LEU:HD11	2.01	0.75
1:A:344:ALA:HB2	1:A:352:LEU:CD2	2.17	0.75
1:B:50:ASP:HA	1:B:92:TRP:CH2	2.21	0.75
1:B:88:LEU:HD22	1:B:92:TRP:CZ3	2.21	0.75
1:B:85:GLU:HG2	1:B:86:PHE:CD1	2.23	0.74
1:B:85:GLU:HG2	1:B:86:PHE:HD1	1.52	0.74
1:B:93:LYS:HD3	1:B:98:THR:OG1	1.88	0.74
1:A:18:MET:HB3	1:A:312:VAL:HG23	1.68	0.73
1:A:214:THR:HG23	1:A:250:LEU:HD11	1.68	0.73
1:B:227:PHE:CE2	1:B:246:TYR:CE1	2.75	0.73
1:A:344:ALA:HB2	1:A:352:LEU:HD23	1.71	0.73
1:B:6:SER:O	1:B:349:ASN:ND2	2.22	0.73
1:B:46:ILE:HG21	1:B:86:PHE:CE2	2.23	0.73
1:B:343:ARG:HG3	1:B:347:ASP:OD2	1.88	0.73
1:B:12:GLU:OE1	1:B:39:LEU:HD21	1.89	0.73
1:B:10:VAL:HG23	1:B:69:VAL:HG12	1.71	0.72
1:A:317:ARG:O	1:A:321:LYS:HD3	1.89	0.72
1:B:249:ARG:HB2	1:B:254:MET:CE	2.19	0.72
1:A:68:ASN:HA	1:A:302:THR:HG23	1.72	0.72
1:A:180:MET:CE	1:A:182:MET:HE3	2.20	0.71
1:B:227:PHE:CD2	1:B:246:TYR:CE1	2.77	0.71
1:B:13:MET:HE1	1:B:64:ILE:HD11	1.72	0.71
1:A:132:ARG:HD2	1:A:275:ASP:N	2.06	0.71
1:A:184:ASN:ND2	1:A:189:ILE:CG1	2.53	0.71
1:B:282:ALA:HB2	1:B:291:MET:SD	2.31	0.70
1:A:13:MET:HG2	1:A:44:LEU:CD1	2.23	0.69
1:A:32:PHE:HA	1:A:35:VAL:O	1.93	0.69
1:A:388:ARG:NH2	1:A:393:ASN:HD21	1.90	0.69
1:B:22:ILE:HD11	1:B:327:THR:HG22	1.73	0.69
1:A:37:LEU:HD11	1:A:39:LEU:HD12	1.75	0.69
1:A:109:ARG:HD3	1:A:278:SER:HB2	1.73	0.69
1:A:210:SER:HB3	1:A:267:TRP:HE1	1.58	0.69
1:B:249:ARG:CB	1:B:254:MET:HE2	2.23	0.69
1:B:129:ILE:HB	1:B:266:ILE:HD13	1.76	0.68
1:B:287:SER:HB3	1:B:290:MET:HG2	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ARG:NH1	1:A:122:SER:O	2.27	0.68
1:A:5:ILE:HB	1:A:35:VAL:CG1	2.24	0.68
1:A:140:ARG:HG2	1:A:183:TYR:OH	1.95	0.67
1:B:359:LEU:HD13	1:B:405:LEU:HD22	1.76	0.67
1:A:255:VAL:HG22	1:B:280:SER:HB2	1.77	0.67
1:A:83:VAL:HG23	1:A:88:LEU:HD11	1.77	0.66
1:A:135:TYR:OH	1:A:183:TYR:HE2	1.78	0.66
1:A:109:ARG:HH21	1:A:308:ALA:CB	2.09	0.66
1:A:109:ARG:HG2	1:A:293:SER:HB2	1.78	0.66
1:A:109:ARG:NH2	1:A:308:ALA:HB1	2.11	0.66
1:A:146:VAL:HB	1:A:177:GLY:H	1.60	0.66
1:B:233:LYS:HD3	1:B:234:GLN:HG3	1.77	0.66
1:A:83:VAL:HA	1:A:88:LEU:HD21	1.77	0.65
1:B:124:TRP:HB3	1:B:285:TYR:CE1	2.31	0.65
1:A:30:LEU:HD21	1:A:401:LEU:HD22	1.78	0.65
1:A:186:ASP:O	1:A:190:GLU:HG3	1.95	0.65
1:A:218:LYS:O	1:A:222:ARG:N	2.28	0.65
1:A:157:THR:OG1	1:A:164:LYS:HE2	1.97	0.65
1:A:318:MET:HE2	1:A:325:THR:HG22	1.78	0.65
1:B:193:ALA:HA	1:B:227:PHE:CE1	2.32	0.65
1:A:222:ARG:O	1:A:226:ILE:HG13	1.97	0.65
1:A:177:GLY:HA2	1:B:186:ASP:OD1	1.97	0.64
1:B:141:ALA:HB2	1:B:182:MET:HB3	1.79	0.64
1:B:307:ALA:HB1	1:B:309:HIS:CE1	2.33	0.64
1:B:130:ILE:HD12	1:B:278:SER:HA	1.78	0.64
1:B:121:VAL:HG11	1:B:124:TRP:CE2	2.32	0.64
1:B:411:GLN:HA	1:B:414:LEU:HD12	1.78	0.63
1:A:22:ILE:HD11	1:A:394:THR:CG2	2.26	0.63
1:B:13:MET:HE1	1:B:64:ILE:CD1	2.29	0.63
1:A:83:VAL:HA	1:A:88:LEU:CD2	2.29	0.63
1:A:162:THR:HG22	1:A:163:GLN:N	2.11	0.63
1:A:388:ARG:NH2	1:A:393:ASN:ND2	2.46	0.62
1:B:180:MET:HE2	1:B:182:MET:HE2	1.80	0.62
1:A:110:GLU:HB2	1:A:129:ILE:HD13	1.81	0.62
1:B:116:ASN:O	1:B:380:ILE:HD11	1.99	0.62
1:B:38:ASP:OD1	1:B:40:HIS:NE2	2.33	0.62
1:B:212:LYS:NZ	1:B:250:LEU:HD21	2.14	0.62
1:A:22:ILE:CD1	1:A:394:THR:HG23	2.29	0.61
1:A:309:HIS:CD2	1:A:331:ALA:HB3	2.34	0.61
1:B:83:VAL:CG2	1:B:91:MET:HG2	2.30	0.61
1:B:96:ASN:HB2	1:B:100:ARG:NH1	2.16	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:PRO:HG2	1:A:205:TRP:CH2	2.35	0.61
1:A:362:VAL:HG21	1:A:405:LEU:HA	1.83	0.61
1:B:388:ARG:HD2	1:B:388:ARG:O	2.00	0.61
1:B:13:MET:CE	1:B:64:ILE:HD11	2.31	0.61
1:A:290:MET:HE2	1:A:330:ILE:HB	1.81	0.61
1:B:388:ARG:NH2	1:B:396:GLU:OE2	2.28	0.61
1:A:324:GLU:OE2	1:A:393:ASN:ND2	2.34	0.60
1:B:9:SER:HA	1:B:38:ASP:HB3	1.83	0.60
1:A:60:ALA:O	1:A:64:ILE:HG12	2.01	0.60
1:A:258:ALA:O	1:A:261:SER:HB3	2.01	0.60
1:A:374:LYS:HG3	1:A:391:TYR:CD2	2.37	0.60
1:A:138:GLN:CG	1:A:182:MET:HE1	2.27	0.60
1:B:79:ASP:OD1	1:B:82:ARG:HG2	2.01	0.60
1:B:20:ARG:HG2	1:B:20:ARG:HH11	1.67	0.60
1:A:96:ASN:HD22	1:A:100:ARG:NH2	1.99	0.60
1:A:132:ARG:CZ	1:A:275:ASP:HB2	2.32	0.60
1:B:388:ARG:NH1	1:B:391:TYR:O	2.35	0.60
1:A:72:LYS:HE2	1:A:75:THR:HG23	1.83	0.60
1:B:46:ILE:HD11	1:B:88:LEU:HD11	1.84	0.60
1:B:132:ARG:CZ	1:B:275:ASP:HB2	2.32	0.59
1:A:65:LYS:HB3	1:A:65:LYS:HZ2	1.66	0.59
1:B:144:PHE:CZ	1:B:179:ALA:HB3	2.37	0.59
1:B:392:LEU:HD12	1:B:397:PHE:HA	1.84	0.59
1:B:381:LYS:HG3	1:B:386:VAL:HG12	1.84	0.59
1:A:16:ASP:OD2	1:A:76:ILE:HB	2.03	0.59
1:A:343:ARG:O	1:A:347:ASP:HB2	2.02	0.58
1:B:76:ILE:HD13	1:B:82:ARG:NH1	2.18	0.58
1:A:4:LYS:CE	1:A:36:GLU:HG3	2.33	0.58
1:A:393:ASN:CG	1:A:396:GLU:HG3	2.27	0.58
1:B:333:ILE:HD11	1:B:398:MET:CE	2.32	0.58
1:A:4:LYS:O	1:A:5:ILE:HG13	2.03	0.58
1:A:410:ALA:O	1:A:413:LYS:HG2	2.04	0.58
1:A:4:LYS:HZ2	1:A:36:GLU:HG3	1.68	0.58
1:A:95:PRO:O	1:A:99:ILE:HG13	2.04	0.58
1:A:383:LEU:O	1:A:383:LEU:HD12	2.03	0.58
1:B:83:VAL:HG21	1:B:91:MET:CG	2.33	0.58
1:B:229:GLU:OE1	1:B:229:GLU:HA	2.01	0.58
1:A:184:ASN:ND2	1:A:189:ILE:HG13	2.18	0.57
1:A:110:GLU:HB2	1:A:129:ILE:CD1	2.35	0.57
1:B:85:GLU:OE2	1:B:86:PHE:HE1	1.88	0.57
1:B:96:ASN:O	1:B:100:ARG:HD2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:PHE:CZ	1:B:231:TYR:HB2	2.39	0.57
1:A:67:HIS:O	1:A:68:ASN:HB2	2.02	0.57
1:A:184:ASN:HD22	1:A:189:ILE:CG1	2.16	0.57
1:A:388:ARG:HH21	1:A:393:ASN:ND2	1.94	0.57
1:B:13:MET:HB3	1:B:44:LEU:HD13	1.87	0.57
1:B:29:LYS:C	1:B:30:LEU:HD22	2.30	0.57
1:B:83:VAL:HG21	1:B:91:MET:HG3	1.86	0.57
1:B:172:PHE:HB3	1:B:175:GLY:O	2.04	0.57
1:A:37:LEU:HD11	1:A:39:LEU:CD1	2.34	0.57
1:A:283:GLN:OE1	1:B:260:LYS:HB2	2.04	0.57
1:B:249:ARG:HG2	1:B:249:ARG:HH11	1.70	0.57
1:B:287:SER:HB3	1:B:290:MET:CG	2.35	0.57
1:A:144:PHE:CZ	1:A:179:ALA:HB3	2.40	0.56
1:B:50:ASP:OD1	1:B:89:LYS:HG2	2.05	0.56
1:A:34:TYR:O	1:A:35:VAL:HG13	2.05	0.56
1:A:197:PHE:O	1:A:201:LEU:HD23	2.06	0.56
1:B:72:LYS:NZ	1:B:75:THR:HG23	2.21	0.56
1:A:65:LYS:HG3	1:A:103:LEU:CD2	2.36	0.56
1:A:184:ASN:ND2	1:A:189:ILE:HG12	2.20	0.56
1:B:12:GLU:HB2	1:B:39:LEU:HD11	1.87	0.56
1:A:289:GLY:O	1:A:331:ALA:HB2	2.06	0.56
1:A:205:TRP:HB3	1:A:206:PRO:HD2	1.86	0.56
1:A:290:MET:HE3	1:A:328:ASN:HD21	1.69	0.56
1:B:247:GLU:OE1	1:B:249:ARG:NH1	2.32	0.56
1:A:65:LYS:HB3	1:A:65:LYS:NZ	2.21	0.55
1:A:387:GLN:N	1:A:390:ASP:OD2	2.36	0.55
1:A:388:ARG:HG3	1:A:388:ARG:O	2.07	0.55
1:A:112:ILE:CG2	1:A:364:ILE:HD11	2.36	0.55
1:B:9:SER:O	1:B:343:ARG:HD3	2.06	0.55
1:B:213:ASN:ND2	1:B:224:LYS:HD3	2.21	0.55
1:B:220:ASP:OD1	1:B:270:LYS:NZ	2.36	0.55
1:B:337:THR:CG2	1:B:359:LEU:HB3	2.37	0.55
1:B:117:ILE:CD1	1:B:376:LEU:HD22	2.37	0.55
1:A:344:ALA:HB2	1:A:352:LEU:HD22	1.89	0.55
1:A:343:ARG:HH12	1:A:346:LEU:HD11	1.69	0.55
1:B:199:MET:HG3	1:B:266:ILE:HD12	1.89	0.55
1:A:22:ILE:HG22	1:A:26:ILE:HD11	1.89	0.55
1:B:7:GLY:HA3	1:B:37:LEU:HD11	1.89	0.55
1:A:178:VAL:HG13	1:B:222:ARG:HG3	1.88	0.55
1:B:231:TYR:CE1	1:B:236:LYS:HA	2.42	0.55
1:A:149:PRO:HB2	1:B:159:SER:OG	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:ILE:HD11	1:A:398:MET:HE1	1.89	0.54
1:B:397:PHE:CE2	1:B:401:LEU:HD11	2.41	0.54
1:A:34:TYR:CD2	1:A:409:LEU:HD12	2.42	0.54
1:B:212:LYS:HE2	1:B:252:ASP:OD2	2.06	0.54
1:A:18:MET:CB	1:A:312:VAL:HG23	2.38	0.54
1:A:46:ILE:HD11	1:A:78:PRO:HG3	1.90	0.54
1:B:141:ALA:CB	1:B:182:MET:HB3	2.37	0.54
1:A:180:MET:HB3	1:B:219:TYR:HD2	1.73	0.54
1:A:367:ILE:HD13	1:A:376:LEU:CD1	2.38	0.54
1:B:76:ILE:HG12	1:B:311:THR:HG21	1.89	0.54
1:A:141:ALA:CB	1:A:182:MET:HB3	2.37	0.54
1:A:158:PRO:HG2	1:A:162:THR:HB	1.90	0.54
1:B:20:ARG:HG2	1:B:20:ARG:NH1	2.20	0.54
1:A:184:ASN:HD22	1:A:189:ILE:HG13	1.72	0.54
1:A:32:PHE:N	1:A:33:PRO:HD2	2.22	0.54
1:A:330:ILE:HG13	1:A:367:ILE:HD11	1.89	0.54
1:B:21:ILE:HD13	1:B:319:TYR:CE2	2.43	0.54
1:B:366:THR:HG22	1:B:371:PHE:HB2	1.89	0.54
1:A:183:TYR:HA	1:B:178:VAL:O	2.08	0.53
1:B:108:PHE:CE1	1:B:199:MET:HG2	2.43	0.53
1:B:277:GLN:O	1:B:281:VAL:HG23	2.08	0.53
1:A:15:GLY:HA3	1:A:73:CYS:SG	2.49	0.53
1:A:388:ARG:O	1:A:388:ARG:NH1	2.41	0.53
1:A:214:THR:HG21	1:A:250:LEU:HD21	1.89	0.53
1:B:227:PHE:HE2	1:B:246:TYR:CE1	2.24	0.53
1:A:110:GLU:OE2	1:A:129:ILE:HD11	2.09	0.53
1:B:83:VAL:HA	1:B:88:LEU:HB2	1.90	0.53
1:A:30:LEU:HD11	1:A:402:GLY:CA	2.38	0.53
1:A:108:PHE:CE1	1:A:199:MET:HG2	2.44	0.53
1:A:155:THR:O	1:B:152:VAL:HA	2.08	0.53
1:A:171:ASN:OD1	1:A:173:GLU:HG2	2.08	0.53
1:B:22:ILE:HG22	1:B:26:ILE:CD1	2.37	0.53
1:B:121:VAL:HG11	1:B:124:TRP:NE1	2.24	0.53
1:A:83:VAL:HG23	1:A:88:LEU:CG	2.39	0.53
1:A:109:ARG:HD3	1:A:278:SER:CB	2.39	0.52
1:B:22:ILE:CD1	1:B:327:THR:HG22	2.39	0.52
1:B:203:LYS:HE3	1:B:203:LYS:O	2.09	0.52
1:A:394:THR:O	1:A:398:MET:HB2	2.08	0.52
1:B:303:VAL:HB	1:B:342:HIS:CD2	2.43	0.52
1:B:296:VAL:HG23	1:B:296:VAL:O	2.09	0.52
1:A:157:THR:HB	1:B:151:LYS:CG	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:THR:OG1	1:A:360:GLU:OE2	2.26	0.52
1:B:19:THR:HG22	1:B:73:CYS:SG	2.49	0.52
1:B:344:ALA:HB2	1:B:352:LEU:HB3	1.90	0.52
1:A:15:GLY:C	1:A:20:ARG:HB2	2.35	0.52
1:A:121:VAL:HG11	1:A:124:TRP:CE2	2.45	0.52
1:A:235:TYR:O	1:A:236:LYS:C	2.53	0.52
1:A:5:ILE:C	1:A:35:VAL:HG12	2.34	0.52
1:A:290:MET:HE1	1:A:376:LEU:HD11	1.90	0.52
1:B:98:THR:O	1:B:102:ILE:HG13	2.10	0.52
1:B:12:GLU:CB	1:B:39:LEU:HD11	2.40	0.52
1:B:68:ASN:ND2	1:B:301:LYS:HE2	2.25	0.52
1:A:83:VAL:HG23	1:A:88:LEU:HG	1.91	0.52
1:A:191:ASP:HB3	1:A:298:PRO:HB3	1.90	0.52
1:B:68:ASN:HA	1:B:302:THR:HG23	1.92	0.52
1:B:364:ILE:O	1:B:368:GLU:HG3	2.10	0.52
1:A:152:VAL:HA	1:B:155:THR:O	2.10	0.52
1:B:46:ILE:HG21	1:B:86:PHE:CD2	2.44	0.51
1:A:364:ILE:HG22	1:A:368:GLU:OE2	2.10	0.51
1:A:11:VAL:HG11	1:A:64:ILE:CD1	2.40	0.51
1:A:392:LEU:HD23	1:A:396:GLU:C	2.35	0.51
1:B:72:LYS:NZ	1:B:73:CYS:O	2.41	0.51
1:B:96:ASN:OD1	2:B:501:A1EOQ:O3	2.27	0.51
1:B:208:TYR:HH	1:B:245:TRP:HZ2	1.56	0.51
1:B:226:ILE:O	1:B:230:ILE:HG13	2.11	0.51
1:B:349:ASN:O	1:B:352:LEU:N	2.44	0.51
1:B:7:GLY:HA3	1:B:37:LEU:CD1	2.41	0.51
1:B:50:ASP:OD1	1:B:92:TRP:HH2	1.93	0.51
1:A:22:ILE:HD12	1:A:329:PRO:HB3	1.93	0.51
1:A:170:HIS:HB2	1:B:183:TYR:CD1	2.45	0.51
1:A:213:ASN:OD1	1:A:248:HIS:CE1	2.63	0.51
1:A:249:ARG:HG2	1:A:249:ARG:HH11	1.75	0.51
1:B:303:VAL:HB	1:B:342:HIS:HD2	1.76	0.51
1:A:109:ARG:HE	1:A:293:SER:HB2	1.76	0.51
1:A:29:LYS:HD3	1:A:399:ASP:OD1	2.11	0.51
1:A:82:ARG:NH1	1:A:85:GLU:OE1	2.43	0.51
1:A:120:LEU:HD13	1:B:259:MET:O	2.11	0.51
1:A:139:TYR:OH	1:A:275:ASP:OD2	2.28	0.51
1:A:343:ARG:HD2	1:A:347:ASP:OD2	2.10	0.51
1:B:46:ILE:CG2	1:B:86:PHE:CE2	2.93	0.51
1:A:6:SER:OG	1:A:36:GLU:O	2.25	0.50
1:A:112:ILE:HD11	1:A:292:THR:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:ARG:O	1:B:318:MET:HG3	2.11	0.50
1:B:26:ILE:HG22	1:B:31:ILE:HG12	1.93	0.50
1:B:403:GLU:O	1:B:407:ILE:HG13	2.10	0.50
1:A:72:LYS:HE2	1:A:75:THR:CG2	2.40	0.50
1:B:117:ILE:HD12	1:B:376:LEU:HD22	1.92	0.50
1:A:15:GLY:O	1:A:20:ARG:HB2	2.11	0.50
1:B:141:ALA:HB1	1:B:181:GLY:O	2.12	0.50
1:B:382:GLY:O	1:B:386:VAL:HG13	2.12	0.50
1:A:141:ALA:HB2	1:A:182:MET:HB3	1.94	0.50
1:B:193:ALA:HA	1:B:227:PHE:HE1	1.76	0.50
1:A:388:ARG:HG3	1:A:388:ARG:HH11	1.77	0.50
1:B:16:ASP:OD1	1:B:45:GLY:HA2	2.11	0.49
1:B:293:SER:HB3	1:B:308:ALA:HB2	1.93	0.49
1:A:70:GLY:O	1:A:304:GLU:HA	2.12	0.49
1:A:144:PHE:HA	1:B:218:LYS:HD2	1.93	0.49
1:A:199:MET:HG3	1:A:266:ILE:HD12	1.92	0.49
1:B:27:LYS:HA	1:B:31:ILE:HB	1.95	0.49
1:B:133:HIS:CD2	1:B:135:TYR:H	2.31	0.49
1:A:149:PRO:HB2	1:B:159:SER:CB	2.43	0.49
1:A:180:MET:SD	1:B:216:LEU:HD22	2.53	0.49
1:A:215:ILE:HD11	2:B:501:A1EOQ:O6	2.11	0.49
1:B:95:PRO:O	1:B:99:ILE:HG13	2.12	0.49
1:B:111:ALA:CA	1:B:291:MET:HG3	2.33	0.49
1:B:250:LEU:O	1:B:253:ASP:HB2	2.12	0.49
1:A:283:GLN:O	1:A:283:GLN:NE2	2.35	0.49
1:A:374:LYS:HG3	1:A:391:TYR:CE2	2.48	0.49
1:B:108:PHE:HE2	1:B:296:VAL:CG2	2.26	0.49
1:B:227:PHE:HD2	1:B:246:TYR:OH	1.95	0.49
1:B:231:TYR:CE1	1:B:246:TYR:HB3	2.47	0.49
1:A:349:ASN:O	1:A:352:LEU:N	2.44	0.49
1:A:133:HIS:O	1:A:271:ASN:HA	2.13	0.49
1:A:217:LYS:O	1:A:221:GLY:HA3	2.12	0.49
1:B:96:ASN:HB2	1:B:100:ARG:HH11	1.77	0.49
1:B:121:VAL:HG21	1:B:124:TRP:CZ2	2.47	0.49
1:B:245:TRP:CD1	1:B:247:GLU:HG3	2.48	0.49
1:A:143:ASP:HB2	1:B:219:TYR:HB2	1.95	0.48
1:A:235:TYR:O	1:A:238:GLN:N	2.46	0.48
1:B:72:LYS:HZ1	1:B:75:THR:HG23	1.77	0.48
1:B:212:LYS:HZ3	1:B:250:LEU:HD21	1.77	0.48
1:B:337:THR:HG21	1:B:359:LEU:HB3	1.94	0.48
1:A:214:THR:CG2	1:A:250:LEU:HD21	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:330:ILE:HD12	1:A:363:SER:HB3	1.94	0.48
1:B:24:GLU:OE2	1:B:27:LYS:NZ	2.45	0.48
1:B:334:PHE:HA	1:B:337:THR:OG1	2.13	0.48
1:B:46:ILE:CD1	1:B:88:LEU:HD11	2.43	0.48
1:B:13:MET:CE	1:B:64:ILE:CD1	2.91	0.48
1:B:106:THR:HB	1:B:108:PHE:CE2	2.49	0.48
1:B:26:ILE:HG12	1:B:333:ILE:CG1	2.44	0.48
1:B:50:ASP:HA	1:B:92:TRP:CZ3	2.48	0.48
1:A:361:GLU:OE1	1:A:408:LYS:NZ	2.41	0.48
1:B:129:ILE:HD12	1:B:266:ILE:HD11	1.95	0.48
1:A:5:ILE:O	1:A:35:VAL:HG12	2.14	0.48
1:A:11:VAL:HB	1:A:64:ILE:CD1	2.44	0.48
1:B:235:TYR:O	1:B:236:LYS:C	2.57	0.48
1:A:7:GLY:HA2	1:A:349:ASN:HD22	1.79	0.48
1:B:10:VAL:HG23	1:B:69:VAL:CG1	2.41	0.48
1:B:254:MET:HE2	1:B:254:MET:HB2	1.81	0.48
1:A:16:ASP:OD1	1:A:16:ASP:N	2.45	0.48
1:A:79:ASP:HA	1:A:91:MET:SD	2.54	0.48
1:B:17:GLU:CD	1:B:76:ILE:HD11	2.39	0.48
1:B:40:HIS:CE1	1:B:67:HIS:NE2	2.82	0.48
1:B:112:ILE:HG22	1:B:364:ILE:HD11	1.96	0.48
1:A:24:GLU:OE2	1:A:27:LYS:NZ	2.28	0.47
1:A:157:THR:HB	1:B:151:LYS:HG2	1.96	0.47
1:B:127:PRO:HD2	1:B:205:TRP:CH2	2.48	0.47
1:B:138:GLN:OE1	1:B:272:TYR:HB2	2.14	0.47
1:A:154:ILE:HA	1:B:153:GLU:O	2.14	0.47
1:A:201:LEU:HD21	1:A:239:PHE:CE1	2.49	0.47
1:A:69:VAL:HG12	1:A:69:VAL:O	2.15	0.47
1:A:291:MET:HE3	1:A:308:ALA:CB	2.45	0.47
1:A:359:LEU:HD13	1:A:405:LEU:HD22	1.96	0.47
1:A:199:MET:HE1	1:A:203:LYS:HE3	1.97	0.47
1:B:50:ASP:OD1	1:B:92:TRP:CH2	2.67	0.47
1:A:19:THR:OG1	1:A:311:THR:HG22	2.13	0.47
1:A:388:ARG:HG3	1:A:388:ARG:NH1	2.30	0.47
1:B:22:ILE:C	1:B:26:ILE:HD12	2.37	0.47
1:B:31:ILE:O	1:B:35:VAL:HG22	2.14	0.47
1:B:110:GLU:O	1:B:291:MET:HG2	2.15	0.47
1:B:227:PHE:CD2	1:B:246:TYR:OH	2.67	0.47
1:B:367:ILE:HG23	1:B:372:MET:HE2	1.97	0.47
1:B:121:VAL:HG21	1:B:124:TRP:CH2	2.49	0.47
1:B:376:LEU:HD23	1:B:376:LEU:HA	1.66	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LEU:HD23	1:A:409:LEU:HA	1.64	0.47
1:B:144:PHE:CE2	1:B:179:ALA:HB3	2.49	0.47
1:B:383:LEU:O	1:B:383:LEU:HD12	2.15	0.47
1:A:12:GLU:OE1	1:A:14:GLN:OE1	2.33	0.47
1:A:162:THR:CG2	1:A:163:GLN:H	2.19	0.47
1:B:173:GLU:O	1:B:174:GLU:CB	2.63	0.47
1:A:155:THR:HG21	1:A:164:LYS:HD3	1.96	0.46
1:B:96:ASN:OD1	1:B:96:ASN:N	2.47	0.46
1:B:393:ASN:CG	1:B:396:GLU:HG3	2.39	0.46
1:A:110:GLU:HG3	1:A:129:ILE:HD13	1.97	0.46
1:A:213:ASN:O	1:A:217:LYS:HD2	2.15	0.46
1:A:393:ASN:OD1	1:A:396:GLU:CG	2.45	0.46
1:B:120:LEU:HD23	1:B:120:LEU:HA	1.58	0.46
1:B:197:PHE:CE1	1:B:231:TYR:HB2	2.49	0.46
1:B:231:TYR:CD1	1:B:246:TYR:HB3	2.51	0.46
1:A:82:ARG:HH11	1:A:86:PHE:HE1	1.63	0.46
1:A:130:ILE:HD11	1:A:281:VAL:HG21	1.96	0.46
1:B:108:PHE:CE2	1:B:296:VAL:HG21	2.50	0.46
1:A:5:ILE:CB	1:A:35:VAL:HG12	2.42	0.46
1:B:64:ILE:O	1:B:68:ASN:N	2.41	0.46
1:B:365:GLU:OE2	1:B:408:LYS:HE3	2.15	0.46
1:B:125:VAL:HG23	1:B:126:LYS:HG2	1.98	0.46
1:B:378:ALA:HA	1:B:386:VAL:HG11	1.98	0.46
1:A:11:VAL:HG11	1:A:64:ILE:HD13	1.97	0.46
1:A:208:TYR:HA	1:A:247:GLU:O	2.16	0.46
1:A:269:CYS:HB3	1:A:273:ASP:HB3	1.97	0.46
1:A:114:CYS:HB2	1:A:117:ILE:HG12	1.96	0.46
1:B:22:ILE:HD11	1:B:327:THR:HG21	1.95	0.46
1:B:71:VAL:O	1:B:71:VAL:HG23	2.16	0.46
1:B:129:ILE:HD12	1:B:266:ILE:CD1	2.46	0.46
1:B:252:ASP:HA	1:B:255:VAL:HG22	1.98	0.46
1:A:140:ARG:O	1:A:140:ARG:HG3	2.15	0.45
1:A:269:CYS:HB3	1:A:273:ASP:CB	2.46	0.45
1:A:303:VAL:HG11	1:A:342:HIS:CG	2.51	0.45
1:B:151:LYS:HG3	1:B:151:LYS:O	2.16	0.45
1:B:173:GLU:O	1:B:174:GLU:HB2	2.16	0.45
1:B:211:THR:O	1:B:250:LEU:HA	2.16	0.45
1:B:212:LYS:HZ2	1:B:250:LEU:HD21	1.80	0.45
1:B:350:LYS:HA	1:B:350:LYS:HD3	1.63	0.45
1:A:31:ILE:C	1:A:33:PRO:HD2	2.42	0.45
1:A:154:ILE:HG21	1:B:144:PHE:HE1	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ASP:OD2	1:B:76:ILE:N	2.49	0.45
1:B:130:ILE:HD12	1:B:278:SER:CA	2.45	0.45
1:A:78:PRO:O	1:A:91:MET:HG2	2.16	0.45
1:A:249:ARG:HG2	1:A:249:ARG:NH1	2.32	0.45
1:A:381:LYS:CD	1:A:385:ASN:O	2.60	0.45
1:B:112:ILE:CG2	1:B:364:ILE:HD11	2.47	0.45
1:B:213:ASN:HD22	1:B:224:LYS:HD3	1.80	0.45
1:B:83:VAL:CG2	1:B:91:MET:CG	2.94	0.45
1:B:193:ALA:O	1:B:197:PHE:CD2	2.70	0.45
1:A:83:VAL:HG13	1:A:84:GLU:N	2.32	0.45
1:A:86:PHE:CD1	1:A:86:PHE:N	2.85	0.45
1:A:135:TYR:OH	1:A:183:TYR:CE2	2.50	0.45
1:B:212:LYS:HB2	1:B:251:ILE:HG22	1.99	0.45
1:A:132:ARG:HD2	1:A:274:GLY:C	2.42	0.45
1:A:303:VAL:HG11	1:A:342:HIS:CD2	2.52	0.45
1:B:269:CYS:HB3	1:B:274:GLY:CA	2.46	0.45
1:A:17:GLU:HA	1:A:316:TYR:CE1	2.51	0.45
1:A:201:LEU:HD21	1:A:239:PHE:CD1	2.51	0.45
1:B:203:LYS:HE3	1:B:203:LYS:CA	2.46	0.45
1:B:292:THR:HG22	1:B:334:PHE:HB3	2.00	0.45
1:A:343:ARG:O	1:A:343:ARG:HD3	2.17	0.44
1:A:8:GLY:O	1:A:37:LEU:HB2	2.17	0.44
1:B:100:ARG:HB3	1:B:134:ALA:HB1	1.99	0.44
1:A:21:ILE:HG21	1:A:319:TYR:CE2	2.52	0.44
1:A:71:VAL:CG1	1:A:339:GLY:HA3	2.47	0.44
1:A:144:PHE:HE2	1:B:154:ILE:CD1	2.31	0.44
1:B:108:PHE:HE2	1:B:296:VAL:HG21	1.81	0.44
1:A:153:GLU:HB3	1:A:167:TYR:O	2.18	0.44
1:B:110:GLU:C	1:B:291:MET:HG2	2.42	0.44
1:A:238:GLN:O	1:A:241:ALA:HB3	2.17	0.44
1:B:11:VAL:O	1:B:70:GLY:HA2	2.18	0.44
1:A:128:ILE:HG13	1:A:285:TYR:OH	2.18	0.44
1:A:290:MET:CE	1:A:328:ASN:HD21	2.29	0.44
1:A:337:THR:CG2	1:A:359:LEU:HD23	2.33	0.44
1:A:149:PRO:HB2	1:B:159:SER:HB3	2.00	0.44
1:A:201:LEU:CD2	1:A:239:PHE:CE1	3.01	0.44
1:A:303:VAL:CG1	1:A:342:HIS:CD2	3.01	0.44
1:A:14:GLN:HB2	1:A:43:ASP:HA	2.00	0.43
1:A:55:GLN:HG3	1:A:59:ASP:OD2	2.18	0.43
1:B:201:LEU:HD22	1:B:242:GLN:OE1	2.18	0.43
1:A:109:ARG:HA	1:A:292:THR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:LEU:HD12	1:B:405:LEU:HD22	2.00	0.43
1:B:145:VAL:CG1	1:B:146:VAL:N	2.81	0.43
1:A:18:MET:HB3	1:A:312:VAL:CG2	2.43	0.43
1:A:152:VAL:HG13	1:B:155:THR:O	2.18	0.43
1:B:17:GLU:O	1:B:20:ARG:N	2.48	0.43
1:B:302:THR:O	1:B:303:VAL:HG23	2.18	0.43
1:A:7:GLY:HA3	1:A:343:ARG:HG3	2.01	0.43
1:A:194:HIS:CE1	1:A:230:ILE:HD13	2.53	0.43
1:A:362:VAL:HG12	1:A:401:LEU:HD23	1.99	0.43
1:B:76:ILE:CG1	1:B:311:THR:HG21	2.48	0.43
1:A:288:LEU:HD22	1:B:256:ALA:HB1	2.01	0.43
1:B:34:TYR:CD2	1:B:409:LEU:HD12	2.54	0.43
1:B:269:CYS:HB3	1:B:274:GLY:N	2.34	0.43
1:A:11:VAL:HB	1:A:64:ILE:HD12	2.01	0.43
1:B:156:TYR:CD1	1:B:157:THR:N	2.87	0.43
1:B:16:ASP:OD1	1:B:46:ILE:N	2.42	0.43
1:B:383:LEU:O	1:B:386:VAL:HG22	2.19	0.43
1:A:11:VAL:CG1	1:A:64:ILE:CD1	2.97	0.42
1:B:93:LYS:CD	1:B:98:THR:OG1	2.64	0.42
1:A:65:LYS:CG	1:A:103:LEU:CD2	2.96	0.42
1:A:110:GLU:CB	1:A:129:ILE:HD13	2.48	0.42
1:A:147:PRO:HD2	1:B:156:TYR:OH	2.19	0.42
1:B:162:THR:HG22	1:B:163:GLN:N	2.27	0.42
1:A:110:GLU:CG	1:A:129:ILE:HD13	2.49	0.42
1:B:76:ILE:HD13	1:B:82:ARG:HH12	1.83	0.42
1:B:108:PHE:CE2	1:B:296:VAL:CG2	3.02	0.42
1:A:20:ARG:O	1:A:23:TRP:HB3	2.20	0.42
1:A:192:PHE:CZ	1:A:268:ALA:HB1	2.54	0.42
1:A:277:GLN:O	1:A:281:VAL:HG23	2.19	0.42
1:B:26:ILE:HG12	1:B:333:ILE:HG13	2.01	0.42
1:B:67:HIS:O	1:B:68:ASN:CB	2.68	0.42
1:A:392:LEU:HG	1:A:396:GLU:HB3	2.01	0.42
1:B:67:HIS:O	1:B:68:ASN:HB2	2.20	0.42
1:B:383:LEU:N	1:B:384:PRO:HD2	2.35	0.42
1:A:115:LYS:HG3	1:A:368:GLU:CD	2.44	0.42
1:A:355:PHE:HD1	1:A:409:LEU:HD11	1.85	0.42
1:A:255:VAL:HG13	1:A:256:ALA:N	2.35	0.42
1:A:340:LEU:O	1:A:352:LEU:HD21	2.20	0.42
1:B:38:ASP:CG	1:B:40:HIS:HE2	2.28	0.42
1:B:52:THR:O	1:B:53:ASN:C	2.63	0.42
1:B:233:LYS:HD3	1:B:234:GLN:CG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:CG2	1:B:280:SER:HB2	2.47	0.42
1:A:281:VAL:O	1:A:285:TYR:HD1	2.03	0.42
1:B:397:PHE:CZ	1:B:401:LEU:HD11	2.55	0.42
1:A:320:GLN:C	1:A:321:LYS:HD2	2.44	0.42
1:B:180:MET:CE	1:B:182:MET:HE2	2.48	0.42
1:A:7:GLY:N	1:A:352:LEU:HD13	2.34	0.41
1:A:32:PHE:N	1:A:33:PRO:CD	2.83	0.41
1:A:140:ARG:O	1:A:183:TYR:HE1	2.03	0.41
1:A:216:LEU:HD23	1:A:216:LEU:N	2.35	0.41
1:B:29:LYS:HB3	1:B:30:LEU:CD2	2.50	0.41
1:B:76:ILE:HG21	1:B:82:ARG:HH11	1.84	0.41
1:B:393:ASN:OD1	1:B:395:PHE:N	2.53	0.41
1:A:155:THR:HG22	1:A:156:TYR:N	2.36	0.41
1:A:194:HIS:HE1	1:A:230:ILE:HD13	1.85	0.41
1:A:295:LEU:HD23	1:A:295:LEU:C	2.46	0.41
1:A:321:LYS:N	1:A:321:LYS:CD	2.83	0.41
1:A:243:LYS:HE3	1:A:243:LYS:HB2	1.85	0.41
1:B:145:VAL:HG12	1:B:146:VAL:N	2.36	0.41
1:B:87:LYS:HD2	1:B:87:LYS:HA	1.84	0.41
1:B:243:LYS:HD3	1:B:243:LYS:N	2.35	0.41
1:A:16:ASP:OD2	1:A:76:ILE:HD12	2.20	0.41
1:A:110:GLU:OE2	1:A:129:ILE:CD1	2.69	0.41
1:B:46:ILE:CG2	1:B:86:PHE:CD2	3.03	0.41
1:B:293:SER:CB	1:B:308:ALA:HB2	2.50	0.41
1:B:393:ASN:OD1	1:B:393:ASN:C	2.62	0.41
1:B:26:ILE:HG12	1:B:333:ILE:HG12	2.03	0.41
1:A:23:TRP:CD2	1:A:73:CYS:HB2	2.56	0.41
1:A:129:ILE:HB	1:A:266:ILE:HD13	2.03	0.41
1:A:180:MET:O	1:B:181:GLY:HA2	2.20	0.41
1:A:261:SER:OG	1:A:262:GLU:N	2.53	0.41
1:B:28:GLU:O	1:B:33:PRO:CG	2.68	0.41
1:B:387:GLN:N	1:B:390:ASP:OD2	2.52	0.41
1:A:28:GLU:O	1:A:33:PRO:CD	2.61	0.41
1:A:144:PHE:HE2	1:B:154:ILE:HD13	1.85	0.41
1:B:76:ILE:HG21	1:B:82:ARG:NH1	2.36	0.41
1:B:376:LEU:O	1:B:379:CYS:HB2	2.21	0.41
1:A:15:GLY:O	1:A:20:ARG:HD2	2.22	0.40
1:A:146:VAL:HG12	1:A:176:GLY:HA2	2.03	0.40
1:A:328:ASN:OD1	1:A:328:ASN:C	2.64	0.40
1:B:22:ILE:CG2	1:B:329:PRO:HB3	2.51	0.40
1:B:36:GLU:O	1:B:37:LEU:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:GLN:O	1:B:243:LYS:HB2	2.21	0.40
1:B:259:MET:HE2	1:B:259:MET:HB2	1.90	0.40
1:B:372:MET:HE2	1:B:372:MET:HB3	1.74	0.40
1:A:65:LYS:HG3	1:A:103:LEU:HD21	2.01	0.40
1:A:293:SER:HB3	1:A:308:ALA:HB2	2.02	0.40
1:A:321:LYS:HD2	1:A:321:LYS:N	2.37	0.40
1:B:78:PRO:O	1:B:91:MET:HE3	2.21	0.40
1:A:270:LYS:O	1:A:271:ASN:C	2.64	0.40
1:B:165:VAL:HG11	1:B:167:TYR:OH	2.21	0.40
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.37	0.40
1:A:269:CYS:HB2	1:A:274:GLY:CA	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	409/443 (92%)	376 (92%)	30 (7%)	3 (1%)	18 46
1	B	409/443 (92%)	383 (94%)	24 (6%)	2 (0%)	24 54
All	All	818/886 (92%)	759 (93%)	54 (7%)	5 (1%)	21 49

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	174	GLU
1	B	174	GLU
1	A	68	ASN
1	B	68	ASN
1	A	382	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	347/372 (93%)	344 (99%)	3 (1%)	70	78
1	B	347/372 (93%)	346 (100%)	1 (0%)	86	85
All	All	694/744 (93%)	690 (99%)	4 (1%)	78	81

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	381	LYS
1	A	393	ASN
1	B	94	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	67	HIS
1	A	101	ASN
1	A	309	HIS
1	A	393	ASN
1	B	48	ASN
1	B	67	HIS
1	B	385	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	A1EOQ	A	501	-	19,19,19	2.75	7 (36%)	25,27,27	2.02	7 (28%)
2	A1EOQ	B	501	-	19,19,19	2.77	7 (36%)	25,27,27	1.75	5 (20%)

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	A1EOQ	A	501	-	-	2/6/35/35	0/2/2/2
2	A1EOQ	B	501	-	-	1/6/35/35	0/2/2/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	A1EOQ	O06-C17	-9.49	1.27	1.45
2	B	501	A1EOQ	O06-C17	-9.30	1.27	1.45
2	B	501	A1EOQ	O06-C18	3.53	1.47	1.35
2	A	501	A1EOQ	O06-C18	3.32	1.47	1.35
2	B	501	A1EOQ	O1-C14	-3.10	1.40	1.44
2	A	501	A1EOQ	O1-C14	-2.92	1.40	1.44
2	B	501	A1EOQ	C16-C18	-2.58	1.45	1.50
2	A	501	A1EOQ	O5-C1	2.47	1.48	1.41
2	B	501	A1EOQ	O5-C1	2.40	1.48	1.41
2	A	501	A1EOQ	C16-C14	-2.34	1.49	1.52
2	A	501	A1EOQ	C3-C2	-2.27	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	A1EOQ	C16-C14	-2.19	1.49	1.52
2	B	501	A1EOQ	O3-C3	2.08	1.47	1.43
2	A	501	A1EOQ	O3-C3	2.06	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	A1EOQ	C1-O1-C14	-5.99	102.66	114.88
2	B	501	A1EOQ	C1-O1-C14	-4.58	105.53	114.88
2	A	501	A1EOQ	C3-C4-C5	4.33	117.96	110.24
2	B	501	A1EOQ	C3-C4-C5	3.64	116.74	110.24
2	B	501	A1EOQ	O06-C18-C16	-3.04	106.48	110.50
2	A	501	A1EOQ	O5-C5-C4	2.92	114.99	109.69
2	A	501	A1EOQ	O06-C18-C16	-2.86	106.72	110.50
2	A	501	A1EOQ	C6-C5-C4	-2.57	106.99	113.00
2	B	501	A1EOQ	C1-O5-C5	-2.48	108.81	113.69
2	A	501	A1EOQ	O08-C18-C16	2.35	132.08	128.98
2	A	501	A1EOQ	O06-C17-C14	2.34	107.57	104.63
2	B	501	A1EOQ	C6-C5-C4	-2.24	107.76	113.00

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	A1EOQ	O5-C5-C6-O6
2	A	501	A1EOQ	C4-C5-C6-O6
2	B	501	A1EOQ	C17-C14-O1-C1

There are no ring outliers.

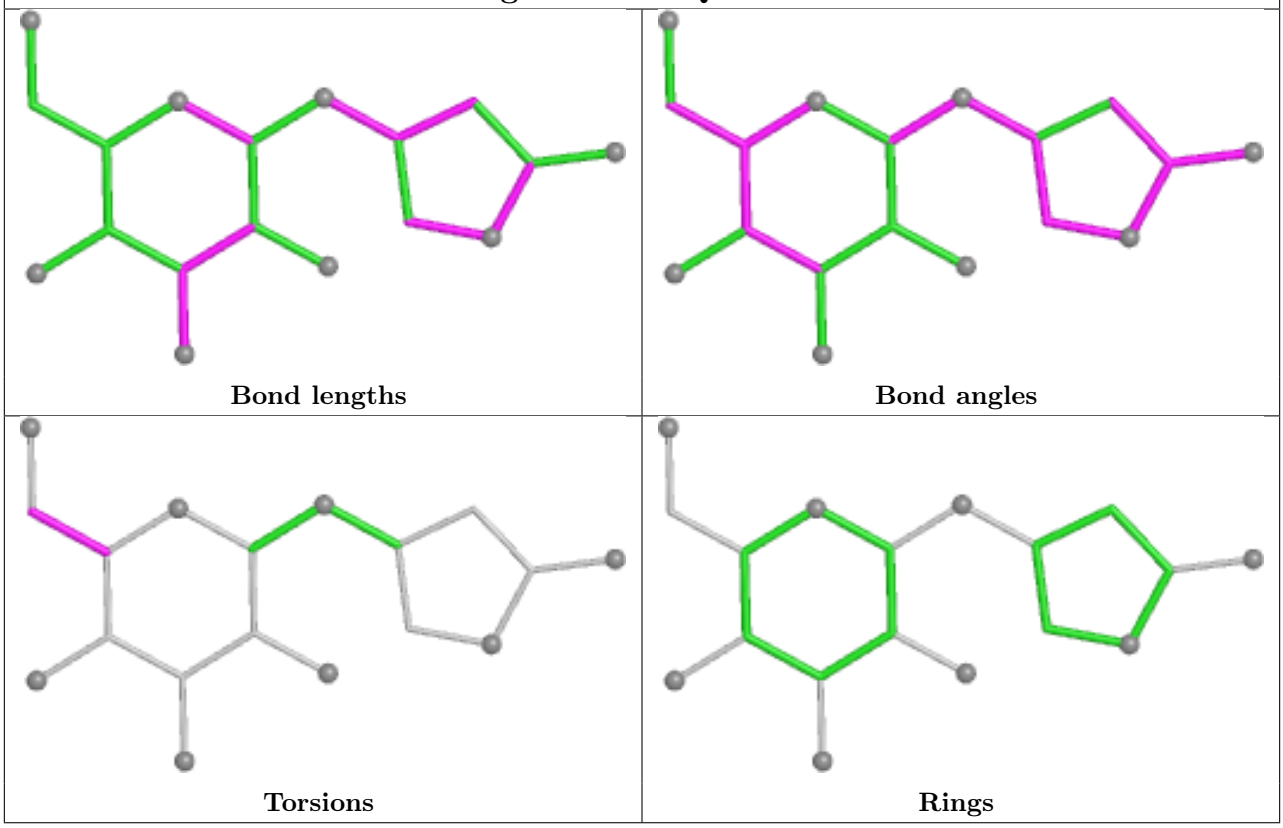
1 monomer is involved in 2 short contacts:

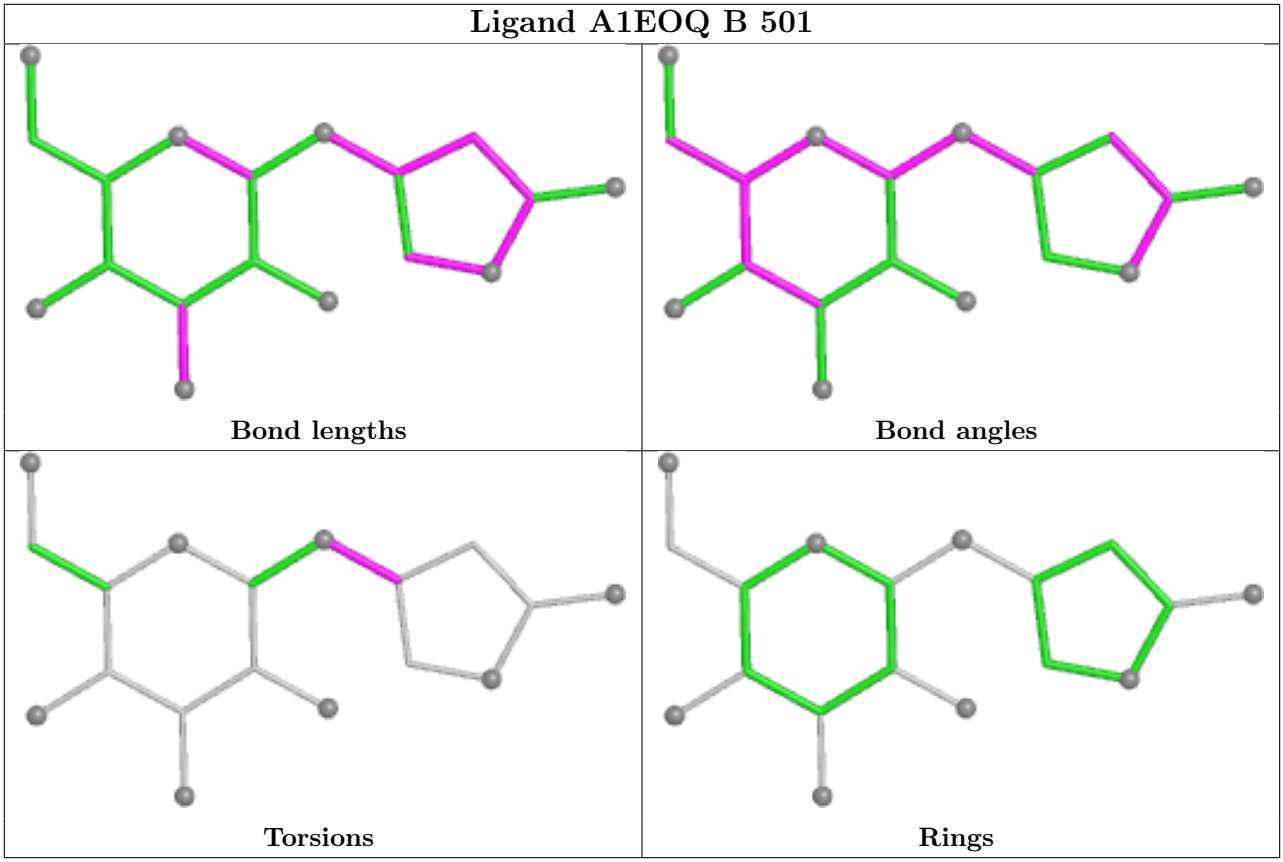
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501	A1EOQ	2	0

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 A1EOQ A 501





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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	411/443 (92%)	0.55	12 (2%)	53	31	32, 66, 96, 107	0
1	B	411/443 (92%)	0.51	9 (2%)	62	40	33, 58, 93, 119	0
All	All	822/886 (92%)	0.53	21 (2%)	57	34	32, 63, 95, 119	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	309	HIS	3.8
1	A	51	ALA	3.7
1	A	154	ILE	3.3
1	B	223	PHE	3.1
1	A	240	GLU	2.8
1	B	107	VAL	2.7
1	B	308	ALA	2.6
1	A	152	VAL	2.5
1	A	308	ALA	2.5
1	B	152	VAL	2.5
1	B	273	ASP	2.4
1	A	205	TRP	2.3
1	A	166	THR	2.3
1	A	96	ASN	2.2
1	B	47	GLU	2.1
1	A	146	VAL	2.1
1	B	96	ASN	2.1
1	A	309	HIS	2.1
1	A	175	GLY	2.1
1	B	227	PHE	2.1
1	A	53	ASN	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 oligosaccharides in this entry.

6.4 Ligands (i)

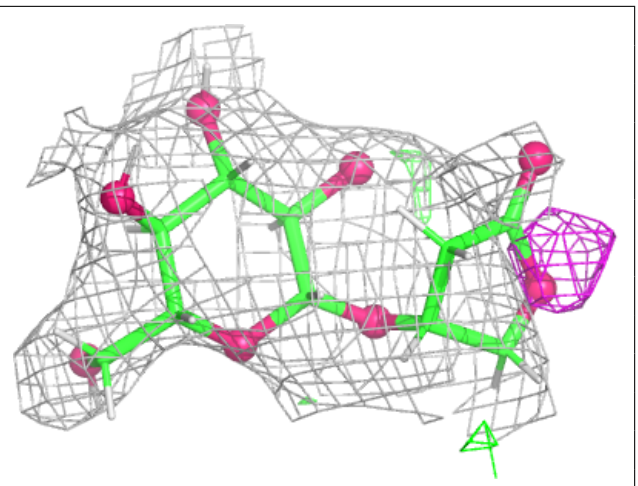
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

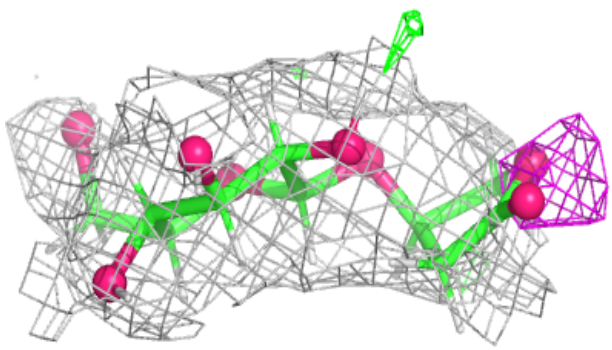
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	A1EOQ	B	501	18/18	0.61	0.15	73,91,113,121	0
2	A1EOQ	A	501	18/18	0.64	0.14	73,85,104,107	0

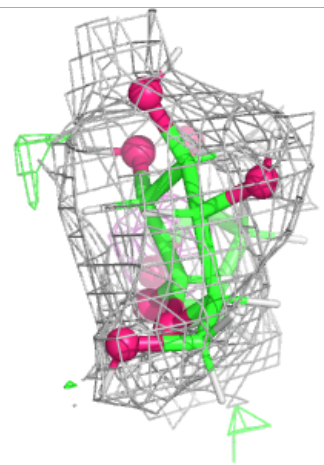
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

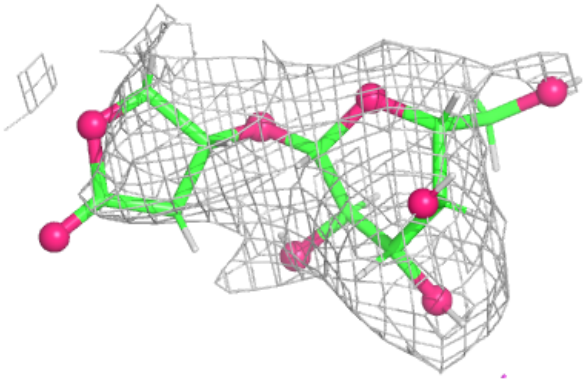
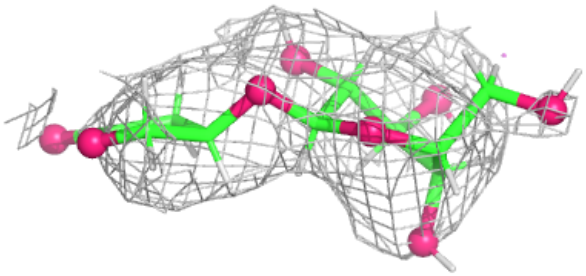
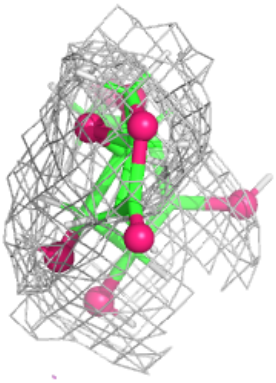
Electron density around A1EOQ B 501:

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







Electron density around A1EOQ A 501: $2mF_o$-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.