



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:25 PM UTC

PDB ID : 7R07 / pdb_00007r07
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

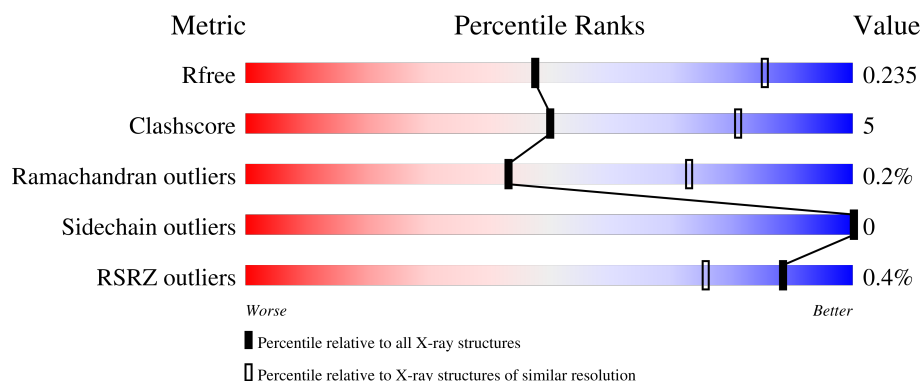
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	601	 87% 12%
1	B	601	 83% 16%
1	C	601	 87% 13%
1	D	601	 85% 14% .
1	E	601	 85% 14% .

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Mol	Chain	Length	Quality of chain
1	F	601	85% 15%
2	G	11	9% 73% 9% 18%
2	H	11	9% 64% 18% 18%
2	I	11	73% 9% 18%
2	J	11	55% 18% 27%
2	K	11	55% 27% 18%
2	L	11	64% 27% 9%

2 Entry composition

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*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 (CCD ID: 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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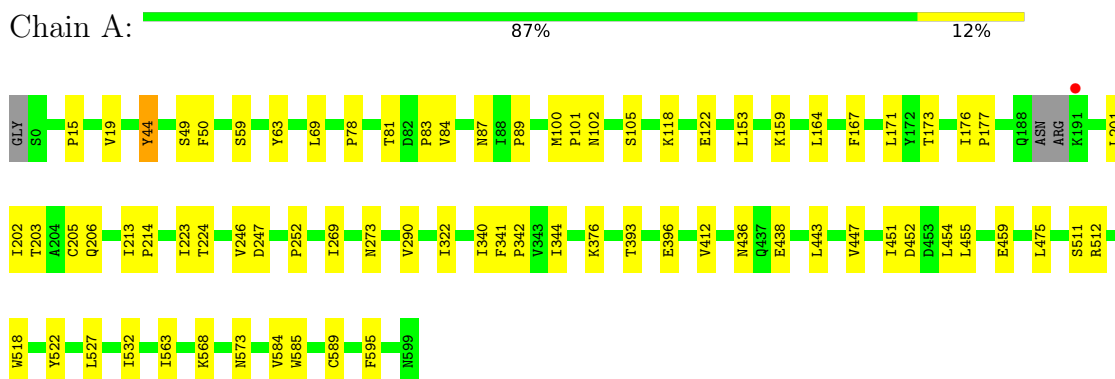
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	3	Total	O	0	0
			3	3		

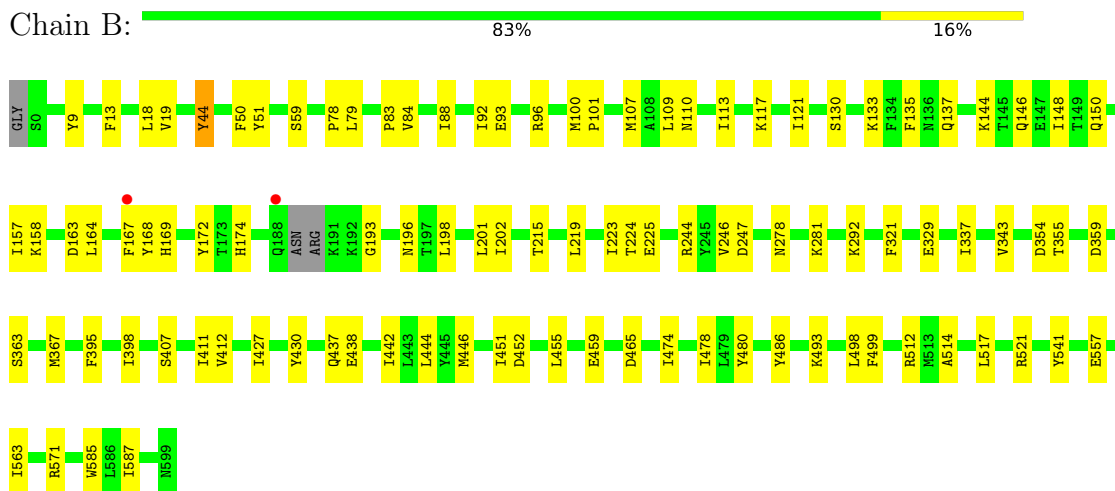
3 Residue-property plots [i](#)

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.

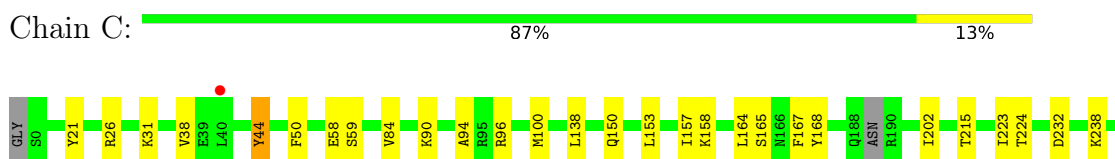
• Molecule 1: AbiK

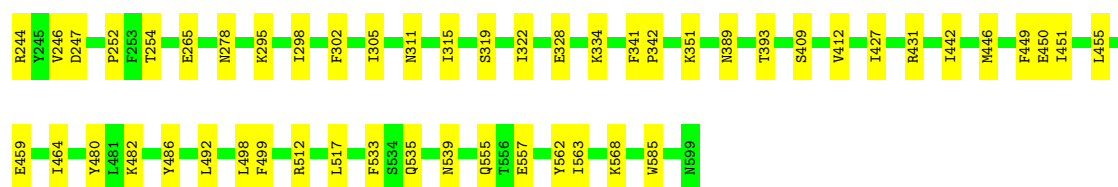


• Molecule 1: AbiK



• Molecule 1: AbiK

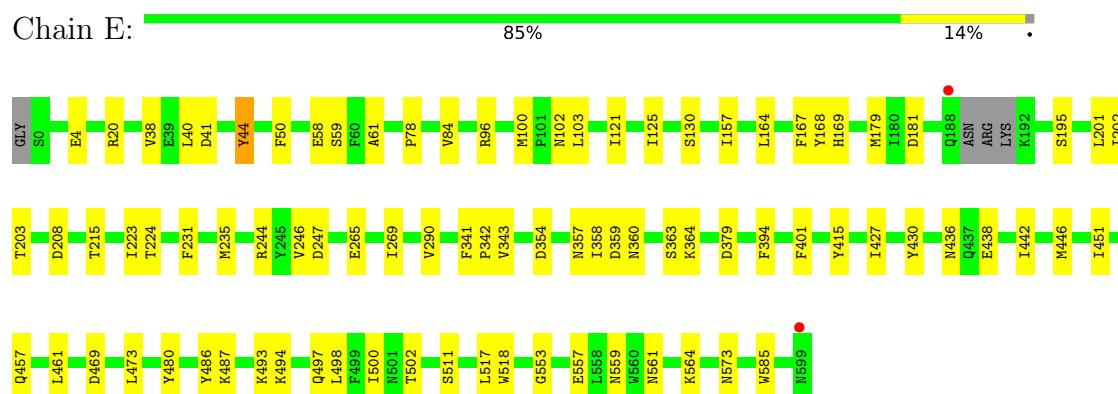




• Molecule 1: AbiK



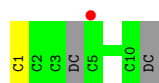
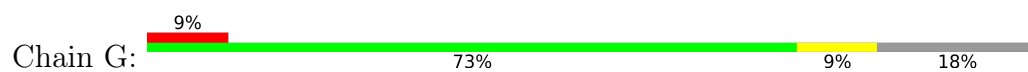
• Molecule 1: AbiK



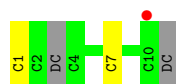
• Molecule 1: AbiK



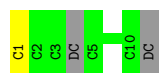
• Molecule 2: DNA (5'-D(*CP*CP*CP*CP*CP*CP*CP*CP*CP*CP*C)-3')



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



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



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



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



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



4 Data and refinement statistics

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 49.63 – 3.10	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.63-3.10) 90.5 (49.63-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.74 (at 3.12Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.189 , 0.232 0.193 , 0.235	Depositor DCC
R_{free} test set	2094 reflections (1.69%)	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)	0.31 , 71.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.12	0/5056	0.31	0/6832
1	B	0.11	0/5030	0.30	0/6802
1	C	0.11	0/5079	0.31	0/6857
1	D	0.11	0/5029	0.29	0/6797
1	E	0.10	0/5055	0.30	0/6828
1	F	0.11	0/5063	0.31	0/6843
2	G	0.21	0/154	0.37	0/233
2	H	0.17	0/180	0.33	0/271
2	I	0.20	0/158	0.37	0/238
2	J	0.13	0/151	0.35	0/227
2	K	0.24	0/167	0.41	0/251
2	L	0.22	0/197	0.42	0/299
All	All	0.11	0/31319	0.31	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 [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	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	62	0
1	C	4977	0	4761	48	0
1	D	4927	0	4670	55	0
1	E	4953	0	4722	57	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	316	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 (316) 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:C:50:PHE:HE2	1:C:100:MET:HE3	1.53	0.73
1:B:18:LEU:HB3	1:B:110:ASN:HD21	1.54	0.72
1:B:50:PHE:HE2	1:B:100:MET:HE3	1.55	0.71
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: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:50:PHE:HE2	1:E:100:MET:HE3	1.64	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:B:367:MET:SD	1:D:0:SER:N	2.75	0.59
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:19:VAL:HB	1:B:107:MET:HE1	1.87	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:C:450:GLU:OE2	1:C:482:LYS:NZ	2.40	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:F:541:TYR:O	1:F:544:SER:OG	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:598:LEU:H	1:D:598:LEU:HD23	1.75	0.51
1:E:50:PHE:CE2	1:E:100:MET:HE3	2.46	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:B:359:ASP:O	1:B:363:SER:OG	2.14	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: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:D:592:ASN:C	1:D:593:GLU:OE2	2.54	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:B:96:ARG:HG3	1:B:169:HIS:HE2	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:81:THR:OG1	1:A:105:SER:OG	2.22	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
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:F:446:MET:HE3	1:F:454:LEU:HB3	1.96	0.46
1:C:232:ASP:OD2	1:C:244:ARG:NH2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:235:MET:HE1	1:E:265:GLU:HB3	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:C:442:ILE:HG22	1:C:446:MET:HE3	1.98	0.45
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
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:465:ASP:HA	1:B:498:LEU:HD11	1.99	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:A:322:ILE:HG23	1:A:340:ILE:HD13	1.98	0.44
1:D:19:VAL:HB	1:D:107:MET:HE1	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:E:493:LYS:HZ2	1:E:497:GLN:HG2	1.84	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
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:E:179:MET:HE1	1:E:231:PHE:HA	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:20:ARG:HD2	1:F:58:GLU:CD	2.44	0.42
1:F:228:MET:HE2	1:F:228:MET:HA	2.00	0.42
1:E:168:TYR:HD2	1:E:215:THR:HB	1.84	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:D:50:PHE:HE2	1:D:100:MET:HE3	1.86	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%)	43	73
1	B	593/601 (99%)	571 (96%)	21 (4%)	1 (0%)	43	73
1	C	594/601 (99%)	577 (97%)	16 (3%)	1 (0%)	43	73
1	D	592/601 (98%)	572 (97%)	19 (3%)	1 (0%)	43	73

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	592/601 (98%)	572 (97%)	19 (3%)	1 (0%)	43	73
1	F	597/601 (99%)	579 (97%)	17 (3%)	1 (0%)	43	73
All	All	3561/3606 (99%)	3443 (97%)	112 (3%)	6 (0%)	43	73

All (6) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	544/569 (96%)	544 (100%)	0	100	100
1	B	537/569 (94%)	537 (100%)	0	100	100
1	C	549/569 (96%)	549 (100%)	0	100	100
1	D	538/569 (95%)	538 (100%)	0	100	100
1	E	545/569 (96%)	545 (100%)	0	100	100
1	F	542/569 (95%)	542 (100%)	0	100	100
All	All	3255/3414 (95%)	3255 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (56) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	HIS

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Mol	Chain	Res	Type
1	A	97	GLN
1	A	196	ASN
1	A	267	ASN
1	A	311	ASN
1	A	555	GLN
1	B	42	ASN
1	B	72	HIS
1	B	139	ASN
1	B	211	HIS
1	B	257	ASN
1	B	280	ASN
1	B	360	ASN
1	B	419	ASN
1	B	497	GLN
1	B	559	ASN
1	B	561	ASN
1	C	161	HIS
1	C	166	ASN
1	C	278	ASN
1	C	350	GLN
1	C	399	ASN
1	C	434	ASN
1	C	566	GLN
1	D	74	ASN
1	D	87	ASN
1	D	257	ASN
1	D	267	ASN
1	D	528	ASN
1	D	535	GLN
1	D	539	ASN
1	D	555	GLN
1	D	566	GLN
1	E	116	ASN
1	E	136	ASN
1	E	230	HIS
1	E	311	ASN
1	E	357	ASN
1	E	360	ASN
1	E	366	ASN
1	E	497	GLN
1	E	559	ASN
1	F	174	HIS

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Mol	Chain	Res	Type
1	F	211	HIS
1	F	230	HIS
1	F	257	ASN
1	F	267	ASN
1	F	273	ASN
1	F	278	ASN
1	F	280	ASN
1	F	357	ASN
1	F	399	ASN
1	F	437	GLN
1	F	462	ASN
1	F	501	ASN
1	F	559	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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	1.24	1 (6%)	17,22,24	0.68	0
1	PTR	A	44	1	15,16,17	1.35	1 (6%)	17,22,24	0.58	0
1	PTR	E	44	1	15,16,17	1.32	1 (6%)	17,22,24	0.58	0
1	PTR	C	44	1	15,16,17	1.22	1 (6%)	17,22,24	0.71	1 (5%)
1	PTR	F	44	1	15,16,17	1.35	1 (6%)	17,22,24	0.49	0
1	PTR	D	44	1	15,16,17	1.34	1 (6%)	17,22,24	0.68	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	E	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	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	-4.50	1.30	1.40
1	B	44	PTR	OH-CZ	-4.48	1.30	1.40
1	F	44	PTR	OH-CZ	-4.44	1.30	1.40
1	D	44	PTR	OH-CZ	-4.43	1.30	1.40
1	E	44	PTR	OH-CZ	-4.39	1.30	1.40
1	C	44	PTR	OH-CZ	-4.38	1.30	1.40

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	44	PTR	O3P-P-OH	2.31	112.16	105.32
1	D	44	PTR	O3P-P-OH	2.22	111.89	105.32

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	C	44	PTR	N-CA-CB-CG
1	B	44	PTR	CA-CB-CG-CD2

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

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	E	44	PTR	2	0
1	C	44	PTR	3	0
1	F	44	PTR	3	0
1	D	44	PTR	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	597/601 (99%)	-0.59	1 (0%) 91 83	74, 108, 164, 231	0
1	B	597/601 (99%)	-0.56	2 (0%) 90 80	79, 122, 171, 239	0
1	C	598/601 (99%)	-0.63	1 (0%) 91 83	71, 99, 149, 250	0
1	D	596/601 (99%)	-0.55	2 (0%) 90 80	80, 118, 174, 235	0
1	E	596/601 (99%)	-0.59	2 (0%) 90 80	71, 106, 161, 222	0
1	F	599/601 (99%)	-0.56	3 (0%) 87 73	74, 112, 166, 221	0
2	G	9/11 (81%)	0.40	1 (11%) 10 5	114, 179, 205, 245	0
2	H	9/11 (81%)	0.23	1 (11%) 10 5	134, 177, 250, 257	0
2	I	9/11 (81%)	-0.05	0 100 100	101, 150, 201, 244	0
2	J	8/11 (72%)	0.02	0 100 100	118, 184, 208, 242	0
2	K	9/11 (81%)	0.35	0 100 100	119, 168, 227, 243	0
2	L	10/11 (90%)	0.13	0 100 100	113, 176, 209, 224	0
All	All	3637/3672 (99%)	-0.57	13 (0%) 88 76	71, 112, 171, 257	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	40	LEU	3.5
2	G	5	DC	3.4
1	E	188	GLN	3.2
1	D	188	GLN	2.6
1	F	187	LYS	2.4
1	F	43	GLU	2.4
1	F	190	ARG	2.3
1	E	599	ASN	2.2
2	H	10	DC	2.2
1	D	41	ASP	2.1
1	B	167	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	191	LYS	2.1
1	B	188	GLN	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	PTR	B	44	16/17	0.68	0.11	176,191,200,203	0
1	PTR	F	44	16/17	0.76	0.12	174,189,202,209	0
1	PTR	D	44	16/17	0.79	0.11	168,196,218,223	0
1	PTR	C	44	16/17	0.86	0.09	153,170,181,181	0
1	PTR	E	44	16/17	0.88	0.09	149,169,177,180	0
1	PTR	A	44	16/17	0.90	0.08	142,154,171,175	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	B	601	1/1	0.25	0.26	182,182,182,182	0
3	MG	D	602	1/1	0.56	0.14	136,136,136,136	0
3	MG	A	601	1/1	0.60	0.14	129,129,129,129	0
3	MG	E	601	1/1	0.68	0.12	128,128,128,128	0
3	MG	I	101	1/1	0.77	0.09	124,124,124,124	0
3	MG	C	601	1/1	0.78	0.12	104,104,104,104	0
3	MG	F	601	1/1	0.80	0.10	125,125,125,125	0
3	MG	D	601	1/1	0.85	0.06	103,103,103,103	0
3	MG	K	101	1/1	0.93	0.06	130,130,130,130	0

6.5 Other polymers [i](#)

There are no such residues in this entry.