



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 06:58 am BST

PDB ID : 2B3T
Title : Structure of complex between E. coli translation termination factor RF1 and the PrmC methyltransferase
Authors : Graille, M.; Heurgue-Hamard, V.; Champ, S.; Mora, L.; Scrima, N.; Ulryck, N.; van Tilbeurgh, H.; Buckingham, R.H.
Deposited on : 2005-09-21
Resolution : 3.10 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 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 : 2.11
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) : 2.11

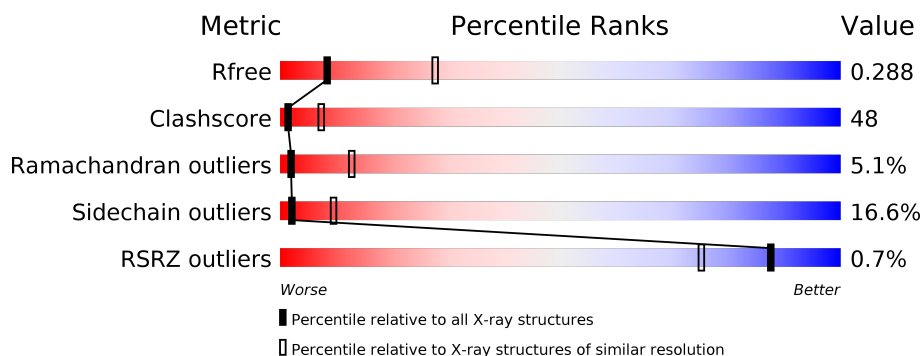
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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 $\leq 5\%$. 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	276	
2	B	360	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4567 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 Protein methyltransferase hemK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	276	Total	C	N	O	S	0	0	0
			2171	1362	388	412	9			

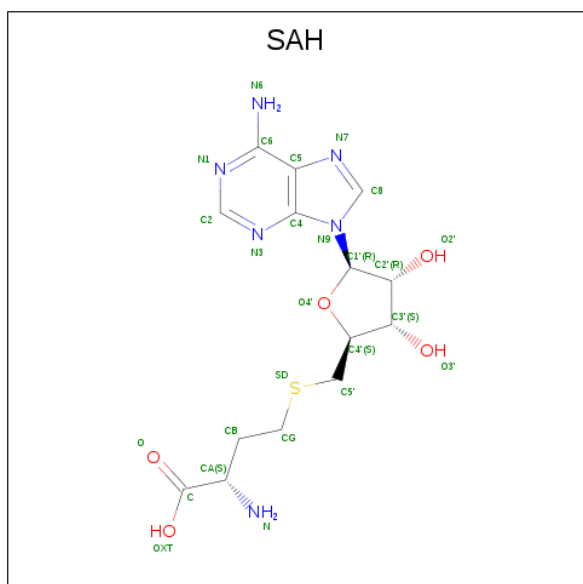
- Molecule 2 is a protein called Peptide chain release factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	300	Total	C	N	O	S	0	0	0
			2370	1457	448	456	9			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	217	VAL	ILE	CONFLICT	UNP P0A7I0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).

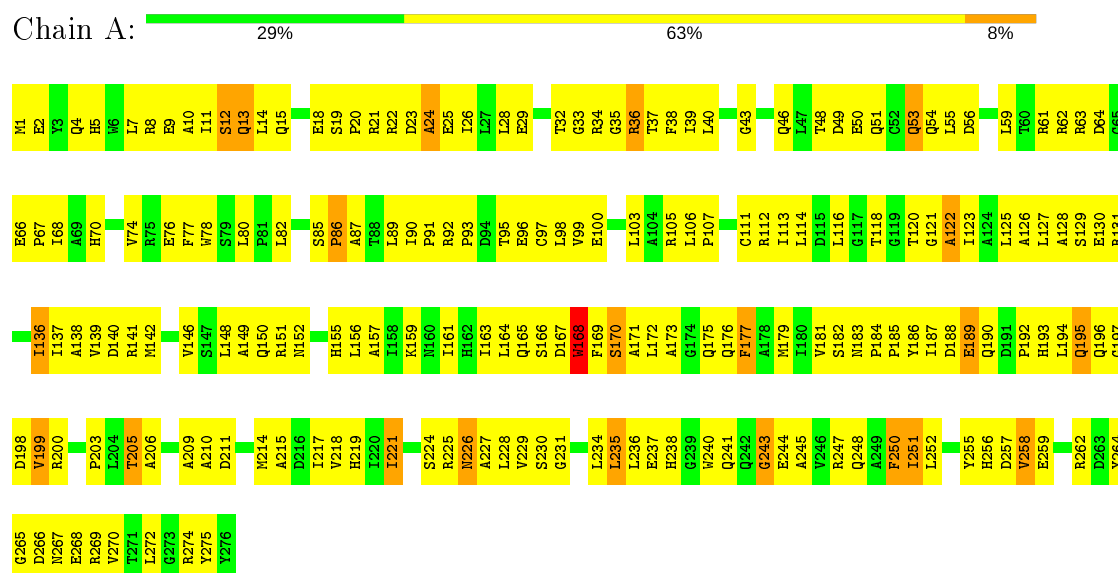


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

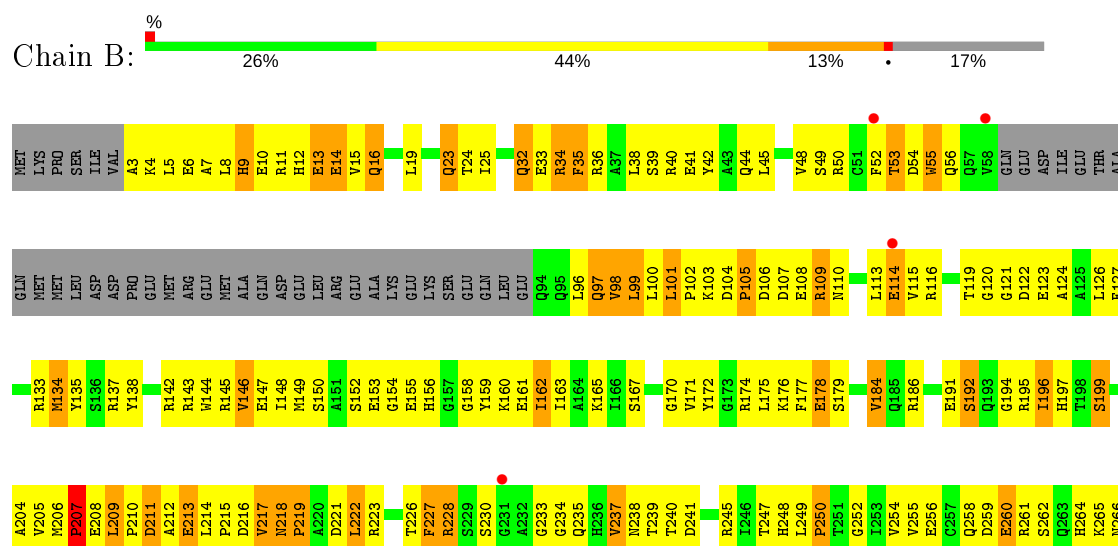
3 Residue-property plots

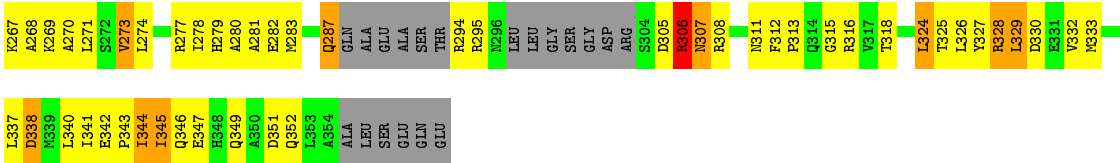
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Protein methyltransferase hemK



• Molecule 2: Peptide chain release factor 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	113.54Å 77.47Å 89.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10 47.94 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-3.10) 99.0 (47.94-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.30 (at 3.12Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.244 , 0.303 0.236 , 0.288	Depositor DCC
R_{free} test set	732 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	67.2	Xtriage
Anisotropy	0.401	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 65.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	4567	wwPDB-VP
Average B, all atoms (Å ²)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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: SAH

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	0.41	0/2216	0.70	0/3014
2	B	0.39	0/2406	0.68	0/3241
All	All	0.40	0/4622	0.69	0/6255

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2171	0	2123	202	0
2	B	2370	0	2317	245	0
3	A	26	0	19	3	0
All	All	4567	0	4459	429	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 48.

All (429) 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)
2:B:23:GLN:HE22	2:B:39:SER:HA	1.12	1.12
1:A:67:PRO:HG3	1:A:198:ASP:HB3	1.44	0.98
2:B:346:GLN:O	2:B:349:GLN:HB3	1.65	0.97
2:B:328:ARG:NE	2:B:328:ARG:HA	1.83	0.92
2:B:97:GLN:HE21	2:B:97:GLN:HA	1.35	0.90
1:A:251:ILE:HD13	1:A:258:VAL:HG21	1.55	0.89
1:A:36:ARG:HG2	2:B:148:ILE:HD12	1.55	0.88
1:A:128:ALA:HB2	1:A:136:ILE:HG13	1.56	0.88
2:B:215:PRO:HG2	2:B:217:VAL:HG13	1.56	0.86
2:B:114:GLU:HG2	2:B:116:ARG:HH22	1.40	0.85
2:B:318:THR:HG23	2:B:325:THR:HG22	1.61	0.82
1:A:187:ILE:HG21	1:A:194:LEU:HD21	1.62	0.82
1:A:95:THR:HG22	1:A:123:ILE:HD11	1.62	0.81
1:A:22:ARG:NH2	2:B:260:GLU:HG3	1.94	0.81
2:B:280:ALA:HA	2:B:283:MET:HE3	1.61	0.80
2:B:34:ARG:N	2:B:34:ARG:HD3	1.95	0.80
2:B:287:GLN:HG3	2:B:295:ARG:HH12	1.49	0.78
1:A:98:LEU:HD21	1:A:181:VAL:HG13	1.67	0.77
1:A:195:GLN:HA	1:A:195:GLN:HE21	1.50	0.76
1:A:50:GLU:HB3	1:A:54:GLN:HE21	1.51	0.76
2:B:104:ASP:OD1	2:B:105:PRO:HD2	1.86	0.76
1:A:244:GLU:HA	1:A:247:ARG:HD2	1.67	0.75
1:A:235:LEU:N	1:A:235:LEU:HD23	2.02	0.75
1:A:197:GLY:O	1:A:200:ARG:HD3	1.85	0.75
2:B:5:LEU:HA	2:B:8:LEU:HD23	1.68	0.75
1:A:265:GLY:HA2	2:B:226:THR:HG21	1.69	0.75
1:A:146:VAL:O	1:A:150:GLN:HG3	1.87	0.74
2:B:114:GLU:CG	2:B:116:ARG:HH22	2.00	0.74
2:B:11:ARG:O	2:B:15:VAL:HG23	1.86	0.74
1:A:106:LEU:HD11	1:A:113:ILE:HD11	1.71	0.73
2:B:23:GLN:NE2	2:B:39:SER:HA	1.97	0.72
2:B:211:ASP:HA	2:B:214:LEU:HG	1.72	0.71
1:A:168:TRP:CE3	1:A:168:TRP:HA	2.25	0.71
2:B:268:ALA:HA	2:B:271:LEU:HD23	1.73	0.71
2:B:110:ASN:HB2	2:B:208:GLU:HG2	1.73	0.70
2:B:50:ARG:NH2	2:B:50:ARG:HB3	2.06	0.70
1:A:22:ARG:HH21	2:B:260:GLU:HG3	1.54	0.70
1:A:106:LEU:HD23	1:A:131:ARG:HG3	1.73	0.69
2:B:3:ALA:HA	2:B:6:GLU:CD	2.12	0.69
2:B:19:LEU:HD23	2:B:19:LEU:O	1.92	0.69
2:B:105:PRO:HG2	2:B:106:ASP:H	1.58	0.68
2:B:261:ARG:HD2	2:B:265:LYS:HE2	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:LEU:HD22	2:B:99:LEU:H	1.57	0.68
2:B:255:VAL:HG21	2:B:274:LEU:HA	1.76	0.68
2:B:13:GLU:HB2	2:B:52:PHE:HD1	1.59	0.68
2:B:7:ALA:O	2:B:11:ARG:HG3	1.94	0.68
2:B:344:ILE:O	2:B:344:ILE:HD13	1.92	0.68
2:B:33:GLU:CG	2:B:34:ARG:H	2.07	0.67
2:B:145:ARG:HB2	2:B:167:SER:HB2	1.77	0.67
2:B:329:LEU:HA	2:B:332:VAL:HG22	1.77	0.67
1:A:112:ARG:HH12	1:A:175:GLN:HB3	1.60	0.67
1:A:114:LEU:HD12	1:A:137:ILE:O	1.95	0.67
2:B:261:ARG:HD2	2:B:265:LYS:CE	2.25	0.67
2:B:97:GLN:O	2:B:99:LEU:HD13	1.95	0.67
2:B:318:THR:CG2	2:B:325:THR:HG22	2.24	0.66
1:A:76:GLU:HG2	2:B:262:SER:HB3	1.78	0.66
2:B:315:GLY:O	2:B:329:LEU:HB2	1.96	0.66
1:A:168:TRP:HE3	1:A:168:TRP:HA	1.61	0.65
2:B:328:ARG:HH11	2:B:330:ASP:HB2	1.62	0.65
2:B:340:LEU:O	2:B:343:PRO:HG2	1.95	0.65
1:A:21:ARG:O	1:A:24:ALA:HB3	1.96	0.65
2:B:134:MET:HG3	2:B:332:VAL:O	1.97	0.64
2:B:329:LEU:HD22	2:B:333:MET:HG2	1.79	0.64
2:B:33:GLU:OE2	2:B:34:ARG:HB2	1.97	0.64
1:A:12:SER:O	1:A:15:GLN:HG2	1.98	0.64
2:B:33:GLU:HG2	2:B:34:ARG:HD3	1.78	0.64
2:B:133:ARG:HG2	2:B:137:ARG:HG3	1.79	0.63
1:A:113:ILE:HB	1:A:136:ILE:HG23	1.81	0.63
1:A:61:ARG:HB3	1:A:66:GLU:OE2	1.99	0.63
2:B:306:ARG:HA	2:B:306:ARG:HE	1.63	0.63
2:B:159:TYR:HB3	2:B:161:GLU:O	1.99	0.62
1:A:166:SER:HB3	1:A:171:ALA:HB3	1.80	0.62
1:A:1:MET:O	1:A:46:GLN:HA	2.00	0.62
1:A:25:GLU:O	1:A:29:GLU:HG3	1.99	0.62
1:A:36:ARG:O	1:A:40:LEU:HD13	2.00	0.62
2:B:241:ASP:HB2	2:B:259:ASP:O	1.99	0.62
1:A:195:GLN:CA	1:A:195:GLN:HE21	2.12	0.62
2:B:327:TYR:O	2:B:328:ARG:HD2	1.98	0.62
2:B:9:HIS:C	2:B:11:ARG:H	2.01	0.62
1:A:182:SER:O	1:A:184:PRO:HD3	1.99	0.62
2:B:40:ARG:O	2:B:44:GLN:HG3	2.00	0.61
1:A:13:GLN:HE21	1:A:63:ARG:HD2	1.66	0.61
1:A:192:PRO:O	1:A:195:GLN:HB2	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:327:TYR:O	2:B:327:TYR:CG	2.53	0.61
2:B:98:VAL:O	2:B:98:VAL:HG23	2.01	0.61
2:B:219:PRO:HD2	2:B:221:ASP:OD1	2.00	0.61
2:B:8:LEU:O	2:B:11:ARG:HB2	2.00	0.61
2:B:305:ASP:O	2:B:306:ARG:C	2.40	0.60
2:B:100:LEU:C	2:B:101:LEU:HD12	2.22	0.60
1:A:210:ALA:H	1:A:215:ALA:HB3	1.66	0.60
1:A:142:MET:SD	1:A:205:THR:HG21	2.42	0.60
1:A:196:GLN:O	1:A:199:VAL:HG12	2.01	0.60
1:A:118:THR:CB	1:A:138:ALA:HB1	2.31	0.60
1:A:96:GLU:O	1:A:100:GLU:HG3	2.02	0.60
1:A:9:GLU:O	1:A:12:SER:HB3	2.01	0.60
1:A:95:THR:CG2	1:A:123:ILE:HD11	2.32	0.59
1:A:195:GLN:HA	1:A:195:GLN:NE2	2.16	0.59
2:B:149:MET:HG2	2:B:269:LYS:HD3	1.83	0.59
1:A:234:LEU:HD11	1:A:236:LEU:HD11	1.84	0.59
2:B:218:ASN:CB	2:B:222:LEU:HD21	2.32	0.59
2:B:306:ARG:CA	2:B:306:ARG:HE	2.16	0.59
1:A:76:GLU:OE1	2:B:261:ARG:HB3	2.03	0.59
1:A:229:VAL:HG12	1:A:230:SER:N	2.18	0.59
2:B:172:TYR:CE2	2:B:176:LYS:HB3	2.38	0.59
1:A:118:THR:HB	1:A:138:ALA:HB1	1.84	0.58
1:A:218:VAL:HA	1:A:221:ILE:HD11	1.85	0.58
1:A:11:ILE:CD1	1:A:21:ARG:HD2	2.33	0.58
1:A:125:LEU:HD12	1:A:161:ILE:HD13	1.85	0.58
2:B:135:TYR:OH	2:B:178:GLU:HG3	2.03	0.58
2:B:110:ASN:OD1	2:B:167:SER:HA	2.04	0.58
1:A:255:TYR:CD2	1:A:274:ARG:O	2.57	0.58
2:B:324:LEU:HD22	2:B:325:THR:N	2.18	0.58
2:B:52:PHE:C	2:B:54:ASP:H	2.07	0.58
1:A:185:PRO:O	1:A:209:ALA:HB2	2.04	0.58
1:A:139:VAL:HG11	1:A:172:LEU:HD21	1.85	0.57
1:A:32:THR:HG22	1:A:51:GLN:NE2	2.19	0.57
2:B:12:HIS:O	2:B:15:VAL:N	2.37	0.57
2:B:196:ILE:HD13	2:B:196:ILE:O	2.03	0.57
1:A:103:LEU:HD11	1:A:130:GLU:HG3	1.85	0.57
1:A:11:ILE:HD11	1:A:21:ARG:HD2	1.87	0.57
2:B:19:LEU:HD23	2:B:19:LEU:C	2.25	0.57
2:B:172:TYR:CD1	2:B:207:PRO:HB3	2.39	0.57
2:B:50:ARG:HB3	2:B:50:ARG:HH21	1.69	0.57
2:B:120:GLY:HA3	2:B:199:SER:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:329:LEU:HD23	2:B:332:VAL:CG2	2.35	0.56
2:B:149:MET:SD	2:B:165:LYS:HB2	2.45	0.56
1:A:92:ARG:CZ	2:B:238:ASN:HB2	2.36	0.56
2:B:33:GLU:CG	2:B:34:ARG:N	2.68	0.56
2:B:54:ASP:C	2:B:56:GLN:N	2.59	0.56
1:A:255:TYR:HD2	1:A:274:ARG:O	1.88	0.56
1:A:4:GLN:HE21	1:A:8:ARG:NH2	2.03	0.56
1:A:186:TYR:CD2	1:A:238:HIS:HA	2.41	0.56
1:A:78:TRP:HA	2:B:264:HIS:ND1	2.20	0.56
2:B:33:GLU:HG2	2:B:34:ARG:N	2.21	0.56
1:A:218:VAL:HG13	1:A:219:HIS:N	2.21	0.55
1:A:248:GLN:HA	1:A:251:ILE:HG12	1.87	0.55
1:A:82:LEU:HD11	1:A:125:LEU:HD23	1.87	0.55
2:B:329:LEU:HA	2:B:332:VAL:CG2	2.36	0.55
2:B:345:ILE:HG22	2:B:346:GLN:N	2.21	0.55
2:B:114:GLU:HG2	2:B:116:ARG:NH2	2.18	0.55
2:B:99:LEU:HD13	2:B:99:LEU:H	1.71	0.55
2:B:210:PRO:O	2:B:213:GLU:N	2.39	0.55
2:B:343:PRO:HA	2:B:346:GLN:NE2	2.22	0.55
2:B:279:HIS:O	2:B:283:MET:HG3	2.07	0.55
2:B:270:ALA:O	2:B:273:VAL:HG23	2.07	0.54
1:A:187:ILE:HG21	1:A:194:LEU:CD2	2.36	0.54
2:B:99:LEU:HD22	2:B:99:LEU:N	2.22	0.54
1:A:166:SER:HB2	1:A:171:ALA:H	1.73	0.54
2:B:148:ILE:O	2:B:149:MET:HG3	2.07	0.54
2:B:269:LYS:O	2:B:273:VAL:HG22	2.08	0.54
2:B:152:SER:HB2	2:B:161:GLU:H	1.73	0.54
1:A:22:ARG:NH2	2:B:260:GLU:CG	2.67	0.54
1:A:77:PHE:CE1	1:A:96:GLU:HG3	2.42	0.53
2:B:12:HIS:C	2:B:14:GLU:N	2.61	0.53
2:B:178:GLU:OE1	2:B:341:ILE:HD11	2.08	0.53
1:A:82:LEU:HD21	1:A:122:ALA:HA	1.91	0.53
1:A:78:TRP:HH2	1:A:100:GLU:HG2	1.71	0.53
2:B:311:ASN:OD1	2:B:313:PRO:HD2	2.08	0.53
1:A:86:PRO:O	1:A:203:PRO:HG3	2.08	0.53
1:A:258:VAL:HG12	1:A:259:GLU:N	2.24	0.53
1:A:206:ALA:HB2	3:A:300:SAH:H3'	1.90	0.53
2:B:329:LEU:HD23	2:B:332:VAL:HG23	1.90	0.53
1:A:85:SER:C	1:A:87:ALA:H	2.13	0.52
2:B:154:GLY:HA3	2:B:158:GLY:H	1.74	0.52
1:A:28:LEU:HA	1:A:55:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:PHE:N	1:A:177:PHE:CD1	2.78	0.52
2:B:210:PRO:C	2:B:212:ALA:N	2.63	0.52
2:B:12:HIS:O	2:B:14:GLU:N	2.43	0.51
2:B:228:ARG:C	2:B:230:SER:N	2.63	0.51
2:B:215:PRO:HG2	2:B:217:VAL:CG1	2.35	0.51
1:A:169:PHE:HA	1:A:172:LEU:HD23	1.93	0.51
2:B:48:VAL:CG2	2:B:49:SER:N	2.73	0.51
1:A:146:VAL:HG21	1:A:165:GLN:HB2	1.91	0.51
2:B:142:ARG:HD2	2:B:144:TRP:CZ2	2.45	0.51
1:A:37:THR:HG21	2:B:146:VAL:HG22	1.91	0.51
2:B:99:LEU:HD13	2:B:99:LEU:N	2.25	0.51
1:A:76:GLU:OE1	2:B:265:LYS:HE2	2.10	0.51
1:A:34:ARG:HD3	1:A:38:PHE:CE2	2.46	0.51
1:A:93:PRO:O	1:A:96:GLU:HB2	2.10	0.51
2:B:249:LEU:N	2:B:250:PRO:HD2	2.26	0.51
1:A:2:GLU:HG2	1:A:43:GLY:O	2.10	0.51
1:A:188:ASP:OD2	1:A:189:GLU:N	2.43	0.51
2:B:116:ARG:HG3	2:B:161:GLU:OE1	2.11	0.51
1:A:92:ARG:NH2	2:B:238:ASN:HB2	2.26	0.50
2:B:98:VAL:HG23	2:B:101:LEU:HD11	1.94	0.50
1:A:106:LEU:HD11	1:A:113:ILE:CD1	2.38	0.50
2:B:114:GLU:N	2:B:114:GLU:CD	2.65	0.50
2:B:210:PRO:C	2:B:212:ALA:H	2.15	0.50
2:B:266:ASN:O	2:B:269:LYS:HB3	2.10	0.50
2:B:270:ALA:HA	2:B:273:VAL:HG23	1.94	0.50
1:A:244:GLU:O	1:A:247:ARG:HB2	2.12	0.50
2:B:134:MET:CG	2:B:337:LEU:HD11	2.41	0.50
1:A:116:LEU:HB2	1:A:182:SER:HB2	1.93	0.50
2:B:342:GLU:HB3	2:B:343:PRO:CD	2.42	0.50
2:B:12:HIS:O	2:B:13:GLU:C	2.50	0.50
1:A:139:VAL:HG12	1:A:164:LEU:HB2	1.94	0.50
2:B:218:ASN:HB3	2:B:222:LEU:HD21	1.93	0.50
2:B:127:PHE:CG	2:B:184:VAL:HG21	2.47	0.50
2:B:215:PRO:CG	2:B:217:VAL:HG13	2.37	0.50
1:A:7:LEU:HD11	1:A:39:ILE:CG2	2.42	0.49
2:B:48:VAL:HG23	2:B:49:SER:N	2.27	0.49
1:A:118:THR:HG21	1:A:138:ALA:HB1	1.94	0.49
1:A:4:GLN:HG3	1:A:5:HIS:N	2.26	0.49
2:B:171:VAL:HG12	2:B:172:TYR:N	2.26	0.49
2:B:52:PHE:O	2:B:54:ASP:N	2.45	0.49
1:A:156:LEU:O	1:A:157:ALA:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:PRO:HG2	1:A:111:CYS:SG	2.52	0.49
2:B:228:ARG:C	2:B:230:SER:H	2.16	0.49
2:B:114:GLU:HB3	2:B:163:ILE:HB	1.93	0.49
2:B:9:HIS:C	2:B:11:ARG:N	2.66	0.49
1:A:112:ARG:O	1:A:177:PHE:HB3	2.13	0.49
2:B:274:LEU:O	2:B:274:LEU:HD23	2.13	0.49
2:B:9:HIS:HB3	2:B:52:PHE:CG	2.47	0.49
1:A:86:PRO:O	1:A:203:PRO:CG	2.61	0.49
2:B:101:LEU:H	2:B:102:PRO:HD2	1.77	0.49
1:A:252:LEU:C	1:A:252:LEU:HD23	2.33	0.48
1:A:99:VAL:HG13	1:A:127:LEU:CD1	2.43	0.48
2:B:177:PHE:CD1	2:B:344:ILE:HD12	2.48	0.48
2:B:9:HIS:O	2:B:11:ARG:N	2.46	0.48
1:A:106:LEU:HD12	1:A:179:MET:HE3	1.96	0.48
1:A:50:GLU:O	1:A:53:GLN:HG3	2.13	0.48
2:B:278:ILE:HG22	2:B:279:HIS:N	2.28	0.48
2:B:227:PHE:HE1	2:B:256:GLU:OE1	1.96	0.48
2:B:49:SER:O	2:B:53:THR:HG22	2.13	0.48
1:A:98:LEU:C	1:A:98:LEU:HD23	2.34	0.48
2:B:175:LEU:O	2:B:178:GLU:HB2	2.13	0.48
2:B:217:VAL:HG23	2:B:217:VAL:O	2.13	0.48
1:A:48:THR:OG1	1:A:51:GLN:HG3	2.13	0.48
2:B:152:SER:O	2:B:159:TYR:HA	2.12	0.48
2:B:4:LYS:O	2:B:7:ALA:HB3	2.14	0.48
1:A:250:PHE:O	1:A:255:TYR:HB2	2.14	0.48
2:B:113:LEU:HD11	2:B:135:TYR:CD2	2.49	0.48
1:A:22:ARG:O	1:A:23:ASP:C	2.50	0.47
1:A:98:LEU:CD2	1:A:98:LEU:C	2.83	0.47
2:B:113:LEU:HD23	2:B:113:LEU:C	2.34	0.47
2:B:35:PHE:O	2:B:39:SER:HB2	2.13	0.47
1:A:262:ARG:HB3	1:A:267:ASN:O	2.14	0.47
2:B:192:SER:C	2:B:194:GLY:H	2.18	0.47
1:A:7:LEU:O	1:A:11:ILE:HG13	2.14	0.47
1:A:19:SER:O	1:A:23:ASP:OD2	2.33	0.47
1:A:53:GLN:C	1:A:53:GLN:NE2	2.68	0.47
2:B:121:GLY:C	2:B:123:GLU:N	2.68	0.47
1:A:234:LEU:C	1:A:235:LEU:HD23	2.35	0.47
2:B:162:ILE:O	2:B:162:ILE:HG23	2.14	0.47
1:A:36:ARG:HG3	1:A:40:LEU:HD13	1.96	0.47
2:B:105:PRO:HG2	2:B:106:ASP:N	2.29	0.47
2:B:329:LEU:CD2	2:B:333:MET:HG2	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:GLY:HA2	1:A:275:TYR:O	2.14	0.47
1:A:50:GLU:O	1:A:53:GLN:N	2.48	0.47
2:B:154:GLY:C	2:B:156:HIS:H	2.17	0.47
1:A:218:VAL:HA	1:A:221:ILE:CG1	2.45	0.47
2:B:172:TYR:C	2:B:174:ARG:H	2.18	0.47
2:B:134:MET:SD	2:B:337:LEU:HD11	2.55	0.47
2:B:97:GLN:NE2	2:B:97:GLN:HA	2.16	0.47
2:B:312:PHE:N	2:B:312:PHE:CD2	2.83	0.47
2:B:101:LEU:HD12	2:B:101:LEU:N	2.29	0.46
1:A:12:SER:C	1:A:14:LEU:H	2.17	0.46
1:A:130:GLU:HA	1:A:130:GLU:OE2	2.14	0.46
1:A:229:VAL:HG12	1:A:230:SER:H	1.80	0.46
1:A:98:LEU:HA	1:A:270:VAL:HG21	1.98	0.46
1:A:99:VAL:HG23	1:A:123:ILE:HG13	1.97	0.46
2:B:108:GLU:HA	2:B:170:GLY:HA2	1.96	0.46
2:B:192:SER:C	2:B:194:GLY:N	2.69	0.46
2:B:213:GLU:OE1	2:B:213:GLU:O	2.33	0.46
1:A:128:ALA:HB2	1:A:136:ILE:CG1	2.38	0.46
1:A:155:HIS:HD2	1:A:156:LEU:HD22	1.80	0.46
1:A:193:HIS:C	1:A:195:GLN:N	2.67	0.46
2:B:186:ARG:O	2:B:197:HIS:N	2.42	0.46
2:B:206:MET:HB3	2:B:207:PRO:HD2	1.98	0.46
1:A:120:THR:O	1:A:149:ALA:HA	2.16	0.46
1:A:247:ARG:O	1:A:251:ILE:HG12	2.16	0.46
2:B:127:PHE:CD2	2:B:184:VAL:HG22	2.50	0.46
2:B:345:ILE:CG2	2:B:346:GLN:N	2.79	0.46
2:B:110:ASN:HB2	2:B:208:GLU:CG	2.44	0.46
2:B:209:LEU:H	2:B:209:LEU:HD12	1.81	0.46
1:A:118:THR:OG1	1:A:121:GLY:HA2	2.15	0.46
1:A:198:ASP:O	1:A:200:ARG:N	2.49	0.46
1:A:91:PRO:HD3	1:A:120:THR:HG21	1.96	0.46
2:B:113:LEU:HD23	2:B:114:GLU:N	2.30	0.46
1:A:224:SER:CB	1:A:234:LEU:HD22	2.46	0.46
1:A:258:VAL:CG1	1:A:259:GLU:N	2.79	0.46
1:A:98:LEU:HD21	1:A:181:VAL:CG1	2.42	0.46
1:A:125:LEU:HD12	1:A:161:ILE:CD1	2.46	0.46
2:B:270:ALA:HA	2:B:273:VAL:CG2	2.46	0.46
2:B:267:LYS:O	2:B:270:ALA:N	2.49	0.45
1:A:105:ARG:NH2	1:A:272:LEU:HD21	2.31	0.45
1:A:152:ASN:O	1:A:156:LEU:HD23	2.16	0.45
1:A:49:ASP:O	1:A:50:GLU:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:GLU:O	2:B:165:LYS:N	2.49	0.45
2:B:324:LEU:HD21	2:B:326:LEU:HD21	1.98	0.45
1:A:218:VAL:HG13	1:A:219:HIS:H	1.81	0.45
2:B:121:GLY:C	2:B:123:GLU:H	2.17	0.45
2:B:19:LEU:HD22	2:B:42:TYR:HD2	1.81	0.45
2:B:328:ARG:HE	2:B:328:ARG:HA	1.73	0.45
1:A:118:THR:CG2	1:A:138:ALA:HB1	2.45	0.45
1:A:193:HIS:O	1:A:194:LEU:C	2.53	0.45
1:A:95:THR:HA	1:A:237:GLU:OE1	2.15	0.45
2:B:135:TYR:O	2:B:138:TYR:HB3	2.17	0.45
2:B:172:TYR:C	2:B:172:TYR:CD2	2.88	0.45
2:B:329:LEU:CA	2:B:332:VAL:HG22	2.46	0.45
1:A:235:LEU:N	1:A:235:LEU:CD2	2.73	0.45
2:B:280:ALA:HA	2:B:283:MET:CE	2.41	0.45
2:B:41:GLU:CG	2:B:45:LEU:HD13	2.46	0.45
2:B:274:LEU:C	2:B:274:LEU:HD23	2.36	0.45
2:B:115:VAL:HB	2:B:162:ILE:CG2	2.47	0.45
2:B:295:ARG:O	2:B:295:ARG:HG3	2.16	0.45
1:A:146:VAL:HG13	1:A:163:ILE:HG22	1.98	0.45
1:A:169:PHE:O	1:A:172:LEU:N	2.49	0.45
1:A:2:GLU:O	1:A:5:HIS:N	2.50	0.45
1:A:198:ASP:C	1:A:200:ARG:H	2.20	0.45
1:A:97:CYS:O	1:A:98:LEU:C	2.54	0.45
2:B:134:MET:HG2	2:B:337:LEU:HD11	1.98	0.45
1:A:125:LEU:CD1	1:A:161:ILE:HD13	2.48	0.44
2:B:216:ASP:O	2:B:218:ASN:N	2.48	0.44
2:B:254:VAL:HG13	2:B:254:VAL:O	2.17	0.44
2:B:5:LEU:O	2:B:8:LEU:HB2	2.17	0.44
2:B:343:PRO:C	2:B:345:ILE:H	2.21	0.44
1:A:210:ALA:HB3	1:A:215:ALA:CB	2.48	0.44
1:A:168:TRP:CD1	1:A:219:HIS:CD2	3.05	0.44
1:A:61:ARG:O	1:A:64:ASP:N	2.49	0.44
1:A:26:ILE:CD1	2:B:260:GLU:HG2	2.47	0.44
2:B:154:GLY:C	2:B:156:HIS:N	2.71	0.44
2:B:55:TRP:HE3	2:B:55:TRP:O	2.00	0.44
1:A:35:GLY:O	1:A:39:ILE:HG13	2.18	0.44
2:B:41:GLU:HG2	2:B:45:LEU:HD13	1.99	0.44
1:A:186:TYR:CZ	2:B:235:GLN:HG3	2.52	0.44
1:A:176:GLN:HG2	1:A:227:ALA:HA	2.00	0.44
1:A:248:GLN:NE2	1:A:251:ILE:HG13	2.32	0.44
2:B:119:THR:O	2:B:124:ALA:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:308:ARG:HA	2:B:318:THR:O	2.18	0.44
2:B:315:GLY:C	2:B:329:LEU:HB2	2.38	0.44
1:A:127:LEU:C	1:A:129:SER:N	2.71	0.43
2:B:233:GLY:O	2:B:234:GLY:C	2.56	0.43
2:B:133:ARG:HG2	2:B:137:ARG:CG	2.48	0.43
1:A:105:ARG:H	1:A:105:ARG:HD2	1.83	0.43
1:A:265:GLY:HA2	2:B:226:THR:CG2	2.43	0.43
2:B:218:ASN:O	2:B:219:PRO:O	2.36	0.43
1:A:68:ILE:HG13	2:B:240:THR:HG21	2.00	0.43
1:A:19:SER:N	1:A:20:PRO:HD3	2.34	0.43
2:B:338:ASP:C	2:B:340:LEU:H	2.19	0.43
1:A:243:GLY:HA3	1:A:268:GLU:OE2	2.18	0.43
1:A:4:GLN:HE21	1:A:8:ARG:HH22	1.66	0.43
2:B:54:ASP:C	2:B:56:GLN:H	2.20	0.43
1:A:172:LEU:HD22	1:A:172:LEU:N	2.32	0.43
1:A:188:ASP:OD2	1:A:189:GLU:HG2	2.19	0.43
2:B:154:GLY:HA3	2:B:158:GLY:N	2.33	0.43
1:A:235:LEU:C	1:A:236:LEU:HD12	2.39	0.43
2:B:32:GLN:O	2:B:33:GLU:HB3	2.17	0.43
2:B:343:PRO:C	2:B:345:ILE:N	2.72	0.43
1:A:18:GLU:O	1:A:18:GLU:HG2	2.18	0.43
1:A:1:MET:HG2	1:A:2:GLU:N	2.34	0.43
2:B:237:VAL:CG2	2:B:238:ASN:N	2.81	0.43
2:B:9:HIS:ND1	2:B:9:HIS:N	2.67	0.43
1:A:116:LEU:HB2	1:A:182:SER:CB	2.49	0.43
1:A:214:MET:O	1:A:214:MET:HG3	2.18	0.43
1:A:218:VAL:HA	1:A:221:ILE:CD1	2.49	0.43
1:A:40:LEU:N	1:A:40:LEU:HD12	2.34	0.43
2:B:308:ARG:NH2	2:B:340:LEU:HD13	2.33	0.43
2:B:341:ILE:O	2:B:345:ILE:HB	2.19	0.43
2:B:50:ARG:O	2:B:54:ASP:OD1	2.37	0.43
2:B:209:LEU:O	2:B:209:LEU:CD1	2.67	0.42
1:A:228:LEU:HD11	1:A:234:LEU:HB2	2.00	0.42
2:B:267:LYS:O	2:B:271:LEU:HD22	2.18	0.42
1:A:126:ALA:O	1:A:129:SER:HB3	2.20	0.42
1:A:217:ILE:O	1:A:221:ILE:HG12	2.20	0.42
1:A:4:GLN:HG2	1:A:43:GLY:O	2.19	0.42
2:B:116:ARG:NH1	2:B:161:GLU:OE1	2.52	0.42
2:B:205:VAL:HG12	2:B:205:VAL:O	2.19	0.42
2:B:278:ILE:HD13	2:B:278:ILE:HA	1.92	0.42
2:B:210:PRO:O	2:B:212:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ASN:N	2:B:219:PRO:HD3	2.34	0.42
1:A:26:ILE:HG12	2:B:260:GLU:HG2	2.01	0.42
1:A:206:ALA:CB	3:A:300:SAH:H3'	2.48	0.42
2:B:145:ARG:HB2	2:B:145:ARG:HE	1.65	0.42
2:B:152:SER:CB	2:B:160:LYS:HB3	2.50	0.42
2:B:45:LEU:N	2:B:45:LEU:HD12	2.35	0.42
2:B:5:LEU:CA	2:B:8:LEU:HD23	2.45	0.42
1:A:95:THR:HG23	1:A:183:ASN:HD22	1.83	0.42
2:B:114:GLU:OE1	2:B:204:ALA:HB3	2.19	0.42
2:B:219:PRO:HD2	2:B:221:ASP:CG	2.40	0.42
2:B:34:ARG:C	2:B:36:ARG:H	2.23	0.42
1:A:169:PHE:O	1:A:170:SER:C	2.57	0.42
2:B:104:ASP:OD1	2:B:105:PRO:CD	2.63	0.42
1:A:12:SER:O	1:A:14:LEU:N	2.48	0.42
2:B:105:PRO:CG	2:B:106:ASP:H	2.24	0.42
2:B:347:GLU:C	2:B:349:GLN:N	2.74	0.42
2:B:52:PHE:C	2:B:54:ASP:N	2.72	0.42
1:A:225:ARG:HG2	1:A:275:TYR:CE1	2.55	0.41
1:A:50:GLU:HB3	1:A:54:GLN:NE2	2.27	0.41
2:B:16:GLN:HB3	2:B:16:GLN:HE21	1.58	0.41
1:A:106:LEU:HD21	1:A:113:ILE:HD11	2.03	0.41
1:A:247:ARG:O	1:A:250:PHE:HB2	2.19	0.41
2:B:245:ARG:HG3	2:B:256:GLU:HB3	2.03	0.41
2:B:248:HIS:O	2:B:252:GLY:HA2	2.20	0.41
2:B:328:ARG:NE	2:B:328:ARG:CA	2.67	0.41
2:B:97:GLN:HE21	2:B:97:GLN:CA	2.13	0.41
2:B:267:LYS:O	2:B:270:ALA:HB3	2.19	0.41
2:B:8:LEU:HD22	2:B:8:LEU:N	2.34	0.41
1:A:59:LEU:O	1:A:63:ARG:HG3	2.21	0.41
1:A:10:ALA:O	1:A:14:LEU:HB2	2.21	0.41
1:A:22:ARG:HA	1:A:22:ARG:HD2	1.76	0.41
2:B:294:ARG:NH2	2:B:351:ASP:OD1	2.52	0.41
2:B:349:GLN:O	2:B:352:GLN:N	2.54	0.41
1:A:193:HIS:O	1:A:195:GLN:N	2.54	0.41
1:A:89:LEU:HG	1:A:90:ILE:N	2.35	0.41
2:B:209:LEU:HD22	2:B:214:LEU:HD23	2.03	0.41
2:B:52:PHE:CZ	2:B:56:GLN:NE2	2.89	0.41
1:A:62:ARG:HD2	1:A:62:ARG:O	2.20	0.41
1:A:186:TYR:CE2	2:B:235:GLN:NE2	2.87	0.41
1:A:140:ASP:O	1:A:165:GLN:HA	2.21	0.41
1:A:183:ASN:OD1	1:A:183:ASN:C	2.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:ILE:HG22	1:A:188:ASP:O	2.21	0.41
1:A:29:GLU:O	1:A:33:GLY:N	2.45	0.41
1:A:141:ARG:HB2	3:A:300:SAH:C6	2.51	0.41
1:A:112:ARG:NH1	1:A:175:GLN:HB3	2.32	0.40
1:A:85:SER:O	1:A:87:ALA:N	2.54	0.40
2:B:179:SER:O	2:B:307:ASN:OD1	2.38	0.40
1:A:167:ASP:C	1:A:167:ASP:OD2	2.59	0.40
1:A:14:LEU:HD13	1:A:59:LEU:HD11	2.03	0.40
2:B:109:ARG:HA	2:B:109:ARG:NE	2.36	0.40
2:B:19:LEU:CD2	2:B:19:LEU:C	2.90	0.40
2:B:223:ARG:HB3	2:B:247:THR:OG1	2.20	0.40
1:A:165:GLN:HG2	1:A:165:GLN:O	2.20	0.40
1:A:196:GLN:HA	1:A:200:ARG:HD2	2.02	0.40
1:A:237:GLU:HG3	1:A:269:ARG:HG3	2.03	0.40
1:A:264:TYR:C	1:A:266:ASP:H	2.23	0.40
2:B:19:LEU:HD21	2:B:38:LEU:HD13	2.04	0.40
2:B:281:ALA:C	2:B:283:MET:H	2.25	0.40
2:B:5:LEU:HD22	2:B:5:LEU:N	2.37	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	274/276 (99%)	226 (82%)	36 (13%)	12 (4%)	2	15
2	B	292/360 (81%)	212 (73%)	63 (22%)	17 (6%)	1	10
All	All	566/636 (89%)	438 (77%)	99 (18%)	29 (5%)	2	13

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	122	ALA
1	A	173	ALA
2	B	105	PRO
2	B	162	ILE
2	B	219	PRO
2	B	250	PRO
1	A	13	GLN
1	A	199	VAL
1	A	226	ASN
1	A	245	ALA
2	B	10	GLU
2	B	53	THR
2	B	96	LEU
2	B	98	VAL
2	B	103	LYS
2	B	217	VAL
2	B	306	ARG
1	A	12	SER
1	A	24	ALA
1	A	243	GLY
1	A	258	VAL
2	B	101	LEU
2	B	150	SER
1	A	168	TRP
2	B	13	GLU
2	B	207	PRO
2	B	228	ARG
1	A	86	PRO
2	B	218	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/229 (100%)	202 (88%)	27 (12%)	5	21
2	B	248/300 (83%)	196 (79%)	52 (21%)	1	5
All	All	477/529 (90%)	398 (83%)	79 (17%)	2	9

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	ARG
1	A	53	GLN
1	A	56	ASP
1	A	70	HIS
1	A	74	VAL
1	A	80	LEU
1	A	136	ILE
1	A	148	LEU
1	A	151	ARG
1	A	159	LYS
1	A	168	TRP
1	A	170	SER
1	A	177	PHE
1	A	189	GLU
1	A	190	GLN
1	A	195	GLN
1	A	205	THR
1	A	211	ASP
1	A	221	ILE
1	A	226	ASN
1	A	235	LEU
1	A	240	TRP
1	A	241	GLN
1	A	250	PHE
1	A	251	ILE
1	A	256	HIS
1	A	257	ASP
2	B	9	HIS
2	B	14	GLU
2	B	16	GLN
2	B	23	GLN
2	B	24	THR
2	B	25	ILE
2	B	32	GLN
2	B	34	ARG
2	B	35	PHE
2	B	55	TRP
2	B	97	GLN
2	B	99	LEU
2	B	107	ASP
2	B	109	ARG
2	B	114	GLU

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Mol	Chain	Res	Type
2	B	122	ASP
2	B	126	LEU
2	B	134	MET
2	B	143	ARG
2	B	146	VAL
2	B	153	GLU
2	B	155	GLU
2	B	178	GLU
2	B	184	VAL
2	B	191	GLU
2	B	192	SER
2	B	195	ARG
2	B	196	ILE
2	B	199	SER
2	B	207	PRO
2	B	209	LEU
2	B	211	ASP
2	B	213	GLU
2	B	222	LEU
2	B	227	PHE
2	B	237	VAL
2	B	239	THR
2	B	258	GLN
2	B	260	GLU
2	B	273	VAL
2	B	277	ARG
2	B	282	GLU
2	B	287	GLN
2	B	306	ARG
2	B	307	ASN
2	B	316	ARG
2	B	324	LEU
2	B	328	ARG
2	B	329	LEU
2	B	338	ASP
2	B	344	ILE
2	B	345	ILE

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

Mol	Chain	Res	Type
1	A	4	GLN

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Mol	Chain	Res	Type
1	A	13	GLN
1	A	15	GLN
1	A	53	GLN
1	A	54	GLN
1	A	155	HIS
1	A	190	GLN
1	A	195	GLN
1	A	196	GLN
1	A	219	HIS
1	A	223	GLN
1	A	226	ASN
1	A	248	GLN
1	A	267	ASN
2	B	16	GLN
2	B	23	GLN
2	B	32	GLN
2	B	44	GLN
2	B	56	GLN
2	B	57	GLN
2	B	94	GLN
2	B	97	GLN
2	B	266	ASN
2	B	279	HIS
2	B	346	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	SAH	A	300	-	21,28,28	1.60	4 (19%)	20,40,40	2.44	8 (40%)

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	SAH	A	300	-	-	0/7/31/31	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	300	SAH	C2-N3	3.94	1.38	1.32
3	A	300	SAH	O4'-C1'	3.31	1.45	1.41
3	A	300	SAH	C8-N7	-2.50	1.30	1.34
3	A	300	SAH	CA-N	2.17	1.51	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	300	SAH	O4'-C1'-C2'	-7.60	95.83	106.93
3	A	300	SAH	CB-CG-SD	-3.58	105.28	113.31
3	A	300	SAH	N3-C2-N1	-3.17	123.72	128.68
3	A	300	SAH	C1'-N9-C4	-2.85	121.63	126.64
3	A	300	SAH	C5-C6-N6	2.58	124.28	120.35
3	A	300	SAH	C2-N1-C6	2.57	123.16	118.75
3	A	300	SAH	C5-C6-N1	-2.36	115.01	120.35
3	A	300	SAH	O4'-C4'-C5'	-2.29	102.95	108.83

There are no chirality outliers.

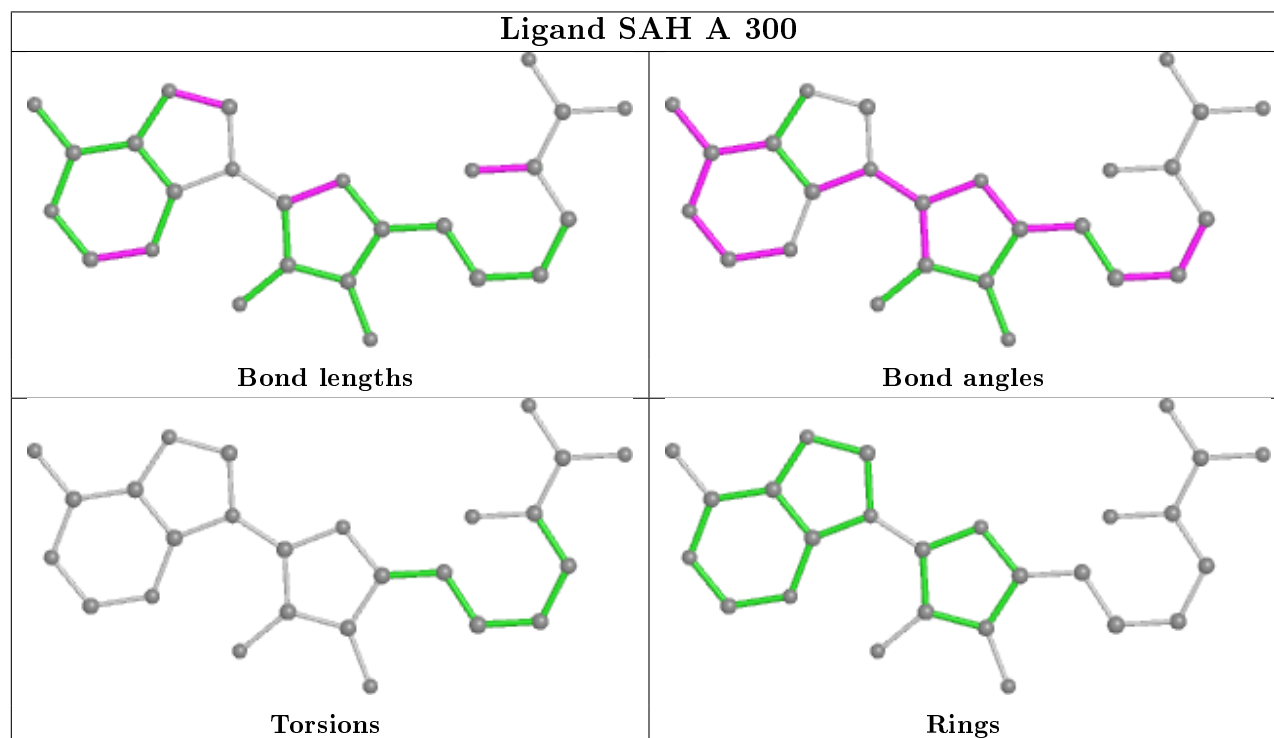
There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	300	SAH	3	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 than 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.



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	276/276 (100%)	-0.24	0 100 100	19, 45, 69, 76	0
2	B	300/360 (83%)	0.00	4 (1%) 77 59	25, 62, 98, 105	0
All	All	576/636 (90%)	-0.11	4 (0%) 87 75	19, 51, 93, 105	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	231	GLY	2.5
2	B	52	PHE	2.2
2	B	114	GLU	2.1
2	B	58	VAL	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](#)

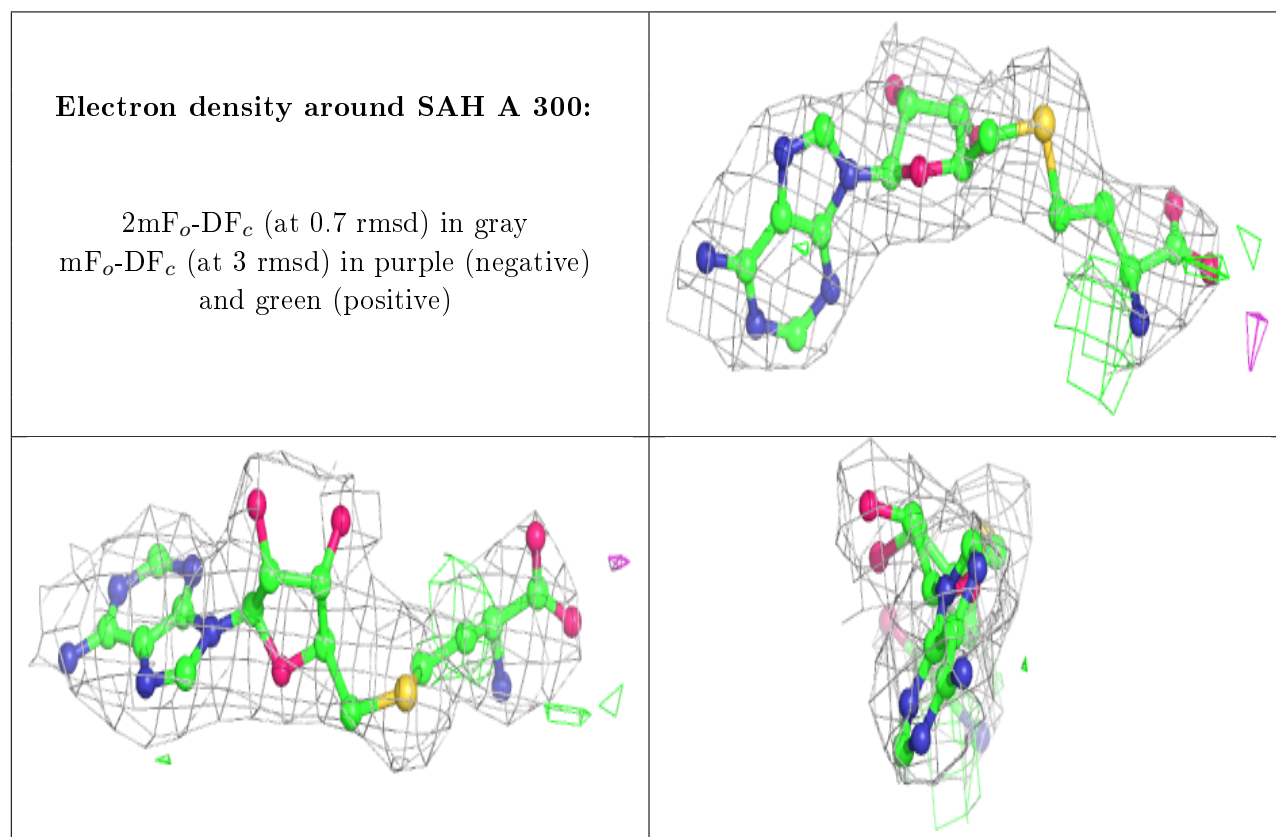
There are no carbohydrates in this entry.

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
3	SAH	A	300	26/26	0.94	0.21	39,45,53,55	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.