



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 12:47 AM UTC

PDB ID : 1ZX4 / pdb_00001zx4
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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

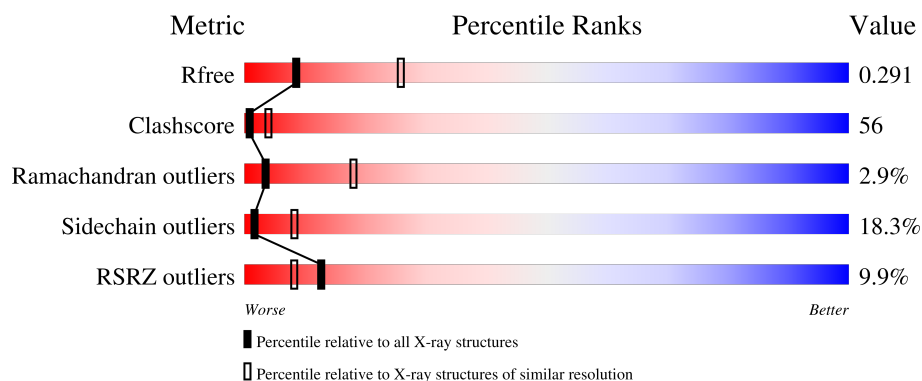
1 Overall quality at a glance

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}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (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 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 $\leq 5\%$. 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	4% 28% 72%
2	S	25	28% 68% .
3	A	192	12% 19% 55% 18% 6%
3	B	192	7% 20% 54% 17% 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:

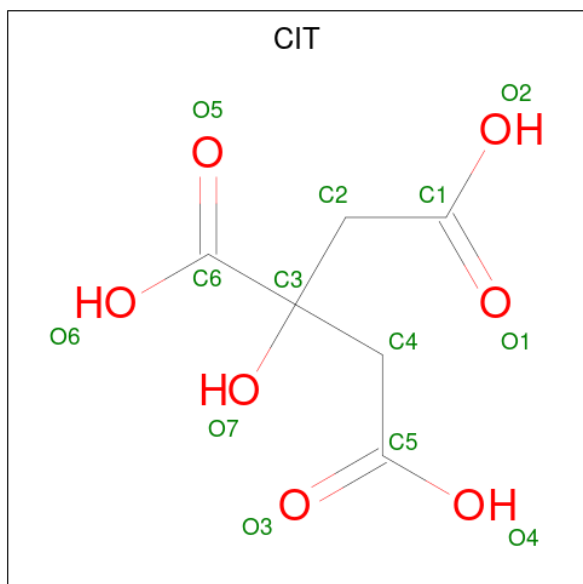
Chain	Residue	Modelled	Actual	Comment	Reference
A	159	MSE	MET	modified residue	UNP Q38420
A	161	MSE	MET	modified residue	UNP Q38420
A	166	MSE	MET	modified residue	UNP Q38420
A	220	MSE	MET	modified residue	UNP Q38420
A	245	ASN	ASP	conflict	UNP Q38420
A	247	MSE	MET	modified residue	UNP Q38420
A	318	MSE	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

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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 (CCD ID: 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

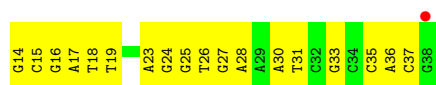
- Molecule 5 is water.

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

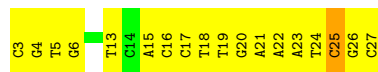
3 Residue-property plots [i](#)

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.

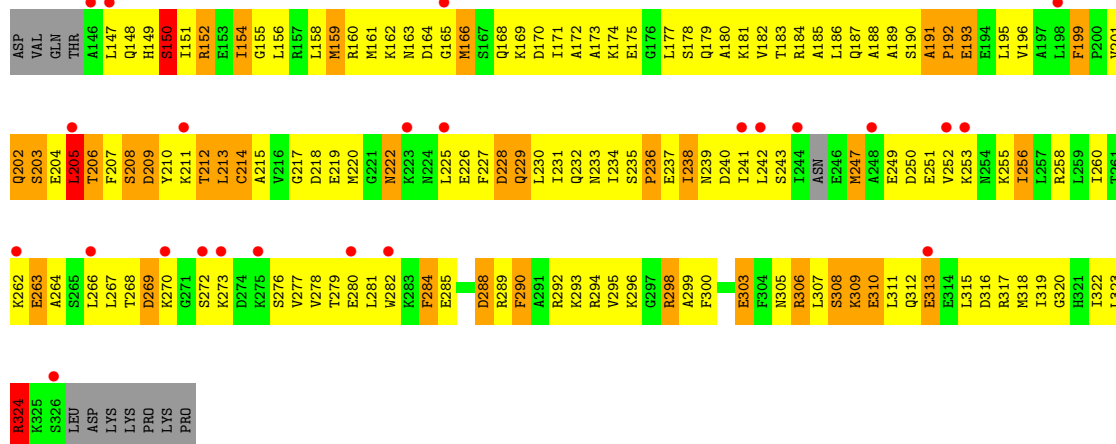
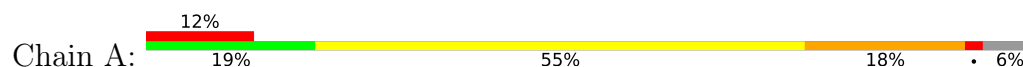
- Molecule 1: parS-small DNA centromere site



- Molecule 2: parS-small DNA centromere site



- Molecule 3: Plasmid Partition par B protein



- Molecule 3: Plasmid Partition par B protein



ASP	ASP	F207	T268	LYS
VAL	VAL	S208	D269	LYS
GLN	GLN	D209	K270	PRO
THR	THR	Y210	G271	LYS
ALA	ALA	K211	SER	PRO
LEU	LEU	T212	LYS	
GLN	GLN	L213	ASP	
HIS	HIS	C214	K275	
S150	S150	A215	S276	
I151	I151	V216	V277	
R152	R152	G217	V278	
E153	E153	D218	T279	
I154	I154	E219	E280	
G155	G155	N220	L281	
L156	L156	G221	W282	
R157	R157	N222	K283	
L158	L158	K223	F284	
M159	M159	N224	E285	
E160	E160	L225	D286	
M161	M161	E226	K287	
K162	K162	F227	D288	
N163	N163	D228	R289	
D164	D164	Q229		
G165	G165	L230	R292	
M166	M166	L231	K293	
		N232	R294	
D170	D170	N233	V295	
I171	I171	L234	K296	
A172	A172	S235	G297	
A173	A173	P236	R298	
K174	K174	E237	A299	
E175	E175	N238	F300	
G176	G176	N239	S301	
L177	L177	D240	Y302	
S178	S178	L241	E303	
Q179	Q179	L242	F304	
A180	A180	S243	N305	
K181	K181	L244	R306	
V182	V182	N245	L307	
T183	T183	E246	S308	
R184	R184	N247	K309	
A185	A185	A248	E310	
L186	L186	E249	L311	
Q187	Q187	N250	G312	
A188	A188	E251	E313	
A189	A189	V252	E314	
S190	S190	K253	L315	
A191	A191	N254	D316	
		K255	R317	
E194	E194	N256	K318	
L195	L195	L257	I319	
L198	L198	R258	G320	
F199	F199	L259	H321	
P200	P200		I322	
V201	V201	K262	L323	
E204	E204	E263	R324	
L205	L205	A264	K325	
T206	T206	S265	S326	
		L266	L327	
		L267	D328	

4 Data and refinement statistics

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α , β , γ	154.60Å 154.60Å 132.30Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	50.61 – 2.98 50.61 – 2.98	Depositor EDS
% Data completeness (in resolution range)	94.4 (50.61-2.98) 90.8 (50.61-2.98)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.93 (at 2.96Å)	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%)	wwPDB-VP
Wilson B-factor (Å ²)	72.7	Xtriage
Anisotropy	0.490	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.44 , 139.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	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, 0.333 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: 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	0.48	0/575	0.92	0/886
2	S	0.51	0/567	0.95	0/873
3	A	0.66	1/1445 (0.1%)	1.24	19/1919 (1.0%)
3	B	0.73	0/1412	1.26	22/1876 (1.2%)
All	All	0.64	1/3999 (0.0%)	1.16	41/5554 (0.7%)

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	205	LEU	CA-C	-5.16	1.46	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	154	ILE	N-CA-C	-9.70	100.93	110.72
3	B	164	ASP	N-CA-C	-8.95	101.62	112.54
3	B	239	ASN	N-CA-C	-8.73	102.06	112.89
3	B	213	LEU	N-CA-C	-8.04	101.80	111.69
3	A	309	LYS	N-CA-C	-7.98	103.68	113.50
3	B	238	ILE	N-CA-C	-7.33	105.50	111.81
3	B	298	ARG	N-CA-C	-7.08	105.46	112.97
3	A	272	SER	N-CA-C	-7.01	104.86	113.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	292	ARG	N-CA-C	6.80	118.45	108.86
3	B	265	SER	N-CA-C	6.50	118.02	111.07
3	A	209	ASP	N-CA-C	-6.36	103.98	111.03
3	A	199	PHE	N-CA-C	6.27	117.79	109.83
3	B	247	MSE	N-CA-C	6.23	118.34	110.24
3	B	162	LYS	N-CA-C	-6.16	104.48	111.07
3	A	183	THR	N-CA-C	-6.11	104.25	111.03
3	B	204	GLU	N-CA-C	6.08	120.70	113.28
3	B	174	LYS	N-CA-C	-6.08	105.96	113.19
3	B	207	PHE	N-CA-C	-6.07	104.30	111.03
3	A	266	LEU	N-CA-C	-5.98	106.52	113.88
3	A	285	GLU	N-CA-C	-5.96	104.86	111.71
3	B	233	ASN	CA-C-N	-5.93	114.69	122.16
3	B	233	ASN	C-N-CA	-5.93	114.69	122.16
3	B	243	SER	N-CA-C	-5.88	106.64	113.88
3	A	199	PHE	CA-C-N	5.83	127.13	119.84
3	A	199	PHE	C-N-CA	5.83	127.13	119.84
3	A	298	ARG	N-CA-C	-5.81	105.85	113.17
3	B	222	ASN	CA-C-N	-5.75	114.60	122.93
3	B	222	ASN	C-N-CA	-5.75	114.60	122.93
3	A	324	ARG	N-CA-C	-5.63	103.94	112.04
3	A	213	LEU	N-CA-C	-5.57	104.60	111.40
3	B	269	ASP	N-CA-C	-5.55	104.74	112.45
3	A	191	ALA	CA-C-N	5.54	126.77	119.84
3	A	191	ALA	C-N-CA	5.54	126.77	119.84
3	B	309	LYS	N-CA-C	-5.43	105.26	111.07
3	B	180	ALA	N-CA-C	-5.38	105.31	111.07
3	A	243	SER	N-CA-C	-5.38	105.33	111.14
3	B	210	TYR	N-CA-C	-5.35	104.69	111.11
3	A	250	ASP	N-CA-C	5.34	116.78	111.07
3	B	226	GLU	N-CA-C	-5.22	107.07	113.50
3	A	240	ASP	N-CA-C	-5.15	105.78	111.71
3	A	290	PHE	N-CA-C	5.05	116.91	108.99

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	36	0
3	A	1437	0	1472	189	1
3	B	1405	0	1444	171	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	404	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 56.

All (404) 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:HD22	3:B:224:ASN:N	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:A:270:LYS:HD2	3:A:277:VAL:HG22	1.54	0.89
3:B:208:SER:O	3:B:212:THR:HG23	1.70	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

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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:17:DC:H2'	2:S:18:DT:H71	1.59	0.83
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:226:GLU:HB3	3:B:277:VAL:HG21	1.63	0.80
3:B:267:LEU:HB3	3:B:277:VAL:HG13	1.61	0.80
2:S:19:DT:H2''	2:S:20:DG:C8	2.15	0.80
3:A:317:ARG:HG3	3:A:317:ARG:HH11	1.47	0.79
3:A:225:LEU:HD13	3:A:225:LEU:O	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
1:T:16:DG:H1	2:S:25:DC:H42	1.34	0.76
3:B:150:SER:N	3:B:153:GLU:HG3	2.01	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:OP1	1:T:24:DG:H4'	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:H5'	1:T:14:DG:C8	2.26	0.70
3:B:183:THR:O	3:B:187:GLN:HG3	1.92	0.70
3:A:152:ARG:HG2	3:A:152:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:323:LEU:C	3:B:327:LEU:HD13	2.17	0.68
3:B:275:LYS:HG2	3:B:276:SER:H	1.59	0.68
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:OE1	3:B:251:GLU:HA	1.93	0.68
1:T:16:DG:H1	2:S:25:DC:N4	1.92	0.67
3:B:324:ARG:HA	3:B:327:LEU:HD21	1.75	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
1:T:14:DG:H5'	1:T:14:DG:H8	1.61	0.66
3:A:270:LYS:HA	3:A:273:LYS:HB2	1.78	0.66
3:A:324:ARG:HG3	3:A:324:ARG:HH11	1.60	0.66
3:A:256:ILE:HD13	3:A:256:ILE:N	2.10	0.66
3:A:306:ARG:HG2	3:A:306:ARG:NH1	2.09	0.66
3:A:318:MSE:SE	3:A:318:MSE:C	2.89	0.65
3:B:177:LEU:CD2	3:B:181:LYS:HG2	2.26	0.65
3:A:256:ILE:HD13	3:A:256:ILE:H	1.61	0.65
3:B:263:GLU:O	3:B:266:LEU:HD23	1.96	0.65
3:B:155:GLY:HA3	3:B:189:ALA:HB2	1.77	0.65
3:B:187:GLN:O	3:B:190:SER:HB3	1.97	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: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
2:S:15:DA:H2'	2:S:15:DA:OP2	1.99	0.63
3:A:208:SER:HB3	4:A:1585:CIT:H21	1.80	0.63
3:A:247:MSE:HE3	3:A:252:VAL:HB	1.80	0.63
3:A:262:LYS:HD2	3:A:262:LYS:C	2.24	0.63
3:B:206:THR:HG22	3:B:207:PHE:N	2.11	0.63
3:A:150:SER:O	3:A:151:ILE:C	2.41	0.63
3:B:152:ARG:NH2	3:B:191:ALA:O	2.32	0.62
3:B:234:ILE:HD13	3:B:234:ILE:H	1.65	0.62
3:B:270:LYS:HB2	3:B:278:VAL:HB	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:T:14:DG:H2''	1:T:15:DC:O5'	2.01	0.61
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:147:LEU:O	3:A:148:GLN:C	2.45	0.60
3:A:201:VAL:HG21	3:A:249:GLU:CD	2.26	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
1:T:35:DC:H2''	1:T:36:DA:C8	2.38	0.59
3:A:270:LYS:CD	3:A:277:VAL:HG22	2.31	0.59
3:A:215:ALA:O	3:A:219:GLU:HG2	2.02	0.59
3:A:232:GLN:NE2	5:A:104:HOH:O	2.34	0.59
3:A:256:ILE:N	3:A:256:ILE:CD1	2.64	0.59
1:T:23:DA:H2''	1:T:24:DG:O5'	2.02	0.59
3:A:206:THR:HB	3:A:209:ASP:OD2	2.02	0.59
3:B:200:PRO:HG2	3:B:242:LEU:HD21	1.84	0.59
3:B:194:GLU:C	3:B:195:LEU:HD23	2.27	0.59
3:A:206:THR:O	3:A:209:ASP:HB2	2.02	0.59
3:B:199:PHE:CD1	3:B:205:LEU:HD21	2.38	0.58
3:B:318:MSE:HE3	3:B:318:MSE:HA	1.84	0.58
3:A:237:GLU:O	3:A:241:ILE:HG13	2.03	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:204:GLU:O	3:A:253:LYS:HD3	2.04	0.57
3:A:290:PHE:CZ	3:A:305:ASN:HB2	2.38	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:A:192:PRO:O	3:A:193:GLU:C	2.48	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
1:T:16:DG:OP2	1:T:16:DG:H8	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:284:PHE:N	3:A:284:PHE:CD2	2.73	0.56
3:B:230:LEU:HD23	3:B:230:LEU:C	2.30	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:208:SER:OG	4:A:1585:CIT:H41	2.06	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
3:A:147:LEU:C	3:A:149:HIS:N	2.60	0.56
3:A:150:SER:C	3:A:152:ARG:N	2.61	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
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:A:276:SER:CB	3:A:296:LYS:HB3	2.36	0.55
3:B:262:LYS:HG3	3:B:263:GLU:N	2.21	0.55
1:T:30:DA:H1'	1:T:31:DT:H5''	1.89	0.55
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
3:B:218:ASP:C	3:B:220:MSE:H	2.16	0.54
1:T:16:DG:H5'	3:A:169:LYS:HD2	1.90	0.54
1:T:24:DG:H2''	1:T:25:DG:O5'	2.08	0.54
1:T:37:DC:OP2	1:T:37:DC:H6	1.91	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
2:S:4:DG:H2''	2:S:5:DT:H5''	1.89	0.54
3:A:281:LEU:HD13	3:A:292:ARG:CA	2.36	0.54
3:B:177:LEU:HD22	3:B:181:LYS:CG	2.31	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:218:ASP:C	3:B:220:MSE:N	2.66	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
3:B:276:SER:HB3	3:B:296:LYS:CE	2.38	0.53
3:A:317:ARG:HG3	3:A:317:ARG:NH1	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:262:LYS:HD2	3:A:263:GLU:N	2.24	0.53
3:B:211:LYS:O	3:B:214:CYS:HB2	2.09	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
3:A:296:LYS:O	3:A:296:LYS:HG3	2.09	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:173:ALA:C	3:B:175:GLU:H	2.18	0.52
3:A:282:TRP:CE2	3:B:327:LEU:HG	2.43	0.51
3:B:175:GLU:O	3:B:176:GLY:C	2.50	0.51
3:B:237:GLU:C	3:B:240:ASP:HB3	2.35	0.51
3:A:262:LYS:CG	3:A:263:GLU:N	2.73	0.51
3:A:262:LYS:HG3	3:A:263:GLU:H	1.75	0.51
3:B:200:PRO:CG	3:B:242:LEU:HD11	2.38	0.51
3:A:147:LEU:O	3:A:149:HIS:N	2.43	0.51
3:A:234:ILE:HG22	3:A:263:GLU:HG3	1.92	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:HG3	3:B:324:ARG:HH11	1.77	0.50
2:S:26:DG:H2''	2:S:27:DC:OP2	2.11	0.50
3:A:152:ARG:HG2	3:A:152:ARG:NH1	2.23	0.50
3:A:284:PHE:CD1	3:A:289:ARG:HB3	2.46	0.50
3:B:228:ASP:OD1	3:B:228:ASP:N	2.40	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:B:172:ALA:HB1	3:B:177:LEU:O	2.12	0.50
3:A:249:GLU:HA	3:A:249:GLU:OE2	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:A:313:GLU:CD	3:A:317:ARG:HH21	2.18	0.50
3:B:323:LEU:O	3:B:327:LEU:HD13	2.11	0.50
1:T:17:DA:H3'	3:A:168:GLN:HE22	1.77	0.50
3:B:172:ALA:HB2	3:B:182:VAL:HG21	1.93	0.50
3:A:154:ILE:O	3:A:158:LEU:HG	2.11	0.50
3:A:188:ALA:C	3:A:190:SER:H	2.20	0.50
3:B:178:SER:O	3:B:181:LYS:HB3	2.11	0.50
2:S:3:DC:H2''	2:S:4:DG:O5'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:242:LEU:O	3:A:242:LEU:HD23	2.12	0.49
3:B:188:ALA:C	3:B:190:SER:N	2.69	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:A:171:ILE:O	3:A:172:ALA:C	2.56	0.49
3:B:287:LYS:HD2	3:B:287:LYS:O	2.13	0.49
3:B:311:LEU:O	3:B:315:LEU:HG	2.12	0.49
3:A:207:PHE:HA	3:A:210:TYR:HD2	1.78	0.49
3:B:199:PHE:CE1	3:B:205:LEU:HD21	2.46	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:A:320:GLY:O	3:A:324:ARG:HD3	2.12	0.48
3:B:224:ASN:ND2	3:B:224:ASN:N	2.31	0.48
3:A:292:ARG:NH1	3:A:303:GLU:OE1	2.45	0.48
3:A:309:LYS:O	3:A:313:GLU:HB2	2.13	0.48
3:A:151:ILE:CG2	3:A:152:ARG:N	2.76	0.48
3:A:156:LEU:HD13	3:A:156:LEU:C	2.39	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:NH1	3:B:289:ARG:HG2	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
2:S:15:DA:OP2	2:S:15:DA:H8	1.96	0.47
3:A:161:MSE:O	3:A:162:LYS:C	2.57	0.47
3:A:249:GLU:O	3:A:252:VAL:HG12	2.13	0.47
3:A:284:PHE:N	3:A:284:PHE:HD2	2.12	0.47
1:T:30:DA:H2''	1:T:31:DT:H5'	1.96	0.47
3:B:226:GLU:HG2	3:B:295:VAL:HG12	1.95	0.47
3:B:263:GLU:HA	3:B:266:LEU:HD21	1.96	0.47
2:S:23:DA:H1'	2:S:24:DT:H5'	1.94	0.47
3:A:281:LEU:H	3:A:292:ARG:HA	1.78	0.47
3:B:233:ASN:HD21	3:B:279:THR:HG21	1.78	0.47
3:A:231:ILE:O	3:A:232:GLN:C	2.57	0.47
2:S:17:DC:C2'	2:S:18:DT:C6	2.97	0.47
3:A:207:PHE:O	3:A:210:TYR:HB2	2.14	0.47
3:B:152:ARG:O	3:B:155:GLY:N	2.47	0.47
3:B:201:VAL:HG21	3:B:249:GLU:HG2	1.96	0.47
3:B:224:ASN:O	3:B:227:PHE:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:192:PRO:HG2	3:A:217:GLY:HA3	1.96	0.47
3:A:232:GLN:O	3:A:236:PRO:HD3	2.14	0.47
3:A:238:ILE:HG22	3:A:239:ASN:N	2.30	0.47
3:B:194:GLU:O	3:B:195:LEU:HD23	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:A:233:ASN:O	3:A:236:PRO:HD2	2.14	0.47
3:B:295:VAL:HG12	3:B:296:LYS:N	2.29	0.47
3:A:289:ARG:HG3	3:A:306:ARG:HB3	1.97	0.46
2:S:17:DC:H2'	2:S:18:DT:C7	2.38	0.46
2:S:20:DG:H2''	2:S:21:DA:H8	1.81	0.46
3:A:276:SER:HA	3:A:296:LYS:HB3	1.97	0.46
3:B:323:LEU:HB3	3:B:327:LEU:CD1	2.45	0.46
3:A:315:LEU:O	3:A:316:ASP:C	2.57	0.46
3:A:230:LEU:HD22	3:A:264:ALA:HB2	1.98	0.46
3:A:312:GLN:HG3	3:B:300:PHE:CZ	2.51	0.46
3:B:253:LYS:HB2	3:B:253:LYS:HZ3	1.81	0.46
3:A:155:GLY:O	3:A:156:LEU:C	2.59	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:B:323:LEU:O	3:B:324:ARG:C	2.59	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
1:T:36:DA:OP2	1:T:36:DA:H8	1.98	0.45
3:A:307:LEU:HD23	3:A:307:LEU:HA	1.63	0.45
3:A:324:ARG:HG3	3:A:324:ARG:NH1	2.30	0.45
3:A:211:LYS:O	3:A:215:ALA:HB2	2.17	0.45
3:A:312:GLN:O	3:A:316:ASP:HB2	2.15	0.45
3:A:317:ARG:HH11	3:A:317:ARG:CG	2.20	0.45
3:A:172:ALA:HB1	3:A:177:LEU:O	2.16	0.45
3:A:315:LEU:HD23	3:B:322:ILE:HG21	1.98	0.45
3:B:188:ALA:C	3:B:190:SER:H	2.23	0.45
3:A:178:SER:O	3:A:181:LYS:N	2.44	0.45
3:A:206:THR:HG23	3:A:207:PHE:N	2.31	0.45
3:B:156:LEU:N	3:B:156:LEU:HD13	2.32	0.45
3:B:289:ARG:HG2	3:B:289:ARG:HH11	1.82	0.45
2:S:5:DT:H2''	2:S:6:DG:C8	2.52	0.45
3:A:229:GLN:CD	3:A:267:LEU:HD13	2.42	0.45
3:B:233:ASN:HD21	3:B:279:THR:CG2	2.30	0.45
3:A:186:LEU:O	3:A:187:GLN:C	2.59	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:286:ASP:C	3:B:288:ASP:H	2.25	0.44
3:B:318:MSE:C	3:B:320:GLY:N	2.73	0.44
3:A:220:MSE:HE3	3:A:226:GLU:C	2.42	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
1:T:33:DG:H5'	1:T:33:DG:C8	2.52	0.44
3:A:151:ILE:HG23	3:A:152:ARG:N	2.31	0.44
3:B:318:MSE:O	3:B:321:HIS:N	2.50	0.44
3:A:252:VAL:O	3:A:256:ILE:HD13	2.18	0.44
1:T:18:DT:H2'	1:T:19:DT:H72	1.99	0.44
3:A:324:ARG:NH1	3:A:324:ARG:CG	2.80	0.44
3:A:158:LEU:CB	3:A:186:LEU:HD21	2.48	0.44
3:B:186:LEU:O	3:B:187:GLN:C	2.59	0.44
3:B:218:ASP:O	3:B:219:GLU:C	2.61	0.44
3:A:262:LYS:CD	3:A:263:GLU:N	2.80	0.44
3:A:269:ASP:O	3:A:273:LYS:HG3	2.18	0.44
3:B:204:GLU:OE1	3:B:249:GLU:C	2.61	0.44
3:B:220:MSE:O	3:B:220:MSE:HG2	2.18	0.44
3:B:297:GLY:C	3:B:299:ALA:H	2.25	0.44
3:B:307:LEU:CD1	3:B:311:LEU:HD13	2.37	0.44
3:A:195:LEU:O	3:A:196:VAL:C	2.59	0.43
3:B:195:LEU:HD23	3:B:195:LEU:N	2.32	0.43
3:A:206:THR:CG2	3:A:207:PHE:N	2.81	0.43
2:S:15:DA:H2''	2:S:16:DC:OP2	2.19	0.43
3:A:159:MSE:HG2	3:A:186:LEU:HD22	1.99	0.43
3:A:165:GLY:O	3:A:166:MSE:HG2	2.18	0.43
3:A:178:SER:C	3:A:180:ALA:N	2.72	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:281:LEU:HD13	3:A:292:ARG:C	2.43	0.43
3:A:298:ARG:HG3	3:B:306:ARG:HA	2.00	0.43
3:B:314:GLU:O	3:B:315:LEU:C	2.61	0.43
3:A:159:MSE:O	3:A:163:ASN:N	2.42	0.43
3:A:238:ILE:HG22	3:A:239:ASN:H	1.83	0.43
3:A:255:LYS:O	3:A:258:ARG:HB2	2.19	0.43
3:B:173:ALA:C	3:B:175:GLU:N	2.73	0.43
3:B:199:PHE:HA	3:B:200:PRO:HD3	1.88	0.43
3:B:221:GLY:O	3:B:222:ASN:CB	2.64	0.43
3:B:226:GLU:OE1	3:B:277:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:225:LEU:HD11	3:B:312:GLN:NE2	2.34	0.43
3:B:175:GLU:HB3	3:B:177:LEU:HD12	2.01	0.43
3:B:188:ALA:O	3:B:190:SER:N	2.52	0.43
3:B:323:LEU:O	3:B:326:SER:N	2.51	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
1:T:16:DG:N2	2:S:25:DC:N3	2.65	0.42
3:A:201:VAL:C	3:A:203:SER:N	2.73	0.42
3:A:208:SER:HB3	4:A:1585:CIT:C2	2.48	0.42
3:B:210:TYR:O	3:B:211:LYS:C	2.61	0.42
3:A:225:LEU:HD21	3:B:312:GLN:HE21	1.85	0.42
3:A:288:ASP:OD1	3:A:288:ASP:N	2.52	0.42
3:A:300:PHE:CE1	3:B:304:PHE:HB2	2.53	0.42
3:A:238:ILE:CD1	3:A:256:ILE:HG13	2.30	0.42
2:S:17:DC:C5'	2:S:17:DC:C6	2.94	0.42
3:B:324:ARG:HA	3:B:327:LEU:CD2	2.48	0.42
3:A:230:LEU:O	3:A:231:ILE:C	2.63	0.42
3:B:253:LYS:HZ3	3:B:253:LYS:CB	2.33	0.42
2:S:4:DG:H2''	2:S:5:DT:H5'	2.00	0.42
3:B:240:ASP:O	3:B:243:SER:N	2.45	0.42
3:B:318:MSE:O	3:B:319:ILE:C	2.61	0.42
2:S:15:DA:OP2	2:S:15:DA:C8	2.73	0.42
3:A:241:ILE:HG22	3:A:241:ILE:O	2.20	0.42
1:T:16:DG:H2''	1:T:17:DA:O5'	2.20	0.41
3:A:226:GLU:OE1	3:A:226:GLU:CA	2.59	0.41
3:A:188:ALA:C	3:A:190:SER:N	2.78	0.41
3:A:251:GLU:O	3:A:255:LYS:HG2	2.21	0.41
3:A:178:SER:O	3:A:179:GLN:C	2.62	0.41
3:A:311:LEU:O	3:A:312:GLN:C	2.62	0.41
3:B:152:ARG:O	3:B:153:GLU:C	2.61	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:220:MSE:HE1	3:B:230:LEU:CD1	2.50	0.41
3:B:267:LEU:HB3	3:B:277:VAL:CG1	2.42	0.41
3:A:322:ILE:HD13	3:A:322:ILE:HA	1.95	0.41
3:B:231:ILE:O	3:B:231:ILE:CG2	2.68	0.41
3:B:276:SER:HB3	3:B:296:LYS:HE3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:209:ASP:O	3:B:210:TYR:C	2.63	0.41
3:A:225:LEU:HD13	3:A:225:LEU:C	2.44	0.40
3:B:166:MSE:SE	3:B:174:LYS:HG3	2.72	0.40
3:B:251:GLU:OE1	3:B:251:GLU:CA	2.66	0.40
3:A:193:GLU:H	3:A:193:GLU:HG2	1.48	0.40
3:A:201:VAL:O	3:A:202:GLN:C	2.63	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: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:207:PHE:O	3:A:210:TYR:N	2.54	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
3:B:323:LEU:C	3:B:327:LEU:CD1	2.91	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%)	5	23
3	B	172/192 (90%)	136 (79%)	30 (17%)	6 (4%)	3	14
All	All	348/384 (91%)	285 (82%)	53 (15%)	10 (3%)	3	18

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 ⓘ

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%)	129 (82%)	29 (18%)	1	8
3	B	154/164 (94%)	126 (82%)	28 (18%)	2	8
All	All	312/328 (95%)	255 (82%)	57 (18%)	2	8

All (57) 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

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Mol	Chain	Res	Type
3	A	228	ASP
3	A	229	GLN
3	A	238	ILE
3	A	247	MSE
3	A	256	ILE
3	A	263	GLU
3	A	269	ASP
3	A	284	PHE
3	A	288	ASP
3	A	303	GLU
3	A	306	ARG
3	A	310	GLU
3	A	313	GLU
3	A	323	LEU
3	A	324	ARG
3	B	156	LEU
3	B	157	ARG
3	B	175	GLU
3	B	190	SER
3	B	204	GLU
3	B	206	THR
3	B	211	LYS
3	B	212	THR
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	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	310	GLU
3	B	313	GLU
3	B	316	ASP
3	B	317	ARG
3	B	318	MSE

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Mol	Chain	Res	Type
3	B	327	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	149	HIS
3	A	222	ASN
3	B	168	GLN
3	B	202	GLN
3	B	224	ASN
3	B	233	ASN
3	B	239	ASN
3	B	312	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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
4	CIT	A	1585	-	12,12,12	1.60	3 (25%)	17,17,17	1.44	1 (5%)
4	CIT	A	1586	-	12,12,12	1.19	1 (8%)	17,17,17	1.29	1 (5%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1585	CIT	C3-C6	3.63	1.57	1.53
4	A	1586	CIT	C4-C3	2.24	1.56	1.54
4	A	1585	CIT	C4-C3	2.24	1.56	1.54
4	A	1585	CIT	C2-C3	2.11	1.56	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1585	CIT	O6-C6-C3	4.12	121.05	113.14
4	A	1586	CIT	O6-C6-C3	3.59	120.03	113.14

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%)	-0.12	1 (4%) 42 26	45, 64, 84, 91	0
2	S	25/25 (100%)	-0.18	0 100 100	47, 62, 82, 90	0
3	A	174/192 (90%)	0.81	24 (13%) 6 4	48, 100, 145, 157	0
3	B	170/192 (88%)	0.74	14 (8%) 17 11	51, 89, 128, 149	0
All	All	394/434 (90%)	0.66	39 (9%) 13 8	45, 89, 142, 157	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	328	ASP	6.1
3	B	271	GLY	6.1
3	A	266	LEU	4.0
3	B	223	LYS	3.6
3	A	275	LYS	3.5
3	B	275	LYS	3.4
3	B	174	LYS	3.4
3	B	285	GLU	3.2
3	A	223	LYS	3.1
3	A	262	LYS	3.1
3	A	244	ILE	3.0
3	A	273	LYS	3.0
3	A	242	LEU	2.9
3	A	147	LEU	2.9
3	A	198	LEU	2.8
3	A	270	LYS	2.8
3	B	284	PHE	2.7
3	A	252	VAL	2.7
3	A	225	LEU	2.6
3	A	241	ILE	2.6
3	B	264	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	A	248	ALA	2.5
3	B	206	THR	2.5
3	A	280	GLU	2.5
3	A	165	GLY	2.4
1	T	38	DG	2.4
3	A	326	SER	2.4
3	B	283	LYS	2.3
3	A	205	LEU	2.3
3	B	165	GLY	2.3
3	B	162	LYS	2.3
3	A	272	SER	2.3
3	A	282	TRP	2.2
3	A	146	ALA	2.2
3	A	211	LYS	2.2
3	B	198	LEU	2.2
3	B	160	ARG	2.1
3	A	313	GLU	2.1
3	A	253	LYS	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
4	CIT	A	1585	13/13	0.54	0.15	153,166,170,172	0
4	CIT	A	1586	13/13	0.78	0.13	164,172,173,176	0

6.5 Other polymers ⓘ

There are no such residues in this entry.