Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2022 – 04:11 pm BST

PDB ID	:	7R07
Title	:	Abortive infection DNA polymerase AbiK from Lactococcus lactis
Authors	:	Figiel, M.; Gapinska, M.; Czarnocki-Cieciura, M.; Zajko, W.; Nowotny, M.
Deposited on	:	2022-02-01
Resolution	:	3.10 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 (i) 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 (1)) were used in the production of this report:

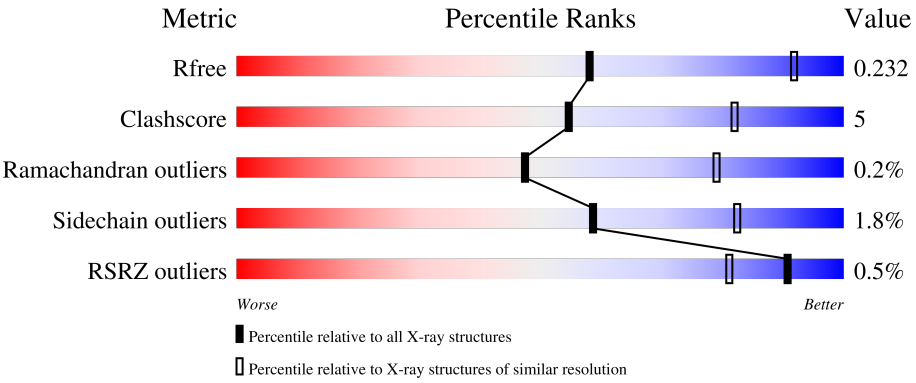
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.30
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0267
CCP4	:	7.1.010 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.30

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 3.10 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	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	601	% 86% 14%
1	B	601	% 82% 17%
1	C	601	86% 13% •
1	D	601	84% 15% ••
1	E	601	84% 15% •

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Mol	Chain	Length	Quality of chain
1	F	601	83% 16%
2	G	11	73% 9% 18%
2	H	11	18% 64% 18% 18%
2	I	11	73% 9% 18%
2	J	11	9% 55% 18% 27%
2	K	11	55% 27% 18%
2	L	11	64% 27% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	602	-	-	-	X

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 30644 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called AbiK.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	598	Total	C	N	O	P	S	0	0	0
			4954	3202	790	941	1	20			
1	B	598	Total	C	N	O	P	S	0	0	0
			4928	3185	785	937	1	20			
1	C	599	Total	C	N	O	P	S	0	0	0
			4977	3220	796	940	1	20			
1	D	597	Total	C	N	O	P	S	0	0	0
			4927	3187	788	931	1	20			
1	E	597	Total	C	N	O	P	S	0	0	0
			4953	3205	790	937	1	20			
1	F	600	Total	C	N	O	P	S	0	0	0
			4960	3210	792	937	1	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q48614
A	0	SER	-	expression tag	UNP Q48614
B	-1	GLY	-	expression tag	UNP Q48614
B	0	SER	-	expression tag	UNP Q48614
C	-1	GLY	-	expression tag	UNP Q48614
C	0	SER	-	expression tag	UNP Q48614
D	-1	GLY	-	expression tag	UNP Q48614
D	0	SER	-	expression tag	UNP Q48614
E	-1	GLY	-	expression tag	UNP Q48614
E	0	SER	-	expression tag	UNP Q48614
F	-1	GLY	-	expression tag	UNP Q48614
F	0	SER	-	expression tag	UNP Q48614

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	9	Total	C	N	O	P	0	0	0
			141	68	22	44	7			
2	H	9	Total	C	N	O	P	0	0	0
			164	81	27	49	7			
2	I	9	Total	C	N	O	P	0	0	0
			145	68	22	47	8			
2	J	8	Total	C	N	O	P	0	0	0
			138	68	22	42	6			
2	K	9	Total	C	N	O	P	0	0	0
			153	73	23	49	8			
2	L	10	Total	C	N	O	P	0	0	0
			179	86	28	56	9			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	2	Total	Mg	0	0
			2	2		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	I	1	Total	Mg	0	0
			1	1		
3	K	1	Total	Mg	0	0
			1	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	C	3	Total	O	0	0
			3	3		
4	D	3	Total	O	0	0
			3	3		
4	E	3	Total	O	0	0
			3	3		

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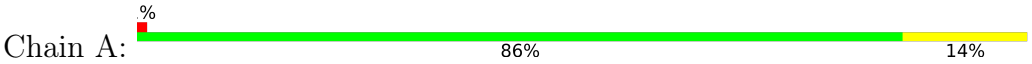
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	F	3	Total O 3 3	0	0

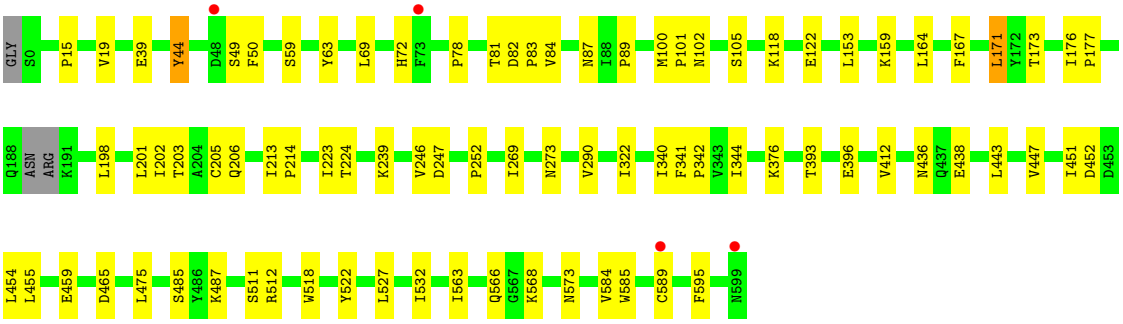
3 Residue-property plots (i)

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: AbiK

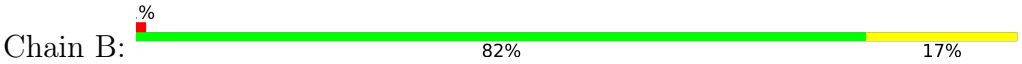
Chain A:

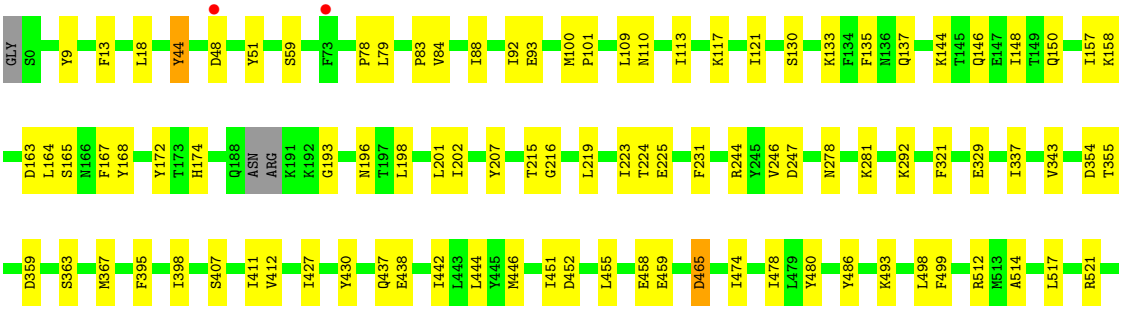




• Molecule 1: AbiK

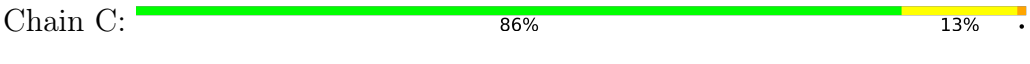
Chain B:

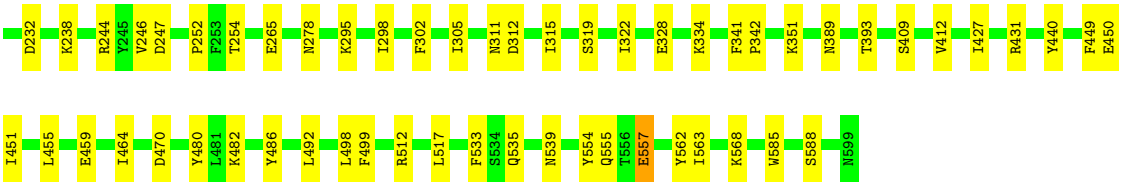




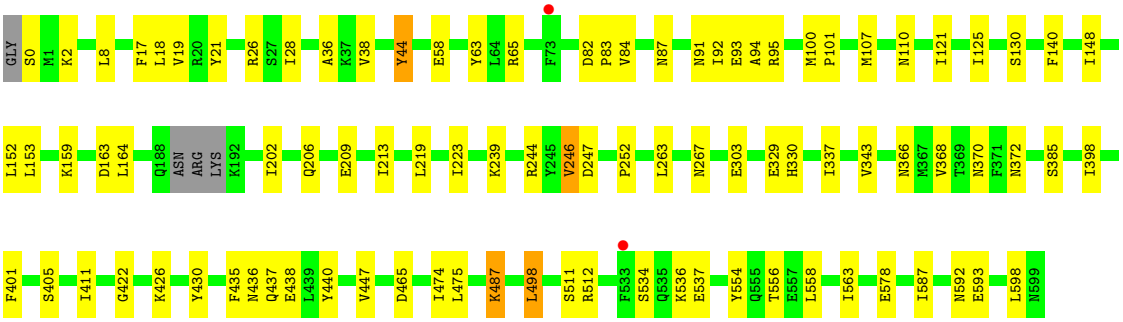
• Molecule 1: AbiK

Chain C:

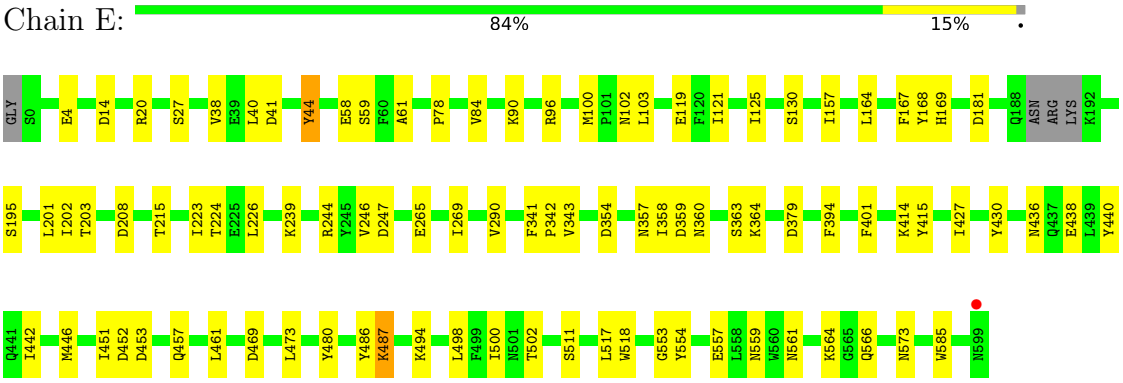




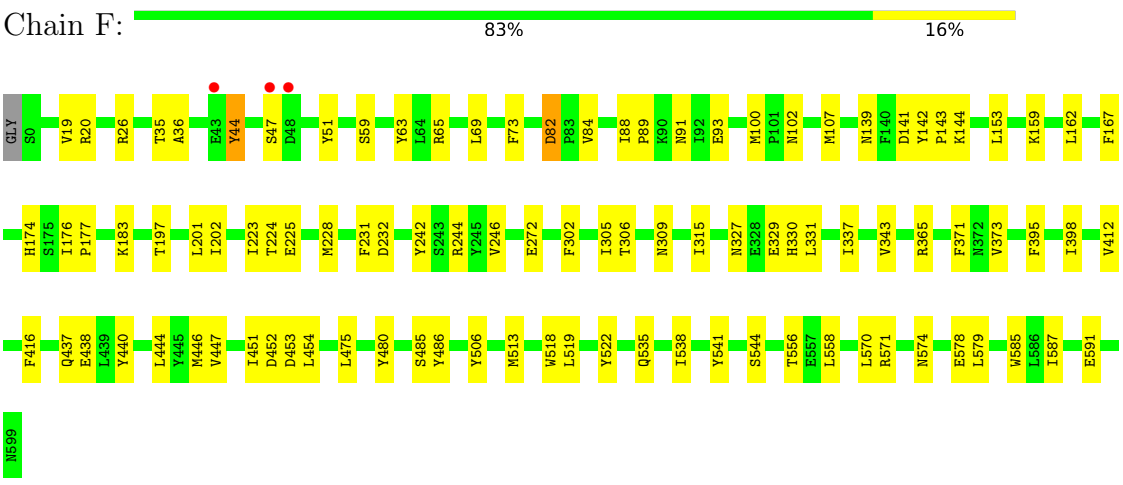
• Molecule 1: AbiK



• Molecule 1: AbiK

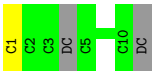


• Molecule 1: AbiK



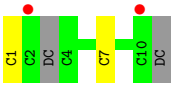
• Molecule 2: DNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')

Chain G:



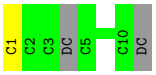
• Molecule 2: DNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')

Chain H:



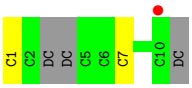
• Molecule 2: DNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')

Chain I:



• Molecule 2: DNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')

Chain J:



• Molecule 2: DNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')

Chain K:

• Molecule 2: DNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')

Chain L:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 62 2 2	Depositor
Cell constants a, b, c, α, β, γ	200.99Å 200.99Å 570.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.63 – 3.10 49.72 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.63-3.10) 90.5 (49.72-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.74 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.189 , 0.232 0.189 , 0.232	Depositor DCC
R_{free} test set	2094 reflections (1.70%)	wwPDB-VP
Wilson B-factor (Å^2)	103.7	Xtriage
Anisotropy	0.140	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	(Not available) , (Not available)	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	30644	wwPDB-VP
Average B, all atoms (Å^2)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.66% 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, PTR

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	0.25	0/5056	0.40	0/6832
1	B	0.25	0/5030	0.39	0/6802
1	C	0.25	0/5079	0.40	0/6857
1	D	0.25	0/5029	0.39	0/6797
1	E	0.25	0/5055	0.39	0/6828
1	F	0.25	0/5063	0.39	0/6843
2	G	0.56	0/154	0.80	0/233
2	H	0.49	0/180	0.75	0/271
2	I	0.57	0/158	0.78	0/238
2	J	0.47	0/151	0.72	0/227
2	K	0.63	0/167	0.82	0/251
2	L	0.60	0/197	0.86	0/299
All	All	0.27	0/31319	0.42	0/42478

There are no bond length outliers.

There are no bond angle outliers.

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	4954	0	4701	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4928	0	4645	60	0
1	C	4977	0	4761	46	0
1	D	4927	0	4670	54	0
1	E	4953	0	4722	52	0
1	F	4960	0	4713	54	0
2	G	141	0	81	2	0
2	H	164	0	100	3	0
2	I	145	0	82	2	0
2	J	138	0	84	3	0
2	K	153	0	91	4	0
2	L	179	0	105	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	I	1	0	0	0	0
3	K	1	0	0	0	0
4	A	4	0	0	0	0
4	C	3	0	0	0	0
4	D	3	0	0	0	0
4	E	3	0	0	0	0
4	F	3	0	0	0	0
All	All	30644	0	28755	306	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 5.

All (306) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:44:PTR:O3P	2:J:1:DC:C5'	1.68	1.42
1:F:44:PTR:O1P	2:L:1:DC:C5'	1.68	1.42
1:C:44:PTR:O3P	2:I:1:DC:C5'	1.68	1.41
1:B:44:PTR:O3P	2:H:1:DC:C5'	1.68	1.40
1:A:44:PTR:O1P	2:G:1:DC:C5'	1.68	1.40
1:E:44:PTR:O3P	2:K:1:DC:C5'	1.68	1.39
1:C:535:GLN:O	1:C:539:ASN:ND2	2.13	0.81
1:C:44:PTR:P	2:I:1:DC:C5'	2.67	0.81
1:D:44:PTR:P	2:J:1:DC:C5'	2.69	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:44:PTR:P	2:H:1:DC:C5'	2.70	0.80
1:C:498:LEU:HD22	1:C:517:LEU:HD11	1.62	0.79
1:D:593:GLU:N	1:D:593:GLU:OE2	2.16	0.77
1:E:44:PTR:P	2:K:1:DC:C5'	2.74	0.76
1:A:44:PTR:P	2:G:1:DC:C5'	2.74	0.75
1:C:238:LYS:HD3	1:C:265:GLU:HG2	1.68	0.75
1:B:9:TYR:HB3	1:B:121:ILE:HD12	1.70	0.74
1:B:18:LEU:HB3	1:B:110:ASN:HD21	1.54	0.72
1:D:246:VAL:HG13	1:D:247:ASP:H	1.54	0.71
1:E:359:ASP:O	1:E:363:SER:OG	2.08	0.71
1:D:202:ILE:HD13	1:D:213:ILE:HD11	1.73	0.70
1:F:44:PTR:P	2:L:1:DC:C5'	2.79	0.70
1:E:202:ILE:HD11	1:E:223:ILE:HD13	1.71	0.70
1:F:232:ASP:OD2	1:F:244:ARG:NH2	2.26	0.68
1:D:92:ILE:HG22	1:D:93:GLU:HG2	1.75	0.68
1:B:88:ILE:HG22	1:B:437:GLN:HB2	1.77	0.67
1:F:535:GLN:HA	1:F:538:ILE:HB	1.77	0.66
1:A:376:LYS:NZ	1:C:150:GLN:OE1	2.29	0.66
1:A:527:LEU:HD22	1:A:532:ILE:HG13	1.79	0.65
1:B:521:ARG:NH2	1:B:557:GLU:OE1	2.30	0.64
1:A:512:ARG:HG3	1:A:563:ILE:HD12	1.78	0.64
1:C:202:ILE:HD11	1:C:223:ILE:HD13	1.79	0.64
1:E:502:THR:HG21	1:E:517:LEU:HD11	1.79	0.64
1:B:446:MET:HA	1:B:451:ILE:HD12	1.78	0.64
1:B:18:LEU:HB3	1:B:110:ASN:ND2	2.13	0.64
1:B:359:ASP:O	1:B:363:SER:OG	2.14	0.64
1:C:498:LEU:HD22	1:C:517:LEU:CD1	2.29	0.63
1:C:157:ILE:HG23	1:C:158:LYS:HG3	1.80	0.63
1:E:78:PRO:HG3	1:E:201:LEU:HD23	1.81	0.62
1:A:412:VAL:HG12	1:A:451:ILE:HD11	1.82	0.61
1:C:84:VAL:HB	1:C:100:MET:HB2	1.82	0.61
1:E:84:VAL:HB	1:E:100:MET:HB2	1.83	0.61
1:D:153:LEU:HA	1:D:252:PRO:HG3	1.83	0.61
1:D:202:ILE:HD11	1:D:223:ILE:HD13	1.83	0.60
1:E:164:LEU:HB2	1:E:247:ASP:HB2	1.82	0.60
1:B:167:PHE:HE2	1:B:224:THR:HG23	1.67	0.60
1:E:343:VAL:HG12	2:K:7:DC:C6	2.38	0.59
1:C:164:LEU:HB2	1:C:247:ASP:HB2	1.84	0.59
1:E:358:ILE:HD12	1:E:401:PHE:HB3	1.85	0.59
1:D:474:ILE:HD13	1:D:587:ILE:HG12	1.84	0.59
1:C:498:LEU:CD2	1:C:517:LEU:HD11	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LYS:O	1:B:121:ILE:HG12	2.03	0.58
1:B:84:VAL:HB	1:B:100:MET:HB2	1.86	0.58
1:F:225:GLU:OE1	1:F:244:ARG:NH1	2.33	0.58
1:C:167:PHE:HE2	1:C:224:THR:HG23	1.69	0.57
1:F:447:VAL:HG11	1:F:475:LEU:HD22	1.86	0.57
1:D:153:LEU:HD13	1:D:159:LYS:HE3	1.87	0.57
1:B:455:LEU:HD22	1:B:459:GLU:HB3	1.87	0.57
1:D:87:ASN:H	1:D:436:ASN:HB2	1.70	0.57
1:B:157:ILE:HG22	1:B:158:LYS:HG3	1.86	0.56
1:C:21:TYR:HE1	1:C:26:ARG:HH21	1.52	0.56
1:C:153:LEU:HA	1:C:252:PRO:HG3	1.87	0.56
1:C:464:ILE:HG22	1:C:498:LEU:HD12	1.88	0.56
1:E:40:LEU:HD12	1:E:41:ASP:N	2.20	0.56
1:F:416:PHE:HD2	1:F:454:LEU:HG	1.69	0.56
1:A:101:PRO:HB3	1:A:205:CYS:HB3	1.87	0.56
1:A:522:TYR:OH	1:A:584:VAL:O	2.18	0.56
1:E:487:LYS:H	1:E:487:LYS:HD2	1.71	0.56
1:A:167:PHE:HE2	1:A:224:THR:HG23	1.71	0.55
1:B:367:MET:SD	1:D:0:SER:N	2.75	0.55
1:B:193:GLY:H	1:B:196:ASN:HB2	1.71	0.55
1:F:343:VAL:HG12	2:L:6:DC:C2	2.42	0.55
1:C:168:TYR:HB3	1:C:215:THR:HG21	1.89	0.54
1:F:183:LYS:HD2	1:F:272:GLU:HG3	1.90	0.54
1:D:84:VAL:HB	1:D:100:MET:HB2	1.88	0.54
1:A:78:PRO:HG3	1:A:201:LEU:HD12	1.89	0.54
1:F:36:ALA:O	1:F:65:ARG:NH2	2.41	0.54
1:F:315:ILE:HG23	1:F:373:VAL:HG13	1.90	0.54
1:B:512:ARG:HB3	1:B:521:ARG:NH1	2.23	0.53
1:A:118:LYS:O	1:A:122:GLU:HG2	2.08	0.53
1:E:436:ASN:HB2	1:E:469:ASP:OD1	2.09	0.53
1:F:59:SER:HB2	1:F:585:TRP:CE2	2.44	0.53
1:B:407:SER:O	1:B:411:ILE:HG12	2.09	0.53
1:B:499:PHE:HB3	1:B:521:ARG:HH21	1.73	0.53
1:A:164:LEU:HB2	1:A:247:ASP:HB2	1.89	0.52
1:C:389:ASN:O	1:C:393:THR:HG23	2.09	0.52
1:D:368:VAL:HG22	1:E:4:GLU:HG3	1.91	0.52
1:A:447:VAL:HG11	1:A:475:LEU:HD22	1.92	0.52
1:D:163:ASP:OD1	1:D:164:LEU:N	2.42	0.52
1:E:500:ILE:HG13	1:E:557:GLU:HG3	1.92	0.52
1:D:405:SER:HB3	1:D:598:LEU:HD12	1.92	0.51
1:E:38:VAL:HG13	1:E:58:GLU:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:598:LEU:H	1:D:598:LEU:HD23	1.75	0.51
1:F:82:ASP:OD2	1:F:506:TYR:OH	2.27	0.51
1:B:146:GLN:O	1:B:150:GLN:HG3	2.10	0.51
1:D:330:HIS:CE1	1:E:290:VAL:HG22	2.46	0.51
1:A:102:ASN:HA	1:A:518:TRP:CE2	2.46	0.51
1:E:181:ASP:OD2	1:E:195:SER:OG	2.25	0.51
1:B:13:PHE:HB3	1:B:117:LYS:HG2	1.93	0.50
1:E:168:TYR:CG	2:K:11:DC:H2"	2.46	0.50
1:B:78:PRO:HA	1:B:571:ARG:HH12	1.76	0.50
1:C:295:LYS:NZ	1:C:334:LYS:O	2.36	0.50
1:D:130:SER:HB2	1:D:244:ARG:NH2	2.27	0.50
1:F:88:ILE:HG22	1:F:437:GLN:HB2	1.93	0.50
1:C:450:GLU:OE2	1:C:482:LYS:NZ	2.40	0.50
1:D:534:SER:HB3	1:D:537:GLU:HB2	1.94	0.50
1:B:92:ILE:HG22	1:B:93:GLU:HG3	1.94	0.50
1:A:63:TYR:HE2	1:A:69:LEU:HD21	1.77	0.50
1:A:213:ILE:HG12	1:A:214:PRO:HD2	1.92	0.50
1:D:512:ARG:HG3	1:D:563:ILE:HD12	1.94	0.50
1:F:20:ARG:NH1	1:F:35:THR:O	2.44	0.49
1:F:102:ASN:HA	1:F:518:TRP:CE2	2.47	0.49
1:F:26:ARG:HG2	1:F:47:SER:HB2	1.94	0.49
1:F:142:TYR:HB3	1:F:143:PRO:HD3	1.94	0.49
1:F:343:VAL:HG12	2:L:6:DC:O2	2.12	0.49
1:F:570:LEU:HD13	1:F:574:ASN:OD1	2.11	0.49
1:B:427:ILE:HD11	1:B:442:ILE:HG21	1.94	0.49
1:C:302:PHE:O	1:C:351:LYS:NZ	2.43	0.49
1:D:83:PRO:HB3	1:D:101:PRO:HA	1.93	0.49
1:F:167:PHE:HE2	1:F:224:THR:HG23	1.76	0.49
1:D:36:ALA:O	1:D:65:ARG:NH1	2.46	0.49
1:E:265:GLU:O	1:E:269:ILE:HG12	2.12	0.49
1:E:498:LEU:O	1:E:502:THR:HG23	2.12	0.49
1:C:90:LYS:HE2	1:C:96:ARG:CZ	2.43	0.49
1:C:409:SER:OG	1:C:449:PHE:O	2.26	0.49
1:D:148:ILE:O	1:D:152:LEU:HD22	2.13	0.49
1:E:40:LEU:HD12	1:E:41:ASP:H	1.78	0.49
1:F:202:ILE:HD11	1:F:223:ILE:HD13	1.95	0.49
1:C:499:PHE:HB3	1:C:557:GLU:HG2	1.95	0.48
1:D:18:LEU:HB2	1:D:110:ASN:HD21	1.78	0.48
1:D:21:TYR:HB3	1:D:26:ARG:HB2	1.95	0.48
1:D:556:THR:HG22	1:D:558:LEU:H	1.78	0.48
1:F:84:VAL:HB	1:F:100:MET:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:427:ILE:HD11	1:E:442:ILE:HG21	1.96	0.48
1:D:38:VAL:HG13	1:D:58:GLU:HB3	1.95	0.48
1:D:263:LEU:O	1:D:267:ASN:ND2	2.46	0.48
1:F:91:ASN:HB2	1:F:93:GLU:H	1.78	0.48
1:B:168:TYR:HB3	1:B:215:THR:HG21	1.96	0.48
1:E:457:GLN:HE22	1:E:487:LYS:HD2	1.79	0.47
1:B:198:LEU:O	1:B:202:ILE:HG12	2.14	0.47
1:B:329:GLU:HB2	1:B:337:ILE:HG13	1.96	0.47
1:C:311:ASN:O	1:C:315:ILE:HG13	2.13	0.47
1:E:360:ASN:O	1:E:364:LYS:HB2	2.14	0.47
1:F:395:PHE:HA	1:F:398:ILE:HG12	1.96	0.47
1:B:79:LEU:HD21	1:B:514:ALA:HB2	1.96	0.47
1:B:354:ASP:OD1	1:B:355:THR:N	2.47	0.47
1:C:44:PTR:HD1	1:C:44:PTR:HA	1.78	0.47
1:C:59:SER:HB2	1:C:585:TRP:CE2	2.49	0.47
1:B:163:ASP:OD1	1:B:164:LEU:N	2.47	0.47
1:B:83:PRO:HB3	1:B:101:PRO:HA	1.96	0.47
1:C:427:ILE:O	1:C:431:ARG:HG3	2.14	0.47
1:E:130:SER:HB2	1:E:244:ARG:NH2	2.30	0.47
1:F:452:ASP:OD1	1:F:453:ASP:N	2.48	0.47
1:A:59:SER:HB2	1:A:585:TRP:CE2	2.49	0.47
1:E:96:ARG:HD2	1:E:169:HIS:NE2	2.30	0.47
1:A:84:VAL:HB	1:A:100:MET:HB2	1.97	0.47
1:A:153:LEU:HA	1:A:252:PRO:HG3	1.97	0.47
1:B:474:ILE:O	1:B:478:ILE:HG13	2.15	0.47
1:A:87:ASN:N	1:A:436:ASN:OD1	2.43	0.46
1:C:568:LYS:HE3	1:C:568:LYS:HB2	1.70	0.46
1:D:366:ASN:O	1:D:370:ASN:N	2.42	0.46
1:D:329:GLU:HB2	1:D:337:ILE:HG13	1.97	0.46
1:E:553:GLY:HA3	1:E:559:ASN:ND2	2.30	0.46
1:C:232:ASP:OD2	1:C:244:ARG:NH2	2.46	0.46
1:A:443:LEU:O	1:A:447:VAL:HG12	2.16	0.46
1:D:536:LYS:HE2	1:D:536:LYS:HB3	1.79	0.46
1:F:365:ARG:HA	1:F:371:PHE:O	2.15	0.46
1:B:130:SER:HB3	1:B:133:LYS:HD3	1.98	0.46
1:E:354:ASP:HB3	1:E:357:ASN:HD22	1.81	0.46
1:A:340:ILE:O	1:A:344:ILE:HG13	2.16	0.46
1:E:167:PHE:HE2	1:E:224:THR:HG23	1.80	0.46
1:F:174:HIS:O	1:F:177:PRO:HD2	2.15	0.46
1:B:278:ASN:OD1	1:B:281:LYS:HG2	2.16	0.45
1:A:290:VAL:HG22	1:F:330:HIS:CE1	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:ILE:HD11	1:C:328:GLU:HG2	1.98	0.45
1:E:203:THR:HB	1:E:208:ASP:HA	1.99	0.45
1:A:176:ILE:HB	1:A:177:PRO:HD3	1.98	0.45
1:B:130:SER:HB2	1:B:244:ARG:NH1	2.32	0.45
1:A:173:THR:HG21	1:A:203:THR:HG23	1.99	0.45
1:A:269:ILE:O	1:A:273:ASN:ND2	2.35	0.45
1:B:164:LEU:HB2	1:B:247:ASP:HB2	1.99	0.45
1:F:446:MET:HA	1:F:451:ILE:HD12	1.99	0.45
1:B:100:MET:HE1	1:B:216:GLY:HA3	1.98	0.45
1:B:465:ASP:HA	1:B:498:LEU:HD11	1.99	0.45
1:D:592:ASN:C	1:D:593:GLU:OE2	2.54	0.45
1:D:430:TYR:CE2	1:D:438:GLU:HB3	2.52	0.44
1:F:480:TYR:CZ	1:F:486:TYR:HB3	2.52	0.44
1:F:541:TYR:O	1:F:544:SER:OG	2.24	0.44
1:A:322:ILE:HG23	1:A:340:ILE:HD13	1.98	0.44
1:B:452:ASP:OD1	1:B:452:ASP:N	2.51	0.44
1:E:121:ILE:O	1:E:125:ILE:HG12	2.18	0.44
1:F:19:VAL:HG21	1:F:107:MET:HE1	2.00	0.44
1:F:519:LEU:HD11	1:F:587:ILE:HD11	2.00	0.44
1:B:44:PTR:HA	1:B:44:PTR:HD1	1.68	0.44
1:C:412:VAL:HG12	1:C:451:ILE:HD11	1.99	0.44
1:D:63:TYR:OH	1:D:578:GLU:OE2	2.17	0.44
1:A:589:CYS:HA	1:A:595:PHE:CE1	2.53	0.44
1:B:517:LEU:O	1:B:521:ARG:HG3	2.18	0.44
1:E:202:ILE:HD11	1:E:223:ILE:HG21	2.00	0.44
1:F:591:GLU:H	1:F:591:GLU:HG2	1.60	0.44
1:C:165:SER:HB2	1:C:278:ASN:HB2	1.99	0.44
1:F:63:TYR:OH	1:F:578:GLU:OE2	2.36	0.44
1:F:197:THR:HG22	1:F:201:LEU:HD23	2.00	0.44
1:A:393:THR:HA	1:A:396:GLU:HB2	2.00	0.43
1:C:168:TYR:HB3	1:C:215:THR:CG2	2.48	0.43
1:A:568:LYS:HB3	1:A:568:LYS:HE3	1.86	0.43
1:B:493:LYS:HG2	1:B:541:TYR:HE1	1.82	0.43
1:C:157:ILE:HG22	1:C:254:THR:HA	1.99	0.43
1:D:19:VAL:HB	1:D:107:MET:HE1	2.00	0.43
1:F:89:PRO:HD3	1:F:438:GLU:OE2	2.17	0.43
1:B:480:TYR:CZ	1:B:486:TYR:HB3	2.54	0.43
1:E:59:SER:HB2	1:E:585:TRP:CE2	2.53	0.43
1:E:461:LEU:O	1:E:494:LYS:HE2	2.18	0.43
1:F:139:ASN:O	1:F:144:LYS:HD3	2.19	0.43
1:A:454:LEU:HD12	1:A:455:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:LEU:HD12	1:B:201:LEU:HB3	2.00	0.43
1:F:522:TYR:OH	1:F:579:LEU:HB3	2.19	0.43
1:C:492:LEU:HD11	1:C:533:PHE:CD1	2.54	0.43
1:F:327:ASN:O	1:F:331:LEU:HD13	2.19	0.43
1:B:59:SER:HB2	1:B:585:TRP:CE2	2.54	0.43
1:C:38:VAL:HG13	1:C:58:GLU:HB3	2.01	0.43
1:F:153:LEU:HD13	1:F:159:LYS:HD3	1.99	0.43
1:B:474:ILE:HD13	1:B:587:ILE:HG12	2.00	0.43
1:F:412:VAL:HG12	1:F:451:ILE:HD11	2.00	0.43
1:B:343:VAL:HG12	2:H:7:DC:C2	2.54	0.43
1:D:487:LYS:H	1:D:487:LYS:HD2	1.84	0.43
1:F:51:TYR:HB2	1:F:444:LEU:HD21	2.01	0.43
1:F:69:LEU:HD13	1:F:73:PHE:HE1	1.84	0.43
1:B:51:TYR:HB2	1:B:444:LEU:HD21	2.01	0.43
1:E:561:ASN:HA	1:E:564:LYS:HE3	2.00	0.43
1:A:49:SER:HB2	1:A:50:PHE:CD2	2.54	0.42
1:B:395:PHE:HA	1:B:398:ILE:HG12	2.01	0.42
1:D:512:ARG:HG3	1:D:563:ILE:HG23	2.01	0.42
1:F:228:MET:HE1	1:F:231:PHE:CD2	2.54	0.42
1:A:452:ASP:OD1	1:A:452:ASP:N	2.53	0.42
1:A:511:SER:HB2	1:A:573:ASN:OD1	2.19	0.42
1:B:557:GLU:HA	1:B:563:ILE:HD11	2.00	0.42
1:C:455:LEU:HD22	1:C:459:GLU:HB3	2.01	0.42
1:D:398:ILE:HA	1:D:401:PHE:HB2	2.02	0.42
1:F:302:PHE:O	1:F:305:ILE:HG22	2.19	0.42
1:B:113:ILE:HD11	1:B:223:ILE:HD11	2.01	0.42
1:C:480:TYR:CZ	1:C:486:TYR:HB3	2.54	0.42
1:D:343:VAL:HG12	2:J:7:DC:C2	2.55	0.42
1:C:90:LYS:HB3	1:C:94:ALA:HB3	2.01	0.42
1:D:8:LEU:HD22	1:D:140:PHE:CE2	2.54	0.42
1:D:206:GLN:O	1:D:209:GLU:HB2	2.19	0.42
1:D:385:SER:HB3	1:D:437:GLN:HG2	2.01	0.42
1:E:511:SER:HB2	1:E:573:ASN:OD1	2.19	0.42
1:A:202:ILE:HD11	1:A:223:ILE:HD13	2.01	0.42
1:E:430:TYR:CE2	1:E:438:GLU:HB3	2.54	0.42
1:E:168:TYR:HD2	1:E:215:THR:HB	1.84	0.42
1:F:232:ASP:OD1	1:F:242:TYR:OH	2.21	0.42
1:B:135:PHE:O	1:B:137:GLN:HG2	2.20	0.42
1:C:555:GLN:HA	1:C:562:TYR:CG	2.55	0.42
1:D:422:GLY:O	1:D:426:LYS:HG3	2.20	0.42
1:A:15:PRO:O	1:A:19:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:LYS:HG3	1:C:138:LEU:HD11	2.02	0.42
1:E:341:PHE:HB3	1:E:394:PHE:HB2	2.02	0.42
1:A:83:PRO:HD3	1:A:206:GLN:HA	2.01	0.41
1:F:329:GLU:HB2	1:F:337:ILE:HG13	2.01	0.41
1:B:292:LYS:HE2	1:B:292:LYS:HB3	1.90	0.41
1:C:341:PHE:HB2	1:C:342:PRO:HD3	2.02	0.41
1:E:20:ARG:NH1	1:E:58:GLU:OE1	2.53	0.41
1:A:171:LEU:HD23	1:A:171:LEU:HA	1.91	0.41
1:C:319:SER:HA	1:C:322:ILE:HD12	2.02	0.41
1:F:44:PTR:HD1	1:F:44:PTR:HA	1.87	0.41
1:D:91:ASN:ND2	1:D:94:ALA:HB3	2.35	0.41
1:A:89:PRO:HG3	1:A:438:GLU:OE1	2.20	0.41
1:A:153:LEU:HD13	1:A:159:LYS:HD3	2.01	0.41
1:D:95:ARG:HD2	1:D:435:PHE:CE1	2.55	0.41
1:D:447:VAL:HG11	1:D:475:LEU:HD22	2.02	0.41
1:E:446:MET:HA	1:E:451:ILE:HG12	2.02	0.41
1:A:81:THR:OG1	1:A:105:SER:OG	2.22	0.41
1:B:225:GLU:OE2	1:B:244:ARG:NH1	2.46	0.41
1:C:302:PHE:O	1:C:305:ILE:HG22	2.21	0.41
1:D:91:ASN:HD21	1:D:94:ALA:HB3	1.86	0.41
1:D:372:ASN:OD1	1:D:411:ILE:HD13	2.20	0.41
1:E:379:ASP:HB2	1:E:415:TYR:CE2	2.56	0.41
1:F:306:THR:N	1:F:309:ASN:OD1	2.45	0.41
1:E:157:ILE:HD13	1:E:157:ILE:HA	1.84	0.41
1:E:341:PHE:HB2	1:E:342:PRO:HD3	2.02	0.41
1:A:438:GLU:OE2	1:A:438:GLU:N	2.52	0.41
1:B:144:LYS:O	1:B:148:ILE:HG13	2.21	0.41
1:B:172:TYR:CE2	1:B:174:HIS:HB2	2.56	0.41
1:D:18:LEU:HD13	1:D:219:LEU:HD21	2.01	0.41
1:D:121:ILE:O	1:D:125:ILE:HG13	2.20	0.41
1:E:103:LEU:HD23	1:E:103:LEU:HA	1.93	0.41
1:A:341:PHE:HB2	1:A:342:PRO:HD3	2.02	0.40
1:C:512:ARG:HG3	1:C:563:ILE:HD12	2.03	0.40
1:D:18:LEU:HB2	1:D:110:ASN:ND2	2.36	0.40
1:D:498:LEU:HD23	1:D:498:LEU:HA	1.93	0.40
1:E:102:ASN:HA	1:E:518:TRP:CE2	2.56	0.40
2:L:4:DC:H6	2:L:4:DC:H2'	1.68	0.40
1:A:455:LEU:HD22	1:A:459:GLU:HB3	2.02	0.40
1:B:219:LEU:HD12	1:B:219:LEU:HA	1.91	0.40
1:B:412:VAL:HG12	1:B:451:ILE:HD11	2.03	0.40
1:E:168:TYR:CE1	1:E:224:THR:HG21	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:379:ASP:HB2	1:E:415:TYR:HE2	1.87	0.40
1:E:480:TYR:CZ	1:E:486:TYR:HB3	2.57	0.40
1:F:556:THR:HG22	1:F:558:LEU:H	1.86	0.40
1:B:430:TYR:CE2	1:B:438:GLU:HB3	2.56	0.40
1:E:20:ARG:HB2	1:E:61:ALA:HB2	2.03	0.40
1:B:321:PHE:CZ	1:B:343:VAL:HG21	2.57	0.40
1:D:17:PHE:HE1	1:D:28:ILE:HD11	1.87	0.40
1:E:473:LEU:HD23	1:E:473:LEU:HA	1.98	0.40
1:F:162:LEU:HD12	1:F:162:LEU:HA	1.86	0.40
1:F:176:ILE:HB	1:F:177:PRO:HD3	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	593/601 (99%)	572 (96%)	20 (3%)	1 (0%)	47 79
1	B	593/601 (99%)	571 (96%)	21 (4%)	1 (0%)	47 79
1	C	594/601 (99%)	577 (97%)	16 (3%)	1 (0%)	47 79
1	D	592/601 (98%)	572 (97%)	19 (3%)	1 (0%)	47 79
1	E	592/601 (98%)	572 (97%)	19 (3%)	1 (0%)	47 79
1	F	597/601 (99%)	579 (97%)	17 (3%)	1 (0%)	47 79
All	All	3561/3606 (99%)	3443 (97%)	112 (3%)	6 (0%)	47 79

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	246	VAL
1	E	246	VAL

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Mol	Chain	Res	Type
1	A	246	VAL
1	B	246	VAL
1	C	246	VAL
1	F	246	VAL

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	544/569 (96%)	534 (98%)	10 (2%)	59	82
1	B	537/569 (94%)	529 (98%)	8 (2%)	65	85
1	C	549/569 (96%)	537 (98%)	12 (2%)	52	78
1	D	538/569 (95%)	528 (98%)	10 (2%)	57	81
1	E	545/569 (96%)	532 (98%)	13 (2%)	49	76
1	F	542/569 (95%)	536 (99%)	6 (1%)	73	89
All	All	3255/3414 (95%)	3196 (98%)	59 (2%)	59	82

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	GLU
1	A	72	HIS
1	A	82	ASP
1	A	171	LEU
1	A	198	LEU
1	A	239	LYS
1	A	465	ASP
1	A	485	SER
1	A	487	LYS
1	A	566	GLN
1	B	48	ASP
1	B	165	SER
1	B	207	TYR
1	B	231	PHE

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Mol	Chain	Res	Type
1	B	458	GLU
1	B	465	ASP
1	B	543	GLN
1	B	546	ASN
1	C	72	HIS
1	C	82	ASP
1	C	96	ARG
1	C	119	GLU
1	C	165	SER
1	C	207	TYR
1	C	312	ASP
1	C	440	TYR
1	C	470	ASP
1	C	554	TYR
1	C	557	GLU
1	C	588	SER
1	D	2	LYS
1	D	82	ASP
1	D	239	LYS
1	D	303	GLU
1	D	440	TYR
1	D	465	ASP
1	D	487	LYS
1	D	498	LEU
1	D	511	SER
1	D	554	TYR
1	E	14	ASP
1	E	27	SER
1	E	90	LYS
1	E	119	GLU
1	E	226	LEU
1	E	239	LYS
1	E	414	LYS
1	E	440	TYR
1	E	452	ASP
1	E	453	ASP
1	E	487	LYS
1	E	554	TYR
1	E	566	GLN
1	F	82	ASP
1	F	141	ASP
1	F	440	TYR

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Mol	Chain	Res	Type
1	F	485	SER
1	F	513	MET
1	F	571	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	257	ASN
1	B	497	GLN
1	F	357	ASN
1	F	370	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

6 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	PTR	B	44	1	15,16,17	1.25	1 (6%)	19,22,24	0.63	0
1	PTR	A	44	1	15,16,17	1.36	1 (6%)	19,22,24	0.56	0
1	PTR	C	44	1	15,16,17	1.24	1 (6%)	19,22,24	0.67	1 (5%)
1	PTR	E	44	1	15,16,17	1.34	1 (6%)	19,22,24	0.63	0
1	PTR	F	44	1	15,16,17	1.36	1 (6%)	19,22,24	0.52	0
1	PTR	D	44	1	15,16,17	1.35	1 (6%)	19,22,24	0.71	1 (5%)

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
1	PTR	B	44	1	-	4/10/11/13	0/1/1/1
1	PTR	A	44	1	-	4/10/11/13	0/1/1/1
1	PTR	C	44	1	-	4/10/11/13	0/1/1/1
1	PTR	E	44	1	-	4/10/11/13	0/1/1/1
1	PTR	F	44	1	-	4/10/11/13	0/1/1/1
1	PTR	D	44	1	-	5/10/11/13	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	PTR	OH-CZ	-4.45	1.30	1.40
1	B	44	PTR	OH-CZ	-4.43	1.30	1.40
1	F	44	PTR	OH-CZ	-4.39	1.30	1.40
1	D	44	PTR	OH-CZ	-4.39	1.30	1.40
1	E	44	PTR	OH-CZ	-4.35	1.30	1.40
1	C	44	PTR	OH-CZ	-4.33	1.30	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	44	PTR	O3P-P-OH	2.21	112.16	105.24
1	D	44	PTR	O3P-P-OH	2.13	111.89	105.24

There are no chirality outliers.

All (25) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	44	PTR	C-CA-CB-CG
1	B	44	PTR	C-CA-CB-CG
1	C	44	PTR	C-CA-CB-CG
1	D	44	PTR	O-C-CA-CB
1	D	44	PTR	C-CA-CB-CG
1	E	44	PTR	C-CA-CB-CG
1	B	44	PTR	CA-CB-CG-CD1
1	A	44	PTR	N-CA-CB-CG
1	B	44	PTR	N-CA-CB-CG
1	B	44	PTR	CA-CB-CG-CD2
1	C	44	PTR	N-CA-CB-CG
1	C	44	PTR	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
1	F	44	PTR	CA-CB-CG-CD1
1	C	44	PTR	CA-CB-CG-CD2
1	F	44	PTR	CA-CB-CG-CD2
1	D	44	PTR	CA-CB-CG-CD1
1	D	44	PTR	CA-CB-CG-CD2
1	D	44	PTR	N-CA-CB-CG
1	E	44	PTR	N-CA-CB-CG
1	F	44	PTR	N-CA-CB-CG
1	A	44	PTR	CA-CB-CG-CD1
1	A	44	PTR	CA-CB-CG-CD2
1	F	44	PTR	C-CA-CB-CG
1	E	44	PTR	CA-CB-CG-CD2
1	E	44	PTR	CA-CB-CG-CD1

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	44	PTR	3	0
1	A	44	PTR	2	0
1	C	44	PTR	3	0
1	E	44	PTR	2	0
1	F	44	PTR	3	0
1	D	44	PTR	2	0

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 9 ligands modelled in this entry, 9 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	597/601 (99%)	-0.27	4 (0%) 87 75	74, 108, 164, 231	0
1	B	597/601 (99%)	-0.23	4 (0%) 87 75	79, 122, 171, 239	0
1	C	598/601 (99%)	-0.37	1 (0%) 95 90	71, 99, 149, 250	0
1	D	596/601 (99%)	-0.22	2 (0%) 94 88	80, 118, 174, 235	0
1	E	596/601 (99%)	-0.31	1 (0%) 95 90	71, 106, 161, 222	0
1	F	599/601 (99%)	-0.30	3 (0%) 91 81	74, 112, 166, 221	0
2	G	9/11 (81%)	-0.12	0 100 100	114, 179, 205, 245	0
2	H	9/11 (81%)	0.43	2 (22%) 0 0	134, 177, 250, 257	0
2	I	9/11 (81%)	-0.09	0 100 100	101, 150, 201, 244	0
2	J	8/11 (72%)	0.44	1 (12%) 3 1	118, 184, 208, 242	0
2	K	9/11 (81%)	0.07	0 100 100	119, 168, 227, 243	0
2	L	10/11 (90%)	0.20	0 100 100	113, 176, 209, 224	0
All	All	3637/3672 (99%)	-0.28	18 (0%) 91 81	71, 112, 171, 257	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	599	ASN	3.9
1	A	599	ASN	3.8
1	F	43	GLU	3.7
2	J	10	DC	3.5
1	D	533	PHE	3.5
1	F	47	SER	3.4
1	B	48	ASP	3.1
1	F	48	ASP	3.1
2	H	10	DC	2.6
1	A	73	PHE	2.3
1	D	73	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	73	PHE	2.2
1	B	554	TYR	2.2
1	B	552	ASN	2.1
1	A	589	CYS	2.1
1	A	48	ASP	2.1
1	B	73	PHE	2.0
2	H	2	DC	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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
1	PTR	B	44	16/17	0.64	0.27	176,191,200,203	0
1	PTR	D	44	16/17	0.65	0.28	168,196,218,223	0
1	PTR	A	44	16/17	0.79	0.21	142,154,171,175	0
1	PTR	E	44	16/17	0.79	0.23	149,169,177,180	0
1	PTR	C	44	16/17	0.82	0.22	153,170,181,181	0
1	PTR	F	44	16/17	0.83	0.23	174,189,202,209	0

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
3	MG	I	101	1/1	0.53	0.32	124,124,124,124	0
3	MG	D	602	1/1	0.67	0.43	136,136,136,136	0
3	MG	E	601	1/1	0.75	0.11	128,128,128,128	0
3	MG	A	601	1/1	0.81	0.27	129,129,129,129	0
3	MG	K	101	1/1	0.91	0.15	130,130,130,130	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	601	1/1	0.92	0.26	104,104,104,104	0
3	MG	F	601	1/1	0.92	0.29	125,125,125,125	0
3	MG	D	601	1/1	0.93	0.34	103,103,103,103	0
3	MG	B	601	1/1	0.93	0.91	182,182,182,182	0

6.5 Other polymers (i)

There are no such residues in this entry.