Full wwPDB X-ray Structure Validation Report ⓘ

Oct 27, 2023 – 12:49 AM EDT

PDB ID	:	3K9F
Title	:	Detailed structural insight into the quinolone-DNA cleavage complex of type IIA topoisomerases
Authors	:	Laponogov, I.; Pan, X.-S.; Veselkov, D.A.; Fisher, L.M.; Sanderson, M.R.
Deposited on	:	2009-10-15
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*
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:

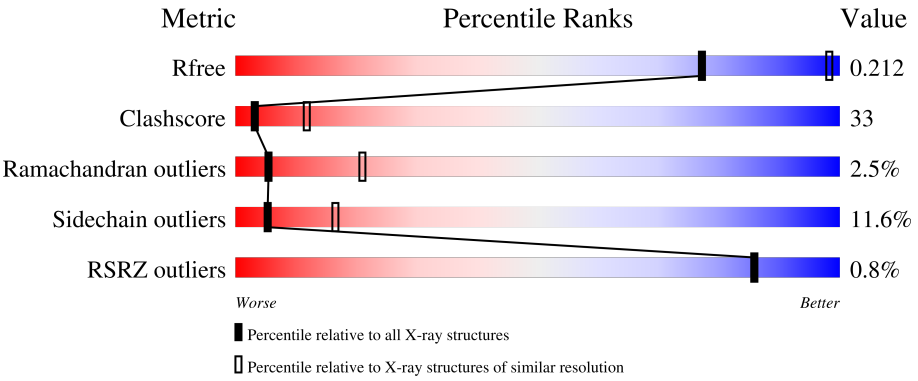
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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))
R_{free}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 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 <=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	57% 33% 6%
1	B	496	59% 32% 5%
2	C	268	43% 32% 7% 17%
2	D	268	42% 32% 8% 17%
3	E	15	20% 27% 53%

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Mol	Chain	Length	Quality of chain
4	F	19	11% 42% 5% 42%
5	G	15	27% 20% 53%
6	H	19	16% 37% 5% 42%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 11559 atoms, of which 40 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	481	Total	C	N	O	S	0	0	0
			3691	2340	643	693	15			
1	B	481	Total	C	N	O	S	0	0	0
			3678	2332	642	689	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
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	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	222	Total	C	N	O	S	0	0	0
			1676	1062	292	314	8			
2	D	222	Total	C	N	O	S	0	0	0
			1676	1062	292	314	8			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	380	MET	-	initiating methionine	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
D	380	MET	-	initiating methionine	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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

- Molecule 3 is a DNA chain called DNA (5'-D(*AP*CP*CP*AP*AP*GP*GP*T*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 DNA (5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*GP*AP*CP*CP*TP*TP*GP*GP*T)-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 DNA (5'-D(*CP*TP*GP*TP*TP*TP*TP*A*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 DNA (5'-D(P*GP*AP*CP*TP*AP*TP*GP*CP*AP*CP*GP*TP*AP*AP*AP*AP*CP*AP*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	C	1	Total	Mg	0	0
			1	1		

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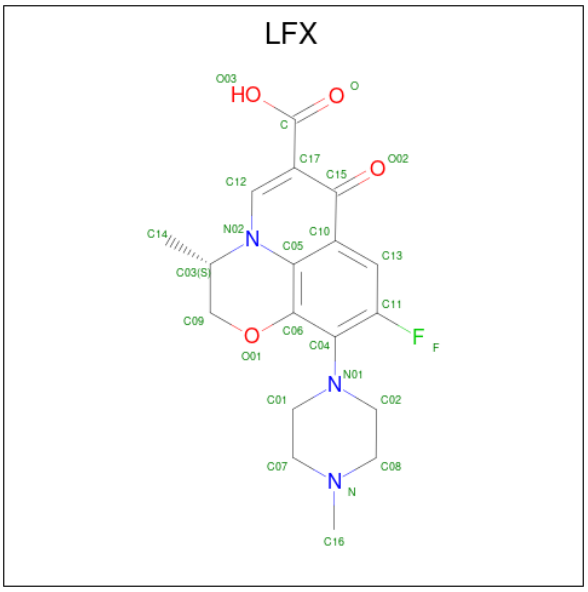
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	D	1	Total Mg 1 1	0	0

- Molecule 8 is (3S)-9-fluoro-3-methyl-10-(4-methylpiperazin-1-yl)-7-oxo-2,3-dihydro-7H-[1,4]oxazino[2,3,4-ij]quinoline-6-carboxylic acid (three-letter code: LFX) (formula: $C_{18}H_{20}FN_3O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	F	1	Total C F H N O 46 18 1 20 3 4	0	0
8	H	1	Total C F H N O 46 18 1 20 3 4	0	0

- Molecule 9 is water.

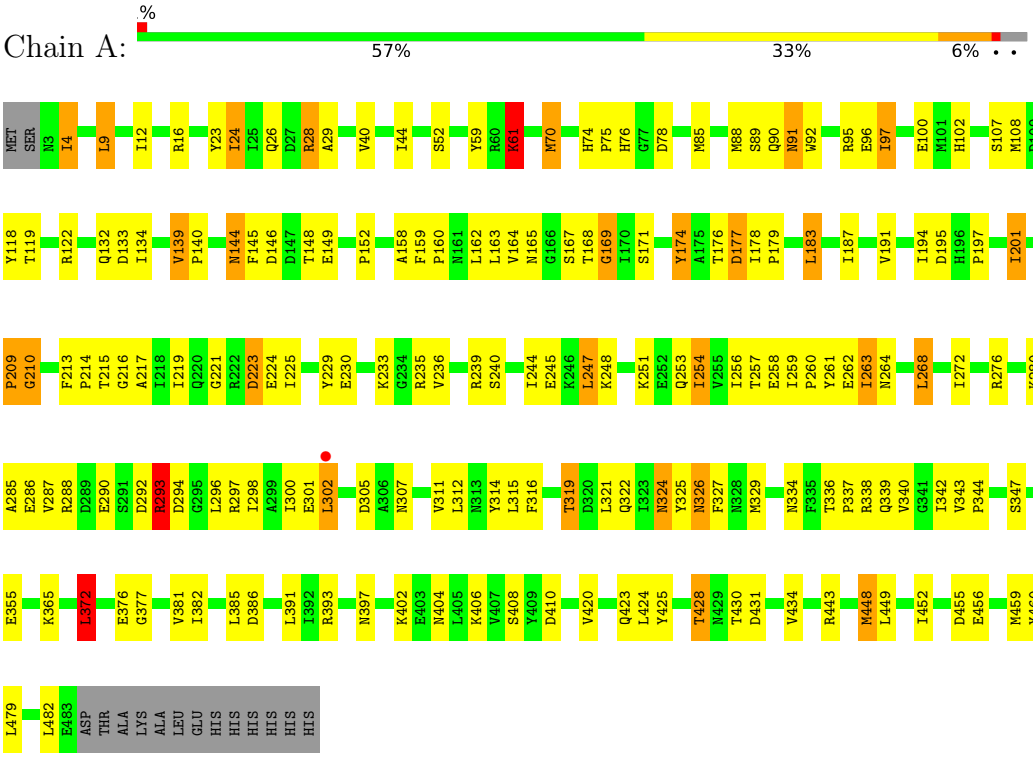
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	7	Total O 7 7	0	0
9	B	6	Total O 6 6	0	0
9	D	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

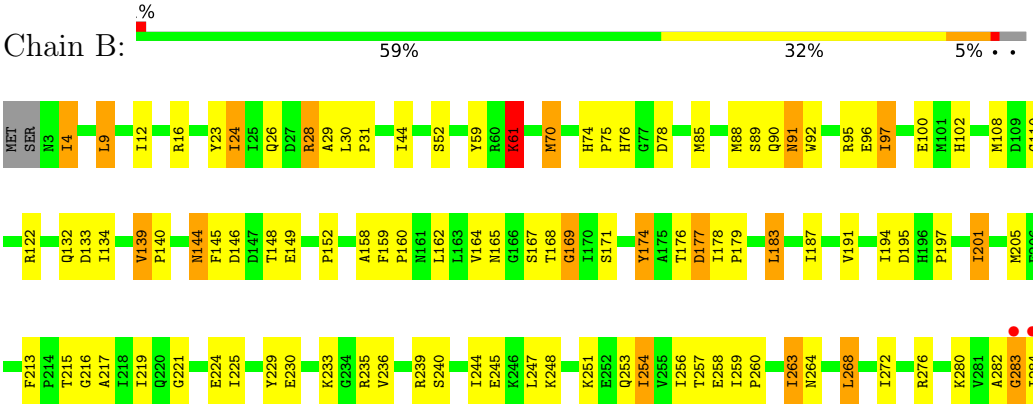
• Molecule 1: DNA topoisomerase 4 subunit A

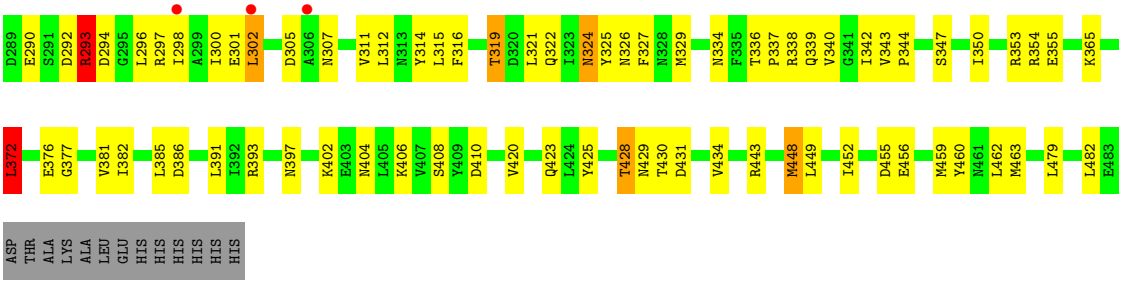
Chain A:



• Molecule 1: DNA topoisomerase 4 subunit A

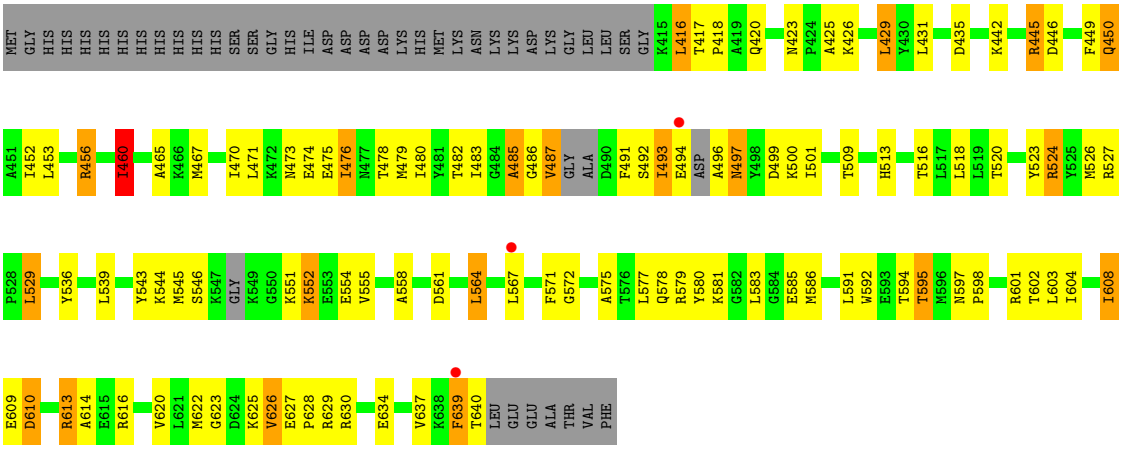
Chain B:





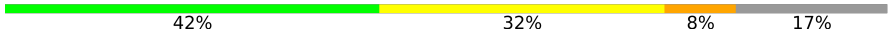
• Molecule 2: DNA topoisomerase 4 subunit B

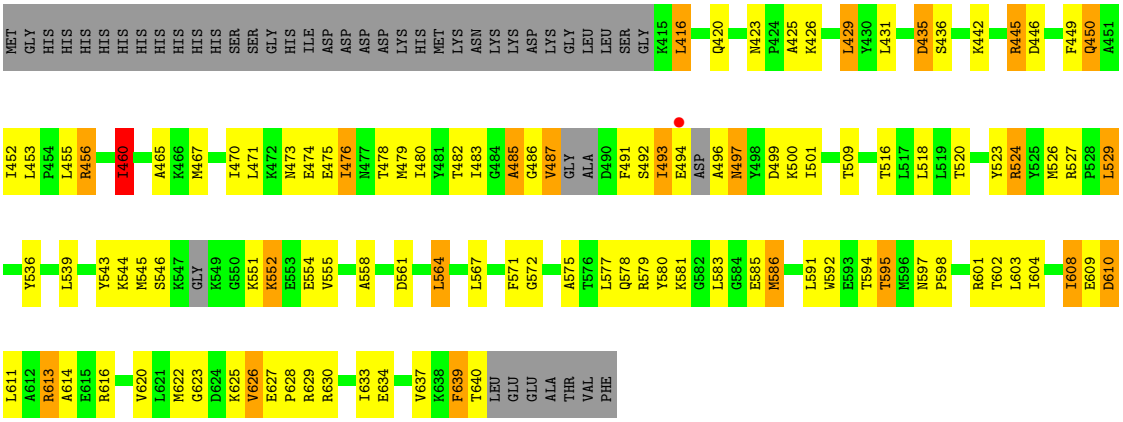
Chain C:



• Molecule 2: DNA topoisomerase 4 subunit B

Chain D:





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

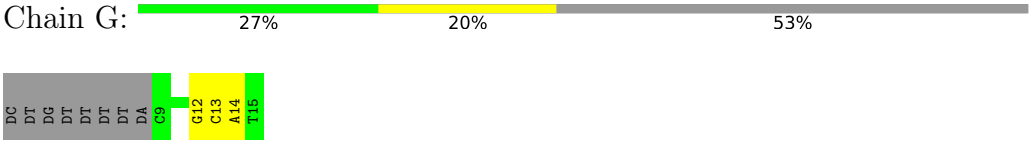
Chain E:

• Molecule 4: DNA (5'-D(P*AP*GP*TP*CP*AP*TP*TP*CP*AP*TP*GP*AP*CP*CP*TP*TP*GP*GP*T)-3')

Chain F:

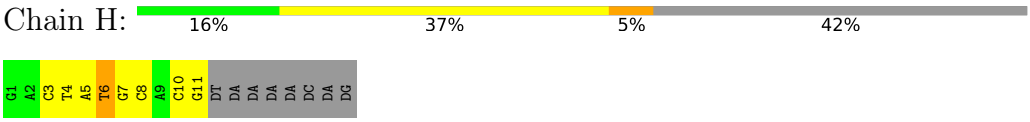
• Molecule 5: DNA (5'-D(*CP*TP*GP*TP*TP*TP*TP*A*CP*GP*TP*GP*CP*AP*T)-3')

Chain G:



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

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	122.41Å 122.41Å 178.29Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	26.73 – 2.90 30.60 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (26.73-2.90) 97.6 (30.60-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.90Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.183 , 0.218 0.178 , 0.212	Depositor DCC
R_{free} test set	6484 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å^2)	80.8	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 60.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.477 for -h,-k,l 0.033 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11559	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, LFX

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	0.50	0/3752	0.70	2/5085 (0.0%)
1	B	0.50	0/3739	0.70	2/5069 (0.0%)
2	C	0.49	0/1702	0.72	1/2307 (0.0%)
2	D	0.48	0/1702	0.72	1/2307 (0.0%)
3	E	0.45	0/157	1.01	0/241
4	F	0.48	0/251	1.16	1/385 (0.3%)
5	G	0.46	0/155	1.05	0/238
6	H	0.46	0/253	1.07	1/388 (0.3%)
All	All	0.49	0/11711	0.74	8/16020 (0.0%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	460	ILE	CB-CA-C	-5.94	99.71	111.60
2	D	460	ILE	CB-CA-C	-5.92	99.75	111.60
1	A	9	LEU	CA-CB-CG	5.17	127.18	115.30
1	B	9	LEU	CA-CB-CG	5.16	127.17	115.30
6	H	6	DT	N3-C4-O4	5.16	122.99	119.90
1	A	372	LEU	CA-CB-CG	5.12	127.09	115.30
1	B	372	LEU	CA-CB-CG	5.12	127.08	115.30
4	F	1	DA	C1'-O4'-C4'	-5.03	105.07	110.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3691	0	3630	215	0
1	B	3678	0	3606	199	0
2	C	1676	0	1617	171	0
2	D	1676	0	1617	178	0
3	E	140	0	78	5	0
4	F	225	0	126	14	0
5	G	139	0	78	3	0
6	H	226	0	124	9	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	F	26	20	19	5	0
8	H	26	20	19	5	0
9	A	7	0	0	2	0
9	B	6	0	0	1	0
9	D	1	0	0	0	0
All	All	11519	40	10914	748	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 33.

All (748) 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)
2:C:492:SER:O	2:C:493:ILE:HG13	1.42	1.19
2:D:492:SER:O	2:D:493:ILE:HG13	1.42	1.17
2:D:520:THR:HG21	2:D:622:MET:HG3	1.18	1.15
2:C:431:LEU:HD13	2:C:479:MET:HE1	1.27	1.14
1:B:146:ASP:HB3	1:B:148:THR:HG23	1.28	1.11
2:C:520:THR:HG21	2:C:622:MET:HG3	1.18	1.10
1:B:28:ARG:HG3	1:B:28:ARG:HH11	1.17	1.09
1:A:285:ALA:HB3	1:A:301:GLU:O	1.53	1.09
1:A:146:ASP:HB3	1:A:148:THR:HG23	1.28	1.08
2:C:613:ARG:HG3	2:C:613:ARG:HH11	0.92	1.08
2:D:613:ARG:HG3	2:D:613:ARG:HH11	0.92	1.07
1:B:285:ALA:HB3	1:B:301:GLU:O	1.53	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:493:ILE:HG22	2:D:494:GLU:H	1.18	1.06
2:D:431:LEU:HD13	2:D:479:MET:HE1	1.34	1.05
1:A:28:ARG:HG3	1:A:28:ARG:HH11	1.17	1.03
2:D:598:PRO:HA	2:D:601:ARG:HE	1.24	1.01
2:C:493:ILE:HG22	2:C:494:GLU:H	1.18	1.01
1:B:283:GLY:HA3	1:B:311:VAL:HG21	1.43	1.00
2:C:520:THR:CG2	2:C:622:MET:HG3	1.91	1.00
1:A:283:GLY:HA3	1:A:311:VAL:HG21	1.43	1.00
2:C:598:PRO:HA	2:C:601:ARG:HE	1.24	1.00
2:C:460:ILE:CD1	2:C:476:ILE:HG13	1.93	0.98
1:A:431:ASP:OD1	1:A:434:VAL:HG23	1.63	0.98
2:D:460:ILE:CD1	2:D:476:ILE:HG13	1.93	0.98
2:D:520:THR:CG2	2:D:622:MET:HG3	1.92	0.98
1:B:431:ASP:OD1	1:B:434:VAL:HG23	1.63	0.98
2:C:431:LEU:HD13	2:C:479:MET:CE	1.95	0.97
2:D:613:ARG:HG3	2:D:613:ARG:NH1	1.72	0.97
1:A:337:PRO:CD	2:C:639:PHE:HE1	1.77	0.96
1:B:337:PRO:CD	2:D:639:PHE:HE1	1.78	0.96
2:D:431:LEU:HD13	2:D:479:MET:CE	1.95	0.96
1:B:354:ARG:HG3	1:B:459:MET:CE	1.97	0.95
1:A:89:SER:O	1:A:97:ILE:HD11	1.67	0.94
2:C:467:MET:HE1	2:C:471:LEU:HD21	1.49	0.94
2:C:456:ARG:NH1	8:F:0:LFX:H08A	1.83	0.94
1:A:354:ARG:HG3	1:A:459:MET:CE	1.97	0.94
2:C:613:ARG:HH11	2:C:613:ARG:CG	1.81	0.93
1:B:169:GLY:HA2	1:B:176:THR:HG22	1.51	0.93
1:B:89:SER:O	1:B:97:ILE:HD11	1.68	0.92
2:D:613:ARG:HH11	2:D:613:ARG:CG	1.81	0.92
2:C:456:ARG:HH12	8:F:0:LFX:H08A	1.31	0.91
1:A:229:TYR:CG	1:A:342:ILE:HD12	2.06	0.91
1:A:169:GLY:HA2	1:A:176:THR:HG22	1.51	0.91
2:D:460:ILE:HD11	2:D:476:ILE:HG13	1.51	0.91
2:D:456:ARG:HH12	8:H:0:LFX:H08A	1.36	0.90
2:C:460:ILE:HD11	2:C:476:ILE:HG13	1.51	0.90
1:B:229:TYR:CG	1:B:342:ILE:HD12	2.06	0.90
1:B:337:PRO:HD3	2:D:639:PHE:HE1	1.35	0.89
1:A:89:SER:C	1:A:97:ILE:HD11	1.93	0.89
1:B:169:GLY:CA	1:B:176:THR:HG22	2.03	0.89
1:B:95:ARG:NH2	1:B:479:LEU:HD12	1.88	0.88
1:A:169:GLY:CA	1:A:176:THR:HG22	2.03	0.88
1:A:95:ARG:NH2	1:A:479:LEU:HD12	1.88	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:89:SER:C	1:B:97:ILE:HD11	1.93	0.88
2:D:480:ILE:HD13	2:D:487:VAL:HG11	1.55	0.88
2:C:480:ILE:HD13	2:C:487:VAL:HG11	1.55	0.88
1:A:144:ASN:HD21	1:A:148:THR:H	1.22	0.88
2:C:616:ARG:O	2:C:620:VAL:HG23	1.75	0.87
2:D:456:ARG:NH1	8:H:0:LFX:H08A	1.89	0.87
1:B:146:ASP:HB3	1:B:148:THR:CG2	2.05	0.87
1:B:337:PRO:HD3	2:D:639:PHE:CE1	2.09	0.87
2:C:613:ARG:HG3	2:C:613:ARG:NH1	1.72	0.87
2:D:543:TYR:CD2	2:D:564:LEU:HD23	2.10	0.87
2:D:467:MET:HE1	2:D:471:LEU:HD21	1.57	0.87
1:A:337:PRO:HD3	2:C:639:PHE:HE1	1.37	0.87
1:B:456:GLU:HG3	1:B:460:TYR:HE2	1.37	0.86
1:A:456:GLU:HG3	1:A:460:TYR:HE2	1.37	0.86
2:D:616:ARG:O	2:D:620:VAL:HG23	1.75	0.86
4:F:1:DA:H4'	4:F:2:DG:OP1	1.74	0.86
1:A:146:ASP:HB3	1:A:148:THR:CG2	2.05	0.86
2:D:486:GLY:C	2:D:487:VAL:HG12	1.96	0.86
1:A:276:ARG:HD2	1:A:285:ALA:O	1.76	0.85
2:C:543:TYR:CD2	2:C:564:LEU:HD23	2.10	0.85
1:A:337:PRO:HD3	2:C:639:PHE:CE1	2.11	0.85
2:D:467:MET:HE3	2:D:471:LEU:HD11	1.59	0.84
2:C:486:GLY:C	2:C:487:VAL:HG12	1.96	0.84
1:B:158:ALA:HA	1:B:353:ARG:NH1	1.91	0.84
1:A:158:ALA:HA	1:A:353:ARG:NH1	1.91	0.84
2:D:552:LYS:HG2	2:D:552:LYS:O	1.76	0.84
1:B:144:ASN:HD21	1:B:148:THR:H	1.22	0.84
1:B:276:ARG:HD2	1:B:285:ALA:O	1.76	0.84
1:B:456:GLU:HG3	1:B:460:TYR:CE2	2.12	0.84
1:A:244:ILE:HD12	1:A:244:ILE:O	1.79	0.83
2:D:478:THR:O	2:D:482:THR:HG23	1.79	0.83
1:A:456:GLU:HG3	1:A:460:TYR:CE2	2.12	0.83
2:C:552:LYS:O	2:C:552:LYS:HG2	1.76	0.83
2:C:478:THR:O	2:C:482:THR:HG23	1.79	0.83
1:B:168:THR:HG22	1:B:177:ASP:HA	1.62	0.82
1:B:268:LEU:HD11	1:B:321:LEU:HD23	1.60	0.82
1:B:337:PRO:CD	2:D:639:PHE:CE1	2.63	0.82
1:B:354:ARG:HG3	1:B:459:MET:HE2	1.61	0.82
1:B:28:ARG:HG3	1:B:28:ARG:NH1	1.93	0.81
1:B:244:ILE:HD12	1:B:244:ILE:O	1.79	0.81
1:A:168:THR:HG22	1:A:177:ASP:HA	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:501:ILE:HD12	2:C:529:LEU:CD1	2.10	0.81
2:D:524:ARG:CG	2:D:524:ARG:HH11	1.92	0.81
2:D:501:ILE:HD12	2:D:529:LEU:CD1	2.11	0.81
1:A:268:LEU:HD11	1:A:321:LEU:HD23	1.61	0.81
1:B:229:TYR:CD2	1:B:342:ILE:HD12	2.16	0.80
2:C:496:ALA:HB1	2:C:497:ASN:HB2	1.63	0.80
2:C:524:ARG:HH11	2:C:524:ARG:CG	1.92	0.80
1:A:229:TYR:CD2	1:A:342:ILE:HD12	2.16	0.80
1:A:337:PRO:CD	2:C:639:PHE:CE1	2.63	0.80
6:H:3:DC:H2"	6:H:4:DT:O5'	1.81	0.80
1:B:285:ALA:CB	1:B:301:GLU:O	2.30	0.80
4:F:3:DT:H2"	4:F:4:DC:O5'	1.81	0.80
2:D:496:ALA:HB1	2:D:497:ASN:HB2	1.63	0.80
1:A:95:ARG:HH22	1:A:479:LEU:HD12	1.47	0.80
1:A:285:ALA:CB	1:A:301:GLU:O	2.30	0.79
2:C:467:MET:HE3	2:C:471:LEU:HD11	1.65	0.78
2:D:460:ILE:HD12	2:D:476:ILE:HG13	1.65	0.78
1:A:354:ARG:HG3	1:A:459:MET:HE1	1.65	0.78
1:B:95:ARG:HH22	1:B:479:LEU:HD12	1.47	0.78
2:D:492:SER:C	2:D:493:ILE:HG13	2.04	0.78
2:C:460:ILE:HD12	2:C:476:ILE:HG13	1.65	0.77
1:B:253:GLN:HG3	1:B:301:GLU:CB	2.14	0.77
1:A:253:GLN:HG3	1:A:301:GLU:CB	2.14	0.77
1:A:70:MET:HE1	1:A:78:ASP:HB3	1.66	0.77
2:C:492:SER:C	2:C:493:ILE:HG13	2.03	0.77
1:A:338:ARG:HD2	1:A:340:VAL:HG12	1.66	0.77
1:B:285:ALA:HB2	1:B:302:LEU:HA	1.67	0.77
1:B:377:GLY:O	1:B:381:VAL:HG23	1.85	0.77
2:C:608:ILE:HD12	2:C:609:GLU:N	2.00	0.77
1:A:285:ALA:HB2	1:A:302:LEU:HA	1.67	0.76
1:A:377:GLY:O	1:A:381:VAL:HG23	1.85	0.76
2:D:485:ALA:HB1	2:D:491:PHE:O	1.85	0.76
1:A:425:TYR:O	1:A:428:THR:HB	1.86	0.76
2:D:608:ILE:HD12	2:D:609:GLU:N	2.01	0.76
1:B:70:MET:HE1	1:B:78:ASP:HB3	1.66	0.76
1:B:338:ARG:HD2	1:B:340:VAL:HG12	1.66	0.76
1:A:24:ILE:HG22	1:A:171:SER:HB2	1.67	0.76
1:B:425:TYR:O	1:B:428:THR:HB	1.86	0.75
2:C:485:ALA:HB1	2:C:491:PHE:O	1.85	0.75
2:D:426:LYS:O	2:D:426:LYS:HG2	1.86	0.75
1:B:24:ILE:HG22	1:B:171:SER:HB2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:426:LYS:O	2:C:426:LYS:HG2	1.85	0.74
1:A:28:ARG:HG3	1:A:28:ARG:NH1	1.93	0.74
2:D:493:ILE:HG22	2:D:494:GLU:N	2.00	0.74
2:C:493:ILE:HG22	2:C:494:GLU:N	2.00	0.74
2:D:625:LYS:O	2:D:626:VAL:HB	1.88	0.74
1:A:263:ILE:HG12	1:A:264:ASN:N	2.02	0.74
1:B:263:ILE:HG12	1:B:264:ASN:N	2.02	0.73
1:A:354:ARG:HG3	1:A:459:MET:HE2	1.70	0.73
1:A:428:THR:HG21	1:B:397:ASN:HA	1.71	0.73
1:A:397:ASN:HA	1:B:428:THR:HG21	1.71	0.73
2:D:524:ARG:HH11	2:D:524:ARG:HG3	1.53	0.72
1:A:283:GLY:O	1:A:302:LEU:HB3	1.89	0.72
1:B:283:GLY:O	1:B:302:LEU:HB3	1.89	0.72
2:C:609:GLU:O	2:C:610:ASP:CB	2.37	0.72
2:D:460:ILE:HG12	2:D:473:ASN:ND2	2.05	0.72
2:C:625:LYS:O	2:C:626:VAL:HB	1.88	0.72
1:B:24:ILE:CG2	1:B:171:SER:HB2	2.20	0.72
2:C:460:ILE:HG12	2:C:473:ASN:ND2	2.04	0.72
2:C:601:ARG:NH1	2:C:603:LEU:HD11	2.05	0.72
2:D:544:LYS:HD3	2:D:580:TYR:OH	1.90	0.72
1:A:91:ASN:N	1:A:91:ASN:HD22	1.87	0.72
2:D:609:GLU:O	2:D:610:ASP:CB	2.37	0.71
2:D:516:THR:HG22	2:D:622:MET:CE	2.20	0.71
2:C:524:ARG:HH11	2:C:524:ARG:HG3	1.53	0.70
1:B:91:ASN:N	1:B:91:ASN:HD22	1.87	0.70
1:B:213:PHE:CE2	1:B:219:ILE:HD11	2.26	0.70
2:D:516:THR:O	2:D:520:THR:HG23	1.91	0.70
1:A:213:PHE:CE2	1:A:219:ILE:HD11	2.26	0.70
1:A:312:LEU:CD2	1:A:316:PHE:CE1	2.75	0.70
2:C:516:THR:O	2:C:520:THR:HG23	1.91	0.70
1:A:24:ILE:CG2	1:A:171:SER:HB2	2.20	0.70
2:D:486:GLY:O	2:D:487:VAL:HG12	1.91	0.70
2:C:493:ILE:CG2	2:C:494:GLU:H	2.00	0.70
2:D:524:ARG:HH11	2:D:524:ARG:CB	2.05	0.70
2:C:486:GLY:O	2:C:487:VAL:HG12	1.91	0.69
1:B:187:ILE:O	1:B:191:VAL:HG23	1.92	0.69
1:B:312:LEU:CD2	1:B:316:PHE:CE1	2.75	0.69
2:C:516:THR:HG22	2:C:622:MET:CE	2.21	0.69
2:D:601:ARG:NH1	2:D:603:LEU:HD11	2.07	0.69
1:A:187:ILE:O	1:A:191:VAL:HG23	1.92	0.69
1:B:213:PHE:CD2	1:B:219:ILE:HD11	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:PHE:CD2	1:A:219:ILE:HD11	2.28	0.69
2:D:491:PHE:O	2:D:492:SER:HB3	1.93	0.69
2:D:592:TRP:CE2	2:D:597:ASN:HB2	2.29	0.68
2:C:544:LYS:HD3	2:C:580:TYR:OH	1.93	0.68
2:C:524:ARG:HH11	2:C:524:ARG:CB	2.05	0.68
2:C:592:TRP:CE2	2:C:597:ASN:HB2	2.29	0.68
2:C:623:GLY:O	2:C:629:ARG:NH2	2.27	0.68
2:C:491:PHE:O	2:C:492:SER:HB3	1.93	0.68
2:C:545:MET:O	2:C:555:VAL:HA	1.94	0.68
1:A:336:THR:HG22	2:C:639:PHE:CD1	2.27	0.68
2:D:516:THR:HG22	2:D:622:MET:HE2	1.76	0.68
2:C:543:TYR:CG	2:C:564:LEU:CD2	2.77	0.68
2:D:543:TYR:CG	2:D:564:LEU:CD2	2.77	0.67
2:C:639:PHE:N	2:C:639:PHE:CD2	2.63	0.67
2:D:639:PHE:N	2:D:639:PHE:CD2	2.62	0.67
2:C:543:TYR:CG	2:C:564:LEU:HD23	2.30	0.66
2:D:543:TYR:CG	2:D:564:LEU:HD23	2.30	0.66
2:D:545:MET:O	2:D:555:VAL:HA	1.94	0.66
2:D:486:GLY:C	2:D:487:VAL:CG1	2.64	0.66
1:B:336:THR:HG22	2:D:639:PHE:HB2	1.78	0.66
1:A:183:LEU:HD21	1:A:187:ILE:HD11	1.78	0.66
2:D:608:ILE:HD11	2:D:610:ASP:O	1.96	0.66
1:A:26:GLN:NE2	2:C:639:PHE:HB3	2.12	0.65
1:B:183:LEU:HD21	1:B:187:ILE:HD11	1.78	0.65
2:C:552:LYS:O	2:C:552:LYS:CG	2.43	0.65
2:C:467:MET:HE1	2:C:471:LEU:CD2	2.26	0.65
2:C:500:LYS:HG2	2:C:536:TYR:CE2	2.32	0.65
1:B:354:ARG:HG3	1:B:459:MET:HE1	1.75	0.65
2:C:446:ASP:O	2:C:450:GLN:HG3	1.96	0.65
2:D:500:LYS:HG2	2:D:536:TYR:CE2	2.32	0.65
2:D:637:VAL:HB	2:D:639:PHE:HE2	1.62	0.64
2:C:486:GLY:C	2:C:487:VAL:CG1	2.63	0.64
2:D:446:ASP:O	2:D:450:GLN:HG3	1.96	0.64
2:D:623:GLY:O	2:D:629:ARG:NH2	2.30	0.64
1:B:26:GLN:NE2	2:D:639:PHE:HB3	2.12	0.64
2:C:501:ILE:HD12	2:C:529:LEU:HD11	1.79	0.64
1:B:336:THR:HG22	2:D:639:PHE:CD1	2.33	0.64
1:A:144:ASN:N	1:A:144:ASN:HD22	1.96	0.64
1:B:260:PRO:O	1:B:263:ILE:HG22	1.97	0.63
1:A:260:PRO:O	1:A:263:ILE:HG22	1.97	0.63
2:C:608:ILE:HD11	2:C:610:ASP:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:VAL:HG12	1:A:344:PRO:HD3	1.79	0.63
1:A:272:ILE:HG22	1:A:287:VAL:HG21	1.81	0.63
2:C:474:GLU:O	2:C:478:THR:HG23	1.99	0.63
2:D:474:GLU:O	2:D:478:THR:HG23	1.99	0.63
6:H:3:DC:H4'	6:H:4:DT:OP1	1.99	0.63
2:C:577:LEU:HD21	2:C:579:ARG:NH1	2.13	0.63
2:D:543:TYR:CB	2:D:564:LEU:HD21	2.28	0.63
6:H:6:DT:H2"	6:H:7:DG:H5'	1.81	0.63
1:B:272:ILE:HG22	1:B:287:VAL:HG21	1.81	0.63
2:C:543:TYR:CB	2:C:564:LEU:HD21	2.28	0.63
2:D:501:ILE:HD12	2:D:529:LEU:HD11	1.79	0.63
1:A:4:ILE:HG23	1:A:4:ILE:O	1.98	0.62
1:B:4:ILE:HG23	1:B:4:ILE:O	1.98	0.62
1:B:44:ILE:HD13	1:B:88:MET:HE1	1.80	0.62
2:D:577:LEU:HD21	2:D:579:ARG:NH1	2.13	0.62
2:C:637:VAL:HB	2:C:639:PHE:HE2	1.63	0.62
2:D:516:THR:CG2	2:D:622:MET:CE	2.77	0.62
1:B:144:ASN:N	1:B:144:ASN:HD22	1.96	0.62
1:B:343:VAL:HG12	1:B:344:PRO:HD3	1.80	0.62
1:A:44:ILE:HD13	1:A:88:MET:CE	2.30	0.62
1:A:404:ASN:O	1:A:408:SER:HB2	2.00	0.62
2:C:598:PRO:HA	2:C:601:ARG:NE	2.07	0.62
1:B:85:MET:HA	1:B:88:MET:HE3	1.80	0.61
1:A:44:ILE:HD13	1:A:88:MET:HE1	1.82	0.61
1:B:44:ILE:HD13	1:B:88:MET:CE	2.30	0.61
2:D:467:MET:HE3	2:D:471:LEU:CD1	2.29	0.61
1:A:336:THR:HG22	2:C:639:PHE:HB2	1.81	0.61
1:B:169:GLY:HA3	1:B:176:THR:HG22	1.81	0.61
1:B:404:ASN:O	1:B:408:SER:HB2	2.00	0.61
2:C:431:LEU:CD1	2:C:479:MET:HE1	2.17	0.61
4:F:3:DT:H4'	4:F:4:DC:OP1	2.00	0.61
1:A:420:VAL:HG13	1:B:425:TYR:HB3	1.83	0.61
2:D:608:ILE:HD11	2:D:610:ASP:C	2.21	0.61
1:A:85:MET:HA	1:A:88:MET:HE3	1.82	0.61
2:D:577:LEU:HD21	2:D:579:ARG:HH12	1.66	0.61
2:C:523:TYR:CZ	2:C:527:ARG:NH1	2.69	0.60
1:B:285:ALA:CB	1:B:302:LEU:HA	2.30	0.60
1:B:448:MET:HE2	1:B:452:ILE:HD11	1.81	0.60
2:C:520:THR:HG21	2:C:622:MET:CG	2.13	0.60
1:A:169:GLY:HA3	1:A:176:THR:O	2.01	0.60
2:C:516:THR:CG2	2:C:622:MET:CE	2.79	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:523:TYR:CZ	2:D:527:ARG:NH1	2.69	0.60
1:A:425:TYR:HB3	1:B:420:VAL:HG13	1.82	0.60
2:D:460:ILE:HD11	2:D:473:ASN:CG	2.22	0.60
1:A:169:GLY:HA3	1:A:176:THR:HG22	1.81	0.60
2:C:577:LEU:HD21	2:C:579:ARG:HH12	1.66	0.60
2:D:446:ASP:H	2:D:450:GLN:HE21	1.49	0.60
1:A:391:LEU:C	1:A:391:LEU:HD23	2.23	0.59
2:C:460:ILE:HD11	2:C:473:ASN:CG	2.22	0.59
2:D:609:GLU:O	2:D:610:ASP:HB2	2.01	0.59
1:B:169:GLY:HA3	1:B:176:THR:O	2.01	0.59
1:B:391:LEU:C	1:B:391:LEU:HD23	2.23	0.59
2:C:446:ASP:H	2:C:450:GLN:HE21	1.49	0.59
2:C:480:ILE:HD13	2:C:487:VAL:CG1	2.30	0.59
2:C:546:SER:HB3	2:C:555:VAL:HG22	1.84	0.59
2:D:552:LYS:O	2:D:552:LYS:CG	2.43	0.59
1:B:75:PRO:HD2	1:B:76:HIS:CD2	2.38	0.59
2:C:609:GLU:O	2:C:610:ASP:HB2	2.02	0.59
2:D:491:PHE:CD1	2:D:492:SER:O	2.55	0.59
2:D:639:PHE:N	2:D:639:PHE:HD2	2.00	0.59
1:A:285:ALA:CB	1:A:302:LEU:HA	2.30	0.59
1:B:59:TYR:CE1	1:B:122:ARG:CZ	2.86	0.59
2:C:491:PHE:CD1	2:C:492:SER:O	2.56	0.59
2:C:546:SER:HA	2:C:554:GLU:O	2.03	0.59
6:H:5:DA:C4	8:H:0:LFX:H01A	2.38	0.59
2:D:546:SER:HA	2:D:554:GLU:O	2.03	0.59
1:A:448:MET:HE2	1:A:452:ILE:HD11	1.83	0.58
1:A:59:TYR:CE1	1:A:122:ARG:CZ	2.86	0.58
1:A:316:PHE:HD2	1:A:322:GLN:HB2	1.68	0.58
2:D:546:SER:HB3	2:D:555:VAL:HG22	1.84	0.58
1:A:75:PRO:HD2	1:A:76:HIS:CD2	2.37	0.58
1:B:316:PHE:HD2	1:B:322:GLN:HB2	1.68	0.58
2:C:608:ILE:HD11	2:C:610:ASP:C	2.23	0.58
1:A:174:TYR:CD2	1:A:174:TYR:N	2.71	0.58
1:B:91:ASN:ND2	1:B:92:TRP:CE3	2.72	0.58
2:C:581:LYS:HE3	2:C:585:GLU:OE2	2.03	0.58
1:B:91:ASN:ND2	1:B:92:TRP:HE3	2.01	0.58
2:D:581:LYS:HE3	2:D:585:GLU:OE2	2.04	0.58
1:B:174:TYR:N	1:B:174:TYR:CD2	2.71	0.58
1:A:91:ASN:ND2	1:A:92:TRP:HE3	2.01	0.57
2:D:429:LEU:HD13	2:D:431:LEU:HD21	1.86	0.57
2:D:453:LEU:C	2:D:453:LEU:HD23	2.24	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASN:ND2	1:A:92:TRP:CE3	2.72	0.57
1:A:207:PHE:O	1:A:209:PRO:HD3	2.04	0.57
1:A:210:GLY:HA2	1:A:225:ILE:HD13	1.87	0.57
2:C:446:ASP:H	2:C:450:GLN:NE2	2.02	0.57
1:A:240:SER:HB3	1:A:259:ILE:HA	1.86	0.57
1:B:343:VAL:HG12	1:B:344:PRO:CD	2.35	0.57
2:C:453:LEU:C	2:C:453:LEU:HD23	2.24	0.57
2:D:446:ASP:H	2:D:450:GLN:NE2	2.02	0.57
2:D:598:PRO:HA	2:D:601:ARG:NE	2.08	0.57
2:C:429:LEU:HD13	2:C:431:LEU:HD21	1.86	0.57
2:D:480:ILE:HD13	2:D:487:VAL:CG1	2.30	0.57
1:A:382:ILE:HG12	1:A:430:THR:HG23	1.87	0.57
1:B:134:ILE:HD11	1:B:152:PRO:HG3	1.87	0.57
4:F:10:DT:H2"	4:F:11:DG:C8	2.40	0.57
1:B:207:PHE:O	1:B:209:PRO:HD3	2.04	0.56
1:B:240:SER:HB3	1:B:259:ILE:HA	1.86	0.56
1:B:382:ILE:HG12	1:B:430:THR:HG23	1.87	0.56
2:D:543:TYR:CG	2:D:564:LEU:HD21	2.40	0.56
1:A:144:ASN:HD22	1:A:144:ASN:H	1.53	0.56
2:D:435:ASP:HB2	4:F:1:DA:C5'	2.35	0.56
1:A:343:VAL:HG12	1:A:344:PRO:CD	2.34	0.56
2:C:526:MET:HE2	2:C:529:LEU:HG	1.86	0.56
2:D:526:MET:HE2	2:D:529:LEU:HG	1.88	0.56
2:C:516:THR:CG2	2:C:622:MET:SD	2.94	0.56
2:D:524:ARG:HG3	2:D:524:ARG:NH1	2.17	0.56
4:F:5:DA:C4	8:F:0:LFX:H01A	2.40	0.56
2:D:456:ARG:NH1	8:H:0:LFX:C08	2.65	0.56
2:D:637:VAL:HG12	2:D:639:PHE:CD2	2.41	0.56
1:A:233:LYS:HA	1:A:327:PHE:O	2.06	0.56
1:A:134:ILE:HD11	1:A:152:PRO:HG3	1.87	0.56
1:A:183:LEU:O	1:A:187:ILE:HG13	2.06	0.56
2:D:558:ALA:HB2	2:D:567:LEU:HD12	1.88	0.56
2:D:516:THR:CG2	2:D:622:MET:SD	2.95	0.55
1:B:210:GLY:HA2	1:B:225:ILE:HD13	1.87	0.55
2:C:630:ARG:O	2:C:634:GLU:HG3	2.07	0.55
1:B:144:ASN:HD22	1:B:144:ASN:H	1.53	0.55
1:B:159:PHE:HB2	1:B:160:PRO:CD	2.37	0.55
2:D:501:ILE:CD1	2:D:529:LEU:HD11	2.36	0.55
1:B:183:LEU:O	1:B:187:ILE:HG13	2.06	0.55
2:C:639:PHE:N	2:C:639:PHE:HD2	2.03	0.55
1:A:132:GLN:O	1:A:133:ASP:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:PHE:CD2	1:A:322:GLN:HB2	2.42	0.55
2:C:456:ARG:NH1	8:F:0:LFX:C08	2.65	0.55
1:B:90:GLN:HG2	1:B:92:TRP:CH2	2.42	0.55
1:B:233:LYS:HA	1:B:327:PHE:O	2.06	0.54
1:B:336:THR:HB	1:B:337:PRO:HD2	1.88	0.54
2:C:423:ASN:OD1	2:C:425:ALA:HB3	2.07	0.54
2:C:501:ILE:CD1	2:C:529:LEU:HD11	2.36	0.54
1:A:159:PHE:HB2	1:A:160:PRO:CD	2.37	0.54
2:D:476:ILE:O	2:D:480:ILE:HG13	2.08	0.54
2:C:445:ARG:O	2:C:445:ARG:HG2	2.04	0.54
1:A:336:THR:HB	1:A:337:PRO:HD2	1.88	0.54
2:D:423:ASN:OD1	2:D:425:ALA:HB3	2.07	0.54
2:D:445:ARG:O	2:D:445:ARG:HG2	2.04	0.54
2:D:630:ARG:O	2:D:634:GLU:HG3	2.08	0.54
2:C:627:GLU:N	2:C:628:PRO:CD	2.70	0.54
1:A:290:GLU:O	1:A:297:ARG:HB3	2.07	0.54
1:B:239:ARG:HG3	1:B:316:PHE:CE2	2.43	0.54
1:B:132:GLN:O	1:B:133:ASP:HB2	2.07	0.54
2:D:456:ARG:HH12	8:H:0:LFX:C08	2.15	0.54
1:B:183:LEU:CD2	1:B:187:ILE:HD11	2.38	0.54
1:B:316:PHE:CD2	1:B:322:GLN:HB2	2.42	0.54
2:C:543:TYR:CB	2:C:564:LEU:CD2	2.86	0.54
2:C:558:ALA:HB2	2:C:567:LEU:HD12	1.88	0.54
2:C:637:VAL:HG12	2:C:639:PHE:CD2	2.42	0.54
1:A:245:GLU:OE2	1:A:297:ARG:NH2	2.41	0.54
1:B:29:ALA:HB3	1:B:171:SER:HB3	1.89	0.54
1:B:290:GLU:O	1:B:297:ARG:HB3	2.07	0.54
2:D:543:TYR:CB	2:D:564:LEU:CD2	2.86	0.54
2:C:476:ILE:O	2:C:480:ILE:HG13	2.08	0.54
2:D:485:ALA:HB3	2:D:491:PHE:CE2	2.43	0.54
1:A:183:LEU:CD2	1:A:187:ILE:HD11	2.38	0.53
2:C:543:TYR:CG	2:C:564:LEU:HD21	2.40	0.53
2:D:483:ILE:HG21	2:D:526:MET:HE3	1.90	0.53
1:A:29:ALA:HB3	1:A:171:SER:HB3	1.89	0.53
1:A:324:ASN:N	1:A:324:ASN:ND2	2.56	0.53
1:A:337:PRO:HD2	2:C:639:PHE:CE1	2.40	0.53
1:B:210:GLY:CA	1:B:225:ILE:HD13	2.38	0.53
2:C:516:THR:HG22	2:C:622:MET:HE2	1.89	0.53
2:D:467:MET:CE	2:D:471:LEU:HD21	2.35	0.53
1:A:210:GLY:CA	1:A:225:ILE:HD13	2.38	0.53
1:A:90:GLN:HG2	1:A:92:TRP:CH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:485:ALA:HB3	2:C:491:PHE:CE2	2.43	0.53
2:D:627:GLU:N	2:D:628:PRO:CD	2.70	0.53
1:B:91:ASN:N	1:B:91:ASN:ND2	2.56	0.53
2:C:429:LEU:CD1	2:C:431:LEU:HD21	2.39	0.53
2:D:429:LEU:CD1	2:D:431:LEU:HD21	2.39	0.53
1:B:324:ASN:HD22	1:B:324:ASN:H	1.57	0.53
1:B:448:MET:CE	1:B:452:ILE:HD11	2.39	0.53
1:A:324:ASN:H	1:A:324:ASN:HD22	1.57	0.53
1:A:448:MET:CE	1:A:452:ILE:HD11	2.39	0.53
1:B:245:GLU:OE2	1:B:297:ARG:NH2	2.41	0.53
3:E:10:DA:H2'	3:E:11:DT:H71	1.89	0.53
1:B:257:THR:O	1:B:258:GLU:HG3	2.09	0.53
2:C:460:ILE:HD12	2:C:476:ILE:CG1	2.39	0.53
1:A:257:THR:O	1:A:258:GLU:HG3	2.09	0.52
1:B:324:ASN:N	1:B:324:ASN:ND2	2.56	0.52
1:A:239:ARG:HG3	1:A:316:PHE:CE2	2.43	0.52
1:B:283:GLY:CA	1:B:311:VAL:HG21	2.30	0.52
1:A:276:ARG:HG3	1:A:284:ILE:CB	2.39	0.52
2:C:524:ARG:HG3	2:C:524:ARG:NH1	2.17	0.52
1:B:276:ARG:HG3	1:B:284:ILE:CB	2.39	0.52
1:B:343:VAL:HG12	1:B:344:PRO:N	2.25	0.52
1:A:91:ASN:N	1:A:91:ASN:ND2	2.56	0.52
1:A:223:ASP:OD1	1:A:223:ASP:N	2.42	0.52
1:B:337:PRO:HD2	2:D:639:PHE:CE1	2.43	0.52
2:D:431:LEU:HD13	2:D:479:MET:HE2	1.86	0.52
1:A:402:LYS:O	1:A:406:LYS:HG3	2.10	0.52
2:D:523:TYR:CE1	2:D:527:ARG:NH1	2.78	0.52
1:B:61:LYS:HE3	1:B:119:THR:O	2.09	0.51
1:B:343:VAL:CG1	1:B:344:PRO:HD3	2.41	0.51
2:C:523:TYR:CE1	2:C:527:ARG:NH1	2.78	0.51
1:A:296:LEU:C	1:A:296:LEU:HD23	2.31	0.51
1:A:343:VAL:HG12	1:A:344:PRO:N	2.24	0.51
3:E:10:DA:H2"	3:E:11:DT:C6	2.45	0.51
1:B:402:LYS:O	1:B:406:LYS:HG3	2.10	0.51
2:D:416:LEU:HD12	2:D:452:ILE:O	2.10	0.51
2:C:416:LEU:HD12	2:C:452:ILE:O	2.10	0.51
1:A:61:LYS:HE3	1:A:119:THR:O	2.10	0.51
1:B:167:SER:O	1:B:168:THR:CG2	2.59	0.51
2:C:446:ASP:N	2:C:450:GLN:HE21	2.09	0.51
1:A:293:ARG:O	1:A:294:ASP:OD2	2.29	0.51
1:A:372:LEU:O	1:A:376:GLU:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:460:ILE:HD12	2:D:476:ILE:CG1	2.39	0.51
2:D:493:ILE:CG2	2:D:494:GLU:H	2.00	0.51
1:A:183:LEU:CD2	1:A:187:ILE:HG13	2.41	0.50
1:A:302:LEU:N	1:A:302:LEU:HD23	2.26	0.50
1:A:343:VAL:CG1	1:A:344:PRO:HD3	2.41	0.50
1:A:292:ASP:O	1:A:293:ARG:C	2.49	0.50
1:A:293:ARG:O	1:A:293:ARG:HG2	2.09	0.50
1:B:296:LEU:C	1:B:296:LEU:HD23	2.31	0.50
2:D:637:VAL:HG12	2:D:639:PHE:HD2	1.77	0.50
6:H:7:DG:H2"	6:H:8:DC:O5'	2.12	0.50
1:B:183:LEU:CD2	1:B:187:ILE:HG13	2.41	0.50
1:B:355:GLU:OE2	1:B:355:GLU:HA	2.11	0.50
1:A:355:GLU:OE2	1:A:355:GLU:HA	2.11	0.50
1:A:423:GLN:HG3	9:A:501:HOH:O	2.11	0.50
2:C:637:VAL:HG12	2:C:639:PHE:HD2	1.75	0.50
2:D:435:ASP:HB3	4:F:2:DG:OP2	2.11	0.50
1:A:167:SER:O	1:A:168:THR:HG23	2.11	0.50
6:H:3:DC:H2'	6:H:4:DT:C6	2.47	0.50
1:B:167:SER:O	1:B:168:THR:HG23	2.11	0.50
1:B:302:LEU:N	1:B:302:LEU:HD23	2.26	0.50
2:D:598:PRO:CA	2:D:601:ARG:HE	2.11	0.50
1:A:261:TYR:CD2	1:A:262:GLU:HG3	2.46	0.50
1:A:315:LEU:HB3	1:A:321:LEU:HD12	1.94	0.50
1:B:372:LEU:O	1:B:376:GLU:HG3	2.11	0.50
1:A:167:SER:O	1:A:168:THR:CG2	2.59	0.50
1:B:195:ASP:O	1:B:197:PRO:HD3	2.12	0.50
2:C:543:TYR:HD1	2:C:577:LEU:HD11	1.77	0.50
2:D:543:TYR:HD1	2:D:577:LEU:HD11	1.77	0.50
2:C:491:PHE:HE2	2:C:526:MET:HE3	1.77	0.49
1:B:293:ARG:O	1:B:294:ASP:OD2	2.29	0.49
1:B:24:ILE:CG2	1:B:171:SER:CB	2.90	0.49
1:B:315:LEU:HB3	1:B:321:LEU:HD12	1.94	0.49
1:B:282:ALA:C	1:B:284:ILE:H	2.16	0.49
2:D:446:ASP:N	2:D:450:GLN:HE21	2.09	0.49
2:D:499:ASP:CG	2:D:499:ASP:O	2.50	0.49
1:A:336:THR:HA	2:C:639:PHE:HD1	1.77	0.49
1:A:195:ASP:O	1:A:197:PRO:HD3	2.12	0.49
1:A:282:ALA:C	1:A:284:ILE:H	2.16	0.49
1:B:224:GLU:HG3	1:B:235:ARG:O	2.13	0.49
2:D:625:LYS:O	2:D:626:VAL:CB	2.60	0.49
1:B:365:LYS:N	1:B:449:LEU:HD13	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:539:LEU:HD21	2:C:604:ILE:CD1	2.42	0.49
2:D:539:LEU:HD21	2:D:604:ILE:CD1	2.42	0.49
2:D:520:THR:O	2:D:524:ARG:HG2	2.13	0.49
2:C:491:PHE:CE2	2:C:526:MET:HE3	2.48	0.49
2:C:499:ASP:CG	2:C:499:ASP:O	2.50	0.49
2:C:609:GLU:O	2:C:610:ASP:HB3	2.13	0.49
2:D:613:ARG:NH1	2:D:613:ARG:CG	2.51	0.49
1:A:324:ASN:ND2	1:A:324:ASN:H	2.10	0.48
1:B:292:ASP:O	1:B:293:ARG:C	2.49	0.48
1:A:224:GLU:HG3	1:A:235:ARG:O	2.13	0.48
1:B:4:ILE:O	1:B:4:ILE:CG2	2.61	0.48
1:B:324:ASN:H	1:B:324:ASN:ND2	2.10	0.48
2:C:467:MET:CE	2:C:471:LEU:HD11	2.37	0.48
1:A:293:ARG:HH12	2:D:445:ARG:N	2.12	0.48
1:B:247:LEU:CB	1:B:251:LYS:O	2.62	0.48
2:C:524:ARG:HH11	2:C:524:ARG:HB3	1.76	0.48
2:C:539:LEU:HD21	2:C:604:ILE:HD11	1.94	0.48
2:D:479:MET:HE1	2:D:518:LEU:HD22	1.95	0.48
1:A:28:ARG:HH11	1:A:28:ARG:CG	2.03	0.48
1:A:247:LEU:CB	1:A:251:LYS:O	2.62	0.48
1:B:230:GLU:OE2	1:B:230:GLU:HA	2.13	0.48
1:B:336:THR:HA	2:D:639:PHE:HD1	1.78	0.48
2:D:520:THR:HG21	2:D:622:MET:CG	2.13	0.48
2:D:524:ARG:HH11	2:D:524:ARG:HB3	1.76	0.48
1:A:286:GLU:OE2	1:A:288:ARG:HD3	2.14	0.48
1:B:194:ILE:CD1	1:B:463:MET:HE2	2.43	0.48
2:C:491:PHE:O	2:C:492:SER:CB	2.61	0.48
1:A:4:ILE:O	1:A:4:ILE:CG2	2.61	0.48
1:A:245:GLU:HB2	1:A:253:GLN:HB3	1.96	0.48
1:A:229:TYR:CD2	1:A:342:ILE:CD1	2.93	0.48
1:A:230:GLU:OE2	1:A:230:GLU:HA	2.13	0.48
4:F:6:DT:C6	4:F:7:DT:H72	2.49	0.48
2:C:520:THR:O	2:C:524:ARG:HG2	2.13	0.48
2:C:442:LYS:O	2:C:445:ARG:HD3	2.14	0.48
2:D:435:ASP:HB2	4:F:1:DA:H5'	1.94	0.48
2:D:539:LEU:HD21	2:D:604:ILE:HD11	1.95	0.48
1:A:40:VAL:HG21	3:E:13:DA:H3'	1.95	0.48
1:A:338:ARG:HD2	1:A:340:VAL:CG1	2.42	0.48
1:B:229:TYR:CD1	1:B:342:ILE:HD12	2.48	0.48
2:C:416:LEU:HD22	2:C:482:THR:CG2	2.44	0.48
2:D:436:SER:HB2	4:F:1:DA:OP2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:442:LYS:O	2:D:445:ARG:HD3	2.14	0.48
1:A:365:LYS:N	1:A:449:LEU:HD13	2.28	0.47
1:B:216:GLY:O	1:B:217:ALA:HB3	2.14	0.47
1:B:245:GLU:HB2	1:B:253:GLN:HB3	1.96	0.47
2:C:544:LYS:NZ	2:C:578:GLN:OE1	2.47	0.47
2:D:460:ILE:H	2:D:460:ILE:HG13	1.46	0.47
2:D:544:LYS:NZ	2:D:578:GLN:OE1	2.47	0.47
1:A:12:ILE:O	1:A:16:ARG:HG2	2.14	0.47
1:A:393:ARG:NH1	1:B:386:ASP:OD1	2.43	0.47
1:A:431:ASP:OD1	1:A:434:VAL:CG2	2.49	0.47
1:B:287:VAL:HG23	1:B:300:ILE:HG23	1.97	0.47
2:C:467:MET:HE3	2:C:471:LEU:CD1	2.39	0.47
2:C:483:ILE:HG21	2:C:526:MET:HE3	1.95	0.47
2:C:598:PRO:CA	2:C:601:ARG:HE	2.10	0.47
1:B:191:VAL:HA	1:B:194:ILE:HD12	1.96	0.47
2:D:608:ILE:CD1	2:D:610:ASP:O	2.61	0.47
1:A:24:ILE:CG2	1:A:171:SER:CB	2.90	0.47
2:D:467:MET:CE	2:D:471:LEU:HD11	2.37	0.47
1:B:12:ILE:O	1:B:16:ARG:HG2	2.14	0.47
1:B:194:ILE:HG13	1:B:350:ILE:CD1	2.45	0.47
2:C:594:THR:OG1	2:C:595:THR:HG22	2.15	0.47
2:D:416:LEU:HD22	2:D:482:THR:CG2	2.44	0.47
1:A:191:VAL:HA	1:A:194:ILE:HD12	1.96	0.47
1:A:382:ILE:HG12	1:A:430:THR:CG2	2.45	0.47
1:B:179:PRO:HG3	1:B:325:TYR:CE1	2.50	0.47
1:A:276:ARG:CD	1:A:285:ALA:O	2.56	0.47
1:B:256:ILE:HD12	1:B:298:ILE:HG22	1.97	0.47
2:C:613:ARG:CG	2:C:613:ARG:NH1	2.52	0.47
1:A:194:ILE:HG13	1:A:350:ILE:CD1	2.45	0.47
1:A:40:VAL:HG21	3:E:13:DA:C3'	2.45	0.46
1:A:169:GLY:HA3	1:A:176:THR:CG2	2.45	0.46
1:A:216:GLY:O	1:A:217:ALA:HB3	2.14	0.46
1:A:28:ARG:NH1	1:A:28:ARG:CG	2.70	0.46
1:A:179:PRO:HG3	1:A:325:TYR:CE1	2.50	0.46
1:A:263:ILE:CD1	1:A:268:LEU:HG	2.45	0.46
1:B:263:ILE:CD1	1:B:268:LEU:HG	2.45	0.46
1:B:286:GLU:OE2	1:B:288:ARG:HD3	2.14	0.46
4:F:5:DA:C5	4:F:6:DT:C4	3.03	0.46
1:B:183:LEU:CD2	1:B:187:ILE:CD1	2.94	0.46
1:B:293:ARG:HH12	2:C:445:ARG:N	2.13	0.46
1:B:315:LEU:HD22	1:B:319:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:499:ASP:O	2:C:500:LYS:HG3	2.15	0.46
2:D:431:LEU:CD1	2:D:479:MET:HE1	2.25	0.46
1:A:336:THR:HG22	2:C:639:PHE:CG	2.50	0.46
1:B:169:GLY:HA3	1:B:176:THR:CG2	2.45	0.46
6:H:10:DC:H2"	6:H:11:DG:C8	2.51	0.46
2:D:426:LYS:O	2:D:426:LYS:CG	2.54	0.46
1:A:95:ARG:O	1:A:95:ARG:HG3	2.15	0.46
2:C:470:ILE:HG23	2:C:476:ILE:HD12	1.98	0.46
2:C:577:LEU:CD2	2:C:579:ARG:HH12	2.29	0.46
1:A:247:LEU:HB3	1:A:251:LYS:CB	2.45	0.46
1:A:287:VAL:HG23	1:A:300:ILE:HG23	1.97	0.46
1:B:95:ARG:O	1:B:95:ARG:HG3	2.15	0.46
1:B:293:ARG:O	1:B:293:ARG:HG2	2.09	0.46
1:B:382:ILE:HG12	1:B:430:THR:CG2	2.45	0.46
1:B:139:VAL:HA	1:B:140:PRO:HD3	1.82	0.46
1:A:256:ILE:HD12	1:A:298:ILE:HG22	1.97	0.45
2:D:483:ILE:O	2:D:497:ASN:HB2	2.16	0.45
1:A:169:GLY:CA	1:A:176:THR:CG2	2.87	0.45
2:D:499:ASP:O	2:D:500:LYS:HG3	2.15	0.45
2:D:594:THR:OG1	2:D:595:THR:HG22	2.17	0.45
1:A:23:TYR:CG	2:C:509:THR:HG21	2.52	0.45
1:A:183:LEU:CD2	1:A:187:ILE:CD1	2.94	0.45
1:B:336:THR:HG22	2:D:639:PHE:CG	2.50	0.45
1:B:423:GLN:HG3	9:B:501:HOH:O	2.17	0.45
2:C:608:ILE:CD1	2:C:610:ASP:O	2.63	0.45
2:C:626:VAL:C	2:C:628:PRO:HD2	2.37	0.45
2:D:629:ARG:HE	2:D:629:ARG:HB2	1.36	0.45
2:C:594:THR:OG1	2:C:595:THR:CG2	2.64	0.45
1:A:163:LEU:HA	1:A:163:LEU:HD23	1.58	0.45
1:A:315:LEU:HD22	1:A:319:THR:HG21	1.97	0.45
1:A:201:ILE:HD11	1:A:229:TYR:O	2.17	0.45
1:B:169:GLY:CA	1:B:176:THR:CG2	2.87	0.45
2:D:616:ARG:HG3	2:D:616:ARG:HH11	1.82	0.45
4:F:5:DA:C2	4:F:6:DT:C2	3.04	0.45
1:A:259:ILE:HB	1:A:260:PRO:CD	2.47	0.45
1:A:229:TYR:CD1	1:A:342:ILE:HD12	2.48	0.45
1:B:23:TYR:CG	2:D:509:THR:HG21	2.52	0.45
2:D:594:THR:OG1	2:D:595:THR:CG2	2.65	0.45
1:A:386:ASP:OD1	1:B:393:ARG:NH1	2.42	0.45
2:D:609:GLU:O	2:D:610:ASP:HB3	2.15	0.45
1:A:382:ILE:HG23	1:A:430:THR:HG22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:343:VAL:CB	1:B:344:PRO:HD3	2.47	0.44
1:B:382:ILE:HG23	1:B:430:THR:HG22	1.99	0.44
1:A:283:GLY:CA	1:A:311:VAL:HG21	2.30	0.44
2:D:449:PHE:O	2:D:449:PHE:CD2	2.71	0.44
1:B:259:ILE:HB	1:B:260:PRO:CD	2.47	0.44
2:D:470:ILE:HG23	2:D:476:ILE:HD12	1.98	0.44
2:D:479:MET:HE1	2:D:518:LEU:CD2	2.47	0.44
1:B:336:THR:HG22	2:D:639:PHE:CB	2.47	0.44
2:C:483:ILE:O	2:C:497:ASN:HB2	2.16	0.44
2:D:455:LEU:HD21	2:D:479:MET:HE3	1.99	0.44
2:D:485:ALA:CB	2:D:491:PHE:CE2	3.01	0.44
1:A:343:VAL:CB	1:A:344:PRO:HD3	2.47	0.44
2:D:616:ARG:HG3	2:D:616:ARG:NH1	2.32	0.44
5:G:12:DG:H4'	5:G:13:DC:OP1	2.18	0.44
1:A:338:ARG:HG2	1:A:339:GLN:N	2.33	0.44
1:A:91:ASN:HD21	1:A:92:TRP:HE3	1.63	0.44
1:B:201:ILE:HD11	1:B:229:TYR:O	2.17	0.44
2:D:626:VAL:C	2:D:628:PRO:HD2	2.38	0.44
1:A:164:VAL:HG12	1:A:165:ASN:N	2.32	0.44
1:A:194:ILE:CD1	1:A:463:MET:HE2	2.48	0.44
1:B:254:ILE:HB	1:B:300:ILE:O	2.18	0.44
1:B:276:ARG:CD	1:B:285:ALA:O	2.56	0.44
1:B:337:PRO:HD3	2:D:639:PHE:CD1	2.51	0.44
2:C:485:ALA:CB	2:C:491:PHE:CE2	3.01	0.44
2:C:516:THR:HG22	2:C:622:MET:HE1	1.97	0.44
2:C:616:ARG:NH1	2:C:616:ARG:HG3	2.33	0.44
4:F:5:DA:C6	4:F:6:DT:C4	3.06	0.44
1:A:463:MET:HE2	1:A:463:MET:HB3	1.84	0.43
2:C:449:PHE:CD2	2:C:449:PHE:O	2.71	0.43
2:C:616:ARG:HG3	2:C:616:ARG:HH11	1.83	0.43
2:D:491:PHE:HE2	2:D:526:MET:HE3	1.82	0.43
1:B:74:HIS:HA	1:B:75:PRO:HD3	1.86	0.43
1:B:338:ARG:HD2	1:B:340:VAL:CG1	2.42	0.43
1:B:338:ARG:HG2	1:B:339:GLN:N	2.33	0.43
2:C:460:ILE:H	2:C:460:ILE:HG13	1.46	0.43
1:A:455:ASP:O	1:A:456:GLU:C	2.57	0.43
1:B:229:TYR:CD2	1:B:342:ILE:CD1	2.94	0.43
2:D:491:PHE:CE2	2:D:526:MET:HE3	2.53	0.43
5:G:13:DC:H2"	5:G:14:DA:O5'	2.18	0.43
1:A:78:ASP:OD2	1:A:78:ASP:N	2.51	0.43
1:A:117:ARG:NH1	9:A:505:HOH:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:491:PHE:CE2	2:C:526:MET:CE	3.01	0.43
2:C:543:TYR:HB2	2:C:564:LEU:CD2	2.49	0.43
2:D:577:LEU:CD2	2:D:579:ARG:HH12	2.30	0.43
1:A:144:ASN:HD21	1:A:148:THR:N	2.02	0.43
2:C:483:ILE:O	2:C:497:ASN:CB	2.67	0.43
2:C:529:LEU:HD23	2:C:529:LEU:HA	1.86	0.43
2:D:491:PHE:CE2	2:D:526:MET:CE	3.01	0.43
6:H:6:DT:C2'	6:H:7:DG:H5'	2.47	0.43
1:A:107:SER:OG	1:A:111:ASP:OD2	2.28	0.43
1:A:219:ILE:HG23	1:A:236:VAL:CG1	2.49	0.43
2:C:426:LYS:O	2:C:426:LYS:CG	2.54	0.43
2:D:608:ILE:HD13	2:D:614:ALA:HB2	2.00	0.43
1:A:24:ILE:HA	1:A:24:ILE:HD12	1.41	0.43
2:D:526:MET:HE2	2:D:526:MET:HB3	1.86	0.43
6:H:5:DA:C2	6:H:6:DT:C2	3.07	0.43
1:B:205:MET:HA	1:B:208:LEU:O	2.19	0.43
2:D:453:LEU:C	2:D:453:LEU:CD2	2.87	0.43
2:D:571:PHE:HB3	2:D:575:ALA:CB	2.49	0.43
1:A:194:ILE:HG13	1:A:350:ILE:HD11	2.01	0.43
1:B:194:ILE:HG13	1:B:350:ILE:HD11	2.01	0.43
1:B:431:ASP:CG	1:B:434:VAL:HG23	2.36	0.43
2:D:543:TYR:HB2	2:D:564:LEU:CD2	2.49	0.43
1:A:28:ARG:CZ	3:E:14:DA:H4'	2.49	0.42
1:A:61:LYS:HZ1	1:A:118:TYR:C	2.21	0.42
1:B:78:ASP:N	1:B:78:ASP:OD2	2.51	0.42
1:B:91:ASN:HD21	1:B:92:TRP:HE3	1.63	0.42
1:B:111:ASP:OD2	1:B:111:ASP:N	2.49	0.42
2:C:456:ARG:HH12	8:F:0:LFX:C08	2.16	0.42
2:C:543:TYR:HB3	2:C:564:LEU:HD21	2.01	0.42
1:A:144:ASN:ND2	1:A:149:GLU:H	2.17	0.42
1:A:254:ILE:HB	1:A:300:ILE:O	2.18	0.42
1:A:256:ILE:HB	1:A:298:ILE:HB	2.01	0.42
2:D:544:LYS:HG3	2:D:555:VAL:HG13	2.00	0.42
1:A:74:HIS:HA	1:A:75:PRO:HD3	1.86	0.42
2:C:608:ILE:HD13	2:C:614:ALA:HB2	2.01	0.42
2:D:483:ILE:O	2:D:497:ASN:CB	2.67	0.42
1:B:164:VAL:HG12	1:B:165:ASN:N	2.32	0.42
1:A:428:THR:CG2	1:B:397:ASN:HA	2.47	0.42
1:B:455:ASP:O	1:B:456:GLU:C	2.57	0.42
1:A:145:PHE:CD1	2:C:581:LYS:HD3	2.54	0.42
1:A:205:MET:HA	1:A:208:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:178:ILE:HA	1:B:179:PRO:HD3	1.81	0.42
1:B:219:ILE:HG23	1:B:236:VAL:CG1	2.49	0.42
1:A:423:GLN:HA	1:B:423:GLN:HA	2.01	0.42
1:B:144:ASN:ND2	1:B:149:GLU:H	2.17	0.42
2:C:544:LYS:HG3	2:C:555:VAL:HG13	2.00	0.42
1:A:144:ASN:H	1:A:144:ASN:ND2	2.18	0.42
1:B:167:SER:C	1:B:168:THR:HG23	2.40	0.42
2:C:571:PHE:HB3	2:C:575:ALA:CB	2.50	0.42
2:D:543:TYR:HB3	2:D:564:LEU:HD21	2.01	0.42
1:B:111:ASP:HA	1:B:112:PRO:HD3	1.86	0.42
1:B:431:ASP:OD1	1:B:434:VAL:CG2	2.49	0.42
1:A:261:TYR:CE2	1:A:262:GLU:HG3	2.55	0.42
1:A:294:ASP:OD2	1:A:294:ASP:C	2.59	0.41
2:C:625:LYS:O	2:C:626:VAL:CB	2.60	0.41
2:D:592:TRP:CD2	2:D:597:ASN:HB2	2.55	0.41
1:B:294:ASP:OD2	1:B:294:ASP:C	2.59	0.41
1:B:329:MET:HB2	1:B:340:VAL:O	2.20	0.41
2:C:592:TRP:CD2	2:C:597:ASN:HB2	2.55	0.41
2:D:610:ASP:OD1	2:D:611:LEU:N	2.47	0.41
1:A:108:MET:C	1:A:110:GLY:H	2.24	0.41
1:A:139:VAL:HA	1:A:140:PRO:HD3	1.82	0.41
1:B:256:ILE:HB	1:B:298:ILE:HB	2.02	0.41
2:D:487:VAL:O	2:D:487:VAL:HG22	2.21	0.41
1:A:213:PHE:CE2	1:A:219:ILE:CD1	3.01	0.41
1:B:30:LEU:HA	1:B:31:PRO:HD3	1.61	0.41
2:C:429:LEU:HD13	2:C:431:LEU:CD2	2.50	0.41
1:A:24:ILE:N	1:A:24:ILE:HD13	2.36	0.41
1:A:178:ILE:HA	1:A:179:PRO:HD3	1.81	0.41
1:A:292:ASP:C	1:A:293:ARG:O	2.57	0.41
1:A:406:LYS:O	1:A:410:ASP:HA	2.21	0.41
1:B:28:ARG:CZ	5:G:14:DA:H4'	2.50	0.41
2:C:453:LEU:C	2:C:453:LEU:CD2	2.87	0.41
2:C:513:HIS:O	2:C:516:THR:HB	2.20	0.41
1:B:108:MET:C	1:B:110:GLY:H	2.24	0.41
1:A:272:ILE:CG2	1:A:287:VAL:HG21	2.49	0.41
1:A:329:MET:HB2	1:A:340:VAL:O	2.20	0.41
1:B:292:ASP:C	1:B:293:ARG:O	2.57	0.41
1:A:213:PHE:HA	1:A:214:PRO:HD3	1.95	0.41
1:B:247:LEU:O	1:B:248:LYS:C	2.59	0.41
1:B:406:LYS:O	1:B:410:ASP:HA	2.21	0.41
2:C:423:ASN:C	2:C:425:ALA:H	2.24	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:608:ILE:HD12	2:C:608:ILE:C	2.41	0.41
1:B:145:PHE:CD1	2:D:581:LYS:HD3	2.55	0.41
2:C:629:ARG:HE	2:C:629:ARG:HB2	1.35	0.41
2:D:480:ILE:CD1	2:D:487:VAL:HG11	2.39	0.41
2:D:536:TYR:CD2	2:D:536:TYR:N	2.89	0.41
1:A:247:LEU:O	1:A:248:LYS:C	2.59	0.41
1:A:336:THR:HG22	2:C:639:PHE:CB	2.49	0.41
1:A:456:GLU:CG	1:A:460:TYR:HE2	2.21	0.41
2:C:583:LEU:HD23	2:C:586:MET:HE3	2.03	0.41
1:A:205:MET:SD	1:A:229:TYR:HD2	2.44	0.40
2:C:417:THR:HA	2:C:418:PRO:HD3	1.80	0.40
2:C:526:MET:HE2	2:C:526:MET:HB3	1.86	0.40
2:D:496:ALA:CB	2:D:497:ASN:HB2	2.43	0.40
2:D:583:LEU:HD23	2:D:586:MET:HE3	2.03	0.40
2:D:633:ILE:HG23	2:D:637:VAL:HG21	2.02	0.40
1:A:111:ASP:OD2	1:A:111:ASP:N	2.49	0.40
1:A:280:LYS:HB3	1:A:314:TYR:OH	2.22	0.40
1:A:326:ASN:OD1	4:F:11:DG:H5"	2.20	0.40
1:B:24:ILE:N	1:B:24:ILE:HD13	2.36	0.40
1:B:209:PRO:O	1:B:482:LEU:HD11	2.22	0.40
1:B:429:ASN:OD1	1:B:429:ASN:C	2.59	0.40
2:D:423:ASN:C	2:D:425:ALA:H	2.24	0.40
1:A:167:SER:C	1:A:168:THR:HG23	2.40	0.40
1:A:293:ARG:NH1	1:A:293:ARG:HB3	2.36	0.40
2:C:479:MET:HE1	2:C:518:LEU:HD22	2.02	0.40
1:A:209:PRO:O	1:A:482:LEU:HD11	2.22	0.40
1:A:247:LEU:HB3	1:A:251:LYS:HB2	2.03	0.40
1:A:282:ALA:O	1:A:284:ILE:N	2.55	0.40
1:B:244:ILE:HD12	1:B:244:ILE:C	2.40	0.40
1:B:282:ALA:O	1:B:284:ILE:N	2.55	0.40
1:A:424:LEU:HD23	1:A:424:LEU:HA	1.91	0.40
1:B:144:ASN:N	1:B:144:ASN:ND2	2.66	0.40
1:B:280:LYS:HB3	1:B:314:TYR:OH	2.22	0.40
1:B:293:ARG:HB3	1:B:293:ARG:NH1	2.36	0.40
1:B:456:GLU:CG	1:B:460:TYR:HE2	2.21	0.40
2:C:496:ALA:CB	2:C:497:ASN:HB2	2.43	0.40
2:C:516:THR:HG23	2:C:622:MET:SD	2.61	0.40
2:D:577:LEU:HD12	2:D:578:GLN:N	2.36	0.40
2:D:637:VAL:CG1	2:D:639:PHE:CE2	3.05	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	479/496 (97%)	435 (91%)	34 (7%)	10 (2%)	7	26
1	B	479/496 (97%)	435 (91%)	34 (7%)	10 (2%)	7	26
2	C	214/268 (80%)	190 (89%)	17 (8%)	7 (3%)	4	15
2	D	214/268 (80%)	189 (88%)	18 (8%)	7 (3%)	4	15
All	All	1386/1528 (91%)	1249 (90%)	103 (7%)	34 (2%)	5	21

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	485	ALA
2	C	493	ILE
2	C	572	GLY
2	C	610	ASP
2	C	626	VAL
2	D	485	ALA
2	D	493	ILE
2	D	572	GLY
2	D	610	ASP
2	D	626	VAL
1	A	210	GLY
1	B	210	GLY
1	A	52	SER
1	A	169	GLY
1	A	209	PRO
1	A	283	GLY
1	A	307	ASN
1	B	52	SER
1	B	169	GLY
1	B	209	PRO
1	B	283	GLY
1	B	307	ASN

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Mol	Chain	Res	Type
2	C	497	ASN
2	D	497	ASN
1	A	305	ASP
1	B	305	ASP
2	C	465	ALA
2	D	465	ALA
1	A	61	LYS
1	A	293	ARG
1	B	61	LYS
1	B	293	ARG
1	A	221	GLY
1	B	221	GLY

5.3.2 Protein sidechains (i)

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	377/431 (88%)	338 (90%)	39 (10%)	7 22
1	B	373/431 (86%)	336 (90%)	37 (10%)	8 24
2	C	163/224 (73%)	139 (85%)	24 (15%)	3 9
2	D	163/224 (73%)	138 (85%)	25 (15%)	2 8
All	All	1076/1310 (82%)	951 (88%)	125 (12%)	5 16

All (125) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ILE
1	A	9	LEU
1	A	24	ILE
1	A	28	ARG
1	A	61	LYS
1	A	70	MET
1	A	91	ASN
1	A	96	GLU
1	A	97	ILE

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Mol	Chain	Res	Type
1	A	100	GLU
1	A	102	HIS
1	A	111	ASP
1	A	139	VAL
1	A	144	ASN
1	A	162	LEU
1	A	174	TYR
1	A	177	ASP
1	A	183	LEU
1	A	201	ILE
1	A	208	LEU
1	A	215	THR
1	A	223	ASP
1	A	247	LEU
1	A	254	ILE
1	A	263	ILE
1	A	268	LEU
1	A	293	ARG
1	A	302	LEU
1	A	319	THR
1	A	324	ASN
1	A	326	ASN
1	A	334	ASN
1	A	347	SER
1	A	372	LEU
1	A	385	LEU
1	A	428	THR
1	A	443	ARG
1	A	448	MET
1	A	462	LEU
1	B	4	ILE
1	B	9	LEU
1	B	24	ILE
1	B	28	ARG
1	B	61	LYS
1	B	70	MET
1	B	91	ASN
1	B	96	GLU
1	B	97	ILE
1	B	100	GLU
1	B	102	HIS
1	B	111	ASP

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Mol	Chain	Res	Type
1	B	139	VAL
1	B	144	ASN
1	B	162	LEU
1	B	174	TYR
1	B	177	ASP
1	B	183	LEU
1	B	201	ILE
1	B	208	LEU
1	B	215	THR
1	B	254	ILE
1	B	263	ILE
1	B	268	LEU
1	B	293	ARG
1	B	302	LEU
1	B	319	THR
1	B	324	ASN
1	B	326	ASN
1	B	334	ASN
1	B	347	SER
1	B	372	LEU
1	B	385	LEU
1	B	428	THR
1	B	443	ARG
1	B	448	MET
1	B	462	LEU
2	C	416	LEU
2	C	420	GLN
2	C	429	LEU
2	C	435	ASP
2	C	445	ARG
2	C	450	GLN
2	C	456	ARG
2	C	460	ILE
2	C	475	GLU
2	C	476	ILE
2	C	487	VAL
2	C	524	ARG
2	C	529	LEU
2	C	551	LYS
2	C	552	LYS
2	C	561	ASP
2	C	564	LEU

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Mol	Chain	Res	Type
2	C	591	LEU
2	C	595	THR
2	C	602	THR
2	C	608	ILE
2	C	613	ARG
2	C	639	PHE
2	C	640	THR
2	D	416	LEU
2	D	420	GLN
2	D	429	LEU
2	D	435	ASP
2	D	445	ARG
2	D	450	GLN
2	D	456	ARG
2	D	460	ILE
2	D	475	GLU
2	D	476	ILE
2	D	487	VAL
2	D	524	ARG
2	D	529	LEU
2	D	551	LYS
2	D	552	LYS
2	D	561	ASP
2	D	564	LEU
2	D	586	MET
2	D	591	LEU
2	D	595	THR
2	D	602	THR
2	D	608	ILE
2	D	613	ARG
2	D	639	PHE
2	D	640	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	GLN
1	A	68	ASN
1	A	91	ASN
1	A	94	ASN
1	A	144	ASN
1	A	324	ASN

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Mol	Chain	Res	Type
1	A	328	ASN
1	A	334	ASN
1	A	352	HIS
1	B	5	GLN
1	B	68	ASN
1	B	91	ASN
1	B	94	ASN
1	B	144	ASN
1	B	324	ASN
1	B	328	ASN
1	B	334	ASN
1	B	352	HIS
2	C	450	GLN
2	D	450	GLN

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

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 2 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	LFX	F	0	-	29,29,29	2.35	8 (27%)	44,44,44	2.19	11 (25%)
8	LFX	H	0	-	29,29,29	2.35	7 (24%)	44,44,44	2.23	13 (29%)

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	LFX	F	0	-	-	2/8/27/27	0/4/4/4
8	LFX	H	0	-	-	2/8/27/27	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	F	0	LFX	O01-C06	-7.07	1.26	1.37
8	H	0	LFX	O01-C06	-7.05	1.26	1.37
8	F	0	LFX	C17-C	-5.57	1.39	1.48
8	H	0	LFX	C17-C	-5.45	1.39	1.48
8	F	0	LFX	O01-C09	-3.79	1.34	1.44
8	H	0	LFX	O01-C09	-3.77	1.34	1.44
8	F	0	LFX	C10-C15	-3.64	1.41	1.48
8	H	0	LFX	C10-C15	-3.54	1.41	1.48
8	H	0	LFX	C03-N02	-2.48	1.44	1.49
8	F	0	LFX	O03-C	-2.23	1.24	1.30
8	F	0	LFX	C03-N02	-2.22	1.45	1.49
8	H	0	LFX	F-C11	-2.18	1.30	1.35
8	H	0	LFX	O03-C	-2.08	1.24	1.30
8	F	0	LFX	C08-N	2.04	1.50	1.46
8	F	0	LFX	F-C11	-2.03	1.30	1.35

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	0	LFX	C09-O01-C06	6.73	127.36	114.11
8	F	0	LFX	C09-O01-C06	6.63	127.16	114.11
8	F	0	LFX	C16-N-C08	6.17	119.90	110.66
8	H	0	LFX	C16-N-C08	5.80	119.33	110.66
8	H	0	LFX	C10-C15-C17	4.69	121.55	115.59
8	H	0	LFX	O03-C-O	-4.51	113.30	123.61
8	F	0	LFX	O03-C-O	-4.40	113.53	123.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	F	0	LFX	C10-C15-C17	4.30	121.06	115.59
8	F	0	LFX	C16-N-C07	3.46	115.84	110.66
8	H	0	LFX	C16-N-C07	3.43	115.80	110.66
8	H	0	LFX	C12-C17-C15	-3.16	117.54	119.88
8	F	0	LFX	C12-C17-C15	-2.72	117.86	119.88
8	H	0	LFX	C17-C12-N02	-2.66	121.51	124.49
8	F	0	LFX	C02-N01-C01	2.64	117.35	111.52
8	H	0	LFX	C08-N-C07	2.45	112.95	109.52
8	F	0	LFX	C17-C12-N02	-2.44	121.75	124.49
8	F	0	LFX	C08-N-C07	2.40	112.89	109.52
8	H	0	LFX	C05-C10-C15	-2.39	118.05	121.08
8	F	0	LFX	C05-C10-C15	-2.35	118.10	121.08
8	H	0	LFX	C02-N01-C01	2.35	116.70	111.52
8	H	0	LFX	O02-C15-C17	-2.32	119.33	123.22
8	F	0	LFX	C06-C04-C11	2.32	117.98	116.02
8	H	0	LFX	C09-C03-N02	2.09	111.48	107.41
8	H	0	LFX	C02-N01-C04	2.03	125.80	119.44

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	F	0	LFX	O03-C-C17-C12
8	F	0	LFX	O03-C-C17-C15
8	H	0	LFX	O03-C-C17-C12
8	H	0	LFX	O03-C-C17-C15

There are no ring outliers.

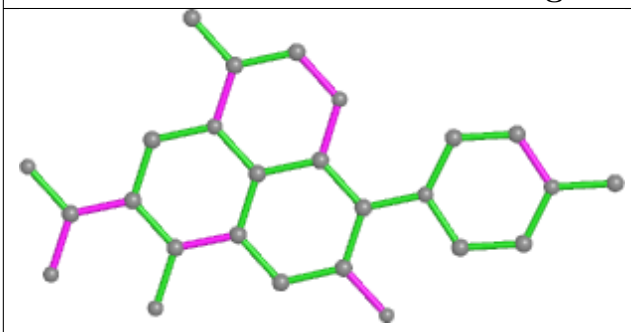
2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	0	LFX	5	0
8	H	0	LFX	5	0

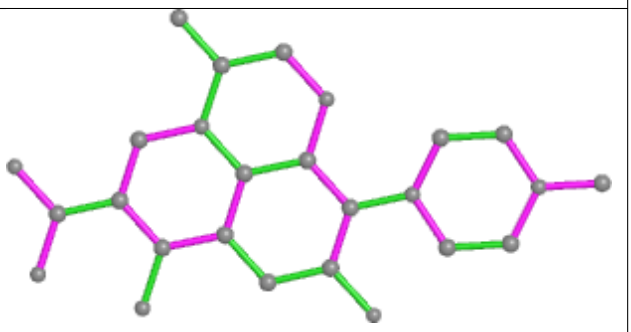
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

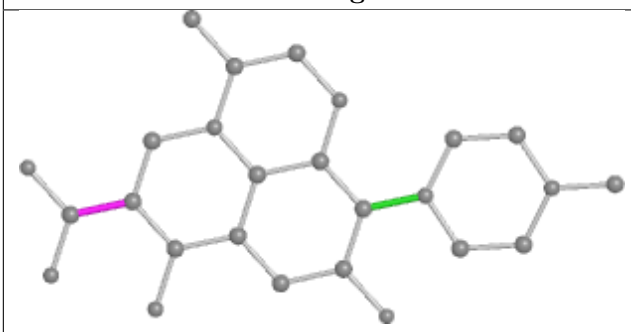
Ligand LFX F 0



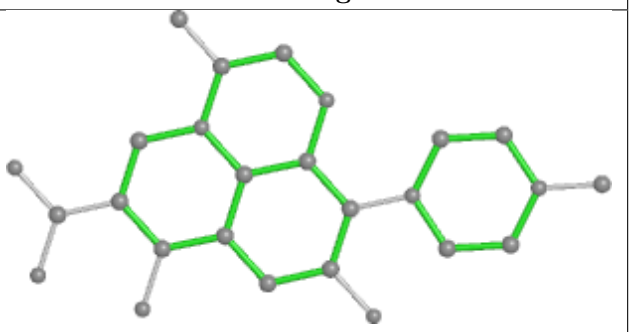
Bond lengths



Bond angles

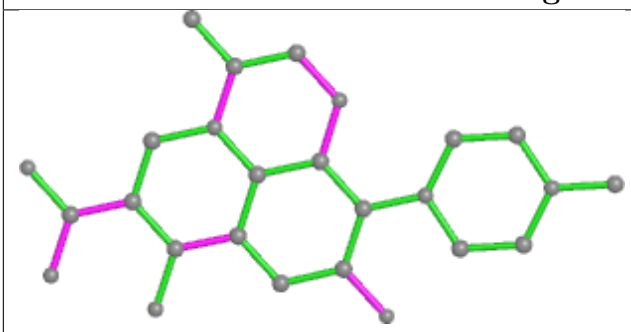


Torsions

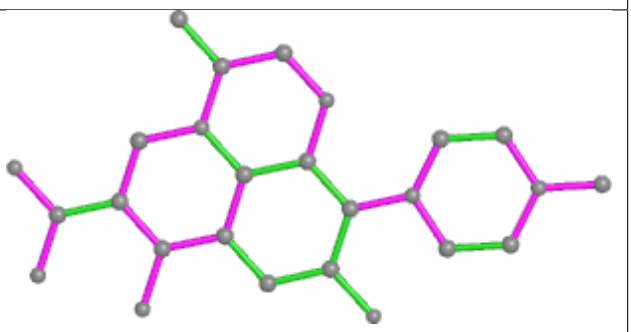


Rings

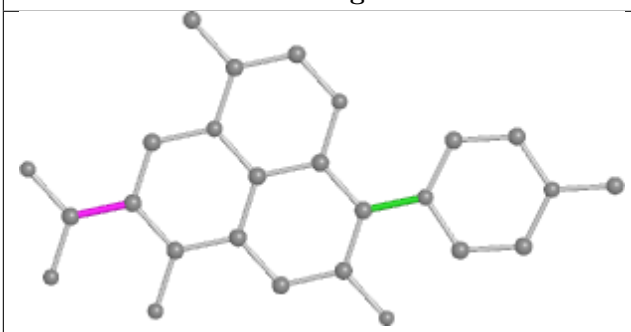
Ligand LFX H 0



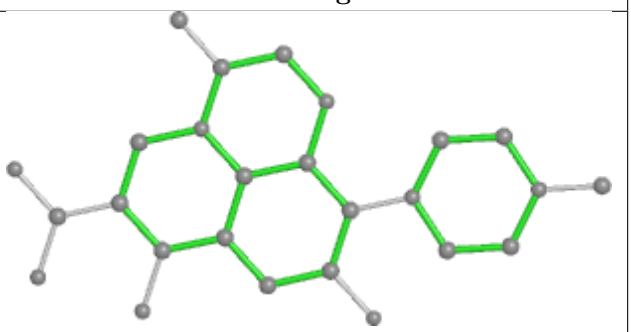
Bond lengths



Bond angles



Torsions



Rings

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

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, 95^{th} 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	481/496 (96%)	0.03	3 (0%) 89 89	45, 82, 134, 194	0
1	B	481/496 (96%)	0.06	5 (1%) 82 82	45, 82, 134, 194	0
2	C	222/268 (82%)	0.07	3 (1%) 75 75	56, 92, 133, 153	0
2	D	222/268 (82%)	0.07	1 (0%) 91 91	56, 92, 133, 153	0
3	E	7/15 (46%)	0.23	0 100 100	60, 69, 105, 156	0
4	F	11/19 (57%)	-0.16	0 100 100	59, 84, 113, 134	0
5	G	7/15 (46%)	0.25	0 100 100	58, 68, 114, 167	0
6	H	11/19 (57%)	-0.21	0 100 100	60, 88, 103, 139	0
All	All	1442/1596 (90%)	0.05	12 (0%) 86 86	45, 85, 134, 194	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	284	ILE	4.5
1	A	283	GLY	4.0
1	A	302	LEU	3.3
1	B	284	ILE	3.0
1	B	283	GLY	2.9
1	B	302	LEU	2.7
2	C	494	GLU	2.2
2	D	494	GLU	2.2
1	B	306	ALA	2.1
2	C	639	PHE	2.1
1	B	298	ILE	2.0
2	C	567	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

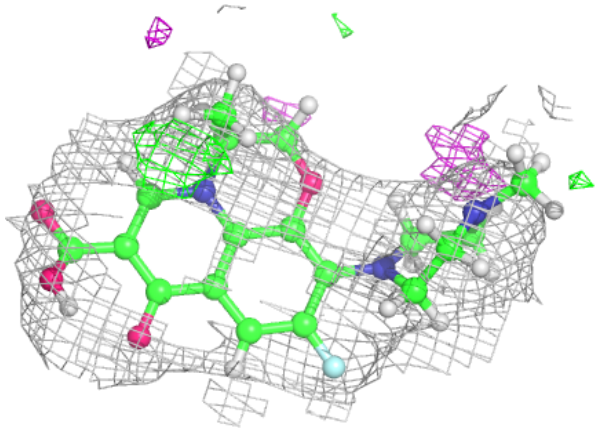
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

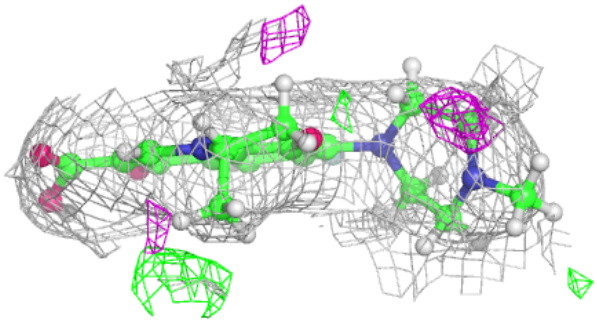
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	MG	C	742	1/1	0.85	0.24	70,70,70,70	0
7	MG	D	742	1/1	0.90	0.22	70,70,70,70	0
8	LFX	F	0	26/26	0.96	0.21	60,102,160,203	0
8	LFX	H	0	26/26	0.96	0.22	61,111,156,209	0

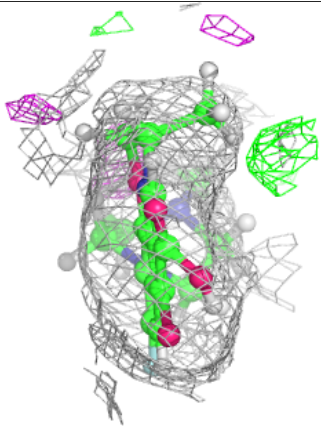
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around LFX F 0:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

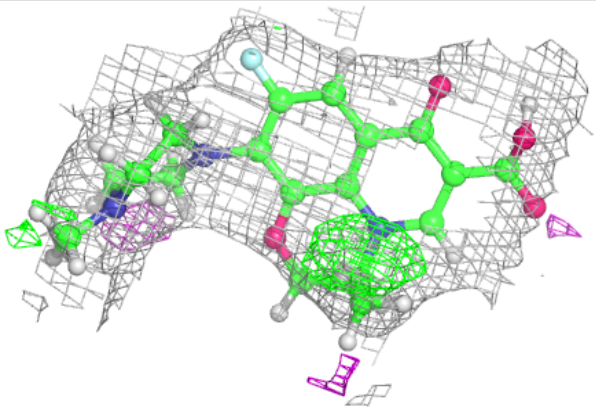


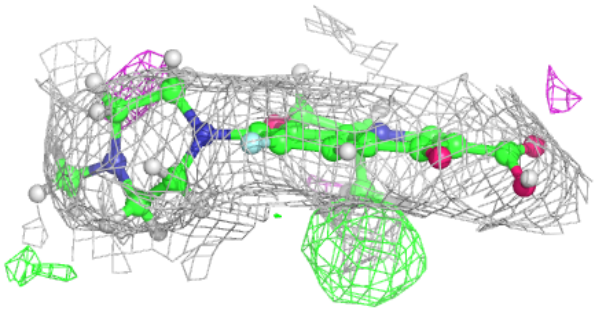


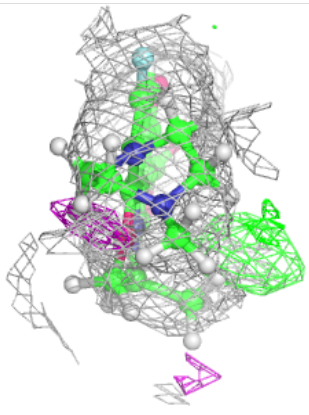


Electron density around LFX H 0:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.