



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:42 pm BST

PDB ID : 6OY7
Title : X-ray crystal structure of a bacterial reiterative transcription complex of pyrG promoter at 7 min
Authors : Shin, Y.; Murakami, K.S.
Deposited on : 2019-05-14
Resolution : 3.04 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 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 : 2.11
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) : 2.11

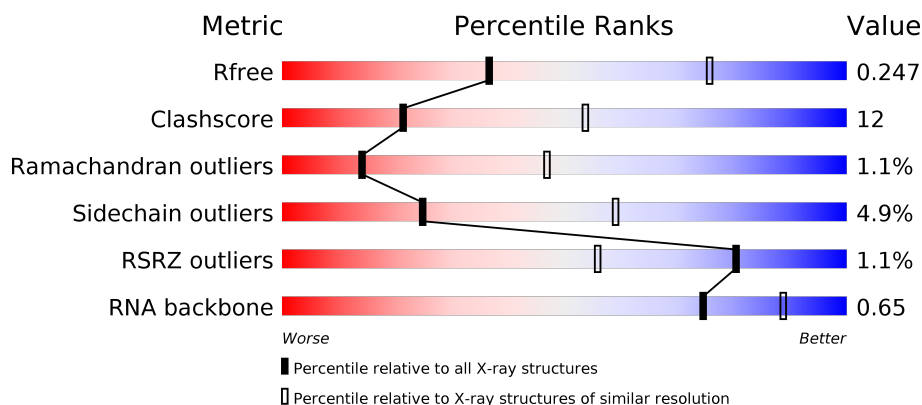
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.04 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	2752 (3.08-3.00)
Clashscore	141614	3096 (3.08-3.00)
Ramachandran outliers	138981	2986 (3.08-3.00)
Sidechain outliers	138945	2988 (3.08-3.00)
RSRZ outliers	127900	2636 (3.08-3.00)
RNA backbone	3102	1034 (3.30-2.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria 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	315	<div> <div>52%</div> <div>17%</div> <div>•</div> <div>28%</div> </div>
1	B	315	<div> <div>51%</div> <div>19%</div> <div>•</div> <div>29%</div> </div>
2	C	1119	<div> <div>%</div> <div>69%</div> <div>28%</div> <div>••</div> </div>
3	D	1524	<div> <div>%</div> <div>71%</div> <div>25%</div> <div>••</div> </div>

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Mol	Chain	Length	Quality of chain
4	E	99	<div><div><div></div><div></div><div></div><div></div></div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>77%17%5%</div></div>
5	F	423	<div><div><div></div><div></div><div></div><div></div></div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>56%23%18%</div></div>
6	G	22	<div><div><div></div><div></div><div></div><div></div></div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>23%50%14%14%</div></div>
7	H	27	<div><div><div></div><div></div><div></div><div></div></div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>22%48%26%</div></div>
8	I	6	<div><div><div></div><div></div><div></div><div></div></div><div>17%</div><div><div></div><div></div><div></div><div></div></div><div>17%33%33%17%</div></div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 28534 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	226	Total	C	N	O	S	0	0	0
			1782	1138	310	332	2			
1	B	224	Total	C	N	O	S	0	0	0
			1767	1129	307	329	2			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0	0
			8745	5534	1555	1632	24			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1485	Total	C	N	O	S	0	0	0
			11729	7435	2066	2193	35			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	94	Total	C	N	O	S	0	0	0
			761	486	132	139	4			

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2790	1760	508	518	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	46	THR	ALA	conflict	UNP Q72L95

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	19	Total	C	N	O	P	0	0	0
			386	183	75	109	19			

- Molecule 7 is a DNA chain called DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*TP*CP*TP*GP*AP*TP*GP*CP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	20	Total	C	N	O	P	0	0	0
			414	198	78	119	19			

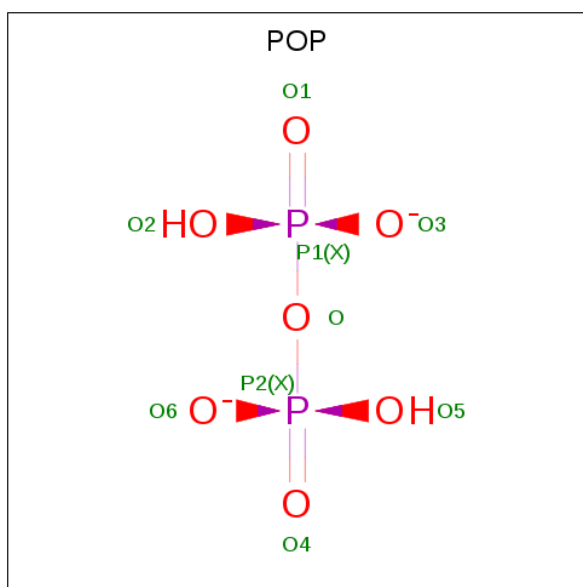
- Molecule 8 is a RNA chain called RNA (5'-D(*(GTP))-R(P*GP*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	I	6	Total	C	N	O	P	0	0	0
			147	60	30	49	8			

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	B	1	Total	Mg	0	0
			1	1		
9	D	1	Total	Mg	0	0
			1	1		

- Molecule 10 is PYROPHOSPHATE 2- (three-letter code: POP) (formula: H₂O₇P₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	D	1	Total	O	P	0	0
			9	7	2		

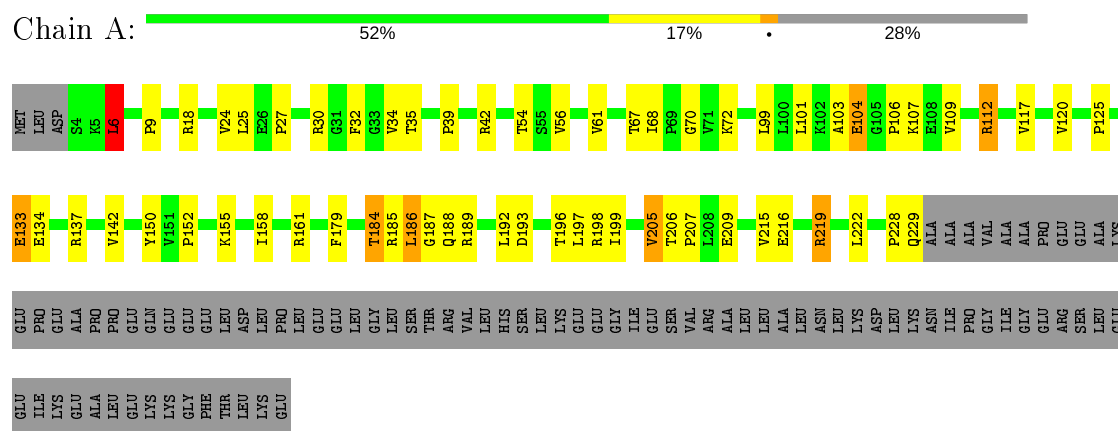
- Molecule 11 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	D	2	Total	Zn	0	0
			2	2		

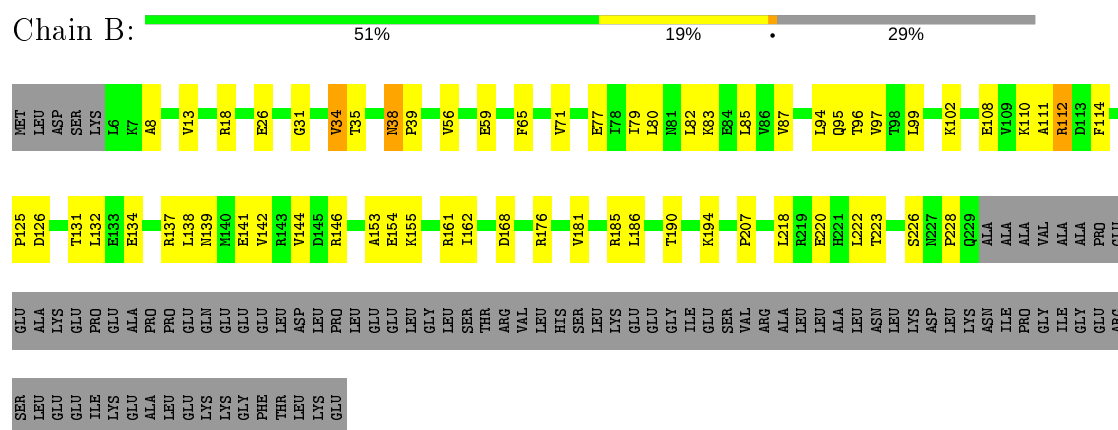
3 Residue-property plots

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

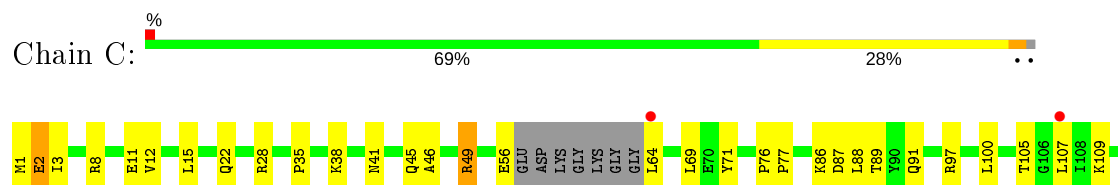
• Molecule 1: DNA-directed RNA polymerase subunit alpha

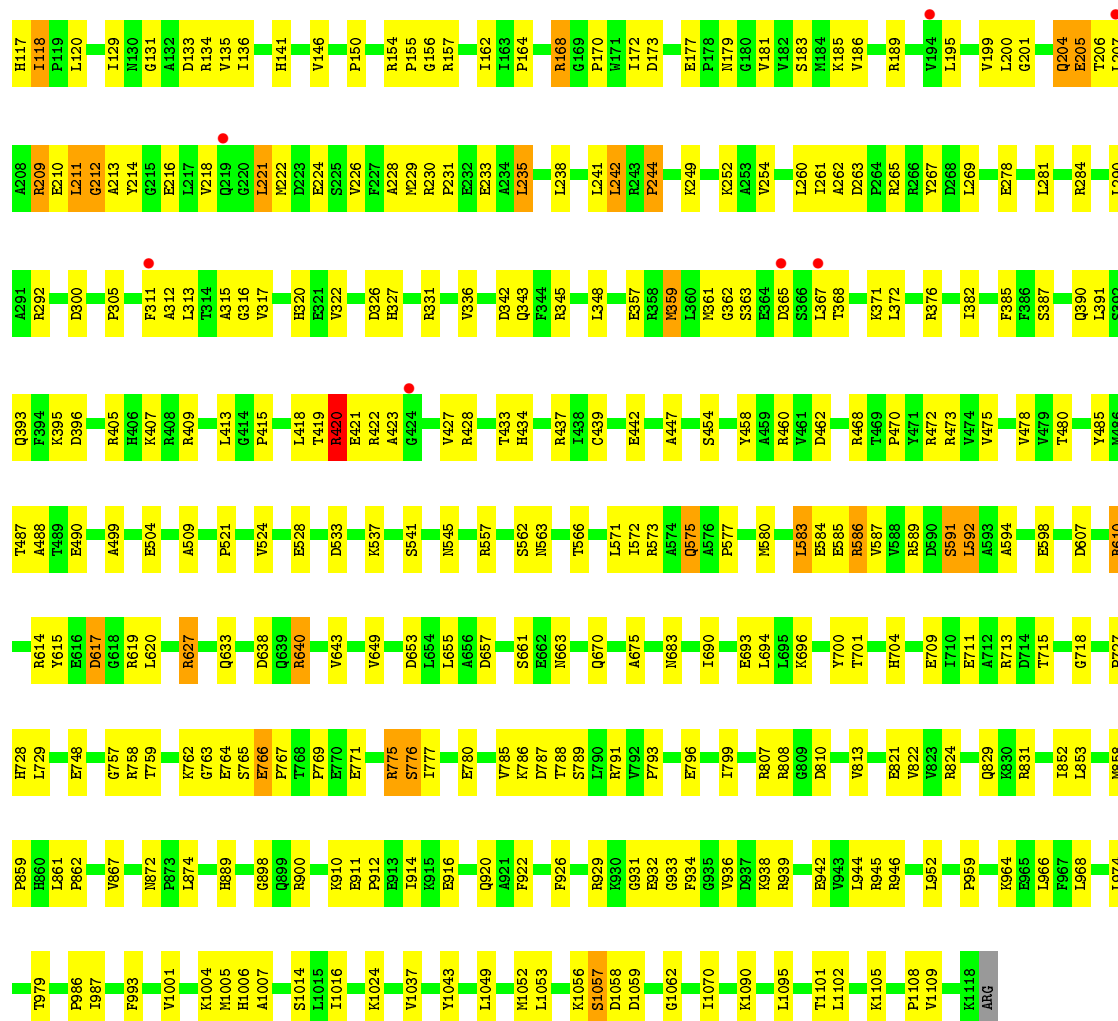


• Molecule 1: DNA-directed RNA polymerase subunit alpha



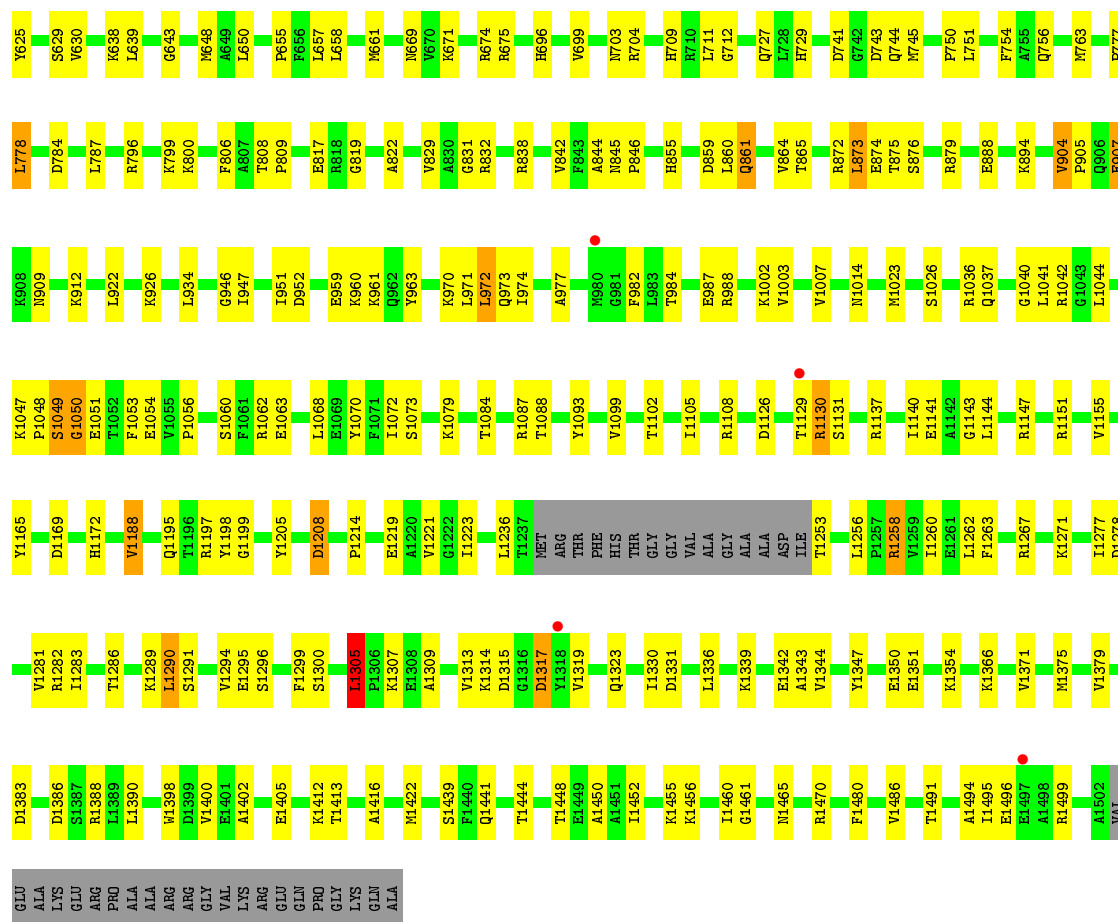
• Molecule 2: DNA-directed RNA polymerase subunit beta



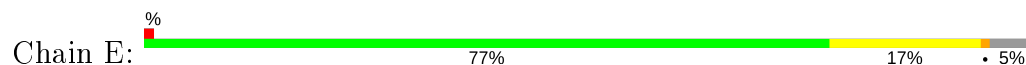


• Molecule 3: DNA-directed RNA polymerase subunit beta'

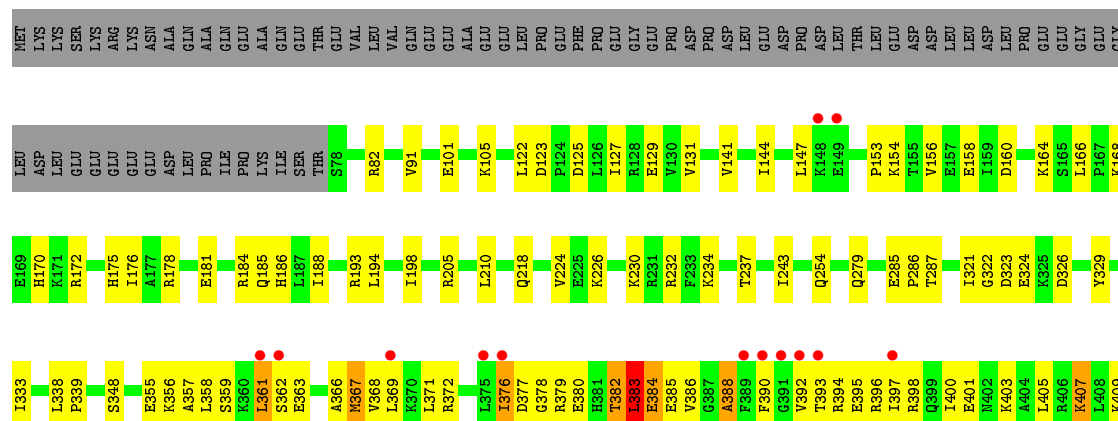


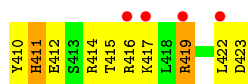


• Molecule 4: DNA-directed RNA polymerase subunit omega

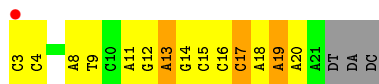


• Molecule 5: RNA polymerase sigma factor SigA

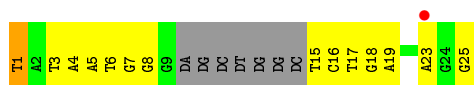




- Molecule 6: DNA (5'-D(P*CP*CP*TP*GP*CP*AP*TP*CP*AP*GP*AP*GP*CP*CP*CP*A
P*AP*AP*A)-3')



- Molecule 7: DNA (5'-D(*TP*AP*TP*AP*AP*TP*GP*GP*GP*TP*CP*TP*GP*AP*TP*GP*CP*AP*GP*G)-3')



- Molecule 8: RNA (5'-D^{*}(GTP))-R(P^{*}GP^{*}GP^{*}GP^{*}GP^{*}G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	185.68Å 101.61Å 295.80Å 90.00° 98.76° 90.00°	Depositor
Resolution (Å)	47.99 – 3.04 47.99 – 3.04	Depositor EDS
% Data completeness (in resolution range)	94.9 (47.99-3.04) 94.9 (47.99-3.04)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.38 (at 3.07Å)	Xtriage
Refinement program	PHENIX (1.14_3260)	Depositor
R, R_{free}	0.207 , 0.247 0.207 , 0.247	Depositor DCC
R_{free} test set	1993 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å ²)	88.5	Xtriage
Anisotropy	0.572	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 42.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	28534	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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

5.1 Standard geometry

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

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	0.58	0/1814	0.89	2/2466 (0.1%)
1	B	0.55	0/1799	0.82	0/2447
2	C	0.55	0/8912	0.82	5/12057 (0.0%)
3	D	0.58	0/11935	0.86	6/16137 (0.0%)
4	E	0.55	0/775	0.80	0/1045
5	F	0.55	0/2835	0.92	6/3816 (0.2%)
6	G	1.45	2/433 (0.5%)	1.33	8/664 (1.2%)
7	H	1.13	1/464 (0.2%)	1.24	2/714 (0.3%)
8	I	1.14	0/129	1.67	4/201 (2.0%)
All	All	0.60	3/29096 (0.0%)	0.88	33/39547 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	G	19	DA	N9-C4	6.14	1.41	1.37
6	G	19	DA	P-O5'	5.88	1.65	1.59
7	H	1	DT	C1'-N1	5.49	1.56	1.49

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	378	GLY	N-CA-C	-10.14	87.75	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	G	19	DA	O4'-C1'-N9	9.01	114.30	108.00
5	F	383	LEU	CA-CB-CG	8.78	135.49	115.30
6	G	17	DC	O4'-C4'-C3'	-8.73	100.76	106.00
2	C	235	LEU	CA-CB-CG	8.10	133.94	115.30
6	G	19	DA	O4'-C4'-C3'	-7.83	101.30	106.00
6	G	15	DC	O5'-P-OP2	-7.68	98.78	105.70
3	D	1305	LEU	CA-CB-CG	7.47	132.47	115.30
5	F	376	ILE	CG1-CB-CG2	-7.03	95.93	111.40
6	G	16	DC	O5'-P-OP2	-6.84	99.54	105.70
3	D	311	LEU	CA-CB-CG	6.25	129.67	115.30
7	H	23	DA	O4'-C1'-N9	6.11	112.28	108.00
2	C	211	LEU	CB-CG-CD2	-6.02	100.77	111.00
6	G	15	DC	OP1-P-OP2	5.90	128.45	119.60
8	I	8	G	N3-C4-N9	-5.84	122.50	126.00
7	H	19	DA	O5'-P-OP2	5.83	117.70	110.70
8	I	8	G	N3-C4-C5	5.81	131.50	128.60
2	C	242	LEU	CA-CB-CG	-5.66	102.28	115.30
5	F	361	LEU	CA-CB-CG	-5.61	102.39	115.30
3	D	873	LEU	CB-CG-CD2	-5.55	101.56	111.00
1	A	6	LEU	CA-CB-CG	5.54	128.03	115.30
5	F	380	GLU	CA-CB-CG	-5.45	101.40	113.40
8	I	7	G	C8-N9-C4	-5.34	104.26	106.40
3	D	12	LEU	CA-CB-CG	-5.32	103.07	115.30
2	C	359	MET	CA-CB-CG	5.29	122.30	113.30
5	F	388	ALA	N-CA-C	5.27	125.22	111.00
3	D	254	GLU	CA-CB-CG	-5.24	101.88	113.40
6	G	16	DC	O4'-C4'-C3'	-5.21	102.42	104.50
3	D	1258	ARG	NE-CZ-NH1	5.19	122.89	120.30
2	C	1095	LEU	CB-CG-CD1	-5.17	102.21	111.00
8	I	5	G	N1-C6-O6	5.07	122.94	119.90
6	G	13	DA	O5'-P-OP2	-5.03	101.17	105.70
1	A	205	VAL	C-N-CA	5.01	134.22	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	420	ARG	Peptide
2	C	766	GLU	Peptide

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	1782	0	1834	46	0
1	B	1767	0	1816	48	0
2	C	8745	0	8828	235	0
3	D	11729	0	11957	287	1
4	E	761	0	778	15	0
5	F	2790	0	2854	103	0
6	G	386	0	212	15	0
7	H	414	0	229	13	0
8	I	147	0	66	24	0
9	B	1	0	0	0	0
9	D	1	0	0	0	0
10	D	9	0	0	0	0
11	D	2	0	0	0	0
All	All	28534	0	28574	682	1

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 12.

All (682) 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)
8:I:3:GTP:N3	8:I:4:G:N2	1.81	1.28
8:I:3:GTP:C2	8:I:4:G:N2	2.16	1.12
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.45	0.97
2:C:946:ARG:HH12	3:D:861:GLN:HE22	1.07	0.92
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.53	0.90
2:C:367:LEU:HA	2:C:371:LYS:HE3	1.54	0.89
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.54	0.87
3:D:500:ARG:HH12	3:D:1390:LEU:HD21	1.39	0.87
1:A:56:VAL:HG22	1:A:142:VAL:HG12	1.56	0.85
3:D:675:ARG:HH22	5:F:423:ASP:HA	1.43	0.84
3:D:952:ASP:HA	3:D:1062:ARG:HH21	1.39	0.84
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.14	0.83
2:C:189:ARG:HH12	2:C:244:PRO:HD3	1.45	0.82
3:D:669:ASN:HD22	5:F:417:LYS:HG2	1.46	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.61	0.80
1:A:30:ARG:HH22	3:D:855:HIS:HD2	1.28	0.80
8:I:3:GTP:N2	8:I:4:G:H21	1.79	0.80
6:G:18:DA:H2'	6:G:19:DA:H5'	1.62	0.79
3:D:500:ARG:NH1	3:D:1390:LEU:HD21	1.98	0.79
5:F:411:HIS:HA	5:F:414:ARG:HH12	1.48	0.78
2:C:683:ASN:HB3	2:C:872:ASN:HD22	1.47	0.78
2:C:769:PRO:HD2	3:D:65:ARG:HH21	1.47	0.77
3:D:1491:THR:HG21	4:E:89:MET:HG2	1.66	0.77
1:B:108:GLU:HG2	1:B:131:THR:HG22	1.67	0.77
1:B:80:LEU:HD22	3:D:844:ALA:HA	1.67	0.77
2:C:390:GLN:HE22	8:I:4:G:H5'	1.49	0.76
1:A:185:ARG:HE	1:A:187:GLY:HA2	1.51	0.76
5:F:361:LEU:HD21	5:F:411:HIS:CG	2.21	0.76
2:C:758:ARG:HH21	2:C:788:THR:HB	1.51	0.76
2:C:769:PRO:HG2	3:D:65:ARG:HE	1.51	0.76
1:B:176:ARG:NH2	3:D:888:GLU:OE1	2.19	0.75
3:D:1282:ARG:NH2	3:D:1295:GLU:OE2	2.18	0.75
2:C:946:ARG:HH12	3:D:861:GLN:NE2	1.85	0.74
2:C:1052:MET:HG3	3:D:623:VAL:HG11	1.68	0.74
1:A:70:GLY:N	2:C:607:ASP:OD1	2.20	0.74
2:C:931:GLY:O	2:C:933:GLY:N	2.21	0.74
5:F:338:LEU:HD23	5:F:339:PRO:HD2	1.70	0.74
3:D:1044:LEU:HD23	3:D:1056:PRO:HB3	1.70	0.74
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.19	0.74
5:F:322:GLY:O	5:F:324:GLU:N	2.20	0.73
5:F:160:ASP:OD2	5:F:164:LYS:NZ	2.20	0.73
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.23	0.72
1:B:77:GLU:HG2	3:D:872:ARG:HH11	1.55	0.72
3:D:272:LEU:HD12	3:D:280:ALA:HB3	1.71	0.72
1:B:110:LYS:HB2	1:B:112:ARG:HH21	1.53	0.72
6:G:3:DC:H42	7:H:25:DG:H1	1.38	0.72
2:C:204:GLN:NE2	2:C:222:MET:SD	2.63	0.72
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.23	0.72
2:C:211:LEU:O	2:C:213:ALA:N	2.20	0.72
5:F:372:ARG:NH1	5:F:401:GLU:OE2	2.23	0.71
2:C:545:ASN:HB3	2:C:583:LEU:HD22	1.72	0.71
2:C:428:ARG:NH2	2:C:447:ALA:O	2.22	0.71
2:C:419:THR:HG22	8:I:3:GTP:H3'	1.72	0.71
3:D:97:THR:HG23	3:D:554:LEU:HD21	1.72	0.70
2:C:711:GLU:HG2	2:C:822:VAL:HG22	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:318:ARG:NH1	3:D:338:GLU:OE1	2.26	0.69
3:D:777:PRO:HG2	3:D:912:LYS:HG3	1.74	0.69
3:D:1126:ASP:O	3:D:1130:ARG:HA	1.92	0.69
1:A:216:GLU:OE2	1:A:219:ARG:NH2	2.25	0.69
3:D:231:VAL:O	3:D:236:TYR:OH	2.11	0.69
2:C:150:PRO:HD3	2:C:322:VAL:HG11	1.74	0.68
2:C:172:ILE:HG12	2:C:186:VAL:HG22	1.74	0.68
3:D:180:LYS:N	3:D:183:GLU:OE1	2.25	0.68
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.73	0.68
3:D:56:TYR:HE1	3:D:69:GLU:HG3	1.57	0.68
5:F:361:LEU:HD13	5:F:407:LYS:HB3	1.76	0.68
2:C:946:ARG:NH1	3:D:861:GLN:HE22	1.88	0.67
2:C:462:ASP:HB3	2:C:468:ARG:HD2	1.77	0.67
3:D:372:ASP:OD1	5:F:232:ARG:NH2	2.27	0.67
1:A:179:PHE:HB3	1:A:197:LEU:HD23	1.77	0.67
3:D:411:THR:HA	3:D:435:VAL:HG12	1.76	0.67
2:C:11:GLU:OE2	2:C:537:LYS:HE2	1.94	0.67
3:D:1386:ASP:OD2	3:D:1412:LYS:HD2	1.94	0.67
2:C:853:LEU:HB2	2:C:858:MET:CE	2.26	0.66
3:D:122:GLU:HG2	3:D:152:LEU:HD11	1.76	0.66
3:D:1281:VAL:HG22	3:D:1317:ASP:H	1.61	0.66
5:F:361:LEU:HD21	5:F:411:HIS:CD2	2.31	0.66
2:C:154:ARG:HE	2:C:157:ARG:HG3	1.61	0.65
3:D:45:PHE:O	3:D:86:ARG:NH2	2.30	0.65
3:D:907:GLU:OE2	3:D:909:ASN:N	2.29	0.65
3:D:1277:ILE:HG13	3:D:1278:ASP:H	1.61	0.65
3:D:179:VAL:O	3:D:205:TYR:OH	2.09	0.65
5:F:358:LEU:HB3	5:F:366:ALA:HB1	1.78	0.65
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.29	0.64
1:B:71:VAL:HG22	1:B:132:LEU:HG	1.79	0.64
1:B:99:LEU:HB3	1:B:114:PHE:CD1	2.33	0.64
2:C:649:VAL:HG13	2:C:653:ASP:HB2	1.79	0.64
3:D:922:LEU:HB3	3:D:926:LYS:HD2	1.79	0.64
5:F:392:VAL:HG22	5:F:397:ILE:CD1	2.28	0.63
2:C:420:ARG:CB	8:I:3:GTP:H2'	2.28	0.63
2:C:715:THR:OG1	2:C:718:GLY:O	2.15	0.63
3:D:658:LEU:HD23	3:D:661:MET:HE3	1.79	0.63
3:D:266:GLU:HG3	3:D:314:PRO:HB3	1.80	0.63
3:D:1281:VAL:CG2	3:D:1317:ASP:H	2.12	0.63
3:D:474:GLU:OE2	3:D:1388:ARG:NH2	2.31	0.63
2:C:109:LYS:HG2	2:C:368:THR:HG22	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:313:LEU:HB2	2:C:320:HIS:HB3	1.81	0.62
8:I:3:GTP:C4	8:I:4:G:N2	2.66	0.62
5:F:122:LEU:HB2	5:F:127:ILE:HD11	1.81	0.62
2:C:420:ARG:CB	8:I:3:GTP:O2'	2.48	0.62
3:D:1137:ARG:O	3:D:1141:GLU:HG3	1.99	0.62
3:D:806:PHE:HB2	3:D:829:VAL:HG22	1.82	0.62
1:A:61:VAL:CG2	1:A:68:ILE:HD11	2.30	0.62
2:C:1006:HIS:CE1	2:C:1024:LYS:HA	2.35	0.62
2:C:1059:ASP:OD1	2:C:1062:GLY:HA3	2.00	0.61
1:B:95:GLN:HE21	1:B:146:ARG:HD2	1.65	0.61
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.82	0.61
3:D:973:GLN:HG2	3:D:974:ILE:HD13	1.80	0.61
3:D:44:LEU:HB3	3:D:525:ARG:HH21	1.65	0.61
3:D:1143:GLY:O	3:D:1147:ARG:HD2	2.01	0.61
2:C:942:GLU:HG2	2:C:945:ARG:HH21	1.65	0.61
8:I:3:GTP:C8	8:I:3:GTP:PA	2.93	0.61
2:C:573:ARG:HB2	2:C:670:GLN:NE2	2.16	0.60
3:D:19:ARG:NE	3:D:94:GLU:OE1	2.29	0.60
2:C:56:GLU:OE2	2:C:64:LEU:N	2.35	0.60
3:D:573:MET:SD	5:F:210:LEU:HD23	2.41	0.60
3:D:1147:ARG:HD3	3:D:1188:VAL:HG11	1.83	0.60
3:D:116:LEU:O	3:D:150:ARG:NH2	2.34	0.60
2:C:987:ILE:HD11	3:D:946:GLY:HA2	1.83	0.60
3:D:1450:ALA:HA	3:D:1455:LYS:HG3	1.83	0.60
3:D:1499:ARG:NH2	4:E:84:ARG:HD2	2.16	0.60
2:C:1006:HIS:ND1	2:C:1024:LYS:HA	2.17	0.60
2:C:214:TYR:C	2:C:216:GLU:H	2.05	0.60
5:F:168:LYS:HG3	5:F:172:ARG:HH21	1.66	0.60
3:D:1129:THR:C	3:D:1131:SER:H	2.06	0.59
3:D:1296:SER:OG	3:D:1299:PHE:O	2.20	0.59
1:B:26:GLU:HB3	1:B:194:LYS:HG3	1.84	0.59
1:B:59:GLU:HB2	1:B:139:ASN:HB3	1.85	0.59
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.84	0.59
3:D:1294:VAL:O	3:D:1300:SER:HB2	2.03	0.59
1:A:206:THR:HB	1:A:209:GLU:OE1	2.02	0.59
2:C:210:GLU:HB3	2:C:211:LEU:HD12	1.85	0.59
2:C:200:LEU:HD13	2:C:300:ASP:HB2	1.84	0.59
2:C:607:ASP:HB3	2:C:610:ARG:H	1.67	0.59
2:C:767:PRO:HB2	2:C:771:GLU:HG2	1.83	0.59
3:D:187:LYS:N	3:D:200:ASP:OD2	2.36	0.59
3:D:44:LEU:HB3	3:D:525:ARG:NH2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:39:VAL:HG21	4:E:72:ARG:HB2	1.84	0.59
5:F:326:ASP:O	6:G:19:DA:N6	2.36	0.59
3:D:171:LEU:HD21	3:D:177:ALA:HB2	1.85	0.59
3:D:669:ASN:HB3	5:F:417:LYS:HE2	1.83	0.59
1:B:18:ARG:O	1:B:207:PRO:HD3	2.03	0.58
2:C:315:ALA:O	2:C:317:VAL:N	2.36	0.58
5:F:144:ILE:HB	5:F:147:LEU:HD22	1.85	0.58
1:B:38:ASN:OD1	2:C:979:THR:HG22	2.02	0.58
3:D:1289:LYS:HG2	3:D:1290:LEU:N	2.17	0.58
3:D:842:VAL:HG22	3:D:865:THR:HB	1.85	0.58
2:C:617:ASP:OD2	2:C:619:ARG:NE	2.37	0.57
5:F:198:ILE:HD13	5:F:243:ILE:HG21	1.85	0.57
2:C:150:PRO:HD3	2:C:322:VAL:CG1	2.34	0.57
5:F:414:ARG:HH11	5:F:414:ARG:HB3	1.69	0.57
3:D:355:VAL:HG11	3:D:385:VAL:HG21	1.84	0.57
2:C:1043:TYR:CD2	3:D:763:MET:HG2	2.39	0.57
3:D:1379:VAL:HG21	3:D:1400:VAL:HG11	1.87	0.57
3:D:658:LEU:HD23	3:D:661:MET:CE	2.35	0.57
3:D:845:ASN:HB2	3:D:846:PRO:HD2	1.86	0.57
3:D:57:GLU:HG3	3:D:64:LYS:HG2	1.86	0.57
3:D:988:ARG:NH2	3:D:1054:GLU:OE1	2.36	0.57
2:C:267:TYR:CE1	2:C:290:LEU:HG	2.40	0.57
2:C:173:ASP:HB2	2:C:185:LYS:HE2	1.86	0.57
2:C:359:MET:HG2	2:C:372:LEU:HD21	1.87	0.57
1:A:198:ARG:HD3	2:C:934:PHE:CZ	2.39	0.57
1:B:65:PHE:CD2	3:D:809:PRO:HB2	2.40	0.56
5:F:394:ARG:HG3	5:F:395:GLU:N	2.19	0.56
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.05	0.56
3:D:205:TYR:CE2	3:D:390:PRO:HG3	2.41	0.56
2:C:229:MET:HB2	2:C:233:GLU:HB2	1.88	0.56
2:C:575:GLN:HG3	2:C:670:GLN:HA	1.88	0.56
3:D:800:LYS:HB3	3:D:822:ALA:HB2	1.88	0.56
8:I:3:GTP:PA	8:I:3:GTP:H8	2.28	0.56
2:C:135:VAL:HG23	2:C:395:LYS:HG3	1.87	0.56
3:D:696:HIS:ND1	4:E:57:ASP:OD1	2.38	0.56
5:F:129:GLU:HG3	5:F:147:LEU:HD21	1.87	0.56
2:C:64:LEU:HD22	2:C:100:LEU:HD11	1.87	0.55
2:C:179:ASN:OD1	2:C:181:VAL:HG12	2.05	0.55
5:F:358:LEU:HD22	5:F:366:ALA:HB1	1.88	0.55
2:C:728:HIS:CE1	2:C:775:ARG:HH11	2.24	0.55
2:C:1070:ILE:HG21	3:D:655:PRO:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:577:PRO:HB3	2:C:993:PHE:CG	2.42	0.55
3:D:907:GLU:HB2	3:D:1026:SER:HA	1.89	0.55
1:A:24:VAL:HG22	1:A:196:THR:HG23	1.89	0.55
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.88	0.55
3:D:65:ARG:HH11	5:F:376:ILE:HA	1.72	0.55
5:F:397:ILE:HD13	5:F:400:ILE:HD11	1.89	0.55
3:D:1271:LYS:HD3	3:D:1331:ASP:HB2	1.88	0.55
5:F:400:ILE:HA	5:F:403:LYS:HB3	1.88	0.55
2:C:214:TYR:O	2:C:218:VAL:HG23	2.07	0.54
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.41	0.54
3:D:625:TYR:CE2	3:D:751:LEU:HD11	2.43	0.54
5:F:226:LYS:HD2	7:H:1:DT:H73	1.89	0.54
3:D:110:SER:O	3:D:114:THR:HG23	2.08	0.54
3:D:704:ARG:HB2	3:D:745:MET:HE2	1.90	0.54
5:F:363:GLU:O	5:F:367:MET:N	2.39	0.54
1:A:112:ARG:HG2	1:A:125:PRO:O	2.08	0.54
2:C:573:ARG:HB2	2:C:670:GLN:HE21	1.72	0.54
2:C:207:LEU:HD13	2:C:221:LEU:HD11	1.90	0.54
2:C:249:LYS:HB3	2:C:252:LYS:HB2	1.89	0.54
3:D:1087:ARG:HG3	3:D:1256:LEU:HD23	1.88	0.54
3:D:1319:VAL:HG12	3:D:1323:GLN:NE2	2.23	0.54
2:C:201:GLY:HA2	2:C:231:PRO:HG3	1.88	0.54
3:D:421:LEU:HD11	3:D:429:SER:HB2	1.90	0.54
3:D:142:LEU:HB2	3:D:161:LEU:HD11	1.90	0.54
1:B:161:ARG:HG3	1:B:162:ILE:O	2.08	0.53
1:B:83:LYS:HE2	1:B:168:ASP:HB2	1.90	0.53
1:A:39:PRO:HG3	1:B:39:PRO:CG	2.38	0.53
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.90	0.53
5:F:411:HIS:HA	5:F:414:ARG:NH1	2.22	0.53
2:C:420:ARG:CB	8:I:3:GTP:C2'	2.85	0.53
2:C:757:GLY:HA2	2:C:789:SER:OG	2.08	0.53
2:C:874:LEU:HD23	3:D:1023:MET:SD	2.48	0.53
3:D:639:LEU:HA	3:D:729:HIS:CD2	2.43	0.53
5:F:394:ARG:NH1	5:F:395:GLU:OE2	2.41	0.53
2:C:598:GLU:N	2:C:615:TYR:OH	2.37	0.53
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.90	0.53
5:F:193:ARG:HB3	7:H:7:DG:H5'	1.89	0.53
2:C:521:PRO:HB3	3:D:1068:LEU:HD21	1.91	0.52
2:C:396:ASP:HA	2:C:633:GLN:NE2	2.25	0.52
2:C:787:ASP:OD2	2:C:791:ARG:NH2	2.42	0.52
5:F:127:ILE:O	5:F:131:VAL:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:556:LYS:NZ	5:F:218:GLN:HE21	2.07	0.52
1:A:133:GLU:HG3	1:A:134:GLU:N	2.23	0.52
3:D:158:TYR:CE1	3:D:454:ALA:HB3	2.45	0.52
2:C:168:ARG:NH1	2:C:345:ARG:HD3	2.24	0.52
2:C:35:PRO:HG2	2:C:38:LYS:HD3	1.91	0.52
2:C:168:ARG:O	2:C:267:TYR:HA	2.10	0.52
2:C:409:ARG:HH21	2:C:409:ARG:HG2	1.74	0.52
3:D:1486:VAL:HG22	4:E:22:VAL:HG13	1.92	0.52
5:F:382:THR:HG22	5:F:383:LEU:HG	1.92	0.52
1:A:30:ARG:HH22	3:D:855:HIS:CD2	2.18	0.52
2:C:759:THR:HB	2:C:785:VAL:HB	1.91	0.52
5:F:168:LYS:O	5:F:172:ARG:HG2	2.10	0.52
3:D:1047:LYS:HB3	3:D:1048:PRO:HD2	1.91	0.52
3:D:619:LEU:HD11	3:D:1439:SER:HB2	1.90	0.52
5:F:230:LYS:O	5:F:232:ARG:HG3	2.10	0.52
1:B:112:ARG:HG3	1:B:125:PRO:O	2.10	0.52
2:C:1102:LEU:HB2	3:D:7:LYS:HB2	1.91	0.52
3:D:1286:THR:HB	3:D:1289:LYS:HB3	1.90	0.52
2:C:931:GLY:C	2:C:933:GLY:H	2.14	0.51
2:C:591:SER:O	2:C:592:LEU:HB2	2.11	0.51
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.90	0.51
3:D:796:ARG:NH2	3:D:859:ASP:OD2	2.40	0.51
1:A:99:LEU:HB2	1:A:142:VAL:HG23	1.91	0.51
2:C:1004:LYS:HD3	3:D:744:GLN:NE2	2.25	0.51
3:D:208:PRO:HG2	3:D:353:VAL:HG21	1.93	0.51
5:F:405:LEU:O	5:F:409:LYS:HG3	2.11	0.51
2:C:419:THR:CG2	8:I:3:GTP:H3'	2.39	0.51
2:C:214:TYR:O	2:C:216:GLU:N	2.43	0.51
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.11	0.51
2:C:1105:LYS:HD2	3:D:3:LYS:NZ	2.25	0.51
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.93	0.51
3:D:1289:LYS:HG2	3:D:1291:SER:H	1.74	0.51
1:A:193:ASP:OD1	2:C:938:LYS:NZ	2.36	0.50
2:C:1101:THR:OG1	2:C:1109:VAL:O	2.29	0.50
2:C:470:PRO:HD3	2:C:485:TYR:CE1	2.45	0.50
3:D:1253:THR:HA	3:D:1258:ARG:HB2	1.93	0.50
6:G:12:DG:N2	7:H:17:DT:O2	2.44	0.50
2:C:762:LYS:HG2	2:C:786:LYS:HD3	1.91	0.50
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.42	0.50
5:F:329:TYR:CE2	5:F:333:ILE:HD11	2.46	0.50
5:F:359:SER:OG	5:F:363:GLU:OE1	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:VAL:HG13	1:B:222:LEU:HD22	1.94	0.50
2:C:45:GLN:HG2	2:C:71:TYR:HE2	1.76	0.50
3:D:171:LEU:HD22	3:D:390:PRO:HG2	1.92	0.50
2:C:150:PRO:HG3	2:C:322:VAL:HG21	1.94	0.50
2:C:580:MET:HB3	2:C:584:GLU:CD	2.32	0.50
3:D:977:ALA:HB1	3:D:982:PHE:HB2	1.94	0.50
2:C:587:VAL:O	2:C:591:SER:HB3	2.12	0.50
5:F:153:PRO:HA	5:F:156:VAL:HG22	1.94	0.50
5:F:361:LEU:HB3	5:F:407:LYS:HE3	1.92	0.50
2:C:281:LEU:HD13	2:C:305:PRO:HB2	1.94	0.50
3:D:800:LYS:NZ	3:D:819:GLY:O	2.44	0.50
5:F:386:VAL:HA	5:F:390:PHE:CZ	2.47	0.50
6:G:12:DG:H8	6:G:12:DG:H5"	1.76	0.50
2:C:224:GLU:CD	2:C:224:GLU:H	2.15	0.50
2:C:41:ASN:OD1	2:C:46:ALA:HA	2.11	0.50
2:C:853:LEU:HB2	2:C:858:MET:HE2	1.93	0.50
3:D:1283:ILE:HG12	3:D:1315:ASP:CG	2.32	0.50
3:D:1102:THR:HG21	3:D:1371:VAL:HG22	1.94	0.50
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.94	0.50
3:D:65:ARG:HD3	5:F:376:ILE:HA	1.93	0.50
1:B:220:GLU:O	1:B:223:THR:OG1	2.26	0.49
2:C:214:TYR:C	2:C:216:GLU:N	2.65	0.49
2:C:487:THR:OG1	2:C:490:GLU:HG3	2.11	0.49
2:C:728:HIS:CE1	2:C:775:ARG:NH1	2.80	0.49
3:D:675:ARG:HH22	5:F:423:ASP:CA	2.17	0.49
2:C:86:LYS:HB2	2:C:88:LEU:HG	1.94	0.49
2:C:926:PHE:HE1	2:C:929:ARG:HH11	1.60	0.49
3:D:1037:GLN:HE21	3:D:1042:ARG:HG3	1.78	0.49
3:D:14:SER:HB3	3:D:511:TRP:CE2	2.46	0.49
3:D:14:SER:HB3	3:D:511:TRP:CZ2	2.47	0.49
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.94	0.49
2:C:235:LEU:HD21	2:C:254:VAL:HG22	1.95	0.49
2:C:952:LEU:HB3	2:C:966:LEU:HD21	1.94	0.49
2:C:675:ALA:HB2	2:C:867:VAL:HG11	1.95	0.49
2:C:1:MET:HB2	2:C:898:GLY:O	2.11	0.49
1:A:103:ALA:HB1	1:A:107:LYS:HE2	1.93	0.49
1:A:39:PRO:HG3	1:B:39:PRO:HG2	1.94	0.49
3:D:1444:THR:O	3:D:1448:THR:HG23	2.13	0.49
3:D:703:ASN:HA	3:D:712:GLY:O	2.12	0.49
1:B:34:VAL:HG12	1:B:181:VAL:HG21	1.94	0.49
2:C:571:LEU:HD22	2:C:700:TYR:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:101:HIS:HB3	3:D:104:PHE:HD2	1.78	0.49
1:A:54:THR:HB	1:A:158:ILE:HD12	1.93	0.49
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.95	0.49
2:C:69:LEU:HB2	2:C:97:ARG:O	2.13	0.49
3:D:491:LYS:NZ	3:D:494:LYS:HE3	2.28	0.49
3:D:1480:PHE:O	4:E:18:ARG:NH2	2.46	0.49
5:F:377:ASP:HB3	5:F:379:ARG:HB2	1.94	0.49
3:D:1277:ILE:HG13	3:D:1278:ASP:N	2.28	0.48
5:F:397:ILE:HA	5:F:400:ILE:HG12	1.95	0.48
2:C:117:HIS:O	2:C:118:ILE:HD13	2.13	0.48
3:D:1105:ILE:HD12	3:D:1199:GLY:HA2	1.95	0.48
2:C:473:ARG:HB3	2:C:480:THR:OG1	2.13	0.48
2:C:922:PHE:CE2	2:C:964:LYS:HB2	2.47	0.48
3:D:1386:ASP:HB2	3:D:1412:LYS:HB3	1.96	0.48
3:D:1386:ASP:OD2	3:D:1413:THR:HG22	2.14	0.48
5:F:168:LYS:HG3	5:F:172:ARG:NH2	2.28	0.48
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.93	0.48
1:B:80:LEU:HD22	3:D:844:ALA:CA	2.38	0.48
2:C:1006:HIS:CD2	2:C:1007:ALA:N	2.81	0.48
3:D:1053:PHE:CE2	3:D:1072:ILE:HG23	2.48	0.48
3:D:959:GLU:HB3	3:D:963:TYR:CE2	2.47	0.48
3:D:984:THR:HG23	3:D:987:GLU:OE2	2.13	0.48
7:H:3:DT:H2''	7:H:4:DA:H5'	1.95	0.48
2:C:226:VAL:O	2:C:229:MET:HG2	2.14	0.48
2:C:861:LEU:HB3	2:C:862:PRO:HD2	1.96	0.48
7:H:17:DT:H2''	7:H:18:DG:H5'	1.96	0.48
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.14	0.48
3:D:322:VAL:HG22	3:D:335:LEU:CD2	2.43	0.48
3:D:210:ARG:HH11	3:D:389:GLU:HG3	1.79	0.48
2:C:1102:LEU:HD23	2:C:1108:PRO:HA	1.96	0.48
3:D:658:LEU:HD11	3:D:674:ARG:HH11	1.78	0.48
3:D:1267:ARG:HD2	3:D:1331:ASP:OD2	2.14	0.48
3:D:1330:ILE:HD13	3:D:1347:TYR:CE1	2.48	0.48
1:B:111:ALA:HB3	1:B:125:PRO:HA	1.95	0.47
2:C:874:LEU:HD12	3:D:784:ASP:OD1	2.14	0.47
5:F:172:ARG:O	5:F:176:ILE:HG12	2.14	0.47
3:D:131:LYS:HD2	3:D:152:LEU:HB3	1.96	0.47
3:D:860:LEU:O	3:D:876:SER:HB2	2.13	0.47
3:D:622:ARG:NH1	6:G:17:DC:OP1	2.45	0.47
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.49	0.47
2:C:1037:VAL:HG13	2:C:1049:LEU:HD11	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:229:MET:HE2	2:C:229:MET:HB3	1.64	0.47
2:C:368:THR:OG1	2:C:371:LYS:HG2	2.14	0.47
2:C:683:ASN:HB3	2:C:872:ASN:HB2	1.96	0.47
5:F:361:LEU:HD23	5:F:361:LEU:HA	1.51	0.47
5:F:410:TYR:C	5:F:412:GLU:H	2.18	0.47
1:B:77:GLU:HG2	3:D:872:ARG:NH1	2.25	0.47
3:D:1283:ILE:HG12	3:D:1315:ASP:HB2	1.97	0.47
3:D:399:ARG:HB3	3:D:401:TYR:CE1	2.50	0.47
5:F:101:GLU:OE1	5:F:105:LYS:HE3	2.14	0.47
8:I:3:GTP:N2	8:I:4:G:N2	2.49	0.47
3:D:132:TYR:HE2	3:D:155:ASP:OD1	1.98	0.47
5:F:377:ASP:CB	5:F:379:ARG:HB2	2.44	0.47
1:A:9:PRO:HB3	1:A:27:PRO:O	2.14	0.47
8:I:3:GTP:N3	8:I:4:G:C2	2.75	0.47
1:A:117:VAL:O	1:A:120:VAL:HG22	2.15	0.47
2:C:683:ASN:HB3	2:C:872:ASN:ND2	2.24	0.47
3:D:1290:LEU:HB3	3:D:1305:LEU:HD23	1.95	0.47
3:D:669:ASN:ND2	5:F:417:LYS:HG2	2.23	0.47
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.97	0.47
3:D:351:MET:HG2	3:D:370:ALA:HB2	1.97	0.47
1:A:61:VAL:HG23	1:A:68:ILE:HD11	1.96	0.47
2:C:475:VAL:O	2:C:478:VAL:HG12	2.14	0.47
3:D:67:ARG:HD2	5:F:377:ASP:OD1	2.15	0.47
1:B:226:SER:O	1:B:228:PRO:HD3	2.15	0.47
2:C:393:GLN:HB3	8:I:5:G:C6	2.50	0.47
2:C:499:ALA:HB2	2:C:533:ASP:HB2	1.96	0.47
5:F:141:VAL:HG21	5:F:153:PRO:HD3	1.95	0.47
2:C:56:GLU:HG3	2:C:64:LEU:O	2.15	0.46
3:D:462:GLN:HB2	3:D:513:ILE:HG21	1.97	0.46
3:D:1495:ILE:HG12	4:E:88:GLU:OE1	2.15	0.46
6:G:18:DA:N6	6:G:19:DA:C4	2.83	0.46
8:I:4:G:H8	8:I:4:G:H3'	1.80	0.46
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.15	0.46
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.50	0.46
2:C:713:ARG:CZ	2:C:715:THR:HG22	2.46	0.46
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.30	0.46
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.97	0.46
3:D:354:VAL:HG22	3:D:367:ILE:O	2.16	0.46
5:F:237:THR:OG1	7:H:4:DA:H8	1.97	0.46
2:C:657:ASP:OD2	2:C:663:ASN:N	2.43	0.46
3:D:205:TYR:CD2	3:D:390:PRO:HG3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:383:LEU:HD12	5:F:384:GLU:OE2	2.16	0.46
3:D:675:ARG:NH2	5:F:423:ASP:HA	2.22	0.46
1:B:99:LEU:HB3	1:B:114:PHE:HD1	1.75	0.46
2:C:189:ARG:HH12	2:C:244:PRO:CD	2.23	0.46
2:C:315:ALA:O	2:C:317:VAL:HG23	2.16	0.46
3:D:1314:LYS:HD2	3:D:1314:LYS:H	1.80	0.46
3:D:208:PRO:HG3	3:D:387:LEU:HD22	1.97	0.46
3:D:216:VAL:HB	3:D:382:GLU:HG2	1.97	0.46
3:D:34:TYR:OH	3:D:35:ARG:NH1	2.48	0.46
3:D:131:LYS:N	3:D:456:MET:HE2	2.31	0.46
5:F:369:LEU:O	5:F:372:ARG:HB2	2.16	0.46
5:F:371:LEU:HD22	5:F:379:ARG:HH21	1.81	0.46
1:B:97:VAL:HG23	1:B:144:VAL:HB	1.98	0.46
3:D:699:VAL:N	3:D:756:GLN:OE1	2.37	0.46
5:F:392:VAL:CG2	5:F:397:ILE:HG12	2.46	0.46
1:B:102:LYS:HG2	1:B:139:ASN:OD1	2.15	0.46
2:C:326:ASP:HA	2:C:331:ARG:HD2	1.97	0.46
3:D:1205:TYR:CE2	3:D:1366:LYS:HE3	2.51	0.46
3:D:485:SER:C	3:D:486:ARG:HG3	2.37	0.46
3:D:437:VAL:HG11	5:F:175:HIS:CE1	2.51	0.46
3:D:787:LEU:HD21	3:D:947:ILE:HG21	1.98	0.45
3:D:972:LEU:HA	3:D:972:LEU:HD13	1.52	0.45
1:B:141:GLU:OE1	1:B:161:ARG:NH2	2.49	0.45
2:C:211:LEU:HD22	2:C:218:VAL:HG13	1.97	0.45
2:C:263:ASP:C	2:C:265:ARG:H	2.20	0.45
2:C:439:CYS:HB2	2:C:541:SER:HB3	1.99	0.45
2:C:763:GLY:C	2:C:765:SER:H	2.19	0.45
3:D:65:ARG:HB2	5:F:377:ASP:O	2.16	0.45
5:F:91:VAL:O	5:F:193:ARG:NH2	2.44	0.45
3:D:960:LYS:NZ	3:D:1063:GLU:OE1	2.49	0.45
3:D:272:LEU:HD11	3:D:282:TYR:CE2	2.51	0.45
6:G:13:DA:H5"	6:G:14:DG:OP1	2.17	0.45
3:D:431:VAL:HG21	3:D:448:GLU:HG2	1.98	0.45
2:C:727:PRO:HB2	2:C:728:HIS:HD2	1.80	0.45
2:C:1057:SER:HB3	2:C:1058:ASP:H	1.49	0.45
5:F:392:VAL:HG22	5:F:397:ILE:HG12	1.99	0.45
2:C:154:ARG:O	2:C:156:GLY:N	2.49	0.45
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.99	0.45
3:D:9:ARG:HB2	3:D:1456:LYS:HG2	1.99	0.45
3:D:186:VAL:HG12	3:D:189:GLN:HB2	1.98	0.45
3:D:439:LEU:HA	3:D:439:LEU:HD23	1.79	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1499:ARG:CZ	4:E:84:ARG:HD2	2.47	0.45
5:F:355:GLU:C	5:F:357:ALA:H	2.20	0.45
2:C:3:ILE:CD1	2:C:900:ARG:HB2	2.47	0.45
2:C:422:ARG:HA	7:H:15:DT:H1'	1.97	0.45
3:D:192:ALA:HB3	3:D:195:VAL:HB	1.98	0.45
3:D:258:VAL:HG12	3:D:273:ARG:O	2.16	0.45
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.99	0.45
2:C:173:ASP:HB2	2:C:185:LYS:HB3	1.99	0.45
2:C:916:GLU:O	2:C:920:GLN:HG3	2.17	0.45
3:D:1342:GLU:CD	3:D:1342:GLU:H	2.19	0.45
5:F:279:GLN:O	5:F:279:GLN:HG2	2.17	0.45
6:G:8:DA:H2''	6:G:9:DT:C6	2.51	0.45
2:C:357:GLU:O	2:C:361:MET:HG2	2.17	0.44
2:C:764:GLU:C	2:C:766:GLU:H	2.19	0.44
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.99	0.44
3:D:65:ARG:HD3	5:F:377:ASP:N	2.33	0.44
5:F:194:LEU:O	5:F:198:ILE:HD12	2.16	0.44
8:I:3:GTP:C8	8:I:3:GTP:O5'	2.70	0.44
2:C:260:LEU:O	2:C:261:ILE:HD12	2.16	0.44
2:C:614:ARG:HE	2:C:620:LEU:HD13	1.82	0.44
3:D:1339:LYS:HB3	3:D:1343:ALA:CB	2.47	0.44
3:D:501:ALA:HB1	3:D:1452:ILE:HG22	1.99	0.44
5:F:398:ARG:O	5:F:401:GLU:HB3	2.17	0.44
6:G:12:DG:H8	6:G:12:DG:C5'	2.30	0.44
2:C:278:GLU:HG2	2:C:284:ARG:HA	1.98	0.44
2:C:807:ARG:HG2	2:C:821:GLU:HB3	1.99	0.44
3:D:658:LEU:HA	3:D:661:MET:HE2	1.99	0.44
5:F:82:ARG:HB2	7:H:8:DG:O6	2.17	0.44
1:B:94:LEU:HD21	1:B:97:VAL:CG1	2.47	0.44
2:C:1016:ILE:O	3:D:87:ARG:NH2	2.40	0.44
3:D:1093:TYR:OH	3:D:1441:GLN:OE1	2.28	0.44
3:D:103:TRP:HB3	3:D:1448:THR:HG21	1.99	0.44
3:D:147:VAL:HG21	3:D:161:LEU:HD21	1.99	0.44
5:F:166:LEU:HA	5:F:166:LEU:HD23	1.80	0.44
5:F:166:LEU:HD13	5:F:170:HIS:HB3	2.00	0.44
5:F:414:ARG:NH1	5:F:414:ARG:HB3	2.32	0.44
8:I:3:GTP:C8	8:I:3:GTP:O1A	2.70	0.44
2:C:118:ILE:HD12	2:C:382:ILE:HG21	2.00	0.44
2:C:205:GLU:O	2:C:209:ARG:HB3	2.18	0.44
2:C:212:GLY:N	2:C:218:VAL:HG11	2.33	0.44
3:D:1042:ARG:HH12	3:D:1073:SER:HB2	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:627:ARG:NH2	2:C:640:ARG:HG3	2.32	0.44
3:D:671:LYS:NZ	3:D:675:ARG:HH21	2.15	0.44
3:D:750:PRO:O	3:D:756:GLN:NE2	2.51	0.44
5:F:168:LYS:HE2	5:F:172:ARG:HH21	1.83	0.44
1:A:186:LEU:HA	1:A:186:LEU:HD12	1.81	0.44
2:C:177:GLU:HG3	2:C:183:SER:HB3	2.00	0.44
2:C:437:ARG:NH2	2:C:488:ALA:HA	2.33	0.44
4:E:73:LEU:HD23	4:E:73:LEU:HA	1.80	0.44
3:D:553:ARG:HD2	3:D:570:GLU:OE2	2.18	0.44
3:D:806:PHE:O	3:D:829:VAL:HA	2.18	0.44
3:D:371:ILE:HB	5:F:232:ARG:NH2	2.32	0.44
2:C:1005:MET:SD	3:D:648:MET:HG3	2.58	0.44
2:C:76:PRO:HG3	2:C:120:LEU:HD12	2.00	0.44
2:C:418:LEU:CB	2:C:423:ALA:HB2	2.48	0.44
3:D:66:GLN:HB3	5:F:376:ILE:HG22	2.00	0.44
5:F:129:GLU:CG	5:F:147:LEU:HD21	2.48	0.44
1:B:153:ALA:C	1:B:155:LYS:H	2.21	0.43
2:C:807:ARG:HB2	2:C:810:ASP:OD2	2.18	0.43
3:D:1198:TYR:CE2	3:D:1460:ILE:HD13	2.53	0.43
1:A:32:PHE:HA	1:A:35:THR:HB	2.00	0.43
1:B:38:ASN:HB3	1:B:39:PRO:HD3	2.00	0.43
2:C:627:ARG:HD2	2:C:638:ASP:OD1	2.18	0.43
3:D:1336:LEU:HB2	3:D:1344:VAL:HG21	1.98	0.43
3:D:483:HIS:O	3:D:489:ARG:HG3	2.18	0.43
1:A:25:LEU:HA	1:A:25:LEU:HD12	1.83	0.43
3:D:1068:LEU:HD12	3:D:1068:LEU:HA	1.84	0.43
3:D:241:ILE:HD13	3:D:310:LEU:HD23	2.00	0.43
3:D:503:LEU:HA	3:D:503:LEU:HD23	1.86	0.43
8:I:4:G:C8	8:I:4:G:H3'	2.53	0.43
3:D:1258:ARG:CZ	3:D:1262:LEU:HD21	2.48	0.43
3:D:12:LEU:HD23	3:D:12:LEU:HA	1.66	0.43
2:C:1105:LYS:HD2	3:D:3:LYS:HZ3	1.83	0.43
3:D:838:ARG:HD3	3:D:874:GLU:CD	2.38	0.43
2:C:15:LEU:HD13	2:C:458:TYR:CZ	2.53	0.43
2:C:439:CYS:CB	2:C:541:SER:HB3	2.48	0.43
3:D:1047:LYS:HD2	3:D:1051:GLU:HG2	2.00	0.43
3:D:711:LEU:HD13	3:D:778:LEU:HD13	1.99	0.43
5:F:392:VAL:HG22	5:F:397:ILE:HD13	1.99	0.43
5:F:393:THR:HG22	5:F:394:ARG:N	2.33	0.43
3:D:1140:ILE:CG2	3:D:1144:LEU:HD12	2.49	0.43
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:437:VAL:HG11	5:F:175:HIS:ND1	2.34	0.43
3:D:438:ASP:OD1	3:D:441:ARG:NH2	2.46	0.43
4:E:37:ASN:HB3	4:E:93:TYR:CD1	2.54	0.43
1:A:39:PRO:HB3	1:B:35:THR:HG23	2.00	0.43
2:C:89:THR:O	2:C:91:GLN:HG2	2.18	0.43
3:D:1263:PHE:O	3:D:1375:MET:HE2	2.18	0.43
3:D:629:SER:OG	3:D:630:VAL:N	2.51	0.43
3:D:963:TYR:CE1	3:D:1002:LYS:HD3	2.54	0.43
6:G:3:DC:H2"	6:G:4:DC:C6	2.54	0.43
1:A:117:VAL:HB	1:A:120:VAL:HG21	2.00	0.43
2:C:212:GLY:CA	2:C:218:VAL:HG21	2.49	0.43
2:C:769:PRO:HG2	3:D:65:ARG:NE	2.27	0.43
3:D:1165:TYR:CZ	3:D:1214:PRO:HB3	2.54	0.43
3:D:963:TYR:CD1	3:D:1002:LYS:HD3	2.54	0.43
1:A:184:THR:O	1:A:192:LEU:HB2	2.18	0.43
2:C:136:ILE:HB	2:C:336:VAL:HG13	2.01	0.43
3:D:1198:TYR:CZ	3:D:1460:ILE:HD13	2.53	0.43
3:D:704:ARG:NH2	8:I:8:G:O2'	2.45	0.43
2:C:164:PRO:HA	2:C:269:LEU:HD12	2.00	0.43
2:C:859:PRO:O	2:C:867:VAL:HG22	2.19	0.43
2:C:952:LEU:HD23	2:C:952:LEU:HA	1.76	0.43
3:D:1049:SER:OG	3:D:1050:GLY:N	2.51	0.43
3:D:1208:ASP:OD1	3:D:1208:ASP:C	2.58	0.43
3:D:66:GLN:HB3	5:F:376:ILE:CG2	2.49	0.43
5:F:172:ARG:HA	5:F:172:ARG:HD3	1.77	0.43
3:D:65:ARG:NH1	5:F:376:ILE:HA	2.33	0.43
1:A:104:GLU:HB3	1:A:137:ARG:CD	2.49	0.42
1:A:39:PRO:HG3	1:B:39:PRO:HG3	2.01	0.42
1:A:42:ARG:NH2	1:B:31:GLY:O	2.44	0.42
3:D:266:GLU:OE2	3:D:315:ARG:HG3	2.19	0.42
3:D:657:LEU:HD12	3:D:657:LEU:HA	1.77	0.42
3:D:236:TYR:CZ	3:D:242:LEU:HD12	2.55	0.42
3:D:741:ASP:OD1	3:D:743:ASP:OD1	2.37	0.42
2:C:420:ARG:HA	8:I:4:G:O6	2.19	0.42
2:C:585:GLU:HG3	2:C:585:GLU:H	1.39	0.42
2:C:655:LEU:HA	2:C:655:LEU:HD23	1.81	0.42
2:C:974:LEU:HA	2:C:974:LEU:HD12	1.69	0.42
3:D:1267:ARG:NH1	3:D:1331:ASP:OD2	2.46	0.42
5:F:123:ASP:OD1	5:F:125:ASP:HB2	2.19	0.42
8:I:3:GTP:HN22	8:I:4:G:H21	1.63	0.42
1:B:56:VAL:HG23	1:B:142:VAL:HG12	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1295:GLU:HA	3:D:1300:SER:HB3	2.01	0.42
3:D:158:TYR:HE1	3:D:454:ALA:HB3	1.84	0.42
3:D:520:LEU:O	3:D:525:ARG:NH1	2.46	0.42
1:B:222:LEU:HA	1:B:222:LEU:HD23	1.82	0.42
2:C:910:LYS:O	2:C:914:ILE:HG13	2.20	0.42
3:D:1260:ILE:HD13	3:D:1260:ILE:HG21	1.78	0.42
3:D:65:ARG:HD3	5:F:376:ILE:C	2.39	0.42
5:F:188:ILE:HG12	5:F:224:VAL:HG21	2.01	0.42
2:C:212:GLY:H	2:C:218:VAL:HG11	1.83	0.42
2:C:763:GLY:C	2:C:765:SER:N	2.73	0.42
2:C:775:ARG:C	2:C:777:ILE:H	2.22	0.42
3:D:1036:ARG:NH2	3:D:1042:ARG:O	2.52	0.42
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.55	0.42
2:C:206:THR:O	2:C:210:GLU:HB2	2.20	0.42
2:C:563:ASN:O	2:C:566:THR:HB	2.20	0.42
3:D:411:THR:HG23	5:F:178:ARG:CB	2.50	0.42
3:D:502:PHE:HD1	3:D:507:ASN:O	2.02	0.42
2:C:694:LEU:HA	2:C:694:LEU:HD23	1.89	0.42
3:D:272:LEU:CD1	3:D:280:ALA:HB3	2.47	0.42
3:D:411:THR:HB	3:D:437:VAL:H	1.85	0.42
4:E:66:LYS:N	4:E:66:LYS:HD2	2.35	0.42
2:C:690:ILE:HG13	2:C:852:ILE:HG23	2.02	0.42
5:F:368:VAL:CG1	5:F:397:ILE:HD12	2.49	0.42
5:F:415:THR:O	5:F:417:LYS:N	2.48	0.42
3:D:1144:LEU:HA	3:D:1144:LEU:HD23	1.72	0.42
3:D:468:LEU:HD23	3:D:468:LEU:HA	1.87	0.42
3:D:934:LEU:HA	3:D:934:LEU:HD23	1.74	0.42
5:F:194:LEU:HB2	7:H:6:DT:C2	2.55	0.42
2:C:189:ARG:NH1	2:C:242:LEU:O	2.53	0.41
2:C:49:ARG:CZ	2:C:49:ARG:HA	2.50	0.41
2:C:701:THR:HA	2:C:831:ARG:O	2.21	0.41
2:C:729:LEU:HD23	2:C:729:LEU:HA	1.63	0.41
2:C:709:GLU:HG3	2:C:824:ARG:HG2	2.02	0.41
3:D:1068:LEU:O	3:D:1072:ILE:HG12	2.20	0.41
3:D:1305:LEU:HG	3:D:1309:ALA:HB3	2.01	0.41
3:D:82:LYS:HB2	3:D:84:ILE:HG22	2.01	0.41
5:F:285:GLU:HA	5:F:286:PRO:HD3	1.91	0.41
1:A:198:ARG:O	1:A:199:ILE:HD13	2.19	0.41
1:B:94:LEU:HD11	1:B:96:THR:O	2.20	0.41
2:C:313:LEU:HD13	2:C:320:HIS:O	2.19	0.41
2:C:348:LEU:HD12	2:C:348:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:889:HIS:CD2	3:D:951:ILE:HG22	2.55	0.41
3:D:1070:TYR:O	3:D:1073:SER:OG	2.33	0.41
2:C:390:GLN:NE2	8:I:4:G:H5'	2.27	0.41
1:A:18:ARG:O	1:A:207:PRO:HD3	2.21	0.41
2:C:312:ALA:HB3	2:C:320:HIS:CD2	2.55	0.41
3:D:1271:LYS:CD	3:D:1331:ASP:HB2	2.48	0.41
4:E:70:THR:OG1	4:E:72:ARG:HG3	2.20	0.41
5:F:154:LYS:O	5:F:158:GLU:HG3	2.20	0.41
6:G:18:DA:N6	6:G:19:DA:C5	2.88	0.41
2:C:195:LEU:O	2:C:199:VAL:HG23	2.19	0.41
3:D:611:GLN:HE22	5:F:326:ASP:HA	1.85	0.41
2:C:460:ARG:HD2	2:C:485:TYR:CE1	2.55	0.41
2:C:589:ARG:HE	2:C:589:ARG:HB2	1.71	0.41
3:D:353:VAL:HG11	3:D:387:LEU:HD21	2.02	0.41
3:D:452:ILE:HD13	3:D:452:ILE:HG21	1.86	0.41
1:A:152:PRO:O	1:A:155:LYS:HB2	2.20	0.41
2:C:129:ILE:HB	2:C:134:ARG:HD2	2.03	0.41
2:C:170:PRO:HD2	2:C:267:TYR:CE2	2.56	0.41
3:D:1286:THR:HB	3:D:1289:LYS:H	1.86	0.41
3:D:1295:GLU:HA	3:D:1300:SER:CB	2.51	0.41
1:B:85:LEU:HG	1:B:87:VAL:HG23	2.01	0.41
2:C:269:LEU:HA	2:C:269:LEU:HD12	1.93	0.41
2:C:391:LEU:HD23	2:C:391:LEU:HA	1.68	0.41
3:D:1290:LEU:HD23	3:D:1307:LYS:O	2.21	0.41
3:D:210:ARG:NH1	3:D:388:HIS:HB3	2.35	0.41
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.92	0.41
5:F:390:PHE:N	5:F:390:PHE:CD2	2.88	0.41
8:I:3:GTP:PA	8:I:3:GTP:O1G	2.79	0.41
1:A:117:VAL:HB	1:A:120:VAL:CG2	2.50	0.41
2:C:238:LEU:O	2:C:241:LEU:HB2	2.21	0.41
2:C:767:PRO:CB	2:C:771:GLU:HG2	2.49	0.41
3:D:1014:ASN:N	3:D:1014:ASN:OD1	2.53	0.41
3:D:1108:ARG:HD2	3:D:1198:TYR:O	2.21	0.41
3:D:1283:ILE:HG12	3:D:1315:ASP:CB	2.51	0.41
5:F:181:GLU:O	5:F:185:GLN:HG2	2.20	0.41
5:F:392:VAL:HG21	5:F:396:ARG:CG	2.50	0.41
3:D:1383:ASP:H	3:D:1416:ALA:HB3	1.84	0.41
3:D:134:VAL:CG2	3:D:151:GLN:H	2.34	0.41
5:F:329:TYR:HE2	5:F:333:ILE:HD11	1.85	0.41
2:C:1056:LYS:HG2	3:D:625:TYR:HD2	1.86	0.41
2:C:263:ASP:O	2:C:265:ARG:N	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:211:LEU:HD23	2:C:311:PHE:HD2	1.85	0.41
2:C:524:VAL:HG22	2:C:528:GLU:HB2	2.03	0.41
3:D:1205:TYR:CZ	3:D:1366:LYS:HE3	2.56	0.41
3:D:335:LEU:HA	3:D:335:LEU:HD23	1.83	0.41
3:D:556:LYS:HZ3	5:F:218:GLN:HE21	1.69	0.41
1:A:104:GLU:HB3	1:A:137:ARG:HD3	2.02	0.41
2:C:327:HIS:CD2	2:C:433:THR:HG21	2.56	0.41
3:D:1084:THR:O	3:D:1088:THR:HG23	2.21	0.41
3:D:1197:ARG:HB2	3:D:1398:TRP:CZ2	2.56	0.41
3:D:671:LYS:NZ	3:D:675:ARG:NH2	2.69	0.41
1:A:228:PRO:HB3	1:B:13:VAL:CG2	2.50	0.40
2:C:572:ILE:HG13	2:C:573:ARG:HG2	2.03	0.40
2:C:586:ARG:HD2	2:C:586:ARG:HA	1.76	0.40
2:C:693:GLU:HA	2:C:696:LYS:HD2	2.02	0.40
2:C:944:LEU:HD23	2:C:944:LEU:HA	1.84	0.40
3:D:638:LYS:HD3	3:D:638:LYS:HA	1.79	0.40
1:B:65:PHE:HD2	3:D:809:PRO:HB2	1.83	0.40
5:F:419:ARG:NH2	5:F:422:LEU:HD12	2.36	0.40
5:F:234:LYS:HD3	7:H:5:DA:OP2	2.21	0.40
2:C:261:ILE:HG22	2:C:262:ALA:N	2.36	0.40
2:C:793:PRO:HB2	2:C:796:GLU:HG3	2.02	0.40
3:D:106:LYS:HA	3:D:106:LYS:HD2	1.96	0.40
3:D:1099:VAL:HG13	3:D:1223:ILE:CD1	2.51	0.40
3:D:172:PRO:HA	3:D:173:PRO:HD3	1.94	0.40
3:D:262:LYS:HD3	3:D:341:GLU:OE1	2.21	0.40
3:D:961:LYS:HE3	3:D:961:LYS:HB2	1.88	0.40
4:E:62:THR:O	4:E:66:LYS:HD3	2.22	0.40
6:G:3:DC:N4	7:H:25:DG:H1	2.13	0.40
1:A:72:LYS:HE3	2:C:643:VAL:O	2.21	0.40
1:B:138:LEU:HA	1:B:138:LEU:HD12	1.92	0.40
1:B:80:LEU:HD21	3:D:842:VAL:HG12	2.03	0.40
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.86	0.40
3:D:1137:ARG:NH2	3:D:1172:HIS:CD2	2.90	0.40
6:G:19:DA:H2''	6:G:20:DA:O5'	2.21	0.40
6:G:11:DA:N6	7:H:16:DC:N4	2.70	0.40
2:C:376:ARG:HA	2:C:376:ARG:HD2	1.69	0.40
2:C:2:GLU:HG3	2:C:3:ILE:N	2.36	0.40
2:C:748:GLU:HA	2:C:799:ILE:HD13	2.04	0.40
2:C:966:LEU:HD13	2:C:986:PRO:HB3	2.03	0.40
3:D:876:SER:OG	3:D:879:ARG:HG3	2.22	0.40
5:F:184:ARG:O	5:F:188:ILE:HG13	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:LEU:HD11	1:A:192:LEU:CD1	2.52	0.40
1:A:39:PRO:CG	1:B:39:PRO:HG2	2.51	0.40
2:C:1053:LEU:HA	3:D:621:LYS:HD2	2.04	0.40
2:C:396:ASP:HA	2:C:633:GLN:HE22	1.84	0.40
2:C:22:GLN:HG3	2:C:407:LYS:HB3	2.03	0.40
2:C:76:PRO:HA	2:C:77:PRO:HD3	1.96	0.40
2:C:775:ARG:HG3	2:C:780:GLU:O	2.22	0.40
2:C:911:GLU:N	2:C:912:PRO:HD2	2.37	0.40
3:D:1054:GLU:HG2	3:D:1054:GLU:H	1.59	0.40
3:D:284:LEU:HD12	3:D:290:PRO:HG3	2.04	0.40
3:D:321:GLN:HB2	3:D:336:PHE:CD2	2.56	0.40
3:D:367:ILE:HD11	3:D:379:ALA:HB2	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:34:TYR:OH	3:D:327:GLU:OE1[4_1359]	2.13	0.07

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	224/315 (71%)	218 (97%)	6 (3%)	0	100	100
1	B	222/315 (70%)	207 (93%)	13 (6%)	2 (1%)	17	52
2	C	1107/1119 (99%)	1055 (95%)	36 (3%)	16 (1%)	11	40
3	D	1481/1524 (97%)	1431 (97%)	40 (3%)	10 (1%)	22	57
4	E	92/99 (93%)	89 (97%)	2 (2%)	1 (1%)	14	47
5	F	344/423 (81%)	311 (90%)	24 (7%)	9 (3%)	5	24
All	All	3470/3795 (91%)	3311 (95%)	121 (4%)	38 (1%)	14	47

All (38) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	212	GLY
2	C	316	GLY
2	C	363	SER
2	C	421	GLU
2	C	932	GLU
3	D	484	PRO
3	D	486	ARG
3	D	1130	ARG
5	F	323	ASP
5	F	388	ALA
5	F	411	HIS
2	C	228	ALA
2	C	362	GLY
2	C	365	ASP
2	C	420	ARG
3	D	1049	SER
5	F	384	GLU
5	F	385	GLU
5	F	416	ARG
2	C	776	SER
5	F	356	LYS
1	B	154	GLU
2	C	105	THR
2	C	594	ALA
3	D	1050	GLY
4	E	94	PRO
2	C	155	PRO
2	C	592	LEU
3	D	320	ALA
3	D	485	SER
5	F	382	THR
1	B	8	ALA
3	D	1494	ALA
3	D	831	GLY
5	F	321	ILE
2	C	244	PRO
2	C	415	PRO
3	D	530	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	199/273 (73%)	185 (93%)	14 (7%)	15	44
1	B	197/273 (72%)	190 (96%)	7 (4%)	35	68
2	C	931/941 (99%)	889 (96%)	42 (4%)	27	62
3	D	1251/1279 (98%)	1183 (95%)	68 (5%)	22	55
4	E	83/88 (94%)	80 (96%)	3 (4%)	35	68
5	F	296/371 (80%)	286 (97%)	10 (3%)	37	70
All	All	2957/3225 (92%)	2813 (95%)	144 (5%)	25	59

All (144) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	34	VAL
1	A	67	THR
1	A	104	GLU
1	A	112	ARG
1	A	133	GLU
1	A	161	ARG
1	A	184	THR
1	A	186	LEU
1	A	188	GLN
1	A	189	ARG
1	A	205	VAL
1	A	219	ARG
1	A	229	GLN
1	B	34	VAL
1	B	38	ASN
1	B	112	ARG
1	B	126	ASP
1	B	134	GLU
1	B	137	ARG
1	B	186	LEU
2	C	2	GLU

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Mol	Chain	Res	Type
2	C	8	ARG
2	C	28	ARG
2	C	49	ARG
2	C	107	LEU
2	C	118	ILE
2	C	133	ASP
2	C	141	HIS
2	C	168	ARG
2	C	204	GLN
2	C	205	GLU
2	C	209	ARG
2	C	221	LEU
2	C	230	ARG
2	C	292	ARG
2	C	342	ASP
2	C	387	SER
2	C	413	LEU
2	C	427	VAL
2	C	434	HIS
2	C	454	SER
2	C	557	ARG
2	C	562	SER
2	C	575	GLN
2	C	583	LEU
2	C	586	ARG
2	C	591	SER
2	C	610	ARG
2	C	617	ASP
2	C	627	ARG
2	C	640	ARG
2	C	661	SER
2	C	775	ARG
2	C	776	SER
2	C	808	ARG
2	C	813	VAL
2	C	829	GLN
2	C	939	ARG
2	C	968	LEU
2	C	1001	VAL
2	C	1014	SER
2	C	1057	SER
3	D	30	GLU

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Mol	Chain	Res	Type
3	D	48	ARG
3	D	68	PHE
3	D	81	THR
3	D	106	LYS
3	D	119	SER
3	D	141	ILE
3	D	142	LEU
3	D	150	ARG
3	D	155	ASP
3	D	161	LEU
3	D	179	VAL
3	D	191	LEU
3	D	198	ARG
3	D	220	ARG
3	D	230	TRP
3	D	231	VAL
3	D	256	GLU
3	D	272	LEU
3	D	273	ARG
3	D	276	ASP
3	D	312	ARG
3	D	325	GLU
3	D	362	GLU
3	D	372	ASP
3	D	421	LEU
3	D	423	ASP
3	D	525	ARG
3	D	548	ILE
3	D	587	ARG
3	D	596	SER
3	D	618	LEU
3	D	650	LEU
3	D	709	HIS
3	D	754	PHE
3	D	778	LEU
3	D	799	LYS
3	D	808	THR
3	D	817	GLU
3	D	832	ARG
3	D	861	GLN
3	D	864	VAL
3	D	873	LEU

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Mol	Chain	Res	Type
3	D	875	THR
3	D	894	LYS
3	D	904	VAL
3	D	907	GLU
3	D	970	LYS
3	D	971	LEU
3	D	972	LEU
3	D	1041	LEU
3	D	1079	LYS
3	D	1151	ARG
3	D	1155	VAL
3	D	1169	ASP
3	D	1188	VAL
3	D	1195	GLN
3	D	1208	ASP
3	D	1219	GLU
3	D	1221	VAL
3	D	1236	LEU
3	D	1290	LEU
3	D	1305	LEU
3	D	1313	VAL
3	D	1317	ASP
3	D	1422	MET
3	D	1470	ARG
3	D	1496	GLU
4	E	15	SER
4	E	66	LYS
4	E	75	PHE
5	F	186	HIS
5	F	205	ARG
5	F	254	GLN
5	F	287	THR
5	F	348	SER
5	F	362	SER
5	F	367	MET
5	F	383	LEU
5	F	407	LYS
5	F	419	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	95	GLN
2	C	390	GLN
2	C	500	ASN
2	C	683	ASN
2	C	834	GLN
3	D	744	GLN
3	D	855	HIS
3	D	861	GLN
3	D	1037	GLN
3	D	1195	GLN
5	F	83	GLN
5	F	218	GLN
5	F	269	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	I	5/6 (83%)	1 (20%)	1 (20%)

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	I	5	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
8	I	4	G

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 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	$\# Z > 2$
10	POP	D	1601	-	6,8,8	0.81	0	13,13,13	1.15	1 (7%)

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
10	POP	D	1601	-	-	0/6/6/6	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	1601	POP	P2-O-P1	-2.99	122.58	132.83

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	226/315 (71%)	-0.35	0	100 100	66, 89, 110, 118	0
1	B	224/315 (71%)	-0.39	0	100 100	65, 93, 117, 134	0
2	C	1111/1119 (99%)	-0.22	9 (0%)	86 65	51, 90, 144, 167	0
3	D	1485/1524 (97%)	-0.29	8 (0%)	91 75	47, 83, 135, 170	0
4	E	94/99 (94%)	-0.34	1 (1%)	80 56	62, 98, 130, 138	0
5	F	346/423 (81%)	-0.10	17 (4%)	29 11	60, 98, 175, 188	0
6	G	19/22 (86%)	-0.15	1 (5%)	26 9	59, 107, 212, 218	0
7	H	20/27 (74%)	-0.34	1 (5%)	28 10	86, 122, 223, 225	0
8	I	5/6 (83%)	0.36	1 (20%)	1 0	62, 68, 90, 154	0
All	All	3530/3850 (91%)	-0.26	38 (1%)	80 56	47, 89, 146, 225	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	F	392	VAL	6.7
5	F	391	GLY	4.9
5	F	389	PHE	4.4
5	F	393	THR	4.0
5	F	390	PHE	4.0
5	F	375	LEU	3.8
5	F	397	ILE	3.6
5	F	376	ILE	3.2
2	C	219	GLN	3.2
5	F	361	LEU	3.1
5	F	416	ARG	2.9
3	D	1318	TYR	2.8
3	D	1497	GLU	2.8
5	F	419	ARG	2.7
2	C	207	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
5	F	149	GLU	2.6
2	C	311	PHE	2.5
5	F	417	LYS	2.5
5	F	148	LYS	2.5
6	G	3	DC	2.5
5	F	422	LEU	2.5
5	F	362	SER	2.5
8	I	4	G	2.4
2	C	365	ASP	2.4
2	C	107	LEU	2.4
2	C	424	GLY	2.3
3	D	142	LEU	2.2
2	C	194	VAL	2.2
2	C	64	LEU	2.2
7	H	23	DA	2.1
3	D	144	GLY	2.1
3	D	1129	THR	2.1
4	E	85	LEU	2.1
3	D	410	SER	2.1
3	D	216	VAL	2.1
2	C	367	LEU	2.1
3	D	980	MET	2.1
5	F	369	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 carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	POP	D	1601	9/9	0.95	0.29	73,86,104,112	0
9	MG	B	1001	1/1	0.97	0.41	66,66,66,66	0
11	ZN	D	1604	1/1	0.98	0.22	84,84,84,84	0
11	ZN	D	1603	1/1	0.98	0.12	111,111,111,111	0
9	MG	D	1602	1/1	0.99	0.29	52,52,52,52	0

6.5 Other polymers [i](#)

There are no such residues in this entry.