Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2023 – 12:15 AM EDT

PDB ID	:	2Q4V
Title	:	Ensemble refinement of the protein crystal structure of thialysine n-acetyltransferase (SSAT2) from Homo sapiens
Authors	:	Levin, E.J.; Kondrashov, D.A.; Wesenberg, G.E.; Phillips Jr., G.N.; Center for Eukaryotic Structural Genomics (CESG)
Deposited on	:	2007-05-31
Resolution	:	1.84 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:

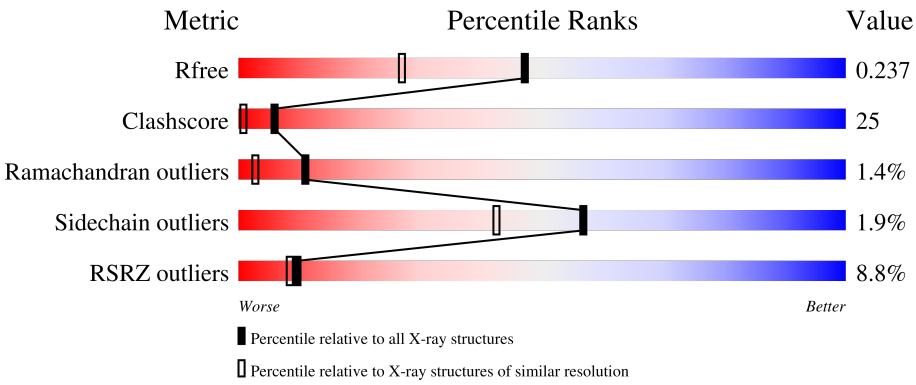
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 1.84 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	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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	1-A	170	8%; 51%, 36%, 5%, 8%
1	1-B	170	8%; 56%, 36%, • 6%
1	2-A	170	8%; 55%, 36%, • 8%
1	2-B	170	8%; 59%, 32%, • 6%

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Mol	Chain	Length	Quality of chain
1	3-A	170	8% 57% 33% 8%
1	3-B	170	8% 59% 34% 6%
1	4-A	170	8% 55% 35% 8%
1	4-B	170	8% 55% 38% 6%
1	5-A	170	8% 45% 45% 8%
1	5-B	170	8% 52% 38% 6%
1	6-A	170	8% 48% 42% 8%
1	6-B	170	8% 35% 54% 5% 6%
1	7-A	170	8% 48% 44% 8%
1	7-B	170	8% 62% 31% 6%
1	8-A	170	8% 60% 31% 8%
1	8-B	170	8% 61% 32% 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23024 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.

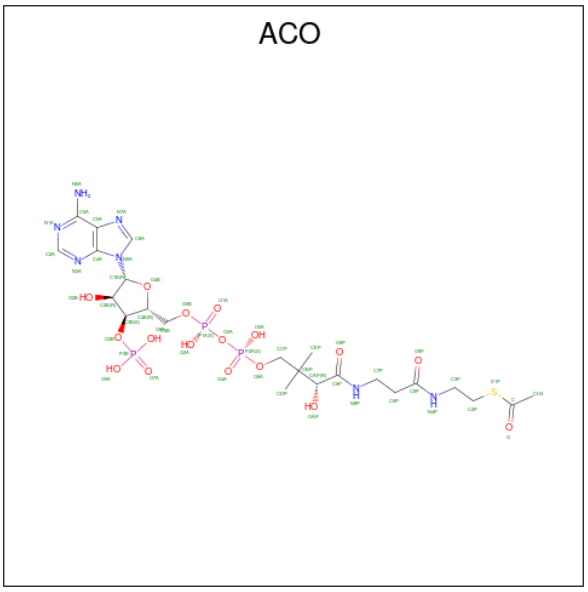
- Molecule 1 is a protein called Diamine acetyltransferase 2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	1-A	156	1248	804	210	227	5	2	0	0	0
1	2-A	156	1248	804	210	227	5	2	0	0	0
1	3-A	156	1248	804	210	227	5	2	0	0	0
1	4-A	156	1248	804	210	227	5	2	0	0	0
1	5-A	156	1248	804	210	227	5	2	0	0	0
1	6-A	156	1248	804	210	227	5	2	0	0	0
1	7-A	156	1248	804	210	227	5	2	0	0	0
1	8-A	156	1248	804	210	227	5	2	0	0	0
1	1-B	159	1274	817	215	235	5	2	0	0	0
1	2-B	159	1274	817	215	235	5	2	0	0	0
1	3-B	159	1274	817	215	235	5	2	0	0	0
1	4-B	159	1274	817	215	235	5	2	0	0	0
1	5-B	159	1274	817	215	235	5	2	0	0	0
1	6-B	159	1274	817	215	235	5	2	0	0	0
1	7-B	159	1274	817	215	235	5	2	0	0	0
1	8-B	159	1274	817	215	235	5	2	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SER	-	expression tag	UNP Q96F10
A	97	MSE	MET	modified residue	UNP Q96F10
A	137	MSE	MET	modified residue	UNP Q96F10
B	1	SER	-	expression tag	UNP Q96F10
B	97	MSE	MET	modified residue	UNP Q96F10
B	137	MSE	MET	modified residue	UNP Q96F10

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
2	1-A	1	51	23	7	17	3	1	0	0
2	2-A	1	51	23	7	17	3	1	0	0
2	3-A	1	51	23	7	17	3	1	0	0
2	4-A	1	51	23	7	17	3	1	0	0
2	5-A	1	51	23	7	17	3	1	0	0
2	6-A	1	51	23	7	17	3	1	0	0
2	7-A	1	51	23	7	17	3	1	0	0
2	8-A	1	51	23	7	17	3	1	0	0

- Molecule 3 is water.

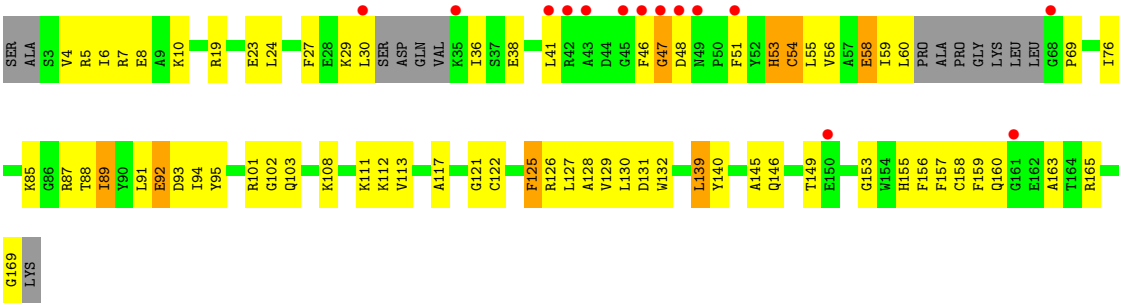
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	1-A	147	147	147	0	0
3	2-A	146	146	146	0	0
3	3-A	146	146	146	0	0
3	4-A	147	147	147	0	0
3	5-A	142	142	142	0	0
3	6-A	152	152	152	0	0
3	7-A	142	142	142	0	0
3	8-A	146	146	146	0	0
3	1-B	158	158	158	0	0
3	2-B	159	159	159	0	0
3	3-B	159	159	159	0	0
3	4-B	158	158	158	0	0
3	5-B	163	163	163	0	0
3	6-B	153	153	153	0	0
3	7-B	163	163	163	0	0
3	8-B	159	159	159	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.

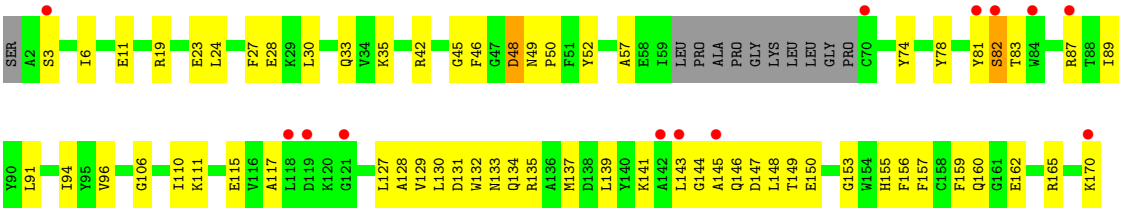
• Molecule 1: Diamine acetyltransferase 2

Chain 1-A:



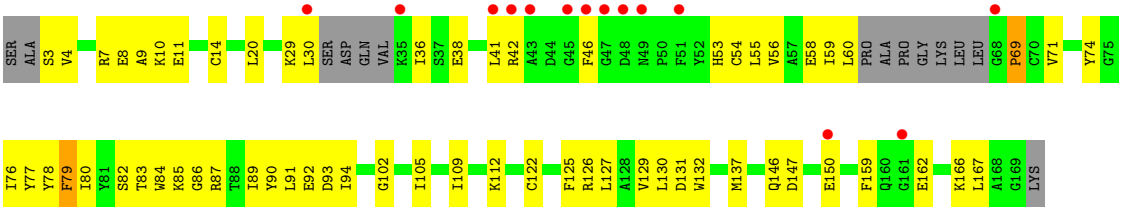
• Molecule 1: Diamine acetyltransferase 2

Chain 1-B:



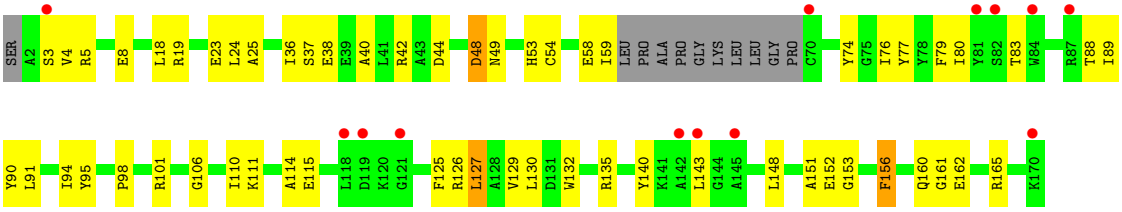
• Molecule 1: Diamine acetyltransferase 2

Chain 2-A:



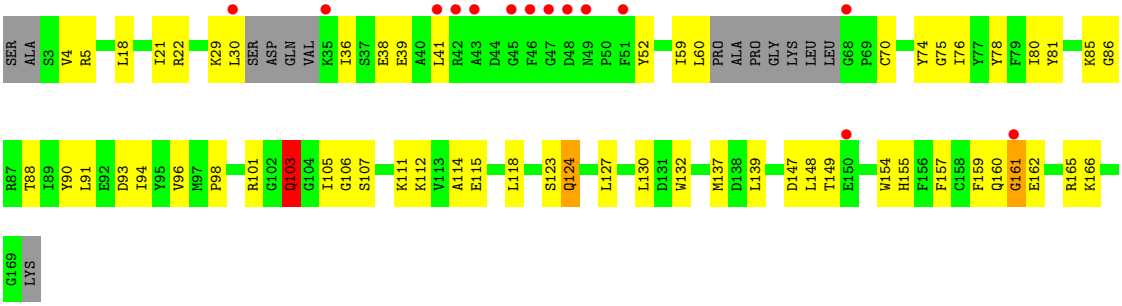
• Molecule 1: Diamine acetyltransferase 2

Chain 2-B:



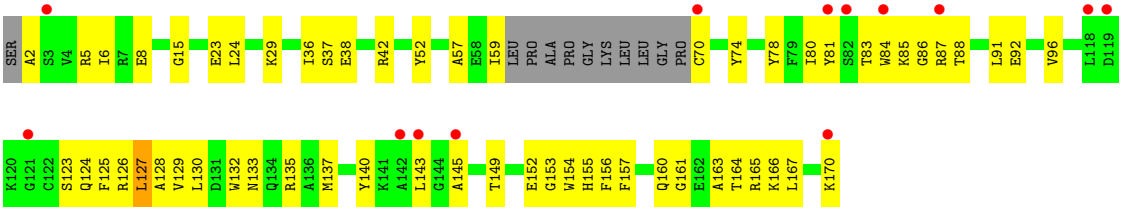
• Molecule 1: Diamine acetyltransferase 2

Chain 3-A:



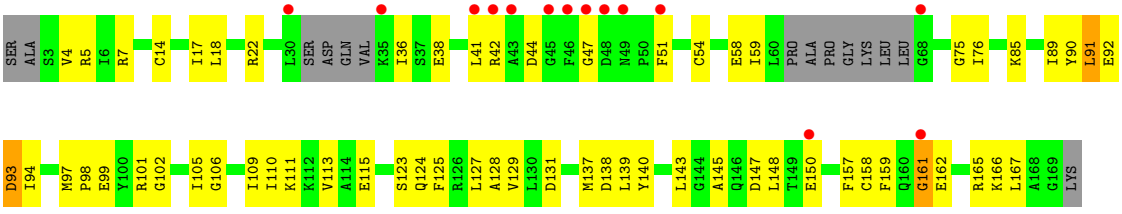
• Molecule 1: Diamine acetyltransferase 2

Chain 3-B:



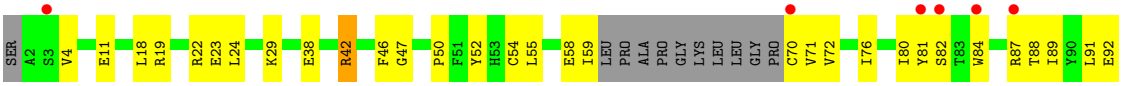
• Molecule 1: Diamine acetyltransferase 2

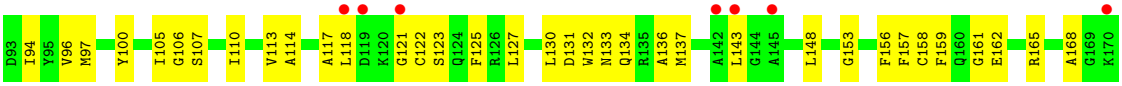
Chain 4-A:



• Molecule 1: Diamine acetyltransferase 2

Chain 4-B:



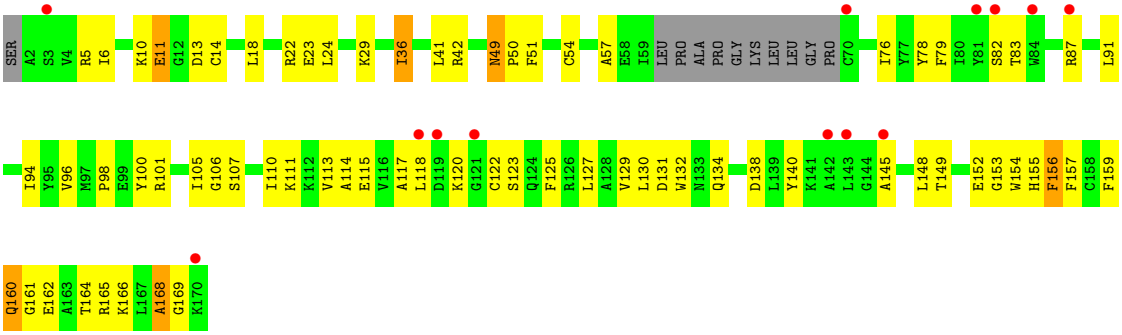


• Molecule 1: Diamine acetyltransferase 2

Chain 5-A:

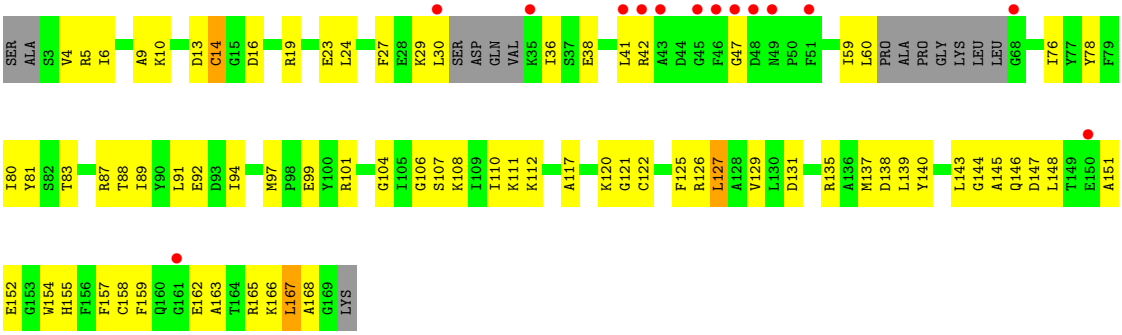
• Molecule 1: Diamine acetyltransferase 2

Chain 5-B:



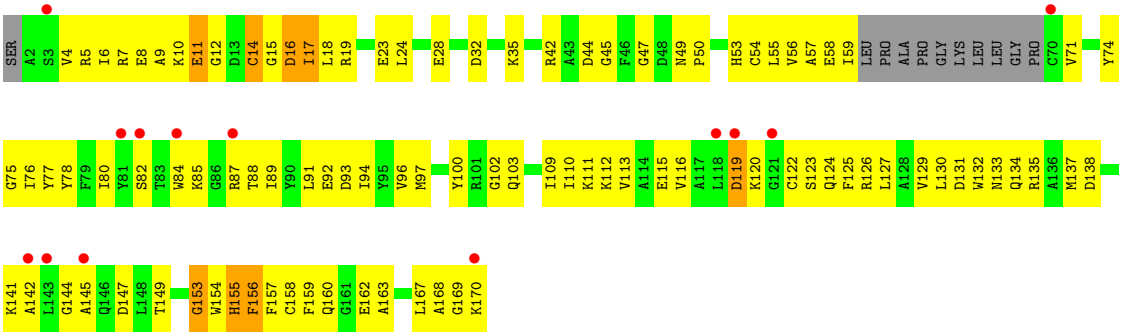
• Molecule 1: Diamine acetyltransferase 2

Chain 6-A:



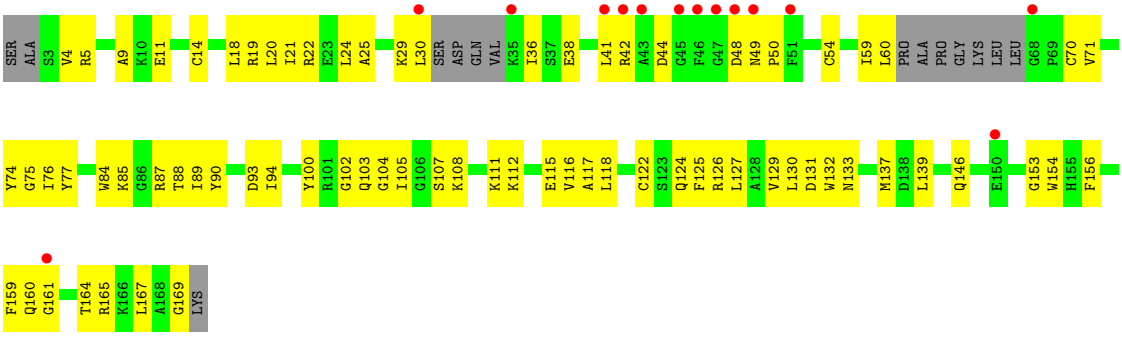
• Molecule 1: Diamine acetyltransferase 2

Chain 6-B:



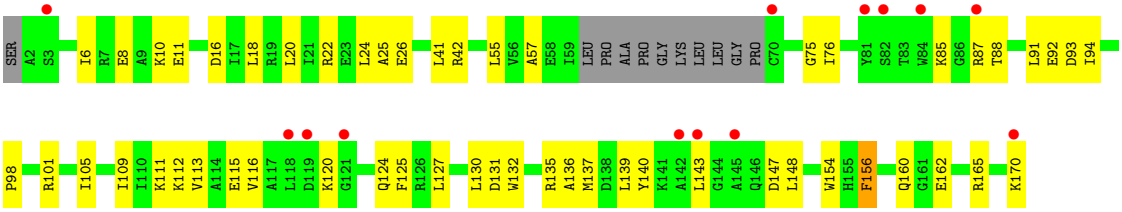
- Molecule 1: Diamine acetyltransferase 2

Chain 7-A:



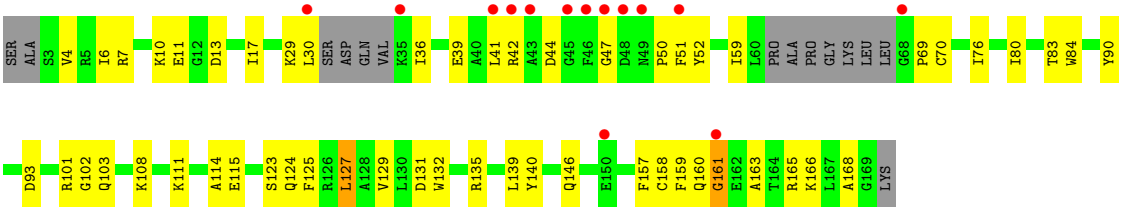
- Molecule 1: Diamine acetyltransferase 2

Chain 7-B:



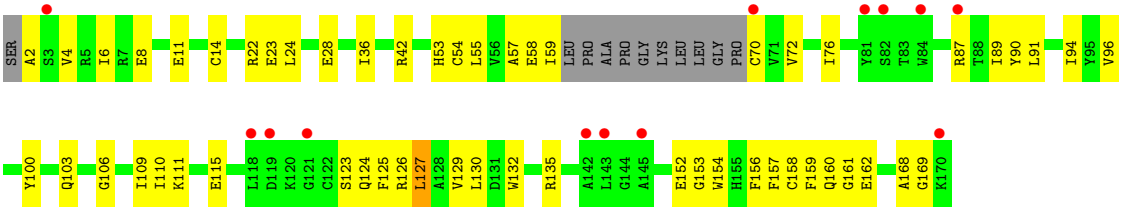
- Molecule 1: Diamine acetyltransferase 2

Chain 8-A:



- Molecule 1: Diamine acetyltransferase 2

Chain 8-B:


SER A2 S3 V4 R5 I6 R7 E8 E11 C14 R22 E23 L24 E28 I36 R42 H53 C54 L55 V56 A57 E58 I59 LEU PRO ALA PRO GLY LYS LEU LEU GLY PRO C70 V71 V72 I76 Y81 S82 T83 W84 R87 T88 I89 Y90 L91 I94 Y95 V96
Y100 Q103 G106 I109 I110 K111 E115 L118 D119 K120 G121 C122 S123 Q124 F125 R126 L127 A128 V129 L130 D131 W132 R135 A142 L143 G144 A145 E152 G153 W154 H155 F156 F157 C158 F159 Q160 G161 E162 A168 G169 K170

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	54.58Å 83.62Å 87.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.52 – 1.84 43.77 – 1.84	Depositor EDS
% Data completeness (in resolution range)	96.5 (40.52-1.84) 96.7 (43.77-1.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.55 (at 1.84Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.183 , 0.234 0.194 , 0.237	Depositor DCC
R_{free} test set	1719 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	27.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	23024	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.50% 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: ACO

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	1-A	0.39	0/1271	0.60	0/1704
1	1-B	0.40	0/1297	0.56	0/1738
1	2-A	0.40	0/1271	0.58	0/1704
1	2-B	0.40	0/1297	0.57	0/1738
1	3-A	0.39	0/1271	0.59	0/1704
1	3-B	0.41	0/1297	0.56	0/1738
1	4-A	0.40	0/1271	0.58	0/1704
1	4-B	0.40	0/1297	0.57	0/1738
1	5-A	0.42	0/1271	0.63	0/1704
1	5-B	0.42	0/1297	0.58	0/1738
1	6-A	0.43	0/1271	0.62	0/1704
1	6-B	0.42	0/1297	0.57	0/1738
1	7-A	0.42	0/1271	0.60	0/1704
1	7-B	0.43	0/1297	0.60	0/1738
1	8-A	0.42	0/1271	0.60	0/1704
1	8-B	0.42	0/1297	0.59	0/1738
All	All	0.41	0/20544	0.59	0/27536

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 (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	1-A	1248	0	1230	77	0
1	1-B	1274	0	1254	65	0
1	2-A	1248	0	1230	72	0
1	2-B	1274	0	1254	55	0
1	3-A	1248	0	1230	73	0
1	3-B	1274	0	1254	75	0
1	4-A	1248	0	1230	65	0
1	4-B	1274	0	1254	84	0
1	5-A	1248	0	1230	88	0
1	5-B	1274	0	1254	79	0
1	6-A	1248	0	1230	74	0
1	6-B	1274	0	1254	118	0
1	7-A	1248	0	1230	80	0
1	7-B	1274	0	1254	58	0
1	8-A	1248	0	1230	58	0
1	8-B	1274	0	1254	53	0
2	1-A	51	0	34	4	0
2	2-A	51	0	34	4	0
2	3-A	51	0	34	3	0
2	4-A	51	0	34	8	0
2	5-A	51	0	34	1	0
2	6-A	51	0	34	8	0
2	7-A	51	0	34	3	0
2	8-A	51	0	34	6	0
3	1-A	147	0	0	10	0
3	1-B	158	0	0	17	0
3	2-A	146	0	0	8	0
3	2-B	159	0	0	12	0
3	3-A	146	0	0	6	0
3	3-B	159	0	0	14	0
3	4-A	147	0	0	8	0
3	4-B	158	0	0	18	0
3	5-A	142	0	0	12	0
3	5-B	163	0	0	16	0
3	6-A	152	0	0	12	0
3	6-B	153	0	0	18	0
3	7-A	142	0	0	8	0
3	7-B	163	0	0	12	0
3	8-A	146	0	0	12	0
3	8-B	159	0	0	9	0
All	All	23024	0	20144	1018	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 25.

All (1018) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLY:HA3	1:B:111:LYS:HE2	1.38	1.06
1:A:154:TRP:HA	1:B:129:VAL:O	1.60	1.01
1:A:80:ILE:HD13	1:A:90:TYR:HB2	1.38	0.99
1:B:11:GLU:HG2	1:B:42:ARG:HH12	1.27	0.98
1:B:59:ILE:HB	1:B:70:CYS:HB3	1.49	0.94
1:A:59:ILE:HB	1:A:70:CYS:SG	2.10	0.92
1:B:11:GLU:HG2	1:B:42:ARG:NH1	1.86	0.90
1:B:42:ARG:HH11	1:B:42:ARG:HG2	1.39	0.87
1:B:87:ARG:HD3	3:B:328:HOH:O	1.76	0.86
1:A:115:GLU:HG3	1:B:168:ALA:HA	1.59	0.85
1:A:130:LEU:HD12	1:A:130:LEU:H	1.42	0.85
1:B:24:LEU:HD23	3:B:290:HOH:O	1.76	0.84
3:A:398:HOH:O	1:B:24:LEU:HD23	1.77	0.84
1:B:87:ARG:HD3	3:B:329:HOH:O	1.77	0.84
1:A:54:CYS:HB3	1:A:76:ILE:HG12	1.57	0.84
1:B:18:LEU:HD23	3:B:205:HOH:O	1.78	0.83
1:A:156:PHE:HB3	1:B:148:LEU:HD12	1.59	0.83
1:A:129:VAL:HG23	3:A:451:HOH:O	1.77	0.83
1:A:146:GLN:HG3	1:B:160:GLN:HE21	1.42	0.83
1:B:165:ARG:HB3	1:B:170:LYS:HB2	1.59	0.83
1:B:87:ARG:HD3	3:B:333:HOH:O	1.78	0.82
1:B:24:LEU:HD23	3:B:289:HOH:O	1.80	0.81
1:B:24:LEU:HD23	3:B:292:HOH:O	1.81	0.79
1:A:101:ARG:NH2	2:A:306:ACO:H72	1.98	0.79
1:B:38:GLU:HG2	1:B:42:ARG:HE	1.45	0.79
1:A:130:LEU:HD22	1:A:132:TRP:HE1	1.46	0.79
2:A:306:ACO:O5A	3:A:321:HOH:O	2.01	0.79
1:A:163:ALA:HB1	1:B:144:GLY:O	1.82	0.78
1:B:91:LEU:HD11	1:B:94:ILE:HG13	1.64	0.78
1:A:4:VAL:HG22	1:A:59:ILE:HD13	1.65	0.78
1:A:115:GLU:HG3	1:B:168:ALA:HA	1.66	0.77
1:B:134:GLN:HB3	3:B:300:HOH:O	1.85	0.77
1:A:153:GLY:HA3	1:B:131:ASP:OD2	1.84	0.77
1:A:92:GLU:HA	3:A:367:HOH:O	1.83	0.77
1:B:127:LEU:HD13	1:B:129:VAL:HG23	1.67	0.76
1:B:125:PHE:HE1	1:B:127:LEU:HD23	1.51	0.76
1:B:42:ARG:NH1	1:B:42:ARG:HG2	1.97	0.76
1:A:102:GLY:O	3:A:392:HOH:O	2.03	0.76
1:B:141:LYS:NZ	1:B:147:ASP:H	1.85	0.76
1:A:102:GLY:O	3:A:396:HOH:O	2.03	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:42:ARG:HH11	1:B:42:ARG:CG	1.99	0.75
1:A:159:PHE:HB2	1:B:125:PHE:HB3	1.68	0.75
1:A:118:LEU:HD11	1:B:165:ARG:HA	1.68	0.75
1:B:91:LEU:HD21	1:B:94:ILE:HD11	1.67	0.75
1:B:10:LYS:HE2	1:B:10:LYS:HA	1.68	0.75
1:A:11:GLU:HB3	3:A:381:HOH:O	1.87	0.75
1:A:126:ARG:HD3	1:B:156:PHE:CZ	2.21	0.75
1:A:4:VAL:HG22	1:A:59:ILE:HD13	1.69	0.75
1:B:54:CYS:HB2	1:B:76:ILE:HG12	1.69	0.74
1:B:13:ASP:OD1	3:B:183:HOH:O	2.04	0.74
1:A:5:ARG:HD3	1:A:60:LEU:HD11	1.68	0.74
1:A:160:GLN:HA	1:B:124:GLN:NE2	2.01	0.74
1:A:155:HIS:NE2	3:A:428:HOH:O	2.21	0.74
1:B:87:ARG:HG3	3:B:305:HOH:O	1.87	0.74
1:B:42:ARG:NE	3:B:191:HOH:O	2.21	0.74
1:A:126:ARG:HG3	1:B:156:PHE:CE2	2.22	0.74
1:A:76:ILE:HB	1:A:93:ASP:HB2	1.70	0.73
1:B:141:LYS:NZ	1:B:147:ASP:HB2	2.04	0.73
1:A:4:VAL:HG13	1:A:58:GLU:O	1.88	0.73
1:B:23:GLU:HG3	3:B:252:HOH:O	1.89	0.73
1:B:130:LEU:HD13	1:B:132:TRP:HE1	1.54	0.72
1:A:11:GLU:HB3	1:A:42:ARG:NH1	2.05	0.72
1:A:22:ARG:HG2	1:A:22:ARG:HH11	1.55	0.72
1:A:130:LEU:HD12	1:A:130:LEU:N	2.04	0.71
1:B:3:SER:HB3	3:B:310:HOH:O	1.90	0.71
1:A:160:GLN:HE22	1:B:85:LYS:HE3	1.54	0.71
1:B:87:ARG:HG3	3:B:310:HOH:O	1.90	0.71
1:A:48:ASP:HA	3:A:445:HOH:O	1.87	0.71
1:B:83:THR:HB	3:B:297:HOH:O	1.90	0.71
1:A:36:ILE:HB	3:A:449:HOH:O	1.90	0.71
1:A:4:VAL:HG22	1:A:59:ILE:HD13	1.73	0.71
1:B:54:CYS:SG	1:B:76:ILE:HA	2.31	0.71
1:A:130:LEU:HD13	1:A:132:TRP:HE1	1.56	0.70
1:B:16:ASP:OD2	3:B:177:HOH:O	2.09	0.70
1:B:38:GLU:HG2	1:B:42:ARG:HE	1.55	0.70
1:A:97:MSE:O	1:A:101:ARG:HG3	1.90	0.70
1:B:54:CYS:SG	1:B:56:VAL:HG13	2.31	0.70
1:A:44:ASP:HB3	1:A:51:PHE:HB2	1.73	0.70
1:B:130:LEU:HD13	1:B:132:TRP:HE1	1.57	0.70
1:B:100:TYR:HB3	1:B:105:ILE:HD12	1.73	0.70
1:B:162:GLU:HG3	3:B:330:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:LEU:HD13	1:B:132:TRP:HE1	1.57	0.69
1:A:83:THR:HG23	3:B:223:HOH:O	1.91	0.69
1:A:127:LEU:HD11	1:B:159:PHE:CD1	2.27	0.69
1:A:115:GLU:HG3	1:B:168:ALA:HA	1.74	0.69
1:A:127:LEU:O	1:B:157:PHE:HB2	1.93	0.69
1:A:168:ALA:O	1:B:115:GLU:HG2	1.93	0.68
1:B:89:ILE:HG22	1:B:125:PHE:HA	1.75	0.68
1:A:94:ILE:HG23	2:A:306:ACO:H31	1.75	0.68
1:A:146:GLN:HG3	1:B:160:GLN:CD	2.14	0.68
1:A:102:GLY:O	3:A:391:HOH:O	2.11	0.68
1:B:38:GLU:CG	1:B:42:ARG:HE	2.06	0.68
1:A:139:LEU:HB2	2:A:306:ACO:O4B	1.94	0.67
1:A:139:LEU:O	1:A:143:LEU:HG	1.93	0.67
1:A:10:LYS:HE3	3:A:385:HOH:O	1.95	0.67
1:A:111:LYS:HE3	3:A:440:HOH:O	1.95	0.67
1:A:54:CYS:HB3	1:A:76:ILE:HG12	1.76	0.67
1:B:18:LEU:HD21	1:B:22:ARG:NH2	2.09	0.67
1:B:11:GLU:HG2	1:B:42:ARG:NH1	2.09	0.67
1:A:29:LYS:O	1:A:30:LEU:HB2	1.93	0.67
1:A:91:LEU:HD21	1:A:94:ILE:HB	1.75	0.67
1:A:159:PHE:HB2	1:B:125:PHE:HB3	1.75	0.67
1:A:161:GLY:O	1:A:165:ARG:HG2	1.95	0.66
1:B:87:ARG:HG3	3:B:308:HOH:O	1.94	0.66
1:B:42:ARG:CZ	3:B:191:HOH:O	2.43	0.66
1:A:7:ARG:CZ	1:A:10:LYS:HE2	2.25	0.66
1:A:92:GLU:HG3	1:A:93:ASP:OD2	1.96	0.66
1:B:19:ARG:O	1:B:23:GLU:HG3	1.95	0.66
1:B:23:GLU:HG3	3:B:253:HOH:O	1.96	0.66
1:A:55:LEU:HD21	3:A:317:HOH:O	1.95	0.66
1:A:14:CYS:HB3	1:A:38:GLU:HG3	1.78	0.65
1:A:129:VAL:HG23	3:A:447:HOH:O	1.96	0.65
1:A:14:CYS:SG	1:A:42:ARG:HG3	2.35	0.65
1:A:158:CYS:HA	1:B:125:PHE:O	1.95	0.65
1:A:54:CYS:CB	1:A:76:ILE:HG12	2.24	0.65
1:B:125:PHE:CE1	1:B:127:LEU:HD23	2.32	0.65
1:B:161:GLY:HA2	3:B:182:HOH:O	1.96	0.65
1:A:41:LEU:HG	3:A:417:HOH:O	1.96	0.65
1:B:91:LEU:HD21	1:B:94:ILE:CD1	2.27	0.65
1:B:94:ILE:CD1	1:B:110:ILE:HG12	2.26	0.65
1:A:152:GLU:HB2	1:A:154:TRP:CD1	2.32	0.65
1:A:145:ALA:HB2	1:B:159:PHE:CE2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:TYR:HB2	1:A:90:TYR:O	1.96	0.65
1:A:127:LEU:HD22	2:A:306:ACO:HH32	1.79	0.65
1:A:36:ILE:HD12	3:B:300:HOH:O	1.97	0.65
1:B:162:GLU:HG2	3:B:319:HOH:O	1.97	0.64
1:A:4:VAL:HG22	1:A:59:ILE:HD13	1.79	0.64
1:A:123:SER:O	1:A:124:GLN:HB3	1.97	0.64
1:A:124:GLN:OE1	1:B:160:GLN:HA	1.98	0.64
1:B:127:LEU:HD13	1:B:129:VAL:HG23	1.79	0.64
1:A:160:GLN:HA	1:B:124:GLN:HE22	1.62	0.64
1:B:130:LEU:O	1:B:137:MSE:HE3	1.98	0.64
1:B:42:ARG:NH1	3:B:190:HOH:O	2.22	0.64
1:B:155:HIS:HB3	1:B:157:PHE:HE1	1.63	0.64
1:B:127:LEU:HD13	1:B:129:VAL:HG23	1.79	0.64
1:A:36:ILE:HG22	1:A:41:LEU:HD12	1.80	0.64
1:B:102:GLY:HA2	3:B:188:HOH:O	1.97	0.64
1:B:135:ARG:HG3	3:B:302:HOH:O	1.97	0.64
1:A:114:ALA:HB1	1:B:164:THR:HG23	1.77	0.64
1:B:11:GLU:O	1:B:14:CYS:SG	2.56	0.64
1:A:101:ARG:O	3:A:354:HOH:O	2.15	0.64
1:B:55:LEU:HD21	3:B:185:HOH:O	1.97	0.64
1:A:9:ALA:CB	1:A:54:CYS:HB2	2.28	0.64
1:A:169:GLY:HA3	1:B:111:LYS:HE2	1.79	0.63
1:B:53:HIS:O	1:B:76:ILE:HG23	1.98	0.63
1:B:91:LEU:HD11	1:B:94:ILE:HG13	1.80	0.63
1:A:124:GLN:CB	1:B:159:PHE:O	2.46	0.63
1:A:139:LEU:C	1:A:139:LEU:HD12	2.19	0.63
1:B:158:CYS:SG	1:B:160:GLN:HG2	2.38	0.63
1:A:127:LEU:HD22	2:A:306:ACO:HH32	1.80	0.63
1:B:98:PRO:HG3	3:B:186:HOH:O	1.97	0.63
1:A:11:GLU:HG3	1:A:42:ARG:HH11	1.64	0.63
3:A:456:HOH:O	1:B:170:LYS:HE2	1.99	0.63
1:B:161:GLY:O	1:B:165:ARG:HG3	1.99	0.62
1:B:29:LYS:HE3	3:B:276:HOH:O	1.98	0.62
1:A:24:LEU:HD13	1:A:95:TYR:HB2	1.80	0.62
1:B:160:GLN:HB2	3:B:247:HOH:O	1.99	0.62
1:A:167:LEU:HG	1:B:114:ALA:HB2	1.79	0.62
1:A:29:LYS:O	1:A:30:LEU:HB2	1.97	0.62
1:A:139:LEU:HD22	2:A:306:ACO:H52A	1.82	0.62
1:A:81:TYR:HB2	1:B:52:TYR:HB3	1.79	0.62
1:B:29:LYS:HE3	3:B:272:HOH:O	1.99	0.62
1:A:165:ARG:HA	1:B:118:LEU:HD11	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:ASP:HA	1:A:137:MSE:CE	2.30	0.62
1:A:88:THR:HG23	1:A:124:GLN:O	1.99	0.62
1:A:18:LEU:HG	1:A:22:ARG:HH12	1.65	0.62
1:A:14:CYS:HB3	1:A:38:GLU:HG3	1.82	0.62
1:B:44:ASP:CG	3:B:256:HOH:O	2.38	0.62
1:B:11:GLU:HG3	1:B:42:ARG:HG2	1.81	0.62
1:A:81:TYR:CB	1:B:52:TYR:HB3	2.30	0.62
1:A:94:ILE:HG23	2:A:306:ACO:H31	1.80	0.62
1:B:133:ASN:HB3	1:B:136:ALA:HB3	1.82	0.62
1:B:98:PRO:HA	1:B:101:ARG:HG2	1.82	0.62
1:A:130:LEU:HD13	1:A:132:TRP:NE1	2.15	0.61
1:A:131:ASP:OD1	1:B:153:GLY:HA3	1.99	0.61
1:A:157:PHE:O	1:B:126:ARG:HA	1.98	0.61
1:B:59:ILE:HB	1:B:70:CYS:CB	2.26	0.61
1:A:137:MSE:HE1	1:B:155:HIS:ND1	2.15	0.61
1:B:91:LEU:HD13	1:B:113:VAL:HG21	1.81	0.61
1:A:94:ILE:HG22	2:A:306:ACO:O	1.99	0.61
1:A:159:PHE:O	1:B:124:GLN:HA	1.99	0.61
1:B:105:ILE:HB	3:B:179:HOH:O	2.00	0.61
1:B:45:GLY:HA2	1:B:50:PRO:HB3	1.81	0.61
1:B:127:LEU:CD1	1:B:129:VAL:HG23	2.29	0.61
1:B:148:LEU:HB3	1:B:154:TRP:CD1	2.35	0.61
1:B:127:LEU:C	1:B:127:LEU:HD12	2.21	0.61
1:B:106:GLY:N	3:B:180:HOH:O	2.27	0.61
1:A:139:LEU:HD22	2:A:306:ACO:H52A	1.83	0.61
1:B:6:ILE:HD13	1:B:57:ALA:HA	1.83	0.61
1:B:162:GLU:HG2	3:B:323:HOH:O	2.00	0.61
1:A:10:LYS:N	1:A:13:ASP:OD2	2.33	0.61
1:A:127:LEU:HB2	1:B:157:PHE:HB2	1.83	0.61
1:B:121:GLY:HA2	3:B:172:HOH:O	2.01	0.61
1:B:169:GLY:HA2	3:B:278:HOH:O	2.01	0.61
1:A:107:SER:O	1:A:111:LYS:HG3	2.01	0.60
1:A:3:SER:OG	1:A:60:LEU:HD12	2.01	0.60
1:A:47:GLY:O	1:A:50:PRO:HD3	2.01	0.60
1:A:128:ALA:O	2:A:306:ACO:HH33	2.02	0.60
1:B:127:LEU:HD12	1:B:128:ALA:N	2.16	0.60
1:A:3:SER:OG	1:A:60:LEU:HD12	2.02	0.60
1:A:127:LEU:HD13	2:A:306:ACO:HH32	1.82	0.60
1:B:96:VAL:HG21	3:B:179:HOH:O	2.01	0.60
1:A:21:ILE:HD11	1:A:76:ILE:HD11	1.83	0.60
1:B:90:TYR:HA	1:B:126:ARG:O	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:ARG:HB3	2:A:306:ACO:H1B	1.84	0.60
1:B:130:LEU:HD13	1:B:132:TRP:HE1	1.66	0.60
1:B:47:GLY:O	1:B:50:PRO:HD3	2.00	0.60
1:A:84:TRP:CH2	1:B:25:ALA:HA	2.35	0.60
1:A:5:ARG:NE	1:A:60:LEU:HD21	2.17	0.60
1:A:106:GLY:HA3	2:A:306:ACO:O6A	2.01	0.60
1:B:152:GLU:HB2	1:B:154:TRP:CD1	2.37	0.59
1:A:18:LEU:O	1:A:22:ARG:HG3	2.03	0.59
1:B:33:GLN:HG3	3:B:233:HOH:O	2.00	0.59
1:B:130:LEU:HD13	1:B:132:TRP:HE1	1.67	0.59
1:B:23:GLU:HG3	3:B:249:HOH:O	2.02	0.59
1:A:48:ASP:HA	3:A:444:HOH:O	2.02	0.59
1:A:130:LEU:H	1:A:130:LEU:CD1	2.12	0.59
1:A:152:GLU:O	1:B:130:LEU:HD22	2.03	0.59
1:B:130:LEU:HD12	1:B:130:LEU:N	2.17	0.59
1:A:11:GLU:HG2	1:A:42:ARG:HG2	1.85	0.59
1:B:91:LEU:HD21	1:B:94:ILE:HD12	1.84	0.59
1:A:131:ASP:OD2	1:B:153:GLY:HA3	2.03	0.59
1:A:152:GLU:HB2	1:A:154:TRP:NE1	2.17	0.59
1:A:160:GLN:HG3	3:B:293:HOH:O	2.03	0.59
1:B:10:LYS:O	1:B:12:GLY:N	2.35	0.59
1:A:146:GLN:HG2	1:B:160:GLN:NE2	2.18	0.59
1:A:153:GLY:HA3	1:B:131:ASP:OD2	2.03	0.59
1:B:141:LYS:HZ3	1:B:147:ASP:H	1.48	0.59
1:A:29:LYS:O	1:A:30:LEU:HB2	2.02	0.59
1:A:160:GLN:NE2	1:B:85:LYS:HE3	2.18	0.59
1:A:54:CYS:HB3	1:A:76:ILE:CG1	2.33	0.59
1:A:157:PHE:HB2	1:B:127:LEU:CD1	2.33	0.59
1:A:131:ASP:HA	1:A:137:MSE:SE	2.53	0.59
1:B:16:ASP:O	1:B:18:LEU:N	2.35	0.59
1:A:11:GLU:HB3	1:A:42:ARG:HH11	1.66	0.59
1:B:96:VAL:HG21	3:B:180:HOH:O	2.02	0.59
1:B:10:LYS:C	1:B:12:GLY:H	2.06	0.58
1:B:94:ILE:CD1	1:B:110:ILE:HG12	2.33	0.58
1:A:157:PHE:HB2	1:B:127:LEU:HD12	1.84	0.58
1:A:83:THR:HG1	1:A:84:TRP:HD1	1.51	0.58
1:B:96:VAL:HG21	3:B:180:HOH:O	2.04	0.58
1:B:107:SER:HB2	3:B:294:HOH:O	2.02	0.58
1:A:59:ILE:HG22	1:A:60:LEU:N	2.18	0.58
1:B:47:GLY:O	1:B:50:PRO:HD3	2.02	0.58
1:A:157:PHE:CZ	1:B:137:MSE:HG2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:ALA:HB2	1:A:54:CYS:HB2	1.86	0.58
1:A:87:ARG:HD3	1:B:44:ASP:OD1	2.04	0.58
1:B:37:SER:O	1:B:40:ALA:HB3	2.03	0.58
1:A:47:GLY:HA3	3:A:423:HOH:O	2.02	0.58
1:A:162:GLU:O	1:A:166:LYS:HD3	2.04	0.58
1:B:24:LEU:O	1:B:28:GLU:HG3	2.04	0.58
1:A:124:GLN:HB2	1:B:159:PHE:O	2.03	0.58
1:A:5:ARG:NE	1:A:60:LEU:HD11	2.19	0.57
1:B:129:VAL:HG12	1:B:130:LEU:N	2.19	0.57
1:B:38:GLU:HG2	1:B:42:ARG:NE	2.17	0.57
1:B:111:LYS:HG2	1:B:115:GLU:OE1	2.04	0.57
1:B:165:ARG:HB3	1:B:165:ARG:NH1	2.20	0.57
1:B:57:ALA:HB2	1:B:109:ILE:HD11	1.87	0.57
1:A:103:GLN:O	1:A:103:GLN:HG3	2.04	0.57
1:B:58:GLU:HG3	1:B:70:CYS:O	2.04	0.57
1:B:16:ASP:O	1:B:19:ARG:N	2.37	0.57
1:A:29:LYS:O	1:A:30:LEU:HB2	2.04	0.57
1:A:4:VAL:HG22	1:A:59:ILE:HD13	1.85	0.57
1:A:14:CYS:HB3	1:A:41:LEU:HD23	1.87	0.57
1:B:4:VAL:HG23	1:B:58:GLU:O	2.04	0.57
1:B:123:SER:C	1:B:124:GLN:HE21	2.08	0.57
1:B:155:HIS:HB3	1:B:157:PHE:CE1	2.39	0.57
1:A:159:PHE:HB3	1:A:164:THR:OG1	2.05	0.57
1:B:161:GLY:HA2	3:B:181:HOH:O	2.03	0.57
1:A:4:VAL:HG22	1:A:59:ILE:CD1	2.35	0.57
1:A:85:LYS:HE3	3:A:416:HOH:O	2.05	0.57
1:B:134:GLN:HG3	1:B:138:ASP:OD2	2.05	0.57
1:B:59:ILE:HG13	1:B:100:TYR:CE1	2.39	0.57
1:A:89:ILE:HG22	1:A:125:PHE:HB2	1.87	0.57
1:A:4:VAL:HG22	1:A:59:ILE:HD13	1.87	0.57
1:B:91:LEU:HD21	1:B:94:ILE:CD1	2.34	0.57
1:B:96:VAL:HG21	3:B:180:HOH:O	2.03	0.57
1:B:166:LYS:HG3	3:B:283:HOH:O	2.05	0.57
1:B:129:VAL:HG12	1:B:130:LEU:O	2.05	0.57
1:A:161:GLY:O	1:A:165:ARG:HG3	2.05	0.57
1:A:126:ARG:HG2	1:A:127:LEU:H	1.69	0.56
1:A:10:LYS:HB3	3:A:401:HOH:O	2.04	0.56
1:A:127:LEU:HD23	1:A:127:LEU:N	2.19	0.56
1:B:35:LYS:HE2	1:B:35:LYS:HA	1.86	0.56
1:B:89:ILE:HG22	1:B:125:PHE:HA	1.87	0.56
1:B:133:ASN:O	1:B:137:MSE:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:ILE:HD11	1:A:140:TYR:HE1	1.69	0.56
1:A:127:LEU:HB2	1:B:157:PHE:CB	2.35	0.56
1:B:59:ILE:HG12	1:B:72:VAL:HG21	1.86	0.56
1:B:130:LEU:O	1:B:133:ASN:HB2	2.05	0.56
1:B:79:PHE:HZ	1:B:120:LYS:HG3	1.69	0.56
1:A:80:ILE:HB	1:B:78:TYR:CZ	2.40	0.56
1:A:133:ASN:O	1:A:137:MSE:HG3	2.04	0.56
1:A:159:PHE:HB2	1:B:125:PHE:HB3	1.87	0.56
1:A:131:ASP:OD1	1:B:153:GLY:HA3	2.05	0.56
1:A:78:TYR:CZ	1:B:80:ILE:HB	2.41	0.56
1:B:135:ARG:HG3	3:B:294:HOH:O	2.05	0.56
1:A:5:ARG:HD3	1:A:60:LEU:HD11	1.87	0.56
1:A:29:LYS:O	1:A:30:LEU:HB3	2.06	0.56
1:B:87:ARG:O	1:B:124:GLN:HB2	2.06	0.56
1:B:23:GLU:OE2	3:B:189:HOH:O	2.17	0.56
1:B:139:LEU:O	1:B:143:LEU:HG	2.04	0.56
1:B:17:ILE:HD11	1:B:54:CYS:SG	2.46	0.56
1:A:166:LYS:HB3	1:B:143:LEU:HD22	1.87	0.56
1:A:162:GLU:O	1:A:166:LYS:HG3	2.06	0.56
1:B:148:LEU:O	1:B:154:TRP:HD1	1.89	0.56
1:B:7:ARG:HH21	1:B:58:GLU:CD	2.09	0.56
1:B:6:ILE:CD1	1:B:57:ALA:HA	2.36	0.56
1:A:146:GLN:HG2	3:A:331:HOH:O	2.06	0.56
1:B:48:ASP:HB2	3:B:180:HOH:O	2.05	0.56
1:A:4:VAL:HG22	1:A:59:ILE:CD1	2.36	0.56
1:A:80:ILE:HG13	1:A:88:THR:HB	1.88	0.56
1:B:134:GLN:HB2	3:B:256:HOH:O	2.06	0.55
1:A:124:GLN:HB3	1:B:159:PHE:O	2.06	0.55
1:A:139:LEU:HB2	2:A:306:ACO:H52A	1.88	0.55
1:A:7:ARG:HB3	3:A:399:HOH:O	2.07	0.55
1:B:80:ILE:HG13	1:B:88:THR:HB	1.88	0.55
1:B:16:ASP:O	1:B:17:ILE:C	2.44	0.55
1:A:130:LEU:HD13	1:A:132:TRP:NE1	2.21	0.55
1:A:130:LEU:HD12	3:A:416:HOH:O	2.06	0.55
1:A:75:GLY:HA2	1:A:93:ASP:O	2.06	0.55
1:A:14:CYS:SG	1:A:38:GLU:O	2.64	0.55
1:A:131:ASP:HA	1:A:137:MSE:SE	2.57	0.55
1:A:145:ALA:HB2	1:B:159:PHE:CD2	2.41	0.55
1:A:36:ILE:HG22	1:A:41:LEU:HG	1.89	0.55
1:A:87:ARG:O	1:A:122:CYS:HA	2.06	0.55
1:A:121:GLY:HA2	3:A:319:HOH:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HB3	1:B:167:LEU:HD21	1.89	0.55
1:B:2:ALA:HB3	1:B:103:GLN:OE1	2.06	0.55
1:A:85:LYS:HE3	3:A:415:HOH:O	2.07	0.55
1:B:91:LEU:HD13	1:B:113:VAL:HG21	1.88	0.55
1:B:50:PRO:HG2	3:B:269:HOH:O	2.07	0.55
1:A:127:LEU:O	1:B:157:PHE:HB2	2.07	0.55
1:A:127:LEU:C	1:A:127:LEU:HD12	2.28	0.55
1:A:41:LEU:HG	3:A:416:HOH:O	2.07	0.55
1:A:103:GLN:HG2	1:A:105:ILE:HG13	1.88	0.55
1:B:129:VAL:HG21	1:B:140:TYR:HE2	1.71	0.55
1:A:159:PHE:CE2	1:B:145:ALA:HB2	2.41	0.55
1:B:109:ILE:O	1:B:113:VAL:HG23	2.06	0.55
1:A:130:LEU:HD13	1:A:132:TRP:HE1	1.70	0.55
1:A:19:ARG:O	1:A:23:GLU:HG2	2.07	0.55
1:B:96:VAL:HG21	3:B:181:HOH:O	2.06	0.55
1:B:14:CYS:SG	1:B:42:ARG:CZ	2.95	0.55
1:A:129:VAL:HG23	3:A:447:HOH:O	2.06	0.55
1:A:91:LEU:HD21	1:A:94:ILE:HB	1.88	0.55
1:B:77:TYR:HB3	1:B:91:LEU:HA	1.88	0.55
1:A:130:LEU:HD13	1:A:132:TRP:CZ2	2.42	0.54
1:A:59:ILE:O	1:A:69:PRO:HA	2.07	0.54
1:B:59:ILE:HG12	1:B:72:VAL:HG21	1.88	0.54
1:A:89:ILE:CG2	1:A:90:TYR:N	2.69	0.54
1:B:142:ALA:HA	3:B:295:HOH:O	2.07	0.54
1:A:7:ARG:NH1	1:A:10:LYS:HE2	2.22	0.54
1:A:17:ILE:HD13	1:A:54:CYS:SG	2.48	0.54
1:A:165:ARG:HH11	1:A:165:ARG:HG3	1.71	0.54
1:A:154:TRP:CZ3	1:B:130:LEU:HG	2.42	0.54
1:A:111:LYS:HE3	3:A:440:HOH:O	2.07	0.54
1:B:75:GLY:HA2	1:B:94:ILE:HG12	1.88	0.54
1:B:89:ILE:HG21	1:B:117:ALA:HB2	1.88	0.54
1:A:126:ARG:HA	1:B:158:CYS:HA	1.89	0.54
1:A:54:CYS:SG	1:A:76:ILE:HG12	2.48	0.54
1:A:5:ARG:CD	1:A:60:LEU:HD21	2.38	0.54
1:B:140:TYR:O	1:B:145:ALA:HB3	2.08	0.54
1:A:111:LYS:O	1:A:115:GLU:HG3	2.07	0.54
1:A:127:LEU:HD11	1:A:140:TYR:CD2	2.42	0.54
1:A:130:LEU:HD13	1:A:132:TRP:HE1	1.72	0.54
1:A:4:VAL:HG22	1:A:59:ILE:CD1	2.38	0.54
1:B:125:PHE:HE1	1:B:127:LEU:HD23	1.72	0.54
1:A:80:ILE:CD1	1:A:90:TYR:HB2	2.26	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:ASP:OD2	1:B:83:THR:HG21	2.07	0.53
1:B:135:ARG:HG3	3:B:301:HOH:O	2.07	0.53
1:A:4:VAL:HG12	1:A:5:ARG:N	2.23	0.53
1:A:41:LEU:HG	3:A:415:HOH:O	2.08	0.53
1:A:160:GLN:H	1:A:163:ALA:HB3	1.72	0.53
1:B:5:ARG:O	1:B:5:ARG:HG3	2.07	0.53
1:B:149:THR:HA	1:B:154:TRP:H	1.72	0.53
1:B:22:ARG:NH2	3:B:290:HOH:O	2.32	0.53
1:A:53:HIS:O	1:A:76:ILE:HG23	2.09	0.53
1:B:162:GLU:O	1:B:165:ARG:HG2	2.07	0.53
1:A:159:PHE:CD2	1:B:145:ALA:HB2	2.44	0.53
1:B:10:LYS:HA	1:B:10:LYS:CE	2.37	0.53
1:A:88:THR:HG23	1:A:124:GLN:O	2.08	0.53
1:B:112:LYS:O	1:B:116:VAL:HG23	2.09	0.53
1:B:156:PHE:HD2	1:B:157:PHE:N	2.06	0.53
1:B:6:ILE:HG22	1:B:55:LEU:HD22	1.89	0.53
1:A:39:GLU:HB2	3:A:421:HOH:O	2.07	0.53
1:B:134:GLN:HG3	1:B:138:ASP:OD2	2.09	0.53
1:B:94:ILE:CD1	1:B:110:ILE:HG12	2.38	0.53
1:A:18:LEU:HD22	1:A:38:GLU:HA	1.91	0.53
1:A:121:GLY:HA2	3:A:319:HOH:O	2.09	0.53
1:A:52:TYR:CE1	1:A:54:CYS:SG	3.02	0.53
1:A:21:ILE:HA	1:A:74:TYR:OH	2.09	0.53
1:A:41:LEU:HA	1:A:52:TYR:OH	2.08	0.53
1:A:85:LYS:HG3	1:A:124:GLN:OE1	2.09	0.53
1:B:87:ARG:O	1:B:124:GLN:HB2	2.09	0.53
1:A:148:LEU:HD21	1:B:158:CYS:HB3	1.90	0.53
1:B:129:VAL:HG11	1:B:137:MSE:HG3	1.91	0.52
1:A:44:ASP:HB2	1:A:52:TYR:OH	2.09	0.52
1:A:78:TYR:CE2	1:A:92:GLU:HB2	2.44	0.52
1:B:53:HIS:O	1:B:54:CYS:SG	2.65	0.52
1:B:89:ILE:HG23	1:B:89:ILE:O	2.09	0.52
1:B:18:LEU:HD21	1:B:22:ARG:NH2	2.23	0.52
1:B:4:VAL:HB	1:B:59:ILE:HD13	1.92	0.52
1:A:91:LEU:HD13	1:A:113:VAL:HG21	1.90	0.52
1:A:139:LEU:HD12	1:A:139:LEU:O	2.09	0.52
1:B:54:CYS:HB2	1:B:76:ILE:HG12	1.89	0.52
1:A:87:ARG:HG3	3:A:325:HOH:O	2.10	0.52
1:A:22:ARG:HG2	1:A:22:ARG:NH1	2.24	0.52
1:A:41:LEU:H	1:A:41:LEU:HD12	1.75	0.52
1:B:169:GLY:HA2	3:B:284:HOH:O	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:VAL:HG11	1:B:157:PHE:CE1	2.45	0.52
1:B:146:GLN:HG2	3:B:301:HOH:O	2.09	0.52
1:A:104:GLY:O	1:A:108:LYS:HG3	2.08	0.52
1:A:24:LEU:O	1:A:27:PHE:HB3	2.10	0.52
1:A:55:LEU:HD21	3:A:317:HOH:O	2.08	0.52
1:A:126:ARG:HD3	1:B:156:PHE:HZ	1.73	0.52
1:A:124:GLN:HB2	1:B:159:PHE:O	2.10	0.52
1:B:15:GLY:O	1:B:18:LEU:HB3	2.10	0.52
1:A:123:SER:HB3	3:A:322:HOH:O	2.09	0.52
1:A:41:LEU:HD12	1:A:52:TYR:OH	2.09	0.52
1:B:162:GLU:HA	1:B:165:ARG:CD	2.40	0.52
1:A:154:TRP:HA	1:A:154:TRP:CE3	2.45	0.52
1:A:126:ARG:HG3	1:B:157:PHE:O	2.10	0.52
1:A:145:ALA:HB2	1:B:159:PHE:CZ	2.44	0.52
1:A:155:HIS:HB2	1:A:157:PHE:HE1	1.74	0.52
1:A:4:VAL:HG22	1:A:59:ILE:CD1	2.38	0.52
1:B:54:CYS:SG	1:B:76:ILE:HG12	2.50	0.52
1:A:111:LYS:HG2	1:B:167:LEU:HD22	1.92	0.52
1:A:85:LYS:HA	1:B:35:LYS:HB2	1.92	0.51
1:A:53:HIS:HB2	1:A:77:TYR:CZ	2.45	0.51
1:A:149:THR:C	1:A:151:ALA:H	2.13	0.51
1:B:148:LEU:HB3	1:B:154:TRP:HB2	1.90	0.51
1:A:167:LEU:HA	1:B:143:LEU:HD13	1.92	0.51
1:A:115:GLU:CG	1:B:168:ALA:HA	2.35	0.51
1:A:111:LYS:HE3	3:A:436:HOH:O	2.09	0.51
1:A:89:ILE:O	1:A:125:PHE:HB2	2.11	0.51
1:B:131:ASP:HA	1:B:137:MSE:HE1	1.92	0.51
1:A:55:LEU:HD22	1:A:112:LYS:HG2	1.92	0.51
1:B:80:ILE:HG12	1:B:88:THR:O	2.10	0.51
1:A:110:ILE:HD11	1:A:140:TYR:CE1	2.45	0.51
1:B:82:SER:C	1:B:84:TRP:H	2.14	0.51
1:A:92:GLU:HG3	1:A:93:ASP:N	2.25	0.51
1:A:160:GLN:CA	1:B:124:GLN:HE22	2.22	0.51
1:A:129:VAL:HG23	3:A:457:HOH:O	2.09	0.51
1:A:126:ARG:HG2	1:A:127:LEU:N	2.25	0.51
1:B:75:GLY:HA2	1:B:93:ASP:O	2.11	0.51
1:B:170:LYS:HE2	3:B:331:HOH:O	2.11	0.51
1:A:59:ILE:HB	1:A:69:PRO:HA	1.93	0.51
1:B:163:ALA:O	1:B:167:LEU:HG	2.11	0.51
1:A:160:GLN:HA	1:B:123:SER:O	2.11	0.51
1:B:162:GLU:HB2	3:B:243:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3:SER:HB3	3:B:312:HOH:O	2.09	0.51
1:A:100:TYR:HB3	1:A:105:ILE:HD12	1.93	0.51
1:A:44:ASP:HB3	1:A:51:PHE:HB2	1.93	0.51
1:B:127:LEU:HD13	1:B:129:VAL:HG23	1.92	0.51
1:B:130:LEU:HD22	1:B:132:TRP:HE1	1.76	0.51
1:B:4:VAL:HG23	1:B:58:GLU:C	2.32	0.51
1:B:162:GLU:HG2	3:B:320:HOH:O	2.10	0.51
1:A:89:ILE:HB	1:A:125:PHE:HB3	1.93	0.50
1:A:124:GLN:O	1:A:124:GLN:HG3	2.11	0.50
1:B:165:ARG:O	1:B:170:LYS:HG2	2.10	0.50
1:A:76:ILE:HB	1:A:93:ASP:HB2	1.94	0.50
1:B:52:TYR:CE2	1:B:54:CYS:HB2	2.45	0.50
1:A:37:SER:O	1:A:41:LEU:HD13	2.12	0.50
1:A:41:LEU:HD12	1:A:52:TYR:OH	2.11	0.50
1:B:100:TYR:HA	1:B:103:GLN:NE2	2.26	0.50
1:B:4:VAL:HB	1:B:59:ILE:HD13	1.94	0.50
1:A:159:PHE:CD2	1:B:145:ALA:HB2	2.47	0.50
1:A:21:ILE:HD11	1:A:76:ILE:HD11	1.93	0.50
1:B:2:ALA:HB1	3:B:313:HOH:O	2.10	0.50
1:B:4:VAL:HG22	1:B:5:ARG:N	2.27	0.50
1:A:160:GLN:HA	1:B:123:SER:O	2.12	0.50
1:B:165:ARG:HH21	1:B:170:LYS:HE3	1.77	0.50
1:A:35:LYS:N	3:A:417:HOH:O	2.45	0.50
1:A:36:ILE:CG2	1:A:41:LEU:HG	2.41	0.50
1:A:139:LEU:HD22	2:A:306:ACO:H52A	1.93	0.50
1:A:8:GLU:HG3	3:A:330:HOH:O	2.12	0.50
1:A:129:VAL:CG1	1:B:155:HIS:HB2	2.41	0.50
1:A:101:ARG:HH22	2:A:306:ACO:H72	1.77	0.50
1:A:102:GLY:HA2	2:A:306:ACO:O1A	2.12	0.50
1:A:88:THR:HG23	1:A:124:GLN:HG3	1.92	0.50
1:A:139:LEU:HB2	2:A:306:ACO:O4B	2.12	0.50
1:B:91:LEU:HD11	1:B:94:ILE:CG1	2.41	0.50
1:B:19:ARG:O	1:B:23:GLU:HG3	2.12	0.50
1:A:82:SER:HB3	1:A:86:GLY:N	2.27	0.50
1:B:2:ALA:HB3	1:B:59:ILE:HD12	1.94	0.50
1:A:145:ALA:HB2	1:B:159:PHE:CE2	2.47	0.50
1:A:41:LEU:HD12	1:A:41:LEU:N	2.27	0.50
1:B:91:LEU:HD21	1:B:94:ILE:CD1	2.42	0.50
1:A:82:SER:HB3	1:A:86:GLY:H	1.76	0.50
1:B:23:GLU:HG3	3:B:250:HOH:O	2.12	0.50
1:B:49:ASN:N	3:B:178:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LYS:HE3	3:A:343:HOH:O	2.12	0.50
1:A:127:LEU:C	1:A:127:LEU:HD12	2.32	0.50
1:A:131:ASP:HB3	1:B:153:GLY:HA3	1.94	0.50
1:B:87:ARG:HD3	3:B:221:HOH:O	2.10	0.50
1:A:83:THR:HG22	1:B:76:ILE:CD1	2.41	0.50
1:A:111:LYS:HE2	1:B:167:LEU:CD2	2.42	0.50
1:A:165:ARG:HG3	1:A:165:ARG:NH1	2.27	0.50
1:B:127:LEU:C	1:B:127:LEU:HD12	2.31	0.50
1:A:6:ILE:HG13	1:A:108:LYS:HB3	1.94	0.50
1:A:10:LYS:HA	1:A:46:PHE:CE2	2.46	0.49
1:B:49:ASN:HB3	3:B:171:HOH:O	2.12	0.49
1:A:57:ALA:O	1:A:71:VAL:HA	2.11	0.49
1:B:11:GLU:HG2	1:B:42:ARG:HH11	1.74	0.49
1:B:54:CYS:CB	1:B:76:ILE:HG12	2.40	0.49
1:A:36:ILE:HG22	1:A:41:LEU:HD12	1.93	0.49
1:A:130:LEU:HD13	1:A:132:TRP:NE1	2.27	0.49
1:B:166:LYS:HG3	3:B:286:HOH:O	2.12	0.49
1:A:126:ARG:HD3	1:B:156:PHE:CE2	2.47	0.49
1:B:131:ASP:OD1	1:B:131:ASP:N	2.45	0.49
1:B:107:SER:HB2	3:B:297:HOH:O	2.11	0.49
1:A:101:ARG:HD3	2:A:306:ACO:H62A	1.78	0.49
1:A:147:ASP:OD2	1:B:155:HIS:ND1	2.46	0.49
1:B:131:ASP:HA	1:B:137:MSE:HE1	1.92	0.49
1:A:44:ASP:O	1:A:50:PRO:HA	2.11	0.49
1:A:75:GLY:HA2	1:A:93:ASP:O	2.12	0.49
1:A:106:GLY:HA3	2:A:306:ACO:O6A	2.11	0.49
1:A:87:ARG:O	1:A:122:CYS:HA	2.13	0.49
1:B:146:GLN:HB3	3:B:307:HOH:O	2.11	0.49
1:A:137:MSE:HE3	1:B:157:PHE:HZ	1.77	0.49
1:A:123:SER:C	1:A:124:GLN:HG3	2.33	0.49
1:A:87:ARG:HB2	1:A:121:GLY:O	2.12	0.49
1:A:14:CYS:HB3	1:A:38:GLU:HG3	1.94	0.49
1:B:11:GLU:O	1:B:11:GLU:HG2	2.13	0.49
1:B:55:LEU:HD13	1:B:112:LYS:CG	2.42	0.49
1:A:11:GLU:HG3	1:A:42:ARG:NH1	2.28	0.49
1:A:89:ILE:HD12	1:A:117:ALA:HA	1.95	0.49
1:A:7:ARG:NH1	1:A:8:GLU:O	2.45	0.49
1:A:98:PRO:HG3	1:A:101:ARG:NH2	2.26	0.49
1:A:160:GLN:CB	1:B:124:GLN:HE22	2.25	0.49
1:B:38:GLU:CG	1:B:42:ARG:HE	2.25	0.49
1:B:98:PRO:HG3	3:B:186:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:GLN:HG3	1:B:160:GLN:NE2	2.19	0.49
1:A:97:MSE:O	1:A:101:ARG:HG3	2.12	0.49
1:B:111:LYS:O	1:B:115:GLU:HG3	2.13	0.49
1:A:167:LEU:O	1:B:111:LYS:HG3	2.13	0.49
1:B:29:LYS:HE3	3:B:274:HOH:O	2.12	0.49
1:B:135:ARG:HG3	3:B:303:HOH:O	2.11	0.49
1:A:6:ILE:HG13	1:A:108:LYS:HB3	1.93	0.48
1:B:84:TRP:NE1	3:B:205:HOH:O	2.35	0.48
1:A:44:ASP:O	1:A:51:PHE:N	2.46	0.48
1:A:89:ILE:HB	1:A:125:PHE:HB3	1.95	0.48
1:A:127:LEU:HD11	1:B:159:PHE:CE1	2.47	0.48
1:B:113:VAL:HG12	1:B:125:PHE:CE2	2.47	0.48
1:A:161:GLY:O	1:A:165:ARG:HG3	2.12	0.48
1:B:106:GLY:O	1:B:110:ILE:HG13	2.13	0.48
1:A:146:GLN:CG	1:B:160:GLN:NE2	2.75	0.48
1:B:49:ASN:N	3:B:180:HOH:O	2.46	0.48
1:A:123:SER:O	1:B:161:GLY:HA2	2.13	0.48
1:B:127:LEU:C	1:B:127:LEU:HD12	2.33	0.48
1:B:111:LYS:O	1:B:115:GLU:HG3	2.12	0.48
1:A:5:ARG:NE	1:A:60:LEU:HD21	2.28	0.48
1:A:76:ILE:HB	1:A:93:ASP:HB2	1.94	0.48
1:A:145:ALA:HB2	1:B:159:PHE:CZ	2.49	0.48
1:B:19:ARG:NH2	1:B:71:VAL:HB	2.28	0.48
1:A:143:LEU:O	3:A:333:HOH:O	2.20	0.48
1:B:98:PRO:HA	1:B:101:ARG:HG2	1.95	0.48
1:A:54:CYS:CB	1:A:76:ILE:HG12	2.43	0.48
1:A:79:PHE:HD1	1:A:122:CYS:HG	1.61	0.48
1:A:127:LEU:HD12	1:B:157:PHE:HB2	1.95	0.48
1:B:11:GLU:HA	1:B:46:PHE:CE2	2.49	0.48
1:A:20:LEU:HB3	1:A:74:TYR:CD1	2.48	0.48
1:B:22:ARG:NE	3:B:217:HOH:O	2.45	0.48
1:A:103:GLN:HG3	3:A:326:HOH:O	2.13	0.48
1:B:84:TRP:CE3	1:B:85:LYS:HE2	2.48	0.48
1:A:75:GLY:HA2	1:A:93:ASP:O	2.13	0.48
1:B:45:GLY:O	1:B:50:PRO:HB3	2.14	0.48
1:A:88:THR:HA	1:A:122:CYS:HB3	1.95	0.48
1:B:24:LEU:HD22	1:B:95:TYR:CD1	2.49	0.48
1:A:107:SER:O	1:A:111:LYS:HG3	2.12	0.48
1:A:99:GLU:CG	3:A:339:HOH:O	2.62	0.48
1:A:105:ILE:O	1:A:109:ILE:HG13	2.13	0.48
1:A:149:THR:O	1:A:151:ALA:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:14:CYS:SG	1:B:42:ARG:NE	2.87	0.48
1:A:103:GLN:O	1:A:103:GLN:HG3	2.14	0.48
1:A:85:LYS:HE3	3:A:418:HOH:O	2.13	0.48
1:B:134:GLN:HA	3:B:308:HOH:O	2.14	0.48
1:B:162:GLU:HB3	3:B:244:HOH:O	2.14	0.48
1:A:146:GLN:HG3	1:B:160:GLN:HE21	1.78	0.48
1:A:6:ILE:O	1:A:112:LYS:HE2	2.14	0.48
1:A:146:GLN:HG3	1:B:160:GLN:HE21	1.79	0.47
1:B:82:SER:C	1:B:84:TRP:H	2.17	0.47
1:B:4:VAL:HB	1:B:59:ILE:CD1	2.44	0.47
1:B:10:LYS:C	1:B:12:GLY:N	2.68	0.47
1:A:11:GLU:HG3	3:A:338:HOH:O	2.14	0.47
1:B:127:LEU:HD12	1:B:127:LEU:C	2.34	0.47
1:A:162:GLU:O	1:A:166:LYS:HG3	2.14	0.47
1:A:94:ILE:HD11	1:A:106:GLY:HA2	1.95	0.47
1:B:162:GLU:OE2	1:B:165:ARG:HD3	2.15	0.47
1:B:149:THR:O	1:B:153:GLY:N	2.45	0.47
1:B:89:ILE:CG2	1:B:125:PHE:HA	2.44	0.47
1:A:111:LYS:O	1:A:115:GLU:HG3	2.14	0.47
1:A:160:GLN:HG2	1:B:124:GLN:OE1	2.13	0.47
1:A:4:VAL:HG22	1:A:59:ILE:HD13	1.96	0.47
1:B:111:LYS:NZ	1:B:115:GLU:OE2	2.47	0.47
1:A:149:THR:HG23	1:B:149:THR:HG21	1.96	0.47
1:B:127:LEU:HD12	1:B:127:LEU:O	2.13	0.47
1:A:9:ALA:O	1:A:46:PHE:HE2	1.98	0.47
1:B:53:HIS:HB2	1:B:77:TYR:CE2	2.49	0.47
1:B:111:LYS:O	1:B:115:GLU:HG3	2.14	0.47
1:A:101:ARG:HD3	2:A:306:ACO:OAP	2.13	0.47
1:A:111:LYS:HE3	3:A:447:HOH:O	2.14	0.47
1:A:127:LEU:C	1:A:127:LEU:HD12	2.35	0.47
1:A:78:TYR:OH	1:A:92:GLU:OE1	2.33	0.47
1:A:145:ALA:HB2	1:B:159:PHE:CD2	2.50	0.47
1:B:18:LEU:HD21	1:B:22:ARG:HH21	1.80	0.47
1:A:99:GLU:HG3	3:A:384:HOH:O	2.14	0.47
1:B:149:THR:O	1:B:153:GLY:HA2	2.15	0.47
1:B:26:GLU:CD	3:B:270:HOH:O	2.53	0.47
1:B:55:LEU:HD13	1:B:112:LYS:HG3	1.97	0.47
1:A:11:GLU:OE1	1:A:42:ARG:HD2	2.14	0.47
1:A:53:HIS:O	1:A:76:ILE:HA	2.15	0.47
1:A:129:VAL:HG11	1:A:137:MSE:HG2	1.96	0.47
1:A:131:ASP:HB3	1:B:153:GLY:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASP:OD2	1:A:150:GLU:HG3	2.14	0.47
1:A:127:LEU:CD1	1:B:157:PHE:HB2	2.45	0.47
1:B:102:GLY:C	3:B:188:HOH:O	2.54	0.47
1:A:70:CYS:SG	1:A:70:CYS:O	2.73	0.47
1:B:8:GLU:HA	1:B:55:LEU:HD23	1.97	0.47
1:A:54:CYS:HB3	1:A:76:ILE:HA	1.97	0.47
1:A:131:ASP:HB3	1:B:153:GLY:CA	2.45	0.47
1:A:131:ASP:HB3	1:B:153:GLY:O	2.15	0.47
1:B:52:TYR:HA	1:B:78:TYR:HB3	1.95	0.47
1:B:38:GLU:O	1:B:42:ARG:HG3	2.15	0.47
1:A:133:ASN:O	1:A:137:MSE:HG3	2.14	0.47
1:A:144:GLY:O	1:B:163:ALA:HB2	2.15	0.47
1:B:6:ILE:HD13	1:B:57:ALA:HA	1.97	0.47
1:B:111:LYS:O	1:B:115:GLU:HG3	2.15	0.47
1:B:127:LEU:C	1:B:127:LEU:HD12	2.35	0.47
1:A:112:LYS:HA	1:A:115:GLU:OE2	2.15	0.47
1:B:133:ASN:O	1:B:137:MSE:HG3	2.15	0.47
1:A:128:ALA:O	1:B:154:TRP:HZ3	1.97	0.47
1:A:157:PHE:HB2	1:B:127:LEU:HD11	1.96	0.47
1:A:148:LEU:HA	1:A:151:ALA:HB3	1.97	0.47
1:B:80:ILE:HD11	1:B:126:ARG:CZ	2.45	0.47
1:B:127:LEU:CD1	1:B:129:VAL:HG23	2.45	0.47
1:B:42:ARG:O	1:B:46:PHE:HB2	2.14	0.47
1:A:36:ILE:HD12	3:B:298:HOH:O	2.15	0.47
1:A:131:ASP:CG	1:B:153:GLY:HA3	2.36	0.47
1:A:103:GLN:HG2	3:A:320:HOH:O	2.14	0.47
1:B:6:ILE:HD13	1:B:57:ALA:HA	1.96	0.46
1:A:93:ASP:OD1	3:A:313:HOH:O	2.20	0.46
1:A:80:ILE:HB	1:B:78:TYR:CZ	2.49	0.46
1:A:93:ASP:OD1	1:B:83:THR:HG21	2.15	0.46
1:A:159:PHE:HB2	1:B:125:PHE:HB3	1.97	0.46
1:B:14:CYS:SG	1:B:42:ARG:HG2	2.55	0.46
1:A:56:VAL:HG23	1:A:56:VAL:O	2.14	0.46
1:A:52:TYR:HE1	1:A:54:CYS:SG	2.39	0.46
1:B:165:ARG:HG2	1:B:170:LYS:HB2	1.97	0.46
1:A:88:THR:HG22	1:A:89:ILE:N	2.29	0.46
1:A:91:LEU:HD11	1:A:94:ILE:HD11	1.98	0.46
1:B:45:GLY:HA2	1:B:50:PRO:CB	2.44	0.46
1:A:105:ILE:O	1:A:109:ILE:HG13	2.14	0.46
1:A:59:ILE:HB	1:A:70:CYS:SG	2.55	0.46
1:B:76:ILE:O	1:B:92:GLU:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:ILE:CD1	1:A:117:ALA:HA	2.44	0.46
1:A:131:ASP:HA	1:A:137:MSE:SE	2.65	0.46
1:B:58:GLU:HA	1:B:70:CYS:O	2.15	0.46
1:A:46:PHE:O	1:A:47:GLY:C	2.53	0.46
1:B:18:LEU:CD2	1:B:22:ARG:NH2	2.78	0.46
1:A:36:ILE:HG22	1:A:37:SER:N	2.30	0.46
1:A:154:TRP:CZ3	1:B:130:LEU:HG	2.51	0.46
1:B:136:ALA:HB1	1:B:140:TYR:CE2	2.50	0.46
1:B:76:ILE:O	1:B:91:LEU:HD12	2.15	0.46
1:B:135:ARG:HG3	3:B:299:HOH:O	2.15	0.46
1:A:139:LEU:O	1:A:143:LEU:HG	2.16	0.46
1:A:100:TYR:O	1:A:103:GLN:HG2	2.16	0.46
1:A:36:ILE:HG22	1:A:41:LEU:HD11	1.98	0.46
1:A:101:ARG:HD3	2:A:306:ACO:N6A	2.30	0.46
1:B:57:ALA:O	1:B:71:VAL:HA	2.15	0.46
1:A:115:GLU:CG	1:B:168:ALA:HA	2.43	0.46
1:A:25:ALA:HB3	3:A:327:HOH:O	2.15	0.46
1:A:94:ILE:HG23	2:A:306:ACO:H31	1.98	0.46
1:A:115:GLU:CG	1:B:168:ALA:HA	2.42	0.46
1:B:146:GLN:HB3	3:B:199:HOH:O	2.16	0.46
1:B:117:ALA:O	1:B:122:CYS:O	2.33	0.46
1:B:49:ASN:HB3	3:B:171:HOH:O	2.15	0.46
1:B:8:GLU:HG3	3:B:272:HOH:O	2.16	0.46
1:A:124:GLN:OE1	3:A:416:HOH:O	2.21	0.46
1:A:59:ILE:HB	1:A:70:CYS:SG	2.56	0.46
1:A:155:HIS:CD2	1:B:131:ASP:HB3	2.50	0.46
1:A:83:THR:HG21	1:B:93:ASP:HB3	1.97	0.46
1:B:4:VAL:HG23	1:B:58:GLU:O	2.16	0.46
1:B:10:LYS:O	1:B:11:GLU:C	2.54	0.46
1:A:59:ILE:HB	1:A:70:CYS:HG	1.77	0.46
1:A:160:GLN:HE22	1:B:85:LYS:CE	2.25	0.46
1:B:22:ARG:NE	3:B:218:HOH:O	2.48	0.46
1:A:137:MSE:HE3	1:B:157:PHE:HZ	1.80	0.46
1:A:162:GLU:HB2	3:A:414:HOH:O	2.15	0.46
1:A:4:VAL:HG12	1:A:5:ARG:H	1.81	0.46
1:B:76:ILE:O	1:B:91:LEU:HD12	2.16	0.45
1:B:8:GLU:HG3	3:B:272:HOH:O	2.15	0.45
1:B:137:MSE:SE	3:B:309:HOH:O	2.84	0.45
1:A:19:ARG:O	1:A:22:ARG:HB2	2.17	0.45
1:B:129:VAL:HG21	1:B:140:TYR:HE2	1.81	0.45
1:A:127:LEU:HD12	1:A:127:LEU:C	2.37	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:ILE:HG13	1:B:100:TYR:CE1	2.51	0.45
1:A:92:GLU:CD	1:B:82:SER:HA	2.37	0.45
1:B:160:GLN:HB2	3:B:248:HOH:O	2.15	0.45
1:B:131:ASP:HA	1:B:137:MSE:CE	2.45	0.45
1:A:36:ILE:HD12	3:B:301:HOH:O	2.16	0.45
1:A:9:ALA:HB2	1:A:56:VAL:HG13	1.99	0.45
1:A:42:ARG:HA	1:A:46:PHE:HD1	1.82	0.45
1:A:18:LEU:O	1:A:22:ARG:HG3	2.17	0.45
1:B:38:GLU:HG2	1:B:42:ARG:NE	2.29	0.45
1:A:86:GLY:HA2	1:B:36:ILE:HD12	1.98	0.45
1:B:127:LEU:CD1	1:B:129:VAL:HG23	2.47	0.45
1:A:117:ALA:HB1	1:A:122:CYS:HB2	1.98	0.45
1:B:87:ARG:O	1:B:122:CYS:SG	2.75	0.45
1:B:82:SER:C	1:B:84:TRP:N	2.70	0.45
1:B:16:ASP:C	1:B:18:LEU:N	2.69	0.45
1:A:88:THR:CG2	1:A:124:GLN:HG3	2.46	0.45
1:B:87:ARG:HD2	3:B:329:HOH:O	2.17	0.45
1:B:23:GLU:OE1	1:B:97:MSE:HE3	2.17	0.45
1:B:117:ALA:O	1:B:122:CYS:HB3	2.16	0.45
1:B:168:ALA:C	1:B:170:LYS:H	2.20	0.45
1:A:83:THR:O	1:B:36:ILE:HG21	2.16	0.45
1:A:76:ILE:O	1:A:91:LEU:HD12	2.16	0.45
1:A:139:LEU:HD13	2:A:306:ACO:H4B	1.98	0.45
1:A:92:GLU:OE1	1:B:82:SER:HA	2.17	0.45
1:A:167:LEU:O	1:B:111:LYS:HG3	2.16	0.45
1:A:91:LEU:CG	1:A:94:ILE:HD11	2.47	0.45
1:B:14:CYS:SG	1:B:42:ARG:HG3	2.56	0.45
1:A:77:TYR:OH	1:A:116:VAL:HG11	2.16	0.45
1:B:111:LYS:HG2	1:B:115:GLU:CD	2.37	0.45
1:A:7:ARG:O	1:A:55:LEU:HA	2.17	0.45
1:A:111:LYS:HE3	3:A:443:HOH:O	2.16	0.45
1:A:147:ASP:OD2	1:B:155:HIS:ND1	2.38	0.45
1:B:102:GLY:CA	3:B:188:HOH:O	2.63	0.45
1:A:101:ARG:HD3	2:A:306:ACO:OAP	2.17	0.45
1:A:69:PRO:HG3	3:A:442:HOH:O	2.16	0.45
1:A:74:TYR:CE2	1:A:76:ILE:HG13	2.52	0.45
1:A:102:GLY:HA2	2:A:306:ACO:O1A	2.17	0.45
1:B:74:TYR:C	1:B:74:TYR:CD1	2.90	0.45
1:B:89:ILE:HG22	1:B:125:PHE:HA	1.99	0.45
1:A:29:LYS:O	1:A:30:LEU:HB2	2.17	0.45
1:B:74:TYR:C	1:B:74:TYR:CD1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:LEU:O	1:A:27:PHE:HB3	2.17	0.45
1:A:78:TYR:HE2	1:A:92:GLU:HB2	1.82	0.45
1:B:116:VAL:O	1:B:119:ASP:HB3	2.16	0.45
1:A:146:GLN:HG2	1:B:160:GLN:HE21	1.81	0.45
1:B:22:ARG:NH1	3:B:236:HOH:O	2.32	0.44
1:A:38:GLU:HG2	1:A:42:ARG:NH1	2.33	0.44
1:A:89:ILE:O	1:A:125:PHE:HA	2.17	0.44
1:B:82:SER:O	1:B:83:THR:HG23	2.18	0.44
1:A:80:ILE:HD11	1:A:126:ARG:HD2	1.98	0.44
1:B:49:ASN:ND2	3:B:325:HOH:O	2.50	0.44
1:B:159:PHE:O	1:B:164:THR:OG1	2.35	0.44
1:B:94:ILE:HD12	1:B:110:ILE:CG1	2.47	0.44
1:A:80:ILE:HB	1:B:78:TYR:CZ	2.52	0.44
1:B:98:PRO:HA	1:B:101:ARG:HG2	1.98	0.44
1:B:132:TRP:CE3	1:B:133:ASN:N	2.86	0.44
1:B:80:ILE:HG12	1:B:88:THR:O	2.17	0.44
1:B:137:MSE:O	1:B:141:LYS:HG3	2.17	0.44
1:B:135:ARG:O	1:B:139:LEU:HB2	2.18	0.44
1:A:52:TYR:HD1	1:A:54:CYS:HG	1.66	0.44
1:B:83:THR:HB	3:B:300:HOH:O	2.16	0.44
2:A:306:ACO:H4B	3:A:365:HOH:O	2.17	0.44
1:A:10:LYS:HG2	3:A:391:HOH:O	2.18	0.44
1:A:84:TRP:CH2	1:B:25:ALA:HA	2.52	0.44
1:A:85:LYS:HE3	3:A:417:HOH:O	2.17	0.44
1:A:91:LEU:HD13	1:A:113:VAL:HG21	1.99	0.44
1:A:127:LEU:HD11	1:B:157:PHE:HB2	2.00	0.44
1:B:88:THR:HG22	1:B:89:ILE:N	2.33	0.44
1:A:70:CYS:HA	3:A:363:HOH:O	2.16	0.44
1:A:139:LEU:HD13	2:A:306:ACO:C5B	2.48	0.44
1:A:7:ARG:NE	1:A:58:GLU:OE1	2.39	0.44
1:A:127:LEU:C	1:A:127:LEU:HD12	2.37	0.44
1:A:114:ALA:O	1:A:118:LEU:HG	2.17	0.44
1:A:159:PHE:CD2	1:B:145:ALA:HB2	2.53	0.44
1:A:36:ILE:HG21	1:A:41:LEU:CD2	2.48	0.44
1:A:44:ASP:O	1:A:50:PRO:HA	2.17	0.44
1:A:13:ASP:O	1:A:17:ILE:HG13	2.18	0.44
1:A:168:ALA:HA	1:B:111:LYS:HG3	1.99	0.44
1:A:126:ARG:O	1:A:127:LEU:HB3	2.17	0.44
1:A:129:VAL:HG23	3:A:451:HOH:O	2.18	0.44
1:A:75:GLY:HA2	1:A:93:ASP:O	2.18	0.44
1:A:78:TYR:CE1	1:A:90:TYR:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:GLY:O	1:B:122:CYS:C	2.57	0.44
1:A:81:TYR:CD1	1:B:51:PHE:HB3	2.53	0.44
1:B:6:ILE:HD12	1:B:57:ALA:HA	1.99	0.44
1:B:162:GLU:HG2	3:B:331:HOH:O	2.17	0.44
1:B:24:LEU:HD22	3:B:309:HOH:O	2.17	0.44
1:B:91:LEU:HD21	1:B:94:ILE:CD1	2.47	0.44
1:B:151:ALA:HB3	1:B:152:GLU:OE1	2.18	0.44
1:B:36:ILE:HG12	1:B:37:SER:N	2.33	0.44
1:A:38:GLU:HG2	1:A:42:ARG:NH1	2.33	0.44
1:A:102:GLY:CA	2:A:306:ACO:O1A	2.65	0.44
1:A:158:CYS:HB2	1:B:148:LEU:HD11	1.99	0.44
1:A:52:TYR:CD1	1:A:54:CYS:SG	3.11	0.44
1:A:155:HIS:O	1:A:157:PHE:HD1	2.01	0.44
1:B:88:THR:HA	1:B:124:GLN:HB2	1.99	0.44
1:B:59:ILE:O	1:B:70:CYS:N	2.50	0.44
1:A:36:ILE:HG22	1:A:41:LEU:CD1	2.47	0.43
1:B:161:GLY:O	1:B:165:ARG:HG3	2.18	0.43
2:A:306:ACO:H10	2:A:306:ACO:O4A	2.18	0.43
1:B:84:TRP:CE2	1:B:85:LYS:HE2	2.53	0.43
1:B:8:GLU:HA	1:B:55:LEU:HD23	2.00	0.43
1:A:147:ASP:OD1	1:A:149:THR:HB	2.18	0.43
1:A:118:LEU:HD12	1:B:168:ALA:HB2	2.00	0.43
1:B:147:ASP:OD1	1:B:147:ASP:C	2.56	0.43
1:A:132:TRP:O	1:A:132:TRP:HE3	2.01	0.43
1:B:23:GLU:HG3	3:B:251:HOH:O	2.18	0.43
1:A:89:ILE:O	1:A:125:PHE:HA	2.18	0.43
1:B:28:GLU:O	1:B:30:LEU:HG	2.18	0.43
1:A:59:ILE:CG2	1:A:60:LEU:N	2.81	0.43
1:B:148:LEU:HA	1:B:152:GLU:OE1	2.17	0.43
1:B:162:GLU:CG	3:B:331:HOH:O	2.66	0.43
1:A:107:SER:HB3	3:A:447:HOH:O	2.18	0.43
1:A:20:LEU:HD11	1:A:71:VAL:HG12	2.01	0.43
1:B:6:ILE:HD13	1:B:57:ALA:HA	2.00	0.43
1:B:74:TYR:C	1:B:74:TYR:CD1	2.91	0.43
1:B:79:PHE:HD1	3:B:214:HOH:O	2.02	0.43
1:B:15:GLY:HA2	1:B:38:GLU:OE1	2.17	0.43
1:B:74:TYR:C	1:B:74:TYR:CD1	2.91	0.43
1:A:42:ARG:HA	1:A:46:PHE:CD1	2.53	0.43
1:A:159:PHE:CD1	1:A:159:PHE:N	2.86	0.43
1:A:38:GLU:HA	1:A:41:LEU:HD13	1.99	0.43
1:A:107:SER:O	1:A:111:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:SER:OG	1:A:124:GLN:HG3	2.18	0.43
1:B:100:TYR:HB3	1:B:105:ILE:CD1	2.48	0.43
1:A:110:ILE:HD11	1:A:140:TYR:HE1	1.83	0.43
1:A:156:PHE:HB3	1:B:148:LEU:HD12	2.00	0.43
1:A:93:ASP:O	1:A:94:ILE:HD13	2.18	0.43
1:A:155:HIS:ND1	1:B:147:ASP:OD2	2.43	0.43
1:A:83:THR:OG1	1:A:84:TRP:CD1	2.69	0.43
1:B:80:ILE:HG13	1:B:88:THR:HB	1.99	0.43
1:B:152:GLU:HB2	1:B:154:TRP:HD1	1.83	0.43
1:A:49:ASN:ND2	3:A:448:HOH:O	2.52	0.43
2:A:306:ACO:H133	2:A:306:ACO:N7A	2.33	0.43
1:B:162:GLU:HG3	3:B:291:HOH:O	2.19	0.43
1:B:6:ILE:CD1	1:B:57:ALA:HA	2.48	0.43
1:B:114:ALA:O	1:B:117:ALA:HB3	2.19	0.43
1:A:89:ILE:O	1:A:125:PHE:HA	2.18	0.43
1:B:149:THR:HA	1:B:154:TRP:H	1.83	0.43
1:B:76:ILE:O	1:B:92:GLU:HB3	2.18	0.43
1:A:123:SER:OG	1:A:124:GLN:N	2.52	0.43
1:A:51:PHE:CE2	1:B:87:ARG:NH2	2.86	0.43
1:A:154:TRP:CE3	1:B:128:ALA:O	2.71	0.43
1:B:96:VAL:HG21	3:B:180:HOH:O	2.18	0.43
1:A:86:GLY:CA	1:B:36:ILE:HD12	2.49	0.43
1:B:87:ARG:HG3	3:B:309:HOH:O	2.17	0.43
1:A:11:GLU:HG3	1:A:46:PHE:CG	2.53	0.43
1:A:81:TYR:O	1:B:92:GLU:HG2	2.19	0.43
1:A:148:LEU:HB3	1:A:154:TRP:CD1	2.54	0.43
1:A:161:GLY:HA2	1:B:123:SER:OG	2.19	0.43
1:A:168:ALA:HB1	1:B:115:GLU:HG2	2.01	0.43
1:A:83:THR:HG22	1:B:76:ILE:HD13	2.01	0.43
1:B:122:CYS:HB2	3:B:323:HOH:O	2.18	0.43
1:B:18:LEU:HB2	1:B:41:LEU:CD1	2.49	0.43
1:A:30:LEU:HG	3:A:427:HOH:O	2.17	0.43
1:A:89:ILE:HD12	1:A:117:ALA:CA	2.49	0.43
1:B:77:TYR:HE2	1:B:79:PHE:CZ	2.37	0.43
1:A:162:GLU:HA	1:A:165:ARG:CG	2.49	0.43
1:A:123:SER:HG	1:A:124:GLN:HE21	1.60	0.43
1:A:22:ARG:HH11	1:A:22:ARG:CG	2.27	0.42
1:A:93:ASP:OD2	1:B:83:THR:HG21	2.19	0.42
1:B:55:LEU:HD23	1:B:55:LEU:HA	1.87	0.42
1:B:103:GLN:N	3:B:178:HOH:O	2.51	0.42
1:B:11:GLU:HG2	1:B:42:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:HIS:C	1:A:54:CYS:SG	2.97	0.42
1:A:91:LEU:HD21	1:A:94:ILE:HD11	2.01	0.42
1:B:134:GLN:O	1:B:134:GLN:HG3	2.19	0.42
1:A:167:LEU:HG	1:B:114:ALA:HB2	2.01	0.42
1:A:86:GLY:HA2	1:B:36:ILE:HD12	2.01	0.42
1:B:38:GLU:OE2	1:B:42:ARG:NH2	2.52	0.42
1:A:13:ASP:O	1:A:16:ASP:N	2.52	0.42
1:A:110:ILE:HD13	1:A:143:LEU:HD12	2.00	0.42
1:B:94:ILE:HD12	1:B:110:ILE:CG1	2.49	0.42
1:B:4:VAL:HG22	1:B:5:ARG:N	2.35	0.42
1:B:75:GLY:CA	1:B:94:ILE:HG12	2.49	0.42
1:A:112:LYS:O	1:A:116:VAL:HG23	2.19	0.42
1:A:123:SER:OG	1:A:124:GLN:HG2	2.20	0.42
1:A:10:LYS:HA	1:A:46:PHE:HE2	1.84	0.42
1:A:83:THR:OG1	1:A:84:TRP:HD1	2.01	0.42
1:B:38:GLU:OE1	1:B:42:ARG:NH2	2.44	0.42
1:B:91:LEU:HD23	1:B:127:LEU:HD23	2.01	0.42
1:A:101:ARG:CZ	2:A:306:ACO:H72	2.49	0.42
1:B:80:ILE:CG1	1:B:88:THR:HB	2.48	0.42
1:A:14:CYS:HB3	1:A:38:GLU:CG	2.48	0.42
1:A:118:LEU:CD1	1:B:170:LYS:HG3	2.49	0.42
1:A:11:GLU:HG2	1:A:42:ARG:CG	2.49	0.42
1:A:59:ILE:HG22	1:A:60:LEU:H	1.85	0.42
1:A:89:ILE:CG2	1:A:90:TYR:N	2.82	0.42
1:A:96:VAL:CG1	1:A:105:ILE:HD12	2.50	0.42
1:B:38:GLU:OE2	1:B:42:ARG:NE	2.52	0.42
1:A:41:LEU:H	1:A:41:LEU:CD1	2.31	0.42
1:B:119:ASP:OD1	1:B:120:LYS:HD3	2.19	0.42
1:B:81:TYR:CE2	1:B:86:GLY:HA2	2.55	0.42
1:A:94:ILE:HG22	2:A:306:ACO:O	2.19	0.42
1:A:131:ASP:HB2	3:A:431:HOH:O	2.19	0.42
1:A:81:TYR:O	1:B:92:GLU:HG2	2.19	0.42
1:A:4:VAL:HG12	1:A:5:ARG:N	2.35	0.42
1:A:139:LEU:O	1:A:139:LEU:HD12	2.19	0.42
1:A:166:LYS:NZ	3:A:438:HOH:O	2.51	0.42
1:A:83:THR:HG22	1:B:76:ILE:HD12	2.00	0.42
1:A:36:ILE:CD1	3:B:298:HOH:O	2.67	0.42
1:A:137:MSE:HE3	1:B:157:PHE:CZ	2.53	0.42
1:B:139:LEU:O	1:B:143:LEU:HG	2.19	0.42
1:A:135:ARG:HB3	2:A:306:ACO:C8A	2.50	0.42
1:A:163:ALA:HB2	1:B:144:GLY:HA3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASP:OD2	1:A:150:GLU:HG3	2.20	0.42
1:A:166:LYS:HD2	3:A:366:HOH:O	2.18	0.42
1:A:36:ILE:HD12	3:B:299:HOH:O	2.20	0.42
1:A:41:LEU:HB3	3:A:423:HOH:O	2.19	0.42
1:B:23:GLU:OE2	1:B:97:MSE:HE3	2.20	0.42
1:A:114:ALA:HB2	1:A:125:PHE:CE1	2.54	0.42
1:B:83:THR:HB	3:B:296:HOH:O	2.20	0.42
1:A:155:HIS:O	1:B:128:ALA:HA	2.20	0.42
1:B:4:VAL:HB	1:B:59:ILE:HD13	2.01	0.42
1:B:52:TYR:HE2	1:B:54:CYS:HB2	1.85	0.42
1:B:106:GLY:O	1:B:110:ILE:HG13	2.19	0.42
1:B:91:LEU:HD11	1:B:94:ILE:CG1	2.42	0.42
1:B:125:PHE:CD1	1:B:126:ARG:N	2.88	0.42
1:B:156:PHE:C	1:B:156:PHE:CD2	2.93	0.42
1:B:94:ILE:HD13	1:B:109:ILE:HB	2.02	0.42
1:B:129:VAL:HG11	1:B:137:MSE:CG	2.50	0.42
1:B:4:VAL:HB	1:B:59:ILE:HD13	2.01	0.42
1:A:30:LEU:C	1:A:30:LEU:HD23	2.39	0.42
1:A:111:LYS:HE2	1:B:167:LEU:HD22	2.00	0.42
1:B:129:VAL:HG21	1:B:140:TYR:CE2	2.54	0.42
1:A:161:GLY:HA2	1:B:123:SER:HB2	2.02	0.42
1:A:89:ILE:HD11	1:A:116:VAL:HG12	2.02	0.42
1:A:165:ARG:HG2	1:A:165:ARG:HH11	1.84	0.41
3:A:418:HOH:O	1:B:160:GLN:HB3	2.19	0.41
1:A:20:LEU:HD11	1:A:71:VAL:HG12	2.02	0.41
1:B:90:TYR:HA	1:B:126:ARG:O	2.20	0.41
1:A:130:LEU:CD2	1:A:132:TRP:HE1	2.23	0.41
1:A:137:MSE:HE3	1:B:155:HIS:HD1	1.85	0.41
1:B:8:GLU:HG2	3:B:222:HOH:O	2.19	0.41
1:A:102:GLY:C	3:A:391:HOH:O	2.54	0.41
1:B:125:PHE:CE1	1:B:127:LEU:HD23	2.54	0.41
1:B:149:THR:O	1:B:153:GLY:HA2	2.20	0.41
1:A:128:ALA:HB3	3:A:367:HOH:O	2.20	0.41
1:A:82:SER:O	1:A:86:GLY:N	2.39	0.41
1:A:123:SER:OG	1:A:124:GLN:NE2	2.36	0.41
1:B:162:GLU:O	1:B:165:ARG:HB3	2.19	0.41
1:B:11:GLU:HG2	1:B:42:ARG:NH1	2.35	0.41
1:B:94:ILE:HD12	1:B:110:ILE:HG12	2.02	0.41
1:B:127:LEU:C	1:B:127:LEU:HD12	2.40	0.41
1:B:130:LEU:HD13	1:B:132:TRP:NE1	2.31	0.41
1:A:7:ARG:HH21	1:A:58:GLU:CD	2.23	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:GLN:HB2	1:B:159:PHE:O	2.20	0.41
1:A:166:LYS:HB3	1:B:143:LEU:HD22	2.03	0.41
1:A:53:HIS:HB2	1:A:77:TYR:CE2	2.55	0.41
1:A:39:GLU:N	3:A:422:HOH:O	2.53	0.41
1:A:91:LEU:HD22	1:A:113:VAL:HG21	2.03	0.41
1:A:89:ILE:CG2	1:A:90:TYR:N	2.83	0.41
1:B:4:VAL:HG23	1:B:58:GLU:C	2.40	0.41
1:B:16:ASP:O	1:B:20:LEU:HG	2.20	0.41
1:B:14:CYS:SG	1:B:42:ARG:HG3	2.60	0.41
1:B:152:GLU:HB2	1:B:154:TRP:CD1	2.55	0.41
1:A:165:ARG:HA	1:B:118:LEU:HD11	2.03	0.41
1:A:76:ILE:O	1:A:92:GLU:N	2.50	0.41
1:B:137:MSE:SE	3:B:303:HOH:O	2.87	0.41
1:A:21:ILE:HA	1:A:74:TYR:OH	2.21	0.41
1:B:105:ILE:HB	3:B:180:HOH:O	2.19	0.41
1:B:116:VAL:O	1:B:120:LYS:HG2	2.21	0.41
1:A:139:LEU:HD13	2:A:306:ACO:H52A	2.01	0.41
1:A:74:TYR:HE2	1:A:76:ILE:HG13	1.86	0.41
1:B:148:LEU:O	1:B:152:GLU:HB2	2.20	0.41
1:A:6:ILE:CG1	1:A:108:LYS:HB3	2.49	0.41
1:A:6:ILE:CG1	1:A:108:LYS:HB3	2.51	0.41
1:B:106:GLY:N	3:B:180:HOH:O	2.53	0.41
1:A:39:GLU:O	1:A:40:ALA:C	2.59	0.41
1:B:91:LEU:HD21	1:B:94:ILE:HD12	2.02	0.41
1:B:106:GLY:O	1:B:110:ILE:HG13	2.21	0.41
1:A:139:LEU:HG	1:A:140:TYR:CD1	2.56	0.41
1:B:165:ARG:NH2	1:B:170:LYS:HE3	2.35	0.41
1:A:160:GLN:OE1	1:B:85:LYS:HE3	2.20	0.41
1:A:18:LEU:HD22	1:A:38:GLU:HA	2.02	0.41
1:B:19:ARG:O	1:B:23:GLU:HG3	2.21	0.41
1:A:81:TYR:CZ	1:A:86:GLY:HA2	2.56	0.41
1:A:19:ARG:O	1:A:23:GLU:HG2	2.21	0.41
1:A:80:ILE:HG13	1:A:88:THR:HB	2.03	0.41
1:A:162:GLU:HA	1:A:165:ARG:HB2	2.03	0.41
1:B:134:GLN:HE21	1:B:138:ASP:CG	2.24	0.41
1:A:20:LEU:HB3	1:A:74:TYR:CE1	2.56	0.41
1:A:24:LEU:HD23	1:A:93:ASP:OD2	2.20	0.41
1:B:24:LEU:O	1:B:28:GLU:HG3	2.20	0.41
1:A:160:GLN:N	3:A:334:HOH:O	2.51	0.41
1:B:24:LEU:O	1:B:27:PHE:HB3	2.21	0.41
1:A:36:ILE:HD12	3:B:297:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:ARG:HD2	3:B:236:HOH:O	2.20	0.41
1:A:104:GLY:O	1:A:108:LYS:HG3	2.21	0.41
1:B:18:LEU:O	1:B:19:ARG:C	2.58	0.41
1:B:130:LEU:N	1:B:130:LEU:CD1	2.83	0.41
1:B:141:LYS:HZ1	1:B:147:ASP:HB2	1.83	0.41
1:A:55:LEU:HD13	1:A:112:LYS:CG	2.51	0.40
1:B:89:ILE:CG2	1:B:125:PHE:HA	2.46	0.40
1:B:81:TYR:CD1	1:B:81:TYR:C	2.94	0.40
1:A:87:ARG:HG2	1:B:51:PHE:CD1	2.57	0.40
1:B:89:ILE:HG21	1:B:117:ALA:HB2	2.03	0.40
1:B:91:LEU:HD21	1:B:94:ILE:HD12	2.03	0.40
1:A:167:LEU:HG	1:B:114:ALA:HB2	2.02	0.40
1:A:107:SER:HB3	3:A:436:HOH:O	2.21	0.40
1:A:49:ASN:CG	3:A:448:HOH:O	2.59	0.40
1:A:139:LEU:HD13	2:A:306:ACO:H4B	2.04	0.40
1:A:38:GLU:HA	1:A:41:LEU:HD13	2.03	0.40
1:A:165:ARG:HH11	1:A:165:ARG:HG3	1.86	0.40
1:B:130:LEU:HD13	1:B:132:TRP:HE1	1.86	0.40
1:A:23:GLU:HB3	1:A:95:TYR:CZ	2.57	0.40
1:B:106:GLY:O	1:B:110:ILE:HG13	2.21	0.40
1:B:18:LEU:CD1	1:B:36:ILE:HG23	2.52	0.40
1:A:159:PHE:CE2	1:B:145:ALA:HB2	2.57	0.40
1:A:111:LYS:HE3	3:A:441:HOH:O	2.21	0.40
1:B:5:ARG:O	1:B:6:ILE:HD13	2.22	0.40
1:B:14:CYS:SG	1:B:41:LEU:HB2	2.62	0.40
1:B:80:ILE:HD11	1:B:126:ARG:NH1	2.36	0.40
1:B:125:PHE:HD1	1:B:126:ARG:N	2.20	0.40
1:A:157:PHE:HB2	1:B:127:LEU:CD1	2.51	0.40
1:A:87:ARG:HG2	1:B:51:PHE:CG	2.57	0.40
1:B:132:TRP:C	1:B:132:TRP:CE3	2.94	0.40
1:A:4:VAL:HG22	1:A:59:ILE:CD1	2.44	0.40
1:B:9:ALA:HB2	1:B:54:CYS:SG	2.62	0.40
1:B:112:LYS:HB2	3:B:297:HOH:O	2.22	0.40
1:B:123:SER:O	1:B:124:GLN:NE2	2.55	0.40
1:A:84:TRP:CE2	3:A:401:HOH:O	2.74	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	1-A	150/170 (88%)	129 (86%)	18 (12%)	3 (2%)	7 1
1	1-B	155/170 (91%)	138 (89%)	15 (10%)	2 (1%)	12 3
1	2-A	150/170 (88%)	140 (93%)	8 (5%)	2 (1%)	12 3
1	2-B	155/170 (91%)	148 (96%)	6 (4%)	1 (1%)	25 12
1	3-A	150/170 (88%)	138 (92%)	9 (6%)	3 (2%)	7 1
1	3-B	155/170 (91%)	150 (97%)	5 (3%)	0	100 100
1	4-A	150/170 (88%)	133 (89%)	13 (9%)	4 (3%)	5 0
1	4-B	155/170 (91%)	147 (95%)	8 (5%)	0	100 100
1	5-A	150/170 (88%)	138 (92%)	8 (5%)	4 (3%)	5 0
1	5-B	155/170 (91%)	143 (92%)	7 (4%)	5 (3%)	4 0
1	6-A	150/170 (88%)	138 (92%)	9 (6%)	3 (2%)	7 1
1	6-B	155/170 (91%)	129 (83%)	22 (14%)	4 (3%)	5 0
1	7-A	150/170 (88%)	144 (96%)	6 (4%)	0	100 100
1	7-B	155/170 (91%)	150 (97%)	5 (3%)	0	100 100
1	8-A	150/170 (88%)	136 (91%)	12 (8%)	2 (1%)	12 3
1	8-B	155/170 (91%)	146 (94%)	8 (5%)	1 (1%)	25 12
All	All	2440/2720 (90%)	2247 (92%)	159 (6%)	34 (1%)	11 3

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	1-A	47	GLY
1	1-B	48	ASP
1	1-A	48	ASP
1	1-A	92	GLU
1	2-B	48	ASP
1	3-A	124	GLN

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Mol	Chain	Res	Type
1	3-A	161	GLY
1	4-A	47	GLY
1	5-A	150	GLU
1	6-A	9	ALA
1	6-A	47	GLY
1	6-B	11	GLU
1	6-B	16	ASP
1	6-B	17	ILE
1	6-B	153	GLY
1	8-A	161	GLY
1	2-A	79	PHE
1	5-B	168	ALA
1	8-A	69	PRO
1	1-B	82	SER
1	4-A	91	LEU
1	5-B	11	GLU
1	5-B	160	GLN
1	6-A	14	CYS
1	3-A	103	GLN
1	5-A	29	LYS
1	5-A	151	ALA
1	2-A	69	PRO
1	5-A	47	GLY
1	5-B	36	ILE
1	5-B	169	GLY
1	4-A	161	GLY
1	4-A	98	PRO
1	8-B	161	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	1-A	126/135 (93%)	118 (94%)	8 (6%)	18 4
1	1-B	129/135 (96%)	126 (98%)	3 (2%)	50 34
1	2-A	126/135 (93%)	126 (100%)	0	100 100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2-B	129/135 (96%)	126 (98%)	3 (2%)	50	34
1	3-A	126/135 (93%)	125 (99%)	1 (1%)	81	75
1	3-B	129/135 (96%)	127 (98%)	2 (2%)	62	49
1	4-A	126/135 (93%)	124 (98%)	2 (2%)	62	49
1	4-B	129/135 (96%)	127 (98%)	2 (2%)	62	49
1	5-A	126/135 (93%)	124 (98%)	2 (2%)	62	49
1	5-B	129/135 (96%)	127 (98%)	2 (2%)	62	49
1	6-A	126/135 (93%)	122 (97%)	4 (3%)	39	21
1	6-B	129/135 (96%)	124 (96%)	5 (4%)	32	14
1	7-A	126/135 (93%)	126 (100%)	0	100	100
1	7-B	129/135 (96%)	128 (99%)	1 (1%)	81	75
1	8-A	126/135 (93%)	125 (99%)	1 (1%)	81	75
1	8-B	129/135 (96%)	127 (98%)	2 (2%)	62	49
All	All	2040/2160 (94%)	2002 (98%)	38 (2%)	57	42

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	1-A	53	HIS
1	1-A	54	CYS
1	1-A	58	GLU
1	1-A	89	ILE
1	1-A	125	PHE
1	1-A	139	LEU
1	1-A	157	PHE
1	1-A	158	CYS
1	1-B	81	TYR
1	1-B	150	GLU
1	1-B	156	PHE
1	2-B	48	ASP
1	2-B	127	LEU
1	2-B	156	PHE
1	3-A	103	GLN
1	3-B	127	LEU
1	3-B	156	PHE
1	4-A	93	ASP
1	4-A	138	ASP

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Mol	Chain	Res	Type
1	4-B	42	ARG
1	4-B	156	PHE
1	5-A	94	ILE
1	5-A	125	PHE
1	5-B	49	ASN
1	5-B	156	PHE
1	6-A	127	LEU
1	6-A	138	ASP
1	6-A	158	CYS
1	6-A	167	LEU
1	6-B	14	CYS
1	6-B	32	ASP
1	6-B	119	ASP
1	6-B	155	HIS
1	6-B	156	PHE
1	7-B	156	PHE
1	8-A	127	LEU
1	8-B	127	LEU
1	8-B	156	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	1-B	160	GLN
1	2-B	53	HIS
1	2-B	160	GLN
1	3-A	103	GLN
1	3-B	124	GLN
1	3-B	146	GLN
1	6-B	124	GLN
1	6-B	134	GLN
1	7-B	160	GLN
1	8-B	160	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)

8 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	ACO	1-A	306	-	45,53,53	1.65	9 (20%)	56,79,79	1.63	6 (10%)
2	ACO	4-A	306	-	45,53,53	1.56	8 (17%)	56,79,79	1.67	10 (17%)
2	ACO	5-A	306	-	45,53,53	1.57	9 (20%)	56,79,79	1.73	9 (16%)
2	ACO	2-A	306	-	45,53,53	1.68	13 (28%)	56,79,79	1.74	7 (12%)
2	ACO	7-A	306	-	45,53,53	1.59	9 (20%)	56,79,79	1.71	9 (16%)
2	ACO	6-A	306	-	45,53,53	1.62	9 (20%)	56,79,79	1.73	8 (14%)
2	ACO	3-A	306	-	45,53,53	1.57	7 (15%)	56,79,79	1.58	7 (12%)
2	ACO	8-A	306	-	45,53,53	1.58	9 (20%)	56,79,79	1.74	8 (14%)

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	ACO	1-A	306	-	-	8/47/67/67	0/3/3/3
2	ACO	4-A	306	-	-	8/47/67/67	0/3/3/3
2	ACO	5-A	306	-	-	7/47/67/67	0/3/3/3
2	ACO	2-A	306	-	-	8/47/67/67	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ACO	7-A	306	-	-	7/47/67/67	0/3/3/3
2	ACO	6-A	306	-	-	10/47/67/67	0/3/3/3
2	ACO	3-A	306	-	-	8/47/67/67	0/3/3/3
2	ACO	8-A	306	-	-	6/47/67/67	0/3/3/3

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1-A	306	ACO	C4A-N3A	3.84	1.41	1.35
2	4-A	306	ACO	C-S1P	-3.75	1.53	1.75
2	5-A	306	ACO	CH3-C	3.72	1.65	1.50
2	1-A	306	ACO	C-S1P	-3.70	1.53	1.75
2	6-A	306	ACO	CH3-C	3.68	1.65	1.50
2	3-A	306	ACO	C-S1P	-3.65	1.53	1.75
2	7-A	306	ACO	CH3-C	3.64	1.65	1.50
2	3-A	306	ACO	CH3-C	3.63	1.65	1.50
2	4-A	306	ACO	CH3-C	3.63	1.65	1.50
2	7-A	306	ACO	C-S1P	-3.62	1.53	1.75
2	8-A	306	ACO	C-S1P	-3.62	1.53	1.75
2	8-A	306	ACO	CH3-C	3.60	1.65	1.50
2	1-A	306	ACO	CH3-C	3.58	1.65	1.50
2	2-A	306	ACO	CH3-C	3.52	1.64	1.50
2	2-A	306	ACO	C-S1P	-3.51	1.54	1.75
2	5-A	306	ACO	C-S1P	-3.51	1.54	1.75
2	3-A	306	ACO	C4A-N3A	3.50	1.40	1.35
2	6-A	306	ACO	C-S1P	-3.43	1.54	1.75
2	2-A	306	ACO	C2A-N3A	3.29	1.37	1.32
2	8-A	306	ACO	C2A-N3A	3.15	1.37	1.32
2	5-A	306	ACO	C2A-N3A	3.05	1.37	1.32
2	7-A	306	ACO	C2A-N3A	3.02	1.37	1.32
2	4-A	306	ACO	C2A-N3A	3.02	1.37	1.32
2	2-A	306	ACO	C4A-N3A	3.01	1.39	1.35
2	6-A	306	ACO	C4A-N3A	3.01	1.39	1.35
2	8-A	306	ACO	C4A-N3A	2.98	1.39	1.35
2	4-A	306	ACO	C4A-N3A	2.98	1.39	1.35
2	6-A	306	ACO	C9P-N8P	2.93	1.40	1.33
2	5-A	306	ACO	C4A-N3A	2.93	1.39	1.35
2	6-A	306	ACO	C2A-N3A	2.89	1.36	1.32
2	1-A	306	ACO	C2A-N3A	2.83	1.36	1.32
2	7-A	306	ACO	C4A-N3A	2.82	1.39	1.35
2	5-A	306	ACO	O-C	2.79	1.34	1.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3-A	306	ACO	C2A-N3A	2.68	1.36	1.32
2	6-A	306	ACO	O-C	2.64	1.33	1.20
2	4-A	306	ACO	O6A-CCP	2.56	1.52	1.43
2	2-A	306	ACO	C9P-N8P	2.55	1.39	1.33
2	3-A	306	ACO	O-C	2.54	1.33	1.20
2	1-A	306	ACO	P3B-O8A	-2.54	1.45	1.54
2	8-A	306	ACO	O-C	2.53	1.33	1.20
2	3-A	306	ACO	P3B-O8A	-2.51	1.45	1.54
2	7-A	306	ACO	O-C	2.51	1.32	1.20
2	6-A	306	ACO	P3B-O8A	-2.49	1.45	1.54
2	1-A	306	ACO	O-C	2.46	1.32	1.20
2	6-A	306	ACO	O4B-C1B	2.46	1.44	1.41
2	8-A	306	ACO	C8A-N7A	-2.46	1.30	1.34
2	2-A	306	ACO	P3B-O8A	-2.44	1.45	1.54
2	7-A	306	ACO	C8A-N7A	-2.43	1.30	1.34
2	5-A	306	ACO	C9P-N8P	2.38	1.38	1.33
2	4-A	306	ACO	C9P-N8P	2.37	1.38	1.33
2	5-A	306	ACO	C8A-N7A	-2.37	1.30	1.34
2	2-A	306	ACO	O-C	2.32	1.32	1.20
2	4-A	306	ACO	O-C	2.32	1.32	1.20
2	8-A	306	ACO	P3B-O8A	-2.31	1.45	1.54
2	8-A	306	ACO	C9P-N8P	2.30	1.38	1.33
2	2-A	306	ACO	C2P-S1P	2.27	1.91	1.81
2	2-A	306	ACO	O5B-C5B	-2.25	1.36	1.44
2	4-A	306	ACO	P3B-O8A	-2.25	1.46	1.54
2	7-A	306	ACO	C9P-N8P	2.23	1.38	1.33
2	1-A	306	ACO	C2B-C3B	2.21	1.57	1.52
2	7-A	306	ACO	P3B-O8A	-2.19	1.46	1.54
2	1-A	306	ACO	C9P-N8P	2.17	1.38	1.33
2	6-A	306	ACO	O6A-CCP	2.17	1.50	1.43
2	2-A	306	ACO	C2B-C1B	2.14	1.57	1.53
2	5-A	306	ACO	P3B-O8A	-2.12	1.46	1.54
2	2-A	306	ACO	O4B-C1B	2.12	1.44	1.41
2	7-A	306	ACO	O6A-CCP	2.12	1.50	1.43
2	1-A	306	ACO	O6A-CCP	2.11	1.50	1.43
2	3-A	306	ACO	C9P-N8P	2.10	1.38	1.33
2	8-A	306	ACO	O6A-CCP	2.02	1.50	1.43
2	5-A	306	ACO	O6A-CCP	2.02	1.50	1.43
2	2-A	306	ACO	P3B-O9A	-2.01	1.47	1.54
2	2-A	306	ACO	C8A-N7A	-2.01	1.31	1.34

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	8-A	306	ACO	C3P-N4P-C5P	6.41	134.73	122.84
2	2-A	306	ACO	C3P-N4P-C5P	6.06	134.09	122.84
2	7-A	306	ACO	C3P-N4P-C5P	5.99	133.95	122.84
2	1-A	306	ACO	C3P-N4P-C5P	5.90	133.78	122.84
2	3-A	306	ACO	C3P-N4P-C5P	5.61	133.26	122.84
2	4-A	306	ACO	C3P-N4P-C5P	5.54	133.11	122.84
2	2-A	306	ACO	O-C-CH3	-5.47	100.62	123.07
2	6-A	306	ACO	C3P-N4P-C5P	5.39	132.85	122.84
2	6-A	306	ACO	O-C-CH3	-5.30	101.34	123.07
2	4-A	306	ACO	O-C-CH3	-5.30	101.34	123.07
2	1-A	306	ACO	O-C-CH3	-5.28	101.42	123.07
2	8-A	306	ACO	O-C-CH3	-5.24	101.56	123.07
2	3-A	306	ACO	O-C-CH3	-5.24	101.57	123.07
2	7-A	306	ACO	O-C-CH3	-5.22	101.64	123.07
2	5-A	306	ACO	O-C-CH3	-5.21	101.70	123.07
2	5-A	306	ACO	C3P-N4P-C5P	5.18	132.46	122.84
2	6-A	306	ACO	O6A-CCP-CBP	4.63	117.99	110.55
2	8-A	306	ACO	O4B-C1B-C2B	-4.09	100.95	106.93
2	2-A	306	ACO	O4B-C1B-C2B	-4.09	100.95	106.93
2	5-A	306	ACO	C5B-C4B-C3B	4.00	127.66	114.40
2	5-A	306	ACO	C2P-C3P-N4P	-3.99	104.04	112.42
2	5-A	306	ACO	O4B-C1B-C2B	-3.90	101.23	106.93
2	8-A	306	ACO	C2P-C3P-N4P	-3.82	104.39	112.42
2	7-A	306	ACO	O4B-C1B-C2B	-3.81	101.36	106.93
2	6-A	306	ACO	O4B-C1B-C2B	-3.74	101.46	106.93
2	7-A	306	ACO	C5B-C4B-C3B	3.59	126.31	114.40
2	7-A	306	ACO	C2P-C3P-N4P	-3.53	104.99	112.42
2	2-A	306	ACO	C5B-C4B-C3B	3.44	125.80	114.40
2	4-A	306	ACO	O6A-CCP-CBP	3.30	115.86	110.55
2	3-A	306	ACO	C2P-C3P-N4P	-3.26	105.58	112.42
2	2-A	306	ACO	C2P-C3P-N4P	-3.19	105.72	112.42
2	1-A	306	ACO	O4B-C1B-C2B	-3.11	102.38	106.93
2	4-A	306	ACO	C5B-C4B-C3B	3.09	124.63	114.40
2	4-A	306	ACO	O4B-C1B-C2B	-2.95	102.62	106.93
2	1-A	306	ACO	C2P-C3P-N4P	-2.89	106.35	112.42
2	8-A	306	ACO	C5B-C4B-C3B	2.75	123.53	114.40
2	6-A	306	ACO	O2B-C2B-C3B	2.73	118.93	111.17
2	6-A	306	ACO	C2P-C3P-N4P	-2.55	107.05	112.42
2	3-A	306	ACO	C3B-C2B-C1B	2.46	105.33	99.89
2	4-A	306	ACO	CEP-CBP-CAP	2.25	112.73	108.82
2	8-A	306	ACO	C3B-C2B-C1B	2.24	104.86	99.89
2	2-A	306	ACO	CH3-C-S1P	2.21	129.52	114.20
2	4-A	306	ACO	C2P-C3P-N4P	-2.15	107.89	112.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	4-A	306	ACO	C6P-C7P-N8P	2.15	116.23	111.90
2	5-A	306	ACO	C2A-N1A-C6A	2.14	122.41	118.75
2	5-A	306	ACO	CEP-CBP-CAP	2.12	112.50	108.82
2	7-A	306	ACO	CEP-CBP-CAP	2.11	112.48	108.82
2	6-A	306	ACO	N3A-C2A-N1A	-2.10	125.40	128.68
2	4-A	306	ACO	CH3-C-S1P	2.09	128.67	114.20
2	7-A	306	ACO	CH3-C-S1P	2.09	128.67	114.20
2	8-A	306	ACO	CH3-C-S1P	2.09	128.62	114.20
2	6-A	306	ACO	CH3-C-S1P	2.08	128.59	114.20
2	1-A	306	ACO	O2B-C2B-C3B	2.08	117.06	111.17
2	1-A	306	ACO	CH3-C-S1P	2.07	128.52	114.20
2	7-A	306	ACO	C2A-N1A-C6A	2.07	122.29	118.75
2	3-A	306	ACO	O4B-C1B-C2B	-2.05	103.93	106.93
2	2-A	306	ACO	C2A-N1A-C6A	2.04	122.24	118.75
2	3-A	306	ACO	CH3-C-S1P	2.03	128.24	114.20
2	5-A	306	ACO	CH3-C-S1P	2.03	128.23	114.20
2	3-A	306	ACO	O9A-P3B-O8A	2.03	115.38	107.64
2	4-A	306	ACO	C2A-N1A-C6A	2.03	122.22	118.75
2	5-A	306	ACO	C3B-C2B-C1B	2.02	104.35	99.89
2	8-A	306	ACO	CEP-CBP-CAP	2.01	112.31	108.82
2	7-A	306	ACO	C3B-C2B-C1B	2.01	104.34	99.89

There are no chirality outliers.

All (62) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	1-A	306	ACO	C5B-O5B-P1A-O1A
2	1-A	306	ACO	C5B-O5B-P1A-O2A
2	2-A	306	ACO	C5B-O5B-P1A-O1A
2	2-A	306	ACO	C5B-O5B-P1A-O2A
2	3-A	306	ACO	C5B-O5B-P1A-O1A
2	3-A	306	ACO	C5B-O5B-P1A-O2A
2	3-A	306	ACO	N8P-C9P-CAP-OAP
2	4-A	306	ACO	C5B-O5B-P1A-O1A
2	4-A	306	ACO	C5B-O5B-P1A-O2A
2	4-A	306	ACO	CBP-CCP-O6A-P2A
2	5-A	306	ACO	C5B-O5B-P1A-O1A
2	5-A	306	ACO	C5B-O5B-P1A-O2A
2	6-A	306	ACO	C4B-C3B-O3B-P3B
2	6-A	306	ACO	C5B-O5B-P1A-O1A
2	6-A	306	ACO	C5B-O5B-P1A-O2A
2	6-A	306	ACO	O9P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
2	6-A	306	ACO	N8P-C9P-CAP-OAP
2	7-A	306	ACO	C5B-O5B-P1A-O1A
2	7-A	306	ACO	C5B-O5B-P1A-O2A
2	8-A	306	ACO	C5B-O5B-P1A-O1A
2	8-A	306	ACO	C5B-O5B-P1A-O2A
2	2-A	306	ACO	C6P-C7P-N8P-C9P
2	4-A	306	ACO	C3B-C4B-C5B-O5B
2	4-A	306	ACO	O4B-C4B-C5B-O5B
2	4-A	306	ACO	C6P-C7P-N8P-C9P
2	5-A	306	ACO	C6P-C7P-N8P-C9P
2	8-A	306	ACO	C6P-C7P-N8P-C9P
2	6-A	306	ACO	O4B-C4B-C5B-O5B
2	3-A	306	ACO	O9P-C9P-CAP-OAP
2	7-A	306	ACO	C6P-C7P-N8P-C9P
2	6-A	306	ACO	C3B-C4B-C5B-O5B
2	1-A	306	ACO	C6P-C7P-N8P-C9P
2	6-A	306	ACO	C5B-O5B-P1A-O3A
2	1-A	306	ACO	P1A-O3A-P2A-O5A
2	2-A	306	ACO	P1A-O3A-P2A-O5A
2	3-A	306	ACO	P1A-O3A-P2A-O5A
2	4-A	306	ACO	P1A-O3A-P2A-O5A
2	5-A	306	ACO	P1A-O3A-P2A-O5A
2	6-A	306	ACO	P1A-O3A-P2A-O5A
2	7-A	306	ACO	P1A-O3A-P2A-O5A
2	8-A	306	ACO	P1A-O3A-P2A-O5A
2	2-A	306	ACO	C3B-C4B-C5B-O5B
2	1-A	306	ACO	C3P-C2P-S1P-C
2	3-A	306	ACO	C3P-C2P-S1P-C
2	1-A	306	ACO	C5P-C6P-C7P-N8P
2	1-A	306	ACO	C5B-O5B-P1A-O3A
2	2-A	306	ACO	C5B-O5B-P1A-O3A
2	3-A	306	ACO	C5B-O5B-P1A-O3A
2	4-A	306	ACO	C5B-O5B-P1A-O3A
2	5-A	306	ACO	C5B-O5B-P1A-O3A
2	7-A	306	ACO	C5B-O5B-P1A-O3A
2	8-A	306	ACO	C5B-O5B-P1A-O3A
2	1-A	306	ACO	P1A-O3A-P2A-O4A
2	3-A	306	ACO	P1A-O3A-P2A-O4A
2	5-A	306	ACO	P1A-O3A-P2A-O4A
2	6-A	306	ACO	P1A-O3A-P2A-O4A
2	7-A	306	ACO	P1A-O3A-P2A-O4A
2	8-A	306	ACO	P1A-O3A-P2A-O4A

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Mol	Chain	Res	Type	Atoms
2	2-A	306	ACO	CBP-CCP-O6A-P2A
2	5-A	306	ACO	CBP-CCP-O6A-P2A
2	7-A	306	ACO	CBP-CCP-O6A-P2A
2	2-A	306	ACO	O4B-C4B-C5B-O5B

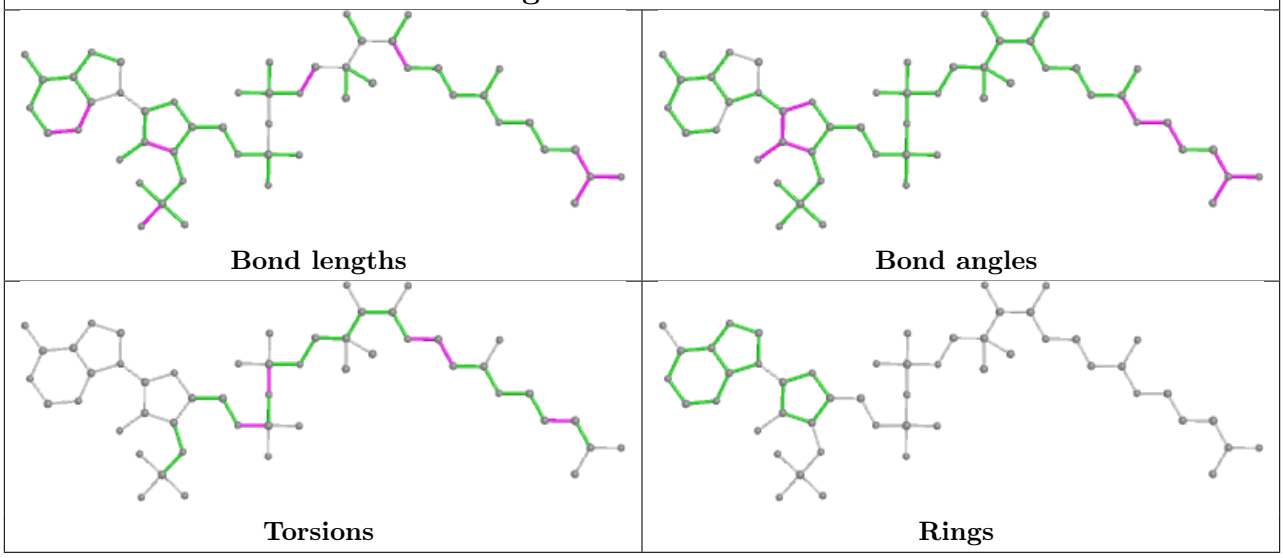
There are no ring outliers.

8 monomers are involved in 37 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	1-A	306	ACO	4	0
2	4-A	306	ACO	8	0
2	5-A	306	ACO	1	0
2	2-A	306	ACO	4	0
2	7-A	306	ACO	3	0
2	6-A	306	ACO	8	0
2	3-A	306	ACO	3	0
2	8-A	306	ACO	6	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 ACO A 306



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	1-A	154/170 (90%)	0.58	14 (9%)	9	8	12, 22, 42, 59	154 (100%)
1	1-B	157/170 (92%)	0.30	13 (8%)	11	10	9, 24, 40, 52	157 (100%)
1	2-A	154/170 (90%)	0.58	14 (9%)	9	8	12, 22, 42, 59	154 (100%)
1	2-B	157/170 (92%)	0.30	13 (8%)	11	10	9, 24, 40, 52	157 (100%)
1	3-A	154/170 (90%)	0.58	14 (9%)	9	8	12, 22, 42, 59	154 (100%)
1	3-B	157/170 (92%)	0.30	13 (8%)	11	10	9, 24, 40, 52	157 (100%)
1	4-A	154/170 (90%)	0.58	14 (9%)	9	8	12, 22, 42, 59	154 (100%)
1	4-B	157/170 (92%)	0.30	13 (8%)	11	10	9, 24, 40, 52	157 (100%)
1	5-A	154/170 (90%)	0.58	14 (9%)	9	8	12, 22, 42, 59	154 (100%)
1	5-B	157/170 (92%)	0.30	13 (8%)	11	10	9, 24, 40, 52	157 (100%)
1	6-A	154/170 (90%)	0.58	14 (9%)	9	8	12, 22, 42, 59	154 (100%)
1	6-B	157/170 (92%)	0.30	13 (8%)	11	10	9, 24, 40, 52	157 (100%)
1	7-A	154/170 (90%)	0.58	14 (9%)	9	8	12, 22, 42, 59	154 (100%)
1	7-B	157/170 (92%)	0.30	13 (8%)	11	10	9, 24, 40, 52	157 (100%)
1	8-A	154/170 (90%)	0.58	14 (9%)	9	8	12, 22, 42, 59	154 (100%)
1	8-B	157/170 (92%)	0.30	13 (8%)	11	10	9, 24, 40, 52	157 (100%)
All	All	2488/2720 (91%)	0.43	216 (8%)	10	9	9, 23, 41, 59	2488 (100%)

All (216) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	1-A	68	GLY	15.1
1	2-A	68	GLY	15.1
1	3-A	68	GLY	15.1
1	4-A	68	GLY	15.1
1	5-A	68	GLY	15.1

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Mol	Chain	Res	Type	RSRZ
1	6-A	68	GLY	15.1
1	7-A	68	GLY	15.1
1	8-A	68	GLY	15.1
1	1-A	47	GLY	10.6
1	2-A	47	GLY	10.6
1	3-A	47	GLY	10.6
1	4-A	47	GLY	10.6
1	5-A	47	GLY	10.6
1	6-A	47	GLY	10.6
1	7-A	47	GLY	10.6
1	8-A	47	GLY	10.6
1	1-A	48	ASP	5.7
1	2-A	48	ASP	5.7
1	3-A	48	ASP	5.7
1	4-A	48	ASP	5.7
1	5-A	48	ASP	5.7
1	6-A	48	ASP	5.7
1	7-A	48	ASP	5.7
1	8-A	48	ASP	5.7
1	1-B	121	GLY	4.9
1	2-B	121	GLY	4.9
1	3-B	121	GLY	4.9
1	4-B	121	GLY	4.9
1	5-B	121	GLY	4.9
1	6-B	121	GLY	4.9
1	7-B	121	GLY	4.9
1	8-B	121	GLY	4.9
1	1-A	49	ASN	4.3
1	2-A	49	ASN	4.3
1	3-A	49	ASN	4.3
1	4-A	49	ASN	4.3
1	5-A	49	ASN	4.3
1	6-A	49	ASN	4.3
1	7-A	49	ASN	4.3
1	8-A	49	ASN	4.3
1	1-A	43	ALA	3.9
1	2-A	43	ALA	3.9
1	3-A	43	ALA	3.9
1	4-A	43	ALA	3.9
1	5-A	43	ALA	3.9
1	6-A	43	ALA	3.9
1	7-A	43	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	8-A	43	ALA	3.9
1	1-B	119	ASP	3.9
1	2-B	119	ASP	3.9
1	3-B	119	ASP	3.9
1	4-B	119	ASP	3.9
1	5-B	119	ASP	3.9
1	6-B	119	ASP	3.9
1	7-B	119	ASP	3.9
1	8-B	119	ASP	3.9
1	1-A	30	LEU	3.6
1	2-A	30	LEU	3.6
1	3-A	30	LEU	3.6
1	4-A	30	LEU	3.6
1	5-A	30	LEU	3.6
1	6-A	30	LEU	3.6
1	7-A	30	LEU	3.6
1	8-A	30	LEU	3.6
1	1-A	35	LYS	3.1
1	2-A	35	LYS	3.1
1	3-A	35	LYS	3.1
1	4-A	35	LYS	3.1
1	5-A	35	LYS	3.1
1	6-A	35	LYS	3.1
1	7-A	35	LYS	3.1
1	8-A	35	LYS	3.1
1	1-B	145	ALA	2.9
1	2-B	145	ALA	2.9
1	3-B	145	ALA	2.9
1	4-B	145	ALA	2.9
1	5-B	145	ALA	2.9
1	6-B	145	ALA	2.9
1	7-B	145	ALA	2.9
1	8-B	145	ALA	2.9
1	1-A	45	GLY	2.7
1	2-A	45	GLY	2.7
1	3-A	45	GLY	2.7
1	4-A	45	GLY	2.7
1	5-A	45	GLY	2.7
1	6-A	45	GLY	2.7
1	7-A	45	GLY	2.7
1	8-A	45	GLY	2.7
1	1-B	84	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
1	2-B	84	TRP	2.6
1	3-B	84	TRP	2.6
1	4-B	84	TRP	2.6
1	5-B	84	TRP	2.6
1	6-B	84	TRP	2.6
1	7-B	84	TRP	2.6
1	8-B	84	TRP	2.6
1	1-B	81	TYR	2.5
1	2-B	81	TYR	2.5
1	3-B	81	TYR	2.5
1	4-B	81	TYR	2.5
1	5-B	81	TYR	2.5
1	6-B	81	TYR	2.5
1	7-B	81	TYR	2.5
1	8-B	81	TYR	2.5
1	1-B	143	LEU	2.5
1	2-B	143	LEU	2.5
1	3-B	143	LEU	2.5
1	4-B	143	LEU	2.5
1	5-B	143	LEU	2.5
1	6-B	143	LEU	2.5
1	7-B	143	LEU	2.5
1	8-B	143	LEU	2.5
1	1-B	118	LEU	2.5
1	2-B	118	LEU	2.5
1	3-B	118	LEU	2.5
1	4-B	118	LEU	2.5
1	5-B	118	LEU	2.5
1	6-B	118	LEU	2.5
1	7-B	118	LEU	2.5
1	8-B	118	LEU	2.5
1	1-B	142	ALA	2.5
1	2-B	142	ALA	2.5
1	3-B	142	ALA	2.5
1	4-B	142	ALA	2.5
1	5-B	142	ALA	2.5
1	6-B	142	ALA	2.5
1	7-B	142	ALA	2.5
1	8-B	142	ALA	2.5
1	1-A	41	LEU	2.4
1	2-A	41	LEU	2.4
1	3-A	41	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	4-A	41	LEU	2.4
1	5-A	41	LEU	2.4
1	6-A	41	LEU	2.4
1	7-A	41	LEU	2.4
1	8-A	41	LEU	2.4
1	1-A	46	PHE	2.3
1	1-A	51	PHE	2.3
1	2-A	46	PHE	2.3
1	2-A	51	PHE	2.3
1	3-A	46	PHE	2.3
1	3-A	51	PHE	2.3
1	4-A	46	PHE	2.3
1	4-A	51	PHE	2.3
1	5-A	46	PHE	2.3
1	5-A	51	PHE	2.3
1	6-A	46	PHE	2.3
1	6-A	51	PHE	2.3
1	7-A	46	PHE	2.3
1	7-A	51	PHE	2.3
1	8-A	46	PHE	2.3
1	8-A	51	PHE	2.3
1	1-A	42	ARG	2.3
1	1-B	170	LYS	2.3
1	2-A	42	ARG	2.3
1	2-B	170	LYS	2.3
1	3-A	42	ARG	2.3
1	3-B	170	LYS	2.3
1	4-A	42	ARG	2.3
1	4-B	170	LYS	2.3
1	5-A	42	ARG	2.3
1	5-B	170	LYS	2.3
1	6-A	42	ARG	2.3
1	6-B	170	LYS	2.3
1	7-A	42	ARG	2.3
1	7-B	170	LYS	2.3
1	8-A	42	ARG	2.3
1	8-B	170	LYS	2.3
1	1-B	82	SER	2.3
1	2-B	82	SER	2.3
1	3-B	82	SER	2.3
1	4-B	82	SER	2.3
1	5-B	82	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	6-B	82	SER	2.3
1	7-B	82	SER	2.3
1	8-B	82	SER	2.3
1	1-B	87	ARG	2.2
1	2-B	87	ARG	2.2
1	3-B	87	ARG	2.2
1	4-B	87	ARG	2.2
1	5-B	87	ARG	2.2
1	6-B	87	ARG	2.2
1	7-B	87	ARG	2.2
1	8-B	87	ARG	2.2
1	1-A	150	GLU	2.1
1	2-A	150	GLU	2.1
1	3-A	150	GLU	2.1
1	4-A	150	GLU	2.1
1	5-A	150	GLU	2.1
1	6-A	150	GLU	2.1
1	7-A	150	GLU	2.1
1	8-A	150	GLU	2.1
1	1-A	161	GLY	2.1
1	2-A	161	GLY	2.1
1	3-A	161	GLY	2.1
1	4-A	161	GLY	2.1
1	5-A	161	GLY	2.1
1	6-A	161	GLY	2.1
1	7-A	161	GLY	2.1
1	8-A	161	GLY	2.1
1	1-B	3	SER	2.1
1	2-B	3	SER	2.1
1	3-B	3	SER	2.1
1	4-B	3	SER	2.1
1	5-B	3	SER	2.1
1	6-B	3	SER	2.1
1	7-B	3	SER	2.1
1	8-B	3	SER	2.1
1	1-B	70	CYS	2.0
1	2-B	70	CYS	2.0
1	3-B	70	CYS	2.0
1	4-B	70	CYS	2.0
1	5-B	70	CYS	2.0
1	6-B	70	CYS	2.0
1	7-B	70	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	8-B	70	CYS	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)

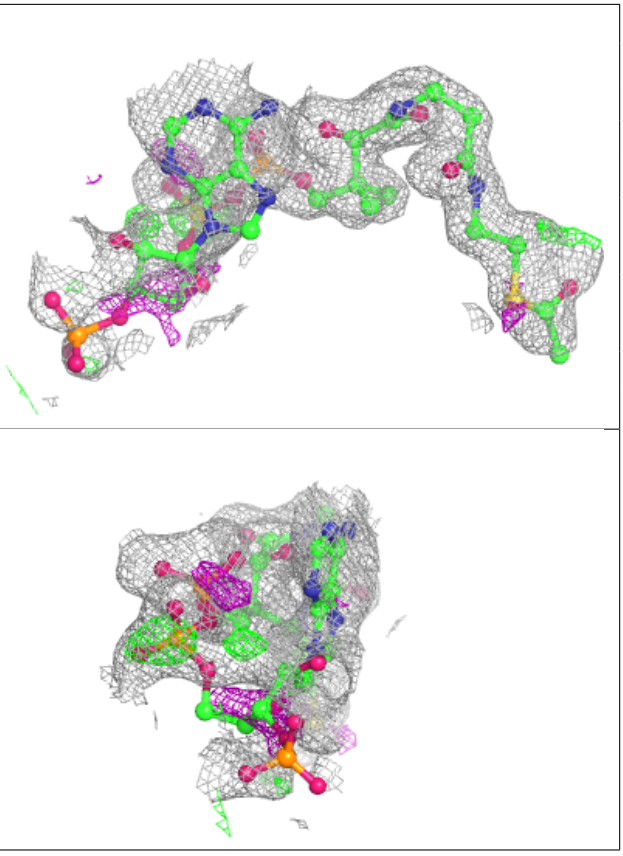
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	ACO	1-A	306	51/51	0.94	0.13	0,19,41,44	51
2	ACO	2-A	306	51/51	0.94	0.13	0,15,36,42	51
2	ACO	3-A	306	51/51	0.94	0.13	13,20,41,45	51
2	ACO	4-A	306	51/51	0.94	0.13	3,14,40,44	51
2	ACO	5-A	306	51/51	0.94	0.13	10,15,38,44	51
2	ACO	6-A	306	51/51	0.94	0.13	4,19,38,44	51
2	ACO	7-A	306	51/51	0.94	0.13	12,18,41,44	51
2	ACO	8-A	306	51/51	0.94	0.13	12,17,41,44	51

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 ACO A 306:

$2mF_o$-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.