Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:24 AM GMT

PDB ID	:	3ANX
Title	:	Crystal structure of triamine/agmatine aminopropyltransferase (SPEE) from thermus thermophilus, complexed with MTA
Authors	:	Ganbe, T.; Ohnuma, M.; Sato, T.; Tanaka, N.; Oshima, T.; Kumasaka, T.
Deposited on	:	2010-09-14
Resolution	:	2.50 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.50 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	Percentile Ranks	Value
Rfree		0.262
Clashscore		32
Ramachandran outliers		2.3%
Sidechain outliers		17.4%
RSRZ outliers		2.2%

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
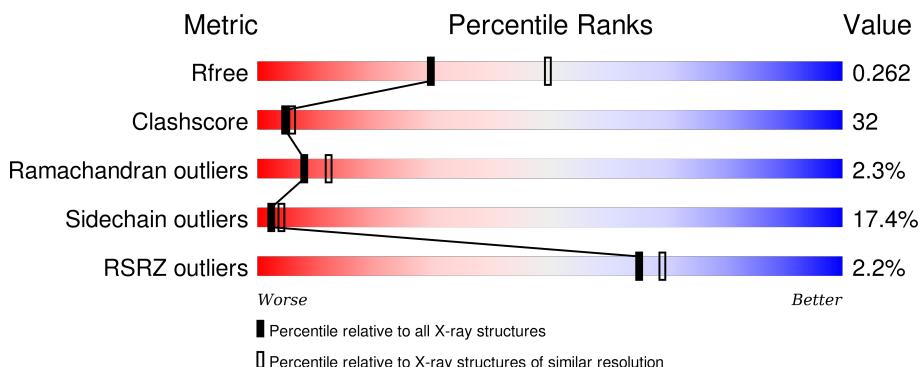
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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	314	% — 44% / 42% / 11% ··
1	B	314	3% — 38% / 48% / 11% ·
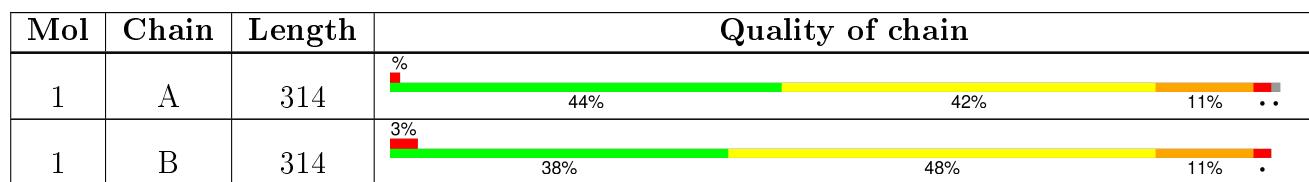
2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5288 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 spermidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	312	Total	C	N	O	S	0	0	0
			2528	1624	434	459	11			
1	B	313	Total	C	N	O	S	0	0	0
			2537	1630	436	460	11			

- Molecule 2 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (three-letter code: MTA) (formula: $C_{11}H_{15}N_5O_3S$).

MTA
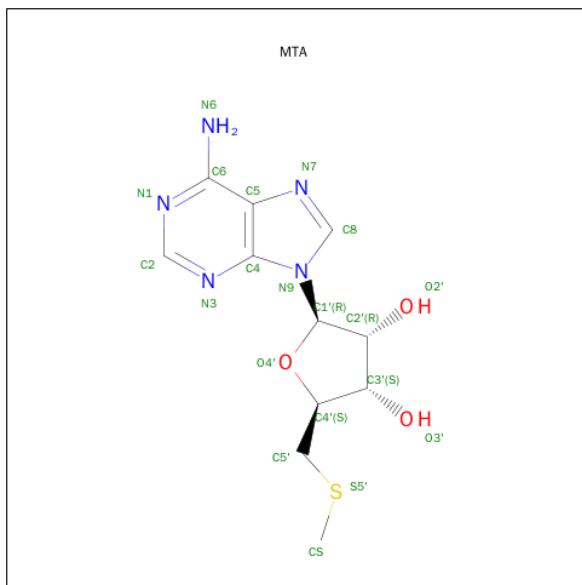
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	2	0
			20	11	5	3	1		
2	B	1	Total	C	N	O	S	2	0
			20	11	5	3	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	102	Total 102	O 102	0	0
3	B	81	Total 81	O 81	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: spermidine synthase

Chain A:

- Molecule 1: spermidine synthase

Chain B:
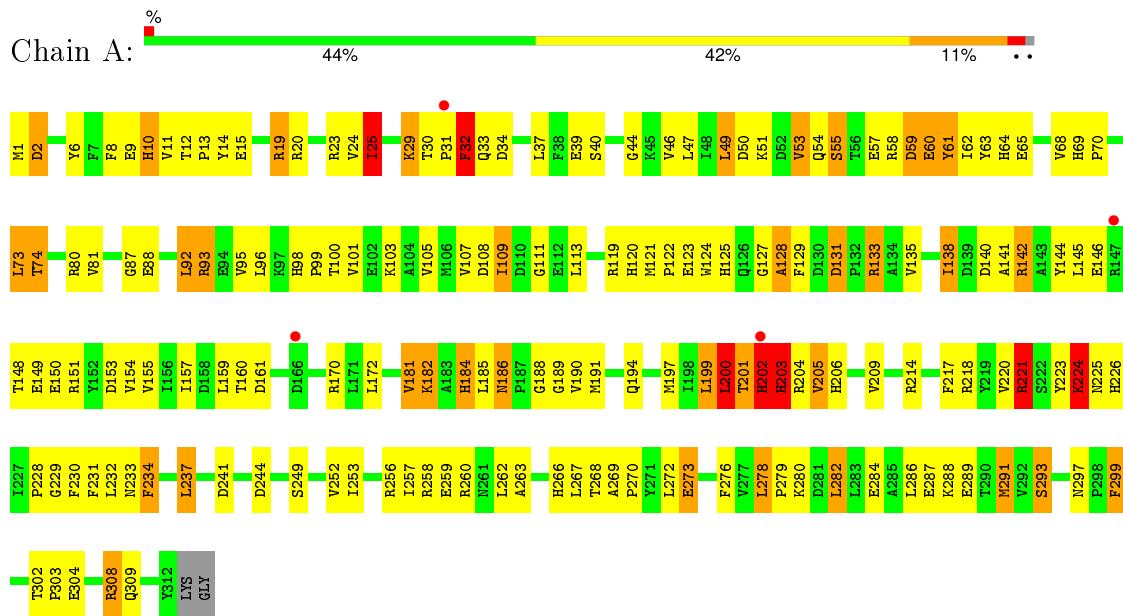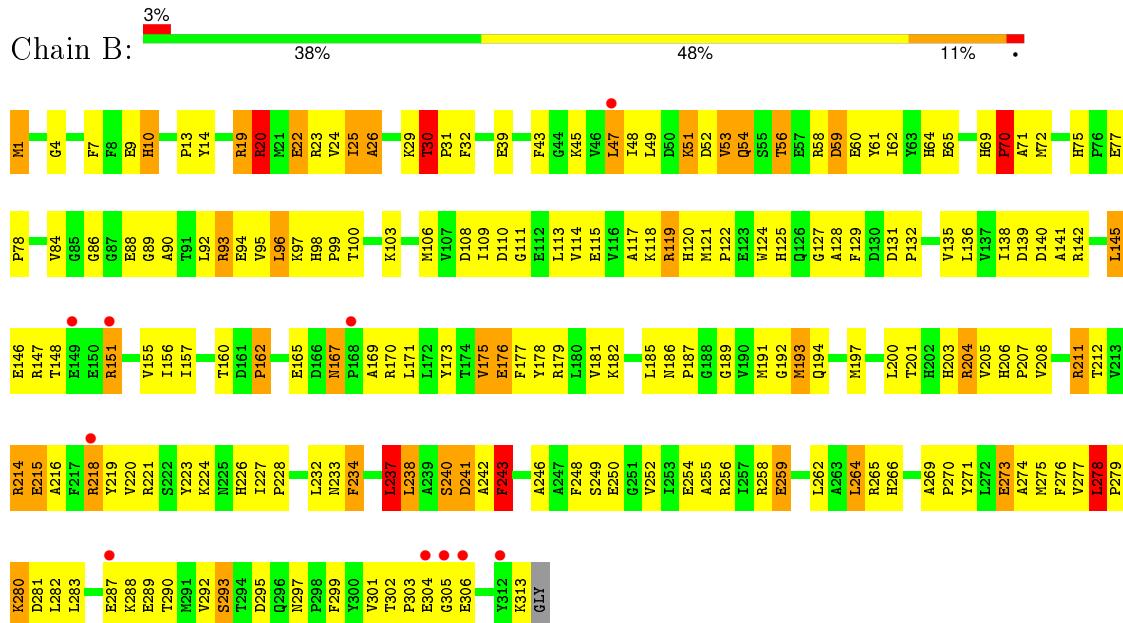
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α, β, γ	88.04Å 88.04Å 191.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 19.99 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.7 (20.00-2.50) 91.7 (19.99-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.180 , 0.263 0.180 , 0.262	Depositor DCC
R_{free} test set	2419 reflections (10.95%)	DCC
Wilson B-factor (Å^2)	35.9	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 58.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.27$	Xtriage
Outliers	0 of 24517 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	5288	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: MTA

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	1.49	14/2594 (0.5%)	1.37	22/3520 (0.6%)
1	B	1.31	4/2603 (0.2%)	1.24	11/3531 (0.3%)
All	All	1.41	18/5197 (0.3%)	1.30	33/7051 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	2
All	All	0	5

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	181	VAL	CB-CG2	9.04	1.71	1.52
1	B	287	GLU	CG-CD	7.99	1.64	1.51
1	B	277	VAL	CB-CG2	6.73	1.67	1.52
1	A	61	TYR	CD2-CE2	6.55	1.49	1.39
1	B	273	GLU	CD-OE2	6.18	1.32	1.25
1	A	61	TYR	C-O	6.15	1.35	1.23
1	A	150	GLU	CG-CD	6.13	1.61	1.51
1	A	129	PHE	CE2-CZ	5.96	1.48	1.37
1	A	284	GLU	CD-OE2	5.75	1.31	1.25
1	A	217	PHE	CE1-CZ	5.63	1.48	1.37
1	A	217	PHE	CE2-CZ	5.58	1.48	1.37
1	A	53	VAL	CA-CB	-5.50	1.43	1.54
1	A	224	LYS	CE-NZ	5.49	1.62	1.49
1	A	209	VAL	CB-CG1	-5.37	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	84	VAL	CA-CB	-5.11	1.44	1.54
1	A	6	TYR	CE1-CZ	5.09	1.45	1.38
1	A	63	TYR	CZ-OH	5.09	1.46	1.37
1	A	289	GLU	CG-CD	5.04	1.59	1.51

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	LEU	CB-CG-CD2	-8.98	95.73	111.00
1	A	49	LEU	CB-CG-CD1	-7.90	97.57	111.00
1	A	308	ARG	NE-CZ-NH1	-7.82	116.39	120.30
1	A	25	ILE	CB-CA-C	-6.99	97.62	111.60
1	B	237	LEU	CA-CB-CG	6.76	130.86	115.30
1	A	209	VAL	CG1-CB-CG2	-6.59	100.35	110.90
1	A	308	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	133	ARG	NE-CZ-NH1	6.33	123.47	120.30
1	A	221	ARG	CG-CD-NE	-6.32	98.52	111.80
1	B	93	ARG	NE-CZ-NH2	6.29	123.45	120.30
1	B	20	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	200	LEU	CB-CG-CD1	6.10	121.38	111.00
1	B	264	LEU	CA-CB-CG	-5.98	101.55	115.30
1	A	93	ARG	NE-CZ-NH1	-5.97	117.32	120.30
1	A	19	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	B	256	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	B	278	LEU	CA-CB-CG	5.84	128.74	115.30
1	A	280	LYS	CD-CE-NZ	-5.78	98.42	111.70
1	B	256	ARG	NE-CZ-NH2	-5.75	117.43	120.30
1	A	159	LEU	CB-CG-CD1	-5.52	101.62	111.00
1	A	105	VAL	N-CA-C	-5.46	96.26	111.00
1	A	73	LEU	CA-CB-CG	-5.33	103.04	115.30
1	A	200	LEU	CA-CB-CG	5.30	127.49	115.30
1	A	32	PHE	CB-CA-C	-5.25	99.89	110.40
1	B	171	LEU	CA-CB-CG	5.25	127.39	115.30
1	A	268	THR	N-CA-C	-5.21	96.94	111.00
1	A	87	GLY	N-CA-C	5.18	126.04	113.10
1	B	19	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	256	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	203	HIS	N-CA-C	5.11	124.80	111.00
1	B	45	LYS	CD-CE-NZ	-5.11	99.95	111.70
1	A	186	ASN	C-N-CD	5.10	139.10	128.40
1	B	47	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	199	LEU	Peptide
1	A	202	HIS	Peptide
1	A	203	HIS	Peptide
1	B	243	PHE	Peptide
1	B	70	PRO	Peptide

5.2   Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2528	0	2491	138	0
1	B	2537	0	2504	193	0
2	A	20	0	13	1	0
2	B	20	0	13	3	0
3	A	102	0	0	20	2
3	B	81	0	0	9	0
All	All	5288	0	5021	322	2

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 32.

All (322) 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:58:ARG:HD2	3:A:390:HOH:O	1.41	1.14
1:B:141:ALA:O	1:B:145:LEU:HD11	1.51	1.11
1:B:141:ALA:O	1:B:145:LEU:CD1	2.04	1.06
1:B:92:LEU:HG	1:B:96:LEU:HD22	1.38	1.05
1:A:202:HIS:HB2	1:A:203:HIS:CD2	1.98	0.99
1:B:176:GLU:HG3	1:B:295:ASP:OD1	1.68	0.93
1:B:145:LEU:HD12	1:B:145:LEU:H	1.30	0.93
1:A:272:LEU:C	1:A:272:LEU:HD23	1.87	0.93
1:A:202:HIS:CB	1:A:203:HIS:CD2	2.52	0.92
1:A:202:HIS:HB3	1:A:203:HIS:HD2	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:HIS:CB	1:A:203:HIS:HD2	1.82	0.91
1:B:108:ASP:OD2	2:B:315:MTA:H1'	1.69	0.91
1:B:221:ARG:HG3	1:B:246:ALA:HB2	1.52	0.91
1:B:218:ARG:HB3	1:B:219:TYR:CE1	2.07	0.90
1:B:175:VAL:HG11	1:B:215:GLU:HB3	1.53	0.87
1:A:201:THR:C	1:B:58:ARG:HH12	1.78	0.87
1:B:48:ILE:O	1:B:49:LEU:HD12	1.73	0.87
1:B:129:PHE:HB2	3:B:344:HOH:O	1.74	0.86
1:A:201:THR:O	1:B:58:ARG:NH1	2.09	0.85
1:A:182:LYS:NZ	1:A:241:ASP:OD1	2.08	0.85
1:B:92:LEU:HG	1:B:96:LEU:CD2	2.08	0.82
1:B:86:GLY:H	2:B:315:MTA:H4'	1.43	0.82
1:B:145:LEU:N	1:B:145:LEU:HD12	1.98	0.79
1:A:278:LEU:HG	1:A:282:LEU:HD13	1.63	0.79
1:B:214:ARG:HA	1:B:220:VAL:HG21	1.65	0.79
1:B:177:PHE:O	1:B:181:VAL:HG23	1.83	0.78
1:B:138:ILE:HG22	1:B:138:ILE:O	1.83	0.78
1:A:293:SER:HB2	1:A:299:PHE:HB3	1.65	0.77
1:A:103:LYS:HE2	1:A:135:VAL:HG21	1.68	0.76
1:B:141:ALA:O	1:B:145:LEU:HD12	1.86	0.76
1:B:221:ARG:HG3	1:B:246:ALA:CB	2.16	0.75
1:B:218:ARG:HB3	1:B:219:TYR:CD1	2.22	0.75
1:A:224:LYS:HE2	3:A:357:HOH:O	1.86	0.75
1:B:22:GLU:HB2	1:B:39:GLU:O	1.87	0.74
1:B:25:ILE:O	1:B:26:ALA:HB2	1.88	0.73
1:A:155:VAL:HG23	1:A:185:LEU:HD21	1.68	0.72
1:A:121:MET:HB3	1:A:124:TRP:CE3	2.25	0.72
1:B:249:SER:HB3	1:B:252:VAL:HG23	1.71	0.72
1:B:157:ILE:HD12	1:B:191:MET:SD	2.30	0.72
1:B:215:GLU:HG2	1:B:292:VAL:HG11	1.71	0.71
1:B:182:LYS:HE2	1:B:241:ASP:OD1	1.90	0.71
1:B:193:MET:CG	1:B:237:LEU:HD22	2.21	0.71
1:A:146:GLU:OE2	3:A:396:HOH:O	2.08	0.71
1:B:259:GLU:OE1	1:B:259:GLU:C	2.30	0.69
1:B:243:PHE:N	1:B:243:PHE:CD1	2.60	0.69
1:B:43:PHE:HB3	1:B:56:THR:CG2	2.22	0.68
1:B:47:LEU:HD12	1:B:54:GLN:HB2	1.75	0.68
1:B:221:ARG:CG	1:B:246:ALA:HB2	2.22	0.68
1:A:12:THR:HB	1:A:13:PRO:HD2	1.75	0.68
1:B:175:VAL:CG1	1:B:215:GLU:HB3	2.22	0.68
1:A:142:ARG:HD3	3:A:396:HOH:O	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ASN:OD1	3:A:317:HOH:O	2.12	0.67
1:A:293:SER:CB	1:A:299:PHE:HB3	2.24	0.67
1:B:243:PHE:N	1:B:243:PHE:HD1	1.91	0.67
1:A:11:VAL:HG12	1:A:12:THR:HG23	1.77	0.67
1:B:98:HIS:CE1	1:B:262:LEU:HD11	2.30	0.67
1:A:272:LEU:CD2	1:A:272:LEU:C	2.64	0.66
1:A:111:GLY:HA2	1:A:138:ILE:CD1	2.25	0.66
1:A:154:VAL:HG22	1:A:190:VAL:HG22	1.77	0.66
1:A:131:ASP:OD1	1:A:133:ARG:N	2.29	0.66
1:A:202:HIS:HB3	1:A:203:HIS:CD2	2.22	0.65
1:B:94:GLU:O	1:B:97:LYS:HB2	1.96	0.65
1:B:43:PHE:HB3	1:B:56:THR:HG23	1.78	0.65
1:B:98:HIS:HE1	1:B:262:LEU:HD11	1.62	0.65
1:B:186:ASN:HB3	1:B:187:PRO:HD2	1.78	0.65
1:A:272:LEU:O	1:A:272:LEU:HD23	1.96	0.64
1:A:278:LEU:HG	1:A:282:LEU:CD1	2.27	0.64
1:B:61:TYR:CE2	1:B:62:ILE:HG12	2.33	0.64
1:B:211:ARG:HD3	1:B:289:GLU:O	1.98	0.64
1:B:47:LEU:HD11	1:B:49:LEU:CD1	2.28	0.64
1:B:47:LEU:CD1	1:B:49:LEU:HD13	2.28	0.64
1:A:53:VAL:HG12	1:A:54:GLN:N	2.11	0.64
1:A:64:HIS:O	1:A:68:VAL:HG23	1.96	0.63
1:B:255:ALA:O	1:B:259:GLU:HB2	1.99	0.63
1:A:99:PRO:HD2	1:A:260:ARG:HG2	1.79	0.63
1:B:186:ASN:HB3	1:B:187:PRO:CD	2.28	0.63
1:A:62:ILE:HG23	1:A:266:HIS:CD2	2.34	0.62
1:B:223:TYR:CD2	1:B:275:MET:HE3	2.34	0.62
1:A:249:SER:HB2	1:A:252:VAL:HG21	1.82	0.61
1:A:120:HIS:C	1:A:122:PRO:HD2	2.21	0.61
1:A:12:THR:HB	1:A:13:PRO:CD	2.30	0.61
1:B:86:GLY:N	2:B:315:MTA:H4'	2.16	0.60
1:B:193:MET:HG2	1:B:237:LEU:CD2	2.30	0.60
1:B:249:SER:HB3	1:B:252:VAL:CG2	2.32	0.60
1:B:182:LYS:CE	1:B:241:ASP:OD1	2.50	0.59
1:A:249:SER:O	1:A:252:VAL:HG23	2.02	0.59
1:A:25:ILE:H	1:A:25:ILE:HD13	1.67	0.59
1:B:155:VAL:HG21	1:B:181:VAL:HG12	1.84	0.59
1:A:9:GLU:CD	1:A:53:VAL:HG23	2.23	0.59
1:A:293:SER:HB2	1:A:299:PHE:H	1.67	0.59
1:B:56:THR:CG2	1:B:59:ASP:OD2	2.51	0.59
1:B:48:ILE:O	1:B:49:LEU:CD1	2.50	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:VAL:O	1:B:255:ALA:HB3	2.03	0.58
1:B:176:GLU:HG3	1:B:295:ASP:CG	2.24	0.58
1:A:151:ARG:HB3	1:A:186:ASN:ND2	2.18	0.58
1:B:194:GLN:OE1	1:B:234:PHE:HE1	1.86	0.58
1:B:219:TYR:CD1	1:B:219:TYR:N	2.70	0.58
1:A:65:GLU:HB3	1:A:267:LEU:HD12	1.86	0.57
1:B:10:HIS:HD2	1:B:52:ASP:OD1	1.87	0.57
1:B:139:ASP:OD2	1:B:140:ASP:N	2.37	0.57
1:B:120:HIS:C	1:B:122:PRO:HD2	2.25	0.57
1:A:201:THR:O	1:B:58:ARG:NH2	2.38	0.57
1:B:282:LEU:O	1:B:282:LEU:HD12	2.04	0.57
1:A:204:ARG:NH2	1:A:291:MET:HE3	2.20	0.57
1:B:151:ARG:HB3	1:B:186:ASN:HD21	1.69	0.57
1:B:175:VAL:HG22	1:B:293:SER:O	2.04	0.56
1:A:233:ASN:HB2	1:B:226:HIS:CD2	2.41	0.56
1:B:203:HIS:ND1	1:B:205:VAL:HG23	2.20	0.56
1:B:269:ALA:HB3	1:B:270:PRO:HD3	1.87	0.56
1:A:279:PRO:HG2	1:A:282:LEU:HB2	1.87	0.56
1:B:211:ARG:O	1:B:211:ARG:NH2	2.38	0.56
1:A:141:ALA:O	1:A:145:LEU:HD12	2.06	0.56
1:A:302:THR:HB	1:A:303:PRO:HD2	1.88	0.56
1:B:203:HIS:HB3	1:B:305:GLY:O	2.05	0.56
1:A:121:MET:N	1:A:122:PRO:CD	2.69	0.56
1:A:197:MET:CE	3:A:375:HOH:O	2.53	0.56
1:A:10:HIS:CG	1:A:11:VAL:N	2.74	0.56
1:B:29:LYS:CG	1:B:29:LYS:O	2.54	0.55
1:B:61:TYR:HB3	3:B:322:HOH:O	2.05	0.55
1:A:99:PRO:CD	1:A:260:ARG:HG2	2.36	0.55
1:B:223:TYR:HE1	1:B:238:LEU:HD13	1.71	0.55
1:A:111:GLY:HA2	1:A:138:ILE:HD12	1.88	0.55
1:A:262:LEU:HA	3:A:339:HOH:O	2.07	0.55
1:B:10:HIS:HB3	1:B:51:LYS:HB2	1.88	0.54
1:B:138:ILE:CG2	1:B:138:ILE:O	2.53	0.54
1:A:214:ARG:HA	1:A:220:VAL:HG21	1.90	0.54
1:B:25:ILE:O	1:B:26:ALA:CB	2.53	0.54
1:A:61:TYR:HB3	3:A:320:HOH:O	2.08	0.54
1:A:121:MET:N	1:A:122:PRO:HD2	2.22	0.54
1:B:95:VAL:C	1:B:97:LYS:H	2.11	0.54
1:B:193:MET:CG	1:B:237:LEU:CD2	2.85	0.54
1:A:146:GLU:HG3	3:A:396:HOH:O	2.08	0.54
1:B:56:THR:HG22	1:B:59:ASP:OD2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:GLU:OE2	1:B:258:ARG:CZ	2.56	0.54
1:B:31:PRO:HG2	1:B:32:PHE:CD2	2.43	0.54
1:A:172:LEU:HD11	2:A:315:MTA:N6	2.24	0.53
1:A:127:GLY:O	1:A:128:ALA:C	2.46	0.53
1:A:37:LEU:HD12	1:A:46:VAL:O	2.07	0.53
1:A:60:GLU:HG3	3:A:320:HOH:O	2.08	0.53
1:A:59:ASP:OD1	1:A:228:PRO:HD2	2.08	0.53
1:B:64:HIS:CE1	1:B:90:ALA:HB3	2.43	0.53
1:B:119:ARG:O	1:B:119:ARG:HG3	2.09	0.53
1:B:89:GLY:HA2	3:B:319:HOH:O	2.08	0.53
1:B:13:PRO:HG2	1:B:14:TYR:CE1	2.44	0.53
1:B:167:ASN:HD22	1:B:169:ALA:H	1.55	0.52
1:B:167:ASN:ND2	1:B:169:ALA:HB3	2.25	0.52
1:B:56:THR:HG22	1:B:59:ASP:H	1.74	0.52
1:A:230:PHE:O	1:A:232:LEU:HB2	2.09	0.52
1:A:81:VAL:HG11	1:A:95:VAL:HG11	1.90	0.52
1:A:263:ALA:N	3:A:339:HOH:O	1.86	0.52
1:A:40:SER:HB3	1:A:44:GLY:O	2.10	0.52
1:B:20:ARG:HH11	1:B:20:ARG:CG	2.23	0.52
1:B:178:TYR:HE2	3:B:318:HOH:O	1.92	0.51
1:B:269:ALA:N	1:B:270:PRO:CD	2.73	0.51
1:B:151:ARG:HB3	1:B:186:ASN:ND2	2.25	0.51
1:B:223:TYR:HD2	1:B:275:MET:HE3	1.75	0.51
1:A:200:LEU:HD11	3:A:365:HOH:O	2.11	0.51
1:B:117:ALA:HA	1:B:121:MET:HB2	1.93	0.51
1:A:33:GLN:NE2	1:A:49:LEU:HD13	2.26	0.51
1:A:123:GLU:HB3	3:A:331:HOH:O	2.10	0.50
1:A:51:LYS:O	1:A:51:LYS:HG3	2.10	0.50
1:B:69:HIS:NE2	1:B:94:GLU:OE1	2.39	0.50
1:A:201:THR:O	1:B:58:ARG:CZ	2.58	0.50
1:B:120:HIS:O	1:B:122:PRO:HD2	2.11	0.50
1:B:109:ILE:HG13	1:B:140:ASP:HA	1.93	0.50
1:B:47:LEU:HD11	1:B:49:LEU:HD11	1.93	0.50
1:B:4:GLY:HA3	1:B:20:ARG:HH12	1.76	0.49
1:B:278:LEU:N	1:B:278:LEU:HD22	2.26	0.49
1:B:47:LEU:HD11	1:B:49:LEU:HD13	1.91	0.49
1:A:145:LEU:O	1:A:184:HIS:NE2	2.46	0.49
1:A:146:GLU:CG	3:A:396:HOH:O	2.60	0.49
1:A:218:ARG:O	1:A:218:ARG:HD2	2.12	0.49
1:B:191:MET:CG	1:B:192:GLY:N	2.75	0.49
1:B:223:TYR:CD2	1:B:275:MET:CE	2.96	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:O	1:A:108:ASP:HB2	2.13	0.49
1:B:75:HIS:HB3	1:B:78:PRO:HG3	1.94	0.49
1:B:10:HIS:CD2	1:B:52:ASP:OD1	2.65	0.49
1:B:47:LEU:CD1	1:B:49:LEU:CD1	2.91	0.49
1:A:160:THR:O	1:A:161:ASP:C	2.50	0.49
1:B:7:PHE:CZ	1:B:48:ILE:HG21	2.48	0.48
1:B:47:LEU:HD12	1:B:54:GLN:CB	2.42	0.48
1:B:49:LEU:HD22	1:B:54:GLN:HG2	1.94	0.48
1:A:32:PHE:CZ	1:A:109:ILE:HG12	2.48	0.48
1:A:194:GLN:HG3	3:A:364:HOH:O	2.12	0.48
1:A:151:ARG:CB	1:A:186:ASN:HD21	2.26	0.48
1:B:61:TYR:CE2	1:B:266:HIS:HB2	2.49	0.48
1:A:98:HIS:O	1:A:101:VAL:HG23	2.13	0.48
1:B:204:ARG:O	1:B:207:PRO:HD2	2.14	0.48
1:B:173:TYR:O	1:B:293:SER:OG	2.31	0.48
1:A:53:VAL:CG1	1:A:54:GLN:N	2.77	0.48
1:B:194:GLN:OE1	1:B:234:PHE:CE1	2.66	0.48
1:B:204:ARG:C	1:B:207:PRO:HD2	2.33	0.47
1:B:274:ALA:O	1:B:275:MET:C	2.50	0.47
1:A:197:MET:HE1	3:A:375:HOH:O	2.12	0.47
1:A:201:THR:C	1:B:58:ARG:NH1	2.59	0.47
1:B:113:LEU:O	1:B:114:VAL:C	2.51	0.47
1:B:142:ARG:O	1:B:146:GLU:HB2	2.14	0.47
1:B:191:MET:HG2	1:B:192:GLY:N	2.30	0.47
1:B:303:PRO:HD3	3:B:356:HOH:O	2.14	0.47
1:A:69:HIS:O	1:A:73:LEU:HB2	2.14	0.47
1:A:25:ILE:HD13	1:A:25:ILE:N	2.30	0.47
1:B:145:LEU:N	1:B:145:LEU:CD1	2.72	0.47
1:B:48:ILE:HG23	1:B:52:ASP:O	2.14	0.47
1:B:111:GLY:O	1:B:115:GLU:HG2	2.15	0.47
1:B:156:ILE:HA	1:B:192:GLY:O	2.15	0.47
1:A:2:ASP:HB2	1:A:20:ARG:NH1	2.29	0.47
1:B:62:ILE:HG23	1:B:266:HIS:CD2	2.50	0.47
1:A:170:ARG:C	1:A:172:LEU:H	2.17	0.47
1:B:280:LYS:HB2	1:B:280:LYS:HE3	1.70	0.47
1:B:47:LEU:O	1:B:54:GLN:N	2.46	0.47
1:A:144:TYR:O	1:A:148:THR:HG22	2.15	0.47
1:B:9:GLU:CD	1:B:53:VAL:HG12	2.35	0.47
1:A:214:ARG:HA	1:A:220:VAL:CG2	2.46	0.46
1:B:264:LEU:HD23	1:B:264:LEU:HA	1.53	0.46
1:B:165:GLU:O	1:B:170:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:157:ILE:CD1	1:B:191:MET:SD	3.03	0.46
1:B:98:HIS:HA	1:B:99:PRO:HD2	1.76	0.46
1:B:274:ALA:C	1:B:276:PHE:N	2.68	0.46
1:A:32:PHE:O	1:A:33:GLN:HB3	2.15	0.46
1:B:162:PRO:HD2	1:B:301:VAL:HG23	1.98	0.46
1:A:269:ALA:HB3	1:A:270:PRO:CD	2.45	0.46
1:A:269:ALA:HB3	1:A:270:PRO:HD3	1.96	0.46
1:A:291:MET:HB2	1:A:291:MET:HE2	1.83	0.46
1:B:29:LYS:O	1:B:30:THR:O	2.33	0.46
1:B:131:ASP:HA	1:B:132:PRO:HD2	1.73	0.46
1:B:106:MET:CE	3:B:319:HOH:O	2.64	0.46
1:B:212:THR:HA	1:B:292:VAL:HG13	1.97	0.46
1:B:182:LYS:O	1:B:185:LEU:HB2	2.16	0.46
1:B:186:ASN:HD22	1:B:186:ASN:N	2.13	0.46
1:B:206:HIS:HB3	1:B:207:PRO:HD3	1.97	0.46
1:A:13:PRO:HG2	1:A:14:TYR:CE1	2.51	0.45
1:B:167:ASN:ND2	1:B:169:ALA:H	2.14	0.45
1:B:211:ARG:HG3	1:B:211:ARG:NH2	2.30	0.45
1:A:25:ILE:HD11	1:A:39:GLU:HG2	1.97	0.45
1:A:9:GLU:OE1	1:A:19:ARG:NH1	2.49	0.45
1:A:297:ASN:O	1:A:309:GLN:HG3	2.17	0.45
1:A:181:VAL:HG11	1:A:191:MET:HG3	1.98	0.45
1:B:179:ARG:HG3	1:B:216:ALA:HB1	1.98	0.45
1:B:302:THR:HG23	1:B:306:GLU:O	2.16	0.45
1:A:24:VAL:O	1:A:24:VAL:HG12	2.16	0.45
1:A:30:THR:HB	1:A:31:PRO:HD2	1.98	0.45
1:B:61:TYR:HE2	1:B:266:HIS:HB2	1.82	0.44
1:B:279:PRO:HD2	1:B:282:LEU:HD23	1.99	0.44
1:A:220:VAL:CG1	1:A:237:LEU:HD22	2.47	0.44
1:A:151:ARG:CB	1:A:186:ASN:ND2	2.81	0.44
1:A:49:LEU:HD21	1:A:113:LEU:HD11	2.00	0.44
1:A:188:GLY:CA	3:A:414:HOH:O	2.65	0.44
1:A:55:SER:HA	3:A:319:HOH:O	2.18	0.44
1:A:73:LEU:HD23	1:A:73:LEU:HA	1.65	0.44
1:B:155:VAL:HG21	1:B:181:VAL:CG1	2.47	0.44
1:B:178:TYR:HA	1:B:181:VAL:HG23	1.98	0.44
1:A:194:GLN:OE1	1:A:234:PHE:CE1	2.71	0.44
1:B:193:MET:SD	1:B:237:LEU:HD22	2.57	0.44
1:A:37:LEU:HA	1:A:46:VAL:O	2.17	0.44
1:A:29:LYS:HG2	1:A:34:ASP:OD1	2.18	0.44
1:B:65:GLU:OE2	1:B:265:ARG:N	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:HIS:N	1:B:70:PRO:CD	2.81	0.44
1:B:93:ARG:O	1:B:97:LYS:HG3	2.17	0.44
1:A:194:GLN:OE1	1:A:234:PHE:HE1	2.00	0.44
1:A:231:PHE:N	1:A:231:PHE:CD1	2.85	0.44
1:A:80:ARG:HD3	1:A:151:ARG:O	2.18	0.44
1:B:167:ASN:HD21	1:B:169:ALA:HB3	1.83	0.44
1:A:282:LEU:HD22	1:A:286:LEU:HG	2.00	0.43
1:B:106:MET:HE2	3:B:319:HOH:O	2.18	0.43
1:B:193:MET:HG3	1:B:237:LEU:HD22	1.98	0.43
1:B:262:LEU:HA	1:B:262:LEU:HD23	1.80	0.43
1:A:92:LEU:O	1:A:93:ARG:C	2.55	0.43
1:A:96:LEU:HB3	1:A:133:ARG:NH2	2.34	0.43
1:A:70:PRO:O	1:A:74:THR:HB	2.19	0.43
1:A:205:VAL:O	1:A:206:HIS:C	2.57	0.43
1:B:77:GLU:HG3	1:B:100:THR:HG21	2.01	0.43
1:A:12:THR:OG1	1:A:15:GLU:HB2	2.18	0.43
1:B:208:VAL:O	1:B:208:VAL:HG12	2.18	0.43
1:B:108:ASP:OD1	1:B:109:ILE:O	2.37	0.43
1:B:259:GLU:OE1	1:B:259:GLU:CA	2.64	0.43
1:A:221:ARG:HD3	1:A:244:ASP:OD1	2.19	0.43
1:B:185:LEU:HD23	1:B:185:LEU:HA	1.61	0.43
1:A:125:HIS:O	1:A:128:ALA:HB2	2.18	0.42
1:B:127:GLY:O	1:B:128:ALA:C	2.57	0.42
1:B:136:LEU:N	3:B:370:HOH:O	2.40	0.42
1:A:223:TYR:HB3	1:A:276:PHE:CD1	2.54	0.42
1:A:96:LEU:HA	1:A:96:LEU:HD23	1.82	0.42
1:B:9:GLU:OE2	1:B:53:VAL:HG12	2.18	0.42
1:A:244:ASP:C	1:A:244:ASP:OD1	2.58	0.42
1:A:131:ASP:HB2	3:A:370:HOH:O	2.19	0.42
1:B:223:TYR:CE2	1:B:275:MET:HE1	2.54	0.42
1:A:88:GLU:N	1:A:88:GLU:OE1	2.50	0.42
1:B:118:LYS:HG2	3:B:383:HOH:O	2.19	0.42
1:B:227:ILE:O	1:B:228:PRO:C	2.57	0.42
1:B:250:GLU:HG2	1:B:250:GLU:O	2.19	0.42
1:B:147:ARG:HG2	1:B:147:ARG:O	2.20	0.42
1:B:49:LEU:HB2	1:B:54:GLN:NE2	2.35	0.41
1:A:160:THR:O	1:A:161:ASP:O	2.39	0.41
1:B:23:ARG:HG2	1:B:24:VAL:O	2.19	0.41
1:A:272:LEU:HD23	1:A:273:GLU:N	2.33	0.41
1:A:279:PRO:HD3	1:B:271:TYR:CE2	2.55	0.41
1:A:153:ASP:O	1:A:189:GLY:HA2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:HIS:ND1	1:B:226:HIS:ND1	2.68	0.41
1:B:278:LEU:H	1:B:278:LEU:HD22	1.86	0.41
1:B:121:MET:HE2	1:B:124:TRP:CD2	2.56	0.41
1:B:278:LEU:HD23	1:B:283:LEU:HD21	2.03	0.41
1:A:8:PHE:HE2	1:B:1:MET:HE1	1.86	0.41
1:A:253:ILE:O	1:A:257:ILE:HG13	2.20	0.41
1:B:145:LEU:HA	1:B:148:THR:HG22	2.03	0.41
1:A:267:LEU:HD22	1:A:272:LEU:HB2	2.03	0.41
1:A:65:GLU:HA	1:A:69:HIS:HD2	1.84	0.41
1:B:47:LEU:HD13	1:B:47:LEU:C	2.41	0.41
1:B:72:MET:CE	1:B:98:HIS:CD2	3.03	0.41
1:B:19:ARG:NH2	1:B:53:VAL:HG11	2.36	0.41
1:B:111:GLY:CA	1:B:138:ILE:HD13	2.51	0.41
1:A:237:LEU:HD12	1:A:237:LEU:C	2.41	0.41
1:A:49:LEU:HD21	1:A:113:LEU:CD1	2.51	0.41
1:B:200:LEU:HD23	1:B:200:LEU:HA	1.89	0.41
1:B:121:MET:N	1:B:122:PRO:CD	2.84	0.40
1:B:227:ILE:N	1:B:227:ILE:HD12	2.35	0.40
1:A:258:ARG:O	1:A:259:GLU:C	2.59	0.40
1:B:157:ILE:HB	1:B:193:MET:CB	2.51	0.40
1:B:122:PRO:HA	1:B:125:HIS:CE1	2.56	0.40
1:A:197:MET:HE2	3:A:375:HOH:O	2.16	0.40
1:B:219:TYR:HD1	1:B:240:SER:O	2.04	0.40
1:B:56:THR:O	1:B:60:GLU:HB3	2.22	0.40
1:B:60:GLU:O	1:B:61:TYR:C	2.59	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:406:HOH:O	3:A:406:HOH:O[7_556]	1.54	0.66
3:A:405:HOH:O	3:A:405:HOH:O[7_556]	2.17	0.03

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	310/314 (99%)	268 (86%)	36 (12%)	6 (2%)	10	16
1	B	311/314 (99%)	261 (84%)	42 (14%)	8 (3%)	7	10
All	All	621/628 (99%)	529 (85%)	78 (13%)	14 (2%)	8	12

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	ALA
1	B	26	ALA
1	B	30	THR
1	A	229	GLY
1	B	71	ALA
1	B	242	ALA
1	B	70	PRO
1	A	50	ASP
1	A	109	ILE
1	B	110	ASP
1	A	32	PHE
1	B	162	PRO
1	A	25	ILE
1	B	189	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	A	269/270 (100%)	227 (84%)	42 (16%)	3	6
1	B	270/270 (100%)	218 (81%)	52 (19%)	2	3
All	All	539/540 (100%)	445 (83%)	94 (17%)	2	4

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ASP
1	A	10	HIS
1	A	23	ARG
1	A	25	ILE
1	A	29	LYS
1	A	47	LEU
1	A	55	SER
1	A	57	GLU
1	A	59	ASP
1	A	60	GLU
1	A	74	THR
1	A	92	LEU
1	A	100	THR
1	A	119	ARG
1	A	131	ASP
1	A	138	ILE
1	A	140	ASP
1	A	142	ARG
1	A	149	GLU
1	A	157	ILE
1	A	182	LYS
1	A	184	HIS
1	A	199	LEU
1	A	200	LEU
1	A	201	THR
1	A	202	HIS
1	A	205	VAL
1	A	221	ARG
1	A	224	LYS
1	A	234	PHE
1	A	237	LEU
1	A	273	GLU
1	A	278	LEU
1	A	282	LEU
1	A	287	GLU
1	A	288	LYS
1	A	291	MET
1	A	293	SER
1	A	299	PHE
1	A	304	GLU
1	A	308	ARG
1	B	1	MET

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Mol	Chain	Res	Type
1	B	10	HIS
1	B	20	ARG
1	B	22	GLU
1	B	25	ILE
1	B	30	THR
1	B	51	LYS
1	B	53	VAL
1	B	54	GLN
1	B	56	THR
1	B	59	ASP
1	B	88	GLU
1	B	96	LEU
1	B	103	LYS
1	B	119	ARG
1	B	135	VAL
1	B	145	LEU
1	B	151	ARG
1	B	160	THR
1	B	167	ASN
1	B	175	VAL
1	B	176	GLU
1	B	193	MET
1	B	197	MET
1	B	201	THR
1	B	204	ARG
1	B	211	ARG
1	B	214	ARG
1	B	215	GLU
1	B	218	ARG
1	B	224	LYS
1	B	232	LEU
1	B	233	ASN
1	B	234	PHE
1	B	237	LEU
1	B	238	LEU
1	B	240	SER
1	B	241	ASP
1	B	243	PHE
1	B	248	PHE
1	B	259	GLU
1	B	273	GLU
1	B	278	LEU

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Mol	Chain	Res	Type
1	B	280	LYS
1	B	281	ASP
1	B	288	LYS
1	B	290	THR
1	B	293	SER
1	B	297	ASN
1	B	299	PHE
1	B	304	GLU
1	B	313	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	54	GLN
1	A	186	ASN
1	A	203	HIS
1	A	297	ASN
1	B	10	HIS
1	B	54	GLN
1	B	126	GLN
1	B	167	ASN
1	B	186	ASN
1	B	233	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	MTA	A	315	-	17,22,22	9.88	3 (17%)	17,32,32	4.75	9 (52%)
2	MTA	B	315	-	17,22,22	12.85	4 (23%)	17,32,32	5.31	9 (52%)

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	MTA	A	315	-	-	0/3/23/23	0/3/3/3
2	MTA	B	315	-	-	0/3/23/23	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	315	MTA	C5'-S5'	-52.37	1.23	1.80
2	A	315	MTA	C5'-S5'	-40.38	1.36	1.80
2	B	315	MTA	C2-N3	2.38	1.36	1.32
2	A	315	MTA	C5-C4	2.61	1.46	1.40
2	A	315	MTA	O4'-C1'	3.04	1.45	1.41
2	B	315	MTA	C5-C4	3.45	1.48	1.40
2	B	315	MTA	O4'-C1'	6.20	1.49	1.41

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	315	MTA	CS-S5'-C5'	-8.19	87.89	101.21
2	B	315	MTA	N3-C2-N1	-6.56	123.87	128.89
2	A	315	MTA	N3-C2-N1	-6.40	123.99	128.89
2	A	315	MTA	C4-C5-N7	-5.54	104.38	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	315	MTA	C4-C5-N7	-3.68	106.10	109.48
2	B	315	MTA	C4'-O4'-C1'	-3.61	105.75	109.72
2	B	315	MTA	O3'-C3'-C2'	-2.89	102.43	111.83
2	A	315	MTA	CS-S5'-C5'	-2.28	97.51	101.21
2	A	315	MTA	O3'-C3'-C4'	-2.23	104.36	111.05
2	A	315	MTA	C2'-C3'-C4'	2.05	106.82	102.61
2	B	315	MTA	C2'-C3'-C4'	2.91	108.58	102.61
2	A	315	MTA	O4'-C4'-C5'	3.10	117.29	108.85
2	A	315	MTA	C4'-O4'-C1'	3.83	113.92	109.72
2	B	315	MTA	O4'-C4'-C5'	4.59	121.36	108.85
2	A	315	MTA	O4'-C1'-N9	5.49	119.60	108.10
2	B	315	MTA	O4'-C1'-N9	5.56	119.75	108.10
2	A	315	MTA	C4'-C5'-S5'	15.30	158.27	113.52
2	B	315	MTA	C4'-C5'-S5'	16.15	160.76	113.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	315	MTA	1	0
2	B	315	MTA	3	0

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	312/314 (99%)	-0.42	4 (1%)	79	82	15, 35, 55, 67	0
1	B	313/314 (99%)	-0.13	10 (3%)	51	56	16, 45, 75, 91	0
All	All	625/628 (99%)	-0.27	14 (2%)	65	69	15, 39, 67, 91	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	149	GLU	3.7
1	B	218	ARG	3.6
1	B	312	TYR	2.9
1	B	151	ARG	2.7
1	B	305	GLY	2.6
1	B	47	LEU	2.6
1	B	306	GLU	2.5
1	B	168	PRO	2.5
1	A	31	PRO	2.3
1	B	287	GLU	2.2
1	B	304	GLU	2.2
1	A	147	ARG	2.2
1	A	202	HIS	2.1
1	A	166	ASP	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 carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å^2)	Q<0.9
2	MTA	B	315	20/20	0.90	0.16	0.62	60,67,87,89	2
2	MTA	A	315	20/20	0.95	0.11	-0.03	45,50,88,89	2

6.5 Other polymers (i)

There are no such residues in this entry.