



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 12:43 AM UTC

PDB ID : 4OIQ / pdb_00004oiq
Title : Crystal structure of Thermus thermophilus transcription initiation complex soaked with GE23077 and rifampicin
Authors : Zhang, Y.; Ebright, R.H.; Arnold, E.
Deposited on : 2014-01-20
Resolution : 3.62 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

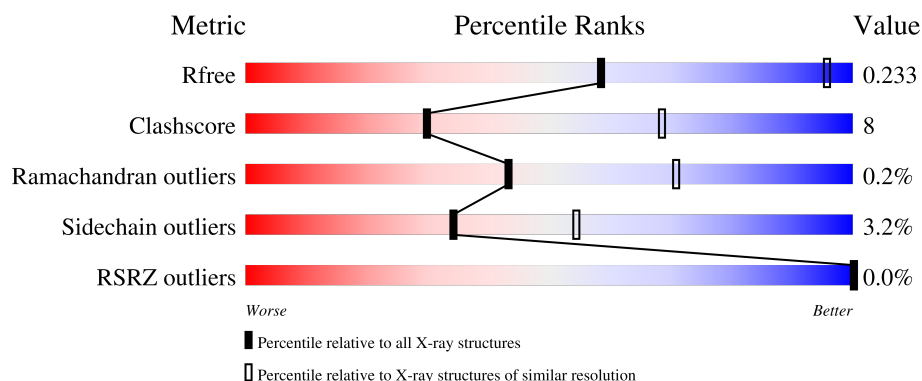
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

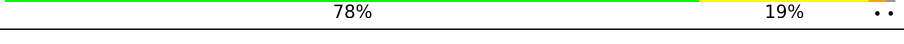
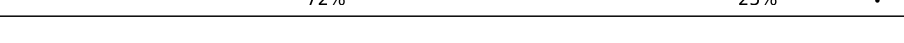
The reported resolution of this entry is 3.62 Å.

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	1062 (3.72-3.52)
Clashscore	190562	1092 (3.72-3.52)
Ramachandran outliers	187476	1057 (3.72-3.52)
Sidechain outliers	187428	1055 (3.72-3.52)
RSRZ outliers	180081	1060 (3.72-3.52)

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	315	
1	B	315	
2	C	1119	
3	D	1524	
4	E	99	

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Mol	Chain	Length	Quality of chain
5	F	443	
6	G	21	
7	H	27	
8	I	7	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 28527 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	231	Total	C	N	O	S	0	0	0
			1809	1155	315	337	2			
1	B	221	Total	C	N	O	S	0	0	0
			1741	1112	302	325	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8774	5550	1565	1635	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1487	Total	C	N	O	S	0	1	0
			11754	7451	2071	2196	36			

- 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
			758	483	132	139	4			

- Molecule 5 is a protein called DNA directed RNA polymerase sigma factor A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	346	Total	C	N	O	S	0	0	0
			2807	1770	509	524	4			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-19	MET	-	expression tag	UNP Q5SKW1
F	-18	GLY	-	expression tag	UNP Q5SKW1
F	-17	SER	-	expression tag	UNP Q5SKW1
F	-16	SER	-	expression tag	UNP Q5SKW1
F	-15	HIS	-	expression tag	UNP Q5SKW1
F	-14	HIS	-	expression tag	UNP Q5SKW1
F	-13	HIS	-	expression tag	UNP Q5SKW1
F	-12	HIS	-	expression tag	UNP Q5SKW1
F	-11	HIS	-	expression tag	UNP Q5SKW1
F	-10	HIS	-	expression tag	UNP Q5SKW1
F	-9	SER	-	expression tag	UNP Q5SKW1
F	-8	SER	-	expression tag	UNP Q5SKW1
F	-7	GLY	-	expression tag	UNP Q5SKW1
F	-6	LEU	-	expression tag	UNP Q5SKW1
F	-5	VAL	-	expression tag	UNP Q5SKW1
F	-4	PRO	-	expression tag	UNP Q5SKW1
F	-3	ARG	-	expression tag	UNP Q5SKW1
F	-2	GLY	-	expression tag	UNP Q5SKW1
F	-1	SER	-	expression tag	UNP Q5SKW1
F	0	HIS	-	expression tag	UNP Q5SKW1

- Molecule 6 is a DNA chain called 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	G	16	Total	C	N	O	P	0	0	0
			328	156	63	94	15			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	H	24	Total	C	N	O	P	0	0	0
			495	236	94	142	23			

- Molecule 8 is a protein called GE23077.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	I	7	Total	C	N	O	0	0	0
			50	26	9	15			

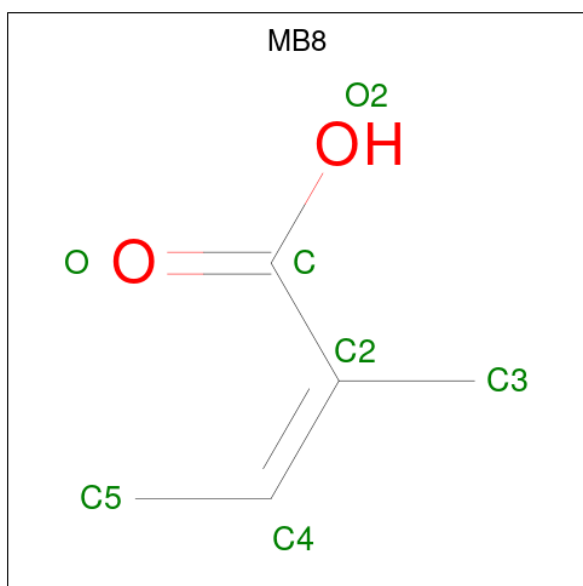
- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	D	3	Total	Mg	0	0
			3	3		
10	F	1	Total	Mg	0	0
			1	1		

- Molecule 11 is (2Z)-2-methylbut-2-enoic acid (CCD ID: MB8) (formula: C₅H₈O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	I	1	Total	C	O	0	0
			2	1	1		

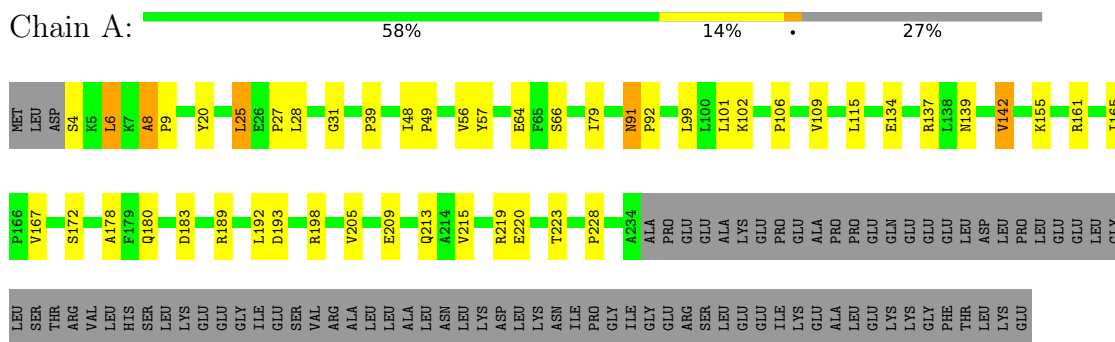
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	D	3	Total	O	0	0
			3	3		

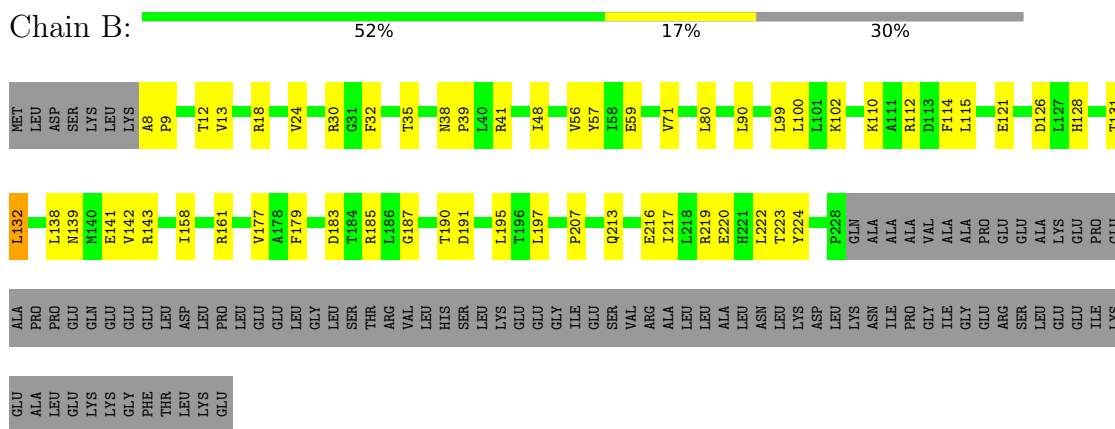
3 Residue-property plots

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

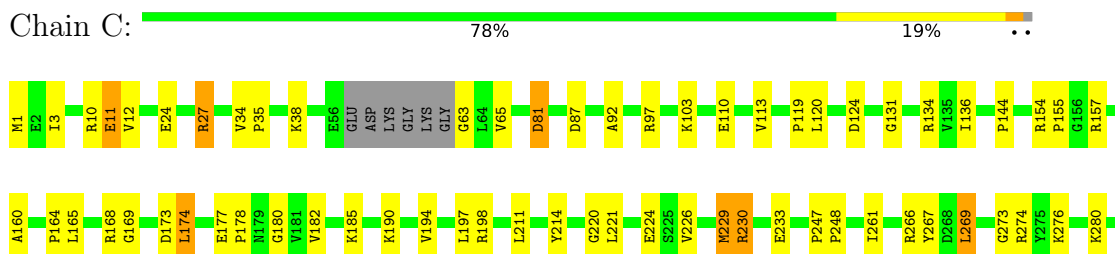
• Molecule 1: DNA-directed RNA polymerase subunit alpha

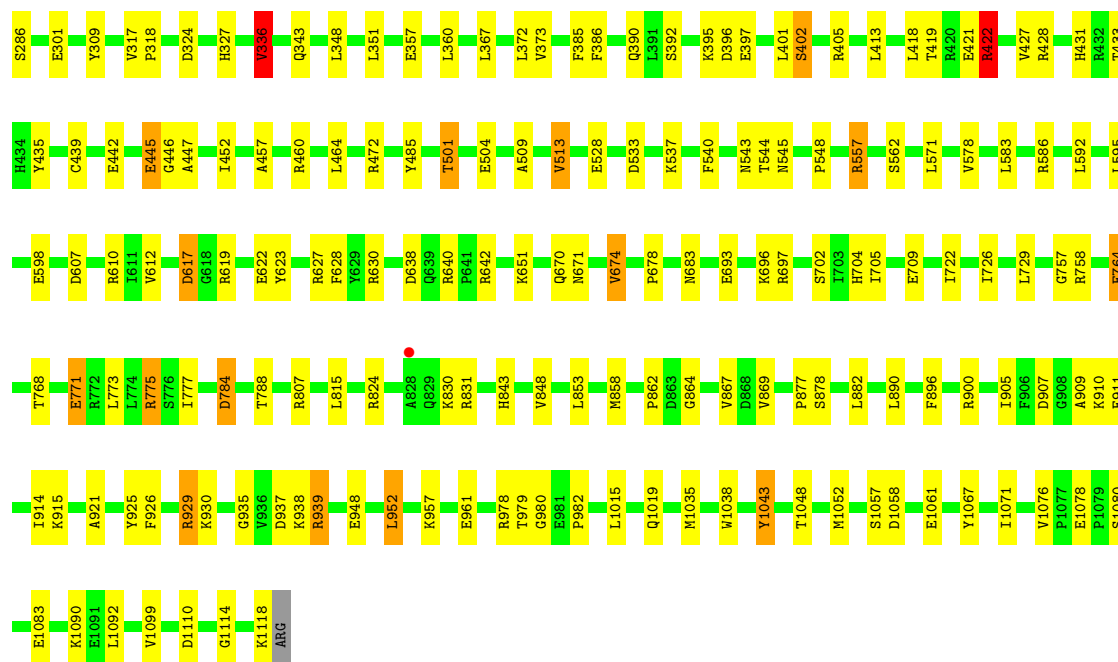


• Molecule 1: DNA-directed RNA polymerase subunit alpha



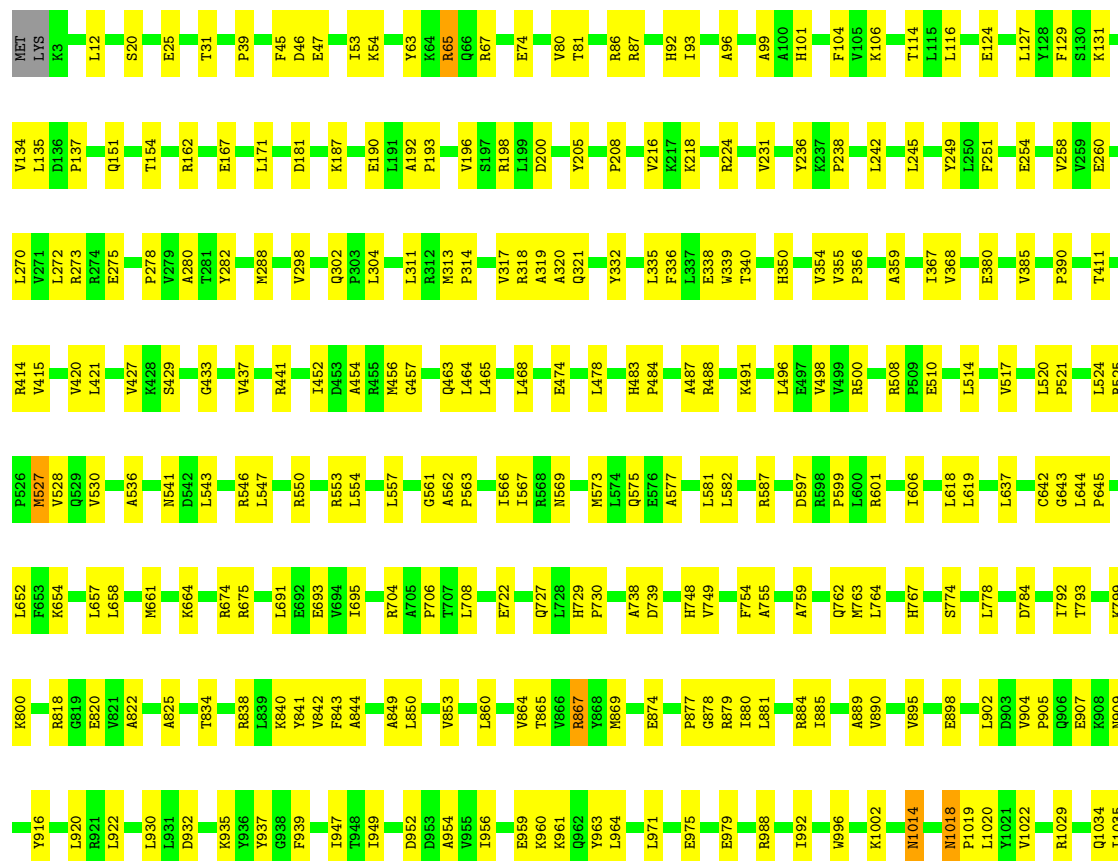
• Molecule 2: DNA-directed RNA polymerase subunit beta

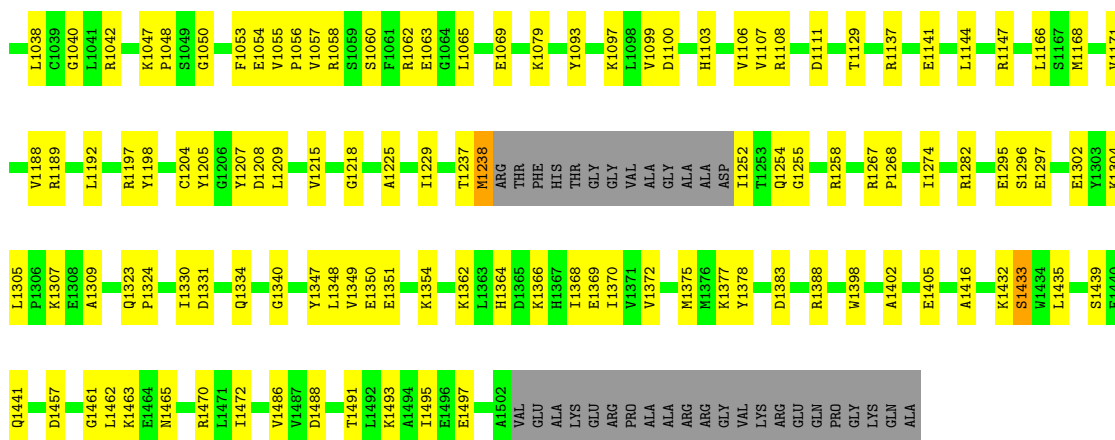




• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 72% 25%





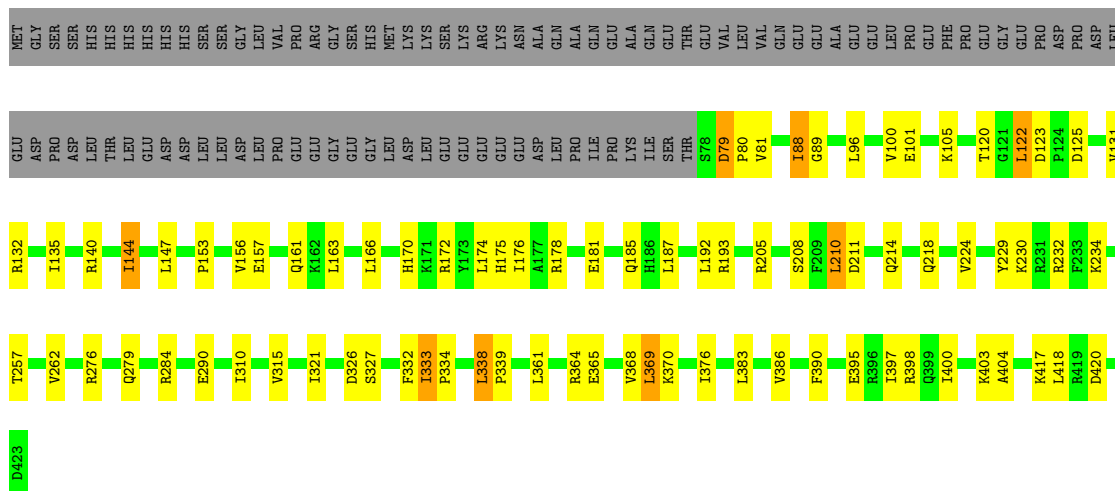
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 79% 16% 5%



- Molecule 5: DNA directed RNA polymerase sigma factor A

Chain F: 60% 17% 22%

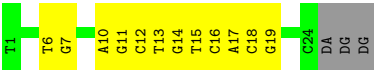


- Molecule 6: 5'-D(*CP*CP*T*GP*CP*AP*TP*CP*CP*GP*TP*GP*AP*GP*TP*CP*GP*AP*GP*GP*G)-3'

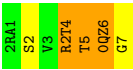
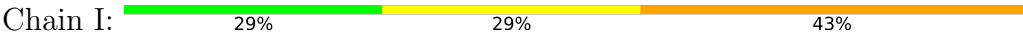
Chain G: 52% 24% 24%



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



● Molecule 8: GE23077



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.84Å 104.18Å 295.32Å 90.00° 98.52° 90.00°	Depositor
Resolution (Å)	48.68 – 3.62 48.68 – 3.62	Depositor EDS
% Data completeness (in resolution range)	91.3 (48.68-3.62) 91.4 (48.68-3.62)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	0.15	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.92 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, R_{free}	0.199 , 0.248 (Not available) , 0.233	Depositor DCC
R_{free} test set	1823 reflections (2.87%)	wwPDB-VP
Wilson B-factor (Å ²)	102.3	Xtriage
Anisotropy	0.506	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28527	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: 2RA, DSN, DVA, R2T, ZN, 2TL, FGL, 0QZ, MB8, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.50	0/1841	0.98	9/2504 (0.4%)
1	B	0.46	0/1773	0.90	4/2413 (0.2%)
2	C	0.54	0/8941	0.96	18/12092 (0.1%)
3	D	0.48	0/11963	0.87	10/16173 (0.1%)
4	E	0.54	0/772	0.90	0/1040
5	F	0.47	0/2852	0.87	6/3837 (0.2%)
6	G	0.28	0/368	0.77	1/567 (0.2%)
7	H	0.26	0/556	0.74	0/858
All	All	0.50	0/29066	0.91	48/39484 (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	1
8	I	0	1
All	All	0	2

There are no bond length outliers.

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	SER	CA-C-N	8.60	128.24	119.56
1	A	172	SER	C-N-CA	8.60	128.24	119.56
2	C	439	CYS	CA-C-N	7.80	127.46	119.19
2	C	439	CYS	C-N-CA	7.80	127.46	119.19
3	D	433	GLY	N-CA-C	7.03	120.04	110.69
1	B	48	ILE	CA-C-N	6.94	128.52	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	48	ILE	C-N-CA	6.94	128.52	119.84
2	C	980	GLY	N-CA-C	-6.69	105.37	115.00
3	D	1018	ASN	CA-C-N	6.38	125.87	119.24
3	D	1018	ASN	C-N-CA	6.38	125.87	119.24
2	C	422	ARG	N-CA-C	6.31	124.25	110.80
2	C	419	THR	N-CA-C	-6.14	101.19	110.28
5	F	333	ILE	N-CA-C	6.07	113.56	107.55
3	D	275	GLU	CB-CA-C	-6.02	109.62	116.54
2	C	169	GLY	CA-C-N	5.98	126.17	120.31
2	C	169	GLY	C-N-CA	5.98	126.17	120.31
2	C	226	VAL	N-CA-C	5.97	117.51	111.00
1	A	8	ALA	CA-C-N	5.90	126.10	120.31
1	A	8	ALA	C-N-CA	5.90	126.10	120.31
2	C	336	VAL	CB-CA-C	-5.86	104.38	111.88
5	F	262	VAL	N-CA-C	5.84	116.58	110.62
1	B	115	LEU	CA-C-N	5.80	125.82	119.90
1	B	115	LEU	C-N-CA	5.80	125.82	119.90
3	D	1050	GLY	N-CA-C	-5.70	107.16	114.85
2	C	501	THR	CA-C-N	5.57	125.89	119.93
2	C	501	THR	C-N-CA	5.57	125.89	119.93
3	D	1255	GLY	N-CA-C	5.54	121.13	111.78
3	D	1340	GLY	CA-C-N	5.50	124.96	119.24
3	D	1340	GLY	C-N-CA	5.50	124.96	119.24
2	C	909	ALA	N-CA-C	-5.47	102.19	110.28
6	G	17	DG	C4'-C3'-O3'	5.39	118.09	110.00
3	D	1331	ASP	CA-C-N	5.38	125.45	119.32
3	D	1331	ASP	C-N-CA	5.38	125.45	119.32
2	C	229	MET	N-CA-C	5.37	121.67	113.61
1	A	165	ILE	N-CA-C	5.32	113.29	107.60
2	C	1043	TYR	N-CA-C	-5.29	106.83	113.28
1	A	91	ASN	CA-C-N	5.27	125.08	119.28
1	A	91	ASN	C-N-CA	5.27	125.08	119.28
5	F	79	ASP	CA-C-N	5.26	125.06	119.28
5	F	79	ASP	C-N-CA	5.26	125.06	119.28
2	C	445	GLU	N-CA-C	5.23	118.12	111.69
2	C	457	ALA	N-CA-C	5.19	117.67	111.71
2	C	269	LEU	N-CA-C	-5.13	102.89	110.48
5	F	144	ILE	CA-C-N	5.11	124.55	119.24
5	F	144	ILE	C-N-CA	5.11	124.55	119.24
2	C	214	TYR	N-CA-C	5.09	116.67	110.41
1	A	115	LEU	CA-C-N	5.02	124.93	119.76
1	A	115	LEU	C-N-CA	5.02	124.93	119.76

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	421	GLU	Peptide
8	I	5	2TL	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	1809	0	1863	29	0
1	B	1741	0	1784	38	0
2	C	8774	0	8877	136	0
3	D	11754	0	11994	245	0
4	E	758	0	770	13	0
5	F	2807	0	2882	57	0
6	G	328	0	181	4	0
7	H	495	0	272	14	0
8	I	50	0	37	5	0
9	D	2	0	0	0	0
10	D	3	0	0	0	0
10	F	1	0	0	0	0
11	I	2	0	0	0	0
12	D	3	0	0	1	0
All	All	28527	0	28660	485	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 8.

All (485) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:628:PHE:H	2:C:638:ASP:HB3	1.32	0.93
2:C:418:LEU:HA	2:C:422:ARG:HH11	1.37	0.89
1:B:190:THR:HG21	3:D:722:GLU:HG3	1.65	0.77
2:C:758:ARG:HH21	2:C:788:THR:HB	1.50	0.77
3:D:1495:ILE:HG12	4:E:88:GLU:HG3	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:81:ASP:OD1	2:C:81:ASP:N	2.20	0.74
3:D:134:VAL:HG22	3:D:151:GLN:H	1.52	0.72
3:D:739:ASP:OD2	12:D:2103:HOH:O	2.07	0.71
2:C:194:VAL:HG22	2:C:221:LEU:HD12	1.72	0.71
8:I:4:R2T:OG1	8:I:4:R2T:N	2.22	0.70
3:D:238:PRO:HD3	3:D:318:ARG:HG3	1.72	0.70
1:A:25:LEU:HD23	1:A:28:LEU:HD21	1.73	0.70
5:F:361:LEU:HB3	5:F:365:GLU:HG3	1.74	0.70
2:C:709:GLU:OE2	2:C:824:ARG:NH1	2.25	0.69
7:H:18:DC:H2'	7:H:19:DG:C8	2.28	0.69
3:D:1208:ASP:HB2	3:D:1215:VAL:HA	1.75	0.69
2:C:418:LEU:HA	2:C:422:ARG:NH1	2.09	0.68
3:D:657:LEU:HG	3:D:661:MET:HE2	1.76	0.67
2:C:3:ILE:HD13	2:C:900:ARG:HB2	1.77	0.67
1:B:59:GLU:OE1	1:B:139:ASN:ND2	2.29	0.66
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.29	0.66
2:C:165:LEU:HB2	2:C:168:ARG:HG3	1.78	0.66
5:F:131:VAL:HG13	5:F:178:ARG:HD3	1.76	0.66
1:A:220:GLU:O	1:A:223:THR:HB	1.97	0.65
2:C:428:ARG:NH2	2:C:447:ALA:O	2.29	0.65
2:C:501:THR:HG21	2:C:513:VAL:HG23	1.79	0.65
2:C:628:PHE:H	2:C:638:ASP:CB	2.07	0.65
2:C:1083:GLU:OE2	3:D:87:ARG:NH2	2.30	0.65
2:C:545:ASN:HB3	2:C:583:LEU:HD23	1.77	0.64
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.26	0.64
3:D:273:ARG:HB3	3:D:278:PRO:HA	1.80	0.64
2:C:628:PHE:N	2:C:638:ASP:HB3	2.10	0.64
1:B:56:VAL:HG22	1:B:142:VAL:HG12	1.79	0.64
7:H:10:DA:H2''	7:H:11:DG:H5''	1.80	0.64
3:D:664:LYS:NZ	3:D:693:GLU:OE1	2.31	0.63
5:F:81:VAL:HG22	5:F:210:LEU:HD21	1.79	0.63
5:F:166:LEU:HD13	5:F:170:HIS:HB3	1.80	0.63
2:C:504:GLU:HG2	2:C:509:ALA:HB2	1.81	0.63
2:C:24:GLU:OE2	2:C:27:ARG:NH2	2.31	0.63
3:D:65:ARG:HB3	3:D:67:ARG:HG2	1.81	0.62
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.81	0.62
2:C:607:ASP:HB2	2:C:610:ARG:NH1	2.15	0.62
4:E:50:THR:HG22	4:E:53:GLY:O	2.00	0.62
3:D:1349:VAL:HG22	3:D:1368:ILE:HG22	1.81	0.61
3:D:1189:ARG:HB3	3:D:1204:CYS:HA	1.83	0.61
3:D:181:ASP:HB2	3:D:205:TYR:CD1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:208:PRO:HA	3:D:390:PRO:HA	1.83	0.60
1:B:80:LEU:HD21	3:D:842:VAL:HG12	1.84	0.60
3:D:39:PRO:HG2	3:D:47:GLU:HG3	1.84	0.60
1:B:128:HIS:HE1	1:B:131:THR:HG23	1.65	0.60
5:F:208:SER:HB3	5:F:211:ASP:OD2	2.01	0.60
3:D:63:TYR:OH	3:D:74:GLU:OE2	2.19	0.59
3:D:1462:LEU:HD22	3:D:1472:ILE:HB	1.84	0.59
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.85	0.59
3:D:218:LYS:HG2	3:D:338:GLU:HG2	1.83	0.59
3:D:1111:ASP:OD1	3:D:1189:ARG:NH2	2.35	0.59
3:D:124:GLU:OE2	3:D:587:ARG:NH2	2.35	0.59
3:D:474:GLU:HG3	3:D:496:LEU:HD11	1.85	0.59
1:A:64:GLU:OE2	2:C:830:LYS:NZ	2.35	0.59
3:D:637:LEU:HD13	3:D:642:CYS:HA	1.85	0.59
3:D:1274:ILE:HD11	3:D:1334:GLN:HB3	1.85	0.58
3:D:1324:PRO:HG3	3:D:1330:ILE:HD11	1.85	0.58
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.38	0.58
2:C:413:LEU:HD12	2:C:452:ILE:HD11	1.85	0.58
2:C:853:LEU:HB2	2:C:858:MET:HE1	1.84	0.58
1:A:183:ASP:HA	2:C:938:LYS:HE3	1.84	0.58
3:D:260:GLU:OE1	3:D:273:ARG:NH1	2.32	0.57
3:D:954:ALA:O	3:D:1062:ARG:NH2	2.36	0.57
5:F:400:ILE:HA	5:F:403:LYS:HG2	1.85	0.57
1:B:220:GLU:O	1:B:223:THR:OG1	2.20	0.57
3:D:864:VAL:HG22	3:D:865:THR:H	1.69	0.57
2:C:134:ARG:NH1	2:C:392:SER:OG	2.37	0.57
1:B:132:LEU:HD21	1:B:138:LEU:HB2	1.87	0.57
2:C:97:ARG:NH2	2:C:110:GLU:OE2	2.36	0.57
2:C:144:PRO:HB2	2:C:273:GLY:HA3	1.87	0.57
2:C:165:LEU:CB	2:C:168:ARG:HG3	2.34	0.57
3:D:1433:SER:O	3:D:1433:SER:OG	2.23	0.57
4:E:18:ARG:NH2	4:E:77:GLU:OE1	2.38	0.57
2:C:229:MET:HB3	2:C:233:GLU:HB2	1.87	0.56
3:D:171:LEU:HD12	3:D:390:PRO:HG2	1.87	0.56
2:C:445:GLU:OE1	8:I:4:R2T:OG1	2.23	0.56
2:C:12:VAL:HG21	2:C:472:ARG:HD3	1.87	0.56
3:D:1377:LYS:HE3	3:D:1378:TYR:CZ	2.41	0.56
5:F:135:ILE:HD11	5:F:178:ARG:HB3	1.87	0.56
3:D:971:LEU:HD21	3:D:992:ILE:HG23	1.88	0.56
3:D:988:ARG:NH2	3:D:1054:GLU:OE2	2.38	0.55
3:D:224:ARG:NE	3:D:254:GLU:OE2	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:840:LYS:HE3	3:D:841:TYR:OH	2.07	0.55
3:D:889:ALA:HB1	3:D:930:LEU:HA	1.88	0.55
1:A:25:LEU:HB3	1:A:28:LEU:HD11	1.87	0.55
2:C:1052:MET:HE1	3:D:748:HIS:HB3	1.89	0.55
2:C:197:LEU:HD12	2:C:221:LEU:HD11	1.89	0.55
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.71	0.55
3:D:224:ARG:H	3:D:251:PHE:HE1	1.55	0.55
1:B:32:PHE:HA	1:B:35:THR:HB	1.88	0.54
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.90	0.54
2:C:704:HIS:CD2	2:C:831:ARG:HD2	2.43	0.54
2:C:939:ARG:HG2	2:C:982:PRO:HD3	1.89	0.54
3:D:1209:LEU:HD11	3:D:1364:HIS:CD2	2.43	0.54
4:E:50:THR:HG23	4:E:52:GLU:N	2.24	0.53
5:F:284:ARG:NH2	5:F:290:GLU:OE2	2.42	0.53
5:F:326:ASP:OD2	6:G:18:DA:N6	2.42	0.53
3:D:563:PRO:HD2	3:D:566:ILE:HD12	1.88	0.53
3:D:437:VAL:HG11	5:F:175:HIS:CD2	2.44	0.53
5:F:88:ILE:HD11	5:F:192:LEU:HD13	1.91	0.53
1:A:57:TYR:CG	1:A:161:ARG:HD2	2.44	0.53
3:D:242:LEU:HB3	3:D:311:LEU:HD12	1.91	0.53
1:A:106:PRO:HG3	1:A:134:GLU:HG2	1.91	0.53
2:C:612:VAL:HG22	2:C:622:GLU:HG3	1.89	0.53
2:C:630:ARG:NH1	2:C:705:ILE:O	2.32	0.53
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.91	0.53
8:I:2:DSN:O	8:I:5:2TL:OG1	2.27	0.53
2:C:1038:TRP:CE2	3:D:1099:VAL:HG11	2.44	0.53
3:D:658:LEU:HA	3:D:661:MET:HE3	1.91	0.53
1:B:100:LEU:HG	1:B:141:GLU:HG2	1.91	0.53
1:B:41:ARG:HA	1:B:177:VAL:HG11	1.90	0.52
2:C:784:ASP:OD1	2:C:784:ASP:N	2.37	0.52
1:A:25:LEU:HD11	1:B:224:TYR:O	2.09	0.52
2:C:35:PRO:HG2	2:C:38:LYS:HD2	1.91	0.52
2:C:168:ARG:O	2:C:267:TYR:HA	2.09	0.52
2:C:726:ILE:HD11	2:C:757:GLY:HA3	1.91	0.52
3:D:272:LEU:HB2	3:D:280:ALA:HB3	1.90	0.52
4:E:45:ARG:NH1	4:E:56:ASP:OD2	2.43	0.52
3:D:956:ILE:HD11	3:D:1062:ARG:HD2	1.91	0.52
1:A:209:GLU:O	1:A:213:GLN:HG2	2.10	0.52
2:C:405:ARG:HD2	2:C:442:GLU:OE2	2.09	0.52
3:D:840:LYS:HE3	3:D:841:TYR:CZ	2.45	0.52
3:D:963:TYR:HE2	3:D:1002:LYS:HD3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:904:VAL:HG22	3:D:905:PRO:HD2	1.91	0.52
2:C:280:LYS:HE3	2:C:309:TYR:CZ	2.45	0.51
3:D:566:ILE:HD11	5:F:192:LEU:HD21	1.92	0.51
2:C:11:GLU:OE1	2:C:537:LYS:HE2	2.10	0.51
3:D:1093:TYR:CZ	3:D:1097:LYS:HE3	2.45	0.51
2:C:177:GLU:HG3	2:C:178:PRO:HD2	1.93	0.51
2:C:937:ASP:OD1	2:C:939:ARG:HD3	2.10	0.51
3:D:652:LEU:HB3	3:D:749:VAL:HG21	1.92	0.51
2:C:1110:ASP:OD2	2:C:1114:GLY:N	2.31	0.51
3:D:569:ASN:ND2	5:F:214:GLN:OE1	2.44	0.51
2:C:435:TYR:OH	2:C:533:ASP:OD2	2.23	0.51
3:D:704:ARG:HD2	3:D:738:ALA:HB2	1.91	0.51
3:D:759:ALA:HA	3:D:763:MET:HB2	1.92	0.51
3:D:99:ALA:HB1	3:D:575:GLN:HE22	1.76	0.51
3:D:1225:ALA:O	3:D:1229:ILE:HG13	2.10	0.51
3:D:1020:LEU:HB3	3:D:1035:ILE:HD12	1.92	0.51
3:D:890:VAL:HB	3:D:922:LEU:HD13	1.93	0.50
5:F:144:ILE:HB	5:F:147:LEU:HD13	1.93	0.50
2:C:224:GLU:CD	2:C:224:GLU:H	2.19	0.50
3:D:500:ARG:NH1	3:D:1388:ARG:O	2.43	0.50
3:D:1305:LEU:HD13	3:D:1309:ALA:HB3	1.93	0.50
1:B:216:GLU:CD	1:B:219:ARG:HH21	2.20	0.50
3:D:844:ALA:HB1	3:D:867:ARG:HH21	1.76	0.50
3:D:314:PRO:HB2	3:D:317:VAL:HG12	1.94	0.50
3:D:1093:TYR:OH	3:D:1441:GLN:NE2	2.40	0.50
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.94	0.50
3:D:96:ALA:HB3	3:D:554:LEU:HD23	1.94	0.50
3:D:784:ASP:HB2	3:D:939:PHE:CE2	2.47	0.50
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.94	0.50
3:D:799:LYS:NZ	3:D:1014:ASN:HA	2.27	0.50
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.94	0.49
3:D:31:THR:HG21	5:F:257:THR:HG22	1.94	0.49
2:C:87:ASP:HA	2:C:131:GLY:HA3	1.94	0.49
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.93	0.49
3:D:561:GLY:HA3	5:F:132:ARG:HD3	1.93	0.49
3:D:784:ASP:HB2	3:D:939:PHE:HE2	1.77	0.49
3:D:1048:PRO:O	3:D:1079:LYS:NZ	2.43	0.49
2:C:422:ARG:NH2	7:H:14:DG:P	2.85	0.49
2:C:1048:THR:HG22	3:D:755:ALA:HB1	1.93	0.49
3:D:134:VAL:HG12	3:D:454:ALA:HB2	1.94	0.49
3:D:93:ILE:HD12	3:D:547:LEU:HD23	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:16:LYS:O	4:E:19:LEU:HB3	2.12	0.49
3:D:190:GLU:HA	3:D:196:VAL:HA	1.94	0.49
5:F:386:VAL:HB	5:F:397:ILE:HG12	1.95	0.49
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.37	0.49
2:C:422:ARG:HH21	7:H:14:DG:P	2.36	0.49
3:D:135:LEU:HD23	3:D:463:GLN:HG2	1.94	0.49
3:D:1042:ARG:HB3	3:D:1057:VAL:HB	1.94	0.49
5:F:395:GLU:OE2	5:F:398:ARG:NH2	2.46	0.49
1:B:71:VAL:HG22	1:B:132:LEU:HD23	1.94	0.49
3:D:483:HIS:CE1	3:D:488:ARG:HD3	2.48	0.49
2:C:764:GLU:OE2	3:D:54:LYS:HE2	2.11	0.49
1:A:99:LEU:HB2	1:A:142:VAL:HG22	1.94	0.49
2:C:911:GLU:O	2:C:915:LYS:HG2	2.13	0.49
3:D:1065:LEU:HD23	3:D:1069:GLU:HB3	1.94	0.48
2:C:878:SER:HA	3:D:1034:GLN:OE1	2.13	0.48
3:D:706:PRO:HB3	6:G:15:DT:H1'	1.95	0.48
3:D:1254:GLN:HB3	3:D:1258:ARG:HB2	1.96	0.48
3:D:1282:ARG:NH2	3:D:1295:GLU:OE2	2.46	0.48
6:G:8:DC:N4	7:H:19:DG:O6	2.46	0.48
1:A:228:PRO:HB3	1:B:13:VAL:HG21	1.96	0.48
2:C:915:LYS:NZ	3:D:952:ASP:OD2	2.41	0.48
2:C:324:ASP:OD2	2:C:431:HIS:NE2	2.36	0.48
3:D:691:LEU:O	3:D:695:ILE:HG23	2.13	0.48
5:F:193:ARG:HB2	7:H:6:DT:H1'	1.96	0.48
1:A:56:VAL:HG23	1:A:167:VAL:HG21	1.96	0.48
2:C:460:ARG:HD2	2:C:485:TYR:CZ	2.48	0.48
3:D:1486:VAL:HG21	4:E:22:VAL:HG13	1.96	0.48
7:H:16:DC:H2'	7:H:17:DA:C8	2.49	0.48
1:B:90:LEU:HD21	1:B:121:GLU:HB2	1.95	0.48
2:C:229:MET:O	2:C:233:GLU:HB2	2.13	0.48
3:D:129:PHE:CD1	3:D:456:MET:HB3	2.49	0.48
2:C:768:THR:O	2:C:771:GLU:N	2.46	0.48
1:B:110:LYS:HD3	1:B:128:HIS:HA	1.96	0.48
2:C:154:ARG:NH1	2:C:178:PRO:HG3	2.28	0.48
2:C:247:PRO:HA	2:C:248:PRO:HD3	1.67	0.48
2:C:607:ASP:HB3	2:C:610:ARG:H	1.78	0.48
2:C:1035:MET:HG2	2:C:1038:TRP:CZ3	2.48	0.48
3:D:101:HIS:CE1	3:D:582:LEU:HD13	2.49	0.48
3:D:411:THR:O	5:F:178:ARG:NH1	2.45	0.48
2:C:882:LEU:HD11	3:D:1038:LEU:HD22	1.94	0.47
3:D:258:VAL:HG12	3:D:273:ARG:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:116:LEU:HD21	3:D:465:LEU:HD23	1.95	0.47
3:D:774:SER:HB2	3:D:1362:LYS:HG2	1.96	0.47
5:F:96:LEU:O	5:F:100:VAL:HG23	2.13	0.47
3:D:557:LEU:HD13	3:D:566:ILE:HG22	1.96	0.47
3:D:601:ARG:NH1	3:D:606:ILE:HG12	2.29	0.47
3:D:961:LYS:HE3	3:D:961:LYS:HB2	1.71	0.47
3:D:1103:HIS:ND1	3:D:1463:LYS:HG3	2.28	0.47
3:D:1461:GLY:O	3:D:1465:ASN:ND2	2.48	0.47
1:B:179:PHE:HB3	1:B:197:LEU:HD13	1.95	0.47
1:B:216:GLU:OE1	1:B:219:ARG:NH2	2.46	0.47
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.95	0.47
3:D:1103:HIS:CG	3:D:1463:LYS:HG3	2.50	0.47
1:A:180:GLN:HE22	2:C:929:ARG:NH1	2.13	0.47
2:C:548:PRO:O	2:C:843:HIS:HE1	1.97	0.47
2:C:773:LEU:O	2:C:777:ILE:HG13	2.14	0.47
3:D:514:LEU:HD13	3:D:517:VAL:HG22	1.97	0.47
3:D:1372:VAL:HA	3:D:1375:MET:HE3	1.97	0.47
2:C:119:PRO:HG2	2:C:386:PHE:CD1	2.49	0.47
2:C:627:ARG:HA	2:C:638:ASP:HB2	1.97	0.47
2:C:890:LEU:HD13	2:C:914:ILE:HG23	1.97	0.47
2:C:930:LYS:NZ	2:C:935:GLY:HA2	2.30	0.47
3:D:116:LEU:HD23	3:D:468:LEU:HD11	1.96	0.47
2:C:640:ARG:HE	2:C:642:ARG:HH22	1.62	0.47
2:C:910:LYS:O	2:C:914:ILE:HG13	2.15	0.47
3:D:1144:LEU:O	3:D:1147:ARG:HG3	2.15	0.47
2:C:1067:TYR:CE2	2:C:1071:ILE:HD13	2.50	0.47
2:C:1090:LYS:HA	2:C:1090:LYS:HD3	1.68	0.47
3:D:137:PRO:HA	3:D:452:ILE:HG13	1.96	0.47
3:D:975:GLU:O	3:D:979:GLU:HG2	2.15	0.47
3:D:134:VAL:CG2	3:D:151:GLN:H	2.26	0.46
3:D:916:TYR:CE2	3:D:920:LEU:HD21	2.51	0.46
5:F:163:LEU:HD13	5:F:174:LEU:HD13	1.96	0.46
5:F:368:VAL:HG21	5:F:400:ILE:HD11	1.98	0.46
1:A:4:SER:O	1:A:189:ARG:NH2	2.39	0.46
2:C:286:SER:OG	2:C:301:GLU:OE2	2.23	0.46
2:C:1019:GLN:HG3	2:C:1058:ASP:HB3	1.96	0.46
3:D:167:GLU:OE2	3:D:198:ARG:NH1	2.47	0.46
4:E:68:LEU:HD12	4:E:68:LEU:HA	1.75	0.46
1:A:20:TYR:OH	1:A:198:ARG:HD2	2.15	0.46
2:C:63:GLY:O	2:C:103:LYS:HG2	2.15	0.46
2:C:571:LEU:HD23	2:C:702:SER:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1350:GLU:O	3:D:1354:LYS:HG3	2.14	0.46
3:D:114:THR:HG21	3:D:498:VAL:HG21	1.97	0.46
3:D:853:VAL:HG11	3:D:860:LEU:HG	1.97	0.46
5:F:321:ILE:HD12	5:F:332:PHE:CE1	2.51	0.46
8:I:4:R2T:NE2	8:I:4:R2T:OB1	2.49	0.46
1:A:27:PRO:HB2	1:A:192:LEU:HD13	1.98	0.46
1:A:101:LEU:HD21	1:A:109:VAL:HG11	1.98	0.46
2:C:1043:TYR:CG	3:D:763:MET:HG2	2.51	0.46
3:D:181:ASP:HB2	3:D:205:TYR:HD1	1.79	0.46
3:D:916:TYR:O	3:D:920:LEU:HG	2.16	0.46
3:D:1493:LYS:O	3:D:1497:GLU:HG2	2.15	0.46
2:C:327:HIS:CE1	2:C:433:THR:HG21	2.51	0.46
2:C:401:LEU:HD21	2:C:543:ASN:ND2	2.31	0.46
3:D:1347:TYR:CZ	3:D:1351:GLU:HG3	2.51	0.46
2:C:445:GLU:OE2	8:I:6:0QZ:N	2.49	0.45
3:D:841:TYR:HB2	3:D:864:VAL:CG2	2.46	0.45
3:D:270:LEU:HD13	3:D:304:LEU:HD13	1.98	0.45
3:D:487:ALA:O	3:D:491:LYS:HG2	2.15	0.45
5:F:81:VAL:HG22	5:F:210:LEU:CD2	2.46	0.45
1:B:213:GLN:O	1:B:217:ILE:HG13	2.17	0.45
2:C:367:LEU:HD13	2:C:372:LEU:HD21	1.98	0.45
2:C:578:VAL:HG23	2:C:671:ASN:CG	2.41	0.45
4:E:50:THR:HG23	4:E:52:GLU:H	1.81	0.45
3:D:483:HIS:CG	3:D:484:PRO:HD2	2.52	0.45
5:F:229:TYR:CZ	5:F:230:LYS:HD3	2.52	0.45
2:C:1038:TRP:NE1	3:D:1099:VAL:HG11	2.31	0.45
3:D:996:TRP:CE2	3:D:1056:PRO:HG3	2.50	0.45
3:D:1465:ASN:OD1	3:D:1470:ARG:NH1	2.50	0.45
1:B:143:ARG:NH1	1:B:158:ILE:HD12	2.31	0.45
2:C:952:LEU:HD12	2:C:952:LEU:HA	1.77	0.45
3:D:520:LEU:HD11	3:D:524:LEU:HD12	1.98	0.45
3:D:963:TYR:CE2	3:D:1002:LYS:HD3	2.51	0.45
3:D:1488:ASP:OD1	3:D:1488:ASP:N	2.43	0.45
3:D:298:VAL:HG12	3:D:302:GLN:NE2	2.32	0.45
1:A:8:ALA:HA	1:A:9:PRO:HD3	1.66	0.45
1:B:18:ARG:O	1:B:207:PRO:HD3	2.17	0.45
3:D:1237:THR:HG22	3:D:1238:MET:N	2.31	0.45
1:A:215:VAL:HG13	1:B:222:LEU:HB3	1.98	0.45
3:D:39:PRO:HB3	3:D:45:PHE:O	2.17	0.45
1:A:31:GLY:N	1:A:193:ASP:OD1	2.49	0.45
2:C:771:GLU:O	2:C:775:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:45:PHE:O	3:D:86:ARG:NH2	2.50	0.44
3:D:317:VAL:HG23	3:D:339:TRP:HB3	1.98	0.44
5:F:417:LYS:HB3	5:F:418:LEU:HD12	1.99	0.44
5:F:193:ARG:HB3	7:H:7:DG:H5''	1.99	0.44
1:B:99:LEU:HB3	1:B:114:PHE:CD1	2.52	0.44
3:D:654:LYS:O	3:D:658:LEU:HG	2.18	0.44
3:D:1491:THR:O	3:D:1495:ILE:HG13	2.17	0.44
5:F:172:ARG:O	5:F:176:ILE:HG12	2.17	0.44
2:C:674:VAL:HG12	2:C:869:VAL:HB	2.00	0.44
2:C:1043:TYR:CD1	3:D:763:MET:HG2	2.52	0.44
2:C:583:LEU:O	2:C:583:LEU:HD12	2.16	0.44
3:D:1383:ASP:HB3	3:D:1416:ALA:HB3	1.99	0.44
3:D:236:TYR:HB2	3:D:319:ALA:HB3	1.99	0.44
3:D:932:ASP:O	3:D:935:LYS:HB3	2.18	0.44
3:D:959:GLU:HB3	3:D:963:TYR:CE1	2.53	0.44
2:C:266:ARG:NH1	7:H:11:DG:O6	2.38	0.44
3:D:550:ARG:HD2	3:D:577:ALA:HB2	1.99	0.44
3:D:573:MET:SD	5:F:210:LEU:HB3	2.58	0.44
3:D:675:ARG:HH22	5:F:420:ASP:HB3	1.83	0.44
3:D:879:ARG:HD3	3:D:902:LEU:O	2.18	0.44
5:F:333:ILE:HA	5:F:334:PRO:HD3	1.80	0.44
1:A:155:LYS:HA	1:A:155:LYS:HD2	1.79	0.44
2:C:198:ARG:NH1	2:C:230:ARG:HA	2.32	0.44
2:C:396:ASP:OD2	2:C:402:SER:HB3	2.18	0.44
2:C:1015:LEU:HD11	3:D:528:VAL:HG21	1.98	0.44
3:D:1209:LEU:HD11	3:D:1364:HIS:HD2	1.83	0.44
2:C:124:ASP:HB3	2:C:592:LEU:HD12	1.99	0.43
3:D:12:LEU:HD21	3:D:104:PHE:CZ	2.53	0.43
3:D:916:TYR:CE1	3:D:920:LEU:HD11	2.53	0.43
3:D:1168:MET:O	3:D:1171:VAL:HB	2.18	0.43
3:D:1296:SER:OG	3:D:1297:GLU:N	2.51	0.43
5:F:321:ILE:O	5:F:327:SER:HB3	2.18	0.43
5:F:383:LEU:HD13	5:F:398:ARG:HB2	2.00	0.43
2:C:1067:TYR:OH	3:D:674[A]:ARG:NH1	2.50	0.43
3:D:1106:VAL:O	3:D:1108:ARG:HG3	2.18	0.43
1:B:110:LYS:HD2	1:B:126:ASP:O	2.18	0.43
3:D:288:MET:HE2	3:D:288:MET:HB3	1.84	0.43
2:C:164:PRO:HA	2:C:269:LEU:HD23	2.00	0.43
2:C:343:GLN:HG3	2:C:385:PHE:HB2	1.99	0.43
3:D:527:MET:HE2	3:D:527:MET:HB2	1.85	0.43
3:D:764:LEU:HD23	3:D:767:HIS:CD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.91	0.43
5:F:153:PRO:HA	5:F:156:VAL:HG22	2.00	0.43
1:B:190:THR:CG2	3:D:722:GLU:HG3	2.42	0.43
3:D:729:HIS:HA	3:D:730:PRO:HD3	1.90	0.43
3:D:907:GLU:OE1	3:D:909:ASN:N	2.50	0.43
2:C:422:ARG:HA	7:H:15:DT:O4'	2.19	0.43
2:C:1092:LEU:HD13	2:C:1099:VAL:HG21	2.01	0.43
3:D:478:LEU:HD21	3:D:500:ARG:NH2	2.33	0.43
3:D:536:ALA:HA	5:F:315:VAL:O	2.18	0.43
2:C:598:GLU:O	2:C:651:LYS:NZ	2.45	0.43
2:C:878:SER:CB	3:D:1029:ARG:HD2	2.49	0.43
3:D:355:VAL:HG11	3:D:385:VAL:HG21	2.01	0.43
3:D:1323:GLN:HA	3:D:1324:PRO:HD3	1.94	0.43
1:B:12:THR:HB	1:B:24:VAL:HB	2.01	0.43
3:D:1402:ALA:O	3:D:1405:GLU:HG2	2.18	0.43
1:B:185:ARG:NH1	1:B:187:GLY:O	2.52	0.43
3:D:236:TYR:CE1	3:D:242:LEU:HD12	2.54	0.43
3:D:963:TYR:CE2	3:D:1002:LYS:HB3	2.53	0.43
5:F:88:ILE:HD11	5:F:192:LEU:CD1	2.48	0.43
5:F:187:LEU:HD23	5:F:224:VAL:HG13	2.00	0.43
2:C:92:ALA:HB2	2:C:120:LEU:HD11	2.00	0.42
3:D:251:PHE:HZ	3:D:282:TYR:CD1	2.37	0.42
3:D:706:PRO:HB2	3:D:708:LEU:HD21	2.00	0.42
1:B:38:ASN:ND2	2:C:979:THR:HG22	2.34	0.42
2:C:557:ARG:HA	2:C:557:ARG:HD2	1.81	0.42
2:C:862:PRO:HD2	2:C:925:TYR:OH	2.19	0.42
3:D:127:LEU:HA	3:D:457:GLY:HA2	2.00	0.42
3:D:192:ALA:HB1	3:D:193:PRO:HD2	2.01	0.42
3:D:1047:LYS:HG2	3:D:1053:PHE:CZ	2.54	0.42
3:D:1302:GLU:OE1	3:D:1304:LYS:HE3	2.19	0.42
2:C:154:ARG:HA	2:C:155:PRO:HD3	1.85	0.42
3:D:350:HIS:HE1	5:F:232:ARG:HB3	1.85	0.42
3:D:597:ASP:O	3:D:599:PRO:HD3	2.19	0.42
3:D:1107:VAL:HB	3:D:1218:GLY:H	1.83	0.42
3:D:1267:ARG:HA	3:D:1268:PRO:HD3	1.83	0.42
3:D:131:LYS:O	3:D:456:MET:HG2	2.19	0.42
3:D:619:LEU:HD11	3:D:1439:SER:HB2	2.01	0.42
3:D:860:LEU:HD23	3:D:877:PRO:HB2	2.01	0.42
3:D:964:LEU:HD23	3:D:964:LEU:HA	1.95	0.42
5:F:276:ARG:O	5:F:279:GLN:HG3	2.19	0.42
5:F:364:ARG:HG3	5:F:390:PHE:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:H:15:DT:H2''	7:H:16:DC:O4'	2.19	0.42
1:A:178:ALA:HB2	2:C:864:GLY:HA3	2.02	0.42
3:D:838:ARG:HD3	3:D:874:GLU:CD	2.44	0.42
3:D:1137:ARG:O	3:D:1141:GLU:HG3	2.20	0.42
3:D:1192:LEU:HG	3:D:1369:GLU:HB3	2.01	0.42
3:D:1366:LYS:O	3:D:1370:ILE:HG12	2.20	0.42
5:F:370:LYS:O	5:F:376:ILE:HG12	2.19	0.42
1:B:57:TYR:CG	1:B:161:ARG:HD2	2.55	0.42
3:D:834:THR:OG1	3:D:838:ARG:HD2	2.19	0.42
3:D:843:PHE:HE1	3:D:864:VAL:HG21	1.84	0.42
3:D:1435:LEU:HB2	3:D:1457:ASP:OD2	2.20	0.42
2:C:595:LEU:HD11	2:C:623:TYR:HB3	2.01	0.42
3:D:224:ARG:HB2	3:D:332:TYR:HD1	1.85	0.42
3:D:245:LEU:HD23	3:D:249:TYR:HB3	2.02	0.42
5:F:181:GLU:O	5:F:185:GLN:HG2	2.20	0.42
1:A:6:LEU:HD11	1:A:27:PRO:HG2	2.02	0.42
2:C:693:GLU:OE1	2:C:696:LYS:HD2	2.20	0.42
2:C:877:PRO:HG2	3:D:1029:ARG:HB3	2.01	0.42
2:C:878:SER:HB3	3:D:1029:ARG:HD2	2.02	0.42
2:C:1118:LYS:HE2	3:D:20:SER:O	2.20	0.42
3:D:525:ARG:HD2	3:D:541:ASN:OD1	2.19	0.42
3:D:557:LEU:HB3	3:D:567:ILE:HD11	2.01	0.42
2:C:180:GLY:O	2:C:220:GLY:HA3	2.20	0.42
2:C:617:ASP:HB2	2:C:619:ARG:HG2	2.00	0.42
2:C:1019:GLN:HG2	2:C:1057:SER:OG	2.19	0.42
3:D:1197:ARG:HB2	3:D:1398:TRP:CH2	2.55	0.42
3:D:99:ALA:HB1	3:D:575:GLN:NE2	2.33	0.42
3:D:869:MET:HE2	3:D:869:MET:HB3	1.94	0.42
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.55	0.42
7:H:16:DC:H2''	7:H:17:DA:O5'	2.19	0.42
1:A:91:ASN:HA	1:A:92:PRO:HD3	1.88	0.41
1:B:110:LYS:NZ	1:B:128:HIS:HB2	2.34	0.41
3:D:421:LEU:HD11	3:D:429:SER:HB2	2.02	0.41
3:D:1018:ASN:O	3:D:1022:VAL:HG23	2.20	0.41
5:F:88:ILE:HA	5:F:88:ILE:HD12	1.77	0.41
5:F:101:GLU:O	5:F:105:LYS:HG3	2.20	0.41
3:D:877:PRO:O	3:D:880:ILE:HB	2.20	0.41
1:B:8:ALA:HA	1:B:9:PRO:HA	1.88	0.41
2:C:34:VAL:HA	2:C:35:PRO:HD2	1.85	0.41
3:D:313:MET:HE3	3:D:313:MET:HB3	1.95	0.41
3:D:367:ILE:HG22	3:D:368:VAL:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:234:LYS:HE2	5:F:234:LYS:HB3	1.77	0.41
1:B:30:ARG:HB2	1:B:191:ASP:HB3	2.02	0.41
3:D:508:ARG:HB3	3:D:510:GLU:CD	2.46	0.41
3:D:520:LEU:HD12	3:D:521:PRO:HD2	2.03	0.41
3:D:949:ILE:HD13	3:D:949:ILE:HA	1.84	0.41
2:C:173:ASP:HB2	2:C:185:LYS:HB3	2.02	0.41
2:C:540:PHE:HB3	2:C:544:THR:HB	2.03	0.41
2:C:693:GLU:O	2:C:697:ARG:HG2	2.20	0.41
3:D:1433:SER:HB2	3:D:1457:ASP:OD1	2.20	0.41
2:C:896:PHE:HB2	2:C:921:ALA:HB1	2.01	0.41
2:C:157:ARG:HA	2:C:157:ARG:HD3	1.87	0.41
3:D:1486:VAL:CG2	4:E:22:VAL:HG13	2.50	0.41
2:C:729:LEU:HD23	2:C:729:LEU:HA	1.94	0.41
3:D:187:LYS:N	3:D:200:ASP:OD1	2.45	0.41
3:D:553:ARG:HG3	5:F:218:GLN:NE2	2.36	0.41
5:F:123:ASP:OD2	5:F:125:ASP:HB2	2.21	0.41
5:F:365:GLU:HB2	5:F:404:ALA:HB2	2.02	0.41
7:H:16:DC:H3'	7:H:17:DA:H2'	2.03	0.41
1:B:24:VAL:HA	1:B:195:LEU:O	2.21	0.41
2:C:586:ARG:HD2	2:C:586:ARG:HA	1.85	0.41
3:D:162:ARG:O	3:D:414:ARG:NH1	2.53	0.41
3:D:216:VAL:HA	3:D:340:THR:HG22	2.02	0.41
3:D:553:ARG:HH12	3:D:573:MET:HE1	1.85	0.41
3:D:562:ALA:O	5:F:140:ARG:NH1	2.46	0.41
3:D:644:LEU:HD12	3:D:645:PRO:HD2	2.01	0.41
3:D:800:LYS:HB3	3:D:822:ALA:HB2	2.03	0.41
4:E:57:ASP:HA	4:E:58:PRO:HD3	1.89	0.41
5:F:157:GLU:O	5:F:161:GLN:HG2	2.21	0.41
5:F:338:LEU:HA	5:F:339:PRO:HD3	1.88	0.41
1:A:48:ILE:HA	1:A:49:PRO:HD3	1.92	0.41
1:A:64:GLU:HG3	1:A:79:ILE:HD12	2.02	0.41
2:C:905:ILE:C	2:C:907:ASP:H	2.28	0.41
3:D:818:ARG:HE	3:D:820:GLU:CD	2.29	0.41
3:D:844:ALA:O	3:D:867:ARG:HB3	2.20	0.41
3:D:860:LEU:HD22	3:D:878:GLY:HA2	2.03	0.41
3:D:881:LEU:O	3:D:885:ILE:HG13	2.21	0.41
3:D:895:VAL:O	3:D:898:GLU:N	2.54	0.41
3:D:959:GLU:HB3	3:D:963:TYR:HE1	1.86	0.41
3:D:1040:GLY:O	3:D:1060:SER:HB3	2.21	0.41
1:A:102:LYS:HE2	1:A:139:ASN:OD1	2.21	0.40
2:C:957:LYS:HB3	2:C:961:GLU:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:464:LEU:HA	3:D:464:LEU:HD23	1.89	0.40
3:D:849:ALA:O	3:D:853:VAL:HG23	2.21	0.40
3:D:885:ILE:HD13	3:D:937:TYR:CG	2.56	0.40
4:E:52:GLU:N	4:E:52:GLU:OE1	2.48	0.40
5:F:369:LEU:HD22	5:F:404:ALA:HB1	2.03	0.40
1:A:219:ARG:HG2	1:B:219:ARG:HG3	2.02	0.40
2:C:442:GLU:OE1	2:C:543:ASN:HB2	2.21	0.40
3:D:850:LEU:HD12	3:D:884:ARG:NH2	2.36	0.40
3:D:25:GLU:HB2	3:D:92:HIS:CE1	2.57	0.40
3:D:46:ASP:OD1	3:D:47:GLU:N	2.54	0.40
3:D:546:ARG:O	3:D:550:ARG:HG3	2.21	0.40
3:D:952:ASP:HA	3:D:1062:ARG:NH1	2.37	0.40
3:D:964:LEU:HD22	3:D:1058:ARG:NH2	2.36	0.40
5:F:89:GLY:HA2	5:F:193:ARG:NH2	2.36	0.40
5:F:120:THR:HG22	5:F:122:LEU:HD13	2.02	0.40
1:B:57:TYR:CD1	1:B:161:ARG:HD2	2.56	0.40
1:B:102:LYS:HG2	1:B:139:ASN:OD1	2.21	0.40
2:C:317:VAL:HA	2:C:318:PRO:HD3	1.85	0.40
2:C:926:PHE:CE2	2:C:930:LYS:HD3	2.56	0.40
3:D:106:LYS:HD2	3:D:106:LYS:HA	1.83	0.40
3:D:321:GLN:HB2	3:D:336:PHE:CD2	2.57	0.40
3:D:822:ALA:HB3	3:D:825:ALA:HB2	2.03	0.40
5:F:386:VAL:HG12	5:F:397:ILE:HD11	2.04	0.40
7:H:12:DC:H2''	7:H:13:DT:C5	2.57	0.40
2:C:858:MET:HG2	2:C:867:VAL:O	2.22	0.40
3:D:1018:ASN:HA	3:D:1019:PRO:HD3	1.89	0.40
3:D:1348:LEU:HD23	3:D:1348:LEU:HA	1.84	0.40
5:F:79:ASP:HA	5:F:80:PRO:HD3	1.88	0.40
6:G:11:DT:H6	6:G:11:DT:H2'	1.76	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	229/315 (73%)	227 (99%)	2 (1%)	0	100	100
1	B	219/315 (70%)	205 (94%)	14 (6%)	0	100	100
2	C	1108/1119 (99%)	1081 (98%)	24 (2%)	3 (0%)	36	64
3	D	1484/1524 (97%)	1410 (95%)	70 (5%)	4 (0%)	36	64
4	E	92/99 (93%)	90 (98%)	2 (2%)	0	100	100
5	F	344/443 (78%)	339 (98%)	5 (2%)	0	100	100
All	All	3476/3815 (91%)	3352 (96%)	117 (3%)	7 (0%)	43	71

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	422	ARG
3	D	320	ALA
2	C	230	ARG
2	C	446	GLY
3	D	154	THR
3	D	1205	TYR
3	D	1166	LEU

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	200/273 (73%)	194 (97%)	6 (3%)	36	56
1	B	194/273 (71%)	191 (98%)	3 (2%)	57	66
2	C	936/941 (100%)	888 (95%)	48 (5%)	21	46
3	D	1255/1279 (98%)	1226 (98%)	29 (2%)	44	61
4	E	82/88 (93%)	81 (99%)	1 (1%)	63	70
5	F	301/388 (78%)	294 (98%)	7 (2%)	44	61
All	All	2968/3242 (92%)	2874 (97%)	94 (3%)	34	54

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	25	LEU
1	A	66	SER
1	A	137	ARG
1	A	142	VAL
1	A	205	VAL
1	B	112	ARG
1	B	132	LEU
1	B	183	ASP
2	C	1	MET
2	C	10	ARG
2	C	11	GLU
2	C	27	ARG
2	C	65	VAL
2	C	81	ASP
2	C	113	VAL
2	C	174	LEU
2	C	182	VAL
2	C	190	LYS
2	C	211	LEU
2	C	261	ILE
2	C	274	ARG
2	C	276	LYS
2	C	336	VAL
2	C	348	LEU
2	C	357	GLU
2	C	360	LEU
2	C	390	GLN
2	C	395	LYS
2	C	397	GLU
2	C	402	SER
2	C	427	VAL
2	C	464	LEU
2	C	513	VAL
2	C	528	GLU
2	C	557	ARG
2	C	562	SER
2	C	617	ASP
2	C	670	GLN
2	C	674	VAL
2	C	722	ILE
2	C	764	GLU
2	C	771	GLU

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Mol	Chain	Res	Type
2	C	775	ARG
2	C	784	ASP
2	C	807	ARG
2	C	815	LEU
2	C	848	VAL
2	C	929	ARG
2	C	939	ARG
2	C	948	GLU
2	C	952	LEU
2	C	978	ARG
2	C	1061	GLU
2	C	1076	VAL
2	C	1078	GLU
2	C	1080	SER
3	D	53	ILE
3	D	65	ARG
3	D	80	VAL
3	D	81	THR
3	D	231	VAL
3	D	335	LEU
3	D	354	VAL
3	D	380	GLU
3	D	415	VAL
3	D	420	VAL
3	D	427	VAL
3	D	527	MET
3	D	530	VAL
3	D	618	LEU
3	D	754	PHE
3	D	762	GLN
3	D	778	LEU
3	D	867	ARG
3	D	947	ILE
3	D	1014	ASN
3	D	1055	VAL
3	D	1100	ASP
3	D	1129	THR
3	D	1188	VAL
3	D	1207	TYR
3	D	1238	MET
3	D	1252	ILE
3	D	1307	LYS

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Mol	Chain	Res	Type
3	D	1433	SER
4	E	93	TYR
5	F	88	ILE
5	F	122	LEU
5	F	205	ARG
5	F	210	LEU
5	F	310	ILE
5	F	338	LEU
5	F	369	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	38	ASN
1	B	128	HIS
1	B	188	GLN
1	B	212	ASN
1	B	221	HIS
2	C	22	GLN
2	C	117	HIS
2	C	498	GLN
2	C	663	ASN
2	C	1047	HIS
3	D	66	GLN
3	D	442	ASN
3	D	463	GLN
3	D	560	GLN
3	D	696	HIS
3	D	714	GLN
3	D	994	GLN
3	D	1046	GLN
3	D	1124	GLN
3	D	1172	HIS
3	D	1441	GLN
5	F	170	HIS
5	F	381	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

7 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
8	2RA	I	1	11,8	4,5,6	0.48	0	1,5,7	0.28	0
8	R2T	I	4	8	8,10,11	2.06	1 (12%)	6,13,15	0.73	0
8	FGL	I	7	8	5,6,7	1.48	1 (20%)	1,7,9	1.26	0
8	0QZ	I	6	8	4,5,6	1.69	1 (25%)	2,5,7	0.33	0
8	2TL	I	5	8	5,6,7	1.22	0	5,7,9	1.34	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	2RA	I	1	11,8	-	2/2/4/6	-
8	R2T	I	4	8	-	6/13/14/16	-
8	FGL	I	7	8	-	0/4/6/8	-
8	0QZ	I	6	8	-	2/3/4/6	-
8	2TL	I	5	8	-	5/5/6/8	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	I	4	R2T	CD-NE2	4.83	1.44	1.32
8	I	6	0QZ	OB-CA	-3.28	1.38	1.43
8	I	7	FGL	OG2-CB	2.19	1.28	1.22

There are no bond angle outliers.

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	I	1	2RA	C-CA-CB-NG
8	I	1	2RA	N-CA-CB-NG
8	I	4	R2T	OB1-CB-CG-CD
8	I	4	R2T	OE1-CD-CG-OG1
8	I	4	R2T	NE2-CD-CG-OG1
8	I	5	2TL	N-CA-CB-OG1
8	I	5	2TL	N-CA-CB-CG2
8	I	5	2TL	C-CA-CB-OG1
8	I	5	2TL	C-CA-CB-CG2
8	I	5	2TL	O-C-CA-CB
8	I	6	0QZ	N-C1-CA-C
8	I	6	0QZ	O-C-CA-C1
8	I	4	R2T	OB1-CB-CG-OG1
8	I	4	R2T	CA-CB-CG-OG1
8	I	4	R2T	CA-CB-CG-CD

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	I	4	R2T	3	0
8	I	6	0QZ	1	0
8	I	5	2TL	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 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	$\# Z > 2$
11	MB8	I	101	8	0,1,6	-	-	-		

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	231/315 (73%)	-0.72	0 100 100	26, 54, 80, 125	0
1	B	221/315 (70%)	-0.78	0 100 100	26, 58, 87, 115	0
2	C	1112/1119 (99%)	-0.66	1 (0%) 92 86	12, 50, 121, 145	0
3	D	1487/1524 (97%)	-0.70	0 100 100	11, 50, 112, 141	1 (0%)
4	E	94/99 (94%)	-0.64	0 100 100	26, 60, 110, 115	0
5	F	346/443 (78%)	-0.60	0 100 100	24, 70, 139, 155	0
6	G	16/21 (76%)	-0.19	0 100 100	84, 107, 178, 180	0
7	H	24/27 (88%)	-0.21	0 100 100	65, 125, 181, 192	0
8	I	0/7	-	-	-	-
All	All	3531/3870 (91%)	-0.68	1 (0%) 100 100	11, 55, 121, 192	1 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	828	ALA	2.3

6.2 Non-standard residues in protein, DNA, RNA chains

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
8	2RA	I	1	6/7	0.87	0.09	40,41,50,55	0
8	FGL	I	7	7/8	0.92	0.08	31,36,41,44	0
8	DVA	I	3	7/8	0.93	0.12	22,25,33,36	0
8	R2T	I	4	11/12	0.93	0.07	25,32,34,34	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	2TL	I	5	7/8	0.95	0.06	27,28,33,37	0
8	DSN	I	2	6/7	0.96	0.04	33,43,50,50	0
8	0QZ	I	6	6/7	0.98	0.05	27,29,29,29	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($\text{\AA}^2$)	Q<0.9
11	MB8	I	101	2/7	0.85	0.15	54,54,54,59	0
10	MG	F	2001	1/1	0.90	0.04	67,67,67,67	0
10	MG	D	2004	1/1	0.97	0.14	11,11,11,11	0
10	MG	D	2005	1/1	0.98	0.03	37,37,37,37	0
9	ZN	D	2002	1/1	0.99	0.02	82,82,82,82	0
9	ZN	D	2001	1/1	1.00	0.01	28,28,28,28	0
10	MG	D	2003	1/1	1.00	0.02	26,26,26,26	0

6.5 Other polymers [i](#)

There are no such residues in this entry.