



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:27 PM GMT

PDB ID : 3RAD
Title : Quinolone(Clinafloxacin)-DNA cleavage complex of type IV topoisomerase from *S. pneumoniae*
Authors : Laponogov, I.; Pan, X.-S.; Veselkov, D.A.; McAuley, K.E.; Fisher, L.M.; Sanderson, M.R.
Deposited on : 2011-03-28
Resolution : 3.35 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

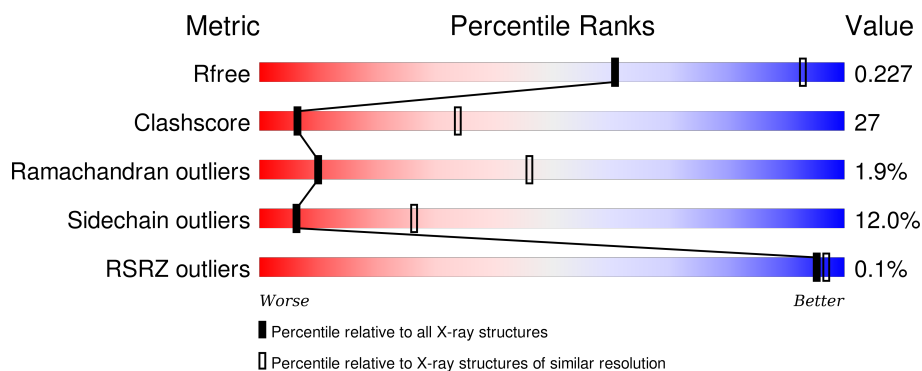
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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.




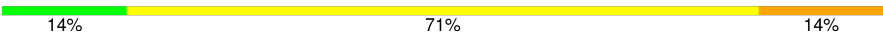

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1005 (3.42-3.30)
Clashscore	102246	1076 (3.42-3.30)
Ramachandran outliers	100387	1059 (3.42-3.30)
Sidechain outliers	100360	1058 (3.42-3.30)
RSRZ outliers	91569	1010 (3.42-3.30)

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	A	496	
1	B	496	
2	C	268	
2	D	268	
3	E	7	

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Mol	Chain	Length	Quality of chain
4	F	11	
5	G	7	
6	H	11	

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
7	MG	A	502	-	-	-	X
8	NFX	H	101	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 11096 atoms, of which 32 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 protein called DNA topoisomerase 4 subunit A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3702	2343	640	706	13			
1	B	482	Total	C	N	O	S	0	0	0
			3696	2345	635	703	13			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	257	THR	ILE	SEE REMARK 999	UNP P72525
A	489	LEU	-	EXPRESSION TAG	UNP P72525
A	490	GLU	-	EXPRESSION TAG	UNP P72525
A	491	HIS	-	EXPRESSION TAG	UNP P72525
A	492	HIS	-	EXPRESSION TAG	UNP P72525
A	493	HIS	-	EXPRESSION TAG	UNP P72525
A	494	HIS	-	EXPRESSION TAG	UNP P72525
A	495	HIS	-	EXPRESSION TAG	UNP P72525
A	496	HIS	-	EXPRESSION TAG	UNP P72525
B	257	THR	ILE	SEE REMARK 999	UNP P72525
B	489	LEU	-	EXPRESSION TAG	UNP P72525
B	490	GLU	-	EXPRESSION TAG	UNP P72525
B	491	HIS	-	EXPRESSION TAG	UNP P72525
B	492	HIS	-	EXPRESSION TAG	UNP P72525
B	493	HIS	-	EXPRESSION TAG	UNP P72525
B	494	HIS	-	EXPRESSION TAG	UNP P72525
B	495	HIS	-	EXPRESSION TAG	UNP P72525
B	496	HIS	-	EXPRESSION TAG	UNP P72525

- Molecule 2 is a protein called DNA topoisomerase 4 subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	209	Total	C	N	O	S	0	0	0
			1429	905	252	266	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	208	Total	C	N	O	S	0	0	0
			1417	898	247	267	5			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	EXPRESSION TAG	UNP Q59961
C	381	GLY	-	EXPRESSION TAG	UNP Q59961
C	382	HIS	-	EXPRESSION TAG	UNP Q59961
C	383	HIS	-	EXPRESSION TAG	UNP Q59961
C	384	HIS	-	EXPRESSION TAG	UNP Q59961
C	385	HIS	-	EXPRESSION TAG	UNP Q59961
C	386	HIS	-	EXPRESSION TAG	UNP Q59961
C	387	HIS	-	EXPRESSION TAG	UNP Q59961
C	388	HIS	-	EXPRESSION TAG	UNP Q59961
C	389	HIS	-	EXPRESSION TAG	UNP Q59961
C	390	HIS	-	EXPRESSION TAG	UNP Q59961
C	391	HIS	-	EXPRESSION TAG	UNP Q59961
C	392	SER	-	EXPRESSION TAG	UNP Q59961
C	393	SER	-	EXPRESSION TAG	UNP Q59961
C	394	GLY	-	EXPRESSION TAG	UNP Q59961
C	395	HIS	-	EXPRESSION TAG	UNP Q59961
C	396	ILE	-	EXPRESSION TAG	UNP Q59961
C	397	ASP	-	EXPRESSION TAG	UNP Q59961
C	398	ASP	-	EXPRESSION TAG	UNP Q59961
C	399	ASP	-	EXPRESSION TAG	UNP Q59961
C	400	ASP	-	EXPRESSION TAG	UNP Q59961
C	401	LYS	-	EXPRESSION TAG	UNP Q59961
C	402	HIS	-	EXPRESSION TAG	UNP Q59961
C	403	MET	-	EXPRESSION TAG	UNP Q59961
C	460	ILE	VAL	SEE REMARK 999	UNP Q59961
C	644	ALA	THR	SEE REMARK 999	UNP Q59961
D	380	MET	-	EXPRESSION TAG	UNP Q59961
D	381	GLY	-	EXPRESSION TAG	UNP Q59961
D	382	HIS	-	EXPRESSION TAG	UNP Q59961
D	383	HIS	-	EXPRESSION TAG	UNP Q59961
D	384	HIS	-	EXPRESSION TAG	UNP Q59961
D	385	HIS	-	EXPRESSION TAG	UNP Q59961
D	386	HIS	-	EXPRESSION TAG	UNP Q59961
D	387	HIS	-	EXPRESSION TAG	UNP Q59961
D	388	HIS	-	EXPRESSION TAG	UNP Q59961
D	389	HIS	-	EXPRESSION TAG	UNP Q59961

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Chain	Residue	Modelled	Actual	Comment	Reference
D	390	HIS	-	EXPRESSION TAG	UNP Q59961
D	391	HIS	-	EXPRESSION TAG	UNP Q59961
D	392	SER	-	EXPRESSION TAG	UNP Q59961
D	393	SER	-	EXPRESSION TAG	UNP Q59961
D	394	GLY	-	EXPRESSION TAG	UNP Q59961
D	395	HIS	-	EXPRESSION TAG	UNP Q59961
D	396	ILE	-	EXPRESSION TAG	UNP Q59961
D	397	ASP	-	EXPRESSION TAG	UNP Q59961
D	398	ASP	-	EXPRESSION TAG	UNP Q59961
D	399	ASP	-	EXPRESSION TAG	UNP Q59961
D	400	ASP	-	EXPRESSION TAG	UNP Q59961
D	401	LYS	-	EXPRESSION TAG	UNP Q59961
D	402	HIS	-	EXPRESSION TAG	UNP Q59961
D	403	MET	-	EXPRESSION TAG	UNP Q59961
D	460	ILE	VAL	SEE REMARK 999	UNP Q59961
D	644	ALA	THR	SEE REMARK 999	UNP Q59961

- Molecule 3 is a DNA chain called 5'-D(*CP*AP*TP*GP*AP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	7	Total	C	N	O	P	0	0	0
			140	69	27	38	6			

- Molecule 4 is a DNA chain called 5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	11	Total	C	N	O	P	0	0	0
			225	108	39	67	11			

- Molecule 5 is a DNA chain called 5'-D(*CP*GP*TP*GP*CP*AP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	7	Total	C	N	O	P	0	0	0
			139	68	25	40	6			

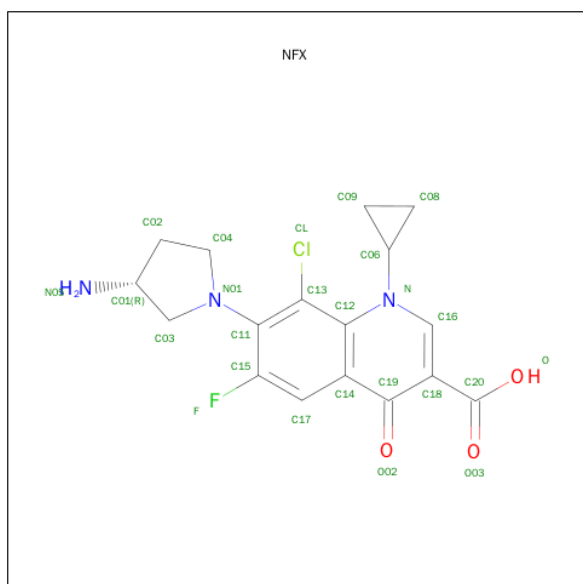
- Molecule 6 is a DNA chain called 5'-D(P*GP*AP*CP*TP*AP*TP*GP*CP*AP*CP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	11	Total	C	N	O	P	0	0	0
			226	107	43	65	11			

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	2	Total Mg 2 2	0	0
7	A	2	Total Mg 2 2	0	0
7	D	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0

- Molecule 8 is 7-[(3R)-3-AMINOPYRROLIDIN-1-YL]-8-CHLORO-1-CYCLOPROPYL-6-FLUORO-4-OXO-1,4-DIHYDROQUINOLINE-3-CARBOXYLIC ACID (three-letter code: NFX) (formula: C₁₇H₁₇ClFN₃O₃).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
8	F	1	Total	C	Cl	F	H	N	O	0	0
			41	17	1	1	16	3	3		
8	H	1	Total	C	Cl	F	H	N	O	0	0
			41	17	1	1	16	3	3		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	18	Total O 18 18	0	0
9	B	11	Total O 11 11	0	0
9	C	2	Total O 2 2	0	0

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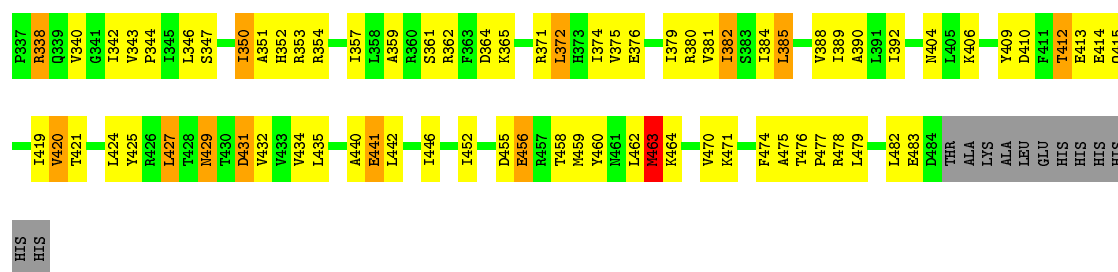
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	E	2	Total	O	0	0
			2	2		
9	G	1	Total	O	0	0
			1	1		

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 ($\text{RSRZ} > 2$). 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.

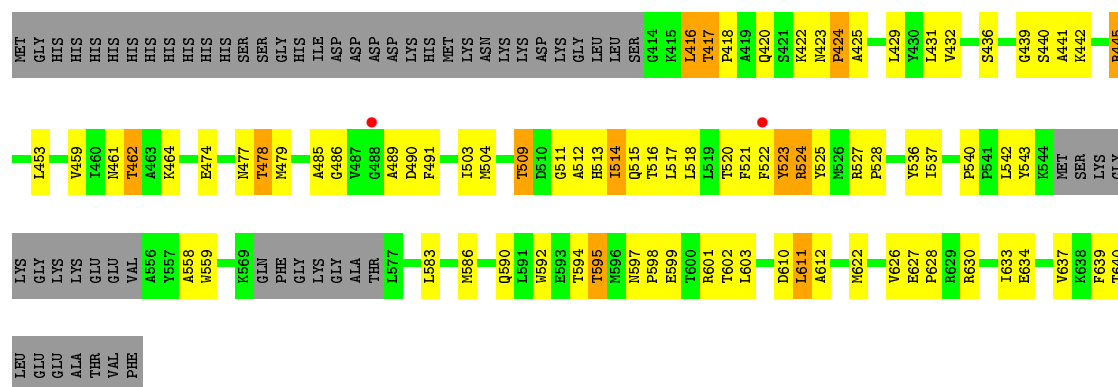
[illegible]

Chain B:

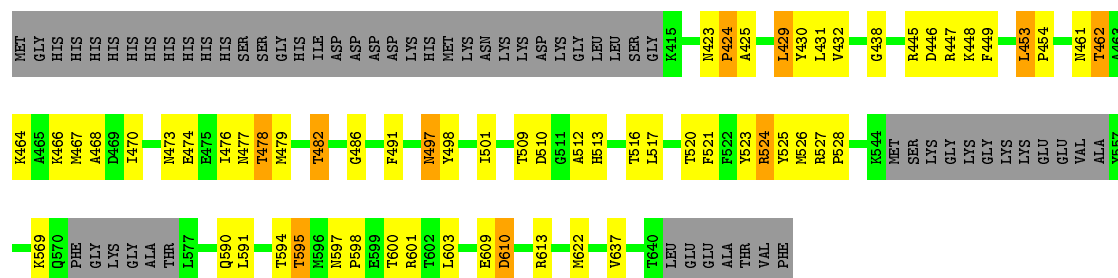
Category	Percentage
P260	1%
Y261	1%
E262	1%
K263	1%
M264	1%
K265	1%
L268	1%
V269	1%
I272	1%
D273	1%
D274	1%
V275	1%
V281	1%
A282	1%
G283	1%
I284	1%
A285	1%
E286	1%
V287	1%
K288	1%
E289	1%
E290	1%
R293	1%
D294	1%
G295	1%
L296	1%
R297	1%
I300	1%
E301	1%
L302	1%
K303	1%
N307	1%
K308	1%
E309	1%
L310	1%
V311	1%
L312	1%
L314	1%
L315	1%
L316	1%
T319	1%
D320	1%
K321	1%
K322	1%
V325	1%
K326	1%
F327	1%
D333	1%
K334	1%
F335	1%
F336	1%
F337	1%
L38	1%
V99	1%
H102	1%
G103	1%
M104	1%
S107	1%
M108	1%
D109	1%
G110	1%
D111	1%
P112	1%
P113	1%
A114	1%
E120	1%
I126	1%
L131	1%
Q132	1%
D133	1%
I134	1%
E135	1%
K136	1%
V139	1%
P140	1%
F141	1%
A142	1%
W143	1%
M144	1%
F145	1%
D146	1%
D147	1%
T148	1%
E149	1%
K150	1%
E151	1%
P152	1%
T153	1%
V154	1%
A157	1%
A158	1%
F159	1%
P160	1%
M161	1%
L162	1%
G163	1%
V164	1%
S167	1%
T168	1%
G169	1%
I170	1%
T176	1%
D177	1%
E187	1%
H188	1%
S189	1%
Q190	1%
N191	1%
W192	1%
R195	1%
E196	1%
T197	1%
MET	7%
N3	1%
I4	1%
L9	1%
Y20	1%
I24	1%
I25	1%
Q26	1%
D27	1%
R28	1%
R34	1%
D35	1%
G36	1%
L37	1%
K38	1%
P39	1%
V40	1%
Q41	1%
R42	1%
R43	1%
I44	1%
N49	1%
N53	1%
S58	1%
Y59	1%
R60	1%
K61	1%
W70	1%
F73	1%
H74	1%
P75	1%
H76	1%
G77	1%
D78	1%
S79	1%
S80	1%
I81	1%
A84	1%
R87	1%
M88	1%
S89	1%
Q90	1%
N91	1%
W92	1%
R95	1%
E96	1%
T97	1%



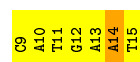
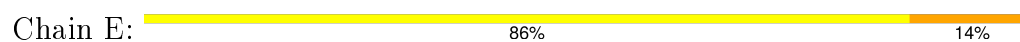
• Molecule 2: DNA topoisomerase 4 subunit B



• Molecule 2: DNA topoisomerase 4 subunit B



• Molecule 3: 5'-D(*CP*AP*TP*GP*AP*AP*T)-3'



• Molecule 4: 5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*G)-3'

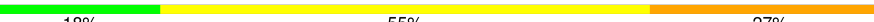


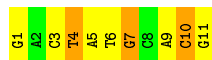
- Molecule 5: 5'-D(*CP*GP*TP*GP*CP*AP*T)-3'

Chain G:  14% 71% 14%



- Molecule 6: 5'-D(P*GP*AP*CP*TP*AP*TP*GP*CP*AP*CP*G)-3'

Chain H:  18% 55% 27%



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	157.13Å 157.13Å 211.09Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	41.67 – 3.35 41.67 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.3 (41.67-3.35) 99.3 (41.67-3.10)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.12 (at 3.12Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.2_869)	Depositor
R, R_{free}	0.177 , 0.228 0.177 , 0.227	Depositor DCC
R_{free} test set	4351 reflections (11.09%)	DCC
Wilson B-factor (Å ²)	77.9	Xtriage
Anisotropy	0.599	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	(Not available) , (Not available)	EDS
Estimated twinning fraction	0.063 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 55080 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	11096	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	A	0.44	0/3763	0.66	1/5104 (0.0%)
1	B	0.44	0/3757	0.64	0/5098
2	C	0.34	0/1455	0.54	0/1991
2	D	0.33	0/1443	0.53	0/1976
3	E	0.76	0/157	1.83	7/241 (2.9%)
4	F	0.89	0/251	2.02	14/385 (3.6%)
5	G	0.84	0/155	1.96	7/238 (2.9%)
6	H	0.77	0/253	1.80	10/388 (2.6%)
All	All	0.46	0/11234	0.80	39/15421 (0.3%)

There are no bond length outliers.

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	14	DA	O4'-C4'-C3'	-13.34	98.00	106.00
4	F	9	DA	O4'-C4'-C3'	-11.62	99.03	106.00
6	H	10	DC	O4'-C4'-C3'	-10.87	99.48	106.00
4	F	10	DT	O4'-C4'-C3'	-9.86	100.09	106.00
4	F	3	DT	O4'-C4'-C3'	-9.75	100.15	106.00
3	E	12	DG	O4'-C4'-C3'	-8.92	100.65	106.00
6	H	4	DT	O4'-C4'-C3'	-7.70	101.38	106.00
5	G	15	DT	N3-C4-O4	7.56	124.44	119.90
5	G	15	DT	O4'-C4'-C3'	-7.44	101.53	104.50
3	E	12	DG	C4'-C3'-C2'	-7.16	96.65	103.10
4	F	1	DA	C3'-C2'-C1'	-7.08	94.00	102.50
6	H	9	DA	O4'-C1'-N9	-6.70	103.31	108.00
3	E	14	DA	O4'-C4'-C3'	-6.55	101.88	104.50
5	G	11	DT	C5-C4-O4	-6.40	120.42	124.90
5	G	15	DT	C5-C4-O4	-6.31	120.48	124.90
4	F	1	DA	O4'-C1'-N9	6.21	112.34	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	7	DT	N3-C2-O2	-6.12	118.63	122.30
4	F	3	DT	O4'-C1'-N1	6.02	112.22	108.00
6	H	7	DG	N3-C4-N9	-6.01	122.39	126.00
6	H	7	DG	N3-C2-N2	-6.00	115.70	119.90
4	F	9	DA	C3'-C2'-C1'	-5.89	95.43	102.50
5	G	15	DT	C4'-C3'-C2'	-5.81	97.87	103.10
5	G	11	DT	N3-C4-O4	5.77	123.36	119.90
4	F	7	DT	N3-C4-O4	5.71	123.32	119.90
4	F	9	DA	C4'-C3'-C2'	-5.58	98.08	103.10
6	H	10	DC	C1'-O4'-C4'	-5.55	104.55	110.10
6	H	4	DT	N3-C4-O4	5.52	123.21	119.90
6	H	4	DT	C5-C4-O4	-5.43	121.10	124.90
3	E	11	DT	C4-C5-C7	5.39	122.24	119.00
4	F	6	DT	N3-C4-O4	5.33	123.10	119.90
3	E	15	DT	N3-C4-O4	5.23	123.04	119.90
4	F	6	DT	C5-C4-O4	-5.21	121.25	124.90
6	H	1	DG	O4'-C1'-N9	5.19	111.63	108.00
3	E	14	DA	C4'-C3'-C2'	-5.17	98.45	103.10
4	F	7	DT	N1-C2-O2	5.11	127.19	123.10
1	A	162	LEU	CA-CB-CG	5.10	127.03	115.30
4	F	1	DA	C1'-O4'-C4'	-5.08	105.02	110.10
3	E	11	DT	C6-C5-C7	-5.03	119.88	122.90
6	H	7	DG	O4'-C1'-N9	5.00	111.50	108.00

There are no chirality outliers.

There are no planarity outliers.

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	A	3702	0	3579	201	0
1	B	3696	0	3589	222	0
2	C	1429	0	1193	80	0
2	D	1417	0	1167	61	0
3	E	140	0	78	6	0
4	F	225	0	126	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	139	0	78	3	0
6	H	226	0	124	7	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	F	25	16	16	4	0
8	H	25	16	16	4	0
9	A	18	0	0	0	0
9	B	11	0	0	1	0
9	C	2	0	0	0	0
9	E	2	0	0	0	0
9	G	1	0	0	0	0
All	All	11064	32	9966	577	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 27.

All (577) 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:B:146:ASP:HB3	1:B:148:THR:HG23	1.27	1.15
1:B:70:MET:HE1	1:B:78:ASP:HB3	1.19	1.11
1:A:70:MET:HE1	1:A:78:ASP:HB3	1.18	1.09
1:B:307:ASN:ND2	1:B:310:LEU:HB2	1.69	1.07
1:A:60:ARG:HB2	1:A:60:ARG:HH11	1.18	1.07
1:B:307:ASN:HD21	1:B:310:LEU:HB2	0.89	1.05
1:B:24:ILE:HD11	1:B:28:ARG:HE	1.16	1.05
1:A:354:ARG:HG3	1:A:459:MET:HE2	1.36	1.04
1:A:443:ARG:HH11	1:A:443:ARG:HG3	0.97	1.04
2:D:462:THR:HG21	2:D:521:PHE:HD2	1.17	1.02
1:A:139:VAL:HG11	1:A:154:VAL:O	1.61	1.00
1:B:24:ILE:HD11	1:B:28:ARG:NE	1.77	0.99
1:A:391:LEU:HD21	1:A:404:ASN:HB3	1.44	0.99
1:A:354:ARG:HG3	1:A:459:MET:CE	1.93	0.99
1:B:307:ASN:HD21	1:B:310:LEU:CB	1.75	0.98
1:A:139:VAL:HG13	1:A:140:PRO:HD2	1.44	0.98
2:C:486:GLY:O	2:C:491:PHE:HD2	1.48	0.96
1:A:21:SER:O	1:A:25:ILE:HG13	1.68	0.93
1:A:222:ARG:HD3	1:A:484:ASP:HA	1.47	0.93
1:A:60:ARG:HH11	1:A:60:ARG:CB	1.82	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:THR:HG23	1:B:415:GLN:NE2	1.82	0.92
1:A:443:ARG:NH1	1:A:443:ARG:HG3	1.77	0.92
1:B:9:LEU:HD23	1:B:9:LEU:O	1.69	0.92
1:A:70:MET:CE	1:A:78:ASP:HB3	2.00	0.91
1:A:443:ARG:HH11	1:A:443:ARG:CG	1.83	0.91
1:B:70:MET:HE1	1:B:78:ASP:CB	2.00	0.89
2:D:462:THR:HG21	2:D:521:PHE:CD2	2.05	0.89
8:H:101:NFX:H03	8:H:101:NFX:CL	2.10	0.89
2:D:474:GLU:O	2:D:478:THR:HG23	1.75	0.87
2:D:524:ARG:HH11	2:D:524:ARG:HB3	1.40	0.87
1:A:91:ASN:HD22	1:A:91:ASN:H	1.23	0.86
1:B:256:ILE:HD13	1:B:321:LEU:HD21	1.57	0.86
1:B:219:ILE:HG23	1:B:236:VAL:HG21	1.57	0.86
1:B:70:MET:CE	1:B:78:ASP:HB3	2.06	0.85
2:D:590:GLN:O	2:D:594:THR:HG23	1.76	0.85
1:A:293:ARG:HB3	1:A:293:ARG:HH11	1.42	0.84
1:A:316:PHE:CE2	1:A:321:LEU:HD13	2.12	0.84
2:D:520:THR:HG21	2:D:622:MET:HG3	1.60	0.84
1:A:334:ASN:O	1:A:336:THR:HG22	1.77	0.84
8:H:101:NFX:CL	8:H:101:NFX:C03	2.64	0.82
1:B:389:ILE:HD11	1:B:427:LEU:HD13	1.60	0.82
1:B:146:ASP:HB3	1:B:148:THR:CG2	2.09	0.82
1:B:41:GLN:HG2	1:B:88:MET:HE2	1.62	0.81
1:B:146:ASP:CB	1:B:148:THR:HG23	2.11	0.81
1:B:243:GLU:O	1:B:244:ILE:HD13	1.80	0.81
1:A:44:ILE:HD12	1:A:88:MET:CE	2.10	0.81
1:B:194:ILE:HD13	1:B:463:MET:HE2	1.63	0.80
1:B:9:LEU:HD23	1:B:9:LEU:C	2.00	0.80
1:A:338:ARG:HD2	1:A:340:VAL:CG1	2.12	0.79
1:A:146:ASP:OD2	1:A:148:THR:HG22	1.82	0.79
1:B:41:GLN:HA	1:B:88:MET:HE1	1.64	0.79
1:B:354:ARG:HG3	1:B:459:MET:HE2	1.64	0.77
2:C:520:THR:HG21	2:C:622:MET:HG3	1.67	0.77
2:C:611:LEU:HD13	2:C:611:LEU:O	1.84	0.77
1:B:254:ILE:HD13	1:B:312:LEU:HD13	1.67	0.77
1:A:139:VAL:HG13	1:A:140:PRO:CD	2.15	0.77
1:B:343:VAL:HB	1:B:344:PRO:HD3	1.66	0.77
1:B:354:ARG:HG3	1:B:459:MET:CE	2.14	0.76
1:B:95:ARG:HA	1:B:214:PRO:HG3	1.66	0.76
1:A:265:LYS:O	1:A:269:VAL:HG23	1.85	0.76
1:B:41:GLN:HA	1:B:88:MET:CE	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:9:DA:O5'	4:F:9:DA:H2'	1.85	0.75
1:B:385:LEU:HD21	1:B:427:LEU:HD22	1.69	0.75
1:A:442:LEU:O	1:A:446:ILE:HG13	1.85	0.75
1:B:24:ILE:CD1	1:B:28:ARG:NE	2.50	0.74
1:A:60:ARG:HB2	1:A:60:ARG:NH1	1.99	0.74
1:B:139:VAL:HG12	1:B:140:PRO:HD2	1.69	0.74
8:F:101:NFX:CL	8:F:101:NFX:H04A	2.25	0.73
1:B:431:ASP:O	1:B:434:VAL:HG12	1.87	0.73
1:B:412:THR:HG23	1:B:415:GLN:HE21	1.50	0.73
1:A:316:PHE:HE2	1:A:321:LEU:HD13	1.52	0.72
1:B:110:GLY:HA3	1:B:264:ASN:HD21	1.54	0.72
2:D:525:TYR:O	2:D:526:MET:HG3	1.89	0.72
2:C:491:PHE:CD1	2:C:528:PRO:HG2	2.25	0.72
1:B:160:PRO:O	1:B:164:VAL:HG23	1.89	0.72
2:C:524:ARG:HB3	2:C:525:TYR:CD1	2.25	0.72
1:B:95:ARG:HB2	1:B:180:PRO:HB3	1.72	0.72
1:B:381:VAL:HG12	1:B:382:ILE:N	2.03	0.72
8:F:101:NFX:CL	8:F:101:NFX:C04	2.75	0.71
1:A:144:ASN:HD21	1:A:148:THR:HG23	1.56	0.71
1:B:219:ILE:HG23	1:B:236:VAL:CG2	2.20	0.71
1:B:38:LYS:H	1:B:41:GLN:NE2	1.88	0.71
2:C:423:ASN:HD21	2:C:425:ALA:HB3	1.56	0.71
1:A:259:ILE:HB	1:A:260:PRO:CD	2.21	0.70
1:B:307:ASN:ND2	1:B:310:LEU:CB	2.44	0.70
1:A:24:ILE:HG22	1:A:171:SER:HB2	1.73	0.70
1:A:252:GLU:OE1	1:A:308:THR:HG21	1.91	0.70
1:B:194:ILE:HD11	1:B:463:MET:HE1	1.73	0.70
1:B:236:VAL:CG2	1:B:237:VAL:N	2.55	0.69
1:B:194:ILE:CD1	1:B:463:MET:HE2	2.22	0.69
2:C:462:THR:HG21	2:C:521:PHE:HD2	1.56	0.69
3:E:9:DC:H2"	3:E:10:DA:H5"	1.75	0.69
2:C:474:GLU:O	2:C:478:THR:HG23	1.92	0.69
1:B:211:PRO:O	1:B:478:ARG:NH2	2.26	0.68
1:B:412:THR:CG2	1:B:415:GLN:NE2	2.56	0.68
1:A:60:ARG:HH11	1:A:60:ARG:CG	2.06	0.68
1:B:43:ARG:HD3	1:B:73:PHE:HB3	1.73	0.68
1:A:412:THR:HG23	1:A:415:GLN:OE1	1.94	0.68
2:D:486:GLY:O	2:D:491:PHE:HD2	1.76	0.68
8:H:101:NFX:CL	8:H:101:NFX:C06	2.78	0.68
8:F:101:NFX:CL	8:F:101:NFX:C06	2.78	0.68
1:A:244:ILE:HD12	1:A:244:ILE:N	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:357:ILE:HD12	1:B:463:MET:HG2	1.76	0.68
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.59	0.68
1:A:28:ARG:CZ	3:E:14:DA:H4'	2.24	0.67
1:A:40:VAL:O	1:A:44:ILE:HG13	1.94	0.67
1:B:389:ILE:HD11	1:B:427:LEU:CD1	2.23	0.67
1:A:338:ARG:HD2	1:A:340:VAL:HG12	1.76	0.67
1:A:169:GLY:HA2	1:A:176:THR:HG22	1.76	0.67
2:D:609:GLU:O	2:D:610:ASP:HB2	1.94	0.67
1:B:194:ILE:HD11	1:B:463:MET:CE	2.25	0.67
2:D:610:ASP:OD1	2:D:613:ARG:HB2	1.95	0.66
1:B:194:ILE:CD1	1:B:463:MET:CE	2.74	0.66
8:H:101:NFX:CL	8:H:101:NFX:C09	2.81	0.66
1:B:9:LEU:CD2	1:B:9:LEU:C	2.64	0.66
8:F:101:NFX:CL	8:F:101:NFX:C09	2.81	0.66
1:A:59:TYR:HB3	1:A:120:GLU:HG3	1.77	0.65
1:B:283:GLY:HA2	1:B:303:LYS:HD2	1.78	0.65
2:C:513:HIS:O	2:C:516:THR:HB	1.97	0.65
2:D:461:ASN:ND2	2:D:464:LYS:HG3	2.12	0.65
1:A:398:LYS:HD2	1:B:425:TYR:CD1	2.32	0.65
1:A:211:PRO:O	1:A:478:ARG:NH2	2.29	0.65
1:B:167:SER:C	1:B:168:THR:HG22	2.15	0.65
2:D:524:ARG:NH1	2:D:524:ARG:HB3	2.11	0.64
1:B:20:TYR:CD1	2:D:513:HIS:HB2	2.32	0.64
1:A:139:VAL:CG1	1:A:140:PRO:HD2	2.24	0.64
1:B:41:GLN:CG	1:B:88:MET:HE2	2.28	0.64
2:D:601:ARG:HH21	2:D:603:LEU:HD11	1.63	0.64
1:A:23:TYR:HB3	2:C:509:THR:HG21	1.78	0.64
1:B:95:ARG:O	1:B:95:ARG:HD2	1.97	0.64
1:A:144:ASN:C	1:A:146:ASP:H	2.01	0.64
1:B:28:ARG:CZ	5:G:14:DA:H4'	2.28	0.64
2:D:478:THR:O	2:D:482:THR:HG23	1.97	0.63
1:B:136:LYS:HE2	1:B:364:ASP:OD1	1.98	0.63
5:G:13:DC:H2''	5:G:14:DA:O5'	1.98	0.63
2:C:630:ARG:O	2:C:634:GLU:HG3	1.98	0.63
2:D:431:LEU:HD13	2:D:479:MET:CE	2.29	0.63
2:C:527:ARG:N	2:C:528:PRO:HD2	2.14	0.63
6:H:10:DC:H2''	6:H:11:DG:H5''	1.81	0.63
1:A:391:LEU:HD21	1:A:404:ASN:CB	2.26	0.63
1:A:169:GLY:O	1:A:170:ILE:HG12	1.99	0.63
2:C:637:VAL:HG12	2:C:639:PHE:CE2	2.34	0.62
1:A:70:MET:HE1	1:A:78:ASP:CB	2.10	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:511:GLY:O	2:C:515:GLN:HG3	1.98	0.62
1:A:22:LYS:O	1:A:26:GLN:HG3	1.99	0.62
1:B:302:LEU:HD12	1:B:308:THR:HG22	1.80	0.62
1:B:139:VAL:HG11	1:B:154:VAL:O	1.99	0.62
1:A:194:ILE:HD11	1:A:463:MET:HE3	1.80	0.62
2:C:461:ASN:ND2	2:C:464:LYS:HG3	2.14	0.62
1:A:22:LYS:HE2	1:A:26:GLN:OE1	2.00	0.62
1:B:139:VAL:HG12	1:B:154:VAL:HG13	1.82	0.61
1:B:259:ILE:HB	1:B:260:PRO:HD2	1.82	0.61
1:B:261:TYR:O	1:B:262:GLU:HB2	1.99	0.61
1:A:222:ARG:HD3	1:A:484:ASP:CA	2.24	0.61
2:C:540:PRO:HA	2:C:595:THR:HG21	1.81	0.61
1:A:194:ILE:HG23	1:A:460:TYR:CD1	2.35	0.61
1:B:259:ILE:HB	1:B:260:PRO:CD	2.31	0.61
2:D:513:HIS:O	2:D:516:THR:HB	2.00	0.61
2:D:431:LEU:HD22	2:D:479:MET:HE3	1.82	0.61
1:B:296:LEU:HD23	1:B:297:ARG:N	2.14	0.61
1:B:139:VAL:CG1	1:B:154:VAL:HG13	2.31	0.61
1:A:389:ILE:HD11	1:A:427:LEU:HD13	1.83	0.61
2:C:416:LEU:HG	2:C:417:THR:N	2.15	0.61
2:C:442:LYS:O	2:C:445:ARG:HD3	2.00	0.61
1:B:389:ILE:HG22	1:B:390:ALA:N	2.15	0.60
1:B:41:GLN:CB	1:B:88:MET:HE2	2.31	0.60
2:C:524:ARG:HB3	2:C:525:TYR:HD1	1.63	0.60
1:B:273:ASP:HA	1:B:287:VAL:HG21	1.83	0.60
1:A:219:ILE:HG23	1:A:236:VAL:HG11	1.84	0.60
1:B:296:LEU:HD23	1:B:296:LEU:C	2.21	0.60
2:C:542:LEU:HB2	2:C:543:TYR:CD2	2.37	0.60
1:A:139:VAL:CG1	1:A:140:PRO:CD	2.80	0.60
2:C:601:ARG:HD2	2:C:603:LEU:HD21	1.83	0.60
1:B:236:VAL:HG23	1:B:237:VAL:H	1.66	0.60
1:A:216:GLY:O	1:A:217:ALA:HB3	2.02	0.59
1:A:443:ARG:NH1	1:A:443:ARG:CG	2.49	0.59
1:A:38:LYS:H	1:A:41:GLN:NE2	1.98	0.59
1:A:144:ASN:O	1:A:146:ASP:N	2.34	0.59
1:B:228:ALA:HA	1:B:233:LYS:O	2.02	0.59
2:C:459:VAL:HG11	2:C:518:LEU:HD23	1.84	0.59
6:H:3:DC:H2'	6:H:4:DT:C6	2.36	0.59
6:H:6:DT:C2'	6:H:7:DG:H5'	2.33	0.59
1:B:412:THR:H	1:B:415:GLN:HE21	1.51	0.58
1:B:431:ASP:C	1:B:431:ASP:OD1	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:LEU:HD22	1:A:389:ILE:HD12	1.85	0.58
1:A:23:TYR:CB	2:C:509:THR:HG21	2.34	0.58
1:B:87:ARG:HA	1:B:90:GLN:HG3	1.85	0.58
1:B:357:ILE:CD1	1:B:463:MET:HG2	2.33	0.58
1:B:126:ILE:HG13	1:B:474:PHE:CD1	2.39	0.58
1:A:285:ALA:HB3	1:A:301:GLU:O	2.04	0.58
1:A:34:ARG:HD2	1:A:352:HIS:ND1	2.19	0.58
1:B:247:LEU:HB2	1:B:251:LYS:O	2.04	0.58
1:A:355:GLU:OE2	1:A:355:GLU:HA	2.04	0.58
2:D:446:ASP:HB3	2:D:449:PHE:CE1	2.39	0.58
2:C:509:THR:O	2:C:512:ALA:HB3	2.04	0.58
1:A:40:VAL:HG13	1:A:41:GLN:N	2.18	0.57
1:A:334:ASN:O	1:A:336:THR:CG2	2.52	0.57
1:A:9:LEU:O	1:A:9:LEU:HD23	2.05	0.57
1:B:84:ALA:O	1:B:88:MET:HG3	2.04	0.57
1:A:350:ILE:HA	1:A:463:MET:HE1	1.87	0.57
2:D:637:VAL:O	2:D:637:VAL:HG12	2.04	0.57
1:A:12:ILE:O	1:A:16:ARG:HG2	2.05	0.57
1:A:377:GLY:O	1:A:381:VAL:HG23	2.05	0.57
2:C:489:ALA:C	2:C:491:PHE:H	2.08	0.57
1:B:236:VAL:CG2	1:B:237:VAL:H	2.18	0.57
6:H:10:DC:C2'	6:H:11:DG:H5''	2.35	0.56
6:H:5:DA:H2''	6:H:6:DT:O5'	2.05	0.56
1:B:210:GLY:HA2	1:B:229:TYR:OH	2.05	0.56
2:C:486:GLY:O	2:C:491:PHE:CD2	2.41	0.56
1:A:190:ALA:O	1:A:194:ILE:HG13	2.06	0.56
2:C:516:THR:HG22	2:C:517:LEU:N	2.20	0.56
1:B:236:VAL:HG22	1:B:237:VAL:N	2.19	0.56
1:A:44:ILE:HD12	1:A:88:MET:HE3	1.86	0.56
2:D:516:THR:O	2:D:520:THR:HG23	2.06	0.56
1:A:391:LEU:HD23	1:A:391:LEU:O	2.06	0.56
2:D:597:ASN:HD22	2:D:600:THR:CB	2.18	0.55
1:A:455:ASP:HB3	1:A:458:THR:HB	1.87	0.55
1:B:406:LYS:HE2	1:B:413:GLU:HA	1.88	0.55
1:A:59:TYR:CB	1:A:120:GLU:HG3	2.36	0.55
1:A:390:ALA:O	1:A:393:ARG:HB3	2.06	0.55
2:C:485:ALA:HB3	2:C:491:PHE:CE2	2.41	0.55
1:A:44:ILE:O	1:A:48:MET:HG3	2.07	0.55
1:B:49:ASN:CB	1:B:131:LEU:HD13	2.36	0.55
1:A:194:ILE:HG23	1:A:460:TYR:HD1	1.70	0.55
2:C:627:GLU:N	2:C:628:PRO:CD	2.69	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:SER:HA	1:B:99:VAL:O	2.06	0.55
2:C:516:THR:CG2	2:C:622:MET:SD	2.95	0.55
1:A:139:VAL:CG1	1:A:154:VAL:O	2.47	0.55
1:A:160:PRO:HG2	1:A:186:VAL:HG12	1.87	0.55
2:C:491:PHE:CE1	2:C:528:PRO:HG2	2.42	0.55
1:B:343:VAL:HB	1:B:344:PRO:CD	2.37	0.55
1:B:43:ARG:CD	1:B:73:PHE:HB3	2.37	0.55
1:A:181:HIS:CD2	1:A:211:PRO:HA	2.42	0.55
1:B:49:ASN:HB2	1:B:131:LEU:HD13	1.89	0.54
1:A:245:GLU:OE2	1:A:297:ARG:NH2	2.39	0.54
1:B:111:ASP:HB2	1:B:112:PRO:HD2	1.89	0.54
1:A:293:ARG:NH1	1:A:293:ARG:HB3	2.18	0.54
1:B:91:ASN:H	1:B:91:ASN:HD22	1.55	0.54
1:B:28:ARG:NH1	1:B:28:ARG:HG3	2.20	0.54
1:A:354:ARG:HG3	1:A:459:MET:HE1	1.87	0.54
3:E:13:DA:H2''	3:E:14:DA:O5'	2.07	0.54
1:B:471:LYS:O	1:B:475:ALA:HB2	2.07	0.54
1:B:35:ASP:O	1:B:161:ASN:HB3	2.07	0.54
2:C:583:LEU:HA	2:C:586:MET:HE3	1.90	0.54
1:A:194:ILE:HD13	1:A:463:MET:HG2	1.89	0.54
1:A:448:MET:O	1:A:452:ILE:HG13	2.06	0.54
2:D:486:GLY:O	2:D:491:PHE:CD2	2.60	0.54
2:D:432:VAL:HG11	2:D:438:GLY:HA2	1.89	0.54
1:B:216:GLY:O	1:B:217:ALA:HB3	2.08	0.54
2:C:516:THR:HG21	2:C:622:MET:SD	2.48	0.53
1:A:167:SER:C	1:A:168:THR:HG22	2.27	0.53
1:B:77:GLY:O	1:B:81:ILE:HG13	2.08	0.53
2:D:431:LEU:CD1	2:D:479:MET:HE2	2.38	0.53
1:A:55:PHE:HA	1:A:122:ARG:HD2	1.90	0.53
2:C:626:VAL:HG11	4:F:9:DA:H3'	1.89	0.53
1:A:259:ILE:HB	1:A:260:PRO:HD2	1.89	0.53
2:D:478:THR:O	2:D:482:THR:CG2	2.57	0.53
2:C:514:ILE:HG22	2:C:515:GLN:N	2.23	0.53
2:C:423:ASN:ND2	2:C:425:ALA:HB3	2.24	0.53
2:C:637:VAL:CG1	2:C:639:PHE:CE2	2.92	0.53
1:A:296:LEU:HD23	1:A:297:ARG:N	2.24	0.53
1:B:456:GLU:HG3	1:B:460:TYR:CE2	2.44	0.53
2:D:509:THR:O	2:D:512:ALA:HB3	2.09	0.53
1:B:381:VAL:O	1:B:384:ILE:N	2.31	0.53
1:A:97:ILE:HG12	1:A:97:ILE:O	2.09	0.53
1:B:75:PRO:HD3	1:B:145:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:9:DC:C2'	3:E:10:DA:H5''	2.38	0.53
2:D:594:THR:OG1	2:D:595:THR:HG22	2.08	0.52
2:D:516:THR:CG2	2:D:622:MET:SD	2.96	0.52
1:B:216:GLY:O	1:B:217:ALA:CB	2.58	0.52
1:B:285:ALA:HB3	1:B:301:GLU:O	2.09	0.52
1:A:20:TYR:CD1	2:C:513:HIS:HB2	2.45	0.52
1:A:329:MET:HE3	1:A:345:ILE:HD11	1.91	0.52
1:A:229:TYR:CD1	1:A:342:ILE:HD13	2.45	0.52
1:A:146:ASP:CG	1:A:148:THR:HG22	2.30	0.52
1:A:139:VAL:HG13	1:A:154:VAL:HG13	1.92	0.52
1:B:219:ILE:CG2	1:B:236:VAL:HG21	2.34	0.52
1:B:351:ALA:O	1:B:354:ARG:HB3	2.09	0.52
1:B:476:THR:HB	1:B:477:PRO:CD	2.38	0.52
1:B:107:SER:OG	1:B:109:ASP:HB2	2.08	0.52
1:B:209:PRO:HB2	1:B:482:LEU:CD1	2.40	0.52
1:B:240:SER:OG	1:B:321:LEU:HD22	2.10	0.52
1:A:44:ILE:HD12	1:A:88:MET:HE2	1.90	0.52
1:B:141:PHE:CE2	1:B:152:PRO:HD3	2.45	0.52
1:B:40:VAL:HG13	1:B:41:GLN:N	2.26	0.51
1:A:201:ILE:O	1:A:205:MET:HG3	2.09	0.51
1:A:40:VAL:CG1	1:A:41:GLN:N	2.73	0.51
2:D:431:LEU:CD1	2:D:479:MET:CE	2.89	0.51
1:B:273:ASP:CA	1:B:287:VAL:HG21	2.40	0.51
1:B:272:ILE:O	1:B:275:VAL:N	2.44	0.51
1:B:190:ALA:O	1:B:194:ILE:HG13	2.10	0.51
1:B:28:ARG:NH1	9:B:606:HOH:O	2.42	0.51
1:B:95:ARG:CD	1:B:95:ARG:O	2.58	0.51
1:A:91:ASN:ND2	1:A:91:ASN:H	2.01	0.51
1:B:96:GLU:OE2	1:B:96:GLU:HA	2.10	0.51
1:B:132:GLN:O	1:B:133:ASP:HB2	2.11	0.51
1:A:213:PHE:CE2	1:A:219:ILE:HD11	2.46	0.51
1:A:164:VAL:HG21	1:A:183:LEU:HD23	1.93	0.51
1:A:132:GLN:O	1:A:133:ASP:HB2	2.10	0.51
1:B:293:ARG:NH2	2:C:592:TRP:CE2	2.80	0.50
1:B:236:VAL:CG1	1:B:327:PHE:HE2	2.24	0.50
1:A:146:ASP:OD2	1:A:148:THR:CG2	2.56	0.50
2:D:446:ASP:O	2:D:448:LYS:N	2.44	0.50
1:B:455:ASP:OD2	1:B:458:THR:HB	2.12	0.50
2:D:453:LEU:HD22	2:D:454:PRO:N	2.26	0.50
1:A:371:ARG:HG3	1:A:371:ARG:O	2.12	0.50
1:A:236:VAL:CG1	1:A:237:VAL:N	2.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:597:ASN:O	2:C:601:ARG:HG2	2.11	0.50
4:F:5:DA:H2'	4:F:6:DT:H71	1.93	0.50
1:B:265:LYS:O	1:B:269:VAL:HG23	2.11	0.50
1:A:23:TYR:CG	2:C:509:THR:HG21	2.46	0.50
1:B:226:LYS:O	1:B:230:GLU:HB2	2.12	0.50
1:A:20:TYR:HA	2:C:509:THR:HG22	1.93	0.50
1:A:194:ILE:HD11	1:A:463:MET:CE	2.42	0.50
1:A:229:TYR:CD1	1:A:342:ILE:CD1	2.95	0.50
1:A:429:ASN:OD1	1:A:430:THR:N	2.44	0.50
1:A:423:GLN:NE2	1:A:425:TYR:HE1	2.10	0.50
1:A:391:LEU:HD23	1:A:391:LEU:C	2.33	0.49
2:D:527:ARG:N	2:D:528:PRO:HD2	2.26	0.49
1:B:187:ILE:O	1:B:191:VAL:HG23	2.12	0.49
2:C:542:LEU:HB3	2:C:543:TYR:CE2	2.47	0.49
1:A:371:ARG:HG2	1:A:442:LEU:HD11	1.95	0.49
1:B:425:TYR:CD2	1:B:425:TYR:C	2.86	0.49
1:A:134:ILE:HG23	1:A:135:GLU:N	2.26	0.49
2:C:479:MET:HE1	2:C:522:PHE:CZ	2.48	0.49
1:B:429:ASN:O	1:B:429:ASN:CG	2.50	0.49
1:A:23:TYR:CD1	2:C:509:THR:HG21	2.47	0.49
1:B:169:GLY:O	1:B:170:ILE:HG12	2.13	0.49
1:A:378:LEU:O	1:A:382:ILE:HG13	2.13	0.49
1:B:44:ILE:HD12	1:B:88:MET:CE	2.43	0.49
1:A:41:GLN:HA	1:A:88:MET:HE1	1.93	0.49
1:A:144:ASN:HD21	1:A:148:THR:CG2	2.24	0.49
1:A:8:SER:HB3	1:A:11:ASP:OD1	2.13	0.49
4:F:9:DA:O5'	4:F:9:DA:C2'	2.60	0.49
2:C:520:THR:CG2	2:C:622:MET:HG3	2.40	0.49
2:C:423:ASN:C	2:C:425:ALA:H	2.16	0.49
1:B:60:ARG:O	1:B:61:LYS:C	2.52	0.49
1:B:143:TRP:CE2	1:B:150:LYS:HE2	2.47	0.49
2:D:597:ASN:ND2	2:D:600:THR:CB	2.76	0.48
1:B:456:GLU:HG3	1:B:460:TYR:HE2	1.77	0.48
2:C:611:LEU:HD13	2:C:611:LEU:C	2.33	0.48
1:B:25:ILE:HG22	1:B:26:GLN:N	2.28	0.48
2:D:423:ASN:O	2:D:425:ALA:N	2.46	0.48
2:D:516:THR:HG22	2:D:517:LEU:N	2.27	0.48
1:B:131:LEU:O	1:B:134:ILE:HG22	2.13	0.48
2:D:429:LEU:HD22	2:D:430:TYR:N	2.28	0.48
1:A:169:GLY:O	1:A:170:ILE:CG1	2.61	0.48
1:A:192:TYR:OH	1:A:203:LYS:HE2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:104:ASN:HB3	1:B:114:ALA:HB2	1.96	0.48
1:A:316:PHE:CD2	1:A:321:LEU:HD13	2.48	0.48
2:C:514:ILE:HA	2:C:517:LEU:HD12	1.94	0.48
1:A:169:GLY:HA3	1:A:176:THR:O	2.12	0.48
2:C:479:MET:CE	2:C:522:PHE:CZ	2.97	0.48
1:B:38:LYS:H	1:B:41:GLN:HE21	1.58	0.48
1:B:243:GLU:C	1:B:244:ILE:HD13	2.32	0.48
1:B:95:ARG:CA	1:B:214:PRO:HG3	2.40	0.48
2:C:626:VAL:HG11	4:F:10:DT:OP2	2.14	0.48
3:E:9:DC:H2''	3:E:10:DA:C5'	2.43	0.48
1:B:283:GLY:CA	1:B:303:LYS:HD2	2.44	0.48
4:F:2:DG:C8	4:F:3:DT:H72	2.49	0.48
1:A:45:LEU:CD2	1:A:123:LEU:HD22	2.43	0.48
1:B:359:ALA:HA	1:B:362:ARG:NH1	2.29	0.48
1:B:452:ILE:HA	1:B:458:THR:HG22	1.96	0.48
1:B:319:THR:OG1	1:B:321:LEU:HB2	2.14	0.48
1:B:194:ILE:HG13	1:B:350:ILE:CD1	2.43	0.48
2:C:540:PRO:HA	2:C:595:THR:CG2	2.44	0.48
1:B:380:ARG:NH2	1:B:409:TYR:O	2.32	0.47
1:B:385:LEU:HD22	1:B:389:ILE:HD12	1.96	0.47
1:A:144:ASN:C	1:A:146:ASP:N	2.67	0.47
2:C:479:MET:CE	2:C:522:PHE:HZ	2.28	0.47
1:A:254:ILE:HD13	1:A:312:LEU:HD12	1.96	0.47
1:A:334:ASN:O	1:A:335:PHE:HB2	2.14	0.47
1:A:452:ILE:HA	1:A:458:THR:HG22	1.95	0.47
1:B:326:ASN:N	1:B:326:ASN:HD22	2.10	0.47
1:A:259:ILE:HB	1:A:260:PRO:HD3	1.94	0.47
1:A:87:ARG:C	1:A:89:SER:H	2.17	0.47
2:C:542:LEU:CB	2:C:543:TYR:CD2	2.96	0.47
2:D:473:ASN:OD1	2:D:476:ILE:HG12	2.14	0.47
1:A:48:MET:HE3	1:A:48:MET:HB3	1.60	0.47
1:B:43:ARG:NH1	1:B:74:HIS:ND1	2.62	0.47
2:D:466:LYS:C	2:D:468:ALA:N	2.68	0.47
2:C:610:ASP:O	2:C:612:ALA:N	2.48	0.47
1:B:34:ARG:HD2	1:B:352:HIS:ND1	2.30	0.47
1:A:337:PRO:HD3	2:C:639:PHE:CE1	2.51	0.46
1:A:350:ILE:HG12	1:A:463:MET:CE	2.45	0.46
1:A:219:ILE:CG2	1:A:236:VAL:HG11	2.44	0.46
1:A:60:ARG:CG	1:A:60:ARG:NH1	2.72	0.46
1:B:288:ARG:NH1	1:B:290:GLU:OE2	2.48	0.46
1:B:159:PHE:HB3	1:B:470:VAL:HG11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:TYR:O	1:A:86:VAL:HG23	2.15	0.46
2:D:432:VAL:HG11	2:D:438:GLY:CA	2.44	0.46
1:A:41:GLN:HA	1:A:88:MET:CE	2.45	0.46
1:B:157:ALA:O	1:B:353:ARG:HD3	2.15	0.46
1:A:36:GLY:CA	1:A:162:LEU:HB2	2.46	0.46
1:A:260:PRO:O	1:A:263:ILE:HB	2.16	0.46
2:C:639:PHE:O	2:C:640:THR:CB	2.63	0.46
2:D:453:LEU:HD22	2:D:453:LEU:C	2.36	0.46
1:B:91:ASN:N	1:B:91:ASN:HD22	2.13	0.46
1:B:440:ALA:C	1:B:442:LEU:N	2.68	0.46
2:C:542:LEU:CB	2:C:543:TYR:CE2	2.98	0.46
1:B:49:ASN:HB2	1:B:131:LEU:CD1	2.46	0.46
1:B:285:ALA:HB3	1:B:301:GLU:HG2	1.97	0.46
1:A:382:ILE:HD12	1:A:432:VAL:HG22	1.98	0.46
1:B:53:ASN:ND2	1:B:60:ARG:HD2	2.31	0.46
1:B:372:LEU:HD22	1:B:376:GLU:HG3	1.98	0.46
1:A:343:VAL:HB	1:A:344:PRO:HD3	1.98	0.46
1:B:338:ARG:HB3	1:B:340:VAL:HG13	1.98	0.46
1:B:307:ASN:ND2	1:B:307:ASN:O	2.49	0.46
1:B:141:PHE:HE2	1:B:152:PRO:HD3	1.81	0.46
1:B:440:ALA:O	1:B:441:GLU:C	2.53	0.46
2:D:598:PRO:HA	2:D:601:ARG:HD3	1.98	0.46
2:D:497:ASN:HB3	2:D:498:TYR:CD2	2.51	0.46
1:A:190:ALA:HB2	1:A:346:LEU:HD22	1.98	0.45
1:A:381:VAL:O	1:A:385:LEU:N	2.49	0.45
1:A:280:LYS:HB3	1:A:280:LYS:HE3	1.60	0.45
1:A:100:GLU:O	1:A:121:ALA:HA	2.16	0.45
1:A:73:PHE:O	1:A:75:PRO:HD3	2.16	0.45
1:A:9:LEU:O	1:A:9:LEU:CD2	2.63	0.45
1:A:187:ILE:O	1:A:191:VAL:HG23	2.16	0.45
1:A:195:ASP:O	1:A:197:PRO:HD3	2.16	0.45
1:A:28:ARG:NH1	3:E:14:DA:H4'	2.31	0.45
1:B:201:ILE:O	1:B:205:MET:HG3	2.17	0.45
2:C:523:TYR:C	2:C:523:TYR:CD2	2.90	0.45
1:B:321:LEU:HD23	1:B:321:LEU:HA	1.75	0.45
1:B:388:VAL:O	1:B:392:ILE:HG13	2.17	0.45
1:B:110:GLY:HA3	1:B:264:ASN:ND2	2.26	0.45
2:C:637:VAL:HG12	2:C:639:PHE:CD2	2.52	0.45
1:B:126:ILE:HG13	1:B:474:PHE:CE1	2.52	0.45
1:A:45:LEU:HD23	1:A:123:LEU:CD2	2.46	0.45
2:C:491:PHE:CD1	2:C:528:PRO:CG	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:412:THR:HG23	1:B:415:GLN:CD	2.33	0.45
1:B:415:GLN:O	1:B:419:ILE:HG13	2.16	0.45
1:A:452:ILE:HA	1:A:458:THR:CG2	2.47	0.45
2:D:467:MET:HA	2:D:470:ILE:HD12	1.99	0.45
2:C:491:PHE:HD1	2:C:528:PRO:CG	2.30	0.45
1:A:24:ILE:HD12	1:A:28:ARG:NE	2.32	0.45
1:B:242:THR:HG21	1:B:312:LEU:HD11	1.99	0.45
1:A:272:ILE:O	1:A:275:VAL:HB	2.17	0.45
1:B:239:ARG:NH1	1:B:316:PHE:CE1	2.84	0.45
6:H:6:DT:H2"	6:H:7:DG:H5'	1.98	0.45
1:A:139:VAL:HG21	1:A:154:VAL:O	2.17	0.45
2:C:597:ASN:C	2:C:599:GLU:H	2.20	0.44
1:A:403:GLU:O	1:A:407:VAL:HG23	2.18	0.44
2:D:431:LEU:HD22	2:D:479:MET:CE	2.46	0.44
1:A:259:ILE:CB	1:A:260:PRO:CD	2.89	0.44
1:A:425:TYR:C	1:A:425:TYR:CD2	2.90	0.44
2:D:497:ASN:HB3	2:D:498:TYR:CE2	2.52	0.44
1:B:371:ARG:O	1:B:375:VAL:HG23	2.17	0.44
1:B:167:SER:O	1:B:168:THR:HG22	2.17	0.44
2:C:417:THR:HA	2:C:418:PRO:HD3	1.70	0.44
1:A:216:GLY:O	1:A:217:ALA:CB	2.65	0.44
1:B:90:GLN:NE2	1:B:92:TRP:CZ2	2.86	0.44
2:D:525:TYR:O	2:D:526:MET:CG	2.62	0.44
1:B:217:ALA:N	1:B:258:GLU:OE1	2.44	0.44
1:B:307:ASN:CG	1:B:307:ASN:O	2.56	0.44
1:B:135:GLU:HG2	1:B:136:LYS:N	2.33	0.44
2:D:477:ASN:C	2:D:479:MET:H	2.21	0.44
2:C:429:LEU:HD11	2:C:431:LEU:HD21	1.98	0.44
1:A:352:HIS:O	1:A:353:ARG:C	2.56	0.44
5:G:9:DC:H2"	5:G:10:DG:C8	2.52	0.44
1:B:462:LEU:O	1:B:464:LYS:N	2.51	0.43
1:B:478:ARG:O	1:B:479:LEU:HD23	2.17	0.43
1:A:389:ILE:CD1	1:A:427:LEU:HD13	2.48	0.43
2:D:453:LEU:HD22	2:D:454:PRO:CD	2.48	0.43
1:A:87:ARG:O	1:A:89:SER:N	2.51	0.43
1:A:276:ARG:HD3	1:A:287:VAL:HG23	1.99	0.43
2:D:523:TYR:C	2:D:523:TYR:CD2	2.91	0.43
1:B:462:LEU:O	1:B:463:MET:C	2.56	0.43
2:D:432:VAL:HG11	2:D:438:GLY:N	2.34	0.43
1:B:288:ARG:HG2	2:C:420:GLN:NE2	2.33	0.43
1:B:346:LEU:O	1:B:350:ILE:CG1	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:GLY:HA2	1:B:176:THR:HG22	2.00	0.43
2:D:466:LYS:O	2:D:468:ALA:N	2.51	0.43
1:B:162:LEU:O	1:B:162:LEU:HD22	2.18	0.43
1:B:375:VAL:HG13	1:B:435:LEU:HD22	2.00	0.43
1:A:412:THR:O	1:A:413:GLU:C	2.55	0.43
1:A:213:PHE:CE2	1:A:219:ILE:CD1	3.01	0.43
1:B:311:VAL:O	1:B:315:LEU:HG	2.18	0.43
1:A:321:LEU:O	1:A:321:LEU:HD22	2.19	0.43
1:A:20:TYR:CZ	1:A:24:ILE:HG13	2.53	0.43
2:D:491:PHE:HD1	2:D:528:PRO:HG2	1.84	0.43
1:B:201:ILE:HD12	1:B:201:ILE:H	1.84	0.43
1:B:385:LEU:HD21	1:B:427:LEU:CD2	2.43	0.43
1:A:144:ASN:OD1	1:A:147:ASP:N	2.52	0.43
1:A:342:ILE:HA	1:A:342:ILE:HD12	1.72	0.43
1:B:342:ILE:HD12	1:B:342:ILE:HA	1.89	0.43
1:B:28:ARG:CG	1:B:28:ARG:HH11	2.31	0.43
1:B:357:ILE:HD12	1:B:463:MET:CG	2.47	0.43
1:A:420:VAL:O	1:A:420:VAL:HG13	2.18	0.43
1:B:236:VAL:HG12	1:B:327:PHE:HE2	1.84	0.43
1:B:375:VAL:O	1:B:379:ILE:HD12	2.19	0.43
1:B:285:ALA:CB	1:B:301:GLU:HG2	2.48	0.43
2:D:466:LYS:O	2:D:470:ILE:HG13	2.19	0.43
2:C:558:ALA:C	2:C:559:TRP:CE3	2.92	0.43
1:B:146:ASP:O	1:B:147:ASP:HB2	2.18	0.43
1:A:244:ILE:N	1:A:244:ILE:CD1	2.79	0.43
1:B:440:ALA:O	1:B:442:LEU:N	2.52	0.43
1:A:187:ILE:O	1:A:188:ASP:C	2.57	0.43
1:B:254:ILE:HB	1:B:300:ILE:HB	2.01	0.42
1:B:442:LEU:O	1:B:446:ILE:HG13	2.18	0.42
1:A:276:ARG:HH11	1:A:276:ARG:HG2	1.84	0.42
2:C:439:GLY:C	2:C:441:ALA:N	2.72	0.42
2:C:536:TYR:C	2:C:537:ILE:HG13	2.39	0.42
2:D:597:ASN:O	2:D:601:ARG:HB3	2.19	0.42
1:A:464:LYS:HB2	1:A:464:LYS:HE2	1.87	0.42
1:B:412:THR:O	1:B:413:GLU:C	2.57	0.42
1:B:167:SER:O	1:B:168:THR:CB	2.67	0.42
1:A:385:LEU:HD23	1:A:385:LEU:HA	1.78	0.42
1:A:185:GLU:OE1	1:A:209:PRO:HD2	2.20	0.42
1:B:41:GLN:CA	1:B:88:MET:CE	2.91	0.42
1:B:476:THR:CB	1:B:477:PRO:CD	2.96	0.42
1:B:361:SER:O	1:B:365:LYS:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ASP:OD1	1:A:56:ASP:N	2.51	0.42
2:C:602:THR:C	2:C:603:LEU:HD23	2.40	0.42
1:A:163:LEU:HG	1:A:345:ILE:HG21	2.00	0.42
1:B:420:VAL:HG12	1:B:421:THR:HG23	2.00	0.42
6:H:3:DC:H4'	6:H:4:DT:OP1	2.19	0.42
1:B:204:LEU:HA	1:B:204:LEU:HD23	1.88	0.42
2:C:524:ARG:CB	2:C:525:TYR:HD1	2.31	0.42
1:A:87:ARG:HA	1:A:90:GLN:CG	2.50	0.42
1:A:471:LYS:O	1:A:475:ALA:HB2	2.20	0.42
1:B:333:ASP:O	1:B:334:ASN:C	2.58	0.42
1:A:240:SER:HB2	1:A:321:LEU:HD22	2.02	0.42
2:D:466:LYS:C	2:D:468:ALA:H	2.23	0.42
1:A:207:PHE:O	1:A:209:PRO:HD3	2.19	0.42
1:B:220:GLN:HA	1:B:483:GLU:O	2.20	0.42
1:B:112:PRO:HA	1:B:113:PRO:HD3	1.84	0.42
1:B:334:ASN:O	1:B:335:PHE:HB2	2.19	0.42
2:C:633:ILE:O	2:C:637:VAL:HB	2.20	0.42
1:A:355:GLU:OE2	1:A:355:GLU:CA	2.67	0.42
1:A:44:ILE:HB	1:A:88:MET:HE1	2.01	0.41
1:B:228:ALA:C	1:B:230:GLU:H	2.23	0.41
1:A:403:GLU:HA	1:A:406:LYS:HD2	2.01	0.41
1:A:326:ASN:OD1	4:F:11:DG:H5"	2.20	0.41
2:C:630:ARG:HG2	2:C:634:GLU:OE2	2.20	0.41
1:A:90:GLN:HE21	1:A:90:GLN:HB3	1.66	0.41
1:A:435:LEU:HA	1:A:435:LEU:HD23	1.64	0.41
1:B:353:ARG:HD2	1:B:353:ARG:HA	1.79	0.41
1:B:434:VAL:CG1	1:B:435:LEU:N	2.83	0.41
1:A:95:ARG:HA	1:A:214:PRO:HB3	2.03	0.41
1:A:29:ALA:HB3	1:A:171:SER:HB3	2.02	0.41
2:D:423:ASN:CG	2:D:423:ASN:O	2.56	0.41
2:C:590:GLN:O	2:C:594:THR:HG23	2.20	0.41
1:B:28:ARG:NH2	2:D:510:ASP:OD2	2.54	0.41
1:A:391:LEU:C	1:A:391:LEU:CD2	2.89	0.41
1:B:9:LEU:CD1	2:D:523:TYR:HD1	2.34	0.41
1:A:24:ILE:HA	1:A:28:ARG:HB2	2.02	0.41
2:C:503:ILE:CG2	2:C:518:LEU:HD12	2.51	0.41
2:D:424:PRO:HA	2:D:497:ASN:O	2.21	0.41
1:B:190:ALA:HB2	1:B:346:LEU:CD2	2.51	0.41
1:B:139:VAL:CG1	1:B:140:PRO:HD2	2.45	0.41
2:C:422:LYS:O	2:C:424:PRO:HD3	2.20	0.41
1:B:37:LEU:HA	1:B:37:LEU:HD23	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:ARG:O	1:B:357:ILE:HG13	2.20	0.41
1:B:168:THR:HA	1:B:169:GLY:HA3	1.74	0.41
1:B:268:LEU:O	1:B:272:ILE:HG13	2.21	0.41
2:C:429:LEU:CD1	2:C:431:LEU:HD21	2.51	0.41
1:B:325:TYR:CD1	1:B:325:TYR:C	2.94	0.41
1:B:424:LEU:HA	1:B:424:LEU:HD23	1.93	0.41
1:A:35:ASP:OD1	1:A:35:ASP:C	2.59	0.41
1:A:96:GLU:OE2	1:A:96:GLU:HA	2.20	0.41
1:B:455:ASP:OD2	1:B:458:THR:CB	2.69	0.41
1:A:168:THR:HA	1:A:169:GLY:HA3	1.77	0.40
1:A:194:ILE:HG12	1:A:463:MET:HE2	2.03	0.40
1:A:159:PHE:HB3	1:A:470:VAL:HG11	2.03	0.40
2:D:423:ASN:C	2:D:425:ALA:H	2.24	0.40
4:F:1:DA:C2	4:F:2:DG:C6	3.09	0.40
1:B:201:ILE:HD12	1:B:201:ILE:N	2.35	0.40
1:B:320:ASP:C	1:B:322:GLN:N	2.74	0.40
1:A:260:PRO:HG2	1:A:320:ASP:O	2.22	0.40
1:B:259:ILE:CB	1:B:260:PRO:CD	2.92	0.40
2:C:417:THR:HG22	2:C:417:THR:O	2.20	0.40
2:C:432:VAL:HA	2:C:504:MET:O	2.21	0.40
1:A:387:GLU:HA	1:A:390:ALA:HB3	2.03	0.40
1:A:337:PRO:HD3	2:C:639:PHE:HE1	1.86	0.40
4:F:3:DT:H4'	4:F:4:DC:OP1	2.22	0.40
1:A:49:ASN:HB2	1:A:131:LEU:HD13	2.02	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
1	A	480/496 (97%)	432 (90%)	40 (8%)	8 (2%)	11 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	480/496 (97%)	414 (86%)	57 (12%)	9 (2%)	10	46
2	C	203/268 (76%)	175 (86%)	23 (11%)	5 (2%)	7	40
2	D	202/268 (75%)	176 (87%)	22 (11%)	4 (2%)	9	45
All	All	1365/1528 (89%)	1197 (88%)	142 (10%)	26 (2%)	10	46

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	145	PHE
1	B	168	THR
1	B	217	ALA
2	D	569	LYS
2	D	610	ASP
1	A	169	GLY
1	A	217	ALA
1	A	305	ASP
2	C	611	LEU
2	D	424	PRO
2	D	447	ARG
1	A	88	MET
1	B	382	ILE
1	B	463	MET
2	C	436	SER
1	A	168	THR
1	B	334	ASN
1	B	427	LEU
2	C	424	PRO
1	A	170	ILE
1	B	441	GLU
2	C	490	ASP
1	B	169	GLY
2	C	598	PRO
1	A	221	GLY
1	B	221	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	
1	A	371/431 (86%)	332 (90%)	39 (10%)	8	33
1	B	372/431 (86%)	321 (86%)	51 (14%)	4	20
2	C	104/224 (46%)	91 (88%)	13 (12%)	6	24
2	D	102/224 (46%)	91 (89%)	11 (11%)	8	32
All	All	949/1310 (72%)	835 (88%)	114 (12%)	6	26

All (114) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	28	ARG
1	A	60	ARG
1	A	70	MET
1	A	90	GLN
1	A	91	ASN
1	A	96	GLU
1	A	97	ILE
1	A	102	HIS
1	A	111	ASP
1	A	117	ARG
1	A	134	ILE
1	A	146	ASP
1	A	154	VAL
1	A	168	THR
1	A	208	LEU
1	A	242	THR
1	A	268	LEU
1	A	279	ASN
1	A	293	ARG
1	A	297	ARG
1	A	321	LEU
1	A	322	GLN
1	A	334	ASN
1	A	336	THR
1	A	338	ARG
1	A	342	ILE
1	A	355	GLU
1	A	366	GLU
1	A	371	ARG

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Mol	Chain	Res	Type
1	A	380	ARG
1	A	385	LEU
1	A	387	GLU
1	A	412	THR
1	A	414	GLU
1	A	420	VAL
1	A	434	VAL
1	A	443	ARG
1	A	462	LEU
1	B	4	ILE
1	B	24	ILE
1	B	26	GLN
1	B	28	ARG
1	B	58	SER
1	B	70	MET
1	B	79	SER
1	B	81	ILE
1	B	90	GLN
1	B	91	ASN
1	B	95	ARG
1	B	96	GLU
1	B	98	LEU
1	B	102	HIS
1	B	120	GLU
1	B	126	ILE
1	B	139	VAL
1	B	146	ASP
1	B	162	LEU
1	B	167	SER
1	B	168	THR
1	B	177	ASP
1	B	198	THR
1	B	202	ASP
1	B	208	LEU
1	B	236	VAL
1	B	238	VAL
1	B	268	LEU
1	B	281	VAL
1	B	294	ASP
1	B	307	ASN
1	B	310	LEU
1	B	321	LEU

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Mol	Chain	Res	Type
1	B	326	ASN
1	B	336	THR
1	B	338	ARG
1	B	347	SER
1	B	350	ILE
1	B	372	LEU
1	B	374	ILE
1	B	385	LEU
1	B	404	ASN
1	B	410	ASP
1	B	412	THR
1	B	414	GLU
1	B	420	VAL
1	B	429	ASN
1	B	431	ASP
1	B	432	VAL
1	B	456	GLU
1	B	463	MET
2	C	416	LEU
2	C	417	THR
2	C	440	SER
2	C	445	ARG
2	C	453	LEU
2	C	462	THR
2	C	477	ASN
2	C	478	THR
2	C	509	THR
2	C	514	ILE
2	C	523	TYR
2	C	524	ARG
2	C	595	THR
2	D	429	LEU
2	D	445	ARG
2	D	453	LEU
2	D	462	THR
2	D	478	THR
2	D	482	THR
2	D	497	ASN
2	D	501	ILE
2	D	524	ARG
2	D	591	LEU
2	D	595	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	53	ASN
1	A	68	ASN
1	A	90	GLN
1	A	91	ASN
1	A	253	GLN
1	A	267	ASN
1	A	328	ASN
1	A	334	ASN
1	A	423	GLN
1	B	41	GLN
1	B	53	ASN
1	B	68	ASN
1	B	76	HIS
1	B	91	ASN
1	B	253	GLN
1	B	264	ASN
1	B	267	ASN
1	B	307	ASN
1	B	313	ASN
1	B	326	ASN
1	B	328	ASN
1	B	415	GLN
1	B	423	GLN
2	C	420	GLN
2	C	423	ASN
2	C	461	ASN
2	C	477	ASN
2	C	597	ASN
2	D	497	ASN
2	D	597	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](#)

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
8	NFX	F	101	7	21,28,28	2.07	4 (19%)	22,43,43	1.63	5 (22%)
8	NFX	H	101	7	21,28,28	2.09	4 (19%)	22,43,43	1.63	5 (22%)

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
8	NFX	F	101	7	-	0/4/23/23	0/3/4/4
8	NFX	H	101	7	-	0/4/23/23	0/3/4/4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	101	NFX	C16-C18	-2.72	1.33	1.38
8	H	101	NFX	C16-C18	-2.70	1.33	1.38
8	F	101	NFX	C11-C13	2.68	1.43	1.40
8	H	101	NFX	C11-C13	2.69	1.43	1.40
8	F	101	NFX	C17-C15	4.17	1.39	1.35
8	H	101	NFX	C17-C15	4.26	1.39	1.35
8	F	101	NFX	C19-C14	6.79	1.50	1.41
8	H	101	NFX	C19-C14	6.85	1.50	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
8	F	101	NFX	C16-N-C06	-4.03	114.67	119.25
8	H	101	NFX	C16-N-C06	-4.03	114.67	119.25
8	H	101	NFX	C18-C19-C14	-2.65	117.37	121.87
8	F	101	NFX	C18-C19-C14	-2.65	117.37	121.87
8	H	101	NFX	C13-C11-C15	-2.15	114.59	117.61
8	F	101	NFX	F-C15-C17	-2.13	116.90	119.74
8	F	101	NFX	C13-C11-C15	-2.13	114.63	117.61
8	H	101	NFX	F-C15-C17	-2.11	116.92	119.74
8	H	101	NFX	C06-N-C12	2.88	124.53	120.94
8	F	101	NFX	C06-N-C12	2.89	124.54	120.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	101	NFX	4	0
8	H	101	NFX	4	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	A	482/496 (97%)	-0.40	0 100 100	55, 80, 119, 141	0
1	B	482/496 (97%)	-0.40	0 100 100	50, 79, 114, 146	0
2	C	209/268 (77%)	-0.61	2 (0%) 84 85	88, 119, 153, 173	0
2	D	208/268 (77%)	-0.53	0 100 100	82, 119, 155, 174	0
3	E	7/7 (100%)	-0.46	0 100 100	86, 91, 128, 158	0
4	F	11/11 (100%)	-0.61	0 100 100	98, 113, 140, 158	0
5	G	7/7 (100%)	-0.37	0 100 100	77, 87, 126, 149	0
6	H	11/11 (100%)	-0.65	0 100 100	90, 104, 130, 145	0
All	All	1417/1564 (90%)	-0.45	2 (0%) 95 97	50, 90, 140, 174	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	488	GLY	2.1
2	C	522	PHE	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
7	MG	A	502	1/1	0.96	0.22	3.13	121,121,121,121	0
8	NFX	H	101	25/25	0.96	0.20	2.89	118,143,190,200	0
8	NFX	F	101	25/25	0.93	0.21	1.58	120,135,161,235	0
7	MG	A	501	1/1	0.88	0.17	-0.75	87,87,87,87	0
7	MG	B	501	1/1	0.80	0.12	-1.73	101,101,101,101	0
7	MG	B	502	1/1	0.96	0.13	-	119,119,119,119	0
7	MG	D	701	1/1	0.90	0.20	-	78,78,78,78	0
7	MG	C	701	1/1	0.93	0.14	-	87,87,87,87	0

6.5 Other polymers [i](#)

There are no such residues in this entry.