Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2023 – 07:24 PM EDT

PDB ID	:	2YY5
Title	:	Crystal Structure of tryptophanyl-tRNA synthetase from Mycoplasma pneumoniae
Authors	:	Ishii, T.; Bessho, Y.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on	:	2007-04-27
Resolution	:	2.55 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:

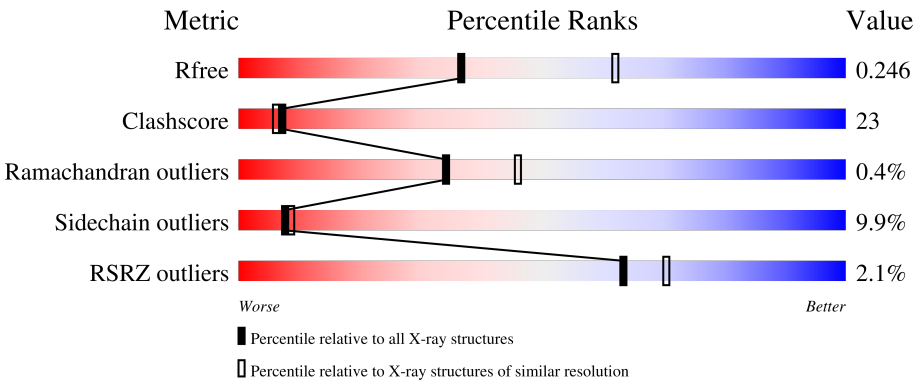
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.55 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	1284 (2.56-2.52)
Clashscore	141614	1332 (2.56-2.52)
Ramachandran outliers	138981	1315 (2.56-2.52)
Sidechain outliers	138945	1315 (2.56-2.52)
RSRZ outliers	127900	1272 (2.56-2.52)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	348	2% 56% 35% 5% •
1	B	348	2% 61% 32% 5% •
1	C	348	2% 57% 34% 6% •
1	D	348	2% 58% 35% 7% •

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	B	1361	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11474 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.

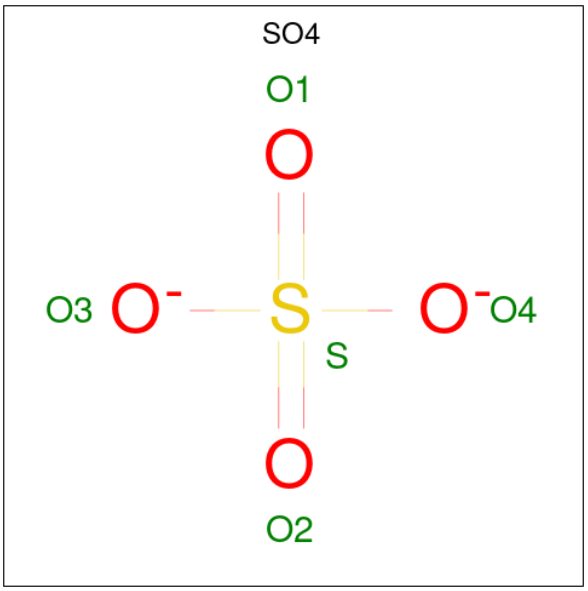
- Molecule 1 is a protein called Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	334	2650	1680	464	492	14	0	0	0
1	B	346	2741	1733	482	511	15	0	0	0
1	C	336	2663	1689	466	494	14	0	0	0
1	D	346	2741	1733	482	511	15	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

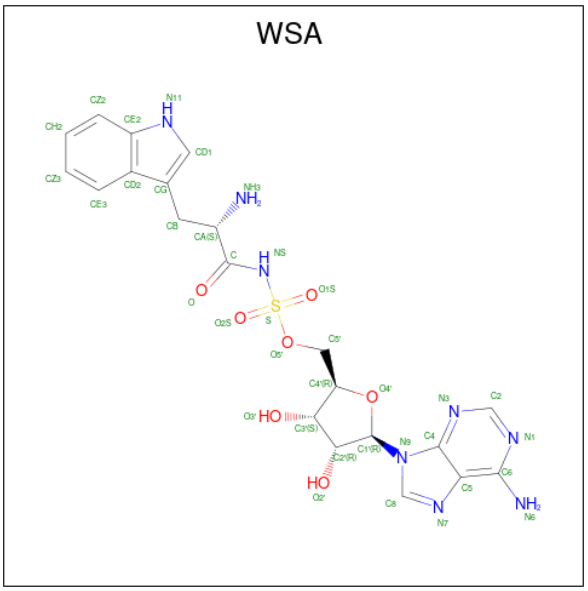
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P75510
A	0	HIS	-	expression tag	UNP P75510
A	240	SER	PRO	engineered mutation	UNP P75510
B	-1	GLY	-	expression tag	UNP P75510
B	0	HIS	-	expression tag	UNP P75510
B	240	SER	PRO	engineered mutation	UNP P75510
C	-1	GLY	-	expression tag	UNP P75510
C	0	HIS	-	expression tag	UNP P75510
C	240	SER	PRO	engineered mutation	UNP P75510
D	-1	GLY	-	expression tag	UNP P75510
D	0	HIS	-	expression tag	UNP P75510
D	240	SER	PRO	engineered mutation	UNP P75510

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O S 5 4 1	0	0
2	A	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	B	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	C	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0
2	D	1	Total O S 5 4 1	0	0

- Molecule 3 is 5'-O-[(L-TRYPTOPHYLAMINO)SULFONYL]ADENOSINE (three-letter code: WSA) (formula: $C_{21}H_{24}N_8O_7S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	37	21	8	7	1	0	0
3	B	1	37	21	8	7	1	0	0
3	C	1	37	21	8	7	1	0	0
3	D	1	37	21	8	7	1	0	0

- Molecule 4 is water.

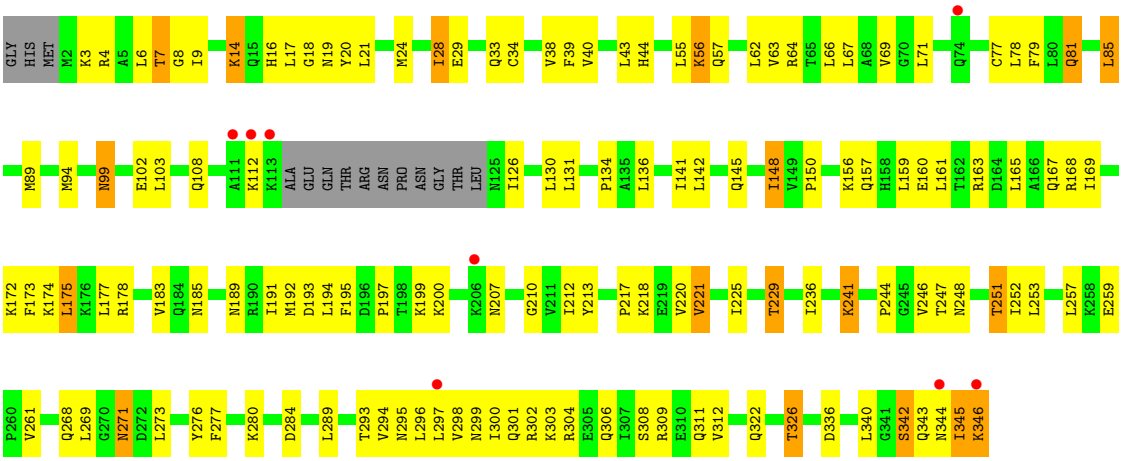
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	121	121	121	0	0
4	B	125	125	125	0	0
4	C	126	126	126	0	0
4	D	119	119	119	0	0

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.

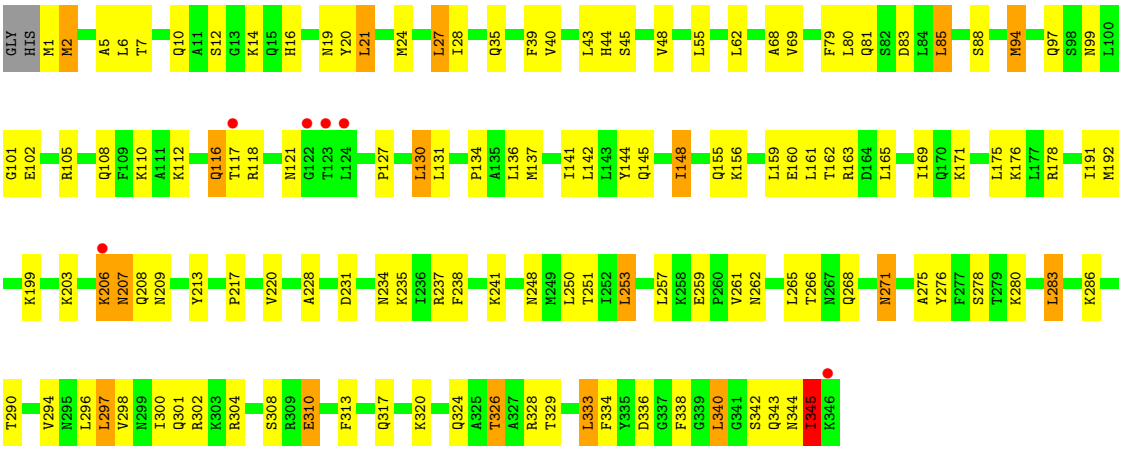
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain A:



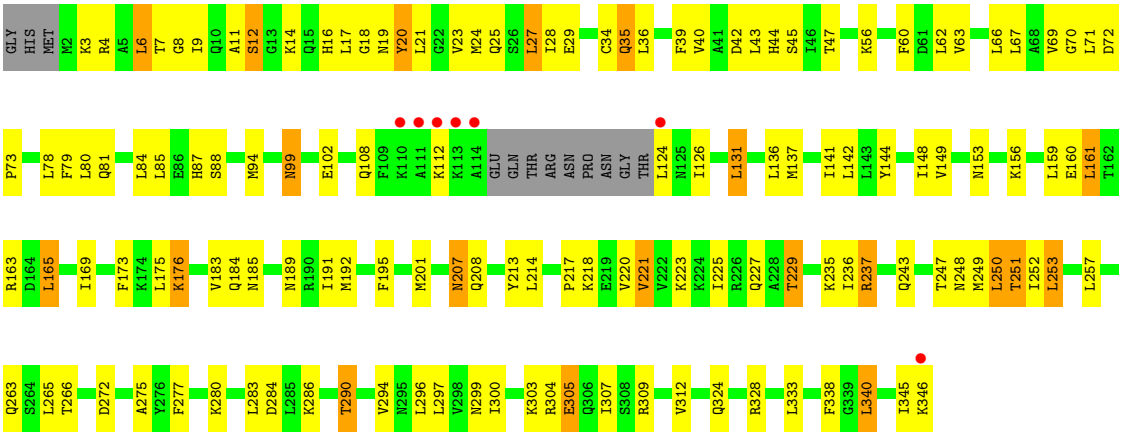
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain B:



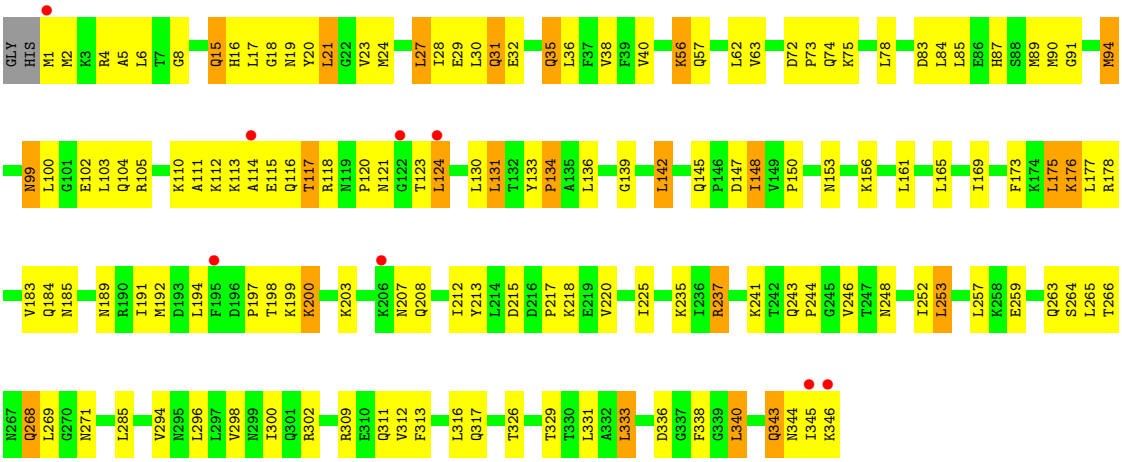
• Molecule 1: Tryptophanyl-tRNA synthetase

Chain C:



- Molecule 1: Tryptophanyl-tRNA synthetase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	88.16Å 52.11Å 194.09Å 90.00° 96.05° 90.00°	Depositor
Resolution (Å)	34.03 – 2.55 34.03 – 2.54	Depositor EDS
% Data completeness (in resolution range)	95.8 (34.03-2.55) 95.5 (34.03-2.54)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$< I/\sigma(I) >$ [1]	4.43 (at 2.54Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.192 , 0.251 0.186 , 0.246	Depositor DCC
R_{free} test set	5664 reflections (9.75%)	wwPDB-VP
Wilson B-factor (Å^2)	24.1	Xtriage
Anisotropy	0.151	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	11474	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% 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: WSA, SO4

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	0.39	0/2686	0.64	1/3615 (0.0%)
1	B	0.38	0/2779	0.65	3/3743 (0.1%)
1	C	0.40	0/2699	0.63	1/3633 (0.0%)
1	D	0.38	0/2779	0.67	2/3743 (0.1%)
All	All	0.39	0/10943	0.65	7/14734 (0.0%)

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

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

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	35	GLN	N-CA-C	-6.99	92.14	111.00
1	B	2	MET	N-CA-C	6.91	129.64	111.00
1	B	345	ILE	CB-CA-C	-6.15	99.30	111.60
1	C	35	GLN	N-CA-C	-5.81	95.32	111.00
1	B	35	GLN	N-CA-C	-5.51	96.13	111.00
1	D	346	LYS	N-CA-C	5.45	125.72	111.00
1	A	345	ILE	N-CA-C	-5.28	96.75	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	20	TYR	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2650	0	2745	132	0
1	B	2741	0	2837	119	0
1	C	2663	0	2761	129	0
1	D	2741	0	2837	138	0
2	A	10	0	0	2	0
2	B	10	0	0	3	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	37	0	24	1	0
3	B	37	0	24	5	0
3	C	37	0	24	3	0
3	D	37	0	24	2	0
4	A	121	0	0	7	0
4	B	125	0	0	11	0
4	C	126	0	0	8	0
4	D	119	0	0	17	0
All	All	11474	0	11276	503	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 23.

All (503) 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:C:56:LYS:HD2	1:D:344:ASN:HB3	1.26	1.13
1:A:345:ILE:O	1:A:346:LYS:HB2	1.53	1.05
1:A:241:LYS:HA	1:A:241:LYS:HE2	1.51	0.91
1:D:94:MET:HE3	1:D:169:ILE:HD11	1.53	0.91
1:D:237:ARG:HH11	1:D:243:GLN:NE2	1.70	0.90
1:A:221:VAL:O	1:A:225:ILE:HD13	1.72	0.89
1:A:309:ARG:HE	1:B:345:ILE:HG22	1.38	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:56:LYS:CD	1:D:344:ASN:HB3	2.03	0.88
1:D:176:LYS:H	1:D:176:LYS:HD2	1.38	0.88
1:A:16:HIS:H	1:A:19:ASN:HD22	1.21	0.88
1:B:283:LEU:HD22	1:B:283:LEU:H	1.39	0.88
1:B:324:GLN:HG2	1:B:328:ARG:HE	1.39	0.88
1:D:124:LEU:H	1:D:124:LEU:HD12	1.39	0.87
1:D:29:GLU:HG3	4:D:1427:HOH:O	1.75	0.87
1:D:194:LEU:HD11	1:D:212:ILE:HD11	1.55	0.86
1:A:56:LYS:HE3	1:A:309:ARG:HH22	1.41	0.85
1:D:1:MET:HG2	1:D:2:MET:N	1.90	0.85
1:A:3:LYS:O	1:A:34:CYS:HB2	1.76	0.85
1:C:346:LYS:HD2	1:D:309:ARG:HE	1.43	0.84
1:D:237:ARG:HH11	1:D:243:GLN:HE22	1.24	0.84
1:B:16:HIS:H	1:B:19:ASN:HD22	1.27	0.83
1:D:263:GLN:O	1:D:266:THR:HG22	1.78	0.82
1:A:191:ILE:HG23	1:A:252:ILE:HD11	1.60	0.81
1:A:71:LEU:HD23	1:A:78:LEU:HD22	1.61	0.81
1:C:165:LEU:O	1:C:169:ILE:HD13	1.80	0.81
1:B:108:GLN:HG2	2:B:1361:SO4:O1	1.82	0.80
1:D:56:LYS:HE3	1:D:309:ARG:NH1	1.98	0.78
1:A:308:SER:OG	1:A:311:GLN:HG3	1.84	0.78
1:D:100:LEU:O	1:D:104:GLN:HG3	1.83	0.78
1:D:246:VAL:HG12	4:D:1461:HOH:O	1.83	0.78
1:C:99:ASN:ND2	1:C:102:GLU:HG3	1.99	0.78
1:A:346:LYS:HB2	1:A:346:LYS:NZ	1.98	0.77
1:C:141:ILE:HD12	1:C:149:VAL:HG21	1.66	0.77
1:A:40:VAL:HG13	1:A:62:LEU:HD23	1.66	0.76
1:D:40:VAL:HG22	1:D:62:LEU:HD23	1.68	0.76
1:A:56:LYS:HE3	1:A:309:ARG:NH2	1.99	0.76
1:D:1:MET:HG2	1:D:2:MET:H	1.51	0.76
1:C:20:TYR:HD2	1:C:21:LEU:HD12	1.51	0.76
1:A:6:LEU:CD2	1:A:141:ILE:HA	2.15	0.76
1:B:5:ALA:HB2	1:B:148:ILE:HD11	1.68	0.75
1:A:63:VAL:HG11	1:A:312:VAL:HG13	1.69	0.75
1:C:108:GLN:O	1:C:112:LYS:HD2	1.87	0.74
1:D:110:LYS:HA	1:D:113:LYS:HG2	1.69	0.74
1:B:261:VAL:O	1:B:262:ASN:HB2	1.87	0.74
1:D:235:LYS:HG2	1:D:237:ARG:CZ	2.17	0.74
1:D:15:GLN:NE2	1:D:62:LEU:HD13	2.03	0.74
1:A:346:LYS:HB2	1:A:346:LYS:HZ2	1.53	0.73
1:A:99:ASN:ND2	1:A:102:GLU:H	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:MET:HA	1:C:27:LEU:CD2	2.18	0.73
1:C:56:LYS:HD2	1:D:344:ASN:CB	2.15	0.72
1:D:94:MET:HB2	4:D:1411:HOH:O	1.87	0.72
1:A:309:ARG:HE	1:B:345:ILE:CG2	2.02	0.72
1:C:225:ILE:HG21	1:C:290:THR:HG22	1.72	0.72
1:A:336:ASP:HA	1:A:344:ASN:HD21	1.54	0.72
1:D:264:SER:HB2	4:D:1463:HOH:O	1.89	0.72
1:D:28:ILE:H	1:D:28:ILE:HD12	1.54	0.71
1:C:40:VAL:HG13	1:C:62:LEU:HD23	1.71	0.71
3:B:1351:WSA:H3'	3:B:1351:WSA:HNS	1.55	0.71
1:B:159:LEU:O	1:B:163:ARG:HG3	1.90	0.71
1:C:16:HIS:H	1:C:19:ASN:HD22	1.39	0.70
1:D:191:ILE:HG23	1:D:252:ILE:HD11	1.73	0.70
1:A:145:GLN:HE22	1:A:178:ARG:H	1.39	0.70
1:B:235:LYS:HG2	1:B:237:ARG:CZ	2.21	0.70
1:D:153:ASN:HD22	1:D:184:GLN:HE22	1.38	0.70
1:C:338:PHE:HB3	1:C:340:LEU:HD22	1.74	0.70
1:C:346:LYS:HD2	1:D:309:ARG:NE	2.05	0.69
1:D:94:MET:CE	1:D:169:ILE:HD11	2.21	0.69
1:C:20:TYR:CD2	1:C:21:LEU:HD12	2.28	0.69
1:B:16:HIS:H	1:B:19:ASN:ND2	1.91	0.69
1:D:16:HIS:H	1:D:19:ASN:HD22	1.37	0.69
1:B:320:LYS:HE3	4:B:1399:HOH:O	1.93	0.68
1:C:44:HIS:O	1:C:47:THR:HB	1.94	0.68
1:D:243:GLN:HB3	1:D:246:VAL:CG1	2.23	0.68
1:C:99:ASN:HD21	1:C:102:GLU:HG3	1.57	0.68
1:C:225:ILE:HD13	1:C:290:THR:HA	1.75	0.68
1:D:199:LYS:HG2	4:D:1457:HOH:O	1.92	0.68
1:C:71:LEU:HD23	1:C:78:LEU:HD22	1.75	0.68
1:C:195:PHE:O	1:C:229:THR:HG21	1.94	0.67
1:C:237:ARG:NH1	1:C:243:GLN:HE22	1.92	0.67
1:A:293:THR:O	1:A:297:LEU:HD13	1.94	0.67
1:D:265:LEU:H	1:D:265:LEU:HD23	1.59	0.67
1:D:72:ASP:HB3	1:D:75:LYS:HG2	1.76	0.67
1:A:4:ARG:O	1:A:148:ILE:HD13	1.94	0.67
1:D:99:ASN:ND2	1:D:102:GLU:H	1.93	0.66
1:A:16:HIS:H	1:A:19:ASN:ND2	1.92	0.66
1:A:85:LEU:HB3	1:B:85:LEU:HB3	1.77	0.66
1:C:16:HIS:HD2	1:C:18:GLY:H	1.40	0.66
1:A:161:LEU:HD13	1:A:165:LEU:HD23	1.76	0.66
1:A:56:LYS:C	1:A:56:LYS:HD2	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:TYR:CZ	1:B:280:LYS:HE3	2.30	0.65
1:C:28:ILE:HD12	1:C:70:GLY:HA3	1.79	0.65
1:A:29:GLU:O	1:A:33:GLN:HG2	1.95	0.65
1:B:207:ASN:HD22	1:B:208:GLN:N	1.94	0.65
1:A:69:VAL:HG22	1:A:300:ILE:HD12	1.77	0.65
1:B:324:GLN:O	1:B:328:ARG:HG3	1.97	0.65
1:C:218:LYS:HD3	1:C:294:VAL:HG11	1.79	0.65
1:A:16:HIS:HD2	1:A:18:GLY:H	1.43	0.64
1:A:248:ASN:O	1:A:252:ILE:HG12	1.97	0.64
1:B:298:VAL:O	1:B:302:ARG:HB2	1.98	0.64
1:D:124:LEU:HD12	1:D:124:LEU:N	2.12	0.64
1:C:159:LEU:O	1:C:163:ARG:HG2	1.97	0.64
1:D:27:LEU:O	1:D:31:GLN:HG2	1.98	0.64
1:C:286:LYS:O	1:C:290:THR:HG23	1.98	0.64
1:B:326:THR:HG22	4:B:1467:HOH:O	1.98	0.64
1:A:217:PRO:HG2	1:A:220:VAL:HG23	1.78	0.64
1:D:16:HIS:HD2	1:D:18:GLY:H	1.45	0.63
1:B:207:ASN:HD22	1:B:207:ASN:C	2.00	0.63
1:C:69:VAL:HG22	1:C:300:ILE:HD12	1.81	0.63
1:A:296:LEU:O	1:A:300:ILE:HG12	1.98	0.63
1:D:90:MET:HG2	4:D:1413:HOH:O	1.99	0.63
1:A:194:LEU:HD11	1:A:212:ILE:HD11	1.80	0.63
1:B:24:MET:O	1:B:27:LEU:HB2	1.98	0.63
1:D:4:ARG:HE	1:D:35:GLN:NE2	1.97	0.62
1:A:342:SER:HB2	1:B:83:ASP:OD1	2.00	0.62
1:C:191:ILE:HG13	1:C:252:ILE:HD11	1.80	0.62
1:B:43:LEU:HD12	1:B:81:GLN:HG2	1.81	0.62
1:C:20:TYR:HD2	1:C:21:LEU:CD1	2.12	0.62
1:C:192:MET:H	1:C:248:ASN:ND2	1.97	0.62
1:D:191:ILE:HD12	1:D:252:ILE:HD13	1.79	0.62
1:D:329:THR:O	1:D:333:LEU:HD22	1.99	0.62
1:A:236:ILE:HD12	1:A:277:PHE:HB3	1.81	0.62
1:C:88:SER:HB3	1:D:89:MET:HE1	1.82	0.61
1:C:290:THR:HG21	4:C:1417:HOH:O	1.99	0.61
1:C:24:MET:HA	1:C:27:LEU:HD23	1.82	0.61
1:B:308:SER:OG	1:B:310:GLU:HG3	2.01	0.61
1:D:148:ILE:HD13	1:D:148:ILE:H	1.65	0.61
1:C:85:LEU:HB3	1:D:85:LEU:HB3	1.82	0.61
1:C:124:LEU:HD22	1:C:126:ILE:HD11	1.82	0.61
1:D:145:GLN:HE22	1:D:178:ARG:H	1.46	0.61
1:A:99:ASN:HD21	1:A:102:GLU:H	1.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:TYR:HA	1:C:24:MET:HB2	1.81	0.61
1:D:133:TYR:CD1	1:D:134:PRO:HD3	2.36	0.61
1:C:43:LEU:HB2	1:C:81:GLN:OE1	2.01	0.61
1:B:165:LEU:O	1:B:169:ILE:HG12	2.01	0.60
1:B:156:LYS:HB2	1:B:156:LYS:NZ	2.17	0.60
1:B:20:TYR:HA	1:B:24:MET:HB2	1.83	0.60
1:A:17:LEU:HD22	1:A:21:LEU:CD2	2.32	0.60
1:A:103:LEU:HD22	1:A:134:PRO:HG2	1.83	0.60
1:D:191:ILE:HD12	1:D:252:ILE:CD1	2.31	0.60
1:B:207:ASN:ND2	1:B:209:ASN:H	2.00	0.60
1:B:343:GLN:HG2	4:B:1419:HOH:O	2.02	0.59
1:D:99:ASN:ND2	1:D:102:GLU:HG2	2.17	0.59
1:A:346:LYS:NZ	1:A:346:LYS:CB	2.65	0.59
1:C:191:ILE:HG13	1:C:252:ILE:CD1	2.33	0.59
1:A:94:MET:CE	1:A:165:LEU:HB3	2.32	0.59
1:D:156:LYS:NZ	1:D:156:LYS:HB2	2.17	0.59
1:D:253:LEU:HD22	1:D:257:LEU:HD11	1.83	0.59
1:C:11:ALA:O	1:C:12:SER:HB3	2.01	0.59
1:D:56:LYS:HE3	1:D:309:ARG:HH12	1.67	0.59
1:C:248:ASN:O	1:C:252:ILE:HG12	2.03	0.59
1:D:185:ASN:O	1:D:189:ASN:HB3	2.02	0.59
1:B:253:LEU:O	1:B:257:LEU:HG	2.03	0.58
1:B:235:LYS:HE3	1:B:235:LYS:HA	1.85	0.58
1:B:6:LEU:CD2	1:B:141:ILE:HA	2.33	0.58
1:B:97:GLN:HG3	1:B:169:ILE:CD1	2.33	0.58
1:A:159:LEU:O	1:A:163:ARG:HG2	2.03	0.58
1:A:303:LYS:HA	1:A:306:GLN:HE21	1.67	0.58
1:D:300:ILE:HD11	4:D:1382:HOH:O	2.03	0.58
1:D:124:LEU:H	1:D:124:LEU:CD1	2.14	0.58
1:A:14:LYS:HG3	1:A:213:TYR:CE1	2.39	0.57
1:A:268:GLN:HG3	4:A:1457:HOH:O	2.02	0.57
1:D:116:GLN:HE22	1:D:130:LEU:CD2	2.17	0.57
1:B:14:LYS:HG3	1:B:213:TYR:CE1	2.40	0.57
1:C:6:LEU:HD13	1:C:144:TYR:CD1	2.39	0.57
1:A:156:LYS:HB2	1:A:156:LYS:NZ	2.19	0.57
1:C:217:PRO:HG2	1:C:220:VAL:HG23	1.85	0.57
1:A:64:ARG:CZ	1:A:304:ARG:HH11	2.17	0.57
1:C:27:LEU:HD12	1:C:36:LEU:HD21	1.86	0.57
1:A:6:LEU:HD22	1:A:141:ILE:HA	1.86	0.57
1:A:43:LEU:HB2	1:A:81:GLN:OE1	2.05	0.57
1:D:20:TYR:HD2	1:D:21:LEU:HD13	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:VAL:CG1	1:A:312:VAL:HG13	2.35	0.56
1:C:4:ARG:HG3	1:C:35:GLN:OE1	2.04	0.56
1:B:261:VAL:O	1:B:262:ASN:CB	2.54	0.56
1:D:237:ARG:NH1	1:D:243:GLN:NE2	2.49	0.56
1:B:40:VAL:HB	1:B:80:LEU:HD12	1.87	0.56
1:C:247:THR:O	1:C:251:THR:HG23	2.06	0.56
1:D:16:HIS:HD2	1:D:18:GLY:N	2.04	0.56
1:D:235:LYS:HG2	1:D:237:ARG:NH1	2.20	0.56
1:A:8:GLY:C	1:A:9:ILE:HD12	2.26	0.56
1:A:199:LYS:HG2	4:A:1446:HOH:O	2.04	0.55
1:D:217:PRO:HG2	1:D:220:VAL:HG23	1.89	0.55
1:A:217:PRO:HG2	1:A:220:VAL:CG2	2.36	0.55
1:D:4:ARG:O	1:D:148:ILE:HD13	2.07	0.55
1:B:217:PRO:HG2	1:B:220:VAL:HG23	1.89	0.55
1:C:9:ILE:N	1:C:9:ILE:HD12	2.21	0.55
1:B:48:VAL:HG13	1:B:130:LEU:HD11	1.89	0.55
1:A:69:VAL:HG12	1:A:69:VAL:O	2.06	0.54
1:D:19:ASN:HD21	1:D:203:LYS:HE3	1.72	0.54
1:C:156:LYS:O	1:C:160:GLU:HG3	2.08	0.54
1:C:338:PHE:HB3	1:C:340:LEU:CD2	2.37	0.54
1:A:345:ILE:O	1:A:346:LYS:NZ	2.40	0.54
1:D:218:LYS:HE3	1:D:294:VAL:HG21	1.90	0.54
1:C:25:GLN:NE2	4:C:1493:HOH:O	2.40	0.54
1:A:28:ILE:HD13	1:A:28:ILE:N	2.23	0.54
1:C:141:ILE:HD11	3:C:1352:WSA:HH2	1.90	0.54
1:D:94:MET:HG3	1:D:165:LEU:HD23	1.90	0.54
1:B:99:ASN:ND2	1:B:102:GLU:H	2.06	0.54
1:A:236:ILE:CD1	1:A:277:PHE:HB3	2.39	0.53
1:D:192:MET:HA	1:D:200:LYS:HA	1.90	0.53
1:D:298:VAL:O	1:D:302:ARG:HB2	2.07	0.53
1:D:28:ILE:HD12	1:D:28:ILE:N	2.21	0.53
1:A:16:HIS:HD2	1:A:18:GLY:N	2.07	0.53
1:A:225:ILE:N	1:A:225:ILE:HD12	2.24	0.53
1:C:99:ASN:ND2	1:C:102:GLU:H	2.07	0.53
1:C:63:VAL:HG11	1:C:312:VAL:HG13	1.90	0.53
1:C:84:LEU:HD21	1:C:324:GLN:HB2	1.90	0.53
1:C:173:PHE:HB2	1:C:175:LEU:HD23	1.90	0.53
1:C:192:MET:H	1:C:248:ASN:HD21	1.55	0.53
1:D:15:GLN:HE21	1:D:62:LEU:HD13	1.73	0.53
1:D:113:LYS:HG3	1:D:114:ALA:N	2.23	0.53
1:D:116:GLN:HE22	1:D:130:LEU:HD23	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:GLY:O	1:B:105:ARG:HD3	2.09	0.53
1:C:60:PHE:HB2	1:D:345:ILE:HD12	1.90	0.53
1:C:225:ILE:CD1	1:C:290:THR:HA	2.38	0.53
1:D:248:ASN:O	1:D:252:ILE:HG12	2.09	0.53
1:A:20:TYR:HA	1:A:24:MET:HB2	1.91	0.53
1:D:176:LYS:O	1:D:176:LYS:HG2	2.09	0.53
1:A:303:LYS:HA	1:A:306:GLN:NE2	2.23	0.52
1:B:206:LYS:HG2	1:B:207:ASN:H	1.74	0.52
1:C:43:LEU:HD12	1:C:81:GLN:HG2	1.91	0.52
1:B:28:ILE:HD11	1:B:69:VAL:O	2.10	0.52
1:B:340:LEU:O	1:B:344:ASN:ND2	2.42	0.52
1:C:236:ILE:HD12	1:C:277:PHE:HB3	1.91	0.52
1:C:280:LYS:HG3	1:C:284:ASP:OD1	2.09	0.52
1:D:197:PRO:HB2	1:D:244:PRO:HB2	1.90	0.52
1:C:207:ASN:C	1:C:207:ASN:HD22	2.11	0.52
1:B:97:GLN:HG3	1:B:169:ILE:HD11	1.90	0.52
1:A:299:ASN:O	1:A:302:ARG:HB3	2.08	0.52
1:A:345:ILE:O	1:A:346:LYS:CB	2.42	0.52
1:B:6:LEU:HG	1:B:7:THR:N	2.24	0.52
1:B:296:LEU:O	1:B:300:ILE:HG12	2.10	0.51
1:C:14:LYS:HD2	1:C:14:LYS:N	2.25	0.51
1:A:253:LEU:HD23	1:A:289:LEU:HA	1.93	0.51
1:D:139:GLY:HA3	4:D:1411:HOH:O	2.10	0.51
1:D:338:PHE:HB3	1:D:340:LEU:HD22	1.93	0.51
1:C:328:ARG:NH2	4:C:1472:HOH:O	2.38	0.51
1:D:111:ALA:O	1:D:115:GLU:HB2	2.10	0.51
1:D:313:PHE:O	1:D:317:GLN:HG2	2.11	0.51
1:C:102:GLU:HG2	4:C:1434:HOH:O	2.10	0.51
1:D:173:PHE:HB2	1:D:175:LEU:HD22	1.93	0.51
1:D:176:LYS:HD2	1:D:176:LYS:N	2.17	0.51
1:D:30:LEU:C	1:D:32:GLU:H	2.14	0.51
1:D:103:LEU:HB3	1:D:131:LEU:HD22	1.93	0.51
1:B:283:LEU:HD22	1:B:283:LEU:N	2.18	0.50
1:C:272:ASP:OD2	1:C:275:ALA:HB2	2.10	0.50
1:A:157:GLN:HA	1:A:160:GLU:OE1	2.12	0.50
1:C:60:PHE:HE2	1:C:309:ARG:HA	1.77	0.50
1:C:247:THR:O	1:C:251:THR:CG2	2.59	0.50
1:D:198:THR:HA	4:D:1484:HOH:O	2.10	0.50
1:A:207:ASN:HB3	4:A:1390:HOH:O	2.11	0.50
1:B:156:LYS:HB2	1:B:156:LYS:HZ3	1.76	0.50
1:C:236:ILE:CD1	1:C:277:PHE:HB3	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:268:GLN:HG2	1:D:269:LEU:HD12	1.93	0.50
1:A:269:LEU:HA	1:A:276:TYR:CD1	2.46	0.50
1:D:148:ILE:HD13	1:D:148:ILE:N	2.27	0.50
1:D:212:ILE:HD11	1:D:225:ILE:HD11	1.93	0.50
1:C:141:ILE:CD1	3:C:1352:WSA:HH2	2.41	0.50
1:D:253:LEU:HD22	1:D:257:LEU:CD1	2.42	0.50
1:D:150:PRO:HA	1:D:183:VAL:O	2.12	0.50
1:D:237:ARG:NH1	1:D:243:GLN:HE22	2.01	0.50
1:B:235:LYS:HG2	1:B:237:ARG:NH2	2.26	0.49
1:A:195:PHE:CG	1:A:207:ASN:ND2	2.80	0.49
1:D:105:ARG:HD3	4:D:1435:HOH:O	2.12	0.49
1:D:173:PHE:HB2	1:D:175:LEU:CD2	2.43	0.49
1:C:195:PHE:O	1:C:229:THR:CG2	2.60	0.49
1:A:99:ASN:ND2	1:A:102:GLU:HB2	2.27	0.49
1:B:12:SER:C	1:B:14:LYS:H	2.15	0.49
1:D:343:GLN:CD	1:D:343:GLN:H	2.14	0.49
1:B:127:PRO:HG2	1:B:130:LEU:HD22	1.95	0.49
1:B:171:LYS:HE2	4:B:1442:HOH:O	2.11	0.49
1:B:290:THR:O	1:B:294:VAL:HG23	2.12	0.49
1:C:208:GLN:HG2	1:C:213:TYR:OH	2.12	0.49
1:A:18:GLY:HA2	1:A:191:ILE:HD13	1.95	0.49
1:A:39:PHE:HA	1:A:79:PHE:O	2.13	0.49
1:A:103:LEU:CD2	1:A:134:PRO:HG2	2.41	0.49
1:D:112:LYS:HA	1:D:115:GLU:HB3	1.95	0.49
1:D:194:LEU:HD11	1:D:212:ILE:CD1	2.35	0.49
1:B:257:LEU:HB3	1:B:266:THR:HB	1.93	0.48
1:C:299:ASN:HD21	1:C:303:LYS:HZ2	1.60	0.48
1:D:121:ASN:OD1	1:D:123:THR:HG22	2.12	0.48
1:A:69:VAL:O	1:A:69:VAL:CG1	2.61	0.48
1:A:191:ILE:H	1:A:191:ILE:HD12	1.78	0.48
1:D:84:LEU:HB2	1:D:87:HIS:HD2	1.76	0.48
1:B:108:GLN:O	1:B:112:LYS:HB2	2.12	0.48
1:B:116:GLN:HE22	1:B:130:LEU:HD21	1.77	0.48
1:B:283:LEU:HD21	4:B:1457:HOH:O	2.13	0.48
1:C:153:ASN:HD22	1:C:184:GLN:HE22	1.61	0.48
1:C:236:ILE:HG23	1:C:250:LEU:HD21	1.94	0.48
1:D:94:MET:CE	1:D:169:ILE:CD1	2.91	0.48
1:B:206:LYS:HZ3	1:B:206:LYS:H	1.62	0.48
1:C:42:ASP:OD1	1:D:340:LEU:HD12	2.13	0.48
1:D:139:GLY:CA	4:D:1411:HOH:O	2.61	0.48
1:B:40:VAL:HG22	1:B:62:LEU:HD23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:6:LEU:HD22	1:C:141:ILE:HA	1.94	0.48
1:B:94:MET:HE2	1:B:165:LEU:HB3	1.95	0.48
1:A:94:MET:HE3	1:A:165:LEU:HB3	1.96	0.47
1:B:145:GLN:HE22	1:B:178:ARG:H	1.60	0.47
1:D:8:GLY:H	3:D:1353:WSA:CE3	2.27	0.47
1:A:326:THR:HG22	4:A:1414:HOH:O	2.13	0.47
1:B:68:ALA:HB2	1:B:304:ARG:HA	1.96	0.47
1:C:305:GLU:C	1:C:307:ILE:H	2.18	0.47
1:A:28:ILE:HD13	1:A:28:ILE:H	1.78	0.47
1:A:241:LYS:HA	1:A:241:LYS:CE	2.32	0.47
1:C:43:LEU:HB2	1:C:81:GLN:CD	2.34	0.47
1:D:17:LEU:HD22	1:D:21:LEU:HD22	1.96	0.47
1:B:259:GLU:HG2	1:B:296:LEU:HD23	1.96	0.47
1:C:225:ILE:HD13	1:C:290:THR:CA	2.41	0.47
1:A:126:ILE:N	1:A:126:ILE:HD12	2.29	0.47
1:A:276:TYR:CZ	1:A:280:LYS:HE3	2.49	0.47
1:C:84:LEU:HB2	1:C:87:HIS:HD2	1.79	0.47
1:C:131:LEU:HD22	1:C:131:LEU:O	2.14	0.47
1:D:115:GLU:O	1:D:115:GLU:HG2	2.15	0.47
1:D:217:PRO:HG2	1:D:220:VAL:CG2	2.45	0.47
1:B:101:GLY:O	1:B:105:ARG:CD	2.63	0.47
1:A:148:ILE:HD13	1:A:148:ILE:H	1.80	0.47
1:B:94:MET:HE3	1:B:169:ILE:HG13	1.97	0.47
1:C:124:LEU:N	1:C:124:LEU:HD12	2.29	0.47
1:D:38:VAL:O	1:D:78:LEU:HA	2.14	0.46
1:D:63:VAL:HG11	1:D:312:VAL:HG13	1.97	0.46
3:D:1353:WSA:O2S	3:D:1353:WSA:O	2.33	0.46
1:A:225:ILE:N	1:A:225:ILE:CD1	2.78	0.46
1:A:294:VAL:O	1:A:298:VAL:HG23	2.15	0.46
1:B:43:LEU:CD1	1:B:81:GLN:HG2	2.44	0.46
1:B:228:ALA:HB3	1:B:286:LYS:HE2	1.97	0.46
1:C:29:GLU:HB2	4:C:1427:HOH:O	2.16	0.46
1:A:17:LEU:HD22	1:A:21:LEU:HD21	1.96	0.46
1:A:276:TYR:CE2	1:A:280:LYS:HE3	2.50	0.46
1:D:120:PRO:HD2	4:D:1396:HOH:O	2.15	0.46
1:C:16:HIS:HD2	1:C:18:GLY:N	2.09	0.46
1:A:38:VAL:O	1:A:78:LEU:HA	2.15	0.46
1:D:194:LEU:HD13	1:D:225:ILE:HD13	1.96	0.46
1:B:342:SER:C	1:B:344:ASN:H	2.17	0.46
1:C:148:ILE:HB	1:C:183:VAL:HG21	1.96	0.46
1:C:263:GLN:O	1:C:266:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LYS:HD2	1:A:173:PHE:CZ	2.51	0.46
1:C:156:LYS:HB2	1:C:156:LYS:NZ	2.30	0.46
1:C:169:ILE:N	1:C:169:ILE:HD12	2.31	0.46
1:A:174:LYS:HA	1:A:174:LYS:HE2	1.97	0.46
1:B:141:ILE:HD12	1:B:162:THR:HG21	1.96	0.46
1:B:203:LYS:HG3	2:B:1360:SO4:S	2.56	0.46
1:A:159:LEU:O	1:A:163:ARG:CG	2.64	0.46
1:B:207:ASN:C	1:B:207:ASN:ND2	2.69	0.46
1:C:94:MET:CE	1:C:165:LEU:HB3	2.46	0.46
1:A:77:CYS:HB2	1:A:322:GLN:OE1	2.16	0.45
1:B:6:LEU:HD22	1:B:141:ILE:HA	1.98	0.45
1:B:155:GLN:NE2	2:B:1361:SO4:O2	2.49	0.45
1:A:112:LYS:O	1:A:112:LYS:HG2	2.16	0.45
1:B:148:ILE:HD13	1:B:148:ILE:H	1.81	0.45
1:D:5:ALA:HB2	1:D:148:ILE:HD11	1.98	0.45
1:B:338:PHE:HB3	1:B:340:LEU:HD22	1.98	0.45
1:D:83:ASP:C	1:D:84:LEU:HD23	2.37	0.45
1:A:56:LYS:C	1:A:56:LYS:CD	2.85	0.45
1:A:99:ASN:HD21	1:A:102:GLU:HB2	1.80	0.45
1:A:108:GLN:HG2	2:A:1363:SO4:O1	2.16	0.45
1:B:12:SER:C	1:B:14:LYS:N	2.70	0.45
1:B:105:ARG:HA	1:B:110:LYS:NZ	2.32	0.45
1:B:192:MET:H	1:B:248:ASN:ND2	2.14	0.45
1:A:297:LEU:O	1:A:301:GLN:NE2	2.50	0.45
1:D:265:LEU:O	1:D:269:LEU:HD13	2.17	0.45
1:B:48:VAL:CG1	1:B:130:LEU:HD11	2.47	0.45
1:D:218:LYS:HD3	1:D:218:LYS:C	2.37	0.45
1:A:195:PHE:O	1:A:229:THR:HG21	2.17	0.45
1:B:44:HIS:CD2	3:B:1351:WSA:HD1	2.52	0.45
1:B:297:LEU:HB3	1:B:301:GLN:NE2	2.32	0.45
1:C:201:MET:HA	4:C:1423:HOH:O	2.16	0.45
1:D:241:LYS:HD3	1:D:241:LYS:O	2.17	0.45
1:A:7:THR:HG22	4:A:1393:HOH:O	2.17	0.45
1:A:102:GLU:OE2	1:A:168:ARG:NH2	2.47	0.45
1:C:23:VAL:O	1:C:27:LEU:HD22	2.16	0.45
1:C:191:ILE:N	1:C:191:ILE:HD12	2.32	0.45
1:D:175:LEU:HB3	1:D:177:LEU:HD13	1.97	0.45
1:D:91:GLY:HA2	4:D:1411:HOH:O	2.16	0.45
1:B:304:ARG:HG2	1:B:304:ARG:NH2	2.32	0.44
1:B:259:GLU:O	1:B:261:VAL:O	2.35	0.44
1:C:253:LEU:O	1:C:257:LEU:HG	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ASP:OD1	1:D:74:GLN:HB2	2.17	0.44
1:B:39:PHE:HB3	1:B:79:PHE:CE2	2.53	0.44
1:C:235:LYS:HD2	1:C:237:ARG:HH12	1.83	0.44
1:C:296:LEU:O	1:C:300:ILE:HG12	2.18	0.44
1:A:247:THR:O	1:A:251:THR:CG2	2.66	0.44
1:B:192:MET:H	1:B:248:ASN:HD21	1.64	0.44
1:B:235:LYS:HA	1:B:235:LYS:CE	2.48	0.44
1:B:304:ARG:HG2	1:B:304:ARG:HH21	1.83	0.44
1:D:99:ASN:HD21	1:D:102:GLU:H	1.64	0.44
1:A:16:HIS:HE1	2:A:1362:SO4:O2	2.00	0.44
1:A:217:PRO:O	1:A:221:VAL:HG12	2.18	0.44
1:B:117:THR:HG22	1:B:118:ARG:N	2.33	0.44
1:B:191:ILE:HD12	1:B:191:ILE:N	2.32	0.44
1:B:296:LEU:HD13	1:B:300:ILE:HG12	1.99	0.44
1:A:77:CYS:HB2	1:A:322:GLN:CD	2.38	0.44
1:B:137:MET:HG3	3:B:1351:WSA:CE2	2.48	0.43
1:B:175:LEU:HD21	1:B:334:PHE:HA	2.00	0.43
1:B:10:GLN:HE21	1:B:45:SER:HA	1.82	0.43
1:C:235:LYS:CD	1:C:237:ARG:HH12	2.31	0.43
1:C:299:ASN:HD21	1:C:303:LYS:NZ	2.15	0.43
1:D:28:ILE:H	1:D:28:ILE:CD1	2.25	0.43
1:A:253:LEU:HD12	1:A:273:LEU:CD1	2.48	0.43
1:A:300:ILE:O	1:A:304:ARG:HG3	2.18	0.43
1:C:6:LEU:HG	1:C:7:THR:N	2.33	0.43
1:C:221:VAL:HG23	1:C:225:ILE:HD11	1.98	0.43
1:C:225:ILE:CG2	1:C:290:THR:HG22	2.42	0.43
1:A:169:ILE:HG23	1:A:173:PHE:CD1	2.53	0.43
1:A:191:ILE:HD12	1:A:191:ILE:N	2.33	0.43
1:A:247:THR:O	1:A:251:THR:HG22	2.19	0.43
1:D:124:LEU:HD11	4:D:1372:HOH:O	2.18	0.43
1:B:20:TYR:HD2	1:B:21:LEU:HD13	1.83	0.43
1:B:217:PRO:HG2	1:B:220:VAL:CG2	2.49	0.43
1:C:4:ARG:NH2	1:C:35:GLN:OE1	2.52	0.43
1:D:133:TYR:N	1:D:134:PRO:CD	2.82	0.43
1:A:343:GLN:HA	1:A:346:LYS:HZ1	1.83	0.43
1:B:156:LYS:O	1:B:160:GLU:HG3	2.17	0.43
1:C:237:ARG:HH11	1:C:243:GLN:HE22	1.63	0.43
1:A:261:VAL:HG22	1:A:295:ASN:HB3	2.00	0.43
1:B:206:LYS:CG	1:B:207:ASN:N	2.82	0.43
1:C:108:GLN:NE2	4:C:1435:HOH:O	2.51	0.43
1:C:286:LYS:O	1:C:290:THR:CG2	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:THR:HG22	1:D:118:ARG:N	2.34	0.43
1:D:259:GLU:HG2	1:D:296:LEU:HD13	2.01	0.43
1:A:197:PRO:HB2	1:A:244:PRO:HB2	2.01	0.43
1:C:217:PRO:HG2	1:C:220:VAL:CG2	2.48	0.43
1:A:7:THR:HG21	1:A:150:PRO:O	2.19	0.42
1:A:253:LEU:C	1:A:253:LEU:HD13	2.40	0.42
1:A:174:LYS:NZ	4:A:1440:HOH:O	2.48	0.42
1:A:280:LYS:HB3	1:A:284:ASP:OD1	2.19	0.42
1:B:21:LEU:HB3	1:B:191:ILE:HD11	2.00	0.42
1:B:329:THR:O	1:B:333:LEU:HD22	2.19	0.42
1:C:191:ILE:HG23	1:C:252:ILE:HD11	2.00	0.42
1:A:108:GLN:O	1:A:112:LYS:HB2	2.19	0.42
1:A:163:ARG:O	1:A:167:GLN:HG3	2.19	0.42
1:A:192:MET:HA	1:A:200:LYS:HA	2.02	0.42
1:B:10:GLN:HB2	3:B:1351:WSA:O1S	2.18	0.42
1:B:134:PRO:HG3	4:B:1375:HOH:O	2.20	0.42
1:B:234:ASN:O	1:B:235:LYS:HE3	2.20	0.42
1:C:39:PHE:HA	1:C:79:PHE:O	2.18	0.42
1:C:176:LYS:HE2	4:C:1441:HOH:O	2.18	0.42
1:C:236:ILE:CG2	1:C:250:LEU:HD21	2.50	0.42
1:D:24:MET:O	1:D:27:LEU:HB2	2.18	0.42
1:D:94:MET:CE	1:D:94:MET:HA	2.50	0.42
1:C:40:VAL:HB	1:C:80:LEU:HD12	2.00	0.42
1:D:90:MET:CG	4:D:1413:HOH:O	2.63	0.42
1:A:9:ILE:HD12	1:A:9:ILE:N	2.35	0.42
1:B:137:MET:HG3	3:B:1351:WSA:N11	2.35	0.42
1:B:159:LEU:HD13	1:B:159:LEU:HA	1.89	0.42
1:D:147:ASP:OD2	1:D:178:ARG:NH2	2.53	0.42
1:B:320:LYS:O	1:B:324:GLN:HB2	2.19	0.42
1:C:137:MET:HG3	3:C:1352:WSA:CE2	2.50	0.42
1:A:172:LYS:HD2	1:A:173:PHE:CE1	2.55	0.42
1:C:72:ASP:HA	1:C:73:PRO:HD2	1.94	0.42
1:B:231:ASP:HB2	4:B:1455:HOH:O	2.20	0.42
1:B:275:ALA:O	1:B:278:SER:HB2	2.20	0.42
1:D:208:GLN:HG2	1:D:213:TYR:OH	2.20	0.42
1:A:218:LYS:O	1:A:221:VAL:HG13	2.20	0.41
1:A:253:LEU:HD11	1:A:257:LEU:HD11	2.02	0.41
1:A:322:GLN:NE2	4:A:1413:HOH:O	2.52	0.41
1:B:283:LEU:CD2	4:B:1457:HOH:O	2.66	0.41
1:C:16:HIS:H	1:C:19:ASN:ND2	2.14	0.41
1:D:156:LYS:HB2	1:D:156:LYS:HZ3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:178:ARG:NE	4:D:1376:HOH:O	2.54	0.41
1:A:271:ASN:N	1:A:271:ASN:HD22	2.18	0.41
1:C:28:ILE:N	1:C:28:ILE:HD13	2.35	0.41
1:D:36:LEU:HG	1:D:38:VAL:HG23	2.02	0.41
1:A:89:MET:CE	1:B:88:SER:HB3	2.51	0.41
1:A:257:LEU:HD11	1:A:269:LEU:HD12	2.03	0.41
1:B:94:MET:HG3	1:B:165:LEU:HD13	2.03	0.41
1:B:238:PHE:CZ	1:B:250:LEU:HG	2.55	0.41
1:B:241:LYS:HB2	4:B:1362:HOH:O	2.20	0.41
1:B:271:ASN:O	1:B:271:ASN:ND2	2.54	0.41
1:C:56:LYS:HD2	1:D:344:ASN:O	2.20	0.41
1:B:296:LEU:HD13	1:B:296:LEU:C	2.41	0.41
1:B:342:SER:O	1:B:345:ILE:HD12	2.21	0.41
1:C:8:GLY:C	1:C:9:ILE:HD12	2.41	0.41
1:C:225:ILE:HD12	1:C:290:THR:HB	2.03	0.41
1:B:6:LEU:HD13	1:B:144:TYR:CD2	2.55	0.41
1:C:28:ILE:CD1	1:C:70:GLY:HA3	2.49	0.41
1:D:142:LEU:C	4:D:1413:HOH:O	2.58	0.41
1:B:199:LYS:HG2	4:B:1448:HOH:O	2.20	0.41
1:B:283:LEU:H	1:B:283:LEU:CD2	2.18	0.41
1:C:185:ASN:O	1:C:189:ASN:HB3	2.20	0.41
1:A:175:LEU:HB3	1:A:177:LEU:HD13	2.01	0.41
1:C:45:SER:C	1:C:47:THR:H	2.23	0.41
1:C:223:LYS:O	1:C:227:GLN:HG3	2.21	0.41
1:C:290:THR:O	1:C:294:VAL:HG23	2.21	0.41
1:A:193:ASP:OD1	1:A:210:GLY:HA3	2.21	0.41
1:D:130:LEU:HA	1:D:130:LEU:HD12	1.78	0.41
1:D:6:LEU:HD13	1:D:6:LEU:C	2.41	0.41
1:A:175:LEU:HD12	1:A:175:LEU:HA	1.90	0.40
1:B:280:LYS:HD3	4:B:1478:HOH:O	2.21	0.40
1:D:72:ASP:HA	1:D:73:PRO:HD2	1.91	0.40
1:A:150:PRO:HA	1:A:183:VAL:O	2.21	0.40
1:A:156:LYS:HB2	1:A:156:LYS:HZ3	1.87	0.40
1:C:17:LEU:HD22	1:C:21:LEU:HD13	2.02	0.40
1:C:88:SER:HB3	1:D:89:MET:CE	2.49	0.40
1:A:185:ASN:O	1:A:189:ASN:HB3	2.21	0.40
1:C:3:LYS:O	1:C:34:CYS:HB3	2.20	0.40
1:C:161:LEU:O	1:C:161:LEU:HD22	2.21	0.40
1:C:249:MET:HE3	1:C:286:LYS:HG2	2.03	0.40
1:C:249:MET:CE	1:C:286:LYS:HG2	2.51	0.40
1:D:176:LYS:O	1:D:177:LEU:HD12	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:HIS:CD2	3:A:1350:WSA:HD1	2.56	0.40
1:A:346:LYS:HD3	1:B:313:PHE:CE2	2.56	0.40
1:D:1:MET:CE	1:D:178:ARG:HH12	2.34	0.40
1:D:184:GLN:NE2	1:D:189:ASN:HB2	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	330/348 (95%)	314 (95%)	16 (5%)	0	100	100
1	B	344/348 (99%)	324 (94%)	19 (6%)	1 (0%)	41	51
1	C	332/348 (95%)	317 (96%)	14 (4%)	1 (0%)	41	51
1	D	344/348 (99%)	322 (94%)	19 (6%)	3 (1%)	17	24
All	All	1350/1392 (97%)	1277 (95%)	68 (5%)	5 (0%)	34	46

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	MET
1	C	12	SER
1	D	117	THR
1	D	31	GLN
1	D	23	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	296/307 (96%)	268 (90%)	28 (10%)	8 10
1	B	306/307 (100%)	275 (90%)	31 (10%)	7 8
1	C	297/307 (97%)	269 (91%)	28 (9%)	8 10
1	D	306/307 (100%)	274 (90%)	32 (10%)	7 7
All	All	1205/1228 (98%)	1086 (90%)	119 (10%)	8 9

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	THR
1	A	14	LYS
1	A	28	ILE
1	A	55	LEU
1	A	56	LYS
1	A	57	GLN
1	A	66	LEU
1	A	67	LEU
1	A	81	GLN
1	A	85	LEU
1	A	99	ASN
1	A	130	LEU
1	A	131	LEU
1	A	136	LEU
1	A	142	LEU
1	A	148	ILE
1	A	175	LEU
1	A	221	VAL
1	A	229	THR
1	A	241	LYS
1	A	246	VAL
1	A	251	THR
1	A	259	GLU
1	A	271	ASN
1	A	326	THR
1	A	340	LEU
1	A	342	SER
1	A	346	LYS
1	B	1	MET
1	B	21	LEU

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Mol	Chain	Res	Type
1	B	27	LEU
1	B	55	LEU
1	B	85	LEU
1	B	94	MET
1	B	116	GLN
1	B	121	ASN
1	B	130	LEU
1	B	131	LEU
1	B	136	LEU
1	B	142	LEU
1	B	148	ILE
1	B	161	LEU
1	B	176	LYS
1	B	206	LYS
1	B	207	ASN
1	B	251	THR
1	B	253	LEU
1	B	265	LEU
1	B	268	GLN
1	B	271	ASN
1	B	283	LEU
1	B	297	LEU
1	B	310	GLU
1	B	317	GLN
1	B	326	THR
1	B	333	LEU
1	B	336	ASP
1	B	340	LEU
1	B	345	ILE
1	C	6	LEU
1	C	27	LEU
1	C	66	LEU
1	C	67	LEU
1	C	99	ASN
1	C	131	LEU
1	C	136	LEU
1	C	142	LEU
1	C	161	LEU
1	C	165	LEU
1	C	176	LYS
1	C	207	ASN
1	C	214	LEU

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Mol	Chain	Res	Type
1	C	221	VAL
1	C	229	THR
1	C	237	ARG
1	C	250	LEU
1	C	251	THR
1	C	253	LEU
1	C	265	LEU
1	C	283	LEU
1	C	290	THR
1	C	297	LEU
1	C	304	ARG
1	C	305	GLU
1	C	333	LEU
1	C	340	LEU
1	C	345	ILE
1	D	15	GLN
1	D	21	LEU
1	D	27	LEU
1	D	56	LYS
1	D	57	GLN
1	D	94	MET
1	D	99	ASN
1	D	124	LEU
1	D	131	LEU
1	D	134	PRO
1	D	136	LEU
1	D	142	LEU
1	D	148	ILE
1	D	161	LEU
1	D	175	LEU
1	D	176	LYS
1	D	200	LYS
1	D	207	ASN
1	D	215	ASP
1	D	237	ARG
1	D	253	LEU
1	D	268	GLN
1	D	271	ASN
1	D	285	LEU
1	D	311	GLN
1	D	316	LEU
1	D	326	THR

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Mol	Chain	Res	Type
1	D	331	LEU
1	D	333	LEU
1	D	336	ASP
1	D	340	LEU
1	D	343	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	16	HIS
1	A	19	ASN
1	A	57	GLN
1	A	74	GLN
1	A	99	ASN
1	A	104	GLN
1	A	145	GLN
1	A	181	GLN
1	A	184	GLN
1	A	207	ASN
1	A	209	ASN
1	A	227	GLN
1	A	271	ASN
1	A	306	GLN
1	A	311	GLN
1	A	314	ASN
1	A	322	GLN
1	A	343	GLN
1	A	344	ASN
1	B	10	GLN
1	B	15	GLN
1	B	19	ASN
1	B	35	GLN
1	B	58	ASN
1	B	99	ASN
1	B	104	GLN
1	B	116	GLN
1	B	145	GLN
1	B	184	GLN
1	B	207	ASN
1	B	208	GLN
1	B	209	ASN

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Mol	Chain	Res	Type
1	B	243	GLN
1	B	248	ASN
1	B	268	GLN
1	B	271	ASN
1	B	301	GLN
1	B	306	GLN
1	B	317	GLN
1	B	322	GLN
1	B	344	ASN
1	C	16	HIS
1	C	19	ASN
1	C	58	ASN
1	C	99	ASN
1	C	104	GLN
1	C	145	GLN
1	C	153	ASN
1	C	181	GLN
1	C	184	GLN
1	C	207	ASN
1	C	243	GLN
1	C	248	ASN
1	C	263	GLN
1	C	267	ASN
1	C	271	ASN
1	C	301	GLN
1	C	317	GLN
1	D	10	GLN
1	D	16	HIS
1	D	19	ASN
1	D	35	GLN
1	D	53	GLN
1	D	58	ASN
1	D	99	ASN
1	D	116	GLN
1	D	119	ASN
1	D	145	GLN
1	D	184	GLN
1	D	207	ASN
1	D	243	GLN
1	D	248	ASN
1	D	263	GLN
1	D	271	ASN

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Mol	Chain	Res	Type
1	D	287	ASN
1	D	299	ASN
1	D	314	ASN
1	D	322	GLN
1	D	344	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

12 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	SO4	A	1363	-	4,4,4	0.27	0	6,6,6	0.15	0
3	WSA	B	1351	-	37,41,41	2.73	6 (16%)	40,61,61	2.29	5 (12%)
2	SO4	C	1367	-	4,4,4	0.25	0	6,6,6	0.15	0
3	WSA	A	1350	-	37,41,41	2.76	6 (16%)	40,61,61	2.18	6 (15%)
2	SO4	A	1362	-	4,4,4	0.24	0	6,6,6	0.17	0
2	SO4	C	1366	-	4,4,4	0.22	0	6,6,6	0.13	0
2	SO4	D	1364	-	4,4,4	0.27	0	6,6,6	0.13	0
2	SO4	D	1365	-	4,4,4	0.23	0	6,6,6	0.07	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SO4	B	1361	-	4,4,4	0.19	0	6,6,6	0.12	0
2	SO4	B	1360	-	4,4,4	0.27	0	6,6,6	0.13	0
3	WSA	D	1353	-	37,41,41	2.73	6 (16%)	40,61,61	2.10	5 (12%)
3	WSA	C	1352	-	37,41,41	2.72	5 (13%)	40,61,61	2.15	6 (15%)

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	WSA	D	1353	-	-	2/17/39/39	0/5/5/5
3	WSA	A	1350	-	-	0/17/39/39	0/5/5/5
3	WSA	C	1352	-	-	2/17/39/39	0/5/5/5
3	WSA	B	1351	-	-	0/17/39/39	0/5/5/5

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1350	WSA	O2S-S	9.56	1.50	1.42
3	C	1352	WSA	O2S-S	9.55	1.50	1.42
3	A	1350	WSA	O1S-S	9.52	1.50	1.42
3	B	1351	WSA	O2S-S	9.48	1.50	1.42
3	D	1353	WSA	O1S-S	9.45	1.50	1.42
3	B	1351	WSA	O1S-S	9.44	1.50	1.42
3	D	1353	WSA	O2S-S	9.40	1.50	1.42
3	C	1352	WSA	O1S-S	9.22	1.50	1.42
3	C	1352	WSA	O5'-S	-7.79	1.43	1.59
3	D	1353	WSA	O5'-S	-7.73	1.43	1.59
3	A	1350	WSA	O5'-S	-7.71	1.43	1.59
3	B	1351	WSA	O5'-S	-7.68	1.43	1.59
3	A	1350	WSA	S-NS	2.29	1.63	1.59
3	B	1351	WSA	C-NS	-2.21	1.33	1.37
3	D	1353	WSA	O4'-C1'	2.21	1.44	1.41
3	A	1350	WSA	C-NS	-2.19	1.33	1.37
3	D	1353	WSA	C-NS	-2.16	1.33	1.37
3	A	1350	WSA	O4'-C1'	2.15	1.44	1.41
3	C	1352	WSA	O4'-C1'	2.14	1.44	1.41
3	B	1351	WSA	O4'-C1'	2.10	1.44	1.41
3	B	1351	WSA	S-NS	2.07	1.63	1.59
3	D	1353	WSA	S-NS	2.04	1.63	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1352	WSA	S-NS	2.03	1.63	1.59

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1351	WSA	C-NS-S	-8.87	110.26	124.61
3	A	1350	WSA	C-NS-S	-8.85	110.29	124.61
3	C	1352	WSA	C-NS-S	-8.01	111.65	124.61
3	B	1351	WSA	O2S-S-O1S	-7.86	108.51	120.76
3	D	1353	WSA	O2S-S-O1S	-7.69	108.78	120.76
3	C	1352	WSA	O2S-S-O1S	-7.44	109.17	120.76
3	A	1350	WSA	O2S-S-O1S	-7.33	109.33	120.76
3	D	1353	WSA	C-NS-S	-7.10	113.11	124.61
3	B	1351	WSA	N3-C2-N1	-4.50	121.64	128.68
3	D	1353	WSA	N3-C2-N1	-4.46	121.71	128.68
3	C	1352	WSA	N3-C2-N1	-4.35	121.88	128.68
3	A	1350	WSA	N3-C2-N1	-4.27	122.01	128.68
3	C	1352	WSA	O4'-C1'-C2'	-3.70	101.52	106.93
3	B	1351	WSA	O5'-C5'-C4'	3.64	114.41	107.62
3	D	1353	WSA	O4'-C1'-C2'	-3.45	101.89	106.93
3	A	1350	WSA	O4'-C1'-C2'	-3.21	102.23	106.93
3	B	1351	WSA	O4'-C1'-C2'	-3.17	102.30	106.93
3	D	1353	WSA	O5'-C5'-C4'	3.01	113.23	107.62
3	A	1350	WSA	C4-C5-N7	-2.30	107.01	109.40
3	A	1350	WSA	O5'-C5'-C4'	2.22	111.76	107.62
3	C	1352	WSA	O5'-C5'-C4'	2.20	111.72	107.62
3	C	1352	WSA	C4-C5-N7	-2.05	107.27	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1352	WSA	O-C-CA-CB
3	C	1352	WSA	NS-C-CA-CB
3	D	1353	WSA	C-NS-S-O1S
3	D	1353	WSA	C5'-O5'-S-NS

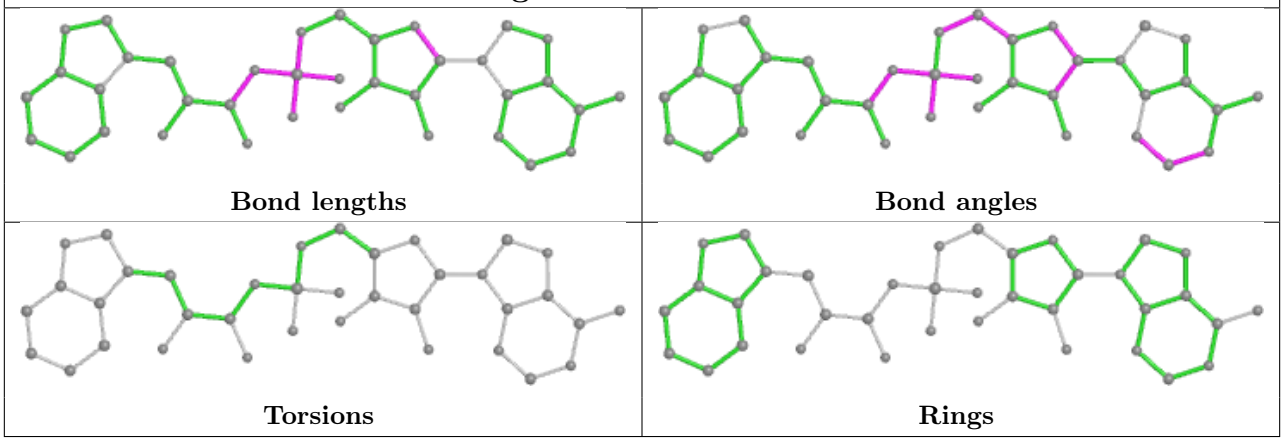
There are no ring outliers.

8 monomers are involved in 16 short contacts:

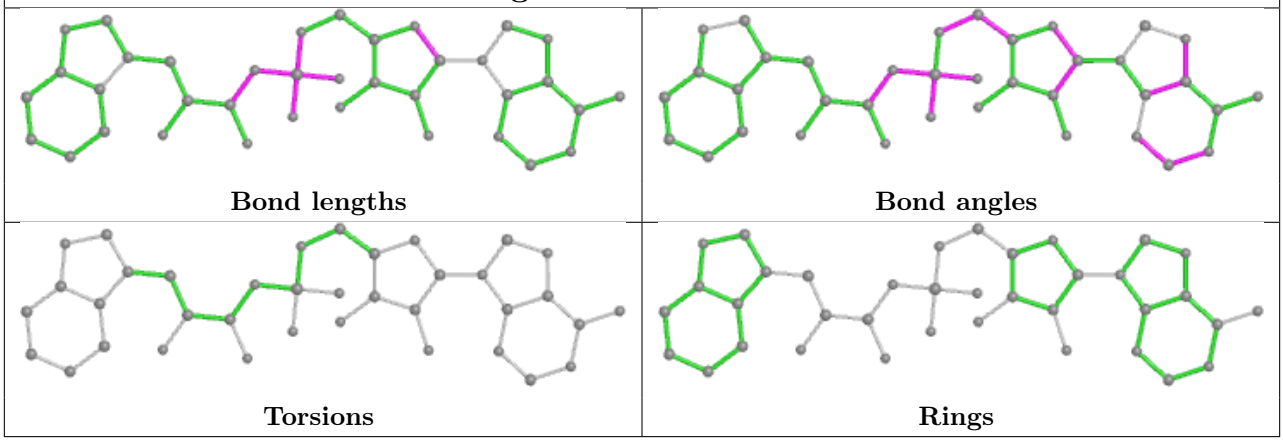
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1363	SO4	1	0
3	B	1351	WSA	5	0
3	A	1350	WSA	1	0
2	A	1362	SO4	1	0
2	B	1361	SO4	2	0
2	B	1360	SO4	1	0
3	D	1353	WSA	2	0
3	C	1352	WSA	3	0

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 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.

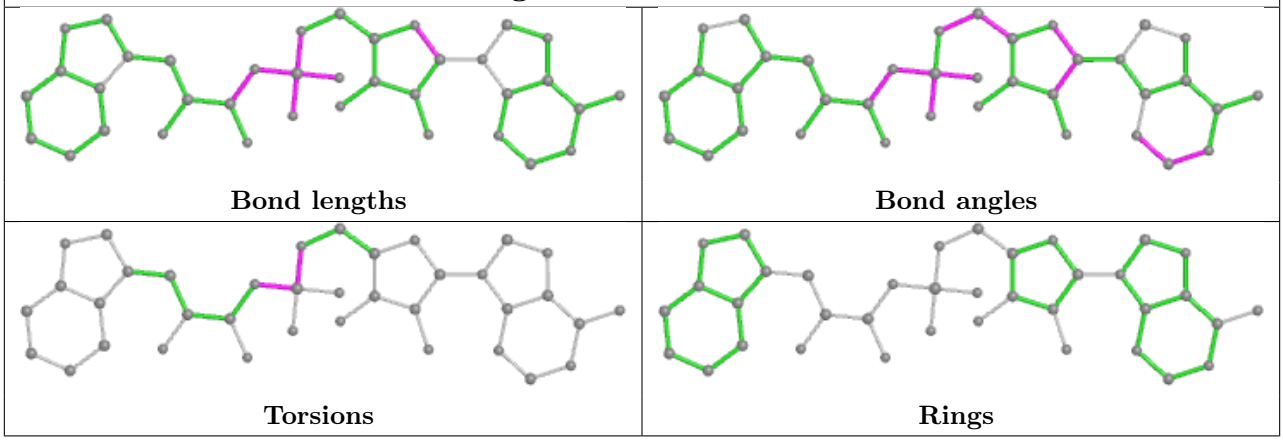
Ligand WSA B 1351



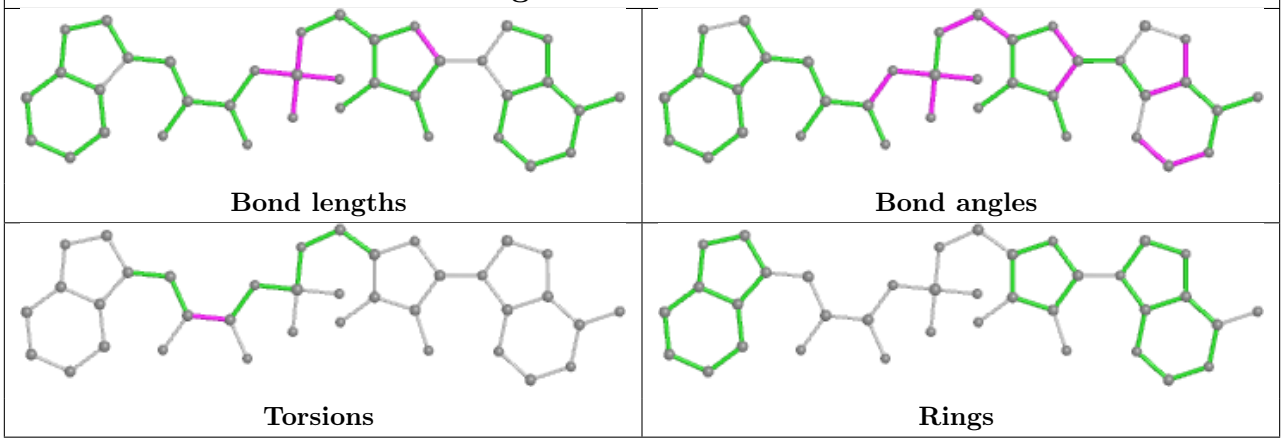
Ligand WSA A 1350



Ligand WSA D 1353



Ligand WSA C 1352



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	334/348 (95%)	-0.33	8 (2%)	59	65	11, 24, 50, 91	0
1	B	346/348 (99%)	-0.33	6 (1%)	70	76	10, 27, 56, 89	0
1	C	336/348 (96%)	-0.38	7 (2%)	63	70	11, 23, 49, 91	0
1	D	346/348 (99%)	-0.22	8 (2%)	60	67	10, 26, 53, 90	0
All	All	1362/1392 (97%)	-0.32	29 (2%)	63	70	10, 25, 53, 91	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	111	ALA	5.8
1	C	113	LYS	5.6
1	D	1	MET	5.2
1	C	124	LEU	4.7
1	C	114	ALA	4.3
1	A	346	LYS	3.6
1	B	123	THR	3.6
1	C	346	LYS	3.2
1	A	113	LYS	2.9
1	B	346	LYS	2.9
1	D	124	LEU	2.8
1	D	114	ALA	2.8
1	B	122	GLY	2.8
1	A	112	LYS	2.7
1	D	345	ILE	2.5
1	C	111	ALA	2.5
1	B	124	LEU	2.4
1	A	206	LYS	2.4
1	A	344	ASN	2.4
1	B	117	THR	2.1
1	D	195	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	206	LYS	2.1
1	C	110	LYS	2.1
1	D	206	LYS	2.1
1	D	346	LYS	2.1
1	D	122	GLY	2.1
1	C	112	LYS	2.1
1	A	74	GLN	2.0
1	A	297	LEU	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.

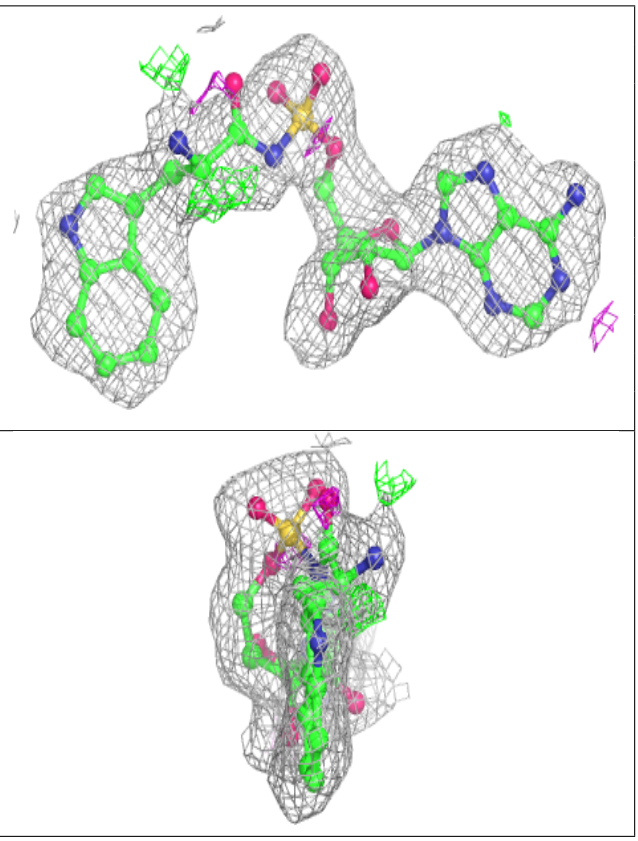
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	WSA	A	1350	37/37	0.96	0.14	8,19,26,39	0
3	WSA	C	1352	37/37	0.97	0.12	13,21,29,30	0
2	SO4	C	1366	5/5	0.98	0.15	43,44,51,59	0
2	SO4	D	1365	5/5	0.98	0.12	37,42,51,51	0
2	SO4	A	1362	5/5	0.98	0.09	18,19,26,29	0
3	WSA	B	1351	37/37	0.98	0.14	5,13,26,36	0
2	SO4	B	1361	5/5	0.98	0.12	43,46,50,52	0
3	WSA	D	1353	37/37	0.98	0.15	4,19,24,33	0
2	SO4	B	1360	5/5	0.99	0.09	12,20,23,23	0
2	SO4	C	1367	5/5	0.99	0.09	13,20,29,30	0
2	SO4	D	1364	5/5	0.99	0.09	11,17,21,22	0
2	SO4	A	1363	5/5	0.99	0.09	29,30,34,37	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers

as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

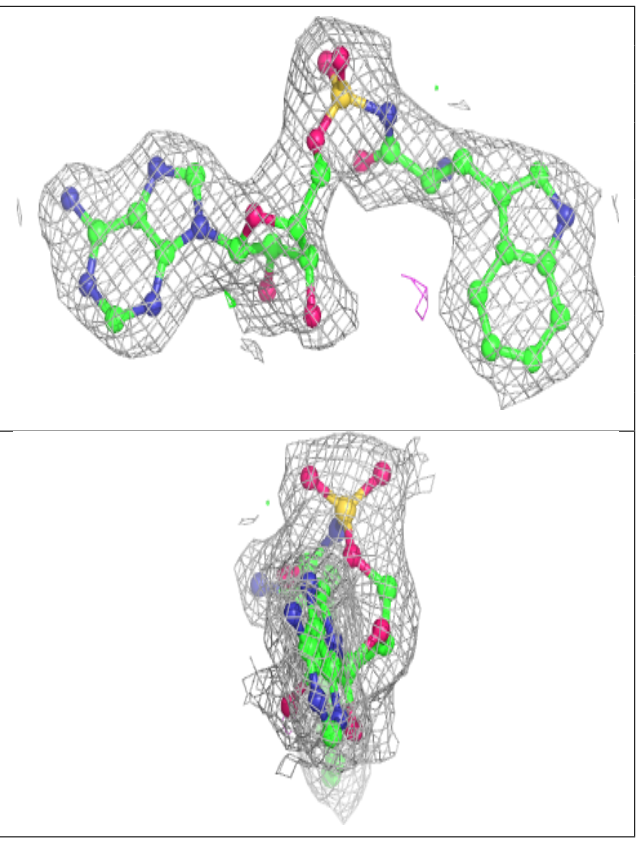
Electron density around WSA A 1350:

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



Electron density around WSA C 1352:

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



Electron density around WSA B 1351:

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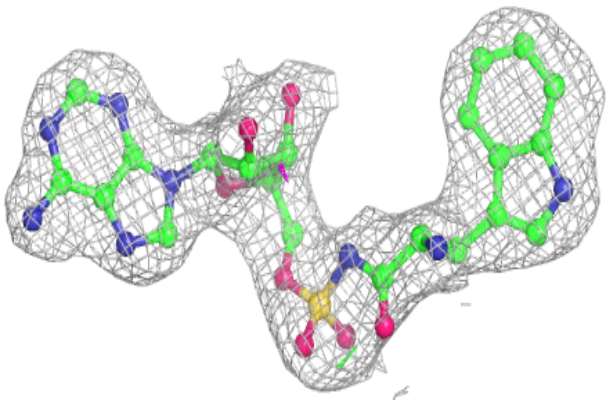
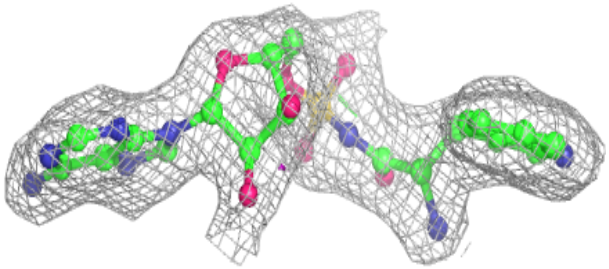
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around WSA D 1353:

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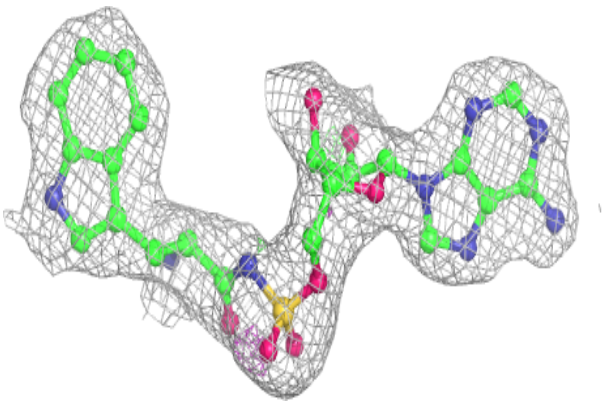
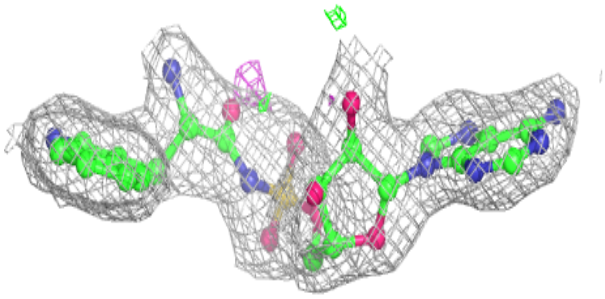
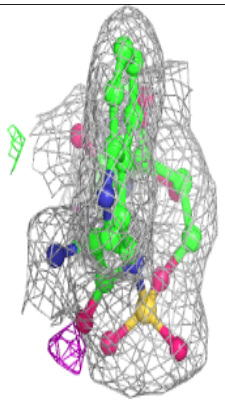
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.