Full wwPDB X-ray Structure Validation Report (i)

Aug 27, 2023 – 09:24 AM EDT

PDB ID	:	3IL5
Title	:	Structure of E. faecalis FabH in complex with 2-({4-bromo-3-[(diethylamino) sulfonyl]benzoyl}amino)benzoic acid
Authors	:	Gajiwala, K.S.; Margosiak, S.; Lu, J.; Cortez, J.; Su, Y.; Nie, Z.; Appelt, K.
Deposited on	:	2009-08-06
Resolution	:	2.60 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:

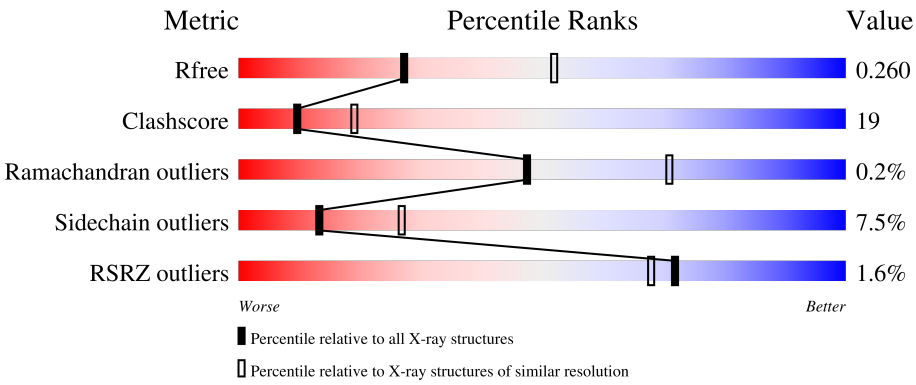
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.60 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

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	343	63% 28% • 7%
1	B	343	% 57% 31% 6% 7%
1	C	343	% 59% 33% • 7%
1	D	343	4% 55% 34% • 7%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 10074 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 3-oxoacyl-[acyl-carrier-protein] synthase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	320	2461	1548	419	482	12	0	0	0
1	B	319	2455	1545	418	480	12	0	0	0
1	C	320	2461	1548	419	482	12	0	0	0
1	D	320	2461	1548	419	482	12	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q820T1
A	-14	GLY	-	expression tag	UNP Q820T1
A	-13	SER	-	expression tag	UNP Q820T1
A	-12	SER	-	expression tag	UNP Q820T1
A	-11	HIS	-	expression tag	UNP Q820T1
A	-10	HIS	-	expression tag	UNP Q820T1
A	-9	HIS	-	expression tag	UNP Q820T1
A	-8	HIS	-	expression tag	UNP Q820T1
A	-7	HIS	-	expression tag	UNP Q820T1
A	-6	HIS	-	expression tag	UNP Q820T1
A	-5	SER	-	expression tag	UNP Q820T1
A	-4	SER	-	expression tag	UNP Q820T1
A	-3	GLY	-	expression tag	UNP Q820T1
A	-2	LEU	-	expression tag	UNP Q820T1
A	-1	VAL	-	expression tag	UNP Q820T1
A	0	PRO	-	expression tag	UNP Q820T1
A	1	ARG	-	expression tag	UNP Q820T1
A	2	GLY	-	expression tag	UNP Q820T1
A	3	SER	-	expression tag	UNP Q820T1
A	4	HIS	-	expression tag	UNP Q820T1
A	326	GLU	-	expression tag	UNP Q820T1

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Chain	Residue	Modelled	Actual	Comment	Reference
A	327	PHE	-	expression tag	UNP Q820T1
B	-15	MET	-	expression tag	UNP Q820T1
B	-14	GLY	-	expression tag	UNP Q820T1
B	-13	SER	-	expression tag	UNP Q820T1
B	-12	SER	-	expression tag	UNP Q820T1
B	-11	HIS	-	expression tag	UNP Q820T1
B	-10	HIS	-	expression tag	UNP Q820T1
B	-9	HIS	-	expression tag	UNP Q820T1
B	-8	HIS	-	expression tag	UNP Q820T1
B	-7	HIS	-	expression tag	UNP Q820T1
B	-6	HIS	-	expression tag	UNP Q820T1
B	-5	SER	-	expression tag	UNP Q820T1
B	-4	SER	-	expression tag	UNP Q820T1
B	-3	GLY	-	expression tag	UNP Q820T1
B	-2	LEU	-	expression tag	UNP Q820T1
B	-1	VAL	-	expression tag	UNP Q820T1
B	0	PRO	-	expression tag	UNP Q820T1
B	1	ARG	-	expression tag	UNP Q820T1
B	2	GLY	-	expression tag	UNP Q820T1
B	3	SER	-	expression tag	UNP Q820T1
B	4	HIS	-	expression tag	UNP Q820T1
B	326	GLU	-	expression tag	UNP Q820T1
B	327	PHE	-	expression tag	UNP Q820T1
C	-15	MET	-	expression tag	UNP Q820T1
C	-14	GLY	-	expression tag	UNP Q820T1
C	-13	SER	-	expression tag	UNP Q820T1
C	-12	SER	-	expression tag	UNP Q820T1
C	-11	HIS	-	expression tag	UNP Q820T1
C	-10	HIS	-	expression tag	UNP Q820T1
C	-9	HIS	-	expression tag	UNP Q820T1
C	-8	HIS	-	expression tag	UNP Q820T1
C	-7	HIS	-	expression tag	UNP Q820T1
C	-6	HIS	-	expression tag	UNP Q820T1
C	-5	SER	-	expression tag	UNP Q820T1
C	-4	SER	-	expression tag	UNP Q820T1
C	-3	GLY	-	expression tag	UNP Q820T1
C	-2	LEU	-	expression tag	UNP Q820T1
C	-1	VAL	-	expression tag	UNP Q820T1
C	0	PRO	-	expression tag	UNP Q820T1
C	1	ARG	-	expression tag	UNP Q820T1
C	2	GLY	-	expression tag	UNP Q820T1
C	3	SER	-	expression tag	UNP Q820T1

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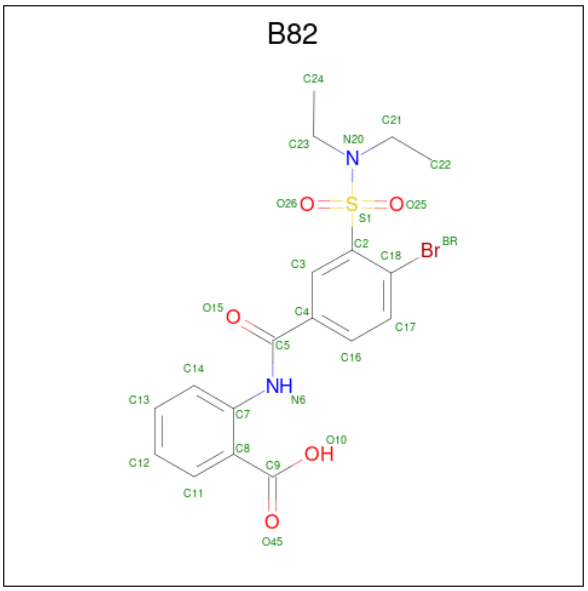
Chain	Residue	Modelled	Actual	Comment	Reference
C	4	HIS	-	expression tag	UNP Q820T1
C	326	GLU	-	expression tag	UNP Q820T1
C	327	PHE	-	expression tag	UNP Q820T1
D	-15	MET	-	expression tag	UNP Q820T1
D	-14	GLY	-	expression tag	UNP Q820T1
D	-13	SER	-	expression tag	UNP Q820T1
D	-12	SER	-	expression tag	UNP Q820T1
D	-11	HIS	-	expression tag	UNP Q820T1
D	-10	HIS	-	expression tag	UNP Q820T1
D	-9	HIS	-	expression tag	UNP Q820T1
D	-8	HIS	-	expression tag	UNP Q820T1
D	-7	HIS	-	expression tag	UNP Q820T1
D	-6	HIS	-	expression tag	UNP Q820T1
D	-5	SER	-	expression tag	UNP Q820T1
D	-4	SER	-	expression tag	UNP Q820T1
D	-3	GLY	-	expression tag	UNP Q820T1
D	-2	LEU	-	expression tag	UNP Q820T1
D	-1	VAL	-	expression tag	UNP Q820T1
D	0	PRO	-	expression tag	UNP Q820T1
D	1	ARG	-	expression tag	UNP Q820T1
D	2	GLY	-	expression tag	UNP Q820T1
D	3	SER	-	expression tag	UNP Q820T1
D	4	HIS	-	expression tag	UNP Q820T1
D	326	GLU	-	expression tag	UNP Q820T1
D	327	PHE	-	expression tag	UNP Q820T1

- Molecule 2 is 2-({[4-bromo-3-(diethylsulfamoyl)phenyl]carbonyl}amino)benzoic acid (three-letter code: B82) (formula: $C_{18}H_{19}BrN_2O_5S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	N	O	S		
2	A	1	27	1	18	2	5	1	0	0
			Total	Br	C	N	O	S		
2	B	1	27	1	18	2	5	1	0	0
			Total	Br	C	N	O	S		
2	C	1	27	1	18	2	5	1	0	0
			Total	Br	C	N	O	S		
2	D	1	27	1	18	2	5	1	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	40	40	40	0	0
			Total	O		
3	B	40	40	40	0	0
			Total	O		
3	C	26	26	26	0	0
			Total	O		
3	D	22	22	22	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: 3-oxoacyl-[acyl-carrier-protein] synthase 3

Chain A: 63% 28% • 7%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET K6 N7 R16 Y17 V18 T24 N25 H26 Q27 L28 S29 D33 T34 I45 R48 R49 I50 V51 T52 S57 H61 L68 K73 Q74 A75 I78 D79 F80

V86 N91 M92 P93 S94 V95 Q98 F109 D112 I113 S114 V121 L124 S125 M126 A127 E128 K129 L132 E145 K149 G165 L170 I171 E172 H178 Q185 G188 W191 G197 Y198 T199 I200 N201 E202 S203 P204 F205 K210 Q211 A212 L216

Q217 M218 R221 S222 I223 F224 D225 F226 A227 I228 Q233 L248 L249 K259 I260 T264 S267 R268 E269 K270 F271 L272 T273 N274 M275 Y278 G279 N280 T281 S282 A283 A284 S285 I286 P287 I288 L289 L290 V294 E295 N296 L299 I300 S303 Q304 Q305 V308 L309 T310

G313 L316 S320 L321 L322 L323 T324 L325 GLU PHE

• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

Chain B: % 57% 31% 6% 7%

MET GLY SER SER HIS HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET K6 N7 Y8 A9 R10 I11 S15 R16 N21 T24 N25 H26 Q27 L28 S29 M32 D33 T34 SER D36 E37 W38 R42 I45 R48 R49 I50 E54 D58

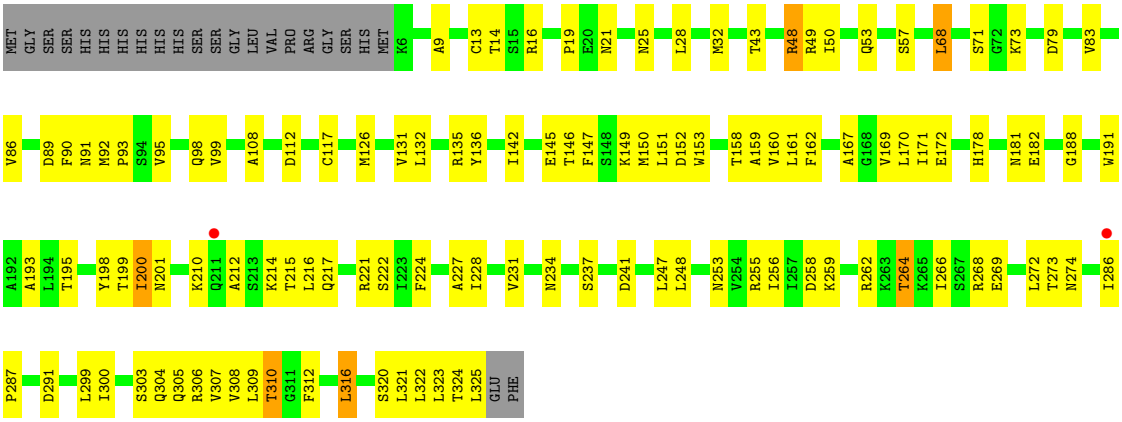
H61 L67 L68 K73 V86 T87 P88 N91 M92 P93 A96 C97 A110 F111 D112 I113 S114 A115 A116 C117 S118 G119 L124 S125 M126 K129 T138 G139 E145 T146 F147 S148 K149 D152 D164 L170 I171 E172 A173 A174 E175 H178 F179 L180 D187

G188 Q189 R190 W191 L194 G197 Y198 T199 I200 N201 F205 Y206 K210 Q211 A212 S213 K214 T215 L216 E219 G220 R221 S222 F226 A227 I228 V231 I235 L247 L248 L249 H250 Q251 A252 N253 V254 R255 K259 I260 T264 K265 I266 S267 R268 E269 K270 F271 L272 T273

N274 M275 G279 S282 I286 P287 I288 L289 L290 V294 I300 S303 Q304 Q305 R306 V307 V308 L309 T310 G311 F312 G313 G314 G315 L316 G319 S320 L321 L322 L323 T324 L325 GLU PHE

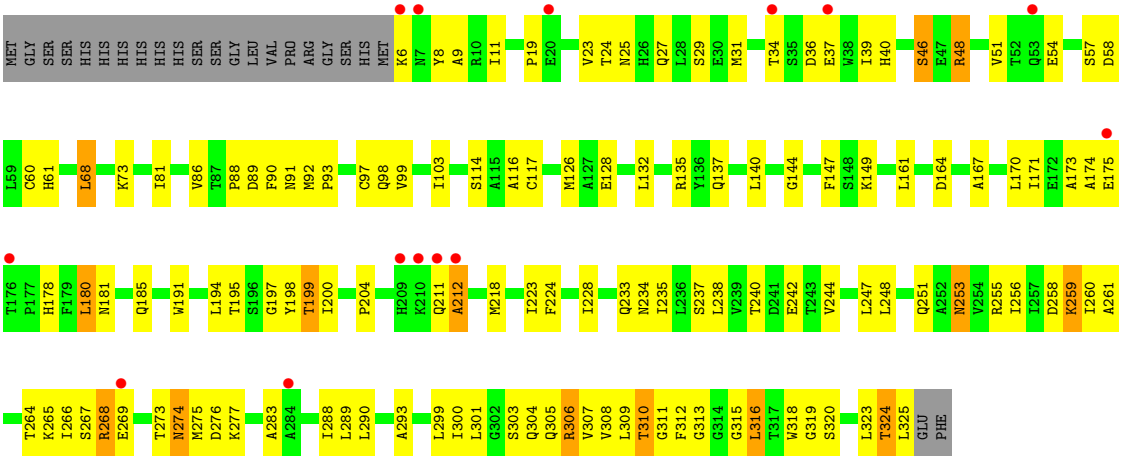
• Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

Chain C: % 59% 33% • 7%



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein] synthase 3

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	66.59Å 84.97Å 114.39Å 90.00° 98.50° 90.00°	Depositor
Resolution (Å)	25.00 – 2.60 24.95 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.4 (25.00-2.60) 94.7 (24.95-2.60)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.07 (at 2.60Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.189 , 0.260 0.191 , 0.260	Depositor DCC
R_{free} test set	3835 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å^2)	39.7	Xtriage
Anisotropy	0.770	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 50.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	10074	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: B82

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	0.34	0/2501	0.52	0/3386
1	B	0.37	0/2494	0.54	0/3375
1	C	0.34	0/2501	0.53	0/3386
1	D	0.32	0/2501	0.52	0/3386
All	All	0.34	0/9997	0.53	0/13533

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	273	THR	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2461	0	2446	93	0
1	B	2455	0	2440	109	0
1	C	2461	0	2446	101	0
1	D	2461	0	2446	118	0
2	A	27	0	18	2	0
2	B	27	0	18	1	0
2	C	27	0	18	1	0
2	D	27	0	18	3	0
3	A	40	0	0	2	0
3	B	40	0	0	2	0
3	C	26	0	0	2	0
3	D	22	0	0	4	0
All	All	10074	0	9850	384	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 19.

All (384) 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:D:211:GLN:HB3	1:D:212:ALA:HB2	1.35	1.09
1:C:200:ILE:HB	1:C:212:ALA:HB2	1.43	1.00
1:D:274:ASN:HB2	1:D:289:LEU:HD13	1.43	0.98
1:C:91:ASN:HB3	1:D:86:VAL:HG22	1.49	0.94
1:A:274:ASN:HB2	1:A:289:LEU:HD13	1.52	0.92
1:A:212:ALA:H	1:C:221:ARG:NH2	1.70	0.88
1:D:306:ARG:HB3	1:D:306:ARG:HH21	1.37	0.87
1:A:200:ILE:HD13	1:A:212:ALA:HB3	1.55	0.86
1:A:300:ILE:H	1:A:305:GLN:HE22	1.20	0.84
1:D:211:GLN:CB	1:D:212:ALA:HB2	2.08	0.83
1:A:126:MET:HB3	1:B:126:MET:HE1	1.61	0.82
1:A:300:ILE:H	1:A:305:GLN:NE2	1.76	0.82
1:C:300:ILE:H	1:C:305:GLN:HE22	1.29	0.81
1:C:178:HIS:HA	1:C:324:THR:HG22	1.62	0.80
1:A:178:HIS:HA	1:A:324:THR:HG22	1.64	0.80
1:C:9:ALA:HB1	1:C:171:ILE:HD11	1.64	0.79
1:C:91:ASN:HD22	1:D:197:GLY:HA3	1.47	0.79
1:D:211:GLN:HB3	1:D:212:ALA:CB	2.12	0.79
1:B:219:GLU:HB3	3:B:362:HOH:O	1.83	0.79
1:A:126:MET:HB3	1:B:126:MET:CE	2.14	0.78
1:D:178:HIS:HA	1:D:324:THR:HG23	1.65	0.77
1:A:248:LEU:HD21	1:A:272:LEU:HD12	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ASP:OD2	1:C:268:ARG:NH2	2.19	0.76
1:A:198:TYR:HD2	1:A:212:ALA:HB1	1.50	0.75
1:C:300:ILE:H	1:C:305:GLN:NE2	1.85	0.74
1:B:38:TRP:O	1:B:42:ARG:HB2	1.87	0.74
1:A:260:ILE:O	1:A:264:THR:HG22	1.88	0.73
1:A:273:THR:HG23	1:A:275:MET:SD	2.29	0.72
1:A:112:ASP:HB2	1:B:114:SER:HB3	1.71	0.72
1:B:36:ASP:N	1:B:38:TRP:HD1	1.88	0.71
1:C:264:THR:HG21	1:C:266:ILE:HD12	1.72	0.71
1:D:274:ASN:HB2	1:D:289:LEU:CD1	2.18	0.71
1:A:86:VAL:HG21	1:B:92:MET:HB2	1.71	0.71
1:A:228:ILE:HD12	1:A:259:LYS:HB2	1.74	0.70
1:C:14:THR:HG22	1:C:169:VAL:HG12	1.74	0.70
1:B:247:LEU:HG	1:B:308:VAL:HG13	1.73	0.70
1:B:255:ARG:CG	1:B:255:ARG:HH21	2.05	0.70
1:A:197:GLY:HA3	1:B:91:ASN:HD22	1.57	0.70
1:B:96:ALA:HB1	1:B:110:ALA:HB1	1.75	0.69
1:D:23:VAL:HG13	1:D:27:GLN:NE2	2.08	0.69
1:C:200:ILE:HB	1:C:212:ALA:CB	2.23	0.68
1:D:303:SER:OG	1:D:305:GLN:HG3	1.93	0.68
1:A:7:ASN:N	1:A:7:ASN:HD22	1.92	0.68
1:A:7:ASN:HD22	1:A:7:ASN:H	1.42	0.67
1:C:228:ILE:HD12	1:C:259:LYS:HB2	1.76	0.67
1:A:248:LEU:HD22	1:A:289:LEU:HG	1.74	0.67
1:A:129:LYS:HB3	1:B:129:LYS:HB3	1.75	0.67
1:A:198:TYR:OH	1:A:210:LYS:HD3	1.95	0.67
1:A:93:PRO:HG3	1:B:191:TRP:HB2	1.76	0.67
1:C:73:LYS:HE3	1:C:172:GLU:OE1	1.95	0.66
1:A:28:LEU:HD11	1:A:48:ARG:NH1	2.11	0.66
1:B:24:THR:OG1	1:B:27:GLN:HG3	1.96	0.66
1:A:200:ILE:HG23	1:A:212:ALA:HB2	1.78	0.66
1:B:250:HIS:CD2	1:B:252:ALA:HB2	2.31	0.66
1:B:214:LYS:HG3	1:B:215:THR:N	2.10	0.65
1:A:303:SER:O	1:A:304:GLN:HB2	1.96	0.65
1:B:206:TYR:OH	1:B:210:LYS:HD2	1.97	0.65
1:D:116:ALA:HB1	3:D:349:HOH:O	1.95	0.65
1:A:299:LEU:HB3	1:A:325:LEU:CD2	2.27	0.65
1:B:10:ARG:HG2	1:B:174:ALA:HB2	1.79	0.65
1:C:181:ASN:HA	1:D:135:ARG:HH12	1.61	0.64
1:D:9:ALA:HB1	1:D:171:ILE:HD11	1.79	0.64
1:B:29:SER:HA	1:B:34:THR:HG22	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:255:ARG:O	1:C:259:LYS:HG2	1.97	0.64
1:C:307:VAL:HG21	1:C:325:LEU:HD22	1.78	0.64
1:D:51:VAL:HG22	1:D:164:ASP:OD2	1.98	0.64
1:D:251:GLN:HB3	1:D:275:MET:HE3	1.80	0.64
1:B:255:ARG:HH21	1:B:255:ARG:HG3	1.61	0.64
1:D:300:ILE:HB	1:D:303:SER:HB3	1.80	0.64
1:B:147:PHE:HE2	1:B:282:SER:HB2	1.63	0.63
1:D:303:SER:O	1:D:304:GLN:HB2	1.98	0.63
1:C:253:ASN:HB3	1:C:256:ILE:HD12	1.81	0.63
1:D:48:ARG:HD3	3:D:348:HOH:O	1.98	0.63
1:B:274:ASN:HB2	1:B:289:LEU:HD13	1.81	0.63
1:A:300:ILE:N	1:A:305:GLN:HE22	1.96	0.63
1:A:52:THR:HG22	1:B:205:PHE:O	1.99	0.62
1:A:281:THR:HB	1:A:284:ALA:HB3	1.81	0.62
1:C:248:LEU:HD21	1:C:272:LEU:HD12	1.81	0.62
1:D:276:ASP:OD2	1:D:277:LYS:HG2	2.00	0.62
1:A:129:LYS:HD2	1:A:129:LYS:N	2.14	0.61
1:D:244:VAL:HG21	1:D:308:VAL:HG12	1.81	0.61
1:A:212:ALA:H	1:C:221:ARG:HH21	1.44	0.61
1:A:200:ILE:HG23	1:A:212:ALA:CB	2.31	0.61
1:D:178:HIS:HA	1:D:324:THR:CG2	2.31	0.60
1:C:90:PHE:CE2	1:D:198:TYR:HB2	2.37	0.60
1:D:132:LEU:HD13	1:D:132:LEU:O	2.01	0.60
1:D:6:LYS:HZ1	1:D:173:ALA:C	2.05	0.60
1:A:267:SER:HB3	1:A:270:LYS:HE3	1.84	0.60
1:B:228:ILE:HD12	1:B:259:LYS:HB2	1.83	0.60
1:C:43:THR:HG22	1:C:161:LEU:HD23	1.83	0.60
1:A:299:LEU:HB3	1:A:325:LEU:HD21	1.84	0.60
1:C:131:VAL:HA	1:C:136:TYR:O	2.02	0.60
1:D:293:ALA:HB1	1:D:299:LEU:HG	1.83	0.59
1:A:48:ARG:HE	1:A:48:ARG:N	2.01	0.59
1:A:308:VAL:HG22	1:A:310:THR:HG22	1.85	0.59
1:B:129:LYS:HD2	1:B:129:LYS:N	2.17	0.59
1:C:86:VAL:HG21	1:D:92:MET:HB2	1.85	0.59
1:A:92:MET:HB2	1:B:86:VAL:HG21	1.83	0.59
1:B:264:THR:HG23	1:B:266:ILE:H	1.67	0.59
1:C:323:LEU:HD12	1:C:323:LEU:O	2.02	0.59
1:C:95:VAL:HA	1:C:98:GLN:HE21	1.66	0.59
1:B:28:LEU:O	1:B:32:MET:HB2	2.02	0.59
1:D:306:ARG:HH21	1:D:306:ARG:CB	2.13	0.59
1:B:49:ARG:O	1:B:50:ILE:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:115:ALA:HB3	1:B:119:GLY:HA2	1.84	0.58
1:A:198:TYR:HD2	1:A:212:ALA:CB	2.14	0.58
1:C:303:SER:OG	1:C:305:GLN:HG3	2.04	0.58
1:C:93:PRO:HG3	1:D:191:TRP:HB2	1.84	0.58
1:D:73:LYS:HG3	1:D:170:LEU:HD11	1.84	0.58
1:C:25:ASN:OD1	1:C:48:ARG:NH2	2.36	0.58
1:A:124:LEU:HB3	1:A:321:LEU:HD11	1.84	0.58
1:C:57:SER:HA	1:C:95:VAL:HG13	1.85	0.58
1:C:198:TYR:OH	1:C:210:LYS:HE2	2.04	0.57
1:A:212:ALA:H	1:C:221:ARG:HH22	1.51	0.57
1:B:300:ILE:H	1:B:305:GLN:HE22	1.52	0.57
1:C:9:ALA:HB1	1:C:171:ILE:CD1	2.34	0.57
1:C:146:THR:O	1:C:149:LYS:HG2	2.04	0.57
1:D:23:VAL:HA	1:D:27:GLN:HE22	1.68	0.57
1:A:310:THR:HB	1:A:320:SER:OG	2.05	0.57
1:D:273:THR:HG23	1:D:275:MET:SD	2.44	0.57
1:D:19:PRO:HG3	1:D:51:VAL:HG12	1.87	0.57
1:B:267:SER:HB3	1:B:270:LYS:HG3	1.87	0.57
1:B:25:ASN:HB2	1:B:37:GLU:OE2	2.04	0.56
1:B:260:ILE:O	1:B:264:THR:HG22	2.05	0.56
1:C:146:THR:OG1	1:C:149:LYS:HE2	2.05	0.56
1:C:264:THR:CG2	1:C:266:ILE:HD12	2.35	0.56
1:A:91:ASN:ND2	1:B:197:GLY:HA3	2.19	0.56
1:C:112:ASP:HB2	1:D:114:SER:HB3	1.88	0.56
1:D:211:GLN:CA	1:D:212:ALA:HB2	2.35	0.56
1:D:323:LEU:HD12	1:D:323:LEU:O	2.05	0.56
1:D:307:VAL:HG21	1:D:325:LEU:HD22	1.88	0.56
1:B:194:LEU:HD23	1:B:314:GLY:N	2.21	0.56
1:C:269:GLU:H	1:C:269:GLU:CD	2.09	0.56
1:C:86:VAL:HG22	1:D:91:ASN:HB3	1.88	0.56
1:C:135:ARG:HD3	3:C:337:HOH:O	2.06	0.56
1:B:308:VAL:CG2	1:B:310:THR:HG22	2.37	0.55
1:C:200:ILE:CB	1:C:212:ALA:HB2	2.26	0.55
1:C:248:LEU:CD2	1:C:272:LEU:HD12	2.36	0.55
1:B:32:MET:O	1:B:33:ASP:HB2	2.06	0.55
1:C:9:ALA:CB	1:C:171:ILE:HD11	2.35	0.55
1:C:92:MET:HB2	1:D:86:VAL:HG21	1.87	0.55
1:D:60:CYS:SG	1:D:144:GLY:HA3	2.47	0.55
1:A:91:ASN:HD22	1:B:197:GLY:HA3	1.70	0.55
1:A:224:PHE:O	1:A:228:ILE:HG12	2.06	0.55
2:D:401:B82:H18	2:D:401:B82:BR	2.61	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:CYS:HB2	1:D:312:PHE:O	2.07	0.54
1:D:299:LEU:HA	1:D:305:GLN:HE22	1.73	0.54
1:B:221:ARG:HG3	1:B:222:SER:N	2.21	0.54
1:C:91:ASN:CB	1:D:86:VAL:HG22	2.33	0.54
1:C:170:LEU:HD23	1:C:171:ILE:N	2.23	0.54
1:B:250:HIS:NE2	1:B:252:ALA:HB2	2.23	0.54
2:A:401:B82:H18	2:A:401:B82:BR	2.62	0.54
1:A:16:ARG:HD2	1:A:288:ILE:HG23	1.90	0.54
1:D:8:TYR:O	1:D:174:ALA:N	2.41	0.54
1:D:81:ILE:HG12	1:D:140:LEU:HD12	1.90	0.54
1:B:303:SER:O	1:B:304:GLN:HB2	2.08	0.54
1:B:247:LEU:HG	1:B:308:VAL:CG1	2.38	0.53
1:D:29:SER:HA	1:D:34:THR:CG2	2.38	0.53
1:A:313:GLY:HA2	2:A:401:B82:H12	1.90	0.53
1:C:151:LEU:HD11	1:C:162:PHE:HB2	1.91	0.53
1:A:198:TYR:CD2	1:A:212:ALA:CB	2.91	0.53
1:A:49:ARG:O	1:A:50:ILE:HD13	2.09	0.53
1:D:235:ILE:HG12	1:D:310:THR:HG21	1.91	0.53
1:A:249:LEU:HG	1:A:310:THR:OG1	2.09	0.53
1:A:128:GLU:O	1:A:132:LEU:HB2	2.09	0.53
1:D:260:ILE:O	1:D:264:THR:HG22	2.09	0.53
1:D:88:PRO:HB2	1:D:90:PHE:O	2.09	0.53
1:B:290:LEU:O	1:B:294:VAL:HG23	2.09	0.52
1:C:221:ARG:HG3	1:C:222:SER:N	2.24	0.52
1:A:216:LEU:HD21	1:A:218:MET:HB2	1.91	0.52
1:A:48:ARG:HB2	1:A:278:TYR:O	2.10	0.52
1:A:114:SER:HB3	1:B:112:ASP:HB2	1.91	0.52
1:D:199:THR:HG22	3:D:340:HOH:O	2.08	0.52
1:A:57:SER:HA	1:A:95:VAL:HG13	1.90	0.52
1:A:171:ILE:O	1:A:171:ILE:HG13	2.08	0.52
1:A:191:TRP:HB2	1:B:93:PRO:HG3	1.92	0.52
1:B:307:VAL:O	1:B:323:LEU:HD12	2.10	0.52
1:C:259:LYS:HD3	1:C:262:ARG:HH12	1.74	0.52
1:B:178:HIS:HA	1:B:324:THR:HG22	1.92	0.52
1:C:178:HIS:HA	1:C:324:THR:CG2	2.36	0.52
1:A:178:HIS:HA	1:A:324:THR:CG2	2.37	0.51
1:B:253:ASN:OD1	1:B:255:ARG:HB2	2.10	0.51
1:C:28:LEU:HB3	1:C:32:MET:HE1	1.93	0.51
1:C:216:LEU:HD23	1:C:217:GLN:N	2.25	0.51
1:B:32:MET:O	1:B:33:ASP:CB	2.58	0.51
1:C:150:MET:O	1:C:215:THR:HA	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:57:SER:HA	1:C:95:VAL:CG1	2.41	0.51
1:C:32:MET:HE1	1:C:160:VAL:HG12	1.92	0.51
1:C:300:ILE:N	1:C:305:GLN:HE22	2.04	0.51
1:C:306:ARG:NH2	1:C:322:LEU:HD21	2.26	0.51
1:C:286:ILE:N	1:C:287:PRO:HD2	2.25	0.51
1:A:303:SER:OG	1:A:305:GLN:HG3	2.10	0.51
1:C:86:VAL:N	1:C:145:GLU:OE2	2.37	0.51
1:C:195:THR:HG22	1:D:93:PRO:HD3	1.93	0.51
1:C:201:ASN:HA	1:D:149:LYS:HB2	1.92	0.51
1:A:29:SER:HB2	1:A:34:THR:O	2.12	0.50
1:A:201:ASN:HA	1:B:149:LYS:HB2	1.94	0.50
1:D:23:VAL:HA	1:D:27:GLN:NE2	2.27	0.50
1:D:273:THR:CG2	1:D:274:ASN:N	2.74	0.50
1:D:261:ALA:O	1:D:264:THR:HG22	2.11	0.50
1:C:91:ASN:ND2	1:D:197:GLY:HA3	2.22	0.50
1:D:25:ASN:HD22	1:D:39:ILE:HB	1.77	0.50
1:D:19:PRO:HG3	1:D:51:VAL:CG1	2.42	0.50
1:B:54:GLU:HG2	1:B:58:ASP:HB3	1.94	0.50
1:B:273:THR:HG23	1:B:275:MET:SD	2.52	0.50
1:D:310:THR:HB	1:D:320:SER:OG	2.12	0.49
1:B:138:THR:HG23	1:B:170:LEU:HD21	1.94	0.49
1:C:308:VAL:HG12	1:C:322:LEU:HD13	1.94	0.49
1:B:86:VAL:N	1:B:145:GLU:OE2	2.44	0.49
1:D:170:LEU:HD23	1:D:171:ILE:N	2.26	0.49
1:A:24:THR:OG1	1:A:27:GLN:HG3	2.13	0.49
1:B:227:ALA:O	1:B:231:VAL:HB	2.12	0.49
1:B:308:VAL:HA	1:B:321:LEU:O	2.12	0.49
1:A:228:ILE:HD12	1:A:259:LYS:CB	2.41	0.49
1:C:224:PHE:CE1	1:C:256:ILE:HG13	2.47	0.49
1:C:227:ALA:O	1:C:231:VAL:HB	2.12	0.49
1:C:193:ALA:HB3	1:C:316:LEU:HD11	1.95	0.48
1:C:83:VAL:HA	1:C:142:ILE:O	2.13	0.48
1:C:247:LEU:HG	1:C:308:VAL:HG22	1.94	0.48
1:D:6:LYS:NZ	1:D:173:ALA:C	2.66	0.48
1:B:16:ARG:HG2	1:B:16:ARG:HH11	1.79	0.48
1:D:40:HIS:C	1:D:40:HIS:HD1	2.15	0.48
1:D:248:LEU:HD11	1:D:290:LEU:HD13	1.95	0.48
1:D:161:LEU:HD12	1:D:218:MET:HE3	1.96	0.48
1:C:57:SER:HB3	1:C:98:GLN:NE2	2.28	0.48
1:C:181:ASN:HA	1:D:135:ARG:NH1	2.29	0.48
1:D:315:GLY:N	1:D:316:LEU:HA	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:THR:HB	1:B:320:SER:OG	2.14	0.48
1:B:198:TYR:HB3	1:B:213:SER:O	2.14	0.47
1:C:300:ILE:HG22	1:C:303:SER:HB3	1.95	0.47
1:D:194:LEU:HD13	1:D:218:MET:HB2	1.96	0.47
1:C:95:VAL:O	1:C:99:VAL:HG23	2.14	0.47
1:B:303:SER:OG	1:B:305:GLN:NE2	2.48	0.47
1:C:126:MET:SD	1:D:126:MET:SD	3.12	0.47
2:C:401:B82:BR	2:C:401:B82:H18	2.70	0.47
1:B:147:PHE:N	1:B:164:ASP:OD1	2.47	0.47
2:B:401:B82:BR	2:B:401:B82:H18	2.70	0.47
1:D:264:THR:HG23	1:D:266:ILE:HB	1.95	0.47
1:A:185:GLN:HA	3:A:363:HOH:O	2.14	0.47
1:B:48:ARG:NE	1:B:48:ARG:H	2.13	0.47
1:B:200:ILE:O	1:B:200:ILE:HG13	2.15	0.47
1:B:214:LYS:HB3	3:B:363:HOH:O	2.14	0.47
1:D:253:ASN:HB3	1:D:256:ILE:HG13	1.97	0.47
1:D:273:THR:HG22	1:D:274:ASN:N	2.29	0.47
1:A:197:GLY:HA3	1:B:91:ASN:ND2	2.28	0.47
1:C:93:PRO:HD3	1:D:195:THR:HG22	1.95	0.47
1:D:24:THR:H	1:D:27:GLN:CD	2.19	0.46
1:D:57:SER:HB3	1:D:98:GLN:NE2	2.31	0.46
1:A:95:VAL:HA	1:A:98:GLN:HE21	1.80	0.46
1:B:7:ASN:N	1:B:7:ASN:ND2	2.62	0.46
1:C:191:TRP:CE3	1:D:93:PRO:HG3	2.50	0.46
1:A:296:ASN:ND2	3:A:332:HOH:O	2.47	0.46
1:B:34:THR:OG1	1:B:38:TRP:HZ2	1.97	0.46
1:C:21:ASN:HB3	1:C:50:ILE:O	2.16	0.46
1:D:11:ILE:O	1:D:301:LEU:HD22	2.16	0.46
1:D:25:ASN:ND2	1:D:39:ILE:HB	2.30	0.46
1:B:21:ASN:HB3	1:B:50:ILE:O	2.15	0.46
1:C:188:GLY:HA3	1:D:97:CYS:O	2.15	0.46
1:C:16:ARG:NH1	1:C:291:ASP:OD2	2.48	0.46
1:B:38:TRP:HZ3	1:B:42:ARG:HD3	1.81	0.46
1:B:139:GLY:O	1:B:170:LEU:HD23	2.16	0.46
1:B:309:LEU:O	1:B:320:SER:HA	2.16	0.46
1:D:228:ILE:HD12	1:D:259:LYS:HB3	1.96	0.46
1:A:7:ASN:N	1:A:7:ASN:ND2	2.59	0.46
1:B:38:TRP:CZ3	1:B:42:ARG:CZ	2.99	0.46
1:C:241:ASP:HA	1:C:266:ILE:HG12	1.98	0.46
1:C:158:THR:HA	1:C:161:LEU:HD12	1.98	0.45
1:D:167:ALA:HB2	1:D:288:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:48:ARG:NH1	1:C:160:VAL:O	2.48	0.45
1:D:9:ALA:CB	1:D:171:ILE:HD11	2.46	0.45
1:C:182:GLU:HB3	1:C:321:LEU:HD23	1.98	0.45
3:C:332:HOH:O	1:D:199:THR:HG21	2.16	0.45
1:D:25:ASN:OD1	1:D:48:ARG:NH2	2.50	0.45
1:A:45:ILE:HD13	1:A:279:GLY:HA2	1.99	0.45
1:D:117:CYS:HB2	1:D:313:GLY:HA3	1.97	0.45
1:D:247:LEU:HG	1:D:308:VAL:CG1	2.47	0.45
1:A:75:ALA:O	1:A:78:ILE:HG12	2.17	0.45
1:A:299:LEU:HA	1:A:305:GLN:HE22	1.81	0.45
1:A:223:ILE:HA	1:A:226:PHE:HB3	1.99	0.45
1:B:11:ILE:HD11	1:B:124:LEU:HD21	1.99	0.45
1:A:28:LEU:CD1	1:A:48:ARG:NH1	2.78	0.45
1:C:201:ASN:CG	1:D:149:LYS:HB3	2.38	0.45
1:C:308:VAL:HG12	1:C:322:LEU:CD1	2.47	0.45
1:A:188:GLY:HA3	1:B:97:CYS:O	2.16	0.44
1:D:99:VAL:O	1:D:103:ILE:HG12	2.17	0.44
1:C:299:LEU:HA	1:C:305:GLN:HE22	1.81	0.44
1:A:68:LEU:HD21	1:A:75:ALA:HB2	2.00	0.44
1:C:13:CYS:HB3	1:C:170:LEU:HB2	1.99	0.44
1:C:153:TRP:CD1	1:D:204:PRO:HD2	2.53	0.44
1:B:86:VAL:HG13	1:B:86:VAL:O	2.16	0.44
1:C:19:PRO:HD2	1:C:49:ARG:CB	2.48	0.44
1:D:29:SER:HA	1:D:34:THR:HG22	1.99	0.44
1:D:128:GLU:O	1:D:132:LEU:HB2	2.18	0.44
1:D:258:ASP:OD2	1:D:268:ARG:NH2	2.51	0.44
1:A:73:LYS:HE3	1:A:172:GLU:OE1	2.17	0.43
1:B:87:THR:OG1	1:B:145:GLU:HG3	2.18	0.43
1:D:6:LYS:HZ2	1:D:173:ALA:HB1	1.83	0.43
1:D:29:SER:HA	1:D:34:THR:HG23	2.00	0.43
1:D:178:HIS:O	1:D:180:LEU:HD13	2.18	0.43
1:A:121:VAL:HG13	1:A:321:LEU:HG	2.01	0.43
1:B:324:THR:HG23	1:B:324:THR:O	2.17	0.43
1:B:178:HIS:HA	1:B:324:THR:CG2	2.48	0.43
1:B:178:HIS:O	1:B:323:LEU:HA	2.18	0.43
1:D:223:ILE:O	2:D:401:B82:H14	2.18	0.43
1:B:7:ASN:ND2	1:B:7:ASN:H	2.15	0.43
1:B:286:ILE:N	1:B:287:PRO:HD2	2.33	0.43
1:D:54:GLU:HB3	1:D:58:ASP:HB2	2.00	0.43
1:A:286:ILE:N	1:A:287:PRO:HD2	2.34	0.43
1:C:79:ASP:O	1:C:108:ALA:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:CYS:HB2	1:C:312:PHE:O	2.18	0.43
1:D:25:ASN:OD1	1:D:46:SER:O	2.36	0.43
1:D:269:GLU:CD	1:D:269:GLU:H	2.22	0.43
1:D:300:ILE:H	1:D:305:GLN:NE2	2.16	0.43
1:B:300:ILE:HB	1:B:303:SER:HB3	2.00	0.43
1:C:310:THR:HB	1:C:320:SER:OG	2.18	0.43
1:A:80:PHE:HA	1:A:109:PHE:O	2.19	0.42
1:B:16:ARG:HG2	1:B:16:ARG:NH1	2.34	0.42
1:B:138:THR:CG2	1:B:170:LEU:HD21	2.49	0.42
1:B:228:ILE:HD12	1:B:259:LYS:CB	2.49	0.42
1:C:300:ILE:CG2	1:C:303:SER:HB3	2.49	0.42
1:A:24:THR:HG1	1:A:27:GLN:HG3	1.84	0.42
1:B:117:CYS:HB2	1:B:312:PHE:O	2.19	0.42
1:D:283:ALA:HB2	3:D:329:HOH:O	2.19	0.42
1:B:308:VAL:HG22	1:B:310:THR:HG22	2.01	0.42
1:C:167:ALA:HB3	1:C:287:PRO:HB2	2.02	0.42
1:A:124:LEU:HD12	1:A:124:LEU:HA	1.83	0.42
1:B:264:THR:HG23	1:B:266:ILE:N	2.34	0.42
1:D:224:PHE:CE1	1:D:256:ILE:HG12	2.54	0.42
1:D:240:THR:O	1:D:244:VAL:HG12	2.20	0.42
1:A:281:THR:O	1:A:284:ALA:HB3	2.19	0.42
1:C:234:ASN:O	1:C:237:SER:HB2	2.20	0.42
1:C:323:LEU:HD12	1:C:323:LEU:C	2.39	0.42
1:A:145:GLU:HG2	1:A:282:SER:HB2	2.01	0.42
1:B:8:TYR:O	1:B:174:ALA:N	2.53	0.42
1:B:9:ALA:HB1	1:B:171:ILE:HD11	2.01	0.42
1:B:308:VAL:HG22	1:B:310:THR:CG2	2.49	0.42
1:C:68:LEU:HD12	1:C:68:LEU:HA	1.63	0.42
1:C:91:ASN:HB3	1:D:86:VAL:CG2	2.36	0.42
1:B:248:LEU:HD21	1:B:272:LEU:HD12	2.01	0.42
1:C:147:PHE:CE1	1:C:216:LEU:HD12	2.55	0.42
1:B:187:ASP:OD1	1:B:189:GLN:HB2	2.20	0.41
1:D:185:GLN:HB2	1:D:318:TRP:CE2	2.55	0.41
1:A:149:LYS:HB2	1:B:201:ASN:HA	2.02	0.41
1:B:178:HIS:O	1:B:180:LEU:HD13	2.20	0.41
1:C:43:THR:HG22	1:C:161:LEU:CD2	2.48	0.41
1:A:198:TYR:HE2	1:A:200:ILE:HG23	1.85	0.41
1:B:273:THR:CG2	1:B:274:ASN:N	2.84	0.41
1:B:34:THR:OG1	1:B:38:TRP:CZ2	2.74	0.41
1:C:152:ASP:O	1:C:159:ALA:HB2	2.20	0.41
1:D:27:GLN:O	1:D:31:MET:HG3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:180:LEU:HD13	1:D:180:LEU:N	2.35	0.41
1:A:290:LEU:O	1:A:294:VAL:HG23	2.21	0.41
1:B:87:THR:N	1:B:88:PRO:CD	2.83	0.41
1:C:71:SER:CB	1:C:170:LEU:HD12	2.50	0.41
1:D:310:THR:HA	1:D:319:GLY:O	2.20	0.41
1:A:18:VAL:HG12	1:A:165:GLY:HA3	2.02	0.41
1:B:15:SER:HB3	1:B:67:LEU:HG	2.02	0.41
1:A:323:LEU:HD12	1:A:323:LEU:C	2.41	0.41
1:B:152:ASP:C	1:B:152:ASP:OD1	2.59	0.41
1:B:210:LYS:H	1:B:210:LYS:HG3	1.54	0.41
1:D:37:GLU:HA	1:D:40:HIS:HB3	2.03	0.41
1:D:68:LEU:HA	1:D:68:LEU:HD12	1.77	0.41
1:D:309:LEU:O	1:D:320:SER:HA	2.21	0.41
1:A:7:ASN:H	1:A:7:ASN:ND2	2.12	0.41
1:A:25:ASN:O	1:A:26:HIS:C	2.59	0.41
1:A:68:LEU:HD12	1:A:68:LEU:HA	1.88	0.41
1:A:73:LYS:HG3	1:A:170:LEU:HD11	2.03	0.41
1:B:45:ILE:HG12	1:B:279:GLY:HA2	2.03	0.41
1:D:180:LEU:HD12	1:D:180:LEU:HA	1.89	0.41
1:D:247:LEU:HG	1:D:308:VAL:HG13	2.01	0.41
1:D:247:LEU:N	1:D:247:LEU:HD12	2.36	0.41
1:B:198:TYR:OH	1:B:210:LYS:HD3	2.21	0.41
1:D:255:ARG:HH21	2:D:401:B82:H22	1.85	0.40
1:D:267:SER:OG	1:D:269:GLU:OE2	2.40	0.40
1:D:311:GLY:O	1:D:318:TRP:HA	2.22	0.40
1:A:200:ILE:H	1:A:200:ILE:HG12	1.37	0.40
1:A:204:PRO:HG2	1:A:205:PHE:CD2	2.56	0.40
1:D:234:ASN:O	1:D:237:SER:HB2	2.21	0.40
1:B:216:LEU:C	1:B:216:LEU:HD23	2.41	0.40
1:D:181:ASN:HD22	1:D:238:LEU:HD22	1.86	0.40
1:B:38:TRP:CZ3	1:B:42:ARG:HD3	2.56	0.40
1:B:73:LYS:HE2	1:B:172:GLU:OE1	2.22	0.40
1:B:235:ILE:HG12	1:B:310:THR:HG21	2.04	0.40
1:B:310:THR:HA	1:B:319:GLY:O	2.22	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	318/343 (93%)	299 (94%)	19 (6%)	0	100	100
1	B	315/343 (92%)	298 (95%)	16 (5%)	1 (0%)	41	64
1	C	318/343 (93%)	299 (94%)	19 (6%)	0	100	100
1	D	318/343 (93%)	297 (93%)	19 (6%)	2 (1%)	25	47
All	All	1269/1372 (92%)	1193 (94%)	73 (6%)	3 (0%)	47	71

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	33	ASP
1	D	212	ALA
1	D	253	ASN

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	268/288 (93%)	251 (94%)	17 (6%)	18	36
1	B	267/288 (93%)	241 (90%)	26 (10%)	8	15
1	C	268/288 (93%)	253 (94%)	15 (6%)	21	42
1	D	268/288 (93%)	246 (92%)	22 (8%)	11	22
All	All	1071/1152 (93%)	991 (92%)	80 (8%)	13	27

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ASN
1	A	33	ASP
1	A	48	ARG
1	A	61	HIS
1	A	68	LEU
1	A	132	LEU
1	A	170	LEU
1	A	199	THR
1	A	200	ILE
1	A	202	GLU
1	A	221	ARG
1	A	233	GLN
1	A	268	ARG
1	A	269	GLU
1	A	275	MET
1	A	310	THR
1	A	316	LEU
1	B	7	ASN
1	B	37	GLU
1	B	42	ARG
1	B	48	ARG
1	B	61	HIS
1	B	68	LEU
1	B	73	LYS
1	B	86	VAL
1	B	145	GLU
1	B	147	PHE
1	B	170	LEU
1	B	171	ILE
1	B	180	LEU
1	B	199	THR
1	B	214	LYS
1	B	221	ARG
1	B	226	PHE
1	B	255	ARG
1	B	265	LYS
1	B	268	ARG
1	B	274	ASN
1	B	275	MET
1	B	308	VAL
1	B	310	THR
1	B	316	LEU
1	B	323	LEU

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Mol	Chain	Res	Type
1	C	48	ARG
1	C	53	GLN
1	C	68	LEU
1	C	89	ASP
1	C	132	LEU
1	C	199	THR
1	C	200	ILE
1	C	214	LYS
1	C	264	THR
1	C	273	THR
1	C	274	ASN
1	C	304	GLN
1	C	309	LEU
1	C	310	THR
1	C	316	LEU
1	D	36	ASP
1	D	46	SER
1	D	48	ARG
1	D	61	HIS
1	D	68	LEU
1	D	89	ASP
1	D	137	GLN
1	D	147	PHE
1	D	175	GLU
1	D	180	LEU
1	D	199	THR
1	D	200	ILE
1	D	233	GLN
1	D	242	GLU
1	D	259	LYS
1	D	265	LYS
1	D	268	ARG
1	D	274	ASN
1	D	306	ARG
1	D	310	THR
1	D	316	LEU
1	D	324	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	ASN

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Mol	Chain	Res	Type
1	A	91	ASN
1	A	98	GLN
1	A	137	GLN
1	A	274	ASN
1	A	304	GLN
1	A	305	GLN
1	B	7	ASN
1	B	74	GLN
1	B	91	ASN
1	B	98	GLN
1	B	189	GLN
1	B	211	GLN
1	B	305	GLN
1	C	53	GLN
1	C	91	ASN
1	C	98	GLN
1	C	189	GLN
1	C	274	ASN
1	C	304	GLN
1	C	305	GLN
1	D	27	GLN
1	D	66	GLN
1	D	98	GLN
1	D	137	GLN
1	D	189	GLN
1	D	211	GLN
1	D	274	ASN
1	D	305	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)

4 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	B82	D	401	-	27,28,28	3.20	15 (55%)	37,40,40	1.37	3 (8%)
2	B82	B	401	-	27,28,28	3.54	17 (62%)	37,40,40	1.34	4 (10%)
2	B82	C	401	-	27,28,28	3.28	15 (55%)	37,40,40	1.24	4 (10%)
2	B82	A	401	-	27,28,28	3.17	13 (48%)	37,40,40	1.30	6 (16%)

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	B82	D	401	-	-	1/28/28/28	0/2/2/2
2	B82	B	401	-	-	1/28/28/28	0/2/2/2
2	B82	C	401	-	-	1/28/28/28	0/2/2/2
2	B82	A	401	-	-	1/28/28/28	0/2/2/2

All (60) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	B82	S1-N20	10.09	1.77	1.63
2	A	401	B82	S1-N20	9.72	1.77	1.63
2	D	401	B82	S1-N20	9.54	1.77	1.63
2	C	401	B82	S1-N20	9.06	1.76	1.63
2	B	401	B82	C2-S1	5.95	1.85	1.78
2	C	401	B82	C2-S1	5.64	1.85	1.78
2	B	401	B82	C8-C7	5.62	1.49	1.41
2	B	401	B82	C3-C4	5.09	1.46	1.39
2	D	401	B82	C8-C7	5.03	1.49	1.41
2	A	401	B82	C2-S1	5.00	1.84	1.78
2	C	401	B82	C3-C2	4.98	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	B82	C8-C7	4.86	1.48	1.41
2	B	401	B82	C3-C2	4.66	1.46	1.39
2	B	401	B82	C11-C8	4.61	1.47	1.39
2	C	401	B82	C8-C7	4.58	1.48	1.41
2	C	401	B82	C3-C4	4.53	1.46	1.39
2	D	401	B82	C11-C8	4.50	1.47	1.39
2	B	401	B82	C14-C7	4.39	1.47	1.39
2	C	401	B82	C11-C8	4.27	1.46	1.39
2	A	401	B82	C3-C4	4.17	1.45	1.39
2	D	401	B82	C3-C2	4.08	1.45	1.39
2	D	401	B82	C14-C7	4.07	1.46	1.39
2	A	401	B82	C11-C8	4.02	1.46	1.39
2	A	401	B82	C3-C2	3.97	1.45	1.39
2	D	401	B82	C17-C18	3.83	1.46	1.38
2	B	401	B82	C17-C18	3.79	1.46	1.38
2	C	401	B82	C17-C18	3.69	1.46	1.38
2	C	401	B82	C14-C7	3.64	1.45	1.39
2	A	401	B82	C14-C7	3.63	1.45	1.39
2	D	401	B82	C16-C4	3.50	1.45	1.39
2	D	401	B82	C2-S1	3.50	1.82	1.78
2	D	401	B82	C3-C4	3.42	1.44	1.39
2	C	401	B82	C16-C4	3.37	1.45	1.39
2	A	401	B82	C17-C18	3.37	1.45	1.38
2	A	401	B82	C16-C4	3.34	1.45	1.39
2	B	401	B82	C16-C4	3.27	1.44	1.39
2	D	401	B82	C16-C17	3.00	1.44	1.38
2	B	401	B82	C16-C17	2.57	1.43	1.38
2	C	401	B82	C16-C17	2.51	1.43	1.38
2	D	401	B82	C8-C9	2.51	1.55	1.49
2	D	401	B82	C12-C11	2.44	1.44	1.38
2	C	401	B82	C5-N6	2.40	1.42	1.35
2	B	401	B82	C21-N20	2.37	1.58	1.48
2	A	401	B82	C21-N20	2.36	1.57	1.48
2	B	401	B82	C5-N6	2.33	1.41	1.35
2	B	401	B82	C7-N6	2.33	1.46	1.41
2	C	401	B82	C13-C14	2.32	1.43	1.38
2	B	401	B82	C13-C14	2.28	1.43	1.38
2	D	401	B82	C21-N20	2.26	1.57	1.48
2	C	401	B82	C21-N20	2.24	1.57	1.48
2	C	401	B82	C7-N6	2.23	1.46	1.41
2	C	401	B82	BR-C18	2.20	1.94	1.89
2	B	401	B82	C12-C11	2.20	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	B82	C12-C11	2.19	1.43	1.38
2	B	401	B82	C12-C13	2.17	1.43	1.38
2	D	401	B82	C13-C14	2.14	1.43	1.38
2	D	401	B82	C12-C13	2.10	1.43	1.38
2	B	401	B82	C8-C9	2.02	1.54	1.49
2	A	401	B82	C8-C9	2.02	1.54	1.49
2	A	401	B82	C5-N6	2.01	1.41	1.35

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	401	B82	O26-S1-N20	4.10	110.42	106.69
2	A	401	B82	O25-S1-N20	3.03	109.45	106.69
2	C	401	B82	O25-S1-N20	2.96	109.39	106.69
2	B	401	B82	O25-S1-N20	2.89	109.33	106.69
2	B	401	B82	C7-C8-C9	2.77	124.99	121.72
2	B	401	B82	BR-C18-C17	-2.63	112.67	117.81
2	A	401	B82	O26-S1-N20	2.59	109.05	106.69
2	A	401	B82	BR-C18-C17	-2.55	112.83	117.81
2	C	401	B82	O26-S1-N20	2.50	108.97	106.69
2	A	401	B82	C7-C8-C9	2.35	124.49	121.72
2	C	401	B82	BR-C18-C17	-2.31	113.30	117.81
2	B	401	B82	O26-S1-N20	2.27	108.76	106.69
2	C	401	B82	C21-N20-S1	-2.21	108.66	117.73
2	D	401	B82	C21-N20-S1	-2.10	109.13	117.73
2	A	401	B82	C21-N20-S1	-2.10	109.14	117.73
2	D	401	B82	C7-C8-C9	2.08	124.18	121.72
2	A	401	B82	O15-C5-N6	2.01	128.30	123.71

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	B82	C22-C21-N20-C23
2	B	401	B82	C22-C21-N20-C23
2	C	401	B82	C22-C21-N20-C23
2	D	401	B82	C22-C21-N20-C23

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	401	B82	3	0
2	B	401	B82	1	0
2	C	401	B82	1	0
2	A	401	B82	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.

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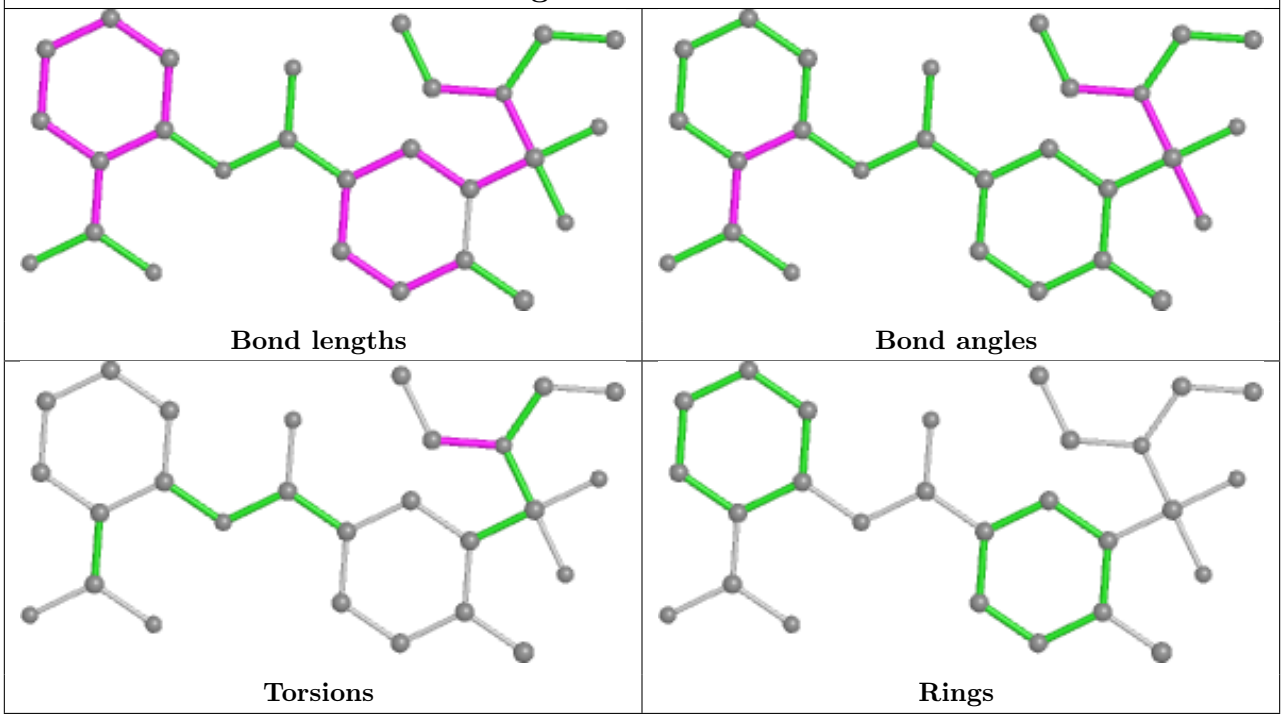
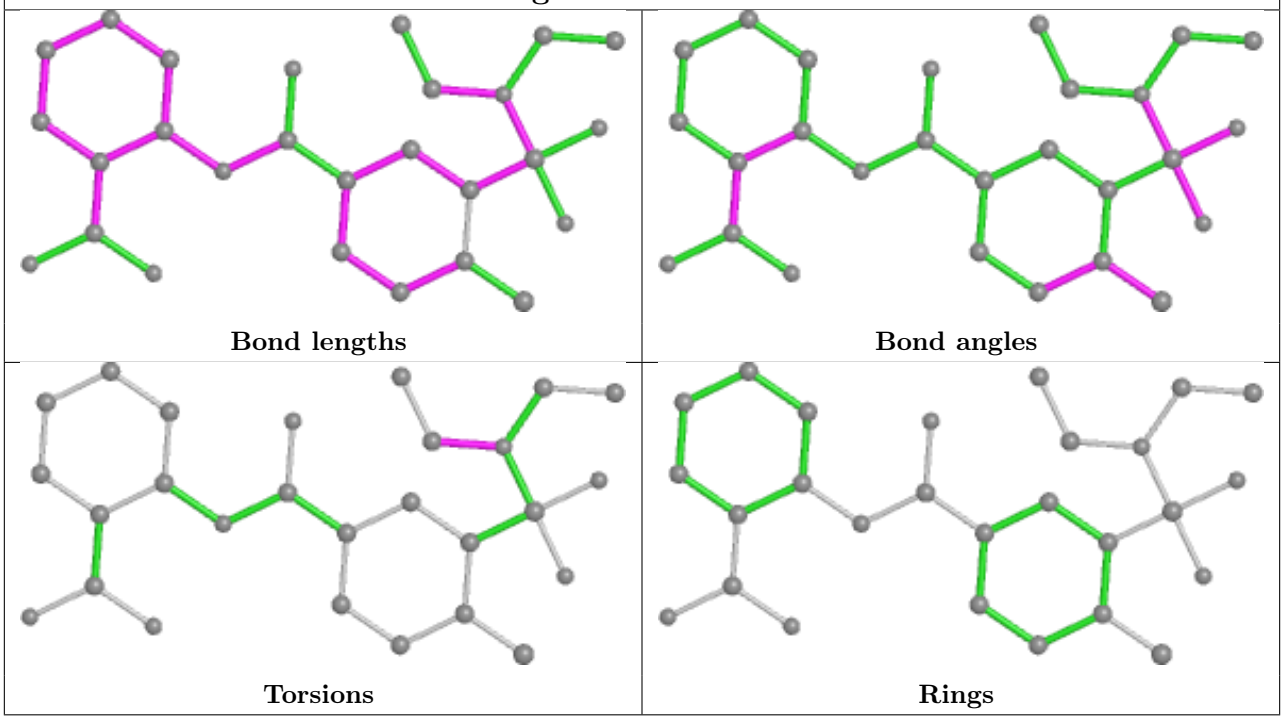
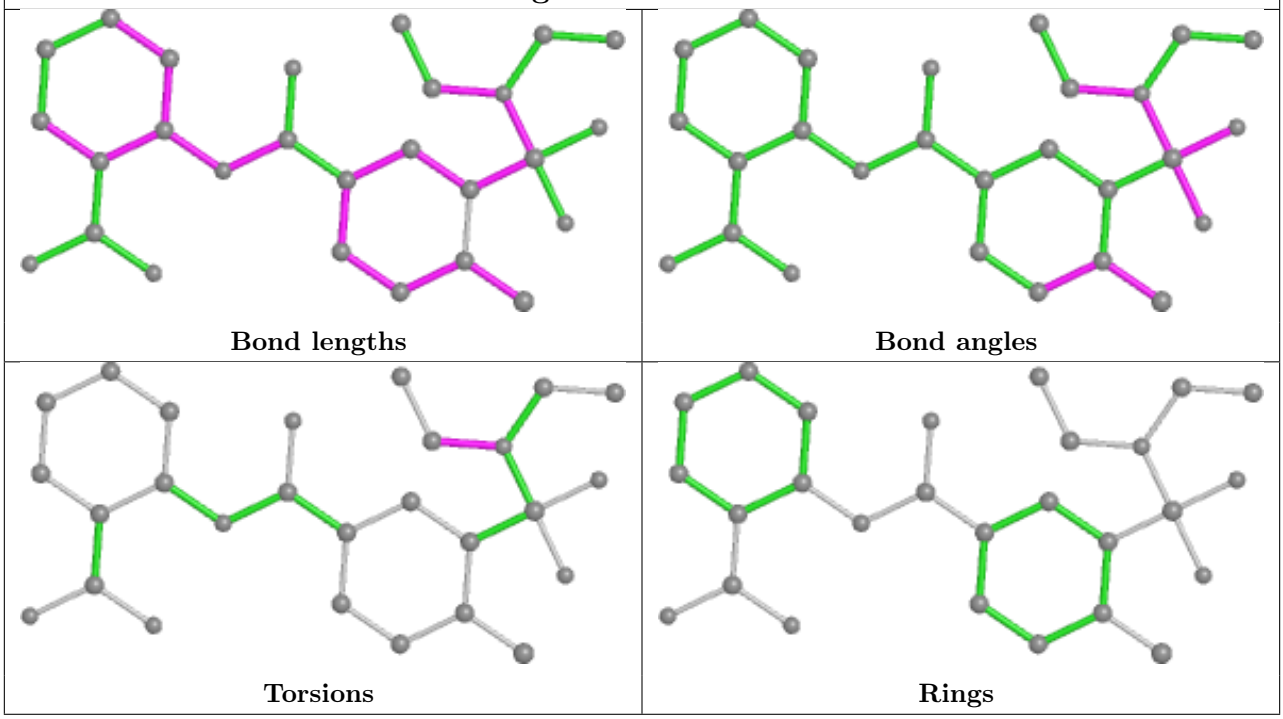


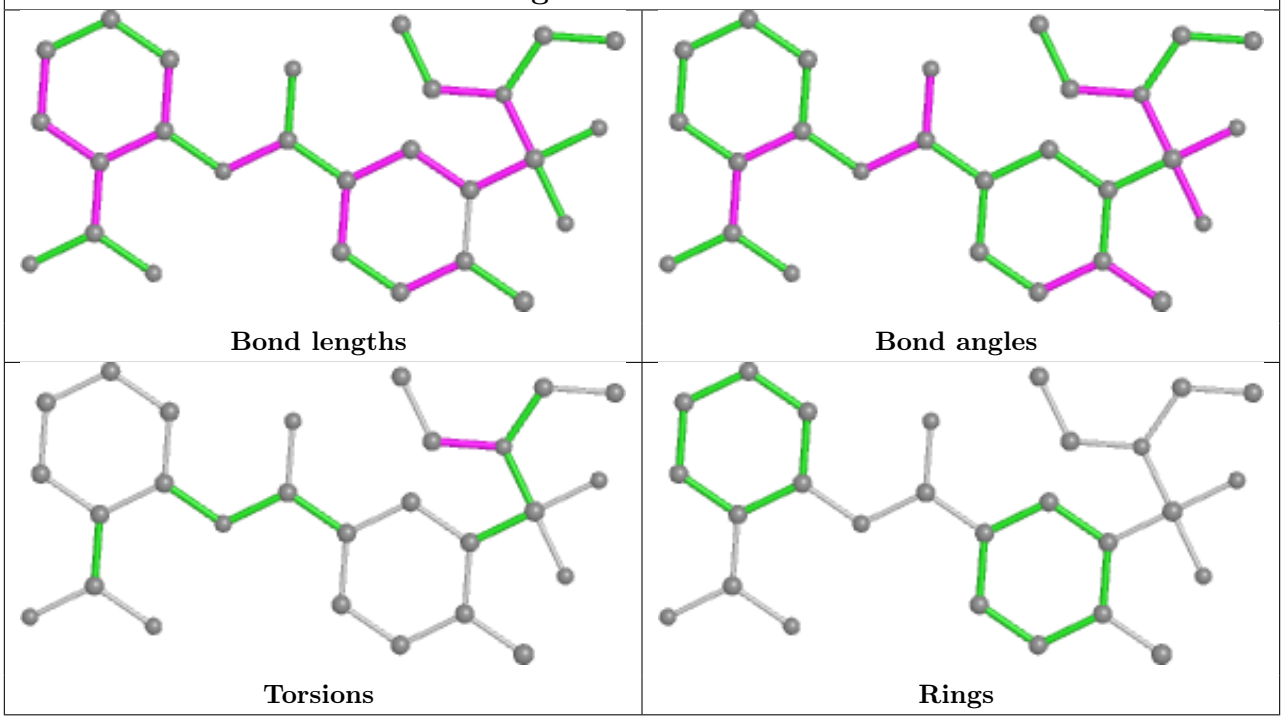
Ligand B82 B 401



Ligand B82 C 401



Ligand B82 A 401



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	320/343 (93%)	-0.23	1 (0%)	94	93	26, 41, 58, 79	0
1	B	319/343 (93%)	-0.37	4 (1%)	77	73	22, 37, 60, 84	0
1	C	320/343 (93%)	-0.29	2 (0%)	89	88	26, 40, 58, 88	0
1	D	320/343 (93%)	0.00	14 (4%)	34	27	27, 46, 76, 96	0
All	All	1279/1372 (93%)	-0.22	21 (1%)	72	68	22, 41, 65, 96	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	209	HIS	4.3
1	A	211	GLN	3.9
1	D	210	LYS	3.8
1	B	175	GLU	3.6
1	D	7	ASN	3.4
1	B	211	GLN	3.1
1	D	37	GLU	3.1
1	D	6	LYS	2.6
1	B	213	SER	2.6
1	C	211	GLN	2.5
1	D	20	GLU	2.4
1	D	53	GLN	2.4
1	D	34	THR	2.4
1	D	212	ALA	2.4
1	B	36	ASP	2.3
1	D	284	ALA	2.3
1	D	211	GLN	2.2
1	C	286	ILE	2.2
1	D	176	THR	2.1
1	D	175	GLU	2.1
1	D	269	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)

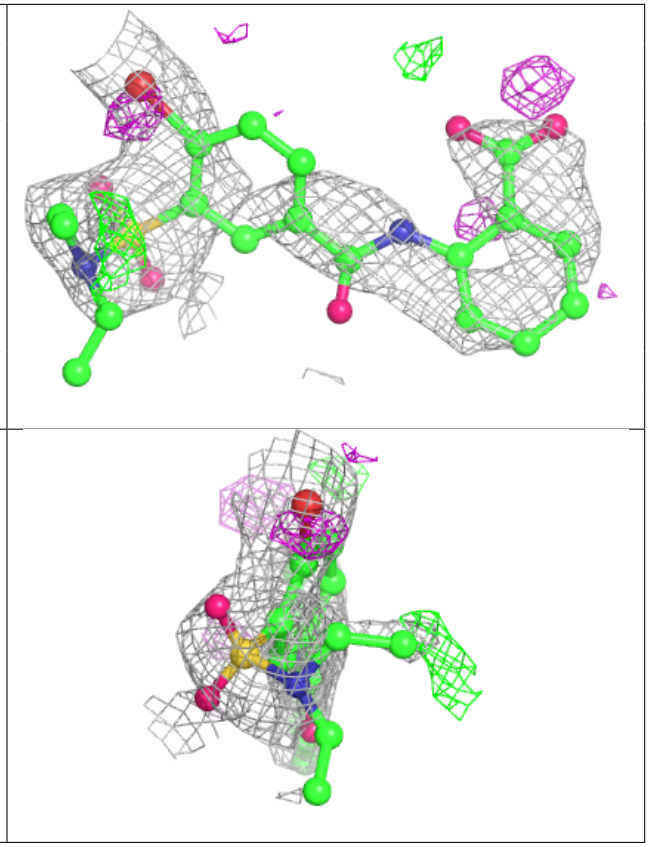
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	B82	B	401	27/27	0.74	0.36	93,108,113,123	0
2	B82	D	401	27/27	0.87	0.26	70,84,91,102	0
2	B82	C	401	27/27	0.89	0.21	46,62,69,86	0
2	B82	A	401	27/27	0.89	0.19	47,69,77,92	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.

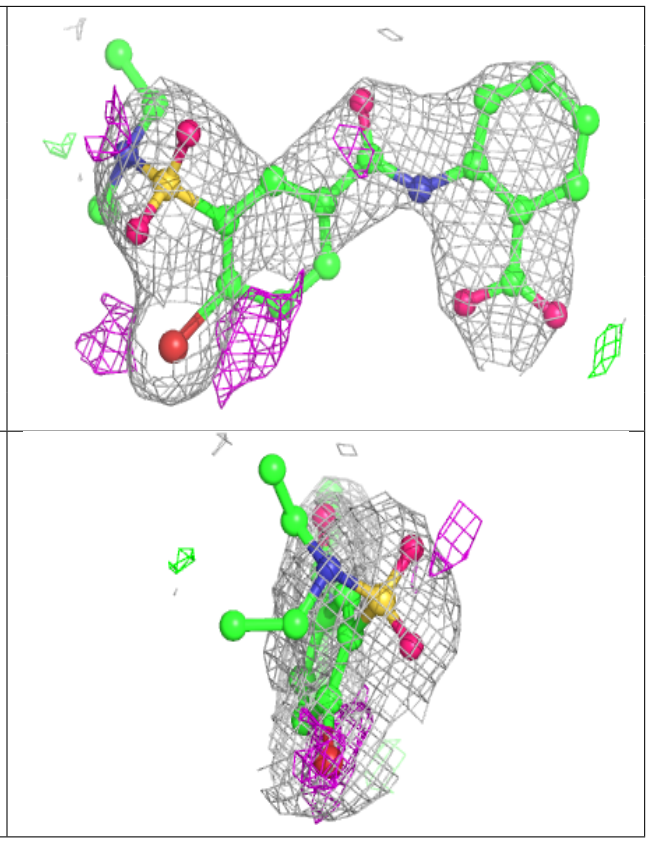
Electron density around B82 B 401:

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



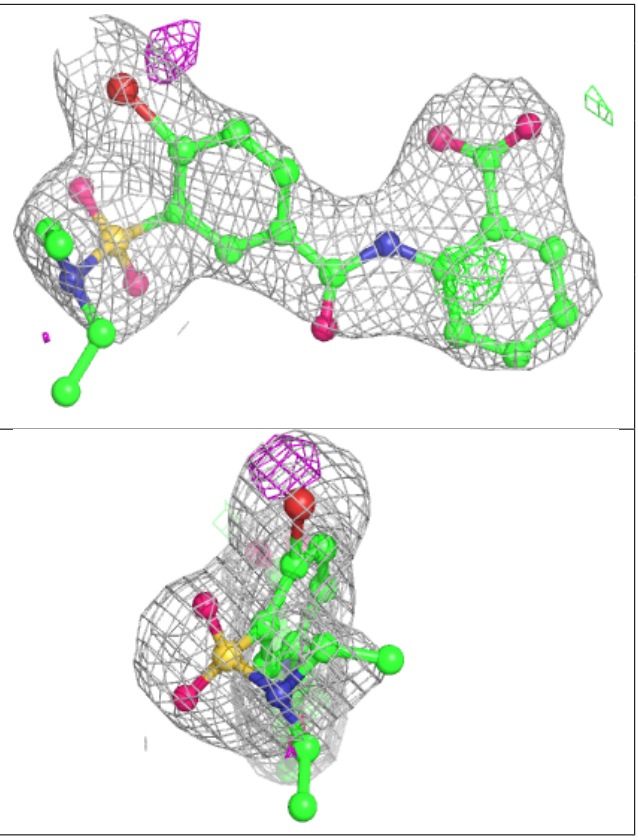
Electron density around B82 D 401:

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



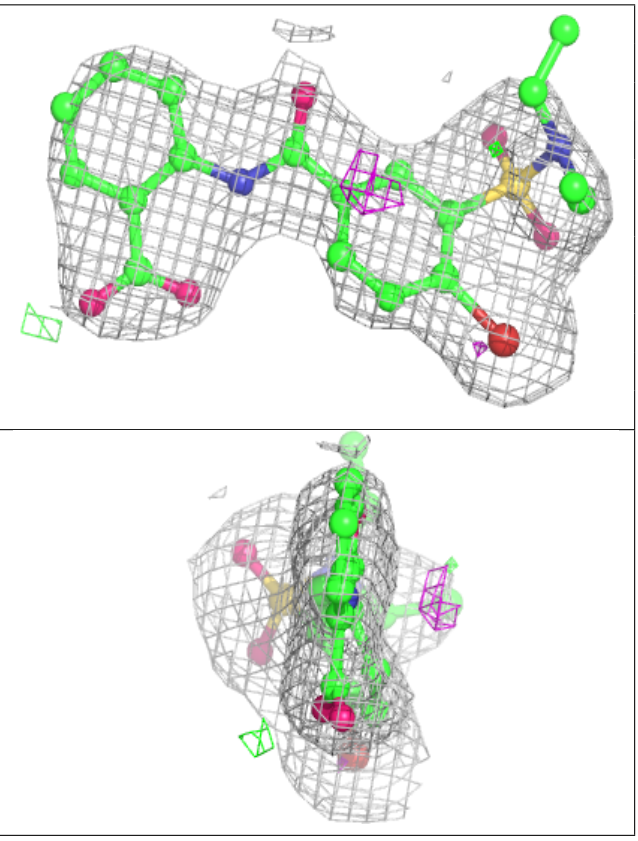
Electron density around B82 C 401:

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



Electron density around B82 A 401:

$2mF_o$-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.