



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 05:37 pm GMT

PDB ID : 1VKX  
Title : CRYSTAL STRUCTURE OF THE NFKB P50/P65 HETERODIMER COM-  
PLEXED TO THE IMMUNOGLOBULIN KB DNA  
Authors : Chen, F.; Huang, D.B.; Ghosh, G.  
Deposited on : 1997-09-17  
Resolution : 2.90 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](mailto: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.

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

MolProbity : 4.02b-467  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

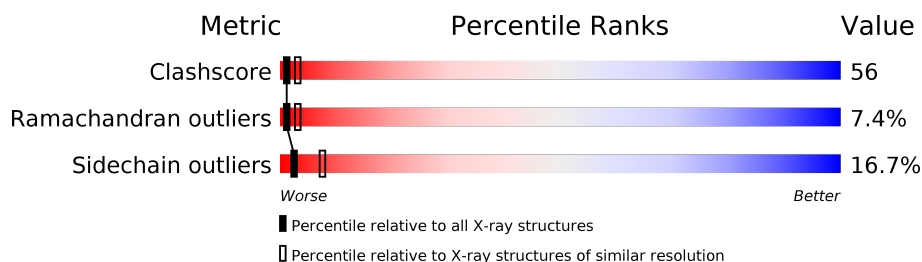
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)

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  $\geq 3$ , 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	12	
2	D	12	
3	A	273	
4	B	312	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5116 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(\*TP\*GP\*GP\*GP\*GP\*AP\*CP\*TP\*TP\*TP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	12	Total	C	N	O	P	0	0	0
			243	117	42	73	11			

- Molecule 2 is a DNA chain called DNA (5'-D(\*AP\*GP\*GP\*AP\*AP\*AP\*GP\*TP\*CP\*CP\*CP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	12	Total	C	N	O	P	0	0	0
			243	116	49	67	11			

- Molecule 3 is a protein called PROTEIN (NF-KAPPA B P65 SUBUNIT).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	273	Total	C	N	O	S	0	0	0
			2176	1356	401	408	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	ALA	PRO	CONFLICT	UNP Q04207

- Molecule 4 is a protein called PROTEIN (NF-KAPPA B P50 SUBUNIT).


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	B	312	Total	C	N	O	S	0	0	0
			2454	1554	428	460	12			

### 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 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.

Note EDS was not executed.

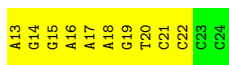
- Molecule 1: DNA (5'-D(\*TP\*GP\*GP\*GP\*GP\*AP\*CP\*TP\*TP\*TP\*CP\*C)-3')

Chain C: 



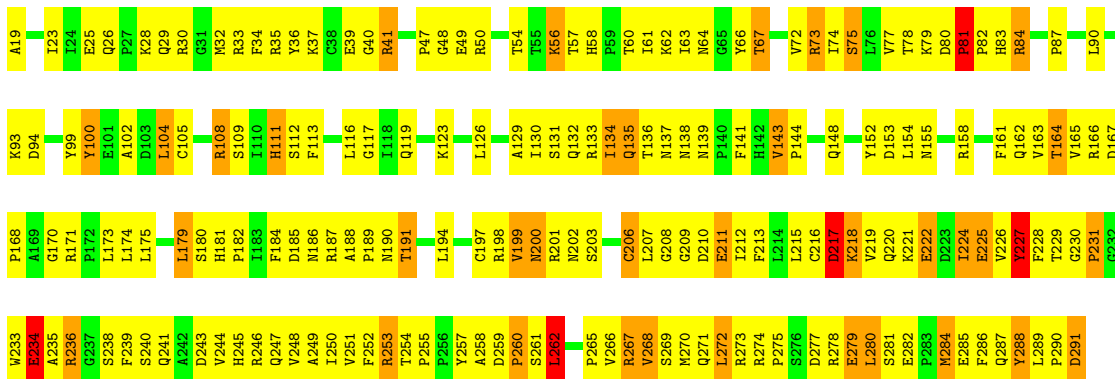
- Molecule 2: DNA (5'-D(\*AP\*GP\*GP\*AP\*AP\*AP\*GP\*TP\*CP\*CP\*CP\*C)-3')

Chain D: 



- Molecule 3: PROTEIN (NF-KAPPA B P65 SUBUNIT)

Chain A: 



- Molecule 4: PROTEIN (NF-KAPPA B P50 SUBUNIT)

Chain B: 



H407	A408	A409	S410	K414	H415	C416	E417	D418	G419	V420	C421	T422	A425	I493	I494	R495	Q496	A497	A498	V499	Q500	G433	F434	A435	H436	L437	G438	I439	K444	V447	F448	L451	R454	H455	T456	E457	A458	C459	T460	R461	G462	Y463	N464	P465	C466	L467	L469	V469	H470	S471	D472	L473	A474	Y475	L476	
Q477	A478	E479	G480	G481	R484	Q485	L486	T487	D488	R489	E490	K491	E492	I493	I494	R495	Q496	A497	A498	V499	Q500	G433	F434	A435	H436	L437	G438	I439	L507	R511	L512	M513	F514	T515	A516	F517	L518	P519	D520	S524	F526	T526	R527	R528	L529	E530	F531	V532	V533	S534	D535	A536	I537	S540	K541	A542
R543	N544	A545	S546	N547	L548	E549	L550	V551	R552	M553	D554	R555	C559	V560	T561	E564	E565	L566	Y567	L568	L569	C570	D571	K572	V573	Q574	K575	D576	D577	L578	Q579	I580	R581	F582	Y583	E584	E585	E586	E587	N588	G589	G590	V591	Y592	E593	G594	D597	F598	S599	P600	T601	D602	Y603	H604	R605	Q606
F607	V610	F611	K612	T613	R614	K615	Y616	K617	D618	V619	N620	I621	T622	K623	P624	A625	S626	V627	F628	V629	Q630	L631	R632	R633	L637	E638	T639	L646	Y647	Y648	P649	E650																								

## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.61Å 106.61Å 206.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.90	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.90)	Depositor
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.208 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5116	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

## 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	0.95	0/271	1.05	3/417 (0.7%)
2	D	0.84	0/273	0.86	0/419
3	A	0.69	0/2228	0.94	4/3021 (0.1%)
4	B	0.66	1/2506 (0.0%)	0.90	1/3384 (0.0%)
All	All	0.70	1/5278 (0.0%)	0.93	8/7241 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	3
3	A	0	1
4	B	0	2
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	385	CYS	CB-SG	-5.05	1.73	1.81

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1	DT	C1'-O4'-C4'	-7.32	102.78	110.10
1	C	1	DT	C3'-C2'-C1'	-7.22	93.83	102.50
1	C	1	DT	O4'-C1'-N1	6.69	112.68	108.00
3	A	262	LEU	CA-CB-CG	5.80	128.64	115.30
3	A	135	GLN	N-CA-C	-5.71	95.59	111.00
3	A	265	PRO	N-CA-C	5.53	126.49	112.10
4	B	527	ARG	N-CA-C	5.38	125.53	111.00
3	A	217	ASP	N-CA-C	-5.06	97.35	111.00

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	227	TYR	Sidechain
4	B	387	TYR	Sidechain
4	B	648	TYR	Sidechain
1	C	1	DT	Sidechain
1	C	3	DG	Sidechain
1	C	9	DT	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	243	0	138	39	0
2	D	243	0	135	42	0
3	A	2176	0	2137	224	0
4	B	2454	0	2449	276	0
All	All	5116	0	4859	554	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 56.

All (554) 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)
4:B:487:THR:HB	4:B:490:GLU:HB2	1.26	1.17
2:D:13:DA:H2''	2:D:14:DG:H5''	1.22	1.16
1:C:2:DG:H2''	1:C:3:DG:C5'	1.82	1.10
4:B:465:PRO:HB2	4:B:467:LEU:HD13	1.32	1.08
1:C:2:DG:H2''	1:C:3:DG:H5'	1.35	1.06
4:B:390:PRO:HA	4:B:426:GLY:HA2	1.36	1.05
3:A:33:ARG:HH21	3:A:35:ARG:HH12	1.07	1.02
4:B:559:CYS:SG	4:B:561:THR:HG23	2.01	0.98
4:B:520:ASP:HB3	4:B:526:THR:HB	1.43	0.97
3:A:33:ARG:HH21	3:A:35:ARG:NH1	1.63	0.95
3:A:200:ASN:HB2	3:A:213:PHE:HB2	1.45	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:DC:C6	1:C:8:DT:H71	2.04	0.92
2:D:13:DA:C2'	2:D:14:DG:H5''	1.99	0.90
4:B:458:ALA:HB1	4:B:464:ASN:HB3	1.54	0.89
4:B:388:VAL:HG21	4:B:518:LEU:HD13	1.52	0.88
4:B:340:PRO:HA	4:B:385:CYS:O	1.73	0.87
4:B:376:LYS:HA	4:B:376:LYS:HE3	1.56	0.87
4:B:579:GLN:HE21	4:B:632:ARG:NH1	1.74	0.86
3:A:23:ILE:HG21	3:A:26:GLN:NE2	1.91	0.86
4:B:390:PRO:HA	4:B:426:GLY:CA	2.06	0.85
3:A:206:CYS:SG	3:A:291:ASP:N	2.48	0.85
4:B:371:SER:HB2	4:B:378:SER:HB3	1.58	0.85
4:B:573:VAL:HB	4:B:578:ILE:HG13	1.57	0.85
1:C:7:DC:C5	1:C:8:DT:H73	2.10	0.85
4:B:448:PHE:HE2	4:B:499:VAL:HG22	1.42	0.84
3:A:23:ILE:HG21	3:A:26:GLN:HE21	1.41	0.84
4:B:527:ARG:HD2	4:B:528:ARG:H	1.41	0.84
4:B:554:ASP:HB2	4:B:567:TYR:H	1.42	0.84
3:A:255:PRO:HG2	3:A:288:TYR:OH	1.77	0.84
4:B:487:THR:CB	4:B:490:GLU:HB2	2.06	0.84
3:A:200:ASN:HB3	3:A:213:PHE:H	1.41	0.83
4:B:388:VAL:H	4:B:430:MET:HE2	1.43	0.83
3:A:221:LYS:HG3	3:A:241:GLN:HE21	1.43	0.83
4:B:481:GLY:HA3	4:B:484:ARG:HD3	1.59	0.82
2:D:20:DT:H1'	2:D:21:DC:H5'	1.60	0.82
3:A:257:TYR:CE2	3:A:266:VAL:HG11	2.15	0.82
3:A:289:LEU:HB3	3:A:290:PRO:HD2	1.62	0.82
4:B:632:ARG:HH11	4:B:632:ARG:HG2	1.43	0.82
4:B:460:ILE:HA	4:B:484:ARG:NH2	1.95	0.81
3:A:78:THR:HG22	3:A:80:ASP:H	1.45	0.81
1:C:1:DT:H4'	4:B:436:ASN:ND2	1.95	0.81
3:A:233:TRP:CD1	3:A:258:ALA:HB2	2.15	0.81
3:A:224:ILE:HD13	3:A:225:GLU:H	1.45	0.81
3:A:245:HIS:CD2	4:B:569:LEU:HB3	2.16	0.81
3:A:221:LYS:HD2	3:A:241:GLN:HB3	1.63	0.81
3:A:224:ILE:HD13	3:A:225:GLU:N	1.97	0.80
3:A:80:ASP:HB3	3:A:81:PRO:HD2	1.65	0.79
4:B:448:PHE:CE2	4:B:499:VAL:HG22	2.17	0.79
4:B:624:PRO:HB2	4:B:646:LEU:HD21	1.64	0.79
4:B:465:PRO:HG3	4:B:467:LEU:HD22	1.64	0.79
1:C:7:DC:C6	1:C:8:DT:C7	2.64	0.79
3:A:284:MET:SD	3:A:285:GLU:N	2.52	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:DG:C8	2:D:20:DT:H73	2.18	0.79
3:A:267:ARG:HD2	3:A:267:ARG:H	1.47	0.78
3:A:139:ASN:HD21	3:A:143:VAL:HG23	1.46	0.78
4:B:371:SER:HB2	4:B:378:SER:CB	2.13	0.77
4:B:463:TYR:HA	4:B:528:ARG:NH1	1.99	0.77
4:B:550:ILE:HD12	4:B:568:LEU:HD11	1.65	0.77
4:B:383:LYS:HG2	4:B:384:ILE:O	1.85	0.76
3:A:273:ARG:HD2	3:A:280:LEU:HD11	1.68	0.76
3:A:246:ARG:HG3	4:B:607:PHE:CE2	2.22	0.75
4:B:460:ILE:HA	4:B:484:ARG:HH21	1.52	0.74
4:B:616:TYR:CG	4:B:617:LYS:N	2.54	0.74
1:C:2:DG:H2''	1:C:3:DG:H5''	1.69	0.74
4:B:388:VAL:HG21	4:B:518:LEU:CD1	2.16	0.74
4:B:632:ARG:NH1	4:B:632:ARG:HG2	2.01	0.74
4:B:465:PRO:HG2	4:B:467:LEU:HB2	1.69	0.74
1:C:2:DG:C2'	1:C:3:DG:C5'	2.64	0.73
4:B:599:SER:OG	4:B:601:THR:HB	1.89	0.73
3:A:132:GLN:HG2	3:A:133:ARG:NH1	2.04	0.73
3:A:33:ARG:NH2	3:A:187:ARG:HH21	1.85	0.73
2:D:19:DG:C8	2:D:20:DT:C7	2.72	0.73
3:A:104:LEU:HD12	3:A:111:HIS:HE2	1.52	0.73
4:B:455:MET:HB3	4:B:469:VAL:HG22	1.71	0.72
3:A:224:ILE:HD11	3:A:272:LEU:HG	1.71	0.71
4:B:470:HIS:CE1	4:B:493:ILE:HB	2.25	0.71
4:B:501:GLN:O	4:B:504:GLU:HG2	1.89	0.71
4:B:579:GLN:NE2	4:B:632:ARG:NH1	2.37	0.71
2:D:14:DG:OP1	2:D:14:DG:H4'	1.88	0.71
3:A:233:TRP:CH2	3:A:288:TYR:HE2	2.07	0.71
4:B:614:PRO:HG2	4:B:647:TYR:OH	1.91	0.71
3:A:104:LEU:HD12	3:A:111:HIS:NE2	2.06	0.71
3:A:49:GLU:HG3	3:A:50:ARG:H	1.54	0.71
3:A:33:ARG:NH2	3:A:35:ARG:HH12	1.86	0.71
4:B:455:MET:SD	4:B:469:VAL:HG13	2.31	0.70
1:C:2:DG:C2'	1:C:3:DG:H5''	2.21	0.70
3:A:111:HIS:N	3:A:111:HIS:ND1	2.38	0.70
4:B:466:GLY:HA3	4:B:473:LEU:HB3	1.73	0.70
3:A:246:ARG:HG3	4:B:607:PHE:CD2	2.27	0.70
1:C:7:DC:N1	1:C:8:DT:H71	2.06	0.70
4:B:395:VAL:HG12	4:B:421:CYS:HB2	1.74	0.69
3:A:56:LYS:HD2	3:A:56:LYS:H	1.57	0.69
4:B:459:CYS:SG	4:B:494:ILE:HD11	2.32	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:190:ASN:HB3	3:A:220:GLN:HE22	1.57	0.69
4:B:560:VAL:HG13	4:B:616:TYR:HB3	1.74	0.69
4:B:581:ARG:HH11	4:B:581:ARG:HG3	1.58	0.69
4:B:548:LEU:HD12	4:B:548:LEU:H	1.58	0.69
4:B:564:GLU:O	4:B:612:LYS:HA	1.93	0.68
4:B:497:ALA:O	4:B:501:GLN:HG3	1.93	0.68
4:B:388:VAL:HG11	4:B:518:LEU:HB3	1.75	0.68
3:A:37:LYS:HB2	3:A:119:GLN:CD	2.14	0.68
3:A:210:ASP:O	3:A:253:ARG:HA	1.94	0.67
1:C:7:DC:C5	1:C:8:DT:C7	2.77	0.67
3:A:73:ARG:NH1	3:A:73:ARG:HG2	2.07	0.67
3:A:202:ASN:HB2	3:A:286:PHE:HA	1.76	0.67
4:B:351:ARG:HH11	4:B:351:ARG:HB3	1.58	0.67
3:A:245:HIS:HD2	4:B:569:LEU:HB3	1.60	0.67
3:A:228:PHE:HE2	3:A:286:PHE:CG	2.13	0.67
4:B:387:TYR:HB2	4:B:430:MET:HG3	1.75	0.67
3:A:219:VAL:HG22	3:A:247:GLN:O	1.94	0.66
3:A:267:ARG:HG3	3:A:267:ARG:HH11	1.60	0.66
3:A:139:ASN:HD21	3:A:143:VAL:H	1.41	0.66
3:A:277:ASP:OD2	3:A:279:GLU:HB2	1.95	0.66
4:B:407:HIS:HE1	4:B:506:ASP:O	1.79	0.66
4:B:353:PHE:CE2	4:B:439:ILE:HD12	2.29	0.66
3:A:87:PRO:HD3	3:A:130:ILE:HD11	1.77	0.66
4:B:416:CYS:O	4:B:417:GLU:HG3	1.95	0.66
4:B:528:ARG:HG3	4:B:528:ARG:HH11	1.60	0.65
3:A:267:ARG:HD2	3:A:267:ARG:N	2.11	0.65
3:A:141:PHE:CZ	3:A:179:LEU:HD11	2.32	0.65
3:A:78:THR:HB	3:A:83:HIS:HA	1.77	0.65
4:B:455:MET:HB3	4:B:469:VAL:CG2	2.26	0.65
4:B:351:ARG:HB3	4:B:351:ARG:NH1	2.11	0.65
2:D:20:DT:H72	4:B:357:TYR:CD1	2.31	0.65
3:A:126:LEU:HD23	3:A:126:LEU:O	1.96	0.65
3:A:238:SER:HB3	3:A:253:ARG:CG	2.27	0.65
4:B:555:ARG:HH11	4:B:555:ARG:HB3	1.61	0.65
4:B:463:TYR:HA	4:B:528:ARG:CZ	2.26	0.65
3:A:203:SER:HB3	3:A:289:LEU:CD1	2.28	0.64
3:A:33:ARG:HB3	3:A:186:ASN:HB3	1.77	0.64
3:A:56:LYS:CD	3:A:56:LYS:H	2.09	0.64
4:B:495:ARG:O	4:B:499:VAL:HG23	1.98	0.64
4:B:527:ARG:HD2	4:B:528:ARG:N	2.12	0.64
4:B:583:TYR:HA	4:B:592:TRP:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:73:ARG:HH11	3:A:73:ARG:HG2	1.61	0.64
2:D:15:DG:H1'	2:D:16:DA:H5''	1.80	0.64
1:C:3:DG:H2''	1:C:4:DG:OP2	1.97	0.63
4:B:367:LEU:HD11	4:B:537:ILE:HD13	1.79	0.63
4:B:514:PHE:HB2	4:B:532:VAL:HG12	1.80	0.63
3:A:245:HIS:HB3	3:A:249:ALA:HB3	1.81	0.63
2:D:14:DG:H2''	2:D:15:DG:O5'	1.98	0.63
3:A:189:PRO:HB3	3:A:218:LYS:HE3	1.80	0.63
3:A:206:CYS:SG	3:A:262:LEU:CB	2.87	0.63
4:B:459:CYS:SG	4:B:473:LEU:HG	2.39	0.63
1:C:2:DG:H1'	1:C:3:DG:H5''	1.81	0.63
3:A:57:THR:HG22	3:A:58:HIS:N	2.13	0.62
4:B:400:ASN:HA	4:B:511:ARG:HE	1.64	0.62
4:B:405:HIS:CE1	4:B:501:GLN:HE22	2.16	0.62
3:A:141:PHE:CE2	3:A:179:LEU:HD11	2.34	0.62
4:B:349:LYS:HZ2	4:B:351:ARG:HG3	1.64	0.62
4:B:625:ALA:O	4:B:647:TYR:N	2.32	0.62
3:A:139:ASN:ND2	3:A:143:VAL:HG23	2.13	0.62
3:A:228:PHE:HB3	3:A:233:TRP:CH2	2.34	0.62
4:B:518:LEU:HB3	4:B:519:PRO:HD2	1.82	0.62
3:A:62:LYS:HD3	3:A:64:ASN:HD21	1.65	0.62
4:B:426:GLY:N	4:B:427:PRO:HD3	2.15	0.62
4:B:551:VAL:HB	4:B:569:LEU:O	1.99	0.61
3:A:104:LEU:HB2	3:A:111:HIS:HD2	1.64	0.61
2:D:20:DT:H5'	2:D:20:DT:H6	1.65	0.61
3:A:25:GLU:OE2	3:A:57:THR:HG21	2.00	0.61
2:D:14:DG:C5'	2:D:14:DG:H8	2.12	0.61
3:A:158:ARG:HG2	3:A:158:ARG:HH11	1.66	0.61
3:A:105:CYS:SG	3:A:108:ARG:NH2	2.74	0.61
3:A:139:ASN:ND2	3:A:143:VAL:H	1.98	0.61
3:A:221:LYS:O	3:A:241:GLN:HG2	2.01	0.61
3:A:206:CYS:SG	3:A:262:LEU:HB2	2.41	0.60
3:A:229:THR:O	3:A:268:VAL:HB	2.02	0.60
4:B:598:PHE:HB2	4:B:602:ASP:HB2	1.83	0.60
3:A:81:PRO:HB2	3:A:82:PRO:HD3	1.83	0.60
4:B:630:GLN:HG3	4:B:630:GLN:O	2.00	0.60
3:A:233:TRP:CG	3:A:234:GLU:N	2.68	0.60
3:A:238:SER:HB3	3:A:253:ARG:HG3	1.82	0.60
3:A:259:ASP:OD2	3:A:262:LEU:HD12	2.01	0.60
4:B:395:VAL:CG1	4:B:421:CYS:HB2	2.31	0.60
3:A:63:ILE:HD12	3:A:163:VAL:HG11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:349:LYS:NZ	4:B:351:ARG:HG3	2.17	0.60
3:A:188:ALA:HB3	3:A:191:THR:HG22	1.83	0.59
3:A:200:ASN:CB	3:A:213:PHE:HB2	2.25	0.59
3:A:208:GLY:O	3:A:210:ASP:N	2.36	0.59
2:D:20:DT:C1'	2:D:21:DC:H5'	2.29	0.59
4:B:495:ARG:HG3	4:B:496:GLN:N	2.17	0.59
1:C:1:DT:H1'	1:C:2:DG:O5'	2.03	0.59
4:B:339:GLY:O	4:B:386:ASN:HB2	2.03	0.59
3:A:143:VAL:HG12	3:A:144:PRO:HD2	1.85	0.59
3:A:217:ASP:O	3:A:219:VAL:HG13	2.03	0.59
3:A:225:GLU:OE2	3:A:227:TYR:HE1	1.84	0.59
4:B:560:VAL:HG11	4:B:619:VAL:HA	1.84	0.59
1:C:7:DC:C4	1:C:8:DT:H73	2.37	0.59
4:B:465:PRO:CG	4:B:467:LEU:HD22	2.32	0.59
3:A:270:MET:HE2	3:A:286:PHE:HB2	1.85	0.58
3:A:203:SER:HB3	3:A:289:LEU:HD12	1.85	0.58
4:B:391:ALA:H	4:B:426:GLY:HA2	1.68	0.58
3:A:133:ARG:O	3:A:134:ILE:HG23	2.03	0.58
4:B:512:LEU:HB2	4:B:534:SER:OG	2.03	0.58
1:C:3:DG:N7	4:B:364:HIS:ND1	2.51	0.58
2:D:14:DG:C8	2:D:14:DG:C5'	2.87	0.58
4:B:632:ARG:HH11	4:B:632:ARG:CG	2.16	0.58
3:A:211:GLU:OE2	3:A:213:PHE:HE1	1.85	0.58
3:A:33:ARG:NH2	3:A:35:ARG:NH1	2.44	0.58
2:D:19:DG:N7	4:B:541:LYS:HE3	2.18	0.58
4:B:383:LYS:NZ	4:B:385:CYS:SG	2.71	0.58
4:B:474:ALA:O	4:B:475:TYR:HB2	2.03	0.58
3:A:227:TYR:CD1	3:A:273:ARG:HD3	2.39	0.58
4:B:384:ILE:O	4:B:385:CYS:SG	2.62	0.57
3:A:239:PHE:HB3	3:A:252:PHE:HA	1.87	0.57
3:A:215:LEU:HD13	4:B:604:HIS:CD2	2.40	0.57
3:A:228:PHE:CG	3:A:255:PRO:HG3	2.39	0.57
3:A:206:CYS:SG	3:A:262:LEU:HB3	2.44	0.57
3:A:208:GLY:HA2	3:A:254:THR:HG22	1.86	0.57
4:B:553:MET:CG	4:B:568:LEU:HD12	2.35	0.57
2:D:19:DG:C2'	2:D:20:DT:H71	2.35	0.57
4:B:599:SER:O	4:B:602:ASP:N	2.37	0.57
4:B:387:TYR:CD1	4:B:387:TYR:C	2.79	0.56
4:B:581:ARG:NH1	4:B:581:ARG:HG3	2.20	0.56
4:B:417:GLU:O	4:B:420:VAL:HG12	2.04	0.56
4:B:467:LEU:HA	4:B:471:SER:OG	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:561:THR:CG2	4:B:650:GLU:HG3	2.35	0.56
3:A:226:VAL:HG21	3:A:252:PHE:CD2	2.40	0.56
2:D:19:DG:P	4:B:444:LYS:HE3	2.45	0.56
4:B:470:HIS:CE1	4:B:473:LEU:HB2	2.41	0.56
3:A:240:SER:O	3:A:243:ASP:N	2.37	0.56
1:C:10:DT:C7	3:A:36:TYR:CD1	2.88	0.56
3:A:113:PHE:CE2	3:A:161:PHE:HE2	2.24	0.56
3:A:228:PHE:N	3:A:235:ALA:O	2.39	0.56
3:A:73:ARG:HH11	3:A:73:ARG:CG	2.18	0.56
3:A:90:LEU:HA	3:A:117:GLY:O	2.06	0.56
3:A:246:ARG:C	3:A:248:VAL:H	2.07	0.55
3:A:123:LYS:HD2	3:A:126:LEU:HD12	1.86	0.55
3:A:287:GLN:O	3:A:287:GLN:HG3	2.07	0.55
4:B:375:ASN:O	4:B:376:LYS:HG2	2.06	0.55
1:C:8:DT:O2	1:C:9:DT:C6	2.60	0.55
3:A:245:HIS:CE1	4:B:570:CYS:O	2.59	0.55
3:A:26:GLN:HA	3:A:26:GLN:HE21	1.72	0.55
3:A:72:VAL:HG13	3:A:72:VAL:O	2.06	0.55
4:B:623:LYS:HG3	4:B:624:PRO:HD2	1.88	0.55
3:A:165:VAL:HG22	3:A:175:LEU:CD1	2.37	0.55
3:A:233:TRP:HD1	3:A:258:ALA:HB2	1.70	0.55
4:B:550:ILE:CD1	4:B:631:LEU:HD13	2.36	0.55
3:A:94:ASP:HB3	3:A:102:ALA:HB2	1.89	0.55
4:B:553:MET:HG3	4:B:568:LEU:HD12	1.87	0.55
4:B:579:GLN:HE21	4:B:632:ARG:HH11	1.50	0.55
3:A:200:ASN:CB	3:A:213:PHE:H	2.15	0.55
3:A:277:ASP:O	3:A:278:ARG:HB2	2.06	0.55
4:B:387:TYR:CD1	4:B:388:VAL:N	2.74	0.54
4:B:542:ALA:HB1	4:B:544:ASN:ND2	2.22	0.54
2:D:15:DG:H2''	2:D:16:DA:C5'	2.37	0.54
4:B:354:ARG:CZ	4:B:356:ARG:NH1	2.71	0.54
4:B:456:THR:O	4:B:460:ILE:HG23	2.07	0.54
3:A:66:TYR:CD1	3:A:67:THR:N	2.75	0.54
4:B:597:ASP:O	4:B:598:PHE:HB3	2.07	0.54
2:D:16:DA:H5'	2:D:16:DA:H8	1.72	0.54
4:B:394:ILE:HG13	4:B:394:ILE:O	2.07	0.54
1:C:2:DG:C1'	1:C:3:DG:H5''	2.36	0.54
3:A:210:ASP:O	3:A:254:THR:N	2.33	0.54
4:B:528:ARG:CG	4:B:528:ARG:HH11	2.21	0.54
3:A:226:VAL:HG21	3:A:252:PHE:CE2	2.43	0.53
4:B:460:ILE:O	4:B:460:ILE:HG13	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:14:DG:H5''	2:D:14:DG:C8	2.42	0.53
1:C:1:DT:H4'	4:B:436:ASN:CG	2.29	0.53
4:B:477:GLN:OE1	4:B:478:ALA:HB3	2.07	0.53
3:A:197:CYS:HB2	3:A:215:LEU:O	2.09	0.53
4:B:459:CYS:SG	4:B:473:LEU:CD1	2.96	0.53
4:B:494:ILE:HG22	4:B:495:ARG:N	2.24	0.53
3:A:166:ARG:HD2	3:A:170:GLY:O	2.09	0.53
4:B:400:ASN:HA	4:B:511:ARG:NE	2.24	0.53
4:B:550:ILE:HD11	4:B:631:LEU:HD13	1.90	0.53
3:A:26:GLN:O	3:A:48:GLY:HA2	2.09	0.53
4:B:410:SER:HB3	4:B:419:GLY:HA3	1.89	0.53
4:B:349:LYS:O	4:B:350:GLN:HB3	2.09	0.52
4:B:388:VAL:HG21	4:B:518:LEU:HD22	1.92	0.52
4:B:353:PHE:CD2	4:B:439:ILE:HD12	2.44	0.52
4:B:542:ALA:HB1	4:B:544:ASN:HD21	1.75	0.52
3:A:33:ARG:CZ	3:A:187:ARG:HE	2.22	0.52
4:B:374:LYS:N	4:B:374:LYS:HD2	2.23	0.52
2:D:19:DG:C8	2:D:20:DT:H71	2.44	0.52
4:B:477:GLN:HG3	4:B:478:ALA:H	1.75	0.52
4:B:586:GLU:O	4:B:587:GLU:HB2	2.10	0.52
3:A:220:GLN:HB3	3:A:222:GLU:OE1	2.10	0.52
3:A:228:PHE:HB2	3:A:235:ALA:O	2.09	0.52
4:B:465:PRO:C	4:B:467:LEU:N	2.62	0.52
3:A:257:TYR:OH	3:A:266:VAL:HG21	2.10	0.52
4:B:425:ALA:HB2	4:B:432:VAL:HB	1.92	0.52
4:B:465:PRO:C	4:B:467:LEU:H	2.12	0.52
2:D:14:DG:H2''	2:D:15:DG:C5'	2.39	0.52
3:A:19:ALA:HA	3:A:64:ASN:O	2.10	0.52
4:B:353:PHE:HE2	4:B:439:ILE:HD12	1.71	0.52
4:B:458:ALA:HB1	4:B:464:ASN:CB	2.34	0.52
2:D:20:DT:C2'	2:D:21:DC:H5'	2.40	0.52
4:B:341:TYR:HA	4:B:529:LEU:HD11	1.92	0.52
4:B:574:GLN:O	4:B:576:ASP:N	2.43	0.52
1:C:4:DG:O6	4:B:364:HIS:CE1	2.63	0.52
3:A:167:ASP:OD1	3:A:171:ARG:N	2.43	0.52
2:D:14:DG:H8	2:D:14:DG:H5'	1.74	0.52
3:A:153:ASP:C	3:A:155:ASN:H	2.14	0.51
3:A:215:LEU:HD13	4:B:604:HIS:CG	2.46	0.51
4:B:470:HIS:CE1	4:B:473:LEU:HD23	2.44	0.51
3:A:226:VAL:O	3:A:236:ARG:HA	2.09	0.51
3:A:233:TRP:CE3	3:A:257:TYR:HE1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:57:THR:CG2	3:A:58:HIS:N	2.73	0.51
3:A:84:ARG:HA	3:A:143:VAL:HG21	1.91	0.51
4:B:384:ILE:HG22	4:B:385:CYS:H	1.76	0.51
4:B:632:ARG:CZ	4:B:637:LEU:HD23	2.40	0.51
3:A:104:LEU:CD1	3:A:111:HIS:HE2	2.22	0.51
3:A:248:VAL:HG21	4:B:605:ARG:HB3	1.90	0.51
2:D:20:DT:H2'	4:B:359:CYS:SG	2.50	0.51
3:A:234:GLU:HG2	3:A:234:GLU:O	2.11	0.51
4:B:387:TYR:HD1	4:B:387:TYR:C	2.13	0.51
4:B:513:MET:HG3	4:B:533:VAL:HG12	1.92	0.51
3:A:233:TRP:O	3:A:234:GLU:HB3	2.09	0.51
3:A:33:ARG:CZ	3:A:187:ARG:HH21	2.24	0.51
3:A:34:PHE:CD1	3:A:34:PHE:N	2.79	0.51
4:B:572:LYS:HG3	4:B:572:LYS:O	2.10	0.51
1:C:7:DC:C2'	1:C:8:DT:H71	2.39	0.51
3:A:33:ARG:HB2	3:A:187:ARG:HG2	1.93	0.51
4:B:404:ILE:HD12	4:B:513:MET:CE	2.41	0.51
4:B:497:ALA:C	4:B:499:VAL:H	2.15	0.51
4:B:559:CYS:SG	4:B:561:THR:CG2	2.87	0.51
3:A:229:THR:HA	3:A:234:GLU:HA	1.93	0.50
3:A:227:TYR:CE1	3:A:273:ARG:HD3	2.46	0.50
3:A:48:GLY:O	3:A:49:GLU:C	2.49	0.50
4:B:342:LEU:HG	4:B:516:ALA:HB2	1.93	0.50
1:C:7:DC:H2'	1:C:8:DT:H71	1.94	0.50
4:B:627:VAL:HG23	4:B:628:PHE:N	2.27	0.50
3:A:258:ALA:O	3:A:260:PRO:HD3	2.11	0.50
4:B:354:ARG:HA	4:B:540:SER:HB3	1.93	0.50
4:B:463:TYR:HB2	4:B:517:PHE:CZ	2.46	0.50
4:B:583:TYR:CE1	4:B:628:PHE:HB2	2.46	0.50
3:A:216:CYS:SG	3:A:248:VAL:O	2.60	0.50
3:A:194:LEU:HD11	3:A:274:ARG:HB2	1.93	0.50
3:A:26:GLN:O	3:A:49:GLU:N	2.42	0.50
3:A:39:GLU:O	3:A:41:ARG:N	2.45	0.50
2:D:16:DA:C8	2:D:16:DA:H5'	2.47	0.50
1:C:6:DA:H3'	3:A:247:GLN:NE2	2.26	0.50
4:B:390:PRO:HA	4:B:426:GLY:C	2.31	0.50
4:B:414:LYS:HE2	4:B:415:HIS:CE1	2.46	0.50
4:B:388:VAL:CG2	4:B:518:LEU:HD22	2.42	0.50
4:B:616:TYR:CD1	4:B:647:TYR:CD2	2.99	0.50
4:B:458:ALA:O	4:B:464:ASN:O	2.30	0.49
4:B:477:GLN:HG3	4:B:479:GLU:OE1	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:34:PHE:N	3:A:185:ASP:OD1	2.45	0.49
3:A:33:ARG:HH21	3:A:187:ARG:HH21	1.55	0.49
3:A:104:LEU:HB2	3:A:111:HIS:CD2	2.46	0.49
4:B:459:CYS:CB	4:B:494:ILE:HD11	2.43	0.49
4:B:378:SER:O	4:B:379:TYR:HB3	2.11	0.49
3:A:100:TYR:CD1	3:A:100:TYR:C	2.85	0.49
3:A:233:TRP:CZ2	3:A:235:ALA:HB3	2.47	0.49
4:B:354:ARG:CA	4:B:540:SER:HB3	2.43	0.49
4:B:388:VAL:H	4:B:430:MET:CE	2.20	0.49
4:B:420:VAL:C	4:B:421:CYS:SG	2.91	0.49
1:C:3:DG:H2''	1:C:4:DG:C8	2.48	0.49
4:B:403:ASN:HD22	4:B:403:ASN:H	1.61	0.48
3:A:90:LEU:HD22	3:A:116:LEU:HD22	1.95	0.48
4:B:632:ARG:HD3	4:B:639:THR:HG22	1.95	0.48
1:C:1:DT:H2''	1:C:2:DG:OP2	2.12	0.48
2:D:15:DG:OP2	4:B:605:ARG:NH2	2.41	0.48
4:B:579:GLN:NE2	4:B:632:ARG:HH12	2.09	0.48
4:B:585:GLU:HA	4:B:591:VAL:HA	1.94	0.48
3:A:79:LYS:HG2	3:A:79:LYS:O	2.13	0.48
4:B:461:ARG:HD2	4:B:463:TYR:CE2	2.49	0.48
1:C:8:DT:O2	1:C:9:DT:N1	2.46	0.48
4:B:616:TYR:HB2	4:B:647:TYR:CD1	2.48	0.48
1:C:1:DT:C2	1:C:2:DG:C5'	2.97	0.48
3:A:49:GLU:HG3	3:A:50:ARG:N	2.24	0.47
3:A:248:VAL:HG13	4:B:604:HIS:NE2	2.29	0.47
4:B:399:THR:HG21	4:B:405:HIS:HB2	1.96	0.47
4:B:495:ARG:O	4:B:498:ALA:HB3	2.14	0.47
1:C:9:DT:H2'	1:C:10:DT:H71	1.95	0.47
3:A:129:ALA:O	3:A:132:GLN:N	2.47	0.47
4:B:387:TYR:CE1	4:B:389:GLY:N	2.77	0.47
1:C:1:DT:C1'	1:C:2:DG:O5'	2.62	0.47
4:B:470:HIS:CD2	4:B:473:LEU:HB2	2.50	0.47
4:B:477:GLN:O	4:B:528:ARG:NH2	2.47	0.47
4:B:399:THR:O	4:B:511:ARG:NE	2.44	0.47
4:B:555:ARG:HH11	4:B:555:ARG:CB	2.26	0.47
3:A:225:GLU:HG3	3:A:225:GLU:O	2.14	0.47
3:A:267:ARG:HG3	3:A:267:ARG:NH1	2.28	0.47
4:B:392:LYS:HD2	4:B:422:THR:CG2	2.45	0.47
4:B:434:PHE:CD2	4:B:514:PHE:HE1	2.33	0.47
4:B:580:ILE:HD13	4:B:611:PHE:CD1	2.49	0.47
1:C:11:DC:H1'	1:C:12:DC:H5'	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:463:TYR:HB2	4:B:517:PHE:CE1	2.49	0.47
3:A:35:ARG:HH11	3:A:187:ARG:NH2	2.12	0.47
4:B:447:VAL:CG1	4:B:502:THR:HG23	2.45	0.47
2:D:20:DT:H2''	2:D:21:DC:H5'	1.97	0.47
4:B:409:HIS:CE1	4:B:507:LEU:HB3	2.49	0.47
3:A:233:TRP:CH2	3:A:288:TYR:CE2	2.97	0.46
3:A:289:LEU:HB3	3:A:290:PRO:CD	2.37	0.46
4:B:589:GLY:O	4:B:590:GLY:O	2.33	0.46
4:B:591:VAL:HG12	4:B:592:TRP:N	2.31	0.46
1:C:1:DT:C2	1:C:2:DG:O5'	2.68	0.46
3:A:257:TYR:CD2	3:A:259:ASP:HB3	2.51	0.46
2:D:20:DT:C7	4:B:357:TYR:CD1	2.99	0.46
3:A:33:ARG:HA	3:A:186:ASN:H	1.80	0.46
3:A:73:ARG:NH1	3:A:162:GLN:NE2	2.64	0.46
4:B:404:ILE:HD12	4:B:513:MET:HE3	1.98	0.46
4:B:465:PRO:CG	4:B:467:LEU:HB2	2.42	0.46
4:B:404:ILE:HG22	4:B:511:ARG:NH2	2.31	0.46
4:B:513:MET:O	4:B:513:MET:HG2	2.15	0.46
4:B:403:ASN:H	4:B:403:ASN:ND2	2.13	0.46
4:B:374:LYS:H	4:B:374:LYS:HD2	1.80	0.46
4:B:447:VAL:HG12	4:B:502:THR:HG23	1.98	0.46
4:B:560:VAL:HG23	4:B:648:TYR:O	2.14	0.46
4:B:388:VAL:O	4:B:390:PRO:N	2.49	0.46
4:B:391:ALA:HB1	4:B:518:LEU:HD23	1.98	0.46
1:C:6:DA:H1'	1:C:7:DC:C6	2.51	0.46
2:D:19:DG:N7	2:D:20:DT:H73	2.30	0.46
3:A:289:LEU:CB	3:A:290:PRO:HD2	2.40	0.45
4:B:384:ILE:HG22	4:B:385:CYS:N	2.31	0.45
3:A:221:LYS:CG	3:A:241:GLN:HE21	2.23	0.45
4:B:394:ILE:HA	4:B:421:CYS:O	2.17	0.45
3:A:60:THR:HG23	3:A:111:HIS:C	2.37	0.45
3:A:199:VAL:O	3:A:199:VAL:HG13	2.16	0.45
4:B:491:LYS:O	4:B:495:ARG:HB3	2.17	0.45
4:B:388:VAL:CG2	4:B:518:LEU:HD13	2.36	0.45
1:C:3:DG:C2'	1:C:4:DG:OP2	2.65	0.45
3:A:158:ARG:NH1	3:A:158:ARG:HG2	2.29	0.45
4:B:560:VAL:CG1	4:B:619:VAL:HA	2.46	0.45
3:A:158:ARG:HH12	3:A:182:PRO:HD3	1.81	0.45
3:A:246:ARG:C	3:A:248:VAL:N	2.70	0.45
4:B:384:ILE:C	4:B:385:CYS:HG	2.18	0.45
4:B:455:MET:CB	4:B:469:VAL:HG22	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:546:SER:O	4:B:633:ARG:NH2	2.48	0.45
4:B:475:TYR:C	4:B:476:LEU:HD22	2.36	0.45
3:A:61:ILE:HG13	3:A:61:ILE:O	2.16	0.44
3:A:84:ARG:HD2	3:A:148:GLN:HA	1.98	0.44
4:B:345:LEU:HD12	4:B:431:VAL:HG22	1.99	0.44
3:A:134:ILE:HG21	3:A:148:GLN:HE22	1.82	0.44
3:A:267:ARG:CD	3:A:267:ARG:N	2.80	0.44
3:A:84:ARG:NE	3:A:152:TYR:CE2	2.83	0.44
2:D:19:DG:N9	2:D:20:DT:H71	2.33	0.44
2:D:21:DC:H2''	2:D:22:DC:O5'	2.16	0.44
3:A:224:ILE:O	3:A:225:GLU:HB3	2.17	0.44
4:B:621:ILE:HG22	4:B:623:LYS:O	2.18	0.44
3:A:104:LEU:HD12	3:A:111:HIS:CD2	2.52	0.44
3:A:198:ARG:HD3	4:B:610:VAL:HG21	1.99	0.44
4:B:487:THR:HG21	4:B:489:ARG:NE	2.32	0.44
3:A:164:THR:HA	3:A:173:LEU:O	2.17	0.44
3:A:210:ASP:HB2	3:A:254:THR:HB	1.99	0.44
3:A:268:VAL:HG23	3:A:269:SER:N	2.33	0.44
4:B:462:GLY:C	4:B:464:ASN:N	2.69	0.44
4:B:461:ARG:C	4:B:463:TYR:H	2.21	0.44
4:B:474:ALA:O	4:B:475:TYR:CB	2.64	0.44
4:B:388:VAL:HG21	4:B:518:LEU:CD2	2.48	0.44
3:A:244:VAL:HG22	3:A:250:ILE:HG12	1.99	0.44
4:B:381:GLN:HB3	4:B:433:GLY:HA2	1.99	0.44
4:B:410:SER:HB3	4:B:419:GLY:CA	2.48	0.44
2:D:19:DG:H2''	2:D:20:DT:H71	2.00	0.44
4:B:460:ILE:HG21	4:B:486:LEU:HD11	1.99	0.44
3:A:248:VAL:HG13	4:B:604:HIS:HE2	1.83	0.44
1:C:1:DT:H1'	1:C:2:DG:P	2.57	0.44
3:A:228:PHE:CE2	3:A:286:PHE:CG	3.00	0.43
4:B:470:HIS:O	4:B:473:LEU:HB2	2.18	0.43
4:B:566:ILE:HG22	4:B:567:TYR:N	2.32	0.43
4:B:616:TYR:CD2	4:B:617:LYS:N	2.86	0.43
4:B:632:ARG:HD2	4:B:637:LEU:HA	1.99	0.43
4:B:416:CYS:SG	4:B:437:LEU:CD2	3.06	0.43
4:B:559:CYS:SG	4:B:560:VAL:N	2.91	0.43
4:B:599:SER:O	4:B:600:PRO:C	2.57	0.43
3:A:123:LYS:O	3:A:126:LEU:HB2	2.19	0.43
3:A:153:ASP:O	3:A:155:ASN:N	2.51	0.43
3:A:37:LYS:O	3:A:37:LYS:HG3	2.18	0.43
4:B:469:VAL:HG12	4:B:470:HIS:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:350:GLN:HG3	4:B:536:ALA:O	2.17	0.43
4:B:597:ASP:O	4:B:598:PHE:CB	2.66	0.43
3:A:30:ARG:HG3	3:A:184:PHE:CD2	2.53	0.43
4:B:344:ILE:HD11	4:B:532:VAL:HG13	2.00	0.43
4:B:451:LEU:HA	4:B:451:LEU:HD12	1.81	0.43
4:B:511:ARG:HG2	4:B:536:ALA:HA	2.00	0.43
2:D:15:DG:H2''	2:D:16:DA:H5'	2.00	0.43
3:A:81:PRO:CB	3:A:82:PRO:HD3	2.47	0.43
4:B:469:VAL:HG11	4:B:494:ILE:HG12	2.01	0.43
1:C:1:DT:C2	1:C:2:DG:H5''	2.53	0.43
3:A:190:ASN:HB3	3:A:220:GLN:NE2	2.29	0.43
3:A:278:ARG:O	3:A:280:LEU:HD12	2.19	0.43
3:A:73:ARG:HH11	3:A:162:GLN:HE21	1.65	0.43
3:A:188:ALA:HA	3:A:189:PRO:HD2	1.70	0.43
3:A:203:SER:HB3	3:A:289:LEU:HD11	1.99	0.43
3:A:228:PHE:HE1	3:A:252:PHE:CE1	2.37	0.43
4:B:358:VAL:O	4:B:358:VAL:HG22	2.19	0.43
4:B:544:ASN:ND2	4:B:544:ASN:H	2.16	0.43
3:A:138:ASN:OD1	3:A:138:ASN:C	2.56	0.42
3:A:84:ARG:NH2	3:A:152:TYR:CD2	2.78	0.42
3:A:163:VAL:HG12	3:A:164:THR:N	2.34	0.42
3:A:30:ARG:HG3	3:A:184:PHE:HD2	1.84	0.42
4:B:354:ARG:N	4:B:540:SER:HB3	2.34	0.42
4:B:555:ARG:HH11	4:B:555:ARG:CG	2.32	0.42
1:C:3:DG:N7	4:B:364:HIS:CE1	2.87	0.42
4:B:477:GLN:O	4:B:528:ARG:NH1	2.52	0.42
4:B:582:PHE:N	4:B:594:GLY:O	2.49	0.42
2:D:13:DA:H8	2:D:13:DA:O5'	2.02	0.42
3:A:141:PHE:HZ	3:A:179:LEU:HD11	1.80	0.42
4:B:454:ARG:HG2	4:B:454:ARG:HH11	1.84	0.42
3:A:84:ARG:NH2	3:A:152:TYR:CG	2.85	0.42
3:A:287:GLN:O	3:A:289:LEU:HG	2.19	0.42
4:B:399:THR:CG2	4:B:405:HIS:HB2	2.49	0.42
3:A:216:CYS:HG	3:A:248:VAL:C	2.18	0.42
3:A:271:GLN:NE2	3:A:281:SER:O	2.52	0.42
4:B:376:LYS:CE	4:B:376:LYS:HA	2.36	0.42
4:B:470:HIS:C	4:B:472:ASP:H	2.23	0.42
4:B:548:LEU:HD23	4:B:578:ILE:HD11	2.01	0.42
2:D:13:DA:H2''	2:D:14:DG:C8	2.55	0.42
3:A:37:LYS:HB2	3:A:119:GLN:OE1	2.19	0.42
4:B:470:HIS:HE2	4:B:494:ILE:HG13	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:454:ARG:HG2	4:B:454:ARG:NH1	2.35	0.42
4:B:388:VAL:HB	4:B:518:LEU:HD22	2.02	0.42
3:A:130:ILE:HD12	3:A:130:ILE:HG23	1.76	0.42
4:B:456:THR:C	4:B:458:ALA:H	2.24	0.42
4:B:579:GLN:NE2	4:B:632:ARG:HH11	2.13	0.42
4:B:598:PHE:HB2	4:B:602:ASP:CB	2.50	0.42
1:C:12:DC:N4	2:D:14:DG:H1	2.18	0.42
4:B:582:PHE:CD2	4:B:629:VAL:HG22	2.55	0.41
4:B:568:LEU:HD21	4:B:631:LEU:CD1	2.50	0.41
3:A:180:SER:O	3:A:181:HIS:C	2.58	0.41
4:B:349:LYS:CB	4:B:368:PRO:HG2	2.50	0.41
4:B:347:GLN:HB3	4:B:348:PRO:HD2	2.01	0.41
3:A:139:ASN:HD21	3:A:143:VAL:N	2.13	0.41
3:A:77:VAL:HG23	3:A:158:ARG:HB2	2.03	0.41
3:A:211:GLU:OE2	3:A:213:PHE:CE1	2.69	0.41
2:D:18:DA:H3'	4:B:444:LYS:NZ	2.36	0.41
2:D:13:DA:C8	2:D:13:DA:O5'	2.72	0.41
3:A:164:THR:O	3:A:164:THR:HG22	2.21	0.41
3:A:216:CYS:HB2	3:A:272:LEU:HD21	2.01	0.41
3:A:74:ILE:HG22	3:A:75:SER:N	2.35	0.41
4:B:623:LYS:CG	4:B:624:PRO:HD2	2.49	0.41
4:B:487:THR:HG22	4:B:489:ARG:HG3	2.03	0.41
4:B:599:SER:C	4:B:601:THR:N	2.73	0.41
3:A:84:ARG:NH2	3:A:152:TYR:CE2	2.86	0.41
4:B:460:ILE:CG2	4:B:486:LEU:HD11	2.51	0.41
4:B:487:THR:O	4:B:490:GLU:HB3	2.20	0.41
2:D:15:DG:C1'	2:D:16:DA:H5''	2.48	0.41
2:D:15:DG:C2'	2:D:16:DA:H5''	2.50	0.41
4:B:646:LEU:CD2	4:B:646:LEU:C	2.88	0.41
3:A:165:VAL:C	3:A:166:ARG:HH11	2.24	0.41
4:B:559:CYS:HA	4:B:648:TYR:CD1	2.56	0.41
2:D:19:DG:H2'	4:B:357:TYR:CE2	2.56	0.41
3:A:163:VAL:CG1	3:A:164:THR:N	2.84	0.41
3:A:93:LYS:HG2	3:A:94:ASP:OD2	2.21	0.41
4:B:432:VAL:O	4:B:432:VAL:HG13	2.21	0.41
3:A:141:PHE:HZ	3:A:179:LEU:CD1	2.34	0.40
3:A:206:CYS:HB3	3:A:262:LEU:HB2	2.02	0.40
4:B:355:PHE:CE1	4:B:439:ILE:HD13	2.56	0.40
1:C:9:DT:C2	1:C:10:DT:C5	3.08	0.40
3:A:236:ARG:HG2	3:A:236:ARG:H	1.56	0.40
4:B:470:HIS:O	4:B:473:LEU:CB	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:524:SER:C	4:B:526:THR:N	2.75	0.40
4:B:511:ARG:NH1	4:B:533:VAL:HG21	2.37	0.40
2:D:17:DA:H2"	2:D:18:DA:C8	2.56	0.40
3:A:261:SER:O	3:A:262:LEU:O	2.39	0.40
3:A:212:ILE:HG22	3:A:213:PHE:N	2.37	0.40
3:A:66:TYR:CD1	3:A:66:TYR:C	2.95	0.40
3:A:74:ILE:O	3:A:99:TYR:HB2	2.22	0.40
4:B:420:VAL:O	4:B:421:CYS:SG	2.79	0.40
4:B:448:PHE:C	4:B:448:PHE:CD1	2.94	0.40
4:B:528:ARG:CG	4:B:528:ARG:NH1	2.85	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	271/273 (99%)	208 (77%)	44 (16%)	19 (7%)	1	3
4	B	310/312 (99%)	241 (78%)	45 (14%)	24 (8%)	1	3
All	All	581/585 (99%)	449 (77%)	89 (15%)	43 (7%)	1	3

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	29	GLN
3	A	40	GLY
3	A	81	PRO
3	A	209	GLY
3	A	231	PRO
3	A	234	GLU
3	A	268	VAL
4	B	373	GLU

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Mol	Chain	Res	Type
4	B	387	TYR
4	B	414	LYS
4	B	427	PRO
4	B	475	TYR
4	B	479	GLU
4	B	575	LYS
3	A	28	LYS
3	A	41	ARG
3	A	134	ILE
3	A	154	LEU
3	A	199	VAL
3	A	262	LEU
4	B	389	GLY
4	B	469	VAL
4	B	478	ALA
4	B	524	SER
4	B	590	GLY
4	B	598	PHE
4	B	647	TYR
3	A	200	ASN
3	A	218	LYS
4	B	375	ASN
4	B	561	THR
4	B	572	LYS
4	B	587	GLU
4	B	606	GLN
3	A	225	GLU
4	B	376	LYS
4	B	530	GLU
4	B	554	ASP
4	B	614	PRO
3	A	230	GLY
4	B	649	PRO
3	A	260	PRO
3	A	275	PRO

### 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	242/242 (100%)	196 (81%)	46 (19%)	2	5
4	B	268/268 (100%)	229 (85%)	39 (15%)	3	11
All	All	510/510 (100%)	425 (83%)	85 (17%)	2	7

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	32	MET
3	A	47	PRO
3	A	54	THR
3	A	56	LYS
3	A	67	THR
3	A	73	ARG
3	A	75	SER
3	A	81	PRO
3	A	84	ARG
3	A	100	TYR
3	A	104	LEU
3	A	108	ARG
3	A	109	SER
3	A	111	HIS
3	A	112	SER
3	A	131	SER
3	A	135	GLN
3	A	136	THR
3	A	137	ASN
3	A	143	VAL
3	A	164	THR
3	A	168	PRO
3	A	174	LEU
3	A	179	LEU
3	A	191	THR
3	A	201	ARG
3	A	206	CYS
3	A	207	LEU
3	A	211	GLU
3	A	217	ASP
3	A	222	GLU
3	A	224	ILE
3	A	227	TYR
3	A	231	PRO

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Mol	Chain	Res	Type
3	A	234	GLU
3	A	236	ARG
3	A	251	VAL
3	A	253	ARG
3	A	267	ARG
3	A	272	LEU
3	A	279	GLU
3	A	280	LEU
3	A	282	GLU
3	A	284	MET
3	A	288	TYR
3	A	291	ASP
4	B	345	LEU
4	B	351	ARG
4	B	364	HIS
4	B	374	LYS
4	B	376	LYS
4	B	387	TYR
4	B	403	ASN
4	B	418	ASP
4	B	420	VAL
4	B	444	LYS
4	B	454	ARG
4	B	460	ILE
4	B	463	TYR
4	B	472	ASP
4	B	473	LEU
4	B	475	TYR
4	B	477	GLN
4	B	479	GLU
4	B	495	ARG
4	B	500	GLN
4	B	515	THR
4	B	518	LEU
4	B	528	ARG
4	B	532	VAL
4	B	533	VAL
4	B	540	SER
4	B	552	ARG
4	B	554	ASP
4	B	555	ARG
4	B	568	LEU

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Mol	Chain	Res	Type
4	B	575	LYS
4	B	578	ILE
4	B	581	ARG
4	B	586	GLU
4	B	605	ARG
4	B	614	PRO
4	B	632	ARG
4	B	637	LEU
4	B	646	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	26	GLN
3	A	64	ASN
3	A	139	ASN
3	A	148	GLN
3	A	162	GLN
3	A	220	GLN
3	A	241	GLN
3	A	271	GLN
4	B	343	GLN
4	B	400	ASN
4	B	403	ASN
4	B	407	HIS
4	B	441	HIS
4	B	500	GLN
4	B	544	ASN
4	B	579	GLN
4	B	606	GLN
4	B	620	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [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 [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

### 6.4 Ligands

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers

EDS was not executed - this section is therefore empty.