



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:09 AM GMT

PDB ID : 1ZX4
Title : Structure of ParB bound to DNA
Authors : Schumacher, M.A.; Funnell, B.E.
Deposited on : 2005-06-06
Resolution : 2.98 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

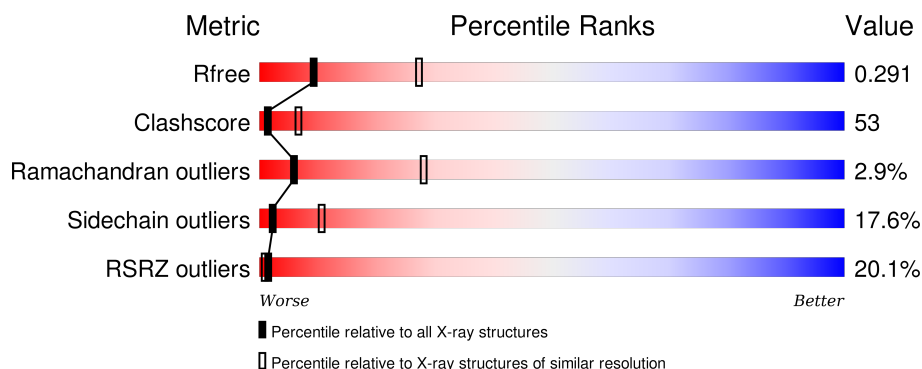
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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}	91344	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	T	25	 8% 28% 72%
2	S	25	 4% 28% 68% •
3	A	192	 23% 25% 54% 15% • 6%
3	B	192	 16% 26% 54% 11% • 8%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 3894 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 DNA chain called parS-small DNA centromere site.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	T	25	Total	C	N	O	P	0	0	0
			512	244	98	146	24			

- Molecule 2 is a DNA chain called parS-small DNA centromere site.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	S	25	Total	C	N	O	P	0	0	0
			507	243	90	150	24			

- Molecule 3 is a protein called Plasmid Partition par B protein.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	180	Total	C	N	O	S	Se	0	0	0
			1437	899	254	277	1	6			
3	B	176	Total	C	N	O	S	Se	0	0	0
			1405	881	247	270	1	6			

There are 14 discrepancies between the modelled and reference sequences:

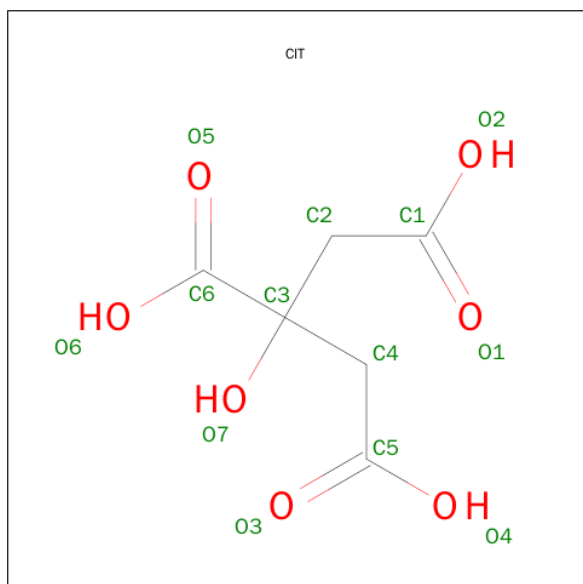
Chain	Residue	Modelled	Actual	Comment	Reference
A	159	MSE	MET	MODIFIED RESIDUE	UNP Q38420
A	161	MSE	MET	MODIFIED RESIDUE	UNP Q38420
A	166	MSE	MET	MODIFIED RESIDUE	UNP Q38420
A	220	MSE	MET	MODIFIED RESIDUE	UNP Q38420
A	245	ASN	ASP	CONFLICT	UNP Q38420
A	247	MSE	MET	MODIFIED RESIDUE	UNP Q38420
A	318	MSE	MET	MODIFIED RESIDUE	UNP Q38420
B	159	MSE	MET	MODIFIED RESIDUE	UNP Q38420
B	161	MSE	MET	MODIFIED RESIDUE	UNP Q38420
B	166	MSE	MET	MODIFIED RESIDUE	UNP Q38420
B	220	MSE	MET	MODIFIED RESIDUE	UNP Q38420
B	245	ASN	ASP	CONFLICT	UNP Q38420

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	247	MSE	MET	MODIFIED RESIDUE	UNP Q38420
B	318	MSE	MET	MODIFIED RESIDUE	UNP Q38420

- Molecule 4 is CITRIC ACID (three-letter code: CIT) (formula: $C_6H_8O_7$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 6 7	0	0
4	A	1	Total C O 13 6 7	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total O 3 3	0	0
5	B	4	Total O 4 4	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.

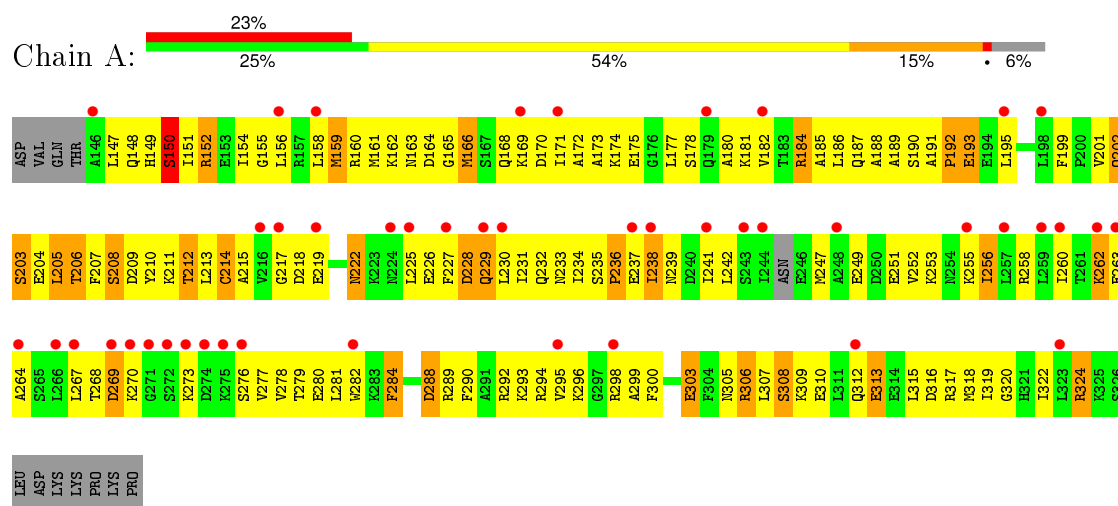
- Molecule 1: parS-small DNA centromere site



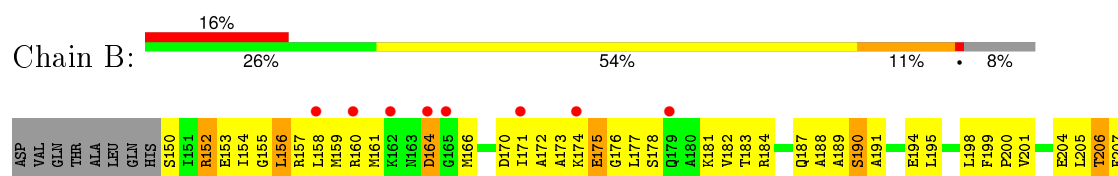
- Molecule 2: parS-small DNA centromere site

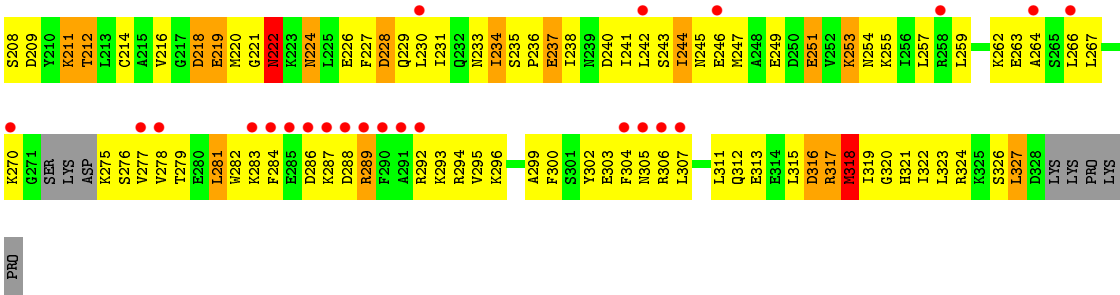


- Molecule 3: Plasmid Partition par B protein



- Molecule 3: Plasmid Partition par B protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.60 Å 154.60 Å 132.30 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.61 – 2.98 50.60 – 2.98	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.61-2.98) 90.8 (50.60-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.96 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.248 , 0.296 0.242 , 0.291	Depositor DCC
R_{free} test set	2158 reflections (12.11%)	DCC
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.43 , 127.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 17816 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	3894	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	T	0.85	0/575	0.91	0/886
2	S	0.87	0/567	1.01	0/873
3	A	0.54	0/1445	0.79	1/1919 (0.1%)
3	B	0.57	0/1412	0.87	2/1876 (0.1%)
All	All	0.66	0/3999	0.88	3/5554 (0.1%)

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
2	S	0	2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	160	ARG	NE-CZ-NH2	-11.17	114.72	120.30
3	B	160	ARG	NE-CZ-NH1	6.24	123.42	120.30
3	A	184	ARG	NE-CZ-NH1	5.05	122.83	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	S	13	DT	Sidechain
2	S	25	DC	Sidechain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	T	512	0	282	33	0
2	S	507	0	284	37	0
3	A	1437	0	1472	179	1
3	B	1405	0	1444	160	0
4	A	26	0	10	3	0
5	A	3	0	0	1	0
5	B	4	0	0	0	0
All	All	3894	0	3492	384	1

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 53.

All (384) 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:T:25:DG:H2''	1:T:26:DT:C5'	1.78	1.13
3:A:278:VAL:HG12	3:A:294:ARG:HB2	1.38	1.05
1:T:25:DG:C2'	1:T:26:DT:H5'	1.91	1.00
3:A:238:ILE:HD11	3:A:256:ILE:HG13	1.41	1.00
3:B:224:ASN:H	3:B:224:ASN:ND2	1.57	0.98
3:A:282:TRP:NE1	3:B:327:LEU:HG	1.78	0.98
3:B:224:ASN:H	3:B:224:ASN:HD22	0.98	0.97
2:S:17:DC:H6	2:S:17:DC:H5'	1.32	0.95
1:T:25:DG:H2''	1:T:26:DT:H5'	0.97	0.94
3:A:192:PRO:HD3	3:A:214:CYS:HA	1.48	0.92
3:B:224:ASN:N	3:B:224:ASN:HD22	1.64	0.92
3:B:161:MSE:HA	3:B:164:ASP:HB2	1.48	0.91
3:B:177:LEU:HD22	3:B:181:LYS:HG2	1.53	0.91
3:B:184:ARG:HB3	3:B:207:PHE:HE2	1.37	0.90
3:B:237:GLU:HA	3:B:240:ASP:HB3	1.53	0.90
3:B:208:SER:O	3:B:212:THR:HG23	1.70	0.89
3:A:270:LYS:HD2	3:A:277:VAL:HG22	1.54	0.89
3:A:306:ARG:HG2	3:A:306:ARG:HH11	1.37	0.87
3:B:307:LEU:HD13	3:B:311:LEU:HD13	1.55	0.87
3:B:184:ARG:HB3	3:B:207:PHE:CE2	2.09	0.87

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:207:PHE:HE1	3:B:211:LYS:HD2	1.39	0.87
3:B:150:SER:O	3:B:154:ILE:HG13	1.76	0.86
2:S:21:DA:H2''	2:S:22:DA:C8	2.14	0.83
3:A:226:GLU:OE1	3:A:226:GLU:HA	1.79	0.82
3:A:305:ASN:OD1	3:B:299:ALA:HB2	1.80	0.82
3:B:206:THR:CG2	3:B:207:PHE:N	2.44	0.80
3:B:267:LEU:HB3	3:B:277:VAL:HG13	1.61	0.80
3:B:226:GLU:HB3	3:B:277:VAL:HG21	1.63	0.80
2:S:19:DT:H2''	2:S:20:DG:C8	2.15	0.80
3:A:317:ARG:HH11	3:A:317:ARG:HG3	1.47	0.79
3:A:225:LEU:O	3:A:225:LEU:HD13	1.83	0.79
3:B:238:ILE:O	3:B:242:LEU:HG	1.82	0.78
3:B:218:ASP:O	3:B:220:MSE:N	2.17	0.78
3:A:161:MSE:HB3	3:A:166:MSE:HE3	1.65	0.78
3:A:281:LEU:HD13	3:A:292:ARG:HA	1.66	0.78
3:A:318:MSE:SE	3:B:318:MSE:HG2	2.34	0.77
3:B:150:SER:N	3:B:153:GLU:HG3	2.01	0.76
1:T:16:DG:H1	2:S:25:DC:H42	1.34	0.76
3:A:233:ASN:OD1	3:A:279:THR:HG22	1.85	0.75
3:A:158:LEU:HD13	3:A:182:VAL:HG13	1.68	0.75
3:B:207:PHE:CE1	3:B:211:LYS:HD2	2.22	0.74
3:B:158:LEU:HA	3:B:161:MSE:HE3	1.69	0.74
3:B:237:GLU:HA	3:B:240:ASP:CB	2.17	0.73
1:T:24:DG:H4'	1:T:24:DG:OP1	1.88	0.73
3:B:200:PRO:HG3	3:B:242:LEU:HD11	1.70	0.73
3:A:262:LYS:HE3	3:A:263:GLU:HG2	1.71	0.73
2:S:4:DG:H1'	2:S:5:DT:H5''	1.71	0.72
3:B:281:LEU:HB2	3:B:292:ARG:HA	1.70	0.72
3:A:299:ALA:HB2	3:B:305:ASN:OD1	1.89	0.71
3:A:208:SER:O	3:A:212:THR:HG23	1.90	0.71
3:A:192:PRO:CD	3:A:214:CYS:HA	2.20	0.71
3:A:195:LEU:HB3	3:A:213:LEU:HD11	1.71	0.71
2:S:21:DA:H2''	2:S:22:DA:H8	1.56	0.71
3:B:221:GLY:O	3:B:222:ASN:HB2	1.90	0.70
1:T:14:DG:C8	1:T:14:DG:H5'	2.26	0.70
3:B:183:THR:O	3:B:187:GLN:HG3	1.92	0.70
3:A:152:ARG:HH11	3:A:152:ARG:HG2	1.57	0.70
2:S:17:DC:H6	2:S:17:DC:C5'	2.06	0.69
3:A:155:GLY:HA3	3:A:189:ALA:HB2	1.75	0.69
3:B:194:GLU:O	3:B:231:ILE:HD11	1.93	0.69
3:B:275:LYS:HG2	3:B:276:SER:H	1.59	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:206:THR:HG23	3:B:207:PHE:H	1.58	0.68
3:A:264:ALA:O	3:A:268:THR:HG23	1.92	0.68
2:S:17:DC:H5'	2:S:17:DC:C6	2.22	0.68
3:A:227:PHE:O	3:A:231:ILE:HG13	1.94	0.68
3:B:251:GLU:HA	3:B:251:GLU:OE1	1.93	0.68
3:B:324:ARG:HA	3:B:327:LEU:HD21	1.75	0.67
1:T:16:DG:H1	2:S:25:DC:N4	1.92	0.67
1:T:36:DA:OP2	1:T:36:DA:H2'	1.95	0.67
3:B:317:ARG:HB2	3:B:317:ARG:NH1	2.10	0.66
3:A:241:ILE:HD12	3:A:256:ILE:HD12	1.77	0.66
1:T:36:DA:H2''	1:T:37:DC:OP2	1.95	0.66
3:A:270:LYS:HA	3:A:273:LYS:HB2	1.78	0.66
1:T:14:DG:H8	1:T:14:DG:H5'	1.61	0.66
3:A:324:ARG:HG3	3:A:324:ARG:HH11	1.60	0.66
3:A:256:ILE:N	3:A:256:ILE:HD13	2.10	0.66
3:A:306:ARG:HG2	3:A:306:ARG:NH1	2.09	0.66
3:B:177:LEU:CD2	3:B:181:LYS:HG2	2.26	0.65
3:A:256:ILE:H	3:A:256:ILE:HD13	1.61	0.65
3:B:263:GLU:O	3:B:266:LEU:HD23	1.96	0.65
3:B:187:GLN:O	3:B:190:SER:HB3	1.97	0.65
3:B:155:GLY:HA3	3:B:189:ALA:HB2	1.77	0.65
3:A:229:GLN:OE1	3:A:267:LEU:HD13	1.97	0.65
3:A:282:TRP:CD1	3:B:327:LEU:HG	2.32	0.65
1:T:26:DT:H2''	1:T:27:DG:C8	2.32	0.65
3:A:151:ILE:HG13	3:A:185:ALA:HA	1.78	0.64
2:S:25:DC:H2''	2:S:26:DG:C8	2.32	0.64
3:A:228:ASP:O	3:A:232:GLN:HG2	1.98	0.64
3:B:323:LEU:C	3:B:327:LEU:HD13	2.17	0.64
3:B:237:GLU:CA	3:B:240:ASP:HB3	2.27	0.64
3:A:293:LYS:HE2	3:A:295:VAL:CG2	2.28	0.64
3:A:247:MSE:HE3	3:A:252:VAL:HB	1.80	0.63
3:A:208:SER:HB3	4:A:1585:CIT:H21	1.80	0.63
2:S:15:DA:H2'	2:S:15:DA:OP2	1.99	0.63
3:B:206:THR:HG22	3:B:207:PHE:N	2.11	0.63
3:B:234:ILE:HD13	3:B:234:ILE:H	1.65	0.62
3:B:152:ARG:NH2	3:B:191:ALA:O	2.32	0.62
3:B:270:LYS:HB2	3:B:278:VAL:HB	1.80	0.62
3:B:312:GLN:O	3:B:316:ASP:HB2	2.00	0.61
2:S:4:DG:C2'	2:S:5:DT:H5''	2.31	0.61
3:A:318:MSE:SE	3:A:318:MSE:C	2.89	0.61
1:T:14:DG:H2''	1:T:15:DC:O5'	2.01	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:206:THR:CG2	3:B:207:PHE:H	2.13	0.60
3:B:216:VAL:HG13	3:B:264:ALA:HB2	1.83	0.60
3:A:280:GLU:HA	3:A:292:ARG:HB3	1.83	0.60
3:B:206:THR:HG22	3:B:208:SER:N	2.16	0.60
3:A:241:ILE:CD1	3:A:256:ILE:HD12	2.32	0.60
2:S:4:DG:H2''	2:S:5:DT:C5'	2.32	0.60
3:B:307:LEU:HD13	3:B:311:LEU:CD1	2.28	0.60
3:B:253:LYS:HG3	3:B:254:ASN:N	2.17	0.59
3:A:270:LYS:CD	3:A:277:VAL:HG22	2.31	0.59
1:T:35:DC:H2''	1:T:36:DA:C8	2.38	0.59
3:A:256:ILE:CD1	3:A:256:ILE:N	2.64	0.59
3:A:232:GLN:NE2	5:A:104:HOH:O	2.34	0.59
3:A:215:ALA:O	3:A:219:GLU:HG2	2.02	0.59
1:T:23:DA:H2''	1:T:24:DG:O5'	2.02	0.59
3:B:200:PRO:HG2	3:B:242:LEU:HD21	1.84	0.59
3:A:206:THR:HB	3:A:209:ASP:OD2	2.02	0.59
3:A:206:THR:O	3:A:209:ASP:HB2	2.02	0.59
3:A:262:LYS:C	3:A:262:LYS:HD2	2.24	0.58
3:B:199:PHE:CD1	3:B:205:LEU:HD21	2.38	0.58
3:B:318:MSE:HA	3:B:318:MSE:HE3	1.84	0.58
3:A:237:GLU:O	3:A:241:ILE:HG13	2.03	0.58
3:A:150:SER:O	3:A:151:ILE:C	2.41	0.58
3:A:263:GLU:O	3:A:267:LEU:HG	2.03	0.58
3:A:238:ILE:CG2	3:A:239:ASN:N	2.66	0.58
3:A:202:GLN:O	3:A:205:LEU:HB2	2.04	0.58
3:B:292:ARG:NH1	3:B:303:GLU:OE1	2.36	0.57
3:A:290:PHE:CZ	3:A:305:ASN:HB2	2.38	0.57
3:A:204:GLU:O	3:A:253:LYS:HD3	2.04	0.57
1:T:25:DG:C2'	1:T:26:DT:C5'	2.67	0.57
3:A:166:MSE:HE1	3:A:174:LYS:HD3	1.86	0.57
1:T:15:DC:H2''	1:T:16:DG:C8	2.39	0.57
3:A:278:VAL:HG12	3:A:294:ARG:CB	2.26	0.57
3:B:230:LEU:HD23	3:B:231:ILE:N	2.20	0.57
3:A:218:ASP:HA	3:A:222:ASN:HB2	1.87	0.57
3:A:191:ALA:HA	3:A:214:CYS:HB2	1.87	0.57
3:A:284:PHE:CD2	3:A:284:PHE:N	2.73	0.56
1:T:16:DG:OP2	1:T:16:DG:H8	1.88	0.56
3:B:244:ILE:HG21	3:B:247:MSE:CE	2.35	0.56
2:S:4:DG:C1'	2:S:5:DT:H5''	2.36	0.56
3:A:235:SER:O	3:A:238:ILE:HG22	2.05	0.56
3:A:299:ALA:HA	3:B:305:ASN:HA	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:208:SER:OG	4:A:1585:CIT:H41	2.06	0.56
3:A:238:ILE:HD11	3:A:256:ILE:CG1	2.26	0.56
3:A:158:LEU:HD12	3:A:185:ALA:HB3	1.86	0.56
3:A:201:VAL:HG21	3:A:249:GLU:CD	2.26	0.55
3:A:147:LEU:O	3:A:148:GLN:C	2.45	0.55
2:S:20:DG:O6	3:A:184:ARG:NH2	2.38	0.55
3:A:230:LEU:HD11	3:A:263:GLU:HB3	1.88	0.55
3:A:230:LEU:CD1	3:A:263:GLU:HB3	2.37	0.55
3:B:259:LEU:O	3:B:262:LYS:HB3	2.07	0.55
2:S:18:DT:H2''	2:S:19:DT:H5'	1.88	0.55
3:B:262:LYS:HG3	3:B:263:GLU:N	2.21	0.55
3:A:276:SER:CB	3:A:296:LYS:HB3	2.36	0.55
1:T:30:DA:H1'	1:T:31:DT:H5''	1.89	0.55
3:B:194:GLU:C	3:B:195:LEU:HD23	2.27	0.54
3:A:289:ARG:HD2	3:A:306:ARG:O	2.07	0.54
3:B:200:PRO:HG2	3:B:242:LEU:CD2	2.37	0.54
1:T:24:DG:H2''	1:T:25:DG:O5'	2.08	0.54
1:T:16:DG:H5'	3:A:169:LYS:HD2	1.90	0.54
3:A:147:LEU:C	3:A:149:HIS:N	2.60	0.54
3:A:284:PHE:HD1	3:A:289:ARG:HE	1.56	0.54
3:B:184:ARG:CB	3:B:207:PHE:HE2	2.17	0.54
1:T:37:DC:H6	1:T:37:DC:OP2	1.91	0.54
3:B:177:LEU:HD22	3:B:181:LYS:CG	2.31	0.54
3:A:281:LEU:HD13	3:A:292:ARG:CA	2.36	0.54
2:S:4:DG:H2''	2:S:5:DT:H5''	1.89	0.54
3:B:154:ILE:HG22	3:B:158:LEU:CD1	2.38	0.54
3:B:170:ASP:O	3:B:174:LYS:HG2	2.08	0.54
3:B:317:ARG:HB2	3:B:317:ARG:HH11	1.71	0.53
1:T:27:DG:H2''	1:T:28:DA:C8	2.43	0.53
3:B:198:LEU:HD11	3:B:231:ILE:HG12	1.89	0.53
2:S:17:DC:H2'	2:S:18:DT:C7	2.38	0.53
3:B:276:SER:HB3	3:B:296:LYS:CE	2.38	0.53
3:A:317:ARG:NH1	3:A:317:ARG:HG3	2.19	0.53
3:B:286:ASP:HB3	3:B:289:ARG:CB	2.39	0.53
3:B:286:ASP:HB3	3:B:289:ARG:HB2	1.91	0.53
3:B:237:GLU:O	3:B:241:ILE:HG13	2.09	0.53
3:B:211:LYS:O	3:B:214:CYS:HB2	2.09	0.53
3:A:262:LYS:HD2	3:A:263:GLU:N	2.24	0.53
3:A:318:MSE:HE2	3:B:322:ILE:CD1	2.39	0.53
3:B:284:PHE:HB2	3:B:289:ARG:O	2.08	0.53
3:A:161:MSE:HE1	3:A:175:GLU:OE2	2.10	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:296:LYS:HG3	3:A:296:LYS:O	2.09	0.52
3:A:192:PRO:O	3:A:193:GLU:C	2.48	0.52
3:A:151:ILE:HA	3:A:154:ILE:HD12	1.90	0.52
3:B:156:LEU:O	3:B:159:MSE:HB2	2.09	0.52
3:B:154:ILE:HG22	3:B:158:LEU:HD11	1.92	0.52
3:B:230:LEU:C	3:B:230:LEU:HD23	2.30	0.52
3:A:282:TRP:CE2	3:B:327:LEU:HG	2.43	0.51
3:A:262:LYS:HG3	3:A:263:GLU:H	1.75	0.51
3:A:262:LYS:CG	3:A:263:GLU:N	2.73	0.51
3:B:200:PRO:CG	3:B:242:LEU:HD11	2.38	0.51
3:A:150:SER:C	3:A:152:ARG:N	2.61	0.51
3:A:234:ILE:HG22	3:A:263:GLU:HG3	1.92	0.51
3:A:147:LEU:O	3:A:149:HIS:N	2.43	0.51
3:A:151:ILE:HD12	3:A:154:ILE:HD12	1.93	0.51
3:A:282:TRP:HE3	3:A:284:PHE:CD2	2.28	0.51
3:B:216:VAL:HA	3:B:219:GLU:OE2	2.11	0.51
1:T:16:DG:C5'	3:A:169:LYS:HD2	2.40	0.51
3:B:324:ARG:HH11	3:B:324:ARG:HG3	1.77	0.50
3:A:284:PHE:CD1	3:A:289:ARG:HB3	2.46	0.50
3:A:152:ARG:NH1	3:A:152:ARG:HG2	2.23	0.50
2:S:26:DG:H2''	2:S:27:DC:OP2	2.11	0.50
3:B:228:ASP:OD1	3:B:228:ASP:N	2.40	0.50
3:B:172:ALA:HB1	3:B:177:LEU:O	2.12	0.50
3:A:307:LEU:O	3:A:308:SER:O	2.29	0.50
3:A:308:SER:OG	3:A:310:GLU:HB2	2.11	0.50
3:A:249:GLU:OE2	3:A:249:GLU:HA	2.12	0.50
3:B:247:MSE:HB2	3:B:251:GLU:HB3	1.93	0.50
2:S:21:DA:C2'	2:S:22:DA:C8	2.93	0.50
3:B:323:LEU:O	3:B:327:LEU:HD13	2.11	0.50
3:B:172:ALA:HB2	3:B:182:VAL:HG21	1.93	0.50
1:T:17:DA:H3'	3:A:168:GLN:HE22	1.77	0.50
3:B:178:SER:O	3:B:181:LYS:HB3	2.11	0.50
3:A:154:ILE:O	3:A:158:LEU:HG	2.11	0.50
3:B:218:ASP:C	3:B:220:MSE:H	2.16	0.49
2:S:3:DC:H2''	2:S:4:DG:O5'	2.12	0.49
3:A:242:LEU:O	3:A:242:LEU:HD23	2.12	0.49
2:S:20:DG:H2''	2:S:21:DA:C8	2.47	0.49
3:A:262:LYS:HG3	3:A:263:GLU:N	2.27	0.49
3:B:311:LEU:O	3:B:315:LEU:HG	2.12	0.49
3:B:287:LYS:O	3:B:287:LYS:HD2	2.13	0.49
3:B:199:PHE:CE1	3:B:205:LEU:HD21	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:207:PHE:HA	3:A:210:TYR:HD2	1.78	0.49
3:B:218:ASP:C	3:B:220:MSE:N	2.66	0.49
3:B:278:VAL:HG22	3:B:294:ARG:HG3	1.95	0.49
3:B:244:ILE:HG21	3:B:247:MSE:HE2	1.94	0.48
3:B:266:LEU:HD23	3:B:266:LEU:H	1.78	0.48
3:A:170:ASP:O	3:A:173:ALA:HB3	2.13	0.48
3:A:278:VAL:CG1	3:A:294:ARG:HB2	2.26	0.48
3:B:224:ASN:N	3:B:224:ASN:ND2	2.31	0.48
3:A:320:GLY:O	3:A:324:ARG:HD3	2.12	0.48
3:A:309:LYS:O	3:A:313:GLU:HB2	2.13	0.48
3:A:292:ARG:NH1	3:A:303:GLU:OE1	2.45	0.48
3:A:151:ILE:CG2	3:A:152:ARG:N	2.76	0.48
3:A:159:MSE:HA	3:A:162:LYS:HB3	1.96	0.48
3:B:251:GLU:O	3:B:255:LYS:HG2	2.13	0.48
3:B:289:ARG:HG2	3:B:289:ARG:NH1	2.29	0.48
3:B:201:VAL:HG21	3:B:249:GLU:CG	2.44	0.48
3:A:290:PHE:CE1	3:A:305:ASN:HB2	2.49	0.48
3:A:249:GLU:O	3:A:252:VAL:HG12	2.13	0.47
3:A:284:PHE:HD2	3:A:284:PHE:N	2.12	0.47
2:S:15:DA:H8	2:S:15:DA:OP2	1.96	0.47
3:B:226:GLU:HG2	3:B:295:VAL:HG12	1.95	0.47
1:T:30:DA:H2''	1:T:31:DT:H5'	1.96	0.47
3:B:263:GLU:HA	3:B:266:LEU:HD21	1.96	0.47
3:A:281:LEU:H	3:A:292:ARG:HA	1.78	0.47
2:S:23:DA:H1'	2:S:24:DT:H5'	1.94	0.47
3:B:233:ASN:HD21	3:B:279:THR:HG21	1.78	0.47
3:B:175:GLU:O	3:B:176:GLY:C	2.50	0.47
2:S:17:DC:C2'	2:S:18:DT:C6	2.97	0.47
3:B:224:ASN:O	3:B:227:PHE:HB2	2.15	0.47
3:B:152:ARG:O	3:B:155:GLY:N	2.47	0.47
3:A:207:PHE:O	3:A:210:TYR:HB2	2.14	0.47
3:B:201:VAL:HG21	3:B:249:GLU:HG2	1.96	0.47
3:A:238:ILE:HG22	3:A:239:ASN:N	2.30	0.47
3:A:192:PRO:HG2	3:A:217:GLY:HA3	1.96	0.47
3:B:237:GLU:C	3:B:240:ASP:HB3	2.35	0.47
3:B:194:GLU:O	3:B:195:LEU:HD23	2.14	0.47
3:A:232:GLN:O	3:A:236:PRO:HD3	2.14	0.47
3:B:204:GLU:OE1	3:B:249:GLU:HB3	2.15	0.47
2:S:19:DT:H2''	2:S:20:DG:N7	2.28	0.47
3:B:295:VAL:HG12	3:B:296:LYS:N	2.29	0.47
3:A:233:ASN:O	3:A:236:PRO:HD2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:289:ARG:HG3	3:A:306:ARG:HB3	1.97	0.46
2:S:17:DC:H2'	2:S:18:DT:H72	1.97	0.46
2:S:20:DG:H2''	2:S:21:DA:H8	1.81	0.46
3:B:323:LEU:HB3	3:B:327:LEU:CD1	2.45	0.46
3:A:276:SER:HA	3:A:296:LYS:HB3	1.97	0.46
3:B:188:ALA:C	3:B:190:SER:N	2.69	0.46
3:B:173:ALA:C	3:B:175:GLU:H	2.18	0.46
3:A:151:ILE:HG23	3:A:152:ARG:N	2.31	0.46
3:A:312:GLN:HG3	3:B:300:PHE:CZ	2.51	0.46
3:A:230:LEU:HD22	3:A:264:ALA:HB2	1.98	0.46
3:B:253:LYS:HZ3	3:B:253:LYS:HB2	1.81	0.46
3:A:191:ALA:HA	3:A:192:PRO:HD3	1.84	0.46
3:B:166:MSE:SE	3:B:171:ILE:HG12	2.65	0.46
3:A:192:PRO:HD3	3:A:214:CYS:CA	2.35	0.46
3:A:225:LEU:HD21	3:B:312:GLN:HG2	1.98	0.45
3:A:228:ASP:HA	3:A:231:ILE:HD12	1.97	0.45
3:A:313:GLU:CD	3:A:317:ARG:HH21	2.18	0.45
1:T:36:DA:OP2	1:T:36:DA:H8	1.98	0.45
3:A:307:LEU:HA	3:A:307:LEU:HD23	1.63	0.45
3:A:324:ARG:HG3	3:A:324:ARG:NH1	2.30	0.45
3:A:317:ARG:HH11	3:A:317:ARG:CG	2.20	0.45
3:A:312:GLN:O	3:A:316:ASP:HB2	2.15	0.45
3:A:211:LYS:O	3:A:215:ALA:HB2	2.17	0.45
3:A:315:LEU:HD23	3:B:322:ILE:HG21	1.98	0.45
3:A:172:ALA:HB1	3:A:177:LEU:O	2.16	0.45
3:A:206:THR:HG23	3:A:207:PHE:N	2.31	0.45
3:B:289:ARG:HG2	3:B:289:ARG:HH11	1.82	0.45
3:B:156:LEU:N	3:B:156:LEU:HD13	2.32	0.45
3:A:178:SER:O	3:A:181:LYS:N	2.44	0.45
2:S:5:DT:H2''	2:S:6:DG:C8	2.52	0.45
3:A:188:ALA:C	3:A:190:SER:H	2.20	0.45
3:B:233:ASN:HD21	3:B:279:THR:CG2	2.30	0.45
3:B:218:ASP:O	3:B:221:GLY:N	2.50	0.45
3:B:236:PRO:O	3:B:240:ASP:N	2.50	0.44
3:A:171:ILE:O	3:A:172:ALA:C	2.56	0.44
3:A:317:ARG:NH1	3:A:317:ARG:CG	2.78	0.44
3:B:231:ILE:O	3:B:235:SER:HB2	2.17	0.44
3:B:318:MSE:O	3:B:321:HIS:N	2.50	0.44
1:T:33:DG:H5'	1:T:33:DG:C8	2.52	0.44
3:A:252:VAL:O	3:A:256:ILE:HD13	2.18	0.44
3:A:324:ARG:NH1	3:A:324:ARG:CG	2.80	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:18:DT:H2'	1:T:19:DT:H72	1.99	0.44
3:A:158:LEU:CB	3:A:186:LEU:HD21	2.48	0.44
3:A:269:ASP:O	3:A:273:LYS:HG3	2.18	0.44
3:B:307:LEU:CD1	3:B:311:LEU:HD13	2.37	0.44
3:B:220:MSE:HG2	3:B:220:MSE:O	2.18	0.44
3:A:262:LYS:CD	3:A:263:GLU:N	2.80	0.44
3:B:195:LEU:HD23	3:B:195:LEU:N	2.32	0.43
3:A:156:LEU:HD13	3:A:156:LEU:C	2.39	0.43
3:A:206:THR:CG2	3:A:207:PHE:N	2.81	0.43
3:A:165:GLY:O	3:A:166:MSE:HG2	2.18	0.43
3:A:159:MSE:HG2	3:A:186:LEU:HD22	1.99	0.43
2:S:15:DA:H2''	2:S:16:DC:OP2	2.19	0.43
3:B:282:TRP:CD1	3:B:283:LYS:N	2.86	0.43
1:T:17:DA:H3'	3:A:168:GLN:NE2	2.33	0.43
3:A:298:ARG:HG3	3:B:306:ARG:HA	2.00	0.43
3:A:238:ILE:HG22	3:A:239:ASN:H	1.83	0.43
3:A:159:MSE:O	3:A:163:ASN:N	2.42	0.43
3:A:255:LYS:O	3:A:258:ARG:HB2	2.19	0.43
3:B:199:PHE:HA	3:B:200:PRO:HD3	1.88	0.43
3:A:161:MSE:O	3:A:162:LYS:C	2.57	0.43
3:B:226:GLU:OE1	3:B:277:VAL:HG23	2.18	0.43
3:B:221:GLY:O	3:B:222:ASN:CB	2.64	0.43
3:B:323:LEU:O	3:B:326:SER:N	2.51	0.43
3:B:175:GLU:HB3	3:B:177:LEU:HD12	2.01	0.43
3:A:225:LEU:HD11	3:B:312:GLN:NE2	2.34	0.43
3:B:188:ALA:O	3:B:190:SER:N	2.52	0.43
1:T:15:DC:H2''	1:T:16:DG:N7	2.34	0.42
3:A:282:TRP:HE3	3:A:284:PHE:CE2	2.36	0.42
3:A:289:ARG:HG3	3:A:306:ARG:CB	2.49	0.42
3:A:231:ILE:O	3:A:232:GLN:C	2.57	0.42
1:T:16:DG:N2	2:S:25:DC:N3	2.65	0.42
3:A:208:SER:HB3	4:A:1585:CIT:C2	2.48	0.42
3:A:225:LEU:HD21	3:B:312:GLN:HE21	1.85	0.42
3:A:300:PHE:CE1	3:B:304:PHE:HB2	2.53	0.42
3:A:288:ASP:OD1	3:A:288:ASP:N	2.52	0.42
2:S:17:DC:C6	2:S:18:DT:H72	2.54	0.42
3:A:238:ILE:CD1	3:A:256:ILE:HG13	2.30	0.42
3:A:178:SER:C	3:A:180:ALA:N	2.72	0.42
2:S:17:DC:C6	2:S:17:DC:C5'	2.94	0.42
3:B:324:ARG:HA	3:B:327:LEU:CD2	2.48	0.42
3:B:173:ALA:C	3:B:175:GLU:N	2.73	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:253:LYS:HZ3	3:B:253:LYS:CB	2.33	0.42
3:B:240:ASP:O	3:B:243:SER:N	2.45	0.42
2:S:4:DG:H2''	2:S:5:DT:H5'	2.00	0.42
3:A:241:ILE:HG22	3:A:241:ILE:O	2.20	0.42
2:S:15:DA:OP2	2:S:15:DA:C8	2.73	0.42
3:A:226:GLU:OE1	3:A:226:GLU:CA	2.59	0.41
1:T:16:DG:H2''	1:T:17:DA:O5'	2.20	0.41
3:A:315:LEU:O	3:A:316:ASP:C	2.57	0.41
3:A:251:GLU:O	3:A:255:LYS:HG2	2.21	0.41
2:S:17:DC:H2''	2:S:18:DT:C6	2.54	0.41
3:A:199:PHE:CZ	3:A:260:ILE:HD12	2.56	0.41
3:B:206:THR:HG22	3:B:208:SER:H	1.86	0.41
3:B:267:LEU:HB3	3:B:277:VAL:CG1	2.42	0.41
3:B:220:MSE:HE1	3:B:230:LEU:CD1	2.50	0.41
3:A:155:GLY:O	3:A:156:LEU:C	2.59	0.41
3:B:323:LEU:O	3:B:324:ARG:C	2.59	0.41
3:B:276:SER:HB3	3:B:296:LYS:HE3	2.01	0.41
3:B:231:ILE:CG2	3:B:231:ILE:O	2.68	0.41
3:A:322:ILE:HD13	3:A:322:ILE:HA	1.95	0.41
3:A:159:MSE:CE	3:A:162:LYS:HD3	2.51	0.41
3:A:212:THR:HA	3:A:215:ALA:HB3	2.02	0.41
3:A:186:LEU:O	3:A:187:GLN:C	2.59	0.41
3:A:201:VAL:C	3:A:203:SER:N	2.73	0.40
3:B:188:ALA:C	3:B:190:SER:H	2.23	0.40
3:B:251:GLU:OE1	3:B:251:GLU:CA	2.66	0.40
3:B:166:MSE:SE	3:B:174:LYS:HG3	2.72	0.40
3:A:193:GLU:HG2	3:A:193:GLU:H	1.48	0.40
3:B:234:ILE:HD13	3:B:234:ILE:N	2.33	0.40
3:B:234:ILE:HG12	3:B:238:ILE:HD11	2.03	0.40
3:A:281:LEU:HD11	3:A:293:LYS:HB2	2.03	0.40
3:B:209:ASP:OD2	3:B:253:LYS:HE3	2.21	0.40
3:B:233:ASN:ND2	3:B:279:THR:HG21	2.36	0.40
3:A:207:PHE:O	3:A:210:TYR:N	2.54	0.40
3:B:318:MSE:C	3:B:320:GLY:N	2.73	0.40
1:T:14:DG:H1	2:S:27:DC:H42	1.68	0.40
3:A:319:ILE:CD1	3:B:302:TYR:CG	3.04	0.40

All (1) 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:160:ARG:NH2	3:A:193:GLU:OE2[7_555]	2.15	0.05

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	
3	A	176/192 (92%)	149 (85%)	23 (13%)	4 (2%)	8	35
3	B	172/192 (90%)	136 (79%)	30 (17%)	6 (4%)	4	23
All	All	348/384 (91%)	285 (82%)	53 (15%)	10 (3%)	6	28

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	150	SER
3	A	308	SER
3	B	219	GLU
3	B	222	ASN
3	B	218	ASP
3	B	318	MSE
3	A	192	PRO
3	B	246	GLU
3	A	236	PRO
3	B	319	ILE

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	
3	A	158/164 (96%)	132 (84%)	26 (16%)	3	12
3	B	154/164 (94%)	125 (81%)	29 (19%)	2	9
All	All	312/328 (95%)	257 (82%)	55 (18%)	2	10

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	150	SER
3	A	152	ARG
3	A	159	MSE
3	A	164	ASP
3	A	166	MSE
3	A	193	GLU
3	A	202	GLN
3	A	203	SER
3	A	205	LEU
3	A	206	THR
3	A	208	SER
3	A	212	THR
3	A	214	CYS
3	A	222	ASN
3	A	228	ASP
3	A	229	GLN
3	A	238	ILE
3	A	256	ILE
3	A	262	LYS
3	A	269	ASP
3	A	284	PHE
3	A	288	ASP
3	A	303	GLU
3	A	306	ARG
3	A	313	GLU
3	A	324	ARG
3	B	152	ARG
3	B	156	LEU
3	B	157	ARG
3	B	164	ASP
3	B	175	GLU
3	B	190	SER
3	B	206	THR
3	B	211	LYS
3	B	212	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	B	222	ASN
3	B	224	ASN
3	B	228	ASP
3	B	229	GLN
3	B	234	ILE
3	B	237	GLU
3	B	244	ILE
3	B	245	ASN
3	B	251	GLU
3	B	253	LYS
3	B	257	LEU
3	B	281	LEU
3	B	288	ASP
3	B	289	ARG
3	B	293	LYS
3	B	313	GLU
3	B	316	ASP
3	B	317	ARG
3	B	318	MSE
3	B	327	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	222	ASN
3	B	202	GLN
3	B	224	ASN
3	B	233	ASN
3	B	312	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\# Z > 2$
4	CIT	A	1585	-	3,12,12	1.12	0	3,17,17	0.85	0
4	CIT	A	1586	-	3,12,12	1.00	0	3,17,17	0.71	0

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
4	CIT	A	1585	-	-	0/6/16/16	0/0/0/0
4	CIT	A	1586	-	-	0/6/16/16	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1585	CIT	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	T	25/25 (100%)	0.46	2 (8%) 15 7	45, 64, 84, 91	0
2	S	25/25 (100%)	0.40	1 (4%) 42 23	47, 62, 82, 90	0
3	A	174/192 (90%)	1.63	45 (25%) 1 1	48, 100, 145, 157	0
3	B	170/192 (88%)	1.32	31 (18%) 2 1	51, 89, 128, 149	0
All	All	394/434 (90%)	1.34	79 (20%) 1 1	45, 89, 142, 157	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	273	LYS	9.1
3	A	270	LYS	8.8
3	B	284	PHE	8.8
3	A	275	LYS	7.9
3	A	266	LEU	7.5
3	A	146	ALA	7.2
3	A	267	LEU	6.4
3	B	287	LYS	6.0
3	B	285	GLU	6.0
3	A	272	SER	5.9
3	A	244	ILE	5.8
3	A	262	LYS	5.8
3	A	216	VAL	5.7
3	B	270	LYS	5.4
3	A	269	ASP	5.2
3	A	241	ILE	5.0
3	A	257	LEU	4.9
3	B	288	ASP	4.8
3	A	243	SER	4.8
3	B	174	LYS	4.7
3	A	274	ASP	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	T	14	DG	4.5
3	A	179	GLN	4.3
3	B	290	PHE	4.3
3	A	263	GLU	4.3
3	B	289	ARG	4.2
3	A	237	GLU	4.2
3	A	229	GLN	4.1
3	A	298	ARG	4.1
3	B	278	VAL	4.1
3	A	227	PHE	4.1
3	B	164	ASP	3.9
3	A	156	LEU	3.9
3	B	165	GLY	3.8
3	A	282	TRP	3.7
3	B	283	LYS	3.7
3	A	195	LEU	3.7
3	B	292	ARG	3.6
3	A	171	ILE	3.6
3	B	160	ARG	3.5
3	A	169	LYS	3.5
3	B	162	LYS	3.5
3	A	260	ILE	3.4
3	A	264	ALA	3.3
3	B	286	ASP	3.2
3	B	307	LEU	3.2
3	B	171	ILE	3.2
3	A	248	ALA	3.2
3	B	242	LEU	3.1
3	A	198	LEU	3.1
3	B	258	ARG	3.1
3	A	219	GLU	3.0
3	B	306	ARG	3.0
2	S	27	DC	2.9
3	B	264	ALA	2.9
3	A	217	GLY	2.9
3	A	225	LEU	2.8
3	A	259	LEU	2.8
3	B	277	VAL	2.8
1	T	15	DC	2.8
3	A	255	LYS	2.8
3	B	305	ASN	2.8
3	A	271	GLY	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	B	266	LEU	2.7
3	A	238	ILE	2.6
3	B	179	GLN	2.6
3	A	295	VAL	2.4
3	B	246	GLU	2.4
3	A	224	ASN	2.4
3	B	230	LEU	2.3
3	A	323	LEU	2.2
3	A	182	VAL	2.2
3	A	230	LEU	2.2
3	A	312	GLN	2.2
3	B	158	LEU	2.1
3	B	291	ALA	2.1
3	A	276	SER	2.1
3	A	158	LEU	2.1
3	B	304	PHE	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(\AA^2)	Q<0.9
4	CIT	A	1585	13/13	0.37	0.35	1.49	153,166,170,172	0
4	CIT	A	1586	13/13	0.67	0.36	0.72	164,172,173,176	0

6.5 Other polymers

There are no such residues in this entry.