Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2022 – 12:19 PM EDT

PDB ID	:	8DB9
Title	:	Adenosine/guanosine nucleoside hydrolase bound to inhibitor
Authors	:	Muellers, S.N.; Allen, K.N.; Stockman, B.J.
Deposited on	:	2022-06-14
Resolution	:	2.89 Å(reported)

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

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

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

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

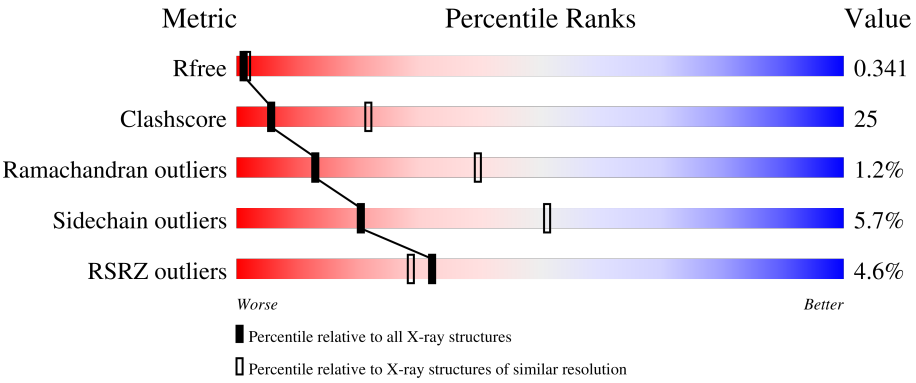
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

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 2.89 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	304	6% 59% 37% .
1	B	304	6% 53% 44% .
1	C	304	4% 60% 37% . .
1	D	304	4% 57% 40% .

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9407 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.

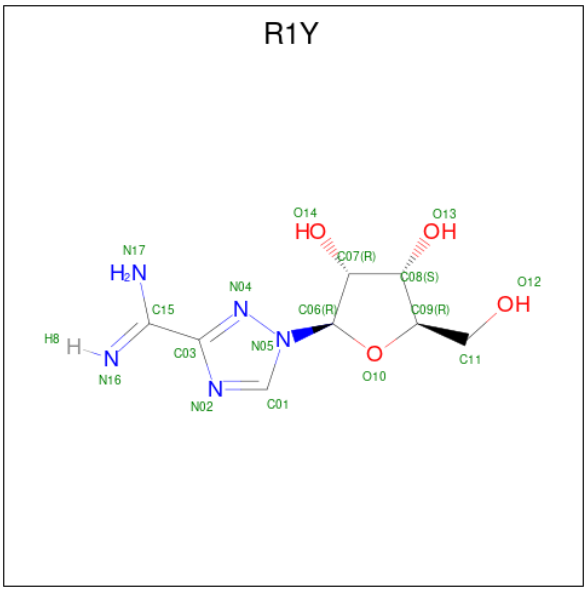
- Molecule 1 is a protein called Inosine-uridine preferring nucleoside hydrolase family protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2341	1492	399	436	14			
1	B	304	Total	C	N	O	S	0	0	0
			2350	1497	401	438	14			
1	C	301	Total	C	N	O	S	0	0	0
			2311	1473	393	432	13			
1	D	304	Total	C	N	O	S	0	0	0
			2350	1497	401	438	14			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Ca	0	0
			1	1		
2	B	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is 1-beta-D-ribofuranosyl-1H-1,2,4-triazole-3-carboximidamide (three-letter code: R1Y) (formula: $C_8H_{13}N_5O_4$) (labeled as "Ligand of Interest" by depositor).



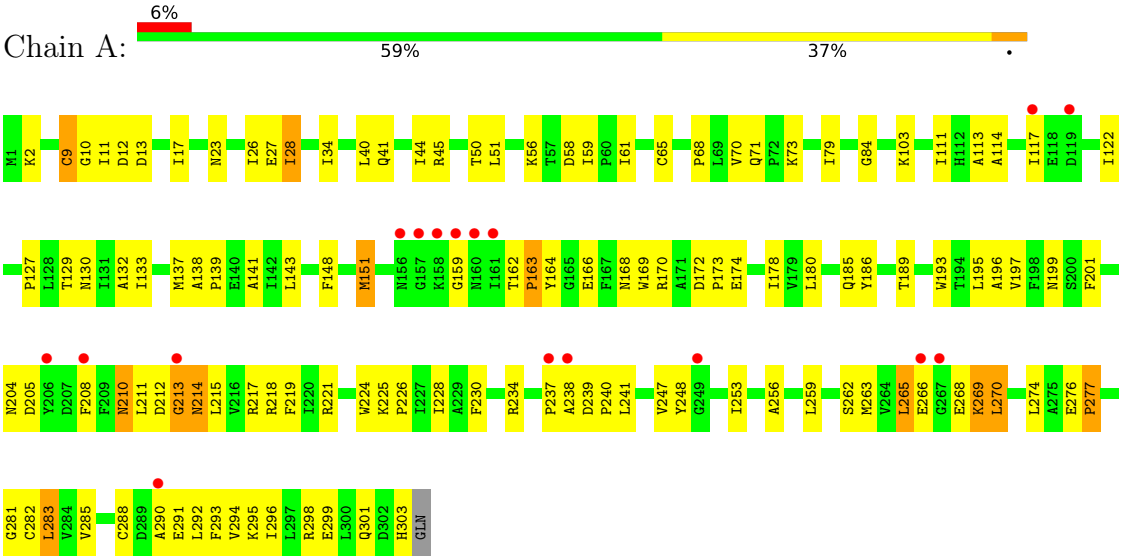
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C N O 17 8 5 4	0	0
3	C	1	Total C N O 17 8 5 4	0	0
3	D	1	Total C N O 17 8 5 4	0	0

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.

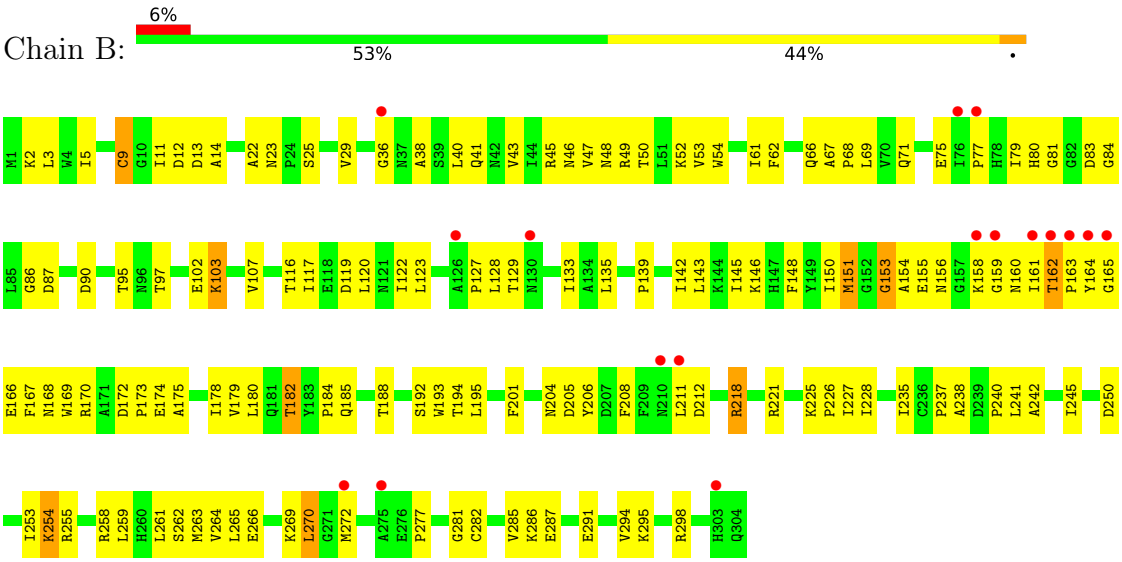
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain A:



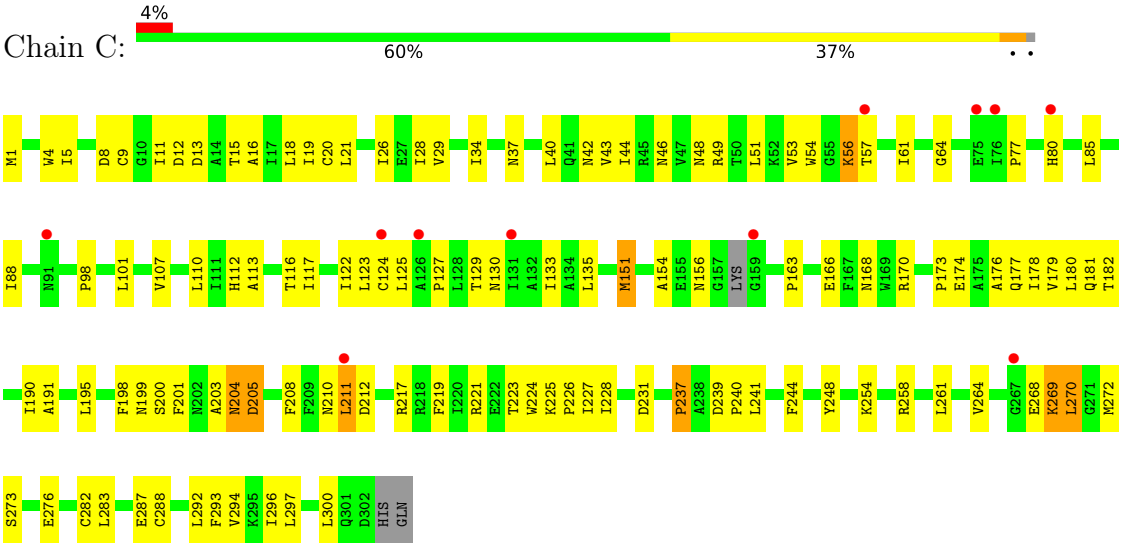
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain B:



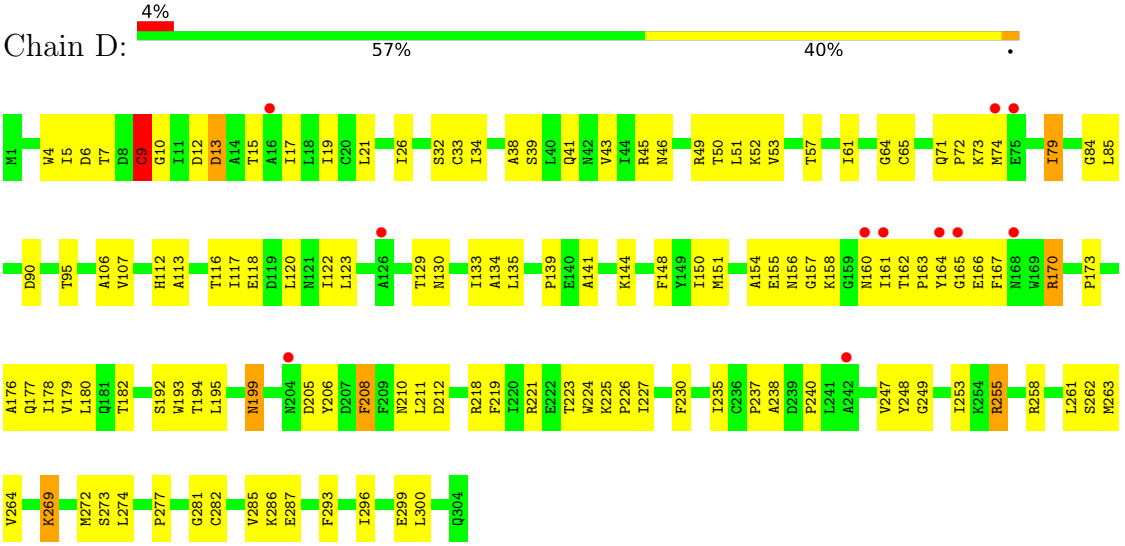
• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain C:



• Molecule 1: Inosine-uridine preferring nucleoside hydrolase family protein

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	50.41Å 75.38Å 88.86Å 65.47° 80.79° 87.32°	Depositor
Resolution (Å)	38.13 – 2.89 38.13 – 2.89	Depositor EDS
% Data completeness (in resolution range)	88.0 (38.13-2.89) 88.0 (38.13-2.89)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 2.90Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660, PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.260 , 0.341 0.261 , 0.341	Depositor DCC
R_{free} test set	1358 reflections (5.87%)	wwPDB-VP
Wilson B-factor (Å^2)	61.3	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 24.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.004 for -h,k,k-l	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	9407	wwPDB-VP
Average B, all atoms (Å^2)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.22% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, R1Y

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	0.50	0/2390	0.64	0/3248
1	B	0.51	0/2399	0.67	1/3260 (0.0%)
1	C	0.55	0/2358	0.69	0/3207
1	D	0.54	0/2399	0.70	1/3260 (0.0%)
All	All	0.52	0/9546	0.67	2/12975 (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	D	9	CYS	N-CA-C	6.04	127.30	111.00
1	B	182	THR	C-N-CA	-5.19	108.72	121.70

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2341	0	2334	132	2
1	B	2350	0	2343	156	0
1	C	2311	0	2292	96	0
1	D	2350	0	2343	106	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	B	17	0	0	1	0
3	C	17	0	0	2	0
3	D	17	0	0	2	0
All	All	9407	0	9312	477	2

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 25.

All (477) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:162:THR:HG22	1:B:163:PRO:CD	1.55	1.36
1:B:237:PRO:HB2	1:B:241:LEU:CD2	1.70	1.22
1:B:162:THR:HG22	1:B:163:PRO:HD2	1.22	1.18
1:B:174:GLU:O	1:B:178:ILE:HG12	1.45	1.15
1:B:237:PRO:HB2	1:B:241:LEU:HD23	1.15	1.12
1:B:161:ILE:CD1	1:B:167:PHE:HA	1.81	1.10
1:C:13:ASP:OD1	1:C:239:ASP:OD2	1.69	1.09
1:B:119:ASP:HA	1:B:146:LYS:HE2	1.36	1.06
1:B:162:THR:HG22	1:B:163:PRO:HD3	1.29	1.06
1:A:218:ARG:HH11	1:A:221:ARG:NH2	1.53	1.05
1:C:269:LYS:HB2	1:C:272:MET:HG3	1.07	1.03
1:B:161:ILE:HD11	1:B:167:PHE:HA	1.36	1.02
1:A:214:ASN:HD22	1:A:303:HIS:CD2	1.77	1.02
1:B:119:ASP:HA	1:B:146:LYS:CE	1.91	1.00
1:B:69:LEU:HD22	1:B:129:THR:HG23	1.42	0.98
1:C:269:LYS:HB2	1:C:272:MET:CG	1.92	0.98
1:A:70:VAL:HG12	1:B:178:ILE:HD11	1.45	0.98
1:B:162:THR:CG2	1:B:163:PRO:CD	2.42	0.98
1:A:212:ASP:OD1	1:A:218:ARG:NH2	1.97	0.96
1:B:139:PRO:O	1:B:143:LEU:HD12	1.64	0.96
1:B:162:THR:CG2	1:B:163:PRO:HD2	1.96	0.95
1:A:218:ARG:HH11	1:A:221:ARG:HH22	0.99	0.95
1:A:218:ARG:HG3	1:A:221:ARG:NH2	1.80	0.95
1:C:269:LYS:CB	1:C:272:MET:HG3	1.98	0.93
1:A:28:ILE:HG21	1:A:59:ILE:HG21	1.50	0.93
1:B:237:PRO:CB	1:B:241:LEU:HD23	2.01	0.90
1:A:214:ASN:HD22	1:A:303:HIS:HD2	1.17	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:163:PRO:HB3	1:C:204:ASN:OD1	1.72	0.88
1:A:26:ILE:HD11	1:A:247:VAL:HG21	1.56	0.87
1:A:12:ASP:HB2	1:A:240:PRO:HD3	1.59	0.84
1:A:295:LYS:NZ	1:A:298:ARG:HD2	1.90	0.83
1:B:69:LEU:CD2	1:B:129:THR:HG23	2.09	0.83
1:B:69:LEU:HD23	1:B:172:ASP:OD2	1.79	0.82
1:A:295:LYS:HZ3	1:A:298:ARG:HD2	1.42	0.81
1:A:218:ARG:NH1	1:A:221:ARG:NH2	2.28	0.80
1:B:161:ILE:HD11	1:B:167:PHE:CA	2.12	0.80
1:B:250:ASP:HA	1:B:253:ILE:HG22	1.65	0.79
1:B:237:PRO:CB	1:B:241:LEU:CD2	2.56	0.79
1:C:211:LEU:HD22	1:C:217:ARG:NH1	1.98	0.79
1:A:214:ASN:OD1	1:A:217:ARG:HG3	1.84	0.77
1:B:83:ASP:CG	1:B:87:ASP:HA	2.05	0.77
1:A:180:LEU:CD1	1:A:263:MET:HG2	2.16	0.76
1:B:162:THR:CG2	1:B:163:PRO:HD3	2.10	0.76
1:B:185:GLN:HE22	1:B:261:LEU:H	1.32	0.76
1:B:161:ILE:HD12	1:B:167:PHE:HA	1.66	0.76
1:B:218:ARG:NH1	1:B:221:ARG:HH22	1.85	0.75
1:A:23:ASN:HB3	1:A:26:ILE:HD12	1.69	0.74
1:D:248:TYR:CE2	1:D:296:ILE:HD13	2.22	0.74
1:D:170:ARG:O	1:D:170:ARG:NE	2.16	0.74
1:A:28:ILE:CG2	1:A:59:ILE:HG21	2.17	0.72
1:A:174:GLU:HG3	1:A:265:LEU:HD11	1.71	0.72
1:B:277:PRO:HB2	1:D:158:LYS:HE3	1.71	0.72
1:D:10:GLY:O	1:D:85:LEU:HD12	1.88	0.72
1:A:218:ARG:HH11	1:A:218:ARG:HG3	1.55	0.71
1:B:161:ILE:HD11	1:B:167:PHE:CD1	2.24	0.71
1:A:210:ASN:HA	1:A:221:ARG:HG3	1.73	0.71
1:C:1:MET:HB3	1:C:26:ILE:HD13	1.73	0.71
1:A:218:ARG:HG3	1:A:221:ARG:HH22	1.56	0.70
1:D:12:ASP:HB2	1:D:240:PRO:HD3	1.73	0.70
1:B:269:LYS:HB3	1:B:272:MET:HG3	1.73	0.70
1:D:15:THR:HG21	1:D:224:TRP:HE1	1.54	0.70
1:A:185:GLN:O	1:A:282:CYS:HA	1.92	0.70
1:D:162:THR:OG1	1:D:165:GLY:O	2.09	0.70
1:B:161:ILE:HD11	1:B:167:PHE:HD1	1.55	0.70
1:A:13:ASP:CG	1:A:239:ASP:OD2	2.29	0.69
1:D:212:ASP:OD1	1:D:218:ARG:NH2	2.25	0.69
1:B:119:ASP:HA	1:B:146:LYS:HE3	1.74	0.69
1:B:208:PHE:HA	1:B:211:LEU:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:ILE:HG22	1:B:237:PRO:HD3	1.74	0.69
1:D:262:SER:O	1:D:274:LEU:HB2	1.93	0.69
1:A:214:ASN:ND2	1:A:303:HIS:CD2	2.56	0.69
1:C:20:CYS:HB3	1:C:28:ILE:HD11	1.75	0.69
1:C:46:ASN:HB3	1:C:85:LEU:HD22	1.74	0.69
1:A:189:THR:HG23	1:A:283:LEU:HB3	1.75	0.68
1:C:211:LEU:HD22	1:C:217:ARG:HH11	1.57	0.68
1:D:156:ASN:HB2	1:D:194:THR:HG21	1.74	0.68
1:B:254:LYS:HB2	1:B:287:GLU:HG3	1.76	0.68
1:A:186:TYR:HA	1:A:281:GLY:O	1.94	0.68
1:B:160:ASN:ND2	3:B:401:R1Y:O12	2.26	0.68
1:B:38:ALA:HB2	1:B:84:GLY:HA3	1.75	0.68
1:D:177:GLN:HB2	1:D:263:MET:HB2	1.76	0.67
1:C:37:ASN:O	1:C:77:PRO:HG2	1.94	0.67
1:B:218:ARG:HH11	1:B:221:ARG:HH22	1.42	0.67
1:A:28:ILE:CG2	1:A:59:ILE:CG2	2.73	0.67
1:B:270:LEU:HG	1:B:270:LEU:O	1.95	0.67
1:A:151:MET:HG3	1:A:238:ALA:O	1.95	0.67
1:B:46:ASN:HA	1:B:49:ARG:HD3	1.77	0.67
1:D:261:LEU:HA	1:D:274:LEU:O	1.96	0.66
1:A:12:ASP:HB2	1:A:239:ASP:HB2	1.77	0.66
1:A:268:GLU:CD	1:A:268:GLU:H	1.98	0.66
1:D:178:ILE:O	1:D:182:THR:OG1	2.14	0.66
1:A:129:THR:OG1	1:A:172:ASP:OD2	2.12	0.66
1:B:9:CYS:HA	1:B:13:ASP:HB2	1.76	0.66
1:D:160:ASN:OD1	1:D:166:GLU:HA	1.95	0.66
1:C:190:ILE:CD1	1:C:282:CYS:HB3	2.25	0.66
1:C:204:ASN:N	1:C:204:ASN:HD22	1.94	0.66
1:C:239:ASP:HB2	1:C:240:PRO:HD3	1.77	0.65
1:C:198:PHE:HE2	1:C:287:GLU:HG3	1.60	0.65
1:B:41:GLN:O	1:B:45:ARG:HG3	1.97	0.65
1:C:190:ILE:HD11	1:C:282:CYS:HB3	1.78	0.65
1:D:32:SER:HB2	1:D:106:ALA:HB1	1.78	0.65
1:B:12:ASP:HB2	1:B:240:PRO:HD3	1.78	0.65
1:B:237:PRO:O	1:B:241:LEU:HD23	1.97	0.65
1:D:107:VAL:HG21	1:D:133:ILE:HG13	1.77	0.65
1:B:148:PHE:HD2	1:B:150:ILE:HD11	1.62	0.64
1:B:264:VAL:HG21	1:B:272:MET:HB2	1.79	0.64
1:D:33:CYS:HB3	1:D:43:VAL:HG12	1.79	0.64
1:A:276:GLU:HG3	1:A:277:PRO:HD2	1.79	0.64
1:C:180:LEU:HD22	1:C:261:LEU:HB2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:241:LEU:N	1:B:241:LEU:HD22	2.12	0.64
1:D:49:ARG:O	1:D:53:VAL:HG13	1.97	0.64
1:D:71:GLN:HG3	1:D:72:PRO:HD2	1.80	0.63
1:C:15:THR:HG21	1:C:224:TRP:HE1	1.62	0.63
1:B:83:ASP:OD1	1:B:87:ASP:HA	1.98	0.63
1:B:69:LEU:CD2	1:B:172:ASP:OD2	2.47	0.62
1:D:170:ARG:HE	1:D:170:ARG:C	2.00	0.62
1:B:5:ILE:HG12	1:B:123:LEU:HD23	1.82	0.62
1:A:218:ARG:CG	1:A:221:ARG:NH2	2.58	0.62
1:A:212:ASP:OD2	1:A:221:ARG:NH2	2.33	0.61
1:B:22:ALA:HA	1:B:54:TRP:CZ2	2.35	0.61
1:A:65:CYS:H	1:A:130:ASN:HD21	1.46	0.61
1:B:127:PRO:HD3	1:B:168:ASN:OD1	2.00	0.61
1:A:212:ASP:OD1	1:A:218:ARG:CZ	2.28	0.61
1:D:51:LEU:HD22	1:D:61:ILE:HD11	1.82	0.61
1:A:295:LYS:HE2	1:A:295:LYS:HA	1.81	0.61
1:C:293:PHE:CE1	1:C:297:LEU:HD21	2.36	0.61
1:B:83:ASP:OD2	1:B:87:ASP:HA	2.01	0.60
1:A:218:ARG:HG3	1:A:218:ARG:NH1	2.15	0.60
1:C:224:TRP:O	1:C:228:ILE:HG13	2.01	0.60
1:B:69:LEU:HD11	1:B:133:ILE:CG1	2.31	0.60
1:B:291:GLU:O	1:B:294:VAL:HG12	2.02	0.60
1:A:133:ILE:HG23	1:B:133:ILE:HG23	1.83	0.59
1:C:29:VAL:HG21	1:C:117:ILE:HD13	1.82	0.59
1:A:28:ILE:HG22	1:A:59:ILE:CG2	2.31	0.59
1:D:160:ASN:HD21	1:D:167:PHE:H	1.49	0.59
1:B:294:VAL:O	1:B:298:ARG:HG3	2.01	0.59
1:A:174:GLU:HA	1:A:265:LEU:HD11	1.82	0.59
1:B:211:LEU:O	1:B:221:ARG:NH1	2.36	0.59
1:D:148:PHE:HD2	1:D:150:ILE:HD11	1.67	0.59
1:D:225:LYS:HB3	1:D:226:PRO:HD3	1.83	0.59
1:A:293:PHE:O	1:A:296:ILE:HG13	2.03	0.59
1:A:253:ILE:HG23	1:A:285:VAL:HG13	1.83	0.59
1:C:129:THR:O	1:C:133:ILE:HG13	2.02	0.59
1:C:239:ASP:CB	1:C:240:PRO:HD3	2.33	0.59
1:A:214:ASN:ND2	1:A:217:ARG:HD2	2.17	0.59
1:C:53:VAL:HG21	1:C:219:PHE:CD2	2.37	0.58
1:C:195:LEU:O	1:C:199:ASN:ND2	2.31	0.58
1:B:81:GLY:HA3	1:B:87:ASP:OD2	2.03	0.58
1:B:212:ASP:OD1	1:B:218:ARG:NH1	2.37	0.58
1:C:244:PHE:HE1	1:C:292:LEU:HD23	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:ALA:H	1:B:166:GLU:HB2	1.69	0.58
1:C:12:ASP:HB2	1:C:239:ASP:HB2	1.85	0.58
1:A:12:ASP:CB	1:A:239:ASP:HB2	2.34	0.58
1:A:68:PRO:HD2	1:A:73:LYS:HA	1.86	0.58
1:A:174:GLU:O	1:A:178:ILE:HG13	2.04	0.58
1:B:41:GLN:CD	1:B:41:GLN:H	2.07	0.58
1:D:195:LEU:O	1:D:199:ASN:HB2	2.03	0.58
1:D:160:ASN:OD1	1:D:160:ASN:N	2.37	0.57
1:A:103:LYS:O	1:A:103:LYS:HG2	2.04	0.57
1:C:51:LEU:HD12	1:C:61:ILE:HD11	1.86	0.57
1:C:151:MET:SD	3:C:401:R1Y:C11	2.92	0.57
1:B:162:THR:CB	1:B:163:PRO:CD	2.82	0.57
1:B:242:ALA:O	1:B:245:ILE:HG13	2.03	0.57
1:B:254:LYS:CB	1:B:287:GLU:HG3	2.34	0.57
1:D:258:ARG:HA	1:D:282:CYS:O	2.05	0.57
1:B:69:LEU:HD23	1:B:175:ALA:HB2	1.87	0.57
1:C:12:ASP:OD2	1:C:80:HIS:HE1	1.88	0.57
1:D:206:TYR:HB3	1:D:208:PHE:CE1	2.40	0.56
1:B:255:ARG:HB3	1:B:287:GLU:OE2	2.05	0.56
1:A:239:ASP:N	1:A:240:PRO:CD	2.68	0.56
1:D:64:GLY:HA3	1:D:130:ASN:HD21	1.69	0.56
1:C:44:ILE:O	1:C:48:ASN:ND2	2.29	0.56
1:C:204:ASN:HD22	1:C:204:ASN:H	1.53	0.56
1:D:79:ILE:HD13	1:D:230:PHE:CZ	2.41	0.56
1:A:214:ASN:HD21	1:A:217:ARG:HD2	1.71	0.56
1:A:217:ARG:HG2	1:A:301:GLN:HB3	1.88	0.56
1:C:268:GLU:HG2	1:C:269:LYS:HD3	1.88	0.56
1:A:180:LEU:HD11	1:A:263:MET:HG2	1.88	0.55
1:D:177:GLN:HA	1:D:180:LEU:HD12	1.87	0.55
1:D:264:VAL:HG11	1:D:269:LYS:HB2	1.88	0.55
1:C:64:GLY:HA3	1:C:130:ASN:HD21	1.71	0.55
1:A:34:ILE:HB	1:A:130:ASN:OD1	2.05	0.55
1:D:154:ALA:HB1	1:D:194:THR:HG23	1.88	0.55
1:D:160:ASN:HB3	1:D:193:TRP:CE2	2.40	0.55
1:C:258:ARG:HA	1:C:282:CYS:O	2.05	0.55
1:D:166:GLU:HG3	1:D:193:TRP:HB2	1.88	0.55
1:D:6:ASP:OD1	1:D:32:SER:OG	2.12	0.55
1:D:218:ARG:NH1	1:D:221:ARG:HH22	2.05	0.55
1:B:212:ASP:OD1	1:B:218:ARG:CZ	2.55	0.55
1:B:46:ASN:O	1:B:50:THR:HG23	2.07	0.55
1:A:217:ARG:NH1	1:A:301:GLN:O	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLU:CD	1:B:266:GLU:HA	2.26	0.55
1:D:135:LEU:HD13	1:D:135:LEU:O	2.07	0.55
1:A:211:LEU:O	1:A:217:ARG:HB3	2.07	0.54
1:C:248:TYR:OH	1:C:296:ILE:HD12	2.07	0.54
1:D:129:THR:O	1:D:133:ILE:HG12	2.07	0.54
1:D:53:VAL:HG11	1:D:219:PHE:CD1	2.42	0.54
1:A:193:TRP:O	1:A:197:VAL:HG23	2.07	0.54
1:A:218:ARG:NH1	1:A:221:ARG:HH22	1.83	0.54
1:A:239:ASP:H	1:A:240:PRO:CD	2.20	0.54
1:C:15:THR:HA	1:C:18:LEU:HD12	1.89	0.54
1:C:11:ILE:HD13	1:C:227:ILE:HG12	1.90	0.54
1:D:73:LYS:O	1:D:74:MET:HG2	2.08	0.54
1:C:211:LEU:HB3	1:C:217:ARG:HD3	1.90	0.54
1:C:61:ILE:O	1:C:101:LEU:HD12	2.08	0.54
1:B:255:ARG:HH12	1:D:286:LYS:NZ	2.05	0.53
1:D:219:PHE:O	1:D:223:THR:HG23	2.08	0.53
1:C:212:ASP:HB2	1:C:221:ARG:NH1	2.24	0.53
1:D:50:THR:O	1:D:53:VAL:HG22	2.08	0.53
1:A:139:PRO:O	1:A:143:LEU:CD1	2.56	0.53
1:A:291:GLU:HA	1:A:291:GLU:OE1	2.08	0.53
1:C:8:ASP:HB3	1:C:34:ILE:HG23	1.90	0.53
1:C:127:PRO:HD3	1:C:168:ASN:OD1	2.08	0.53
1:D:240:PRO:HB2	1:D:293:PHE:HZ	1.73	0.53
1:B:237:PRO:HB2	1:B:241:LEU:HD21	1.81	0.53
1:B:258:ARG:O	1:B:259:LEU:HD23	2.09	0.53
1:A:10:GLY:HA2	1:A:84:GLY:O	2.09	0.53
1:C:112:HIS:CE1	1:C:116:THR:HG21	2.44	0.53
1:A:23:ASN:HB3	1:A:26:ILE:CD1	2.38	0.53
1:C:264:VAL:O	1:C:270:LEU:O	2.27	0.53
1:C:223:THR:O	1:C:226:PRO:HD2	2.08	0.53
1:D:162:THR:OG1	1:D:165:GLY:C	2.47	0.53
1:B:185:GLN:HE22	1:B:261:LEU:N	2.05	0.52
1:D:113:ALA:O	1:D:117:ILE:HG12	2.09	0.52
1:B:255:ARG:HH22	1:D:286:LYS:HD2	1.75	0.52
1:C:125:LEU:HB3	1:C:239:ASP:OD1	2.10	0.52
1:B:258:ARG:NH1	1:B:281:GLY:O	2.39	0.52
1:B:14:ALA:HB1	1:B:50:THR:HG21	1.91	0.52
1:B:195:LEU:HD22	1:B:285:VAL:HG23	1.90	0.52
1:C:191:ALA:HA	1:C:195:LEU:HD23	1.92	0.52
1:D:166:GLU:OE2	3:D:401:R1Y:O12	2.28	0.52
1:A:41:GLN:OE1	1:A:45:ARG:NH1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:LEU:O	1:A:270:LEU:HG	2.10	0.52
1:D:155:GLU:HA	1:D:273:SER:HB2	1.92	0.52
1:A:195:LEU:HG	1:A:241:LEU:HD13	1.92	0.52
1:C:4:TRP:HB3	1:C:122:ILE:HD13	1.92	0.51
1:D:38:ALA:HB2	1:D:84:GLY:HA3	1.92	0.51
1:D:135:LEU:HD22	1:D:139:PRO:HA	1.92	0.51
1:B:119:ASP:CA	1:B:146:LYS:CE	2.79	0.51
1:B:9:CYS:HA	1:B:13:ASP:CB	2.41	0.51
1:D:10:GLY:HA2	1:D:84:GLY:O	2.10	0.51
1:D:163:PRO:HB2	1:D:164:TYR:CD1	2.45	0.51
1:B:52:LYS:HE2	1:B:97:THR:HG21	1.93	0.51
1:A:51:LEU:HD12	1:A:61:ILE:HD11	1.92	0.51
1:B:241:LEU:CD2	1:B:241:LEU:N	2.74	0.51
1:C:227:ILE:O	1:C:231:ASP:HB2	2.10	0.51
1:A:28:ILE:HG22	1:A:28:ILE:O	2.09	0.51
1:D:41:GLN:O	1:D:45:ARG:HG3	2.11	0.51
1:A:218:ARG:CG	1:A:221:ARG:HH22	2.21	0.51
1:A:224:TRP:O	1:A:228:ILE:HG13	2.10	0.51
1:B:159:GLY:HA3	1:B:165:GLY:O	2.10	0.51
1:C:212:ASP:HB2	1:C:221:ARG:HH12	1.76	0.51
1:D:170:ARG:O	1:D:173:PRO:HD3	2.11	0.51
1:C:135:LEU:HD13	1:C:182:THR:HB	1.93	0.51
1:D:4:TRP:HB3	1:D:122:ILE:HD13	1.92	0.51
1:B:135:LEU:HD13	1:B:182:THR:HB	1.92	0.50
1:D:210:ASN:O	1:D:211:LEU:HD23	2.11	0.50
1:A:185:GLN:HB3	1:A:282:CYS:SG	2.51	0.50
1:A:217:ARG:CG	1:A:301:GLN:HB3	2.41	0.50
1:C:244:PHE:CE1	1:C:292:LEU:HD23	2.46	0.50
1:A:295:LYS:NZ	1:A:298:ARG:CD	2.70	0.50
1:B:155:GLU:OE2	1:B:286:LYS:NZ	2.43	0.50
1:A:166:GLU:O	1:A:170:ARG:NH2	2.45	0.50
1:A:166:GLU:OE2	1:A:168:ASN:HB2	2.12	0.50
1:A:70:VAL:HG12	1:B:178:ILE:CD1	2.31	0.50
1:A:51:LEU:CD1	1:A:61:ILE:HD11	2.41	0.49
1:D:26:ILE:HG13	1:D:247:VAL:HG13	1.94	0.49
1:A:111:ILE:HG12	1:A:138:ALA:HB3	1.94	0.49
1:A:132:ALA:HB1	1:A:178:ILE:HD12	1.94	0.49
1:A:180:LEU:HD12	1:A:263:MET:HG2	1.92	0.49
1:A:28:ILE:HG22	1:A:59:ILE:HG23	1.95	0.49
1:B:264:VAL:O	1:B:270:LEU:HA	2.13	0.49
1:A:127:PRO:HD3	1:A:168:ASN:OD1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:11:ILE:HG21	1:A:224:TRP:HA	1.93	0.49
1:D:33:CYS:O	1:D:64:GLY:N	2.39	0.49
1:B:170:ARG:O	1:B:170:ARG:HD3	2.12	0.49
1:D:218:ARG:HH11	1:D:221:ARG:HH22	1.60	0.49
1:D:164:TYR:HB3	1:D:272:MET:SD	2.52	0.49
1:A:9:CYS:HA	1:A:13:ASP:HB2	1.93	0.49
1:B:161:ILE:HD11	1:B:167:PHE:CB	2.43	0.49
1:A:65:CYS:SG	1:A:130:ASN:ND2	2.86	0.49
1:C:190:ILE:HD12	1:C:190:ILE:N	2.27	0.49
1:D:135:LEU:HD11	1:D:182:THR:HB	1.95	0.49
1:B:103:LYS:O	1:B:103:LYS:HD3	2.13	0.48
1:B:23:ASN:OD1	1:B:25:SER:HB3	2.14	0.48
1:A:174:GLU:HA	1:A:265:LEU:CD1	2.42	0.48
1:D:34:ILE:HD12	1:D:65:CYS:O	2.13	0.48
1:A:139:PRO:O	1:A:143:LEU:HD13	2.14	0.48
1:B:50:THR:HA	1:B:53:VAL:HG12	1.94	0.48
1:A:13:ASP:O	1:A:17:ILE:HG12	2.14	0.48
1:B:86:GLY:HA2	1:B:226:PRO:HG2	1.94	0.48
1:B:237:PRO:CB	1:B:241:LEU:HD21	2.40	0.48
1:C:156:ASN:HB2	1:C:163:PRO:HG3	1.96	0.48
1:D:71:GLN:HG2	1:D:170:ARG:NH2	2.29	0.48
1:D:255:ARG:HD2	1:D:287:GLU:OE2	2.13	0.48
1:A:262:SER:O	1:A:262:SER:OG	2.31	0.48
1:B:119:ASP:CG	1:B:146:LYS:HE3	2.35	0.48
1:D:151:MET:HB3	1:D:151:MET:HE3	1.69	0.47
1:A:34:ILE:HD11	1:A:129:THR:HB	1.95	0.47
1:B:75:GLU:N	1:B:75:GLU:OE1	2.48	0.47
1:C:198:PHE:CE2	1:C:287:GLU:HG3	2.46	0.47
1:B:142:ILE:HG23	1:B:145:ILE:HD12	1.95	0.47
1:A:12:ASP:CG	1:A:239:ASP:HB2	2.35	0.47
1:A:137:MET:HE3	1:B:107:VAL:HB	1.97	0.47
1:A:239:ASP:H	1:A:240:PRO:HD2	1.78	0.47
1:B:40:LEU:HD23	1:B:66:GLN:HG3	1.97	0.47
1:C:15:THR:O	1:C:19:ILE:HG13	2.15	0.47
1:C:40:LEU:O	1:C:43:VAL:HB	2.15	0.47
1:C:123:LEU:HD11	1:C:125:LEU:HD21	1.97	0.47
1:D:79:ILE:HG23	1:D:230:PHE:CD2	2.49	0.47
1:B:67:ALA:HB1	1:B:68:PRO:CD	2.45	0.47
1:B:255:ARG:HD2	1:B:287:GLU:OE2	2.15	0.47
1:B:206:TYR:HB3	1:B:208:PHE:CE2	2.50	0.47
1:C:231:ASP:OD2	3:C:401:R1Y:N16	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:223:THR:O	1:D:226:PRO:HD2	2.15	0.47
1:C:201:PHE:CD2	1:C:208:PHE:HZ	2.32	0.46
1:C:28:ILE:HD12	1:C:28:ILE:H	1.80	0.46
1:C:88:ILE:HG13	1:C:88:ILE:O	2.16	0.46
1:C:239:ASP:CB	1:C:240:PRO:CD	2.93	0.46
1:D:117:ILE:HD11	1:D:120:LEU:HD13	1.96	0.46
1:D:49:ARG:HG2	1:D:95:THR:HG21	1.98	0.46
1:B:174:GLU:HG3	1:B:265:LEU:CD2	2.45	0.46
1:B:151:MET:HG3	1:B:238:ALA:O	2.16	0.46
1:D:107:VAL:HG21	1:D:133:ILE:CG1	2.45	0.46
1:D:90:ASP:HB3	1:D:95:THR:C	2.36	0.46
1:B:36:GLY:O	1:B:77:PRO:HG3	2.16	0.46
1:B:119:ASP:CA	1:B:146:LYS:HE3	2.43	0.46
1:B:11:ILE:HD12	1:B:80:HIS:ND1	2.31	0.46
1:C:21:LEU:HB3	1:C:54:TRP:CD1	2.50	0.46
1:A:79:ILE:HG12	1:A:230:PHE:CE1	2.50	0.45
1:B:69:LEU:HD11	1:B:133:ILE:HG13	1.98	0.45
1:C:42:ASN:O	1:C:46:ASN:ND2	2.49	0.45
1:B:3:LEU:HD11	1:B:123:LEU:HB2	1.98	0.45
1:B:180:LEU:HD22	1:B:261:LEU:HB2	1.99	0.45
1:A:13:ASP:OD2	1:A:239:ASP:OD2	2.34	0.45
1:C:16:ALA:HB2	1:C:239:ASP:HB3	1.98	0.45
1:B:218:ARG:HH11	1:B:221:ARG:NH2	2.11	0.45
1:B:119:ASP:CA	1:B:146:LYS:HE2	2.27	0.45
1:A:40:LEU:O	1:A:44:ILE:HG13	2.17	0.45
1:C:237:PRO:O	1:C:241:LEU:HD12	2.15	0.45
1:A:166:GLU:OE1	1:A:169:TRP:HB2	2.17	0.45
1:D:263:MET:HE1	1:D:272:MET:O	2.17	0.45
1:D:273:SER:O	1:D:274:LEU:HD23	2.17	0.45
1:C:227:ILE:HD13	1:C:227:ILE:HA	1.69	0.45
1:D:51:LEU:CD2	1:D:61:ILE:HD11	2.46	0.45
1:B:68:PRO:HG2	1:B:71:GLN:O	2.17	0.44
1:A:71:GLN:HG3	1:A:173:PRO:HD2	1.99	0.44
1:A:239:ASP:N	1:A:240:PRO:HD2	2.32	0.44
1:B:237:PRO:CG	1:B:241:LEU:HD21	2.47	0.44
1:B:277:PRO:HD2	1:D:164:TYR:CE2	2.52	0.44
1:C:190:ILE:HD13	1:C:282:CYS:HB3	1.97	0.44
1:B:43:VAL:O	1:B:47:VAL:HG13	2.17	0.44
1:C:122:ILE:HG22	1:C:124:CYS:SG	2.57	0.44
1:D:151:MET:SD	1:D:238:ALA:HB1	2.57	0.44
1:A:114:ALA:HB1	1:A:141:ALA:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLU:CG	1:B:266:GLU:HA	2.47	0.44
1:B:156:ASN:HB2	1:B:194:THR:HG21	1.98	0.44
1:A:256:ALA:HB1	1:A:283:LEU:HD22	1.99	0.44
1:B:122:ILE:HG22	1:B:148:PHE:HA	1.99	0.44
1:B:154:ALA:HB2	1:B:193:TRP:HB3	1.98	0.44
1:B:188:THR:OG1	1:B:282:CYS:SG	2.73	0.44
1:D:227:ILE:HD11	3:D:401:R1Y:N02	2.32	0.44
1:D:33:CYS:HB3	1:D:43:VAL:CG1	2.46	0.44
1:B:174:GLU:CD	1:B:265:LEU:HD23	2.38	0.44
1:C:64:GLY:CA	1:C:130:ASN:HD21	2.31	0.44
1:A:199:ASN:O	1:A:237:PRO:HD2	2.17	0.44
1:B:11:ILE:HD13	1:B:227:ILE:HB	2.00	0.44
1:A:139:PRO:O	1:A:143:LEU:HD12	2.17	0.43
1:A:214:ASN:OD1	1:A:217:ARG:CG	2.60	0.43
1:D:107:VAL:HG21	1:D:133:ILE:CD1	2.48	0.43
1:A:56:LYS:HE3	1:A:56:LYS:HB2	1.80	0.43
1:B:250:ASP:HA	1:B:253:ILE:CG2	2.42	0.43
1:A:28:ILE:N	1:A:28:ILE:CD1	2.79	0.43
1:B:146:LYS:HE2	1:B:146:LYS:HB2	1.87	0.43
1:C:56:LYS:HB2	1:C:56:LYS:HE3	1.25	0.43
1:C:98:PRO:HG2	1:D:74:MET:HB3	2.00	0.43
1:C:170:ARG:O	1:C:173:PRO:HD3	2.18	0.43
1:D:160:ASN:HD21	1:D:166:GLU:HG2	1.83	0.43
1:A:122:ILE:HG22	1:A:148:PHE:HA	1.99	0.43
1:B:90:ASP:OD1	1:B:95:THR:OG1	2.31	0.43
1:A:151:MET:CG	1:A:238:ALA:O	2.64	0.43
1:C:21:LEU:HB3	1:C:54:TRP:NE1	2.33	0.43
1:C:107:VAL:O	1:C:110:LEU:HB3	2.19	0.43
1:C:176:ALA:O	1:C:180:LEU:HD12	2.18	0.43
1:A:213:GLY:N	1:A:217:ARG:HD3	2.34	0.43
1:B:48:ASN:O	1:B:52:LYS:HG2	2.18	0.43
1:B:295:LYS:HD3	1:B:295:LYS:HA	1.68	0.43
1:C:297:LEU:O	1:C:300:LEU:HG	2.18	0.43
1:B:201:PHE:CD1	1:B:208:PHE:HZ	2.37	0.43
1:D:46:ASN:HA	1:D:49:ARG:HD2	2.01	0.43
1:D:79:ILE:HD13	1:D:230:PHE:CE2	2.54	0.43
1:A:180:LEU:CD1	1:A:263:MET:CG	2.94	0.43
1:B:116:THR:O	1:B:116:THR:HG22	2.19	0.43
1:B:161:ILE:CD1	1:B:167:PHE:HD1	2.28	0.43
1:B:269:LYS:HB3	1:B:272:MET:CG	2.46	0.42
1:C:46:ASN:HA	1:C:49:ARG:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:GLN:NE2	1:C:181:GLN:HB3	2.33	0.42
1:D:176:ALA:O	1:D:179:VAL:HG22	2.19	0.42
1:C:135:LEU:CD1	1:C:179:VAL:HA	2.49	0.42
1:C:205:ASP:OD2	1:C:205:ASP:N	2.51	0.42
1:D:141:ALA:O	1:D:144:LYS:HB2	2.19	0.42
1:A:28:ILE:N	1:A:28:ILE:HD13	2.35	0.42
1:A:241:LEU:HD21	1:A:288:CYS:SG	2.59	0.42
1:B:61:ILE:O	1:B:102:GLU:HG2	2.19	0.42
1:B:143:LEU:HD23	1:B:184:PRO:HD3	2.01	0.42
1:C:210:ASN:OD1	1:C:221:ARG:HD3	2.19	0.42
1:B:2:LYS:NZ	1:B:29:VAL:HG11	2.34	0.42
1:B:173:PRO:HG3	1:B:270:LEU:HD11	2.02	0.42
1:A:214:ASN:HD21	1:A:217:ARG:HH11	1.67	0.42
1:A:266:GLU:HG2	1:B:266:GLU:CG	2.50	0.42
1:A:290:ALA:O	1:A:294:VAL:HG22	2.19	0.42
1:B:14:ALA:CB	1:B:50:THR:HG21	2.49	0.42
1:B:128:LEU:HD22	1:B:179:VAL:HG21	2.01	0.42
1:B:221:ARG:O	1:B:225:LYS:HG3	2.19	0.42
1:B:237:PRO:CG	1:B:241:LEU:CD2	2.97	0.42
1:A:50:THR:HG22	1:A:219:PHE:CZ	2.55	0.42
1:A:248:TYR:CE2	1:A:296:ILE:HG21	2.55	0.42
1:B:69:LEU:HD11	1:B:133:ILE:HG12	2.02	0.42
1:D:15:THR:O	1:D:19:ILE:HG13	2.19	0.42
1:A:269:LYS:H	1:A:269:LYS:HG2	1.65	0.42
1:B:80:HIS:HB3	1:B:84:GLY:O	2.20	0.42
1:C:177:GLN:HE21	1:C:181:GLN:HB3	1.84	0.42
1:D:95:THR:HG22	1:D:95:THR:O	2.20	0.42
1:B:169:TRP:HB3	1:B:263:MET:HE1	2.02	0.42
1:D:112:HIS:O	1:D:116:THR:HG23	2.19	0.42
1:B:153:GLY:O	1:B:192:SER:HB2	2.20	0.41
1:C:204:ASN:H	1:C:204:ASN:ND2	2.16	0.41
1:A:196:ALA:HB2	1:A:238:ALA:HA	2.01	0.41
1:B:228:ILE:HD11	1:B:235:ILE:HG12	2.02	0.41
1:D:17:ILE:O	1:D:21:LEU:HD13	2.20	0.41
1:D:133:ILE:HD13	1:D:133:ILE:HG21	1.81	0.41
1:B:2:LYS:HE3	1:B:117:ILE:HG23	2.03	0.41
1:C:174:GLU:O	1:C:178:ILE:HG12	2.20	0.41
1:D:107:VAL:HG13	1:D:134:ALA:HB2	2.03	0.41
1:D:135:LEU:HD13	1:D:135:LEU:C	2.40	0.41
1:A:34:ILE:CD1	1:A:129:THR:HB	2.50	0.41
1:A:174:GLU:CG	1:A:265:LEU:HD11	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:PHE:CD2	1:A:208:PHE:HZ	2.37	0.41
1:B:148:PHE:HB2	1:B:188:THR:HG22	2.03	0.41
1:C:5:ILE:HD13	1:C:123:LEU:HB3	2.01	0.41
1:D:57:THR:O	1:D:57:THR:OG1	2.36	0.41
1:C:254:LYS:HE3	1:C:288:CYS:O	2.21	0.41
1:B:117:ILE:HG21	1:B:120:LEU:HD13	2.02	0.41
1:B:172:ASP:HB3	1:B:175:ALA:HB3	2.03	0.41
1:B:228:ILE:HD11	1:B:235:ILE:CG1	2.51	0.41
1:D:5:ILE:HD12	1:D:123:LEU:HD23	2.02	0.41
1:D:7:THR:OG1	1:D:13:ASP:HB3	2.20	0.41
1:A:50:THR:HG22	1:A:219:PHE:HZ	1.84	0.41
1:A:58:ASP:OD1	1:A:58:ASP:N	2.54	0.41
1:A:151:MET:HE3	1:A:238:ALA:O	2.21	0.41
1:B:62:PHE:CE2	1:B:102:GLU:HG3	2.56	0.41
1:B:162:THR:CB	1:B:163:PRO:HD2	2.46	0.41
1:B:264:VAL:CG2	1:B:272:MET:HB2	2.49	0.41
1:C:56:LYS:O	1:C:56:LYS:HG3	2.20	0.41
1:C:283:LEU:HA	1:C:283:LEU:HD12	1.81	0.41
1:D:26:ILE:HG21	1:D:247:VAL:HG22	2.03	0.41
1:A:166:GLU:O	1:A:170:ARG:CZ	2.68	0.41
1:A:174:GLU:CA	1:A:265:LEU:HD11	2.51	0.41
1:C:57:THR:O	1:C:57:THR:OG1	2.30	0.41
1:A:295:LYS:HZ1	1:A:298:ARG:NE	2.18	0.40
1:C:294:VAL:HA	1:C:297:LEU:HG	2.03	0.40
1:D:12:ASP:HB2	1:D:240:PRO:CD	2.46	0.40
1:A:225:LYS:HB2	1:A:226:PRO:HD3	2.03	0.40
1:B:2:LYS:NZ	1:B:2:LYS:HB3	2.36	0.40
1:B:169:TRP:HB3	1:B:263:MET:CE	2.52	0.40
1:D:34:ILE:HD13	1:D:130:ASN:OD1	2.21	0.40
1:D:154:ALA:O	1:D:273:SER:OG	2.36	0.40
1:A:113:ALA:O	1:A:117:ILE:HB	2.21	0.40
1:B:228:ILE:HD13	1:B:228:ILE:HA	1.90	0.40
1:C:154:ALA:HB2	1:C:166:GLU:HB2	2.03	0.40
1:D:9:CYS:H	1:D:43:VAL:HG13	1.87	0.40
1:D:79:ILE:H	1:D:79:ILE:HG12	1.69	0.40
1:D:235:ILE:O	1:D:237:PRO:HD3	2.21	0.40
1:D:253:ILE:HG23	1:D:285:VAL:HG13	2.02	0.40
1:C:110:LEU:O	1:C:113:ALA:HB3	2.21	0.40
1:C:210:ASN:HA	1:C:221:ARG:HB2	2.03	0.40
1:D:192:SER:O	1:D:195:LEU:HB3	2.22	0.40

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

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:LEU:N	1:A:276:GLU:OE2[1_655]	1.92	0.28
1:A:215:LEU:CB	1:A:276:GLU:OE2[1_655]	2.12	0.08

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	301/304 (99%)	272 (90%)	24 (8%)	5 (2%)	9 31
1	B	302/304 (99%)	271 (90%)	29 (10%)	2 (1%)	22 54
1	C	297/304 (98%)	266 (90%)	28 (9%)	3 (1%)	15 45
1	D	302/304 (99%)	270 (89%)	27 (9%)	5 (2%)	9 31
All	All	1202/1216 (99%)	1079 (90%)	108 (9%)	15 (1%)	13 40

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	163	PRO
1	D	9	CYS
1	A	9	CYS
1	B	9	CYS
1	C	9	CYS
1	C	203	ALA
1	D	157	GLY
1	D	249	GLY
1	A	213	GLY
1	A	277	PRO
1	B	153	GLY
1	D	277	PRO
1	D	281	GLY
1	A	159	GLY
1	C	237	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	249/250 (100%)	230 (92%)	19 (8%)	13	36
1	B	250/250 (100%)	238 (95%)	12 (5%)	25	58
1	C	244/250 (98%)	233 (96%)	11 (4%)	27	61
1	D	250/250 (100%)	235 (94%)	15 (6%)	19	49
All	All	993/1000 (99%)	936 (94%)	57 (6%)	20	51

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	27	GLU
1	A	28	ILE
1	A	151	MET
1	A	162	THR
1	A	164	TYR
1	A	204	ASN
1	A	205	ASP
1	A	210	ASN
1	A	214	ASN
1	A	234	ARG
1	A	259	LEU
1	A	265	LEU
1	A	269	LYS
1	A	270	LEU
1	A	274	LEU
1	A	283	LEU
1	A	292	LEU
1	A	299	GLU
1	B	79	ILE
1	B	103	LYS
1	B	151	MET
1	B	158	LYS
1	B	162	THR

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Mol	Chain	Res	Type
1	B	164	TYR
1	B	204	ASN
1	B	205	ASP
1	B	218	ARG
1	B	254	LYS
1	B	262	SER
1	B	270	LEU
1	C	56	LYS
1	C	151	MET
1	C	200	SER
1	C	204	ASN
1	C	205	ASP
1	C	211	LEU
1	C	225	LYS
1	C	269	LYS
1	C	270	LEU
1	C	273	SER
1	C	276	GLU
1	D	9	CYS
1	D	13	ASP
1	D	39	SER
1	D	52	LYS
1	D	79	ILE
1	D	118	GLU
1	D	161	ILE
1	D	170	ARG
1	D	199	ASN
1	D	205	ASP
1	D	208	PHE
1	D	255	ARG
1	D	269	LYS
1	D	299	GLU
1	D	300	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	210	ASN
1	A	303	HIS
1	B	42	ASN
1	B	185	GLN

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Mol	Chain	Res	Type
1	B	260	HIS
1	C	46	ASN
1	C	130	ASN
1	C	202	ASN
1	D	91	ASN
1	D	96	ASN
1	D	156	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	R1Y	D	401	2	15,18,18	5.06	10 (66%)	14,26,26	2.41	5 (35%)
3	R1Y	B	401	2	15,18,18	5.13	10 (66%)	14,26,26	2.83	6 (42%)
3	R1Y	C	401	2	15,18,18	5.22	11 (73%)	14,26,26	2.37	1 (7%)

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
3	R1Y	D	401	2	-	2/2/26/26	0/2/2/2
3	R1Y	B	401	2	-	2/2/26/26	0/2/2/2
3	R1Y	C	401	2	-	0/2/26/26	0/2/2/2

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	401	R1Y	O10-C06	11.08	1.56	1.41
3	D	401	R1Y	O10-C06	10.83	1.56	1.41
3	B	401	R1Y	O10-C06	10.46	1.55	1.41
3	B	401	R1Y	C08-C07	-8.56	1.29	1.53
3	C	401	R1Y	C08-C07	-8.46	1.30	1.53
3	D	401	R1Y	C08-C07	-8.37	1.30	1.53
3	B	401	R1Y	C15-N17	6.49	1.50	1.33
3	B	401	R1Y	C03-C15	6.42	1.56	1.48
3	B	401	R1Y	C08-C09	6.13	1.68	1.53
3	D	401	R1Y	C15-N17	6.10	1.49	1.33
3	C	401	R1Y	C03-C15	6.01	1.56	1.48
3	D	401	R1Y	C08-C09	5.82	1.67	1.53
3	C	401	R1Y	C03-N04	-5.76	1.28	1.34
3	C	401	R1Y	C08-C09	5.73	1.67	1.53
3	B	401	R1Y	O10-C09	-5.63	1.32	1.45
3	D	401	R1Y	O10-C09	-5.53	1.32	1.45
3	D	401	R1Y	C03-C15	5.50	1.55	1.48
3	C	401	R1Y	O10-C09	-5.15	1.33	1.45
3	D	401	R1Y	C03-N04	-5.10	1.29	1.34
3	C	401	R1Y	C15-N16	5.08	1.49	1.28
3	B	401	R1Y	C03-N04	-4.95	1.29	1.34
3	C	401	R1Y	C07-C06	4.83	1.61	1.53
3	D	401	R1Y	C07-C06	4.54	1.60	1.53
3	C	401	R1Y	C15-N17	-4.04	1.23	1.33
3	B	401	R1Y	C07-C06	3.35	1.58	1.53
3	B	401	R1Y	C01-N02	-2.93	1.30	1.35
3	C	401	R1Y	C01-N05	-2.83	1.30	1.33
3	B	401	R1Y	C01-N05	-2.82	1.30	1.33
3	D	401	R1Y	C01-N02	-2.75	1.30	1.35
3	C	401	R1Y	C01-N02	-2.74	1.30	1.35
3	D	401	R1Y	C01-N05	-2.39	1.31	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	401	R1Y	N04-C03-N02	-8.20	107.92	114.72
3	B	401	R1Y	N04-C03-N02	-8.05	108.05	114.72
3	D	401	R1Y	N04-C03-N02	-6.53	109.31	114.72
3	B	401	R1Y	C08-C07-C06	4.21	107.32	100.98
3	D	401	R1Y	C08-C07-C06	3.61	106.41	100.98
3	D	401	R1Y	C11-C09-C08	-3.09	107.64	115.09
3	D	401	R1Y	C07-C08-C09	3.03	108.52	102.64
3	B	401	R1Y	C07-C08-C09	2.68	107.86	102.64
3	B	401	R1Y	O10-C09-C08	2.16	109.39	105.11
3	B	401	R1Y	O10-C09-C11	-2.06	104.77	109.21
3	B	401	R1Y	O14-C07-C06	-2.05	103.28	110.85
3	D	401	R1Y	O10-C09-C08	2.02	109.11	105.11

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	401	R1Y	O10-C09-C11-O12
3	D	401	R1Y	C08-C09-C11-O12
3	B	401	R1Y	C08-C09-C11-O12
3	B	401	R1Y	O10-C09-C11-O12

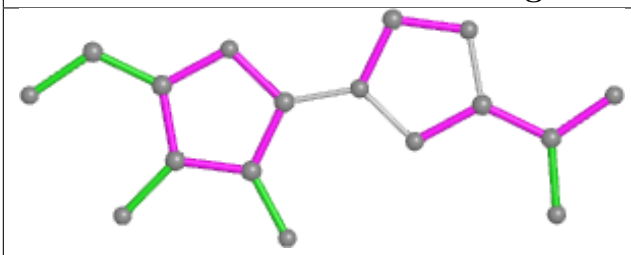
There are no ring outliers.

3 monomers are involved in 5 short contacts:

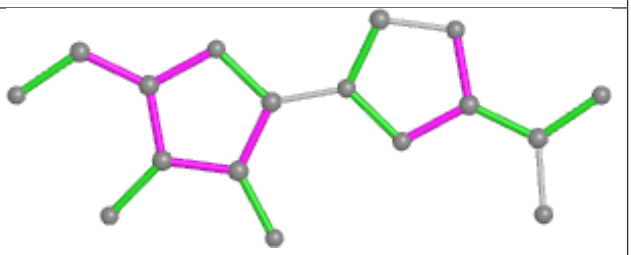
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	401	R1Y	2	0
3	B	401	R1Y	1	0
3	C	401	R1Y	2	0

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.

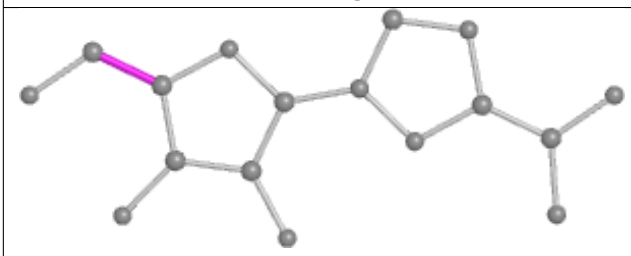
Ligand R1Y D 401



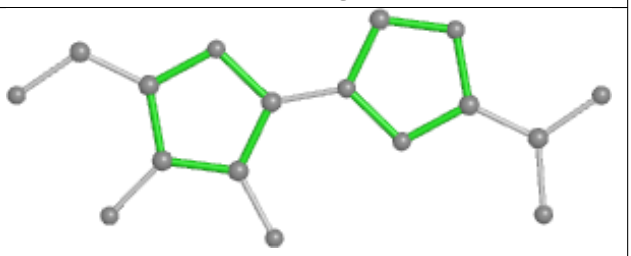
Bond lengths



Bond angles

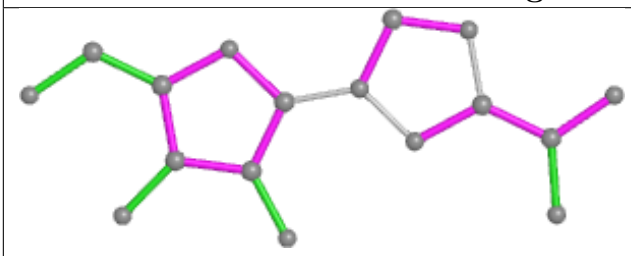


Torsions

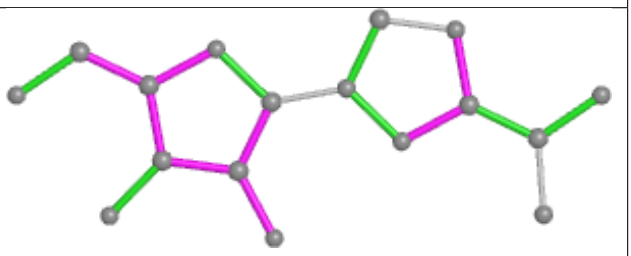


Rings

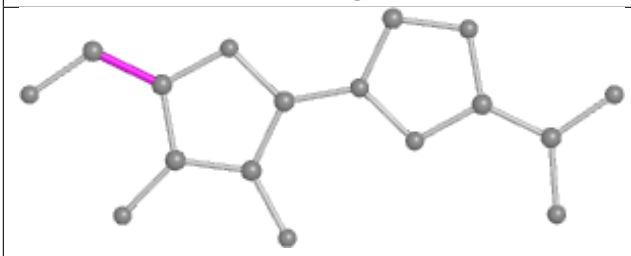
Ligand R1Y B 401



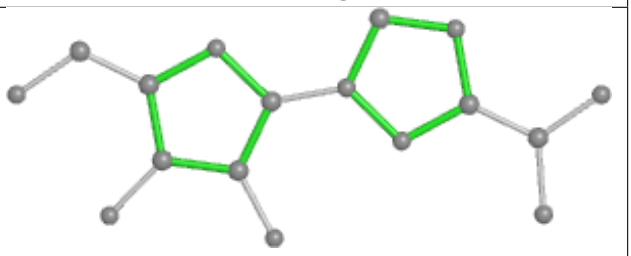
Bond lengths



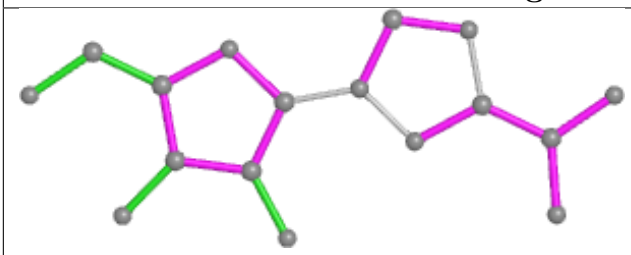
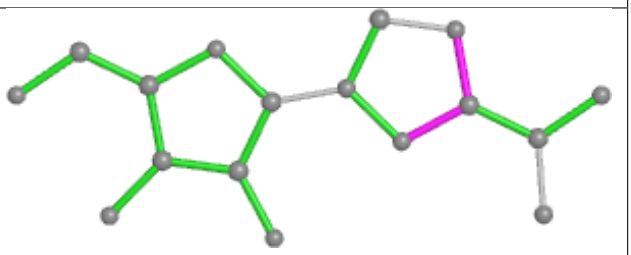
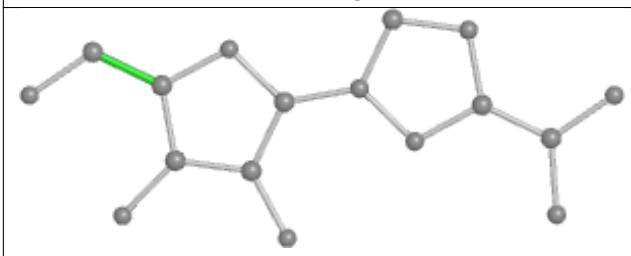
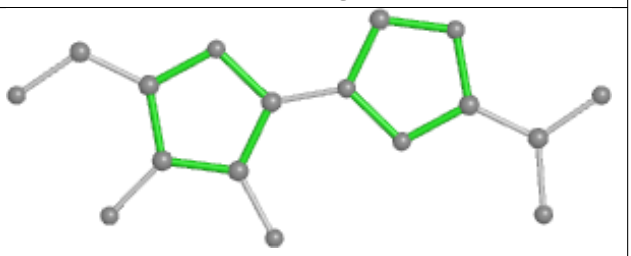
Bond angles



Torsions



Rings

Ligand R1Y C 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	303/304 (99%)	0.36	17 (5%)	24	20	42, 51, 70, 140	0
1	B	304/304 (100%)	0.45	17 (5%)	24	20	41, 56, 76, 98	0
1	C	301/304 (99%)	0.26	11 (3%)	41	37	40, 50, 62, 84	0
1	D	304/304 (100%)	0.35	11 (3%)	42	37	42, 54, 75, 99	0
All	All	1212/1216 (99%)	0.36	56 (4%)	32	29	40, 52, 73, 140	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	159	GLY	11.5
1	B	164	TYR	6.6
1	A	157	GLY	5.1
1	B	163	PRO	5.0
1	C	76	ILE	4.3
1	D	164	TYR	4.0
1	A	156	ASN	3.8
1	D	161	ILE	3.7
1	B	76	ILE	3.6
1	B	165	GLY	3.5
1	D	75	GLU	3.3
1	A	267	GLY	3.3
1	C	159	GLY	3.2
1	A	290	ALA	3.2
1	B	126	ALA	2.9
1	A	249	GLY	2.9
1	D	160	ASN	2.9
1	B	159	GLY	2.8
1	D	168	ASN	2.8
1	A	160	ASN	2.7
1	A	266	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	237	PRO	2.7
1	A	213	GLY	2.7
1	A	119	ASP	2.7
1	B	210	ASN	2.6
1	C	267	GLY	2.6
1	A	158	LYS	2.6
1	C	211	LEU	2.5
1	D	204	ASN	2.5
1	A	238	ALA	2.5
1	C	75	GLU	2.5
1	B	77	PRO	2.5
1	B	303	HIS	2.4
1	A	206	TYR	2.4
1	B	36	GLY	2.3
1	D	74	MET	2.3
1	C	126	ALA	2.3
1	A	161	ILE	2.3
1	C	57	THR	2.3
1	D	126	ALA	2.2
1	D	165	GLY	2.2
1	B	275	ALA	2.2
1	A	208	PHE	2.2
1	B	272	MET	2.2
1	B	161	ILE	2.1
1	C	124	CYS	2.1
1	B	211	LEU	2.1
1	B	162	THR	2.1
1	D	242	ALA	2.1
1	C	80	HIS	2.0
1	C	131	ILE	2.0
1	C	91	ASN	2.0
1	A	117	ILE	2.0
1	D	16	ALA	2.0
1	B	130	ASN	2.0
1	B	158	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

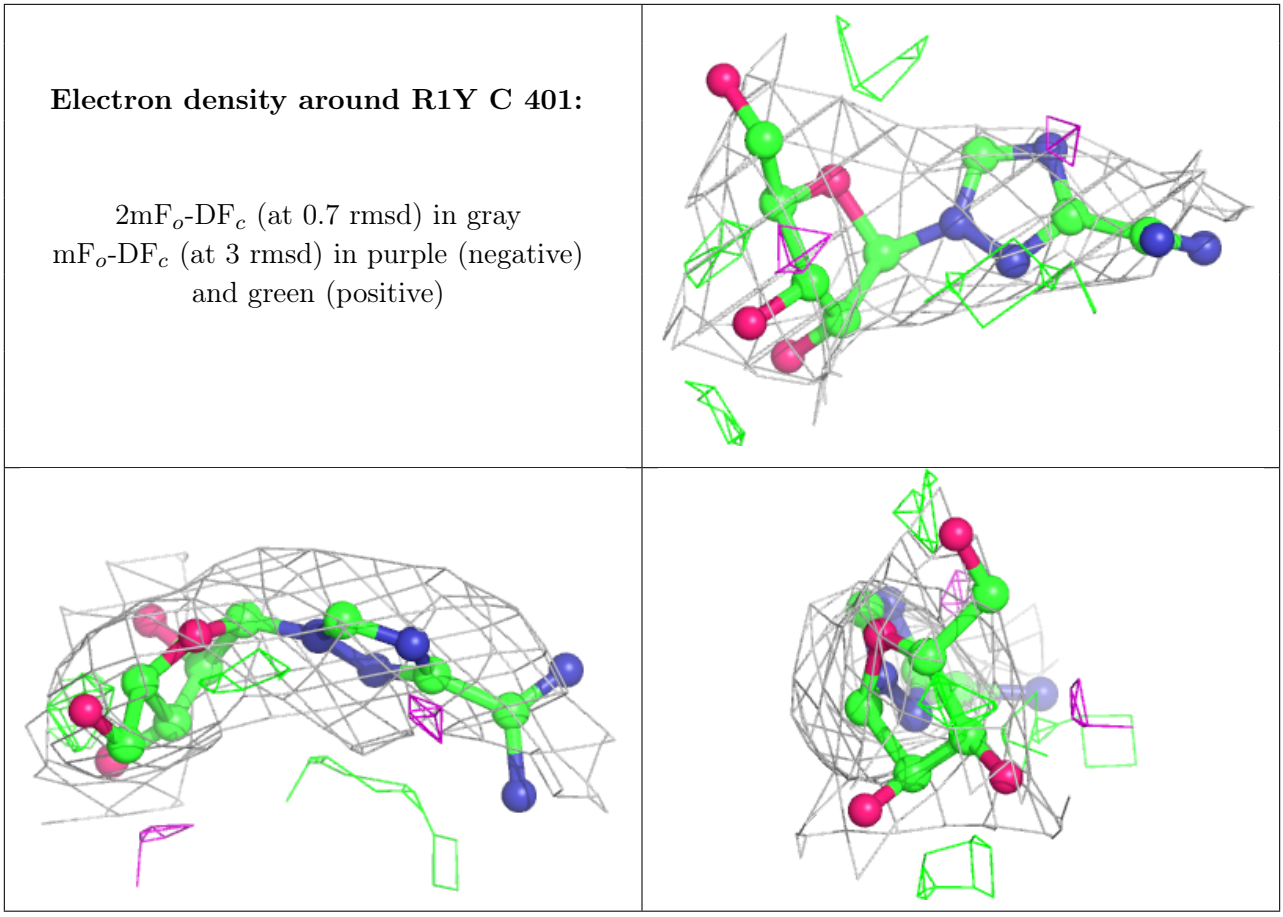
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	R1Y	C	401	17/17	0.80	0.33	53,55,65,66	0
3	R1Y	B	401	17/17	0.85	0.26	54,59,60,62	0
3	R1Y	D	401	17/17	0.85	0.31	54,59,64,68	0
2	CA	A	401	1/1	0.94	0.28	45,45,45,45	0
2	CA	C	402	1/1	0.96	0.32	50,50,50,50	0
2	CA	D	402	1/1	0.97	0.28	51,51,51,51	0
2	CA	B	402	1/1	0.97	0.18	52,52,52,52	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.

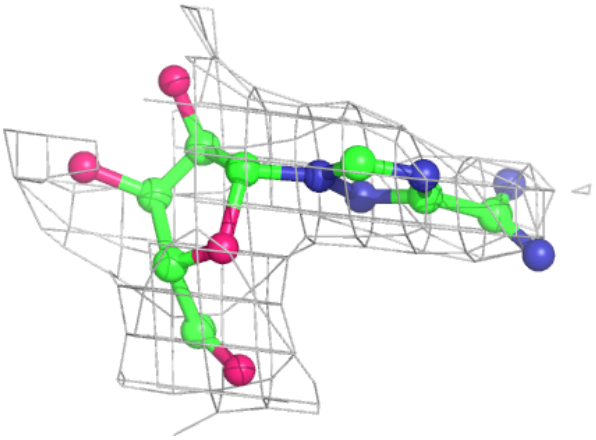
Electron density around R1Y C 401:

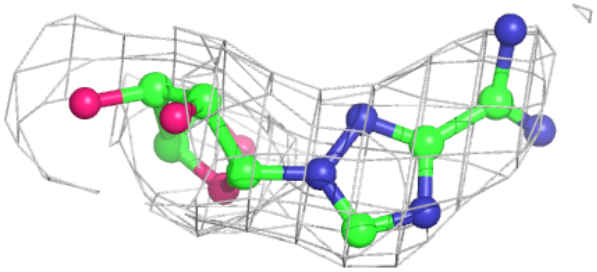
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

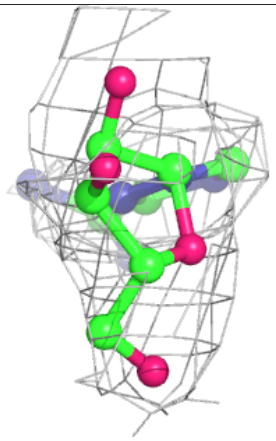


Electron density around R1Y B 401:

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

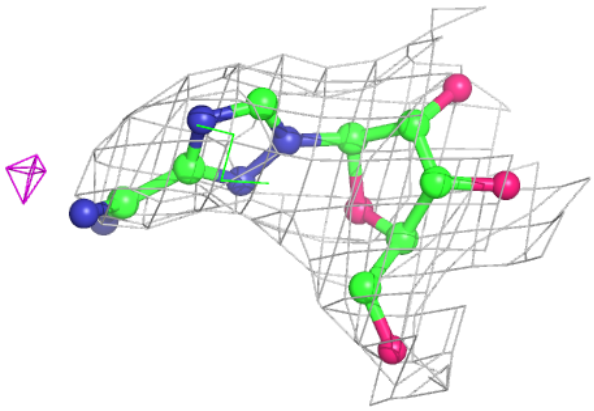


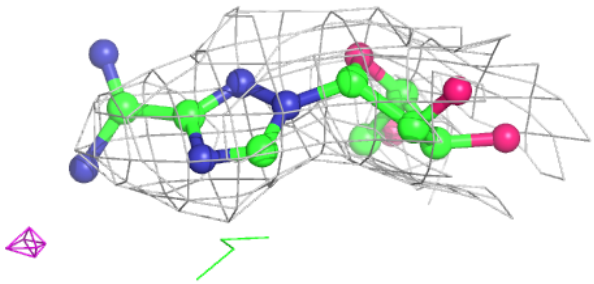


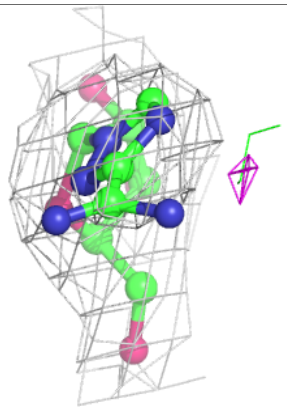


Electron density around R1Y D 401:

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







6.5 Other polymers (i)

There are no such residues in this entry.