



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:05 AM UTC

PDB ID : 1RAM / pdb_00001ram
Title : A NOVEL DNA RECOGNITION MODE BY NF-KB P65 HOMODIMER
Authors : Chen, Y.-Q.; Ghosh, S.; Ghosh, G.
Deposited on : 1997-11-22
Resolution : 2.70 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

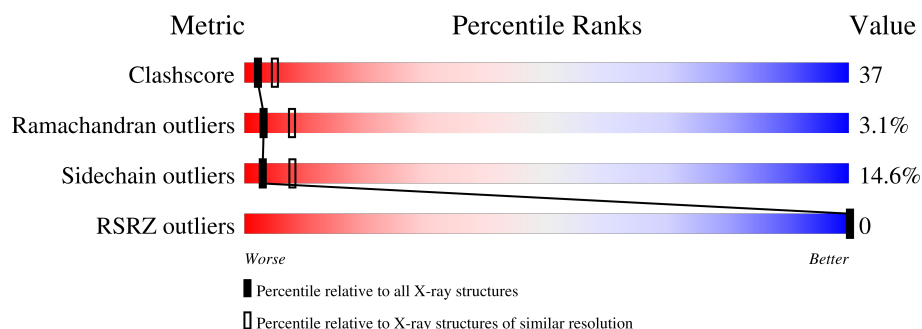
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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))
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	C	20	
1	D	20	
2	A	273	
2	B	273	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	DTT	A	1	X	-	-	-
3	DTT	B	2	X	-	-	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5202 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.

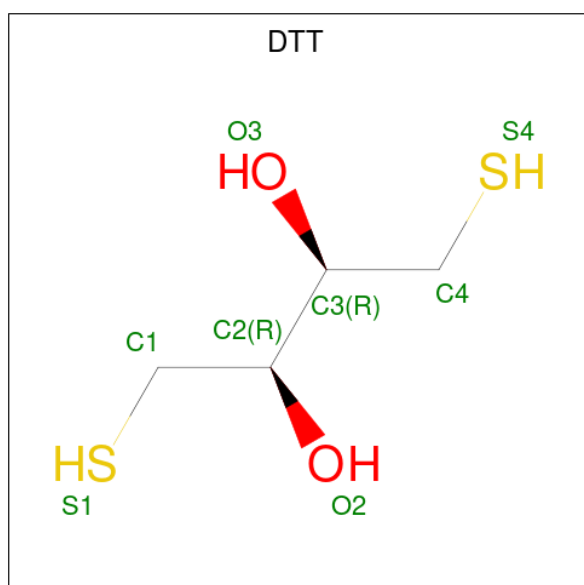
- Molecule 1 is a DNA chain called DNA (5'-D(*CP*GP*GP*CP*TP*GP*GP*AP*AP*AP*TP*TP*TP*CP*CP*AP*GP*CP*CP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	20	Total	C	N	O	P	0	0	0
			407	194	76	118	19			
1	D	20	Total	C	N	O	P	0	0	0
			407	194	76	118	19			

- Molecule 2 is a protein called PROTEIN (TRANSCRIPTION FACTOR NF-KB P65).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	273	Total	C	N	O	S	0	0	0
			2178	1358	401	408	11			
2	B	273	Total	C	N	O	S	0	0	0
			2178	1358	401	408	11			

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: DTT) (formula: C₄H₁₀O₂S₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	S	0	0
			8	4	2	2		
3	B	1	Total	C	O	S	0	0
			8	4	2	2		

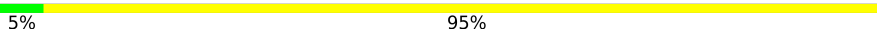
- Molecule 4 is water.

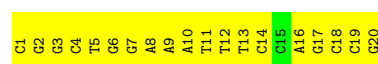
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	3	Total	O	0	0
			3	3		
4	D	2	Total	O	0	0
			2	2		
4	A	5	Total	O	0	0
			5	5		
4	B	6	Total	O	0	0
			6	6		

3 Residue-property plots

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.

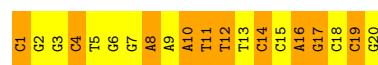
- Molecule 1: DNA (5'-D(*CP*GP*GP*CP*TP*GP*GP*AP*AP*AP*TP*TP*TP*CP*CP*AP*GP*CP*CP*G)-3')

Chain C: 



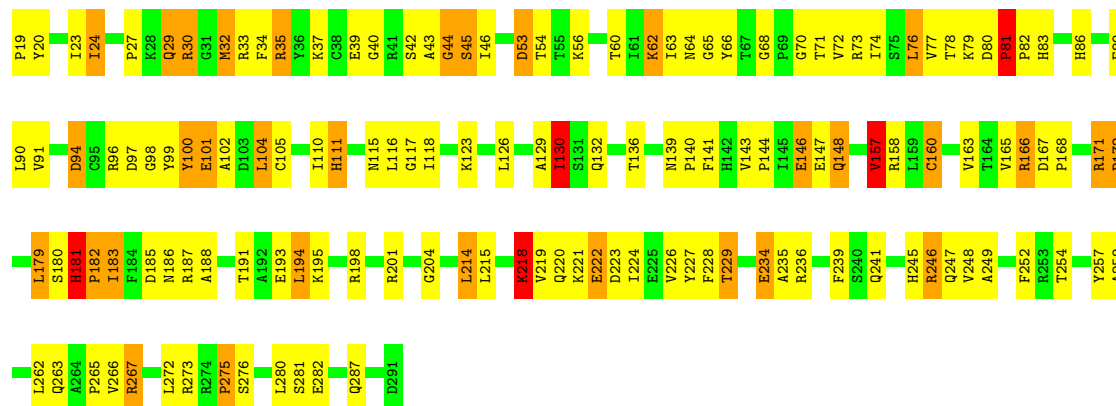
- Molecule 1: DNA (5'-D(*CP*GP*GP*CP*TP*GP*GP*AP*AP*AP*TP*TP*TP*CP*CP*AP*GP*CP*CP*G)-3')

Chain D: 



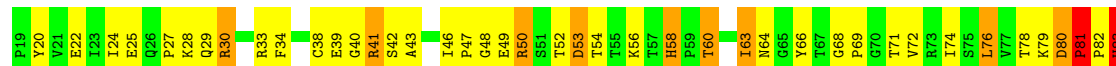
- Molecule 2: PROTEIN (TRANSCRIPTION FACTOR NF-KB P65)

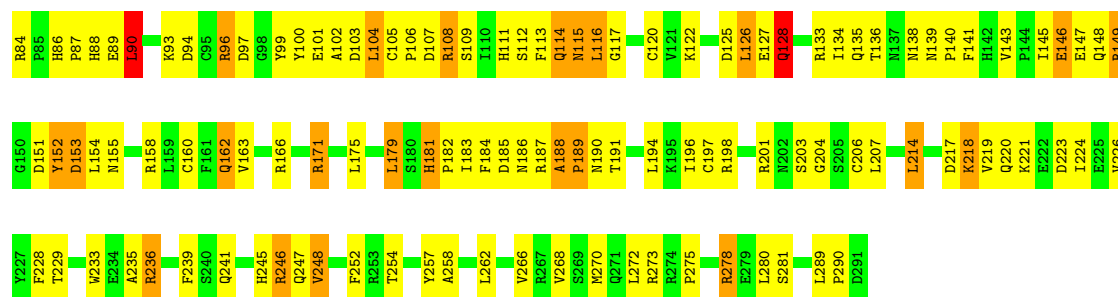
Chain A: 



- Molecule 2: PROTEIN (TRANSCRIPTION FACTOR NF-KB P65)

Chain B: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.69Å 81.08Å 167.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	6.00 – 2.70 6.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	91.2 (6.00-2.70) 87.4 (6.00-2.70)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.51Å)	Xtriage
Refinement program	X-PLOR 3.843	Depositor
R, R_{free}	0.222 , 0.324 0.229 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	65.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 103.7	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	5202	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.85% 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

5.1 Standard geometry

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

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	0.51	0/456	0.89	0/702
1	D	0.55	0/456	1.23	6/702 (0.9%)
2	A	0.80	0/2231	1.26	23/3025 (0.8%)
2	B	0.69	0/2231	1.24	22/3025 (0.7%)
All	All	0.72	0/5374	1.22	51/7454 (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
1	C	0	1
1	D	0	5
2	B	0	2
All	All	0	8

There are no bond length outliers.

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	80	ASP	CA-C-N	12.95	133.72	120.38
2	B	80	ASP	C-N-CA	12.95	133.72	120.38
2	B	81	PRO	N-CA-C	10.67	123.72	110.70
2	A	81	PRO	N-CA-C	8.85	121.50	110.70
2	A	183	ILE	N-CA-C	-8.57	96.17	108.17
2	A	30	ARG	N-CA-C	8.03	121.11	109.14
2	A	80	ASP	CA-C-N	7.85	128.47	120.38
2	A	80	ASP	C-N-CA	7.85	128.47	120.38
2	B	183	ILE	N-CA-C	-7.16	98.09	109.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	DT	N1-C1'-C2'	7.02	124.03	113.50
2	A	229	THR	N-CA-C	7.01	119.83	108.76
2	B	268	VAL	N-CA-C	-6.98	100.01	108.53
2	B	246	ARG	N-CA-C	6.83	120.91	111.90
2	B	90	LEU	N-CA-C	-6.66	98.84	109.76
2	B	229	THR	N-CA-C	6.63	119.40	108.99
2	A	80	ASP	N-CA-C	6.57	118.35	110.07
2	B	82	PRO	N-CA-C	-6.49	105.58	114.80
2	A	254	THR	CA-C-N	6.41	126.98	120.38
2	A	254	THR	C-N-CA	6.41	126.98	120.38
1	D	1	DC	O5'-C5'-C4'	6.32	120.28	110.80
2	A	111	HIS	N-CA-C	6.11	118.37	108.41
2	B	80	ASP	N-CA-C	5.97	117.33	109.93
2	B	197	CYS	N-CA-C	5.94	117.56	111.14
2	A	181	HIS	N-CA-C	-5.91	102.65	110.40
2	A	81	PRO	CA-C-N	-5.79	112.60	119.84
2	A	81	PRO	C-N-CA	-5.79	112.60	119.84
2	B	58	HIS	N-CA-C	5.64	114.79	108.25
2	B	43	ALA	N-CA-C	-5.56	107.14	114.31
1	D	8	DA	C4'-C3'-O3'	-5.54	101.69	110.00
2	B	163	VAL	N-CA-C	5.52	116.72	109.21
1	D	8	DA	N9-C1'-C2'	5.46	121.69	113.50
2	A	76	LEU	N-CA-C	-5.44	100.16	109.24
2	B	188	ALA	CA-C-N	5.42	126.61	119.84
2	B	188	ALA	C-N-CA	5.42	126.61	119.84
1	D	16	DA	N9-C1'-C2'	5.40	121.61	113.50
2	B	254	THR	CA-C-N	5.40	125.94	120.38
2	B	254	THR	C-N-CA	5.40	125.94	120.38
2	A	157	VAL	N-CA-CB	-5.40	104.96	112.52
2	A	236	ARG	NE-CZ-NH2	-5.40	114.34	119.20
2	B	83	HIS	N-CA-C	5.37	122.23	110.80
1	D	11	DT	N1-C1'-C2'	5.35	121.52	113.50
2	A	130	ILE	N-CA-C	5.32	117.70	111.05
2	A	180	SER	N-CA-C	-5.28	101.67	109.86
2	A	83	HIS	N-CA-C	5.25	117.74	109.39
2	A	68	GLY	CA-C-N	5.20	125.20	119.90
2	A	68	GLY	C-N-CA	5.20	125.20	119.90
2	B	128	GLN	N-CA-C	-5.20	106.45	112.89
2	A	148	GLN	N-CA-C	-5.16	107.12	113.41
2	B	236	ARG	NE-CZ-NH2	-5.08	114.63	119.20
2	B	207	LEU	N-CA-C	-5.04	107.14	113.28
2	A	105	CYS	N-CA-C	-5.03	102.11	109.50

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	152	TYR	Sidechain
2	B	66	TYR	Sidechain
1	C	14	DC	Sidechain
1	D	10	DA	Sidechain
1	D	14	DC	Sidechain
1	D	17	DG	Sidechain
1	D	19	DC	Sidechain
1	D	4	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	C	407	0	226	56	0
1	D	407	0	226	57	0
2	A	2178	0	2140	116	0
2	B	2178	0	2140	154	0
3	A	8	0	10	0	0
3	B	8	0	10	3	0
4	A	5	0	0	0	0
4	B	6	0	0	0	0
4	C	3	0	0	0	0
4	D	2	0	0	1	0
All	All	5202	0	4752	356	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 37.

All (356) 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:D:1:DC:H5'	1:D:2:DG:C8	1.78	1.19
1:C:8:DA:H2''	1:C:9:DA:C5'	1.79	1.11
1:D:1:DC:H5'	1:D:2:DG:H8	1.10	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:8:DA:H2''	1:C:9:DA:H5'	1.31	1.08
2:B:89:GLU:HG2	2:B:133:ARG:HH22	1.19	1.07
2:A:33:ARG:HH21	2:A:187:ARG:HH22	1.06	0.98
1:C:19:DC:N4	1:D:2:DG:H1	1.62	0.97
1:C:19:DC:H42	1:D:2:DG:H1	1.01	0.96
2:B:86:HIS:HD2	2:B:88:HIS:H	1.03	0.93
2:A:166:ARG:HG2	2:A:166:ARG:HH11	1.32	0.92
2:B:33:ARG:HE	2:B:187:ARG:HB2	1.36	0.91
1:D:2:DG:H2'	1:D:3:DG:C8	2.05	0.91
1:C:17:DG:H1	1:D:4:DC:H42	1.10	0.90
1:D:3:DG:H2''	1:D:4:DC:O5'	1.69	0.89
2:A:33:ARG:HH21	2:A:187:ARG:NH2	1.71	0.89
2:A:89:GLU:HB2	2:A:98:GLY:HA2	1.55	0.89
2:B:86:HIS:CD2	2:B:88:HIS:H	1.90	0.88
1:D:6:DG:H2''	1:D:7:DG:O5'	1.73	0.86
1:D:13:DT:H2''	1:D:14:DC:O5'	1.75	0.86
1:C:1:DC:O5'	1:C:2:DG:H5'	1.76	0.86
1:C:6:DG:H2'	1:C:7:DG:C8	2.12	0.85
1:D:3:DG:H2''	1:D:4:DC:C5'	2.07	0.85
1:D:16:DA:H2'	1:D:17:DG:C8	2.11	0.84
2:B:84:ARG:H	2:B:84:ARG:HD3	1.43	0.84
1:C:11:DT:H5''	2:A:123:LYS:HE2	1.58	0.84
2:B:33:ARG:HG2	2:B:187:ARG:H	1.44	0.82
2:A:29:GLN:HG3	2:A:182:PRO:O	1.79	0.82
1:C:3:DG:H2''	1:C:4:DC:OP2	1.78	0.82
1:C:17:DG:H2''	1:C:18:DC:OP2	1.80	0.81
2:B:46:ILE:HG13	2:B:116:LEU:O	1.79	0.81
2:A:132:GLN:O	2:A:136:THR:HG22	1.80	0.81
2:B:33:ARG:NE	2:B:187:ARG:HB2	1.96	0.81
1:D:18:DC:C2'	1:D:19:DC:H5'	2.10	0.81
1:C:1:DC:H4'	1:C:2:DG:O4'	1.82	0.80
1:C:8:DA:C2'	1:C:9:DA:C5'	2.59	0.80
1:C:8:DA:C2'	1:C:9:DA:H5''	2.14	0.78
1:D:20:DG:H1'	4:D:317:HOH:O	1.83	0.78
2:B:33:ARG:HG3	2:B:186:ASN:HB3	1.66	0.78
1:C:20:DG:H1	1:D:1:DC:H42	1.30	0.78
2:A:126:LEU:HD23	2:A:130:ILE:HD11	1.63	0.78
2:A:160:CYS:SG	2:A:160:CYS:O	2.41	0.77
2:B:41:ARG:CZ	2:B:41:ARG:H	1.97	0.77
2:B:146:GLU:HA	2:B:149:ARG:HH21	1.48	0.77
2:B:189:PRO:HB3	2:B:220:GLN:NE2	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:DA:H2''	1:D:11:DT:O5'	1.83	0.77
1:C:19:DC:N3	1:D:2:DG:N2	2.32	0.77
2:B:134:ILE:HD11	2:B:148:GLN:HG3	1.67	0.76
1:C:8:DA:H2''	1:C:9:DA:H5''	1.67	0.75
1:D:15:DC:H2'	1:D:16:DA:C8	2.22	0.75
2:A:141:PHE:CE2	2:A:179:LEU:HD11	2.20	0.75
1:C:1:DC:H4'	1:C:2:DG:C5'	2.17	0.75
1:C:6:DG:C2'	1:C:7:DG:C8	2.69	0.75
1:D:2:DG:H2''	1:D:3:DG:O5'	1.88	0.74
1:C:3:DG:N2	1:D:18:DC:N3	2.33	0.74
2:B:206:CYS:HB3	2:B:262:LEU:HD12	1.69	0.74
2:A:62:LYS:HD3	2:A:110:ILE:HD11	1.69	0.73
2:A:141:PHE:HE2	2:A:179:LEU:HD11	1.53	0.73
2:A:194:LEU:H	2:A:194:LEU:HD22	1.52	0.73
1:C:17:DG:H1	1:D:4:DC:N4	1.85	0.73
1:D:18:DC:H2'	1:D:19:DC:H5'	1.71	0.71
1:D:1:DC:C5'	1:D:2:DG:C8	2.68	0.70
2:B:89:GLU:CG	2:B:133:ARG:HH22	2.01	0.70
2:B:257:TYR:CZ	2:B:266:VAL:HG11	2.26	0.70
2:B:94:ASP:HB2	2:B:100:TYR:CE1	2.27	0.69
2:B:89:GLU:HG2	2:B:133:ARG:NH2	2.01	0.69
2:B:140:PRO:HG3	2:B:162:GLN:HE22	1.55	0.69
1:D:3:DG:H8	1:D:3:DG:OP2	1.76	0.69
1:D:19:DC:H2''	1:D:20:DG:H5'	1.73	0.69
2:B:30:ARG:HD2	2:B:191:THR:HG22	1.73	0.69
1:C:4:DC:H2''	1:C:5:DT:OP2	1.94	0.68
2:B:171:ARG:HG2	2:B:171:ARG:HH11	1.57	0.68
1:C:8:DA:H1'	1:C:9:DA:H5''	1.75	0.68
2:A:76:LEU:HD13	2:A:90:LEU:HD13	1.76	0.68
2:B:86:HIS:HD2	2:B:88:HIS:N	1.86	0.67
2:B:76:LEU:HD13	2:B:90:LEU:HD22	1.76	0.67
1:C:8:DA:C1'	1:C:9:DA:H5''	2.24	0.67
1:D:4:DC:H5'	2:A:44:GLY:HA2	1.76	0.67
2:B:107:ASP:C	2:B:108:ARG:HD3	2.21	0.66
2:A:89:GLU:HB2	2:A:98:GLY:CA	2.26	0.66
2:B:151:ASP:HB3	3:B:2:DTT:O3	1.96	0.65
1:C:2:DG:N1	1:D:18:DC:N4	2.44	0.65
2:B:217:ASP:O	2:B:219:VAL:HG13	1.97	0.65
2:A:144:PRO:O	2:A:148:GLN:HG3	1.97	0.64
2:B:25:GLU:HB3	2:B:60:THR:H	1.62	0.64
1:C:19:DC:H2''	1:C:20:DG:OP2	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:GLY:HA2	2:B:106:PRO:HB3	1.80	0.64
2:B:105:CYS:SG	2:B:108:ARG:HG2	2.38	0.64
2:A:45:SER:HA	2:A:116:LEU:O	1.97	0.63
2:B:33:ARG:HG2	2:B:187:ARG:N	2.10	0.63
2:A:144:PRO:HB2	2:A:147:GLU:OE1	1.98	0.63
2:A:228:PHE:O	2:A:229:THR:HG23	1.98	0.63
2:B:141:PHE:CZ	2:B:179:LEU:HD23	2.32	0.63
1:C:17:DG:C4	1:C:18:DC:C5	2.86	0.63
2:A:239:PHE:HB3	2:A:252:PHE:CB	2.29	0.63
2:A:126:LEU:CD2	2:A:130:ILE:HD11	2.28	0.62
2:B:146:GLU:HA	2:B:149:ARG:NH2	2.13	0.62
2:B:218:LYS:HE3	2:B:247:GLN:OE1	1.98	0.62
2:A:76:LEU:CD1	2:A:90:LEU:HD13	2.30	0.62
1:C:2:DG:N2	1:D:19:DC:N3	2.44	0.62
2:A:86:HIS:CD2	2:A:157:VAL:HG23	2.35	0.61
1:C:20:DG:H1	1:D:1:DC:N4	1.98	0.61
2:B:141:PHE:HZ	2:B:179:LEU:HD23	1.66	0.61
2:B:105:CYS:SG	2:B:108:ARG:NE	2.74	0.60
1:C:2:DG:H2''	1:C:3:DG:C8	2.36	0.60
2:B:60:THR:HA	2:B:111:HIS:O	2.00	0.60
1:D:7:DG:H2''	1:D:8:DA:O5'	2.00	0.60
2:B:58:HIS:CE1	2:B:114:GLN:HB3	2.36	0.60
2:B:104:LEU:HD22	2:B:111:HIS:NE2	2.16	0.60
2:B:239:PHE:HB3	2:B:252:PHE:CB	2.31	0.60
2:B:84:ARG:HG3	2:B:143:VAL:HG11	1.83	0.60
1:C:6:DG:N2	1:D:16:DA:C2	2.70	0.60
2:B:24:ILE:HG13	2:B:60:THR:HG22	1.82	0.60
2:B:149:ARG:HD3	2:B:149:ARG:N	2.17	0.60
1:D:10:DA:C2'	1:D:11:DT:O5'	2.50	0.59
2:A:100:TYR:CD1	2:A:101:GLU:N	2.71	0.59
2:B:140:PRO:HB2	2:B:141:PHE:CD1	2.37	0.59
2:A:262:LEU:HD13	2:A:266:VAL:HG23	1.83	0.59
1:C:1:DC:H4'	1:C:2:DG:H5'	1.84	0.59
2:A:19:PRO:HG3	2:A:65:GLY:O	2.03	0.59
2:A:70:GLY:C	2:A:104:LEU:HB2	2.28	0.58
2:B:155:ASN:HD22	2:B:185:ASP:HB3	1.68	0.58
2:B:187:ARG:HB3	2:B:187:ARG:NH1	2.18	0.58
1:C:3:DG:N1	1:D:18:DC:N4	2.51	0.58
1:D:19:DC:H2''	1:D:20:DG:C5'	2.34	0.58
2:B:30:ARG:HD3	2:B:184:PHE:HB2	1.86	0.58
2:B:71:THR:HG22	2:B:103:ASP:HA	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:DA:H2''	1:D:9:DA:O5'	2.03	0.57
2:A:74:ILE:HB	2:A:100:TYR:HB3	1.86	0.57
2:B:136:THR:HG22	2:B:136:THR:O	2.04	0.57
2:A:224:ILE:HD11	2:A:272:LEU:HD22	1.86	0.57
1:C:2:DG:C6	1:D:18:DC:N4	2.72	0.57
2:A:267:ARG:O	2:A:267:ARG:HG2	2.04	0.57
2:B:88:HIS:CE1	2:B:154:LEU:HD22	2.40	0.57
2:A:60:THR:CG2	2:A:110:ILE:HG23	2.34	0.57
1:C:2:DG:H1	1:D:19:DC:H42	1.52	0.57
1:C:1:DC:C4'	1:C:2:DG:O4'	2.53	0.56
1:D:15:DC:H2''	1:D:16:DA:O4'	2.05	0.56
2:A:70:GLY:O	2:A:104:LEU:HB2	2.04	0.56
2:A:239:PHE:HB3	2:A:252:PHE:HB3	1.88	0.56
1:C:17:DG:C5	1:C:18:DC:C5	2.93	0.56
1:C:3:DG:H1	1:D:18:DC:N4	2.02	0.56
2:B:86:HIS:CG	2:B:87:PRO:HD2	2.41	0.56
2:B:166:ARG:HG3	2:B:166:ARG:HH11	1.70	0.56
2:B:27:PRO:O	2:B:181:HIS:HE1	1.88	0.56
2:A:166:ARG:HG2	2:A:166:ARG:NH1	2.06	0.55
2:B:171:ARG:HG2	2:B:171:ARG:NH1	2.21	0.55
2:A:218:LYS:HG3	2:A:247:GLN:NE2	2.21	0.55
2:B:41:ARG:H	2:B:41:ARG:NE	2.04	0.55
2:A:222:GLU:HB3	2:A:241:GLN:OE1	2.07	0.55
2:B:29:GLN:HG2	2:B:182:PRO:O	2.06	0.55
2:B:194:LEU:HB3	2:B:281:SER:HB3	1.88	0.55
1:C:8:DA:H5'	1:C:8:DA:H8	1.72	0.55
1:D:2:DG:C2'	1:D:3:DG:C8	2.85	0.55
2:A:60:THR:HG21	2:A:110:ILE:HG23	1.87	0.55
2:A:193:GLU:HG3	2:A:193:GLU:O	2.07	0.55
2:B:187:ARG:HB3	2:B:187:ARG:HH11	1.72	0.55
2:B:80:ASP:OD1	3:B:2:DTT:S1	2.62	0.55
1:D:15:DC:C2'	1:D:16:DA:C8	2.90	0.54
2:B:140:PRO:HB2	2:B:141:PHE:HD1	1.72	0.54
2:B:145:ILE:HA	2:B:148:GLN:HG2	1.88	0.54
2:A:185:ASP:OD2	2:A:187:ARG:HB2	2.07	0.54
2:B:78:THR:OG1	2:B:83:HIS:HA	2.08	0.54
2:B:239:PHE:HB3	2:B:252:PHE:HB3	1.89	0.54
2:A:97:ASP:HB2	2:A:99:TYR:CE2	2.43	0.54
1:C:1:DC:C4'	1:C:2:DG:H5'	2.37	0.54
2:B:60:THR:OG1	2:B:112:SER:HB3	2.08	0.54
2:A:267:ARG:HA	2:A:287:GLN:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:ARG:HH11	2:B:191:THR:HG22	1.73	0.53
2:B:40:GLY:HA3	2:B:41:ARG:NH1	2.23	0.53
2:A:77:VAL:CG1	2:A:140:PRO:HG3	2.38	0.53
2:A:166:ARG:HH11	2:A:166:ARG:CG	2.14	0.53
1:C:17:DG:C6	1:C:18:DC:N4	2.76	0.53
2:B:52:THR:C	2:B:54:THR:H	2.16	0.53
2:B:20:TYR:HE1	2:B:22:GLU:HG3	1.74	0.53
2:B:245:HIS:CE1	2:B:246:ARG:HG2	2.44	0.53
2:B:214:LEU:C	2:B:214:LEU:HD23	2.34	0.53
1:D:1:DC:H2'	1:D:1:DC:O2	2.07	0.52
2:B:104:LEU:HD22	2:B:111:HIS:CE1	2.45	0.52
2:A:257:TYR:CD1	2:A:258:ALA:N	2.77	0.52
1:D:1:DC:O2	1:D:1:DC:C2'	2.57	0.52
2:A:43:ALA:HB3	2:A:117:GLY:HA3	1.91	0.52
2:B:149:ARG:HD3	2:B:149:ARG:H	1.74	0.52
2:B:257:TYR:OH	2:B:266:VAL:HG11	2.10	0.52
2:B:257:TYR:CG	2:B:258:ALA:N	2.78	0.52
2:B:58:HIS:ND1	2:B:114:GLN:HB3	2.26	0.51
2:A:81:PRO:HB2	2:A:82:PRO:HD3	1.92	0.51
2:B:33:ARG:CG	2:B:186:ASN:HB3	2.39	0.51
2:B:93:LYS:HB2	2:B:115:ASN:ND2	2.26	0.51
1:C:1:DC:H4'	1:C:2:DG:C4'	2.41	0.51
2:B:63:ILE:HD13	2:B:175:LEU:HD11	1.92	0.51
2:B:94:ASP:HB2	2:B:100:TYR:HE1	1.75	0.51
1:C:6:DG:H2''	1:C:7:DG:C8	2.44	0.50
2:A:100:TYR:CE1	2:A:102:ALA:HB3	2.46	0.50
2:B:226:VAL:HG12	2:B:228:PHE:CE1	2.47	0.50
1:C:8:DA:H5'	1:C:8:DA:C8	2.46	0.50
2:A:77:VAL:HG11	2:A:140:PRO:HG3	1.92	0.50
2:B:90:LEU:HD12	2:B:117:GLY:O	2.11	0.50
2:A:158:ARG:CZ	2:A:182:PRO:HD3	2.41	0.50
2:B:257:TYR:CD1	2:B:258:ALA:N	2.76	0.50
2:A:181:HIS:C	2:A:181:HIS:HD1	2.18	0.50
2:B:79:LYS:HA	2:B:158:ARG:HD2	1.93	0.50
2:B:33:ARG:HH21	2:B:187:ARG:NE	2.10	0.50
2:B:86:HIS:NE2	2:B:88:HIS:CD2	2.80	0.50
2:A:188:ALA:HB3	2:A:191:THR:OG1	2.11	0.49
1:C:2:DG:H1	1:D:19:DC:N4	2.10	0.49
1:C:17:DG:N2	1:D:4:DC:N3	2.50	0.49
2:A:144:PRO:HD2	2:A:147:GLU:CG	2.42	0.49
2:B:47:PRO:HA	2:B:58:HIS:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:69:PRO:HB2	2:B:166:ARG:HD2	1.94	0.49
2:B:125:ASP:O	2:B:128:GLN:HG3	2.11	0.49
1:C:1:DC:O5'	1:C:2:DG:C5'	2.56	0.49
2:A:72:VAL:HB	2:A:104:LEU:HD13	1.93	0.49
2:A:257:TYR:OH	2:A:266:VAL:HG11	2.13	0.49
2:B:289:LEU:HB3	2:B:290:PRO:HD2	1.95	0.49
2:B:139:ASN:HD21	2:B:143:VAL:N	2.11	0.49
2:B:181:HIS:HD1	2:B:181:HIS:C	2.20	0.48
2:B:20:TYR:CE1	2:B:64:ASN:ND2	2.74	0.48
2:B:28:LYS:HD3	2:B:48:GLY:O	2.14	0.48
1:D:12:DT:OP1	2:B:122:LYS:HD2	2.13	0.48
2:A:262:LEU:HD13	2:A:266:VAL:CG2	2.43	0.48
1:D:19:DC:H2'	1:D:20:DG:C8	2.48	0.48
1:D:9:DA:H2'	1:D:10:DA:O4'	2.13	0.48
2:B:141:PHE:CD1	2:B:141:PHE:N	2.82	0.48
2:B:233:TRP:CH2	2:B:235:ALA:HB3	2.49	0.48
1:D:12:DT:H2''	1:D:13:DT:O5'	2.14	0.48
2:B:34:PHE:CD1	2:B:34:PHE:N	2.81	0.48
2:B:46:ILE:HD12	2:B:116:LEU:HD13	1.95	0.48
2:B:33:ARG:HE	2:B:187:ARG:CB	2.19	0.47
2:A:100:TYR:CD1	2:A:100:TYR:C	2.92	0.47
2:B:58:HIS:HB3	2:B:113:PHE:O	2.14	0.47
2:B:86:HIS:CD2	2:B:87:PRO:HD2	2.50	0.47
2:B:88:HIS:ND1	2:B:120:CYS:HA	2.29	0.47
2:B:219:VAL:HG22	2:B:247:GLN:O	2.14	0.47
1:D:6:DG:O6	2:A:35:ARG:NH2	2.47	0.47
2:B:107:ASP:O	2:B:108:ARG:HD3	2.13	0.47
2:B:166:ARG:HH11	2:B:166:ARG:CG	2.28	0.47
2:A:74:ILE:HG22	2:A:90:LEU:HD21	1.97	0.47
2:B:140:PRO:HB3	2:B:160:CYS:SG	2.54	0.47
2:A:27:PRO:O	2:A:181:HIS:HE1	1.98	0.47
2:A:146:GLU:HB2	2:A:147:GLU:OE1	2.15	0.47
2:B:41:ARG:NE	2:B:42:SER:H	2.13	0.47
2:A:20:TYR:CE1	2:A:64:ASN:OD1	2.68	0.47
2:A:166:ARG:NH1	2:A:166:ARG:CG	2.75	0.47
2:A:273:ARG:HG3	2:A:280:LEU:HD23	1.97	0.47
2:A:218:LYS:HD2	2:A:247:GLN:OE1	2.15	0.46
2:B:76:LEU:HD12	2:B:76:LEU:HA	1.80	0.46
2:A:34:PHE:CD2	2:A:185:ASP:HB2	2.50	0.46
2:B:47:PRO:HA	2:B:58:HIS:HD2	1.80	0.46
2:B:72:VAL:O	2:B:101:GLU:HA	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:DG:H2''	1:D:4:DC:H5''	1.91	0.46
2:A:44:GLY:O	2:A:45:SER:CB	2.64	0.46
2:A:228:PHE:HB2	2:A:235:ALA:O	2.14	0.46
2:A:248:VAL:HG21	2:B:246:ARG:HB2	1.97	0.46
2:B:138:ASN:C	2:B:138:ASN:OD1	2.57	0.46
1:D:4:DC:H2'	1:D:5:DT:O4'	2.16	0.46
2:A:227:TYR:CE2	2:A:229:THR:HG21	2.51	0.46
2:A:139:ASN:HD21	2:A:143:VAL:N	2.14	0.46
2:B:224:ILE:HD11	2:B:272:LEU:HD22	1.97	0.46
2:A:91:VAL:HG23	2:A:91:VAL:O	2.16	0.46
2:B:30:ARG:HD2	2:B:191:THR:CG2	2.44	0.46
2:B:96:ARG:HE	2:B:97:ASP:CG	2.24	0.46
2:B:189:PRO:HB3	2:B:220:GLN:HE22	1.76	0.46
2:A:214:LEU:C	2:A:214:LEU:HD23	2.41	0.45
2:B:146:GLU:HA	2:B:149:ARG:HE	1.80	0.45
1:C:16:DA:H2''	1:C:17:DG:C8	2.52	0.45
2:B:99:TYR:CD1	2:B:99:TYR:C	2.95	0.45
2:A:62:LYS:HD3	2:A:110:ILE:CD1	2.44	0.45
2:A:126:LEU:O	2:A:129:ALA:HB3	2.16	0.45
2:B:74:ILE:HB	2:B:100:TYR:HB3	1.99	0.45
1:C:9:DA:OP1	2:A:221:LYS:HE3	2.17	0.45
2:A:257:TYR:CZ	2:A:266:VAL:HG11	2.52	0.45
2:A:40:GLY:C	2:A:42:SER:H	2.25	0.45
2:A:215:LEU:HB3	2:B:245:HIS:CD2	2.51	0.45
2:A:227:TYR:CE2	2:A:229:THR:CG2	3.00	0.45
2:B:221:LYS:HE2	2:B:241:GLN:HE21	1.82	0.45
2:A:37:LYS:C	2:A:39:GLU:H	2.25	0.44
1:C:18:DC:OP2	1:C:18:DC:H2'	2.17	0.44
2:B:188:ALA:HB3	2:B:191:THR:OG1	2.17	0.44
2:B:223:ASP:OD1	2:B:275:PRO:HD2	2.17	0.44
2:B:273:ARG:HG3	2:B:280:LEU:HD23	1.98	0.44
2:A:62:LYS:HG3	2:A:63:ILE:N	2.33	0.44
2:B:53:ASP:HA	2:B:56:LYS:HE3	2.00	0.44
1:C:1:DC:C5'	1:C:2:DG:H5'	2.47	0.44
1:C:1:DC:N3	1:D:20:DG:O6	2.50	0.44
2:A:226:VAL:HG11	2:A:252:PHE:CZ	2.52	0.44
2:B:52:THR:O	2:B:56:LYS:HD2	2.18	0.44
2:B:233:TRP:CZ2	2:B:235:ALA:HB3	2.53	0.44
2:A:72:VAL:HG23	2:A:163:VAL:HG22	2.00	0.44
2:A:245:HIS:CD2	2:A:246:ARG:HG2	2.53	0.44
2:B:246:ARG:O	2:B:248:VAL:HG13	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:46:ILE:HD11	2:A:118:ILE:CD1	2.48	0.43
2:B:201:ARG:NH2	2:B:204:GLY:HA2	2.33	0.43
2:B:273:ARG:HH12	2:B:278:ARG:HG2	1.83	0.43
2:A:46:ILE:HD11	2:A:118:ILE:HD11	2.01	0.43
2:A:72:VAL:O	2:A:72:VAL:HG13	2.18	0.43
2:A:245:HIS:HB3	2:A:249:ALA:HB3	2.00	0.43
2:B:196:ILE:O	2:B:196:ILE:HG22	2.18	0.43
2:B:246:ARG:C	2:B:248:VAL:H	2.26	0.43
1:C:12:DT:H2''	1:C:13:DT:H5'	2.01	0.43
1:D:3:DG:C2'	1:D:4:DC:O5'	2.53	0.43
2:A:201:ARG:NH2	2:A:204:GLY:HA2	2.33	0.43
2:B:104:LEU:HD22	2:B:111:HIS:CD2	2.53	0.43
2:B:233:TRP:CD1	2:B:258:ALA:HB2	2.53	0.43
2:A:171:ARG:HG3	2:A:172:PRO:HD2	2.00	0.43
2:A:275:PRO:O	2:A:276:SER:C	2.62	0.43
2:A:62:LYS:HE2	2:A:64:ASN:HD21	1.84	0.43
2:B:126:LEU:HG	2:B:127:GLU:OE1	2.19	0.43
1:D:3:DG:C2'	1:D:4:DC:C5'	2.91	0.43
2:A:141:PHE:CZ	2:A:179:LEU:HD11	2.53	0.43
2:A:97:ASP:HA	2:A:132:GLN:HE22	1.83	0.43
2:A:220:GLN:HB3	2:A:222:GLU:OE2	2.19	0.43
2:B:24:ILE:CG1	2:B:60:THR:HG22	2.46	0.43
2:B:201:ARG:NE	2:B:203:SER:O	2.44	0.42
1:D:19:DC:C2'	1:D:20:DG:O4'	2.67	0.42
2:B:149:ARG:N	2:B:149:ARG:CD	2.81	0.42
2:B:39:GLU:CD	2:B:187:ARG:HH21	2.27	0.42
1:C:1:DC:O2	1:C:1:DC:O4'	2.37	0.42
1:C:10:DA:C2	1:D:12:DT:O2	2.72	0.42
2:A:60:THR:HA	2:A:111:HIS:O	2.19	0.42
2:B:87:PRO:HD3	2:B:152:TYR:CD1	2.55	0.42
2:B:153:ASP:HB2	3:B:2:DTT:O2	2.19	0.42
2:A:144:PRO:HD2	2:A:147:GLU:HG2	2.02	0.42
1:C:12:DT:H72	2:A:187:ARG:HD3	2.02	0.42
1:C:12:DT:H2''	1:C:13:DT:C5'	2.50	0.42
2:A:24:ILE:HD13	2:A:24:ILE:N	2.34	0.41
2:A:79:LYS:HA	2:A:158:ARG:HD2	2.02	0.41
2:B:49:GLU:HB3	2:B:50:ARG:HD2	2.02	0.41
2:B:147:GLU:C	2:B:149:ARG:H	2.28	0.41
2:A:32:MET:HE3	2:A:32:MET:HB3	1.66	0.41
2:A:66:TYR:CE1	2:A:165:VAL:HB	2.55	0.41
2:B:80:ASP:HA	2:B:81:PRO:HD3	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:62:LYS:HE2	2:A:64:ASN:ND2	2.35	0.41
2:A:181:HIS:C	2:A:181:HIS:ND1	2.78	0.41
2:B:27:PRO:O	2:B:181:HIS:CE1	2.72	0.41
2:B:226:VAL:HG11	2:B:252:PHE:CZ	2.55	0.41
2:A:257:TYR:CG	2:A:258:ALA:N	2.89	0.41
2:B:228:PHE:CZ	2:B:270:MET:HG3	2.56	0.41
2:A:73:ARG:HE	2:A:101:GLU:CD	2.28	0.41
2:A:94:ASP:HB3	2:A:101:GLU:O	2.21	0.41
2:A:143:VAL:HA	2:A:144:PRO:HD3	1.85	0.41
2:A:227:TYR:HE1	2:A:234:GLU:OE2	2.02	0.41
2:B:93:LYS:H	2:B:115:ASN:HD22	1.67	0.41
2:A:37:LYS:C	2:A:39:GLU:N	2.79	0.41
2:A:118:ILE:HD11	2:A:183:ILE:HD12	2.02	0.41
2:A:157:VAL:O	2:A:182:PRO:HA	2.21	0.41
2:A:34:PHE:CE2	2:A:185:ASP:HB2	2.56	0.41
2:B:147:GLU:C	2:B:149:ARG:N	2.75	0.41
2:B:29:GLN:HG3	2:B:181:HIS:CE1	2.56	0.40
2:B:72:VAL:HG12	2:B:102:ALA:O	2.21	0.40
2:A:257:TYR:CE2	2:A:266:VAL:HG11	2.56	0.40
2:B:221:LYS:HG3	2:B:241:GLN:NE2	2.36	0.40
1:D:15:DC:H2'	1:D:16:DA:N7	2.37	0.40
2:A:281:SER:O	2:A:282:GLU:C	2.62	0.40
2:B:96:ARG:HG2	2:B:97:ASP:OD1	2.22	0.40
2:B:20:TYR:CE1	2:B:22:GLU:HG3	2.53	0.40
2:B:126:LEU:O	2:B:126:LEU:HD12	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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
2	A	271/273 (99%)	234 (86%)	28 (10%)	9 (3%)	3 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	271/273 (99%)	227 (84%)	36 (13%)	8 (3%)	3	8
All	All	542/546 (99%)	461 (85%)	64 (12%)	17 (3%)	3	8

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	44	GLY
2	A	45	SER
2	A	81	PRO
2	B	81	PRO
2	B	83	HIS
2	A	94	ASP
2	A	223	ASP
2	B	115	ASN
2	A	53	ASP
2	A	219	VAL
2	B	53	ASP
2	B	153	ASP
2	A	218	LYS
2	B	104	LEU
2	B	218	LYS
2	A	246	ARG
2	B	38	CYS

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	
2	A	243/243 (100%)	201 (83%)	42 (17%)	2	5
2	B	243/243 (100%)	214 (88%)	29 (12%)	5	13
All	All	486/486 (100%)	415 (85%)	71 (15%)	3	8

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	23	ILE
2	A	24	ILE
2	A	29	GLN
2	A	30	ARG
2	A	32	MET
2	A	35	ARG
2	A	53	ASP
2	A	54	THR
2	A	56	LYS
2	A	62	LYS
2	A	71	THR
2	A	78	THR
2	A	81	PRO
2	A	96	ARG
2	A	100	TYR
2	A	101	GLU
2	A	104	LEU
2	A	115	ASN
2	A	130	ILE
2	A	146	GLU
2	A	157	VAL
2	A	160	CYS
2	A	166	ARG
2	A	167	ASP
2	A	168	PRO
2	A	171	ARG
2	A	172	PRO
2	A	179	LEU
2	A	181	HIS
2	A	182	PRO
2	A	186	ASN
2	A	194	LEU
2	A	195	LYS
2	A	198	ARG
2	A	214	LEU
2	A	218	LYS
2	A	222	GLU
2	A	234	GLU
2	A	263	GLN
2	A	265	PRO
2	A	267	ARG
2	A	275	PRO
2	B	30	ARG

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Mol	Chain	Res	Type
2	B	41	ARG
2	B	50	ARG
2	B	60	THR
2	B	63	ILE
2	B	76	LEU
2	B	81	PRO
2	B	90	LEU
2	B	96	ARG
2	B	108	ARG
2	B	109	SER
2	B	114	GLN
2	B	116	LEU
2	B	126	LEU
2	B	128	GLN
2	B	135	GLN
2	B	146	GLU
2	B	149	ARG
2	B	162	GLN
2	B	171	ARG
2	B	179	LEU
2	B	181	HIS
2	B	189	PRO
2	B	190	ASN
2	B	198	ARG
2	B	214	LEU
2	B	236	ARG
2	B	248	VAL
2	B	278	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	29	GLN
2	A	86	HIS
2	A	119	GLN
2	A	132	GLN
2	A	263	GLN
2	B	86	HIS
2	B	114	GLN
2	B	115	ASN
2	B	132	GLN
2	B	135	GLN

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Mol	Chain	Res	Type
2	B	155	ASN
2	B	220	GLN
2	B	241	GLN
2	B	287	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	$\# Z > 2$
3	DTT	B	2	-	7,7,7	0.61	0	4,8,8	0.41	0
3	DTT	A	1	-	7,7,7	0.94	0	4,8,8	0.68	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
3	DTT	B	2	-	2/2/2/2	1/8/8/8	-
3	DTT	A	1	-	2/2/2/2	4/8/8/8	-

There are no bond length outliers.

There are no bond angle outliers.

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1	DTT	C2
3	A	1	DTT	C3
3	B	2	DTT	C2
3	B	2	DTT	C3

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1	DTT	C1-C2-C3-O3
3	A	1	DTT	C1-C2-C3-C4
3	A	1	DTT	O2-C2-C3-O3
3	A	1	DTT	O2-C2-C3-C4
3	B	2	DTT	O3-C3-C4-S4

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2	DTT	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	20/20 (100%)	-0.47	0 100 100	25, 51, 83, 84	0
1	D	20/20 (100%)	-0.36	0 100 100	20, 43, 74, 85	0
2	A	273/273 (100%)	-0.85	0 100 100	14, 37, 64, 87	0
2	B	273/273 (100%)	-0.58	0 100 100	16, 48, 87, 100	0
All	All	586/586 (100%)	-0.69	0 100 100	14, 42, 75, 100	0

There are no RSRZ outliers to report.

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(Å ²)	Q<0.9
3	DTT	B	2	8/8	0.84	0.11	75,80,83,91	0
3	DTT	A	1	8/8	0.96	0.09	39,64,80,88	0

6.5 Other polymers [i](#)

There are no such residues in this entry.