



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 09:37 PM GMT

PDB ID : 1PVQ
Title : BASIS FOR A SWITCH IN SUBSTRATE SPECIFICITY: CRYSTAL STRUCTURE OF SELECTED VARIANT OF CRE SITE-SPECIFIC RECOMBINASE, LNSGG BOUND TO THE ENGINEERED RECOGNITION SITE LOXM7
Authors : Baldwin, E.P.; Martin, S.S.; Abel, J.; Gelato, K.A.; Kim, H.; Schultz, P.G.; Santoro, S.W.
Deposited on : 2003-06-28
Resolution : 2.75 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

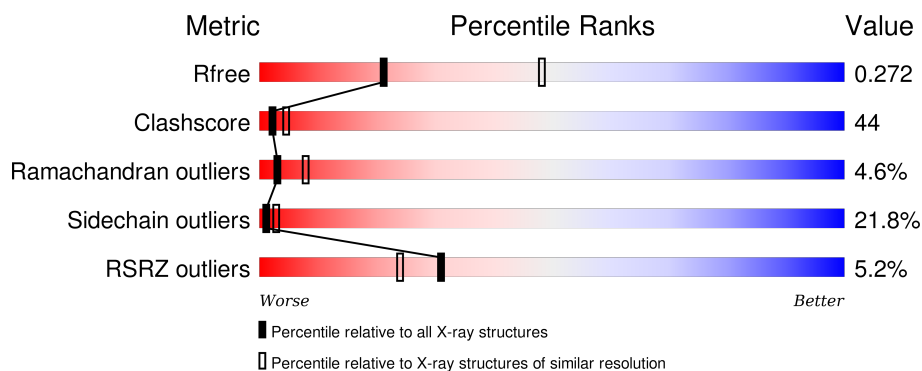
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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	C	34	<div> <div>9%</div> <div>12% 47% 38% .</div> </div>
2	D	34	<div> <div>3%</div> <div>24% 59% 18%</div> </div>
3	A	349	<div> <div>8%</div> <div>34% 42% 15% . 7%</div> </div>
3	B	349	<div> <div>%</div> <div>40% 42% 9% . 9%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6633 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 34-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	34	Total	C	N	O	P	0	4	0
			737	357	129	216	35			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	7	DC	T	ENGINEERED	GB 215623
C	8	DT	C	ENGINEERED	GB 215623
C	9	DA	G	ENGINEERED	GB 215623
C	26	DT	C	ENGINEERED	GB 215623
C	27	DA	G	ENGINEERED	GB 215623
C	28	DG	A	ENGINEERED	GB 215623

- Molecule 2 is a DNA chain called 34-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	34	Total	C	N	O	P	0	5	0
			774	375	138	224	37			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	7	DC	T	ENGINEERED	GB 215626
D	8	DT	C	ENGINEERED	GB 215626
D	9	DA	G	ENGINEERED	GB 215626
D	26	DT	C	ENGINEERED	GB 215626
D	27	DA	G	ENGINEERED	GB 215626
D	28	DG	A	ENGINEERED	GB 215626

- Molecule 3 is a protein called Recombinase CRE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	323	Total 2543	C 1579	N 485	O 464	S 15	38	0	0
3	B	319	Total 2512	C 1561	N 481	O 455	S 15	4	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	Initiating Methionine	UNP P06956
A	-4	HIS	-	EXPRESSION TAG	UNP P06956
A	-3	HIS	-	EXPRESSION TAG	UNP P06956
A	-2	HIS	-	EXPRESSION TAG	UNP P06956
A	-1	HIS	-	EXPRESSION TAG	UNP P06956
A	0	HIS	-	EXPRESSION TAG	UNP P06956
A	1	HIS	-	EXPRESSION TAG	UNP P06956
A	174	LEU	ILE	ENGINEERED	UNP P06956
A	258	ASN	THR	ENGINEERED	UNP P06956
A	259	SER	ARG	ENGINEERED	UNP P06956
A	262	GLY	GLU	ENGINEERED	UNP P06956
A	266	GLY	GLU	ENGINEERED	UNP P06956
B	-5	MET	-	Initiating Methionine	UNP P06956
B	-4	HIS	-	EXPRESSION TAG	UNP P06956
B	-3	HIS	-	EXPRESSION TAG	UNP P06956
B	-2	HIS	-	EXPRESSION TAG	UNP P06956
B	-1	HIS	-	EXPRESSION TAG	UNP P06956
B	0	HIS	-	EXPRESSION TAG	UNP P06956
B	1	HIS	-	EXPRESSION TAG	UNP P06956
B	174	LEU	ILE	ENGINEERED	UNP P06956
B	258	ASN	THR	ENGINEERED	UNP P06956
B	259	SER	ARG	ENGINEERED	UNP P06956
B	262	GLY	GLU	ENGINEERED	UNP P06956
B	266	GLY	GLU	ENGINEERED	UNP P06956

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	22	Total 22	O 22	0	0
4	B	30	Total 30	O 30	0	0
4	C	7	Total 7	O 7	0	0
4	D	8	Total 8	O 8	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.

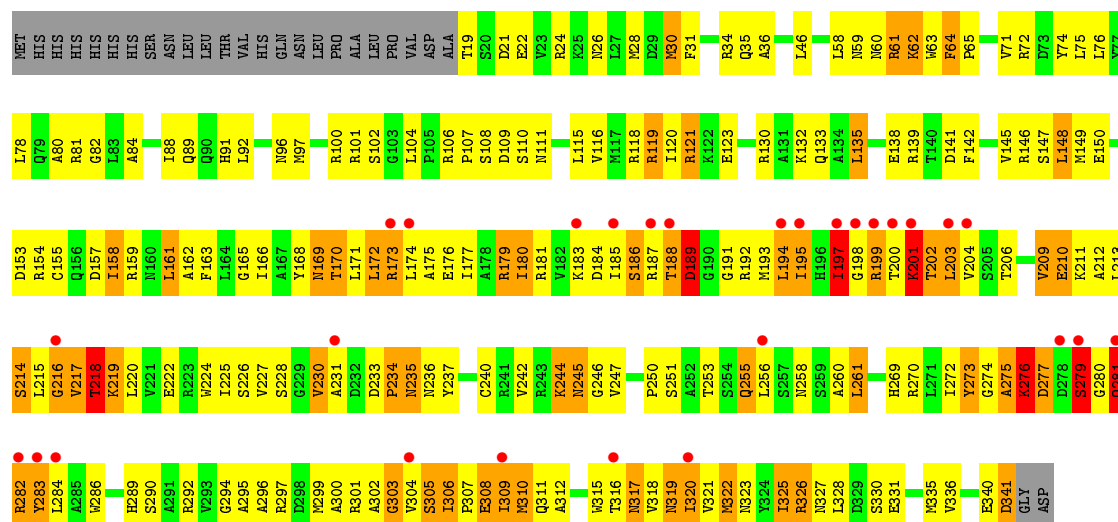
- Molecule 1: 34-MER

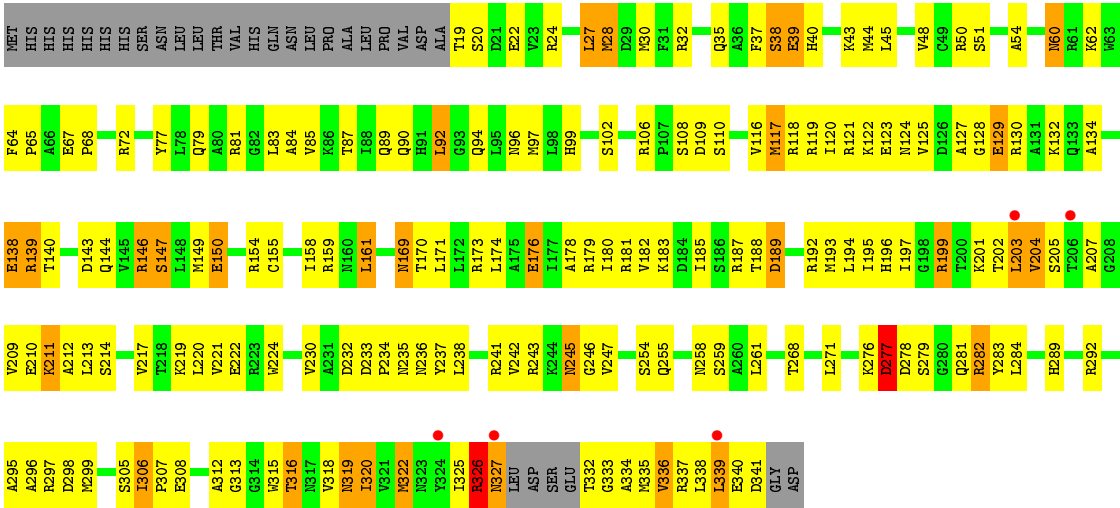


- Molecule 2: 34-MER



- Molecule 3: Recombinase CRE





4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	107.41Å 121.35Å 180.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.75 90.31 – 2.75	Depositor EDS
% Data completeness (in resolution range)	97.0 (5.00-2.75) 95.6 (90.31-2.75)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.70 (at 2.73Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.224 , 0.281 0.216 , 0.272	Depositor DCC
R_{free} test set	1190 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 88.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 29661 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6633	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.19% 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

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	C	0.67	1/826 (0.1%)	2.47	28/1274 (2.2%)
2	D	0.62	0/868	1.36	8/1337 (0.6%)
3	A	0.37	0/2584	0.77	7/3484 (0.2%)
3	B	0.45	0/2552	0.72	1/3439 (0.0%)
All	All	0.48	1/6830 (0.0%)	1.21	44/9534 (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	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	18[B]	DA	O3'-P	8.00	1.70	1.61

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	18[B]	DA	O3'-P-O5'	36.17	172.72	104.00
1	C	16[A]	DG	OP2-P-O3'	-25.79	48.46	105.20
1	C	16[B]	DG	OP2-P-O3'	-25.79	48.46	105.20
1	C	16[A]	DG	O3'-P-O5'	23.03	147.76	104.00
1	C	16[B]	DG	O3'-P-O5'	23.03	147.76	104.00
1	C	18[B]	DA	OP2-P-O3'	-18.37	64.80	105.20
1	C	18[B]	DA	OP1-P-O3'	-11.86	79.11	105.20
1	C	20	DG	C4-N9-C1'	-8.73	115.15	126.50
3	A	64	PHE	C-N-CD	-7.97	103.07	120.60
3	A	235	ASN	N-CA-C	-7.80	89.95	111.00
1	C	20	DG	C8-N9-C1'	7.65	136.95	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	4	DA	O4'-C1'-N9	7.58	113.31	108.00
1	C	34	DT	O4'-C1'-N1	7.31	113.12	108.00
1	C	27	DA	O4'-C1'-N9	7.21	113.05	108.00
1	C	17[B]	DT	P-O5'-C5'	-7.15	109.46	120.90
2	D	10	DT	C3'-C2'-C1'	-7.11	93.97	102.50
1	C	28	DG	O4'-C1'-N9	7.00	112.90	108.00
1	C	18[B]	DA	C8-N9-C4	6.79	108.52	105.80
3	A	319	ASN	N-CA-C	-6.76	92.74	111.00
3	A	326	ARG	N-CA-C	6.75	129.23	111.00
2	D	21	DT	C1'-O4'-C4'	-6.61	103.49	110.10
3	A	189	ASP	N-CA-C	6.59	128.80	111.00
1	C	9	DA	C8-N9-C4	6.53	108.41	105.80
3	B	326	ARG	N-CA-C	6.43	128.36	111.00
2	D	13	DA	P-O5'-C5'	-6.30	110.82	120.90
1	C	25	DA	P-O5'-C5'	-6.25	110.89	120.90
2	D	20[A]	DA	P-O3'-C3'	-6.25	112.20	119.70
1	C	18[B]	DA	C4-N9-C1'	-6.24	115.06	126.30
3	A	281	GLN	N-CA-C	6.20	127.74	111.00
1	C	17[B]	DT	C1'-O4'-C4'	-5.98	104.12	110.10
2	D	7	DC	C6-N1-C2	5.95	122.68	120.30
1	C	26	DT	P-O3'-C3'	-5.90	112.62	119.70
1	C	3	DA	P-O5'-C5'	-5.80	111.61	120.90
1	C	14	DA	C3'-C2'-C1'	-5.61	95.77	102.50
2	D	21	DT	P-O5'-C5'	-5.44	112.19	120.90
1	C	18[B]	DA	N9-C1'-C2'	5.36	122.78	112.60
1	C	32	DT	P-O5'-C5'	-5.32	112.39	120.90
2	D	4	DA	O4'-C1'-N9	5.28	111.70	108.00
1	C	24	DT	C6-N1-C2	5.12	123.86	121.30
1	C	25	DA	O4'-C4'-C3'	-5.12	102.45	104.50
1	C	27	DA	C3'-C2'-C1'	-5.08	96.40	102.50
3	A	183	LYS	N-CA-C	-5.06	97.33	111.00
2	D	1	DA	O4'-C1'-N9	-5.01	104.49	108.00
1	C	9	DA	C4-N9-C1'	-5.01	117.28	126.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	16[A]	DG	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	C	737	0	414	51	0
2	D	774	0	424	76	0
3	A	2543	0	2563	281	0
3	B	2512	0	2536	192	0
4	A	22	0	0	4	0
4	B	30	0	0	3	0
4	C	7	0	0	0	0
4	D	8	0	0	0	0
All	All	6633	0	5937	544	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (544) 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)
3:A:171:LEU:HD13	3:A:312:ALA:HB1	1.20	1.11
3:A:325:ILE:HG23	3:A:331:GLU:HG3	1.22	1.11
3:A:201:LYS:HE3	3:A:201:LYS:HA	1.33	1.08
3:A:213:LEU:HB3	3:A:217:VAL:HG23	1.33	1.06
2:D:33:DA:H2"	2:D:34:DT:H5"	1.36	1.05
3:B:178:ALA:HB2	3:B:261:LEU:HD11	1.39	1.00
3:A:145:VAL:HG22	3:A:272:ILE:HD11	1.42	0.99
1:C:5:DC:H2"	1:C:6:DT:H5"	1.44	0.96
3:A:217:VAL:HG23	3:A:218:THR:H	1.30	0.95
3:A:209:VAL:HG22	3:A:210:GLU:H	1.32	0.94
3:B:313:GLY:HA3	3:B:315:TRP:CZ3	2.05	0.92
2:D:15:DC:H2'	2:D:16[B]:DA:C8	2.04	0.92
3:A:258:ASN:HA	3:A:261:LEU:HD12	1.51	0.92
3:A:299:MET:HG3	3:B:335:MET:HE1	1.51	0.90
3:A:214:SER:HB3	3:B:339:LEU:HD12	1.54	0.90
3:B:79:GLN:HG3	3:B:120:ILE:HG23	1.54	0.90
3:A:310:MET:HG3	3:A:315:TRP:HB2	1.55	0.89
3:B:193:MET:HE1	3:B:221:VAL:HG11	1.54	0.89
3:B:83:LEU:HD13	3:B:87:THR:HG21	1.55	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:130:ARG:HG2	3:B:130:ARG:HH11	1.39	0.87
3:A:171:LEU:HD13	3:A:312:ALA:CB	2.04	0.87
3:A:172:LEU:HD11	3:A:197:ILE:CD1	2.05	0.86
3:B:161:LEU:HD13	3:B:220:LEU:HD22	1.57	0.85
3:B:178:ALA:HB2	3:B:261:LEU:CD1	2.06	0.84
3:A:62:LYS:HD3	3:A:63:TRP:N	1.91	0.84
3:B:199:ARG:HB2	3:B:204:VAL:HG12	1.61	0.83
3:A:297:ARG:HH21	3:A:301:ARG:HH22	1.22	0.83
1:C:5:DC:H2''	1:C:6:DT:C5'	2.07	0.83
3:A:62:LYS:HD3	3:A:63:TRP:H	1.44	0.82
2:D:5:DC:H2'	2:D:6:DT:C6	2.14	0.82
1:C:17[B]:DT:N3	2:D:18[B]:DA:N1	2.28	0.82
2:D:15:DC:H2'	2:D:16[B]:DA:N7	1.95	0.82
3:A:306:ILE:HG22	3:A:307:PRO:HD3	1.62	0.81
3:A:187:ARG:CD	3:A:193:MET:HG2	2.11	0.80
1:C:14:DA:N3	3:B:201:LYS:NZ	2.27	0.80
3:A:203:LEU:HA	3:B:130:ARG:HD3	1.63	0.80
3:B:45:LEU:HD22	3:B:97:MET:CE	2.11	0.79
3:A:159:ARG:HB2	3:A:224:TRP:CZ3	2.17	0.79
2:D:18[B]:DA:C2'	2:D:19[B]:DC:H5''	2.13	0.79
3:A:213:LEU:HB3	3:A:217:VAL:CG2	2.13	0.78
3:B:161:LEU:HD13	3:B:220:LEU:CD2	2.13	0.78
3:A:24:ARG:O	3:A:28:MET:HG3	1.84	0.78
1:C:28:DG:H2''	1:C:29:DA:H8	1.49	0.78
2:D:7:DC:H1'	2:D:8:DT:H5''	1.65	0.78
3:A:171:LEU:HA	3:A:292:ARG:HG3	1.66	0.77
3:A:179:ARG:HA	3:A:255:GLN:NE2	1.99	0.77
3:A:158:ILE:CD1	3:A:224:TRP:HA	2.15	0.77
3:B:154:ARG:O	3:B:158:ILE:HD12	1.85	0.76
3:A:217:VAL:HA	3:A:220:LEU:HD12	1.68	0.76
2:D:14:DG:H2''	2:D:15:DC:H6	1.51	0.76
2:D:15:DC:C2'	2:D:16[B]:DA:C8	2.69	0.75
3:B:277:ASP:HB2	3:B:284:LEU:HD13	1.67	0.75
3:A:19:THR:N	3:A:22:GLU:HB2	2.01	0.75
3:A:203:LEU:CA	3:B:130:ARG:HD3	2.16	0.75
3:B:193:MET:HE1	3:B:221:VAL:CG1	2.17	0.75
3:A:297:ARG:HH21	3:A:301:ARG:NH2	1.84	0.75
3:A:194:LEU:CD2	3:A:210:GLU:HG2	2.17	0.74
3:B:233:ASP:O	3:B:236:ASN:HB2	1.87	0.74
3:A:308:GLU:O	3:A:311:GLN:HB2	1.86	0.74
3:A:188:THR:HG21	3:A:194:LEU:HD13	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17[A]:DT:H3'	3:B:121:ARG:NE	2.03	0.73
3:A:158:ILE:HG13	3:A:159:ARG:N	2.03	0.73
3:A:96:ASN:HD21	3:A:108:SER:CB	2.01	0.72
3:A:149:MET:HB2	3:A:161:LEU:HD21	1.71	0.72
3:A:121:ARG:HH11	3:A:121:ARG:HG3	1.54	0.72
3:A:158:ILE:HD11	3:A:224:TRP:HE3	1.54	0.72
3:A:201:LYS:HE3	3:B:130:ARG:NH2	2.05	0.72
3:B:116:VAL:O	3:B:120:ILE:HG13	1.89	0.72
3:A:297:ARG:CZ	3:A:328:LEU:HD21	2.19	0.72
3:A:310:MET:CE	3:A:318:VAL:HG22	2.21	0.71
3:A:270:ARG:HH11	3:A:270:ARG:HG3	1.55	0.71
3:A:306:ILE:HG22	3:A:307:PRO:CD	2.19	0.71
1:C:28:DG:H2''	1:C:29:DA:C8	2.25	0.71
3:A:166:ILE:HG22	3:A:177:ILE:CD1	2.20	0.70
3:A:176:GLU:O	3:A:180:ILE:HG13	1.92	0.70
3:A:308:GLU:OE2	3:B:334:ALA:HB2	1.92	0.69
2:D:17[B]:DT:H6	2:D:17[B]:DT:H5''	1.56	0.69
3:A:72:ARG:HH11	3:A:72:ARG:HG2	1.55	0.69
1:C:25:DA:H5'	1:C:25:DA:C8	2.27	0.69
3:B:180:ILE:HD13	3:B:195:ILE:HG21	1.74	0.69
2:D:23:DA:H2'	2:D:24:DT:H71	1.75	0.69
3:B:19:THR:N	3:B:22:GLU:HB2	2.09	0.68
1:C:32:DT:H2''	1:C:33:DA:C8	2.29	0.68
3:B:217:VAL:O	3:B:221:VAL:HG23	1.94	0.68
2:D:18[B]:DA:C3'	2:D:19[B]:DC:H5''	2.23	0.68
2:D:23:DA:H5'	3:B:201:LYS:HG3	1.76	0.68
3:A:187:ARG:HD2	3:A:193:MET:HG2	1.74	0.68
3:A:209:VAL:HG23	3:B:327:ASN:ND2	2.08	0.68
3:A:141:ASP:O	3:A:145:VAL:HG23	1.94	0.67
3:A:188:THR:HB	3:A:189:ASP:OD1	1.93	0.67
3:B:146:ARG:O	3:B:150:GLU:HB2	1.94	0.67
3:A:295:ALA:HB1	3:B:335:MET:HE3	1.77	0.67
3:A:325:ILE:CG2	3:A:331:GLU:HG3	2.13	0.67
3:A:233:ASP:O	3:A:235:ASN:N	2.27	0.67
1:C:18[B]:DA:H1'	1:C:19[B]:DT:O5'	1.94	0.67
3:B:79:GLN:HG3	3:B:120:ILE:CG2	2.24	0.67
3:A:170:THR:OG1	3:A:172:LEU:HD12	1.94	0.67
3:A:219:LYS:O	3:A:222:GLU:N	2.28	0.67
3:B:117:MET:HE3	3:B:117:MET:HA	1.75	0.67
3:B:128:GLY:O	3:B:130:ARG:NH1	2.27	0.67
3:A:217:VAL:O	3:A:219:LYS:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:297:ARG:NH1	3:A:327:ASN:OD1	2.28	0.66
2:D:15:DC:OP1	2:D:15:DC:H4'	1.95	0.66
3:A:181:ARG:HA	3:A:237:TYR:HA	1.76	0.66
3:A:245:ASN:N	3:A:245:ASN:HD22	1.94	0.66
3:B:90:GLN:NE2	3:B:94:GLN:HE21	1.93	0.66
3:B:319:ASN:OD1	3:B:319:ASN:N	2.29	0.66
3:A:175:ALA:O	3:A:179:ARG:HB2	1.96	0.65
3:A:202:THR:O	3:A:204:VAL:N	2.29	0.65
1:C:21:DC:H2''	1:C:22:DT:O5'	1.95	0.65
3:A:304:VAL:HG12	3:A:308:GLU:HG2	1.79	0.65
3:A:165:GLY:CA	3:A:217:VAL:HG12	2.26	0.65
3:A:165:GLY:HA3	3:A:217:VAL:HG12	1.78	0.65
3:B:92:LEU:HD22	3:B:96:ASN:ND2	2.12	0.65
3:B:72:ARG:HH11	3:B:72:ARG:HG2	1.61	0.65
3:B:333:GLY:O	3:B:337:ARG:HG2	1.97	0.65
3:A:58:LEU:HD23	3:A:59:ASN:HD21	1.62	0.65
2:D:16[A]:DA:H2''	2:D:17[A]:DT:H71	1.79	0.64
3:A:214:SER:OG	3:A:215:LEU:N	2.29	0.64
3:A:209:VAL:HG22	3:A:210:GLU:N	2.08	0.64
3:B:194:LEU:CD2	3:B:212:ALA:HB2	2.27	0.64
1:C:16[A]:DG:C5'	3:B:202:THR:HB	2.28	0.64
3:A:187:ARG:HD3	3:A:193:MET:HG2	1.78	0.64
3:A:224:TRP:HZ2	3:A:240:CYS:HG	1.45	0.64
3:A:304:VAL:CG1	3:A:308:GLU:HG2	2.28	0.64
3:A:201:LYS:HA	3:A:201:LYS:CE	2.17	0.64
2:D:11:DA:H2''	2:D:12:DT:O5'	1.97	0.64
3:A:236:ASN:HD21	3:A:250:PRO:HB3	1.62	0.64
1:C:4:DA:H2''	1:C:5:DC:H5''	1.78	0.64
3:B:313:GLY:HA3	3:B:315:TRP:CE3	2.32	0.64
3:B:305:SER:O	3:B:308:GLU:N	2.30	0.64
3:B:196:HIS:HB2	3:B:210:GLU:OE2	1.97	0.63
3:A:176:GLU:OE2	3:A:199:ARG:HA	1.98	0.63
3:A:297:ARG:NH2	3:A:301:ARG:HH22	1.95	0.63
3:A:304:VAL:O	3:A:305:SER:HB3	1.98	0.63
1:C:17[B]:DT:O4	2:D:18[B]:DA:N6	2.31	0.63
3:A:106:ARG:NH1	3:A:109:ASP:OD1	2.32	0.63
3:B:332:THR:OG1	3:B:333:GLY:N	2.31	0.62
2:D:5:DC:H2''	2:D:6:DT:H5'	1.79	0.62
3:A:217:VAL:HG23	3:A:218:THR:N	2.08	0.62
2:D:11:DA:N3	3:A:282:ARG:NH2	2.46	0.62
1:C:23:DA:H2''	1:C:24:DT:C5'	2.30	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:23:DA:H2''	1:C:24:DT:H5'	1.82	0.62
3:B:124:ASN:ND2	4:B:345:HOH:O	2.28	0.62
3:A:310:MET:HE3	3:A:318:VAL:HG22	1.82	0.62
3:A:194:LEU:HD23	3:A:210:GLU:OE2	2.00	0.62
3:A:146:ARG:O	3:A:150:GLU:HB2	1.99	0.62
3:A:211:LYS:NZ	3:A:312:ALA:O	2.31	0.61
3:A:279:SER:O	3:A:281:GLN:N	2.26	0.61
3:A:171:LEU:CA	3:A:292:ARG:HG3	2.30	0.61
2:D:16[A]:DA:H4'	2:D:17[A]:DT:OP1	2.00	0.61
3:A:299:MET:HG3	3:B:335:MET:CE	2.28	0.61
3:A:146:ARG:HD3	3:A:150:GLU:OE2	2.00	0.61
3:B:279:SER:HB2	3:B:281:GLN:HG3	1.82	0.61
2:D:33:DA:C2'	2:D:34:DT:H5''	2.22	0.61
3:A:299:MET:O	3:A:304:VAL:HG23	2.00	0.61
3:B:117:MET:HA	3:B:117:MET:CE	2.29	0.61
3:B:237:TYR:CZ	3:B:255:GLN:HG2	2.36	0.61
3:A:213:LEU:HD22	3:A:217:VAL:HG21	1.81	0.61
3:A:158:ILE:HD12	3:A:224:TRP:HA	1.83	0.61
1:C:19[B]:DT:H2''	1:C:20:DG:C8	2.36	0.61
3:A:310:MET:HE1	3:A:318:VAL:HG22	1.83	0.61
1:C:16[A]:DG:H5'	3:B:202:THR:HB	1.82	0.61
3:A:297:ARG:HH12	3:A:327:ASN:ND2	1.98	0.60
3:A:171:LEU:HD11	3:B:335:MET:HE2	1.83	0.60
3:A:340:GLU:O	3:A:341:ASP:HB2	2.01	0.60
3:B:155:CYS:HB3	3:B:242:VAL:HG11	1.84	0.60
3:B:27:LEU:O	3:B:30:MET:HB3	2.01	0.60
2:D:7:DC:H1'	2:D:8:DT:C5'	2.31	0.60
3:A:159:ARG:HB2	3:A:224:TRP:CE3	2.36	0.60
3:A:166:ILE:HG22	3:A:177:ILE:HD13	1.83	0.60
3:B:195:ILE:O	3:B:211:LYS:N	2.32	0.60
3:A:172:LEU:HD11	3:A:197:ILE:HD12	1.83	0.60
3:A:222:GLU:O	3:A:225:ILE:HB	2.02	0.60
3:A:138:GLU:OE2	3:A:301:ARG:NH2	2.33	0.60
3:B:185:ILE:HD11	3:B:238:LEU:HD22	1.84	0.60
3:B:40:HIS:HD2	3:B:43:LYS:NZ	2.00	0.60
3:B:237:TYR:CE2	3:B:255:GLN:HG2	2.37	0.60
3:A:201:LYS:HE3	3:B:130:ARG:HH22	1.66	0.59
3:B:134:ALA:HA	3:B:283:TYR:CD1	2.37	0.59
2:D:16[A]:DA:H2''	2:D:17[A]:DT:C7	2.32	0.59
1:C:9:DA:H2''	1:C:10:DT:C6	2.38	0.59
3:A:163:PHE:CZ	3:A:261:LEU:HB3	2.38	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:297:ARG:HE	3:A:301:ARG:NH2	2.01	0.59
1:C:18[B]:DA:O4'	1:C:18[B]:DA:N3	2.31	0.59
3:A:212:ALA:O	3:A:213:LEU:HD23	2.03	0.59
3:A:297:ARG:HH12	3:A:327:ASN:HD21	1.49	0.59
3:A:256:LEU:HD22	3:A:260:ALA:CB	2.33	0.59
3:B:173:ARG:NH1	3:B:176:GLU:OE2	2.35	0.58
3:A:222:GLU:O	3:A:225:ILE:N	2.35	0.58
3:A:188:THR:CG2	3:A:194:LEU:HD13	2.33	0.58
3:A:325:ILE:HG23	3:A:331:GLU:CG	2.15	0.58
3:A:245:ASN:H	3:A:245:ASN:HD22	1.52	0.58
2:D:18[B]:DA:H2''	2:D:19[B]:DC:O4'	2.04	0.58
3:A:158:ILE:CD1	3:A:224:TRP:HE3	2.16	0.58
3:B:140:THR:O	3:B:144:GLN:HG3	2.03	0.58
3:A:35:GLN:NE2	3:B:123:GLU:OE2	2.36	0.58
3:A:322:MET:HE3	3:A:325:ILE:HD12	1.84	0.58
1:C:19[A]:DT:H2''	1:C:20:DG:C8	2.38	0.58
3:B:90:GLN:HE21	3:B:94:GLN:HE21	1.51	0.58
3:B:278:ASP:OD1	3:B:278:ASP:N	2.37	0.58
3:A:194:LEU:HD23	3:A:210:GLU:HG2	1.85	0.58
3:A:65:PRO:HG3	3:A:104:LEU:HD13	1.85	0.58
2:D:16[B]:DA:H2''	2:D:17[B]:DT:OP2	2.03	0.57
3:A:256:LEU:HD22	3:A:260:ALA:HB3	1.85	0.57
1:C:29:DA:H2''	1:C:30:DG:H8	1.67	0.57
3:A:174:LEU:HD22	3:A:261:LEU:HB2	1.86	0.57
2:D:23:DA:H2'	2:D:24:DT:C6	2.39	0.57
3:B:45:LEU:HD22	3:B:97:MET:HE1	1.87	0.57
3:A:158:ILE:HD11	3:A:224:TRP:CE3	2.38	0.57
3:A:245:ASN:ND2	3:A:247:VAL:H	2.02	0.57
2:D:17[A]:DT:OP2	3:A:202:THR:HB	2.04	0.57
3:A:306:ILE:O	3:A:309:ILE:HB	2.04	0.57
3:B:276:LYS:HD2	3:B:284:LEU:HB2	1.87	0.57
3:A:310:MET:HE3	3:A:317:ASN:O	2.05	0.56
3:B:194:LEU:HD23	3:B:212:ALA:HB2	1.87	0.56
3:A:199:ARG:CG	3:A:199:ARG:HH11	2.18	0.56
3:B:106:ARG:O	3:B:109:ASP:HB2	2.05	0.56
3:A:217:VAL:O	3:A:218:THR:C	2.43	0.56
1:C:16[B]:DG:O6	2:D:18[B]:DA:N6	2.39	0.56
3:B:130:ARG:HG2	3:B:130:ARG:NH1	2.16	0.56
3:B:139:ARG:O	3:B:139:ARG:HG3	2.06	0.56
3:A:121:ARG:HG3	3:A:121:ARG:NH1	2.20	0.56
3:A:169:ASN:OD1	3:B:339:LEU:HD11	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:154:ARG:O	3:A:157:ASP:N	2.38	0.56
3:A:132:LYS:HB2	3:A:283:TYR:CE2	2.41	0.56
3:A:247:VAL:HG21	4:A:355:HOH:O	2.06	0.56
3:B:159:ARG:HB2	3:B:224:TRP:CZ3	2.41	0.56
3:B:45:LEU:HD22	3:B:97:MET:HE3	1.88	0.55
3:B:279:SER:CB	3:B:281:GLN:HG3	2.36	0.55
3:B:179:ARG:HG2	3:B:255:GLN:NE2	2.21	0.55
3:A:224:TRP:HZ2	3:A:240:CYS:SG	2.29	0.55
3:A:195:ILE:HG22	3:A:197:ILE:HG12	1.88	0.55
3:A:179:ARG:HA	3:A:255:GLN:HE21	1.69	0.55
3:A:96:ASN:HD21	3:A:108:SER:HB2	1.72	0.55
3:A:315:TRP:HE1	3:A:320:ILE:HG21	1.72	0.55
3:A:145:VAL:HG22	3:A:272:ILE:CD1	2.29	0.55
3:A:224:TRP:CE3	3:A:228:SER:HB3	2.42	0.55
2:D:4:DA:H2"	2:D:5:DC:H5"	1.88	0.55
3:A:297:ARG:HH12	3:A:327:ASN:CG	2.11	0.55
3:A:78:LEU:O	3:A:81:ARG:HB2	2.06	0.55
1:C:15:DT:H5"	3:B:320:ILE:CD1	2.36	0.54
3:A:297:ARG:NH2	3:A:328:LEU:HD21	2.21	0.54
3:A:166:ILE:HG22	3:A:177:ILE:HD11	1.87	0.54
2:D:23:DA:H5'	3:B:201:LYS:CG	2.36	0.54
3:B:306:ILE:HG22	3:B:307:PRO:HD3	1.90	0.54
2:D:15:DC:H2'	2:D:16[A]:DA:N7	2.22	0.54
3:A:201:LYS:HA	3:B:130:ARG:NH2	2.23	0.54
3:A:209:VAL:HG23	3:B:327:ASN:HD22	1.73	0.54
3:B:24:ARG:O	3:B:28:MET:HB2	2.08	0.54
3:A:272:ILE:HB	3:A:273:TYR:CD1	2.43	0.54
3:B:193:MET:CE	3:B:213:LEU:HD12	2.37	0.54
3:A:119:ARG:O	3:A:123:GLU:HG3	2.08	0.54
3:A:195:ILE:HG22	3:A:197:ILE:CG1	2.38	0.53
3:A:213:LEU:HB3	3:A:218:THR:H	1.73	0.53
3:B:197:ILE:HG12	3:B:211:LYS:HG2	1.90	0.53
3:A:132:LYS:HB2	3:A:283:TYR:HE2	1.72	0.53
3:B:169:ASN:C	3:B:169:ASN:HD22	2.10	0.53
3:B:243:ARG:O	3:B:246:GLY:N	2.29	0.53
3:A:30:MET:CE	3:A:101:ARG:HB2	2.38	0.53
3:A:158:ILE:HD11	3:A:224:TRP:HA	1.89	0.53
3:A:270:ARG:NH1	3:A:270:ARG:HG3	2.23	0.53
3:B:64:PHE:HA	3:B:65:PRO:C	2.28	0.53
2:D:4:DA:H5"	3:A:242:VAL:O	2.08	0.53
3:A:274:GLY:O	3:A:275:ALA:O	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:193:MET:HE2	3:B:213:LEU:HD12	1.90	0.53
3:B:193:MET:HE1	3:B:221:VAL:CB	2.39	0.53
3:A:224:TRP:CD2	3:A:228:SER:HB3	2.43	0.53
1:C:26:DT:H2''	1:C:27:DA:C8	2.43	0.53
1:C:25:DA:H2''	1:C:26:DT:O5'	2.07	0.53
3:B:40:HIS:HD2	3:B:43:LYS:HZ3	1.55	0.52
3:A:173:ARG:CG	3:A:173:ARG:HH11	2.22	0.52
3:A:272:ILE:HB	3:A:273:TYR:HD1	1.73	0.52
1:C:6:DT:H5'	1:C:6:DT:C6	2.44	0.52
3:B:332:THR:HG23	3:B:333:GLY:N	2.24	0.52
3:A:72:ARG:HG2	3:A:72:ARG:NH1	2.22	0.52
3:B:335:MET:C	3:B:338:LEU:H	2.12	0.52
3:B:40:HIS:CD2	3:B:43:LYS:NZ	2.77	0.52
3:B:119:ARG:O	3:B:123:GLU:HG3	2.08	0.52
1:C:6:DT:H5'	1:C:6:DT:H6	1.72	0.52
1:C:16[B]:DG:C6	2:D:18[B]:DA:N6	2.78	0.52
3:B:48:VAL:HG11	3:B:94:GLN:HB2	1.92	0.52
3:A:236:ASN:ND2	3:A:250:PRO:HB3	2.25	0.52
3:A:139:ARG:HB2	3:A:168:TYR:OH	2.10	0.52
3:B:48:VAL:HG21	3:B:94:GLN:HG3	1.92	0.52
2:D:12:DT:H2''	2:D:13:DA:C8	2.45	0.52
3:B:196:HIS:HB2	3:B:210:GLU:CD	2.29	0.52
3:A:171:LEU:HB3	3:A:292:ARG:HG2	1.91	0.52
3:A:170:THR:OG1	3:A:172:LEU:HB2	2.10	0.52
3:B:306:ILE:HG22	3:B:307:PRO:CD	2.40	0.52
3:B:318:VAL:O	3:B:322:MET:HG2	2.09	0.52
3:A:58:LEU:HD23	3:A:59:ASN:ND2	2.23	0.51
3:B:306:ILE:HG22	3:B:307:PRO:N	2.25	0.51
3:B:128:GLY:O	3:B:129:GLU:O	2.28	0.51
1:C:16[B]:DG:H5''	3:B:316:THR:OG1	2.10	0.51
3:A:245:ASN:H	3:A:245:ASN:ND2	2.07	0.51
3:A:281:GLN:O	3:A:282:ARG:HB2	2.11	0.51
3:B:297:ARG:O	3:B:298:ASP:C	2.48	0.51
3:A:180:ILE:O	3:A:237:TYR:HD1	1.94	0.51
3:A:201:LYS:CE	3:B:130:ARG:HH22	2.22	0.51
3:A:204:VAL:O	3:A:204:VAL:HG22	2.10	0.51
3:B:83:LEU:HD13	3:B:87:THR:CG2	2.35	0.51
3:A:76:LEU:HD21	3:A:116:VAL:CG2	2.41	0.51
3:A:30:MET:HE2	3:A:101:ARG:CB	2.40	0.51
3:A:275:ALA:O	3:A:276:LYS:O	2.29	0.51
3:A:31:PHE:CE1	3:A:34:ARG:NH1	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:308:GLU:HB2	4:A:356:HOH:O	2.10	0.51
3:A:165:GLY:O	3:A:217:VAL:HG11	2.10	0.51
3:A:216:GLY:O	3:A:217:VAL:O	2.28	0.51
3:B:276:LYS:O	3:B:277:ASP:O	2.29	0.51
3:A:247:VAL:HG11	4:A:355:HOH:O	2.10	0.51
3:B:77:TYR:O	3:B:81:ARG:HG3	2.11	0.51
3:B:170:THR:O	3:B:171:LEU:HB2	2.11	0.51
3:B:335:MET:O	3:B:338:LEU:N	2.38	0.50
3:A:219:LYS:O	3:A:220:LEU:C	2.50	0.50
3:A:201:LYS:HA	3:B:130:ARG:HH21	1.76	0.50
1:C:5:DC:H2'	1:C:6:DT:H72	1.93	0.50
1:C:16[B]:DG:OP1	3:B:316:THR:N	2.43	0.50
2:D:14:DG:C4	2:D:15:DC:C6	2.99	0.50
2:D:23:DA:C4'	3:B:201:LYS:HG3	2.41	0.50
3:A:158:ILE:HD13	3:A:227:VAL:HB	1.93	0.50
3:B:188:THR:HG23	3:B:192:ARG:O	2.12	0.50
3:B:299:MET:CE	3:B:312:ALA:HB2	2.42	0.50
2:D:2:DT:H2''	2:D:3:DA:C8	2.46	0.50
3:B:79:GLN:CG	3:B:120:ILE:HG23	2.36	0.50
1:C:14:DA:H2'	1:C:14:DA:O5'	2.12	0.50
3:B:179:ARG:HG2	3:B:255:GLN:HE22	1.76	0.50
3:A:76:LEU:HD23	3:A:120:ILE:HD11	1.94	0.50
3:B:35:GLN:HA	3:B:35:GLN:HE21	1.77	0.50
3:A:172:LEU:HD23	3:A:176:GLU:OE1	2.12	0.49
2:D:2:DT:H2''	2:D:3:DA:N7	2.26	0.49
3:A:273:TYR:N	3:A:273:TYR:CD1	2.79	0.49
3:B:125:VAL:C	3:B:127:ALA:H	2.15	0.49
3:A:318:VAL:HG12	3:A:322:MET:HB2	1.94	0.49
2:D:10:DT:H2'	2:D:10:DT:O5'	2.13	0.49
3:B:194:LEU:HD23	3:B:212:ALA:CB	2.42	0.49
3:A:171:LEU:HD21	3:A:295:ALA:HB3	1.93	0.49
3:A:146:ARG:O	3:A:150:GLU:N	2.45	0.49
3:A:138:GLU:HG2	3:A:294:GLY:CA	2.42	0.49
3:B:282:ARG:O	3:B:283:TYR:HB2	2.13	0.49
2:D:15:DC:N3	2:D:16[B]:DA:N6	2.61	0.49
3:B:27:LEU:HD12	3:B:27:LEU:HA	1.61	0.49
1:C:15:DT:H5''	3:B:320:ILE:HD11	1.95	0.49
1:C:1:DA:H8	1:C:1:DA:O5'	1.95	0.48
3:B:281:GLN:HB2	3:B:284:LEU:HD21	1.95	0.48
3:B:245:ASN:OD1	3:B:247:VAL:HG23	2.13	0.48
3:B:268:THR:O	3:B:271:LEU:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:DG:C2'	2:D:15:DC:H6	2.22	0.48
2:D:6:DT:H1'	2:D:7:DC:H5'	1.94	0.48
3:A:34:ARG:C	3:A:36:ALA:H	2.17	0.48
3:A:189:ASP:OD1	3:A:189:ASP:N	2.35	0.48
3:A:166:ILE:CG2	3:A:177:ILE:HD13	2.44	0.48
3:A:279:SER:O	3:A:281:GLN:HG3	2.14	0.48
3:A:195:ILE:HG22	3:A:197:ILE:HD11	1.95	0.48
3:A:201:LYS:HE3	3:A:201:LYS:CA	2.23	0.48
2:D:17[B]:DT:C6	2:D:17[B]:DT:H5''	2.44	0.48
1:C:29:DA:H2''	1:C:30:DG:C8	2.46	0.48
3:A:277:ASP:OD2	3:A:284:LEU:HB3	2.14	0.48
3:B:72:ARG:HG2	3:B:72:ARG:NH1	2.27	0.48
3:A:188:THR:OG1	3:A:194:LEU:HD13	2.14	0.48
3:A:169:ASN:C	3:A:169:ASN:HD22	2.17	0.48
3:A:142:PHE:O	3:A:146:ARG:HB2	2.12	0.48
3:A:245:ASN:ND2	3:A:245:ASN:N	2.60	0.48
3:B:132:LYS:HB2	3:B:283:TYR:HE2	1.78	0.48
3:B:67:GLU:HB3	4:B:357:HOH:O	2.13	0.48
3:A:302:ALA:O	3:A:303:GLY:O	2.32	0.48
2:D:18[A]:DA:H8	2:D:18[A]:DA:O5'	1.96	0.48
3:A:169:ASN:CG	3:B:339:LEU:HD11	2.35	0.47
3:A:274:GLY:C	3:A:275:ALA:O	2.53	0.47
3:B:39:GLU:H	3:B:39:GLU:HG3	1.29	0.47
2:D:23:DA:C5'	3:B:201:LYS:HG3	2.41	0.47
3:A:218:THR:CG2	3:A:219:LYS:N	2.78	0.47
3:A:158:ILE:CD1	3:A:227:VAL:HB	2.44	0.47
3:A:233:ASP:N	3:A:234:PRO:CD	2.78	0.47
3:A:135:LEU:O	3:A:290:SER:HB3	2.15	0.47
3:A:171:LEU:CD2	3:A:295:ALA:HB3	2.45	0.47
2:D:18[B]:DA:P	2:D:18[B]:DA:H8	2.38	0.47
3:A:214:SER:CB	3:B:339:LEU:HD12	2.35	0.47
3:A:315:TRP:NE1	3:A:320:ILE:HG21	2.30	0.47
3:B:138:GLU:HB2	4:B:363:HOH:O	2.14	0.47
1:C:16[A]:DG:P	3:B:316:THR:HG1	2.38	0.47
2:D:18[A]:DA:OP2	3:B:121:ARG:NE	2.48	0.47
3:A:270:ARG:NH1	3:A:270:ARG:CG	2.78	0.46
3:A:30:MET:HE1	3:A:101:ARG:HB2	1.97	0.46
3:A:173:ARG:HG2	3:A:173:ARG:HH11	1.80	0.46
3:A:320:ILE:CD1	3:A:320:ILE:N	2.79	0.46
3:A:158:ILE:HD12	3:A:224:TRP:CA	2.45	0.46
1:C:29:DA:C2	1:C:30:DG:C4	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:245:ASN:HD22	3:A:246:GLY:N	2.14	0.46
3:B:188:THR:O	3:B:189:ASP:HB2	2.15	0.46
3:B:40:HIS:CD2	3:B:43:LYS:HZ1	2.33	0.46
2:D:23:DA:OP2	3:B:38:SER:HB2	2.15	0.46
1:C:11:DA:OP1	3:B:81:ARG:NH2	2.37	0.46
1:C:16[A]:DG:OP1	3:B:315:TRP:HA	2.15	0.46
3:A:273:TYR:N	3:A:273:TYR:HD1	2.14	0.46
3:B:130:ARG:CG	3:B:130:ARG:HH11	2.15	0.46
1:C:16[B]:DG:O6	2:D:19[B]:DC:N4	2.43	0.46
2:D:15:DC:H2''	2:D:16[B]:DA:C8	2.50	0.46
3:A:119:ARG:CG	3:A:120:ILE:N	2.79	0.46
3:A:84:ALA:O	3:A:88:ILE:HG13	2.16	0.46
3:B:85:VAL:HG12	3:B:89:GLN:OE1	2.16	0.46
3:B:276:LYS:HD2	3:B:284:LEU:HD12	1.97	0.46
3:B:197:ILE:CG1	3:B:211:LYS:HG2	2.45	0.46
3:A:162:ALA:O	3:A:165:GLY:N	2.47	0.45
3:A:224:TRP:CZ2	3:A:240:CYS:SG	3.08	0.45
3:A:96:ASN:ND2	3:A:108:SER:HB2	2.30	0.45
2:D:3:DA:H2'	2:D:3:DA:O5'	2.17	0.45
3:A:100:ARG:HG3	3:A:106:ARG:HD2	1.98	0.45
3:A:275:ALA:C	3:A:276:LYS:O	2.52	0.45
3:B:296:ALA:O	3:B:299:MET:HB2	2.17	0.45
3:A:315:TRP:NE1	3:A:320:ILE:CG2	2.79	0.45
3:B:203:LEU:HD12	3:B:203:LEU:C	2.37	0.45
3:B:338:LEU:HA	3:B:338:LEU:HD12	1.72	0.45
3:B:193:MET:CE	3:B:221:VAL:HB	2.46	0.45
1:C:10:DT:OP2	3:B:50:ARG:NH1	2.49	0.45
3:A:171:LEU:O	3:A:292:ARG:HD2	2.16	0.45
2:D:15:DC:O2	2:D:16[B]:DA:C5	2.69	0.45
3:A:71:VAL:O	3:A:75:LEU:HG	2.16	0.45
2:D:21:DT:H2''	2:D:22:DT:H5'	1.98	0.45
3:A:203:LEU:O	3:B:130:ARG:HA	2.17	0.45
3:A:188:THR:HB	3:A:189:ASP:H	1.40	0.45
2:D:16[B]:DA:H2'	2:D:16[B]:DA:OP2	2.17	0.45
3:B:279:SER:OG	3:B:281:GLN:HG3	2.17	0.45
2:D:2:DT:O2	3:A:244:LYS:NZ	2.35	0.45
3:A:306:ILE:HD11	3:A:322:MET:CE	2.47	0.45
1:C:9:DA:H2'	1:C:10:DT:H71	1.99	0.45
3:A:111:ASN:O	3:A:115:LEU:HG	2.17	0.45
3:A:138:GLU:HG2	3:A:294:GLY:HA2	1.98	0.45
2:D:9:DA:H2''	2:D:10:DT:O5'	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:196:HIS:HA	3:B:210:GLU:HA	1.99	0.45
3:A:306:ILE:HG22	3:A:307:PRO:N	2.31	0.45
3:B:214:SER:OG	3:B:217:VAL:HG23	2.16	0.45
3:A:149:MET:HB3	3:A:149:MET:HE2	1.83	0.45
2:D:8:DT:H2''	2:D:9:DA:C8	2.52	0.45
3:A:74:TYR:HH	3:A:91:HIS:CE1	2.31	0.45
3:A:185:ILE:HG12	3:A:195:ILE:CG1	2.47	0.44
3:B:143:ASP:O	3:B:147:SER:HB3	2.16	0.44
3:B:336:VAL:O	3:B:340:GLU:OE1	2.36	0.44
3:A:297:ARG:NH2	3:A:328:LEU:CD2	2.80	0.44
3:B:187:ARG:NH2	3:B:222:GLU:OE2	2.42	0.44
3:A:161:LEU:O	3:A:162:ALA:C	2.56	0.44
2:D:5:DC:H2'	2:D:6:DT:C5	2.52	0.44
1:C:13:DA:H2''	1:C:14:DA:O5'	2.17	0.44
1:C:23:DA:H2''	1:C:24:DT:O5'	2.18	0.44
3:A:154:ARG:HB2	3:A:157:ASP:HB2	1.99	0.44
3:A:107:PRO:O	3:A:110:SER:OG	2.29	0.44
3:A:209:VAL:HG23	3:B:327:ASN:HB2	2.00	0.44
3:A:158:ILE:HG13	3:A:159:ARG:H	1.77	0.44
3:B:238:LEU:O	3:B:238:LEU:HD12	2.18	0.44
3:A:173:ARG:CG	3:A:173:ARG:NH1	2.79	0.44
3:A:171:LEU:HD11	3:B:335:MET:CE	2.48	0.44
3:A:195:ILE:HG22	3:A:197:ILE:CD1	2.48	0.44
3:A:306:ILE:CG2	3:A:307:PRO:HD3	2.41	0.44
3:A:185:ILE:HG12	3:A:195:ILE:HG12	2.00	0.43
3:A:186:SER:C	3:A:187:ARG:HG2	2.38	0.43
3:B:60:ASN:HA	3:B:60:ASN:HD22	1.62	0.43
3:B:128:GLY:O	3:B:129:GLU:C	2.57	0.43
3:B:173:ARG:O	3:B:174:LEU:C	2.56	0.43
1:C:2:DT:H2''	1:C:3:DA:N7	2.33	0.43
3:B:149:MET:O	3:B:150:GLU:C	2.56	0.43
3:A:170:THR:O	3:A:171:LEU:C	2.56	0.43
3:B:306:ILE:N	3:B:307:PRO:HD2	2.32	0.43
2:D:1:DA:H2'	2:D:2:DT:C6	2.53	0.43
3:A:253:THR:O	3:A:253:THR:HG22	2.17	0.43
3:A:184:ASP:OD1	3:A:184:ASP:N	2.52	0.43
2:D:18[B]:DA:H2'	2:D:19[B]:DC:C6	2.53	0.43
3:B:320:ILE:H	3:B:320:ILE:HG12	1.64	0.43
3:A:171:LEU:HD21	3:A:295:ALA:CB	2.49	0.43
3:A:219:LYS:O	3:A:222:GLU:HB2	2.18	0.43
3:B:68:PRO:HB3	3:B:110:SER:OG	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:182:VAL:HB	3:B:234:PRO:HA	2.01	0.43
3:A:310:MET:HE1	3:A:318:VAL:CG2	2.48	0.42
2:D:17[A]:DT:H3'	3:B:121:ARG:CZ	2.49	0.42
1:C:23:DA:H2'	1:C:24:DT:C6	2.54	0.42
2:D:11:DA:C2	3:A:282:ARG:NH2	2.83	0.42
3:A:311:GLN:OE1	3:A:311:GLN:HA	2.19	0.42
2:D:15:DC:H2'	2:D:16[A]:DA:C8	2.54	0.42
1:C:15:DT:H5''	3:B:320:ILE:HD12	2.01	0.42
3:A:31:PHE:O	3:A:34:ARG:NH1	2.46	0.42
3:B:99:HIS:O	3:B:102:SER:HB2	2.19	0.42
3:A:296:ALA:O	3:A:300:ALA:N	2.53	0.42
3:A:187:ARG:HA	3:A:193:MET:HA	2.02	0.42
3:B:67:GLU:HA	3:B:68:PRO:HD2	1.90	0.42
3:A:186:SER:O	3:A:187:ARG:HG2	2.19	0.42
3:A:72:ARG:CG	3:A:72:ARG:NH1	2.82	0.42
3:B:305:SER:O	3:B:306:ILE:C	2.57	0.42
3:A:30:MET:HE2	3:A:101:ARG:HB3	2.00	0.42
3:A:269:HIS:HD2	3:A:286:TRP:CD2	2.37	0.42
1:C:1:DA:H2''	1:C:2:DT:O5'	2.19	0.42
3:B:92:LEU:HD22	3:B:96:ASN:HD21	1.80	0.42
3:B:295:ALA:O	3:B:296:ALA:C	2.56	0.42
3:B:35:GLN:CA	3:B:35:GLN:HE21	2.29	0.42
3:A:154:ARG:O	3:A:155:CYS:C	2.58	0.42
3:A:307:PRO:O	3:A:311:GLN:HG2	2.19	0.42
3:A:233:ASP:N	3:A:234:PRO:HD3	2.35	0.42
3:A:74:TYR:O	3:A:78:LEU:HG	2.20	0.42
3:B:35:GLN:HA	3:B:35:GLN:NE2	2.34	0.42
3:A:194:LEU:HD23	3:A:210:GLU:CG	2.49	0.41
3:B:84:ALA:O	3:B:87:THR:N	2.52	0.41
3:A:179:ARG:HA	3:A:255:GLN:HE22	1.80	0.41
3:A:199:ARG:NH1	3:A:199:ARG:CG	2.79	0.41
3:A:209:VAL:CG2	3:A:210:GLU:H	2.14	0.41
3:B:217:VAL:O	3:B:220:LEU:HB2	2.20	0.41
1:C:25:DA:C5'	1:C:25:DA:C8	2.99	0.41
3:B:188:THR:CG2	3:B:192:ARG:HB2	2.49	0.41
3:A:310:MET:SD	3:A:321:VAL:HG21	2.61	0.41
3:A:217:VAL:CG2	3:A:218:THR:N	2.80	0.41
3:A:179:ARG:CG	3:A:255:GLN:HE22	2.33	0.41
3:A:26:ASN:HB3	3:A:102:SER:HA	2.01	0.41
3:A:80:ALA:C	3:A:82:GLY:H	2.22	0.41
3:B:38:SER:OG	3:B:40:HIS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17[A]:DT:H3'	3:B:121:ARG:CD	2.50	0.41
3:A:62:LYS:HA	3:A:62:LYS:HD3	1.85	0.41
3:B:306:ILE:O	3:B:307:PRO:C	2.59	0.41
3:B:181:ARG:HD3	3:B:235:ASN:O	2.21	0.41
3:B:51:SER:O	3:B:54:ALA:HB3	2.20	0.41
3:A:148:LEU:HD13	3:A:148:LEU:HA	1.79	0.41
3:A:199:ARG:HG2	4:A:349:HOH:O	2.20	0.41
3:B:161:LEU:HD13	3:B:220:LEU:HD21	1.96	0.41
3:A:62:LYS:HD2	3:A:64:PHE:H	1.86	0.41
1:C:14:DA:H1'	3:B:201:LYS:HZ2	1.86	0.41
2:D:23:DA:H5'	3:B:201:LYS:CB	2.50	0.41
3:B:211:LYS:HE2	3:B:211:LYS:HB3	1.72	0.41
3:B:181:ARG:HA	3:B:237:TYR:HA	2.03	0.41
3:B:183:LYS:HG2	3:B:234:PRO:O	2.20	0.41
3:A:191:GLY:O	3:A:192:ARG:HG3	2.21	0.41
3:A:304:VAL:HG11	3:A:308:GLU:HG2	2.00	0.41
3:B:48:VAL:HG21	3:B:94:GLN:CG	2.51	0.41
3:A:171:LEU:HB3	3:A:292:ARG:CG	2.52	0.40
3:A:199:ARG:HG3	3:A:199:ARG:NH1	2.36	0.40
3:A:193:MET:HG3	3:A:218:THR:OG1	2.21	0.40
2:D:14:DG:C4	2:D:15:DC:C5	3.09	0.40
3:A:60:ASN:C	3:A:61:ARG:HG2	2.41	0.40
2:D:16[B]:DA:O5'	2:D:16[B]:DA:H2'	2.21	0.40
3:A:336:VAL:O	3:A:340:GLU:HG3	2.21	0.40
1:C:11:DA:N3	3:B:282:ARG:NH2	2.69	0.40
2:D:5:DC:C6	2:D:6:DT:H72	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	A	321/349 (92%)	264 (82%)	34 (11%)	23 (7%)	1	2
3	B	315/349 (90%)	284 (90%)	25 (8%)	6 (2%)	10	28
All	All	636/698 (91%)	548 (86%)	59 (9%)	29 (5%)	3	8

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	188	THR
3	A	189	ASP
3	A	217	VAL
3	A	218	THR
3	A	234	PRO
3	A	275	ALA
3	A	276	LYS
3	A	280	GLY
3	A	282	ARG
3	A	305	SER
3	A	319	ASN
3	B	129	GLU
3	B	277	ASP
3	A	216	GLY
3	A	303	GLY
3	B	189	ASP
3	B	207	ALA
3	A	279	SER
3	A	283	TYR
3	A	203	LEU
3	A	281	GLN
3	B	150	GLU
3	A	201	LYS
3	A	231	ALA
3	B	326	ARG
3	A	197	ILE
3	A	209	VAL
3	A	230	VAL
3	A	198	GLY

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	268/291 (92%)	203 (76%)	65 (24%)	1	2
3	B	264/291 (91%)	213 (81%)	51 (19%)	2	4
All	All	532/582 (91%)	416 (78%)	116 (22%)	1	3

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	21	ASP
3	A	30	MET
3	A	46	LEU
3	A	61	ARG
3	A	62	LYS
3	A	89	GLN
3	A	92	LEU
3	A	97	MET
3	A	118	ARG
3	A	119	ARG
3	A	121	ARG
3	A	130	ARG
3	A	133	GLN
3	A	135	LEU
3	A	147	SER
3	A	148	LEU
3	A	153	ASP
3	A	158	ILE
3	A	161	LEU
3	A	169	ASN
3	A	170	THR
3	A	172	LEU
3	A	173	ARG
3	A	179	ARG
3	A	180	ILE
3	A	186	SER
3	A	189	ASP
3	A	194	LEU
3	A	195	ILE
3	A	197	ILE
3	A	199	ARG
3	A	200	THR
3	A	201	LYS

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Mol	Chain	Res	Type
3	A	202	THR
3	A	206	THR
3	A	210	GLU
3	A	214	SER
3	A	218	THR
3	A	219	LYS
3	A	226	SER
3	A	230	VAL
3	A	244	LYS
3	A	245	ASN
3	A	251	SER
3	A	255	GLN
3	A	261	LEU
3	A	273	TYR
3	A	276	LYS
3	A	277	ASP
3	A	279	SER
3	A	289	HIS
3	A	306	ILE
3	A	308	GLU
3	A	309	ILE
3	A	310	MET
3	A	316	THR
3	A	317	ASN
3	A	320	ILE
3	A	322	MET
3	A	323	ASN
3	A	325	ILE
3	A	326	ARG
3	A	330	SER
3	A	335	MET
3	A	341	ASP
3	B	20	SER
3	B	27	LEU
3	B	28	MET
3	B	32	ARG
3	B	37	PHE
3	B	38	SER
3	B	39	GLU
3	B	44	MET
3	B	60	ASN
3	B	62	LYS

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Mol	Chain	Res	Type
3	B	92	LEU
3	B	108	SER
3	B	117	MET
3	B	118	ARG
3	B	122	LYS
3	B	138	GLU
3	B	139	ARG
3	B	146	ARG
3	B	147	SER
3	B	161	LEU
3	B	169	ASN
3	B	176	GLU
3	B	199	ARG
3	B	203	LEU
3	B	204	VAL
3	B	205	SER
3	B	209	VAL
3	B	211	LYS
3	B	219	LYS
3	B	230	VAL
3	B	232	ASP
3	B	241	ARG
3	B	245	ASN
3	B	254	SER
3	B	258	ASN
3	B	259	SER
3	B	277	ASP
3	B	282	ARG
3	B	289	HIS
3	B	292	ARG
3	B	306	ILE
3	B	316	THR
3	B	319	ASN
3	B	320	ILE
3	B	322	MET
3	B	325	ILE
3	B	326	ARG
3	B	327	ASN
3	B	336	VAL
3	B	339	LEU
3	B	341	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such

sidechains are listed below:

Mol	Chain	Res	Type
3	A	59	ASN
3	A	90	GLN
3	A	94	GLN
3	A	196	HIS
3	A	245	ASN
3	A	255	GLN
3	A	269	HIS
3	B	26	ASN
3	B	35	GLN
3	B	40	HIS
3	B	60	ASN
3	B	90	GLN
3	B	133	GLN
3	B	255	GLN
3	B	327	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

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	C	34/34 (100%)	0.35	3 (8%) 12 8	29, 52, 85, 94	2 (5%)
2	D	34/34 (100%)	0.08	1 (2%) 55 48	31, 46, 70, 90	0
3	A	322/349 (92%)	0.61	28 (8%) 13 8	23, 67, 98, 99	13 (4%)
3	B	319/349 (91%)	0.13	5 (1%) 74 70	20, 43, 90, 99	1 (0%)
All	All	709/766 (92%)	0.36	37 (5%) 31 24	20, 53, 96, 99	16 (2%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	A	282	ARG	8.8
3	A	283	TYR	6.5
3	A	281	GLN	6.3
1	C	17[B]	DT	5.3
3	B	327	ASN	4.8
1	C	18[B]	DA	4.7
3	A	279	SER	4.6
3	A	198	GLY	4.6
3	A	199	ARG	4.1
3	A	204	VAL	4.0
3	A	183	LYS	3.9
3	B	339	LEU	3.8
3	A	320	ILE	3.7
3	A	200	THR	3.4
3	A	185	ILE	3.3
3	A	197	ILE	3.2
3	A	173	ARG	3.1
3	A	174	LEU	2.9
1	C	16[A]	DG	2.9
3	A	203	LEU	2.8
3	A	201	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
3	A	304	VAL	2.5
3	A	309	ILE	2.5
3	A	195	ILE	2.5
3	A	188	THR	2.4
3	A	216	GLY	2.4
3	A	278	ASP	2.4
3	A	284	LEU	2.3
3	A	316	THR	2.3
3	A	231	ALA	2.3
3	A	187	ARG	2.2
3	A	194	LEU	2.2
3	A	256	LEU	2.2
3	B	203	LEU	2.1
2	D	17[A]	DT	2.1
3	B	324	TYR	2.1
3	B	206	THR	2.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.