



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:15 PM UTC

PDB ID : 5VI5 / pdb_00005vi5
Title : Structure of Mycobacterium smegmatis transcription initiation complex with a full transcription bubble
Authors : Darst, S.A.; Campbell, E.A.; Lilic, M.
Deposited on : 2017-04-14
Resolution : 3.20 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

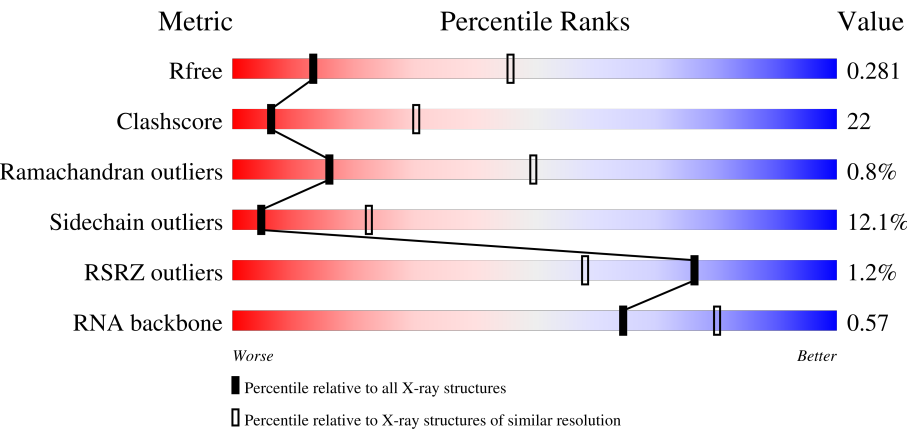
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	O	50	22%76%
2	P	50	40%48%12%
3	Q	4	50%50%
4	A	350	%36%22%5%37%

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Mol	Chain	Length	Quality of chain
4	B	350	
5	C	1169	
6	D	1317	
7	E	107	
8	F	466	
9	J	114	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	SO4	C	1201	-	-	X	-
10	SO4	F	502	-	-	X	-

2 Entry composition [i](#)

There are 13 unique types of molecules in this entry. The entry contains 26574 atoms, of which 16 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 DNA chain called DNA (49-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	O	49	Total	C	N	O	P	0	0	0
			1009	481	188	292	48			

- Molecule 2 is a DNA chain called DNA (44-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	44	Total	C	N	O	P	0	0	0
			903	430	167	262	44			

- Molecule 3 is a RNA chain called RNA (5'-R(*UP*CP*GP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	Q	4	Total	C	N	O	P	0	0	0
			82	38	15	26	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	220	Total	C	N	O	S	0	0	0
			1617	1022	278	315	2			
4	B	233	Total	C	N	O	S	0	0	0
			1660	1050	287	321	2			

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	C	1113	Total	C	N	O	S	0	0	0
			8138	5103	1427	1573	35			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	238	ASN	GLN	conflict	UNP P60281

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	D	1238	Total	C	N	O	S	0	0	0
			9391	5885	1699	1767	40			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	663	GLU	ALA	conflict	UNP A0QS66
D	1272	ASN	GLN	conflict	UNP A0QS66

- Molecule 7 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	E	76	Total	C	N	O		0	0	0
			592	378	100	114				

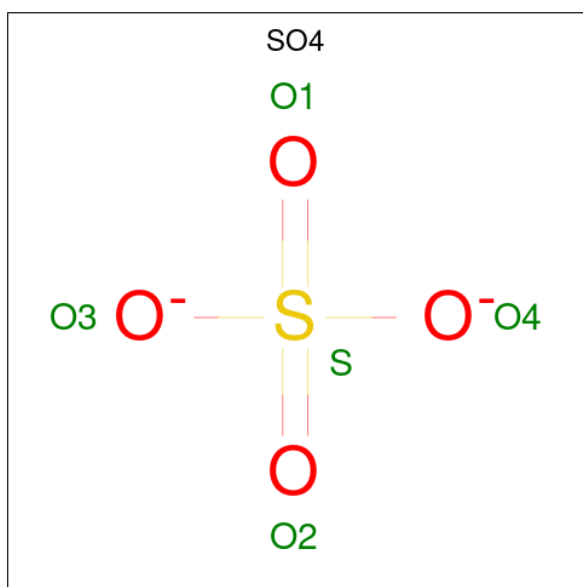
- Molecule 8 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	314	Total	C	N	O	S	0	0	0
			2461	1542	442	470	7			

- Molecule 9 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	J	86	Total	C	N	O	S	0	0	0
			663	414	122	125	2			

- Molecule 10 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

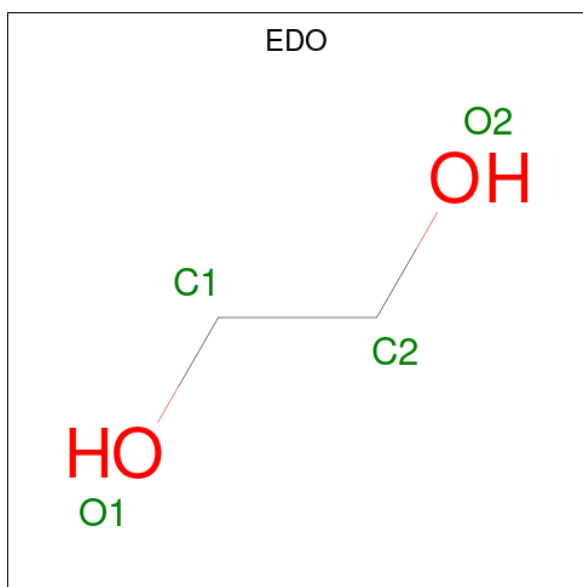


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	C	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	D	1	Total	O	S	0	0
			5	4	1		
10	F	1	Total	O	S	0	0
			5	4	1		
10	F	1	Total	O	S	0	0
			5	4	1		

- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 12 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	D	1	Total	C	H	O	0	0
			10	2	6	2		
12	F	1	Total	C	H	O	0	0
			10	2	6	2		

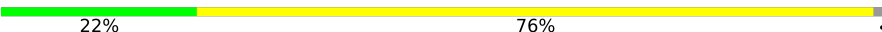
- Molecule 13 is water.

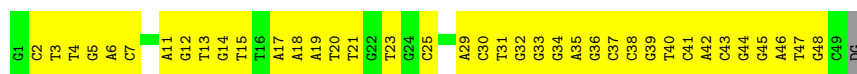
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
13	C	1	Total	H	O	0	0
			3	2	1		
13	D	1	Total	H	O	0	0
			3	2	1		

3 Residue-property plots

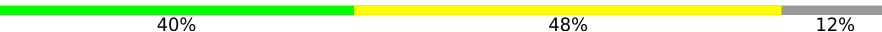
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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.

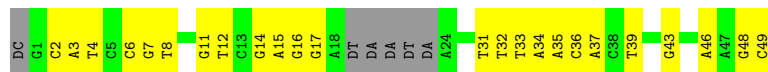
- Molecule 1: DNA (49-MER)

Chain O: 



- Molecule 2: DNA (44-MER)

Chain P: 

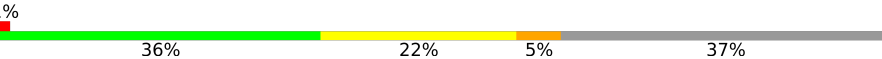


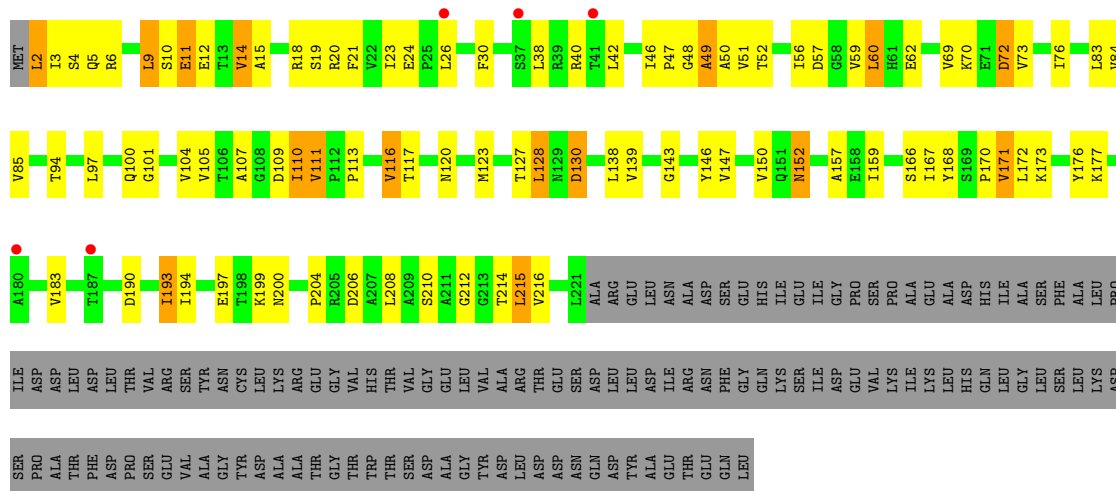
- Molecule 3: RNA (5'-R(*UP*CP*GP*A)-3')

Chain Q: 

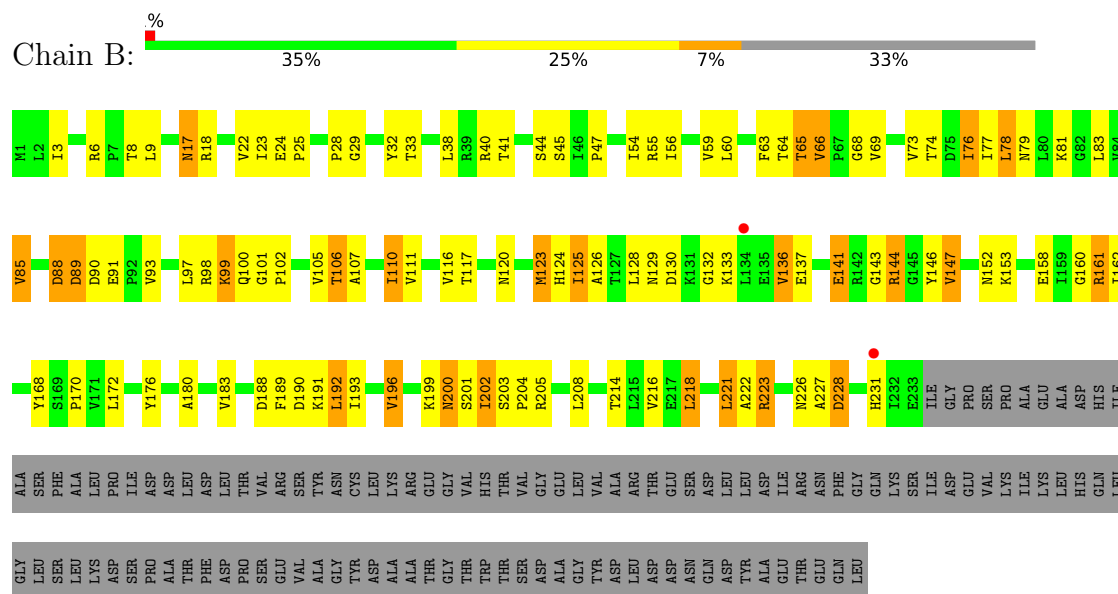


- Molecule 4: DNA-directed RNA polymerase subunit alpha

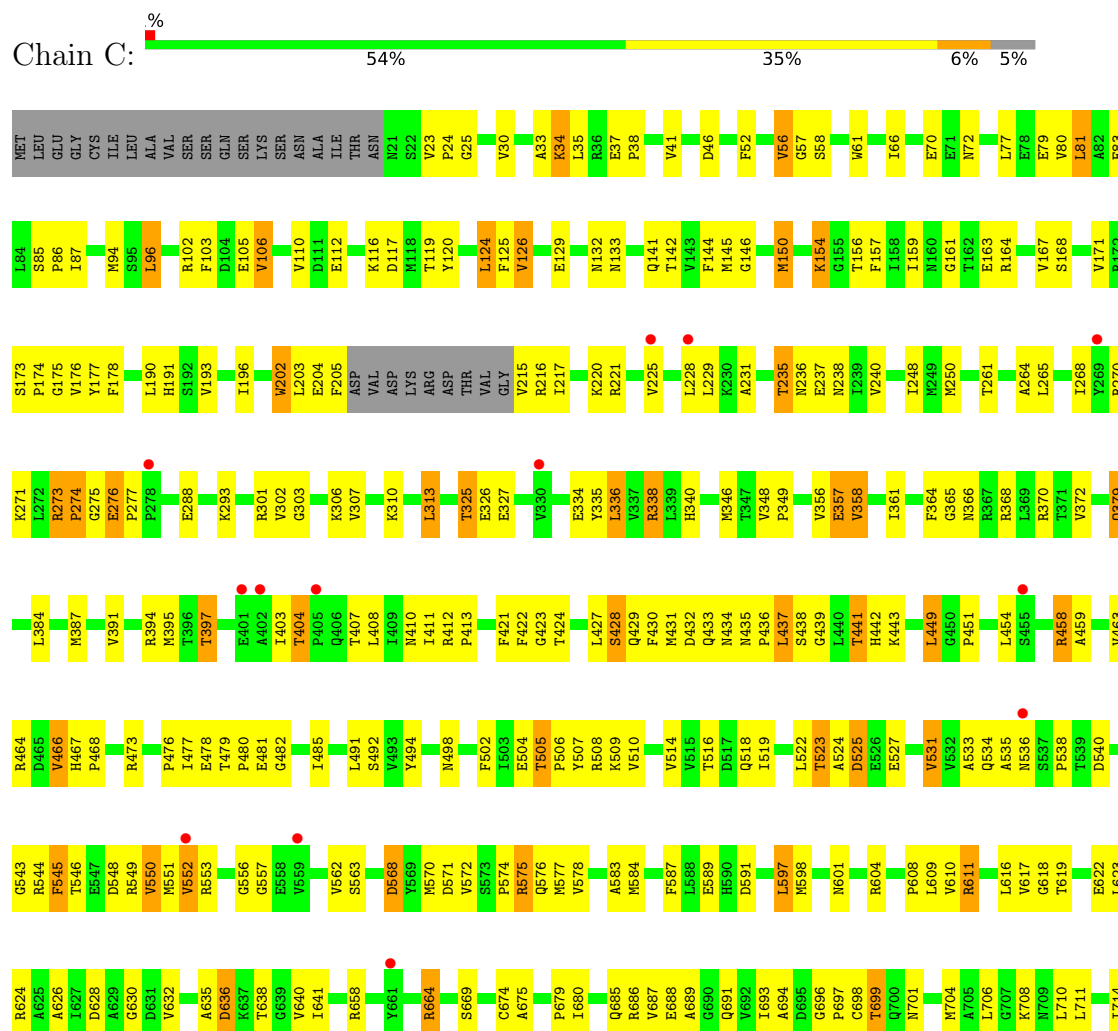
Chain A: 

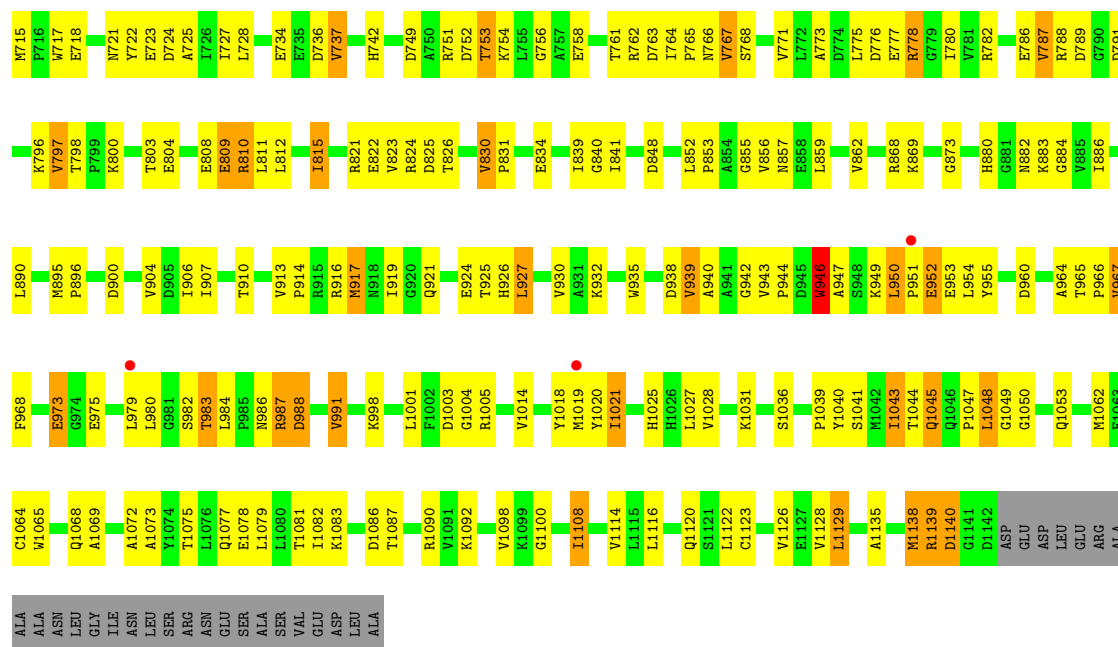


• Molecule 4: DNA-directed RNA polymerase subunit alpha

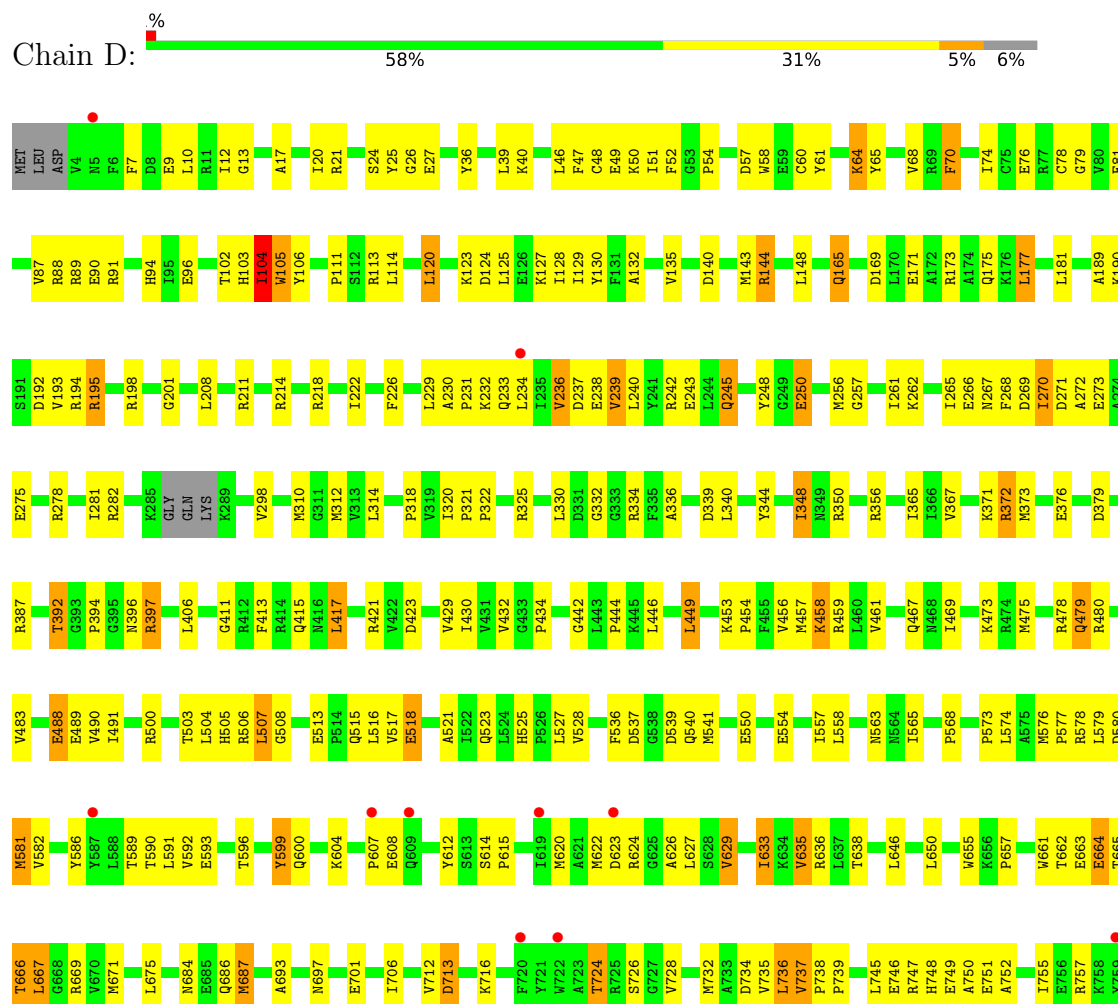


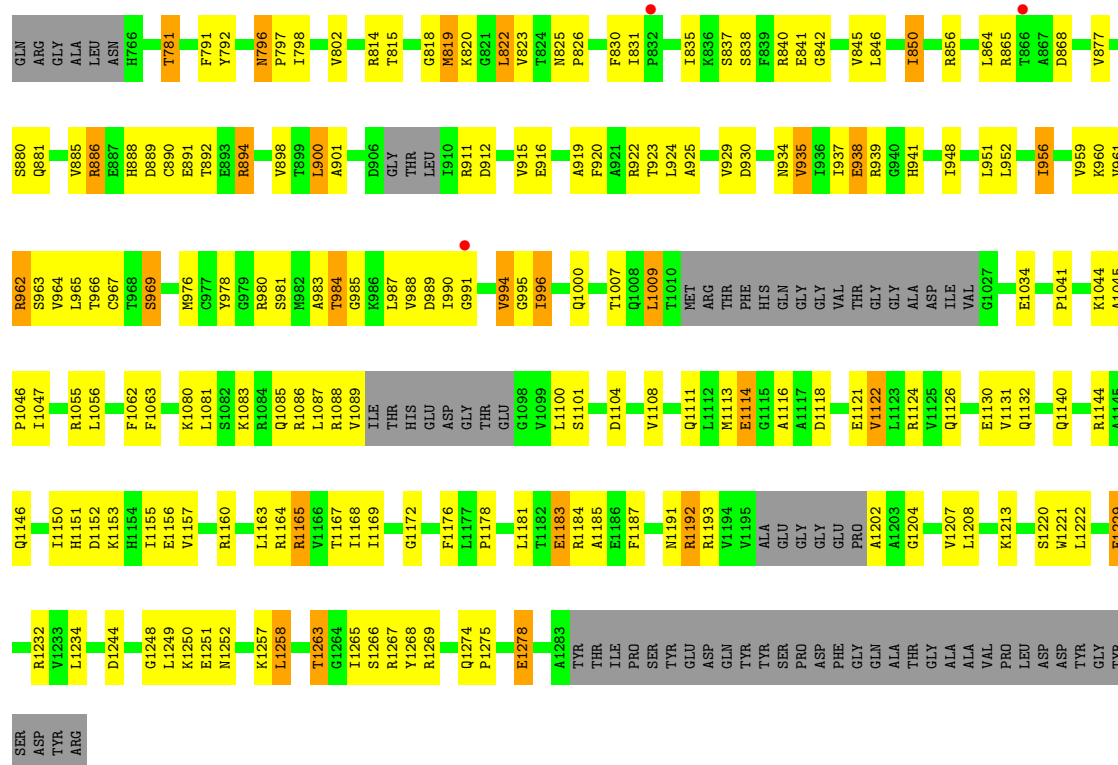
• Molecule 5: DNA-directed RNA polymerase subunit beta





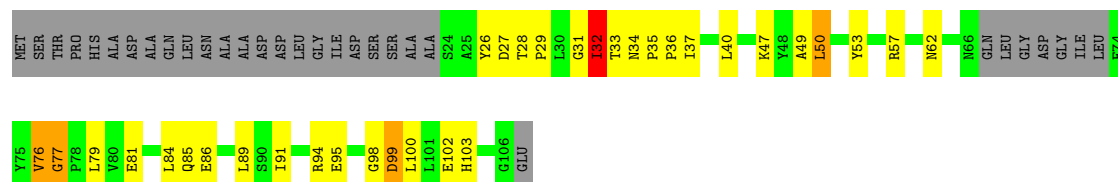
• Molecule 6: DNA-directed RNA polymerase subunit beta'





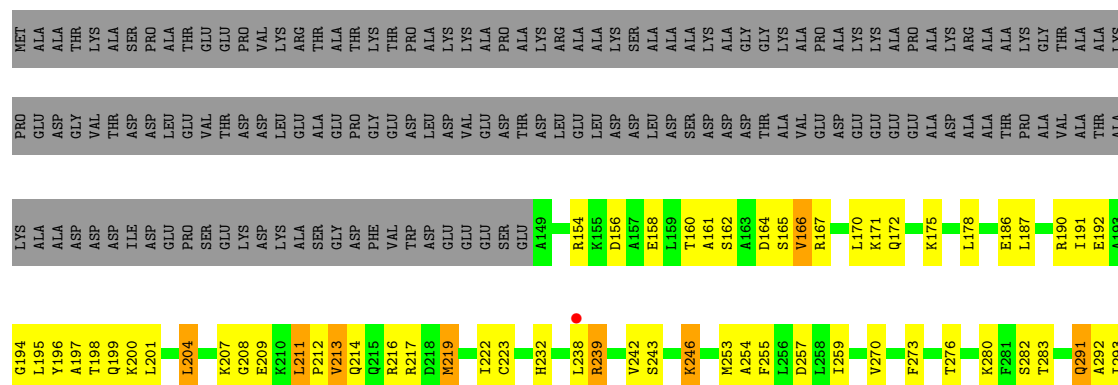
• Molecule 7: DNA-directed RNA polymerase subunit omega

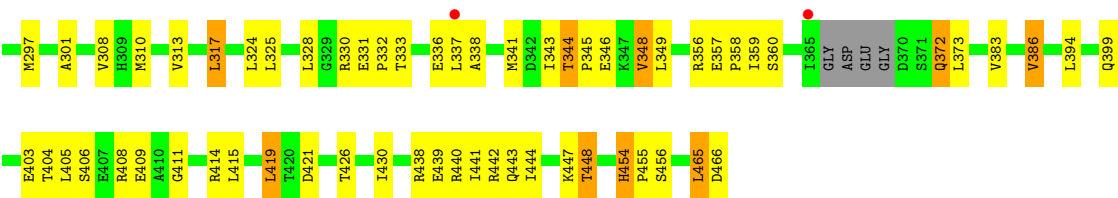
Chain E: 39% 27% 29%



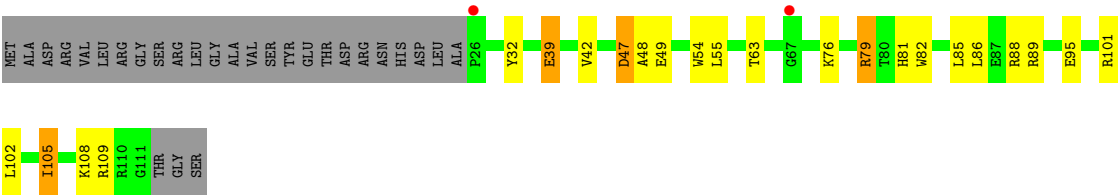
• Molecule 8: RNA polymerase sigma factor SigA

Chain F: 41% 23% 33%





● Molecule 9: RNA polymerase-binding protein RbpA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	132.06Å 163.56Å 139.96Å 90.00° 107.90° 90.00°	Depositor
Resolution (Å)	50.02 – 3.20 50.02 – 3.20	Depositor EDS
% Data completeness (in resolution range)	93.5 (50.02-3.20) 93.5 (50.02-3.20)	Depositor EDS
R_{merge}	0.22	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.19Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155)	Depositor
R, R_{free}	0.253 , 0.280 0.253 , 0.281	Depositor DCC
R_{free} test set	1992 reflections (2.13%)	wwPDB-VP
Wilson B-factor (Å ²)	85.8	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 43.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	26574	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% 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: SO4, ZN, EDO

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	O	0.20	0/1133	0.38	0/1749
2	P	0.19	0/1012	0.36	0/1557
3	Q	0.05	0/91	0.18	0/140
4	A	0.09	0/1643	0.30	0/2242
4	B	0.10	0/1686	0.34	0/2308
5	C	0.17	0/8285	0.34	4/11285 (0.0%)
6	D	0.12	0/9540	0.30	0/12930
7	E	0.11	0/604	0.39	0/822
8	F	0.19	0/2491	0.36	2/3365 (0.1%)
9	J	0.10	0/677	0.30	0/920
All	All	0.15	0/27162	0.33	6/37318 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	949	LYS	N-CA-C	-6.66	105.13	112.72
8	F	161	ALA	N-CA-C	6.06	117.68	111.14
8	F	165	SER	N-CA-C	6.04	117.94	111.36
5	C	950	LEU	CA-C-N	-5.43	114.33	119.76
5	C	950	LEU	C-N-CA	-5.43	114.33	119.76
5	C	946	TRP	N-CA-C	-5.03	106.25	112.38

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	O	1009	0	554	85	0
2	P	903	0	497	30	0
3	Q	82	0	45	1	0
4	A	1617	0	1616	85	0
4	B	1660	0	1624	97	0
5	C	8138	0	7718	416	1
6	D	9391	0	9221	387	1
7	E	592	0	583	31	0
8	F	2461	0	2467	98	0
9	J	663	0	619	18	0
10	C	5	0	0	2	0
10	D	15	0	0	1	0
10	F	10	0	0	3	0
11	D	2	0	0	0	0
12	D	4	6	6	3	0
12	F	4	6	6	0	0
13	C	1	2	0	1	0
13	D	1	2	0	0	0
All	All	26558	16	24956	1128	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 22.

All (1128) 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)
6:D:732:MET:O	6:D:840:ARG:NH1	1.85	1.10
6:D:981:SER:HB3	6:D:984:THR:OG1	1.53	1.08
4:A:48:GLY:HA2	4:A:49:ALA:HB3	1.39	1.04
5:C:935:TRP:CH2	5:C:954:LEU:CD2	2.40	1.04
5:C:935:TRP:HH2	5:C:954:LEU:HD22	1.18	1.03
1:O:40:DT:H2''	1:O:41:DC:H5'	1.34	1.02
4:B:55:ARG:NH1	4:B:160:GLY:O	1.91	1.02
5:C:763:ASP:O	5:C:821:ARG:NH1	1.92	1.00
8:F:330:ARG:NH1	8:F:336:GLU:OE2	1.95	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:414:ARG:HA	8:F:419:LEU:HD12	1.46	0.97
6:D:111:PRO:O	6:D:113:ARG:NH1	2.00	0.95
6:D:577:PRO:HA	6:D:581:MET:HE2	1.48	0.94
5:C:154:LYS:O	5:C:443:LYS:NZ	1.99	0.94
5:C:935:TRP:HH2	5:C:954:LEU:CD2	1.78	0.94
1:O:13:DT:H3	2:P:37:DA:H61	0.93	0.93
8:F:357:GLU:HG3	8:F:358:PRO:HD2	1.51	0.92
5:C:215:VAL:HG21	5:C:225:VAL:HA	1.51	0.91
5:C:935:TRP:CH2	5:C:954:LEU:HD22	2.03	0.91
5:C:572:VAL:HG22	5:C:576:GLN:HE21	1.32	0.90
1:O:12:DG:H2''	1:O:13:DT:H5'	1.54	0.89
5:C:895:MET:HG3	5:C:896:PRO:HD2	1.55	0.89
5:C:534:GLN:HE21	5:C:536:ASN:H	1.21	0.86
6:D:47:PHE:O	6:D:88:ARG:NH2	2.10	0.84
5:C:641:ILE:HD11	5:C:687:VAL:HG13	1.58	0.84
5:C:751:ARG:HD2	6:D:332:GLY:HA3	1.60	0.84
5:C:935:TRP:CZ2	5:C:954:LEU:CD2	2.60	0.83
5:C:751:ARG:HG2	5:C:856:VAL:HG12	1.58	0.83
1:O:38:DC:H1'	1:O:39:DG:H5''	1.60	0.82
5:C:379:GLN:HG2	5:C:421:PHE:HB2	1.62	0.82
4:B:55:ARG:HH11	4:B:160:GLY:C	1.88	0.82
8:F:211:LEU:HD23	8:F:211:LEU:H	1.44	0.82
9:J:47:ASP:OD2	9:J:47:ASP:N	2.13	0.81
6:D:488:GLU:HG2	6:D:516:LEU:HD12	1.61	0.81
6:D:622:MET:HE1	6:D:629:VAL:HG13	1.60	0.81
1:O:32:DG:N7	8:F:239:ARG:NH1	2.28	0.81
5:C:708:LYS:NZ	5:C:737:VAL:O	2.13	0.81
4:B:24:GLU:HG2	4:B:191:LYS:HB2	1.63	0.80
4:A:177:LYS:HG3	4:A:193:ILE:HG23	1.62	0.80
6:D:892:THR:OG1	6:D:894:ARG:NH1	2.13	0.80
5:C:1040:TYR:HE2	5:C:1090:ARG:HD2	1.45	0.80
1:O:4:DT:O4	2:P:46:DA:N6	2.16	0.79
4:B:97:LEU:HB3	4:B:136:VAL:HG13	1.65	0.79
2:P:17:DG:H2''	5:C:430:PHE:CZ	2.18	0.79
6:D:573:PRO:HG2	6:D:576:MET:HE2	1.65	0.79
6:D:432:VAL:HG22	6:D:434:PRO:HD3	1.63	0.78
6:D:47:PHE:HD1	6:D:322:PRO:HB3	1.47	0.78
5:C:538:PRO:HB2	5:C:546:THR:HB	1.66	0.78
4:A:48:GLY:CA	4:A:49:ALA:HB3	2.13	0.77
1:O:19:DA:H2''	1:O:20:DT:O5'	1.83	0.77
8:F:158:GLU:O	8:F:171:LYS:NZ	2.12	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:981:SER:CB	6:D:984:THR:OG1	2.32	0.77
4:B:6:ARG:O	4:B:25:PRO:HD2	1.84	0.77
6:D:822:LEU:HD12	6:D:822:LEU:H	1.48	0.77
1:O:32:DG:C8	8:F:239:ARG:HD3	2.20	0.76
6:D:507:LEU:HD23	6:D:574:LEU:HD23	1.66	0.76
6:D:889:ASP:OD2	6:D:891:GLU:N	2.15	0.76
8:F:465:LEU:HD13	8:F:466:ASP:H	1.49	0.75
4:A:48:GLY:HA2	4:A:49:ALA:CB	2.16	0.75
5:C:102:ARG:HB2	5:C:125:PHE:HB2	1.69	0.75
6:D:978:TYR:CE1	6:D:994:VAL:HG11	2.22	0.75
5:C:306:LYS:NZ	5:C:366:ASN:OD1	2.20	0.75
5:C:624:ARG:NH1	5:C:628:ASP:OD2	2.20	0.75
5:C:38:PRO:HG3	5:C:508:ARG:HD2	1.67	0.75
5:C:313:LEU:HD12	5:C:327:GLU:OE2	1.87	0.74
6:D:981:SER:HB3	6:D:984:THR:HG1	1.48	0.74
5:C:916:ARG:NH2	10:C:1201:SO4:O4	2.20	0.74
6:D:20:ILE:HD13	6:D:318:PRO:HD3	1.68	0.74
6:D:190:LYS:HZ2	6:D:192:ASP:HB3	1.52	0.74
5:C:788:ARG:N	5:C:791:ASP:OD2	2.21	0.74
5:C:852:LEU:HB3	5:C:856:VAL:HG23	1.68	0.74
6:D:190:LYS:NZ	6:D:192:ASP:HB3	2.03	0.74
1:O:38:DC:H2'	1:O:38:DC:O2	1.87	0.74
5:C:954:LEU:O	5:C:954:LEU:HD23	1.86	0.74
1:O:31:DT:H6	1:O:31:DT:H5'	1.51	0.73
1:O:46:DA:H61	2:P:4:DT:H3	1.33	0.73
5:C:773:ALA:O	5:C:782:ARG:NH2	2.21	0.73
5:C:434:ASN:OD1	5:C:1025:HIS:ND1	2.14	0.73
4:B:99:LYS:NZ	4:B:100:GLN:H	1.85	0.73
1:O:32:DG:H2''	1:O:33:DG:OP2	1.87	0.73
5:C:41:VAL:O	5:C:624:ARG:NH2	2.20	0.73
5:C:758:GLU:HG2	5:C:798:THR:HG22	1.68	0.73
1:O:40:DT:C2'	1:O:41:DC:H5'	2.14	0.73
6:D:865:ARG:NH1	6:D:1007:THR:O	2.22	0.73
5:C:680:ILE:HG12	5:C:693:ILE:O	1.89	0.73
6:D:1087:LEU:HD23	6:D:1113:MET:HG2	1.70	0.73
1:O:40:DT:H5''	1:O:40:DT:H6	1.53	0.72
5:C:636:ASP:OD1	5:C:636:ASP:N	2.21	0.72
6:D:128:ILE:HD12	6:D:135:VAL:HB	1.71	0.72
2:P:14:DG:OP2	6:D:421:ARG:NH2	2.22	0.72
5:C:1108:ILE:HD13	5:C:1108:ILE:H	1.53	0.72
4:A:105:VAL:HG23	4:A:128:LEU:HD11	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:525:HIS:HE1	6:D:527:LEU:HD12	1.52	0.72
7:E:84:LEU:HD12	7:E:84:LEU:H	1.53	0.72
5:C:714:ILE:HG22	5:C:910:THR:HG22	1.69	0.72
6:D:1140:GLN:HG2	6:D:1155:ILE:HD12	1.70	0.72
5:C:809:GLU:OE1	5:C:810:ARG:N	2.23	0.72
8:F:232:HIS:ND1	10:F:502:SO4:O2	2.23	0.72
5:C:935:TRP:CH2	5:C:954:LEU:HD23	2.24	0.71
5:C:1045:GLN:HG2	5:C:1087:THR:HG22	1.71	0.71
5:C:1140:ASP:OD1	6:D:25:TYR:OH	2.04	0.71
5:C:1027:LEU:O	5:C:1031:LYS:HG3	1.91	0.71
5:C:800:LYS:HG2	5:C:822:GLU:O	1.90	0.71
6:D:47:PHE:CD1	6:D:322:PRO:HB3	2.25	0.71
6:D:781:THR:HG22	6:D:814:ARG:HD2	1.72	0.71
1:O:37:DC:H2''	1:O:38:DC:O5'	1.89	0.71
5:C:23:VAL:HG13	5:C:24:PRO:HD2	1.73	0.71
4:A:56:ILE:HB	4:A:59:VAL:HG22	1.71	0.71
1:O:13:DT:H3	2:P:37:DA:N6	1.79	0.70
4:B:68:GLY:O	4:B:129:ASN:N	2.21	0.70
5:C:1043:ILE:HD12	5:C:1044:THR:H	1.57	0.70
5:C:535:ALA:HB2	5:C:571:ASP:HB2	1.72	0.70
4:A:26:LEU:HB2	4:A:190:ASP:O	1.92	0.70
5:C:880:HIS:NE2	5:C:924:GLU:OE2	2.23	0.70
5:C:562:VAL:HG22	5:C:563:SER:H	1.56	0.70
6:D:880:SER:O	6:D:995:GLY:HA3	1.91	0.70
5:C:1072:ALA:HB1	6:D:554:GLU:OE2	1.92	0.69
8:F:213:VAL:O	8:F:217:ARG:HG2	1.92	0.69
4:A:48:GLY:O	4:A:143:GLY:N	2.24	0.69
4:A:60:LEU:HD12	4:A:60:LEU:H	1.57	0.69
6:D:189:ALA:HB1	6:D:194:ARG:NH1	2.08	0.69
6:D:365:ILE:HD12	6:D:365:ILE:H	1.57	0.69
5:C:1129:LEU:HA	5:C:1135:ALA:HA	1.74	0.69
6:D:344:TYR:O	6:D:348:ILE:HG22	1.92	0.69
5:C:473:ARG:NH1	5:C:524:ALA:H	1.90	0.69
6:D:411:GLY:O	6:D:415:GLN:HB3	1.93	0.69
6:D:846:LEU:HD12	6:D:846:LEU:H	1.58	0.68
1:O:11:DA:H2''	1:O:12:DG:H5''	1.73	0.68
4:A:21:PHE:HB2	4:A:194:ILE:HG22	1.74	0.68
6:D:165:GLN:NE2	6:D:169:ASP:OD2	2.26	0.68
5:C:766:ASN:ND2	8:F:466:ASP:OD2	2.27	0.68
5:C:952:GLU:OE1	5:C:953:GLU:N	2.27	0.68
6:D:901:ALA:HA	6:D:911:ARG:C	2.18	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:48:DG:OP1	6:D:123:LYS:HG2	1.94	0.68
5:C:70:GLU:HG2	5:C:72:ASN:H	1.58	0.68
5:C:478:GLU:OE2	5:C:604:ARG:NH2	2.27	0.68
5:C:1049:GLY:O	5:C:1053:GLN:NE2	2.25	0.68
4:B:102:PRO:HG3	4:B:130:ASP:HA	1.75	0.67
6:D:475:MET:HE2	6:D:480:ARG:HH21	1.58	0.67
8:F:344:THR:OG1	8:F:346:GLU:HG2	1.94	0.67
4:A:20:ARG:HB3	4:A:193:ILE:HD11	1.76	0.67
5:C:789:ASP:HA	5:C:830:VAL:HG22	1.76	0.67
5:C:947:ALA:HB1	5:C:950:LEU:CB	2.25	0.67
6:D:231:PRO:O	6:D:232:LYS:HB2	1.95	0.67
4:B:65:THR:O	4:B:66:VAL:HG23	1.94	0.67
1:O:32:DG:H5'	8:F:239:ARG:CG	2.25	0.67
1:O:37:DC:H2''	1:O:38:DC:C5'	2.25	0.67
5:C:685:GLN:HG2	5:C:686:ARG:H	1.60	0.67
5:C:939:VAL:HG13	5:C:943:VAL:HG22	1.75	0.67
6:D:444:PRO:HG3	6:D:521:ALA:O	1.95	0.67
1:O:32:DG:H8	8:F:239:ARG:HD3	1.60	0.66
5:C:608:PRO:HA	5:C:698:CYS:SG	2.35	0.66
2:P:34:DA:H4'	2:P:35:DA:OP1	1.94	0.66
8:F:454:HIS:NE2	8:F:456:SER:OG	2.21	0.66
8:F:190:ARG:NH1	10:F:502:SO4:O3	2.28	0.66
5:C:231:ALA:HA	5:C:265:LEU:HD22	1.77	0.66
5:C:708:LYS:HG3	5:C:737:VAL:HG23	1.77	0.66
8:F:454:HIS:HD1	8:F:455:PRO:HD2	1.60	0.66
6:D:1275:PRO:HG3	7:E:76:VAL:HG21	1.75	0.66
6:D:1183:GLU:OE1	6:D:1185:ALA:N	2.29	0.66
5:C:1047:PRO:HD2	6:D:421:ARG:O	1.96	0.66
5:C:896:PRO:HB2	5:C:1001:LEU:HD13	1.78	0.65
5:C:235:THR:OG1	5:C:238:ASN:OD1	2.11	0.65
8:F:243:SER:HA	8:F:246:LYS:HD2	1.78	0.65
5:C:724:ASP:OD1	5:C:916:ARG:NH1	2.30	0.65
6:D:991:GLY:HA2	6:D:1265:ILE:HD11	1.77	0.65
5:C:454:LEU:HD13	5:C:459:ALA:HB2	1.79	0.65
8:F:444:ILE:O	8:F:448:THR:OG1	2.14	0.65
1:O:32:DG:H5'	8:F:239:ARG:HG2	1.79	0.65
5:C:551:MET:O	5:C:552:VAL:HG13	1.97	0.65
6:D:1086:ARG:O	6:D:1087:LEU:HD23	1.96	0.65
4:A:40:ARG:HH12	4:B:32:TYR:HB2	1.62	0.65
5:C:531:VAL:HG12	5:C:568:ASP:OD1	1.97	0.65
4:A:146:TYR:HD2	4:A:167:ILE:HG12	1.61	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:766:ASN:O	5:C:767:VAL:HG13	1.97	0.64
1:O:38:DC:C1'	1:O:39:DG:H5''	2.26	0.64
5:C:728:LEU:HD11	5:C:886:ILE:HD13	1.78	0.64
4:A:46:ILE:HG22	4:A:170:PRO:HG2	1.78	0.64
6:D:103:HIS:O	6:D:104:ILE:HG22	1.97	0.64
8:F:211:LEU:HB2	8:F:212:PRO:HD2	1.79	0.64
6:D:65:TYR:HB3	6:D:70:PHE:CE2	2.33	0.64
5:C:583:ALA:O	5:C:619:THR:HG21	1.98	0.64
6:D:268:PHE:CZ	6:D:273:GLU:HG3	2.33	0.64
6:D:925:ALA:O	6:D:939:ARG:HD2	1.97	0.64
4:B:29:GLY:HA2	4:B:190:ASP:OD2	1.97	0.64
6:D:237:ASP:O	6:D:238:GLU:HB3	1.96	0.64
6:D:1249:LEU:HD12	6:D:1250:LYS:N	2.13	0.64
5:C:935:TRP:CZ2	5:C:954:LEU:HD21	2.31	0.64
5:C:952:GLU:OE1	5:C:953:GLU:HB2	1.96	0.64
6:D:270:ILE:HD13	6:D:270:ILE:H	1.63	0.64
4:A:9:LEU:HB2	4:A:23:ILE:HG12	1.78	0.64
4:A:50:ALA:HB3	4:A:168:TYR:CD1	2.32	0.64
7:E:40:LEU:HB3	7:E:50:LEU:HD11	1.79	0.64
6:D:1047:ILE:HD13	6:D:1122:VAL:HG12	1.78	0.64
6:D:796:ASN:HD21	6:D:798:ILE:HG23	1.63	0.63
6:D:1034:GLU:OE2	6:D:1041:PRO:HA	1.98	0.63
5:C:94:MET:HE3	5:C:395:MET:HE2	1.81	0.63
4:A:97:LEU:HB2	4:A:110:ILE:HG23	1.80	0.63
5:C:568:ASP:OD1	5:C:568:ASP:N	2.29	0.63
6:D:706:ILE:HG13	7:E:36:PRO:HB3	1.79	0.63
5:C:306:LYS:O	5:C:310:LYS:HB3	1.98	0.63
6:D:12:ILE:HG12	6:D:13:GLY:H	1.64	0.63
5:C:117:ASP:HA	5:C:161:GLY:HA3	1.81	0.63
4:B:22:VAL:HG12	4:B:193:ILE:HG12	1.80	0.63
5:C:482:GLY:O	5:C:485:ILE:HG13	1.98	0.63
5:C:916:ARG:NH2	10:C:1201:SO4:S	2.72	0.63
6:D:1121:GLU:OE2	6:D:1124:ARG:NH2	2.32	0.63
1:O:6:DA:H2''	1:O:7:DC:H5'	1.80	0.63
4:B:200:ASN:OD1	4:B:200:ASN:N	2.24	0.63
5:C:664:ARG:NH1	5:C:675:ALA:HB1	2.14	0.63
6:D:1266:SER:HA	6:D:1269:ARG:NH1	2.14	0.63
6:D:242:ARG:NH1	6:D:245:GLN:OE1	2.31	0.62
4:A:176:TYR:HB3	4:A:194:ILE:HG13	1.81	0.62
5:C:476:PRO:HG2	5:C:477:ILE:HD12	1.81	0.62
6:D:1046:PRO:HG2	6:D:1081:LEU:HD21	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:1088:ARG:HH11	6:D:1111:GLN:HB3	1.62	0.62
6:D:1118:ASP:HB3	6:D:1121:GLU:HB2	1.80	0.62
1:O:33:DG:H5''	8:F:246:LYS:HE2	1.80	0.62
2:P:43:DG:O6	8:F:438:ARG:NH1	2.32	0.62
5:C:986:ASN:C	5:C:988:ASP:H	2.07	0.62
6:D:713:ASP:OD1	6:D:716:LYS:NZ	2.32	0.62
5:C:467:HIS:CG	5:C:468:PRO:HD2	2.35	0.62
5:C:618:GLY:O	5:C:964:ALA:HA	1.99	0.62
8:F:345:PRO:O	8:F:348:VAL:HG13	1.99	0.62
4:A:206:ASP:OD1	4:B:226:ASN:ND2	2.33	0.62
6:D:446:LEU:HD12	6:D:446:LEU:H	1.63	0.62
5:C:423:GLY:O	5:C:424:THR:OG1	2.14	0.62
5:C:480:PRO:O	5:C:485:ILE:HG12	2.00	0.62
5:C:824:ARG:HE	5:C:825:ASP:H	1.48	0.62
6:D:1172:GLY:HA2	6:D:1202:ALA:HB2	1.82	0.62
5:C:145:MET:O	5:C:411:ILE:HD12	2.00	0.62
5:C:752:ASP:OD1	5:C:857:ASN:ND2	2.33	0.62
6:D:237:ASP:OD1	6:D:239:VAL:HG13	1.99	0.61
4:B:41:THR:O	4:B:45:SER:HB3	2.00	0.61
6:D:978:TYR:CD2	6:D:988:VAL:HG21	2.35	0.61
1:O:32:DG:C5'	8:F:239:ARG:HG2	2.30	0.61
2:P:43:DG:OP2	8:F:426:THR:OG1	2.15	0.61
5:C:178:PHE:CE1	5:C:193:VAL:HG13	2.34	0.61
6:D:114:LEU:HG	6:D:312:MET:HE2	1.82	0.61
6:D:189:ALA:HB1	6:D:194:ARG:HH11	1.64	0.61
5:C:935:TRP:HZ2	5:C:954:LEU:HD21	1.66	0.61
5:C:473:ARG:HH11	5:C:524:ALA:H	1.46	0.61
5:C:216:ARG:HG3	5:C:220:LYS:O	2.01	0.61
5:C:882:ASN:HD21	5:C:1019:MET:HE1	1.66	0.61
4:B:101:GLY:N	4:B:132:GLY:O	2.30	0.61
6:D:589:THR:HG21	6:D:687:MET:SD	2.41	0.61
5:C:1043:ILE:O	6:D:89:ARG:NH2	2.34	0.61
2:P:34:DA:H2''	2:P:35:DA:O5'	2.01	0.60
5:C:715:MET:HE3	5:C:717:TRP:HD1	1.66	0.60
5:C:935:TRP:CB	5:C:982:SER:HB2	2.31	0.60
5:C:710:LEU:HD13	5:C:1021:ILE:HD11	1.83	0.60
4:B:56:ILE:HG13	4:B:136:VAL:HB	1.83	0.60
1:O:18:DA:H2''	1:O:19:DA:C8	2.36	0.60
2:P:12:DT:H4'	5:C:1062:MET:HE2	1.81	0.60
4:B:17:ASN:OD1	4:B:17:ASN:N	2.33	0.60
4:B:66:VAL:HG12	4:B:69:VAL:HG22	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:172:LEU:O	6:D:620:MET:HE2	2.01	0.60
5:C:1031:LYS:NZ	13:C:1301:HOH:O	2.24	0.60
6:D:951:LEU:HB3	6:D:956:ILE:HD11	1.82	0.60
1:O:43:DC:H2''	1:O:44:DG:OP2	2.01	0.60
5:C:1040:TYR:CE2	5:C:1090:ARG:HD2	2.32	0.60
9:J:108:LYS:O	9:J:108:LYS:HD3	2.01	0.60
4:A:12:GLU:O	4:A:19:SER:HB2	2.01	0.60
4:B:88:ASP:OD2	4:B:88:ASP:N	2.32	0.60
6:D:894:ARG:HH11	6:D:894:ARG:HB2	1.66	0.60
4:B:158:GLU:OE1	4:B:161:ARG:NH1	2.35	0.60
1:O:44:DG:H2''	1:O:45:DG:OP2	2.01	0.60
6:D:748:HIS:HA	6:D:751:GLU:HG2	1.84	0.60
6:D:796:ASN:OD1	6:D:798:ILE:HG22	2.01	0.60
8:F:194:GLY:HA2	8:F:222:ILE:HG22	1.84	0.60
1:O:19:DA:H4'	1:O:20:DT:OP1	2.02	0.60
5:C:144:PHE:CZ	5:C:146:GLY:HA2	2.37	0.60
5:C:1139:ARG:HG2	6:D:90:GLU:CD	2.27	0.60
4:A:46:ILE:HB	4:A:170:PRO:HD2	1.84	0.59
5:C:796:LYS:HB3	5:C:826:THR:O	2.02	0.59
1:O:2:DC:H2''	1:O:3:DT:O5'	2.02	0.59
4:A:159:ILE:HD12	4:A:159:ILE:H	1.67	0.59
5:C:698:CYS:O	5:C:699:THR:HG23	2.01	0.59
5:C:572:VAL:HG22	5:C:576:GLN:NE2	2.11	0.59
6:D:64:LYS:NZ	6:D:64:LYS:HB3	2.17	0.59
6:D:230:ALA:HB1	6:D:231:PRO:HD2	1.84	0.59
6:D:397:ARG:HH11	6:D:397:ARG:HB2	1.67	0.59
6:D:1085:GLN:HB2	6:D:1113:MET:HE2	1.83	0.59
5:C:429:GLN:OE1	5:C:442:HIS:NE2	2.28	0.59
5:C:675:ALA:HA	5:C:697:PRO:HG3	1.83	0.59
6:D:181:LEU:HD23	6:D:181:LEU:O	2.01	0.59
5:C:574:PRO:O	5:C:575:ARG:HG2	2.02	0.59
5:C:193:VAL:HB	5:C:205:PHE:HB2	1.84	0.59
5:C:853:PRO:O	5:C:856:VAL:HG22	2.02	0.59
5:C:1041:SER:HB3	5:C:1044:THR:O	2.03	0.59
1:O:31:DT:H5'	1:O:31:DT:C6	2.37	0.59
4:A:177:LYS:CG	4:A:193:ILE:HG23	2.33	0.59
4:B:170:PRO:HA	4:B:199:LYS:HE2	1.84	0.59
5:C:464:ARG:HD3	5:C:485:ILE:O	2.03	0.59
5:C:967:VAL:HG23	5:C:968:PHE:H	1.67	0.59
1:O:12:DG:C2'	1:O:13:DT:H5'	2.30	0.59
5:C:1073:ALA:H	6:D:1263:THR:HG23	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:104:ILE:HD12	6:D:379:ASP:HB3	1.84	0.59
6:D:339:ASP:OD1	8:F:360:SER:OG	2.20	0.59
8:F:409:GLU:HB3	8:F:448:THR:HG21	1.84	0.59
7:E:29:PRO:HB2	7:E:33:THR:HG23	1.84	0.58
6:D:525:HIS:CE1	6:D:527:LEU:HD12	2.36	0.58
5:C:507:TYR:OH	5:C:553:ARG:NH2	2.36	0.58
6:D:106:TYR:HB3	6:D:113:ARG:HB2	1.85	0.58
6:D:1088:ARG:NH1	6:D:1111:GLN:H	2.01	0.58
7:E:31:GLY:C	7:E:33:THR:H	2.10	0.58
5:C:458:ARG:O	5:C:458:ARG:HG3	2.03	0.58
6:D:666:THR:HG23	6:D:669:ARG:HD2	1.84	0.58
5:C:154:LYS:NZ	5:C:154:LYS:HB3	2.18	0.58
8:F:254:ALA:HB3	8:F:257:ASP:OD2	2.04	0.58
5:C:812:LEU:HA	5:C:815:ILE:HG23	1.84	0.58
6:D:24:SER:HB2	6:D:94:HIS:HB3	1.85	0.58
6:D:818:GLY:O	6:D:838:SER:HB3	2.03	0.58
8:F:465:LEU:HD22	8:F:466:ASP:N	2.18	0.58
5:C:574:PRO:HB2	5:C:968:PHE:HB2	1.84	0.58
6:D:103:HIS:ND1	6:D:105:TRP:HB2	2.18	0.58
7:E:76:VAL:O	7:E:77:GLY:O	2.21	0.58
5:C:1139:ARG:HG2	6:D:90:GLU:OE2	2.04	0.58
6:D:1267:ARG:HG3	6:D:1268:TYR:N	2.19	0.58
6:D:796:ASN:HD21	6:D:798:ILE:CG2	2.17	0.57
4:B:9:LEU:HD21	4:B:208:LEU:HD21	1.87	0.57
6:D:622:MET:HE2	6:D:629:VAL:HG22	1.85	0.57
6:D:892:THR:HG1	6:D:894:ARG:HH12	1.44	0.57
1:O:35:DA:H2''	1:O:36:DG:C4'	2.34	0.57
6:D:978:TYR:CZ	6:D:994:VAL:HG11	2.39	0.57
6:D:1087:LEU:HA	6:D:1113:MET:HA	1.85	0.57
5:C:25:GLY:HA3	5:C:691:GLN:HG3	1.86	0.57
5:C:196:ILE:O	5:C:196:ILE:HG23	2.04	0.57
5:C:454:LEU:HD12	5:C:454:LEU:O	2.05	0.57
5:C:611:ARG:O	5:C:708:LYS:HE2	2.04	0.57
6:D:737:VAL:HG13	6:D:840:ARG:CD	2.35	0.57
8:F:454:HIS:ND1	8:F:455:PRO:HD2	2.19	0.57
1:O:39:DG:O5'	1:O:39:DG:H8	1.87	0.57
4:A:3:ILE:HD12	4:A:3:ILE:O	2.04	0.57
6:D:262:LYS:HG3	6:D:310:MET:HE1	1.86	0.57
6:D:1140:GLN:HG2	6:D:1155:ILE:CD1	2.34	0.57
1:O:35:DA:H2''	1:O:36:DG:O4'	2.04	0.57
4:B:141:GLU:OE2	4:B:168:TYR:OH	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:394:ARG:CB	5:C:408:LEU:HD23	2.34	0.57
6:D:728:VAL:HG23	6:D:797:PRO:HB3	1.84	0.57
5:C:273:ARG:O	5:C:275:GLY:N	2.38	0.57
6:D:963:SER:OG	6:D:1156:GLU:OE1	2.20	0.57
6:D:459:ARG:NE	6:D:489:GLU:OE2	2.37	0.57
3:Q:4:A:OP1	5:C:883:LYS:NZ	2.25	0.57
4:A:42:LEU:O	4:A:171:VAL:HG11	2.04	0.57
5:C:1019:MET:HG2	5:C:1020:TYR:H	1.70	0.57
8:F:186:GLU:OE2	9:J:101:ARG:NH2	2.31	0.57
2:P:3:DA:H2''	2:P:4:DT:C5	2.40	0.56
4:B:221:LEU:HD12	4:B:222:ALA:N	2.20	0.56
5:C:946:TRP:CD1	5:C:946:TRP:C	2.83	0.56
6:D:453:LYS:HB3	6:D:454:PRO:HD3	1.86	0.56
4:A:130:ASP:OD1	4:A:130:ASP:N	2.32	0.56
5:C:1048:LEU:HD12	5:C:1053:GLN:HB3	1.86	0.56
5:C:491:LEU:HD23	5:C:492:SER:N	2.21	0.56
5:C:216:ARG:HE	5:C:221:ARG:HA	1.70	0.56
7:E:31:GLY:O	7:E:33:THR:N	2.33	0.56
6:D:922:ARG:NH2	6:D:1156:GLU:OE2	2.39	0.56
4:B:64:THR:O	4:B:65:THR:HG22	2.06	0.56
7:E:35:PRO:HG2	7:E:40:LEU:HD11	1.86	0.56
8:F:219:MET:HE2	8:F:219:MET:HA	1.88	0.56
6:D:114:LEU:HD21	6:D:265:ILE:HD11	1.87	0.56
5:C:177:TYR:HE1	5:C:306:LYS:HZ3	1.54	0.56
6:D:1251:GLU:N	6:D:1251:GLU:OE1	2.39	0.56
5:C:913:VAL:HB	5:C:914:PRO:HD3	1.87	0.55
6:D:747:ARG:O	6:D:751:GLU:HG2	2.05	0.55
5:C:752:ASP:N	5:C:855:GLY:O	2.34	0.55
5:C:762:ARG:O	5:C:762:ARG:HG2	2.06	0.55
6:D:612:TYR:HD1	6:D:633:ILE:HD13	1.70	0.55
6:D:663:GLU:HG2	6:D:664:GLU:H	1.70	0.55
6:D:1221:TRP:CD1	6:D:1244:ASP:HB2	2.41	0.55
5:C:167:VAL:HG22	5:C:168:SER:H	1.70	0.55
5:C:950:LEU:CB	5:C:951:PRO:HD2	2.37	0.55
6:D:148:LEU:HD13	6:D:148:LEU:O	2.06	0.55
6:D:500:ARG:NH2	6:D:539:ASP:OD2	2.30	0.55
4:A:210:SER:OG	4:B:228:ASP:OD1	2.25	0.55
5:C:125:PHE:HE1	5:C:144:PHE:HB2	1.71	0.55
6:D:646:LEU:O	6:D:646:LEU:HD23	2.07	0.55
6:D:1257:LYS:HG2	6:D:1258:LEU:H	1.72	0.55
1:O:2:DC:H2'	1:O:3:DT:H71	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:152:ASN:O	4:B:153:LYS:HB2	2.05	0.55
5:C:852:LEU:HB3	5:C:856:VAL:CG2	2.36	0.55
6:D:74:ILE:HD12	9:J:42:VAL:HG13	1.88	0.55
6:D:124:ASP:HB3	6:D:234:LEU:CD1	2.37	0.55
6:D:593:GLU:OE1	6:D:593:GLU:N	2.35	0.55
1:O:35:DA:O3'	1:O:36:DG:H4'	2.07	0.55
6:D:76:GLU:CD	6:D:76:GLU:H	2.15	0.55
6:D:1248:GLY:O	6:D:1252:ASN:ND2	2.38	0.55
4:A:152:ASN:OD1	4:A:152:ASN:N	2.40	0.55
5:C:70:GLU:OE1	5:C:72:ASN:HB3	2.06	0.55
5:C:728:LEU:HD11	5:C:886:ILE:CD1	2.37	0.55
5:C:947:ALA:CA	5:C:950:LEU:CB	2.84	0.55
6:D:442:GLY:HA3	6:D:523:GLN:HB2	1.87	0.55
5:C:533:ALA:HB3	5:C:570:MET:HB2	1.89	0.55
5:C:797:VAL:HG13	5:C:823:VAL:HB	1.89	0.55
6:D:592:VAL:HG21	12:D:2006:EDO:H12	1.89	0.55
5:C:518:GLN:O	5:C:519:ILE:HD12	2.06	0.55
4:B:170:PRO:HB2	4:B:202:ILE:HD12	1.89	0.55
4:B:214:THR:O	4:B:218:LEU:HB2	2.06	0.55
5:C:1040:TYR:HE2	5:C:1090:ARG:CD	2.19	0.55
6:D:825:ASN:CB	6:D:826:PRO:HD2	2.37	0.55
7:E:49:ALA:O	7:E:53:TYR:HB2	2.07	0.55
1:O:39:DG:OP1	5:C:458:ARG:HD2	2.06	0.54
6:D:751:GLU:O	6:D:755:ILE:HG13	2.06	0.54
6:D:1167:THR:O	6:D:1204:GLY:HA3	2.07	0.54
7:E:26:TYR:HB3	7:E:29:PRO:HD3	1.90	0.54
1:O:21:DT:OP2	6:D:36:TYR:OH	2.23	0.54
4:B:89:ASP:O	4:B:90:ASP:HB2	2.07	0.54
5:C:1087:THR:HA	5:C:1090:ARG:NE	2.22	0.54
8:F:253:MET:HG2	8:F:301:ALA:HB2	1.89	0.54
5:C:788:ARG:HG2	5:C:789:ASP:OD1	2.08	0.54
5:C:932:LYS:O	5:C:960:ASP:N	2.35	0.54
5:C:174:PRO:HA	5:C:196:ILE:HG23	1.90	0.54
5:C:718:GLU:H	6:D:724:THR:CG2	2.20	0.54
5:C:947:ALA:HA	5:C:950:LEU:CB	2.37	0.54
6:D:1220:SER:OG	6:D:1244:ASP:OD2	2.25	0.54
2:P:11:DG:H2''	2:P:12:DT:H5'	1.88	0.54
4:B:99:LYS:HZ3	4:B:100:GLN:H	1.51	0.54
5:C:947:ALA:CB	5:C:950:LEU:CB	2.86	0.54
7:E:98:GLY:C	7:E:100:LEU:HD12	2.32	0.54
5:C:190:LEU:C	5:C:191:HIS:HD1	2.15	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:124:ASP:HB3	6:D:234:LEU:HD13	1.89	0.54
6:D:911:ARG:HG2	6:D:912:ASP:H	1.72	0.54
6:D:1009:LEU:HD12	6:D:1146:GLN:HG3	1.89	0.54
4:B:221:LEU:HD12	4:B:222:ALA:H	1.73	0.54
6:D:60:CYS:HB2	6:D:78:CYS:SG	2.48	0.54
6:D:1086:ARG:O	6:D:1113:MET:HE3	2.07	0.54
1:O:6:DA:H2''	1:O:7:DC:OP2	2.07	0.53
6:D:1183:GLU:OE1	6:D:1184:ARG:N	2.41	0.53
1:O:40:DT:OP1	5:C:458:ARG:NH1	2.34	0.53
4:B:100:GLN:HA	4:B:133:LYS:HA	1.90	0.53
6:D:190:LYS:HB3	6:D:193:VAL:HG12	1.90	0.53
4:B:170:PRO:HB3	4:B:201:SER:HB2	1.90	0.53
5:C:572:VAL:H	5:C:576:GLN:NE2	2.06	0.53
6:D:978:TYR:CZ	6:D:1153:LYS:HD3	2.43	0.53
4:A:48:GLY:HA3	4:A:168:TYR:HB3	1.90	0.53
5:C:504:GLU:HG2	5:C:523:THR:HB	1.90	0.53
5:C:626:ALA:HB2	5:C:704:MET:HG2	1.90	0.53
5:C:796:LYS:HG2	5:C:797:VAL:H	1.74	0.53
6:D:195:ARG:HH21	6:D:198:ARG:HD2	1.73	0.53
8:F:406:SER:HB3	8:F:409:GLU:HG3	1.88	0.53
5:C:939:VAL:CG1	5:C:943:VAL:HG22	2.37	0.53
5:C:968:PHE:CG	6:D:845:VAL:HG22	2.43	0.53
6:D:48:CYS:SG	6:D:50:LYS:HB3	2.49	0.53
6:D:336:ALA:HA	8:F:359:ILE:O	2.07	0.53
5:C:742:HIS:CD2	5:C:868:ARG:HG3	2.44	0.53
6:D:922:ARG:HH22	6:D:1156:GLU:CD	2.15	0.53
8:F:373:LEU:C	8:F:373:LEU:HD23	2.34	0.53
1:O:38:DC:C2'	1:O:39:DG:H5''	2.38	0.53
1:O:45:DG:H2''	1:O:46:DA:C8	2.44	0.53
5:C:102:ARG:NH2	5:C:142:THR:HG23	2.24	0.53
6:D:1087:LEU:CD2	6:D:1113:MET:HG2	2.38	0.53
8:F:404:THR:O	8:F:405:LEU:HG	2.09	0.53
4:A:40:ARG:HH12	4:B:32:TYR:CB	2.21	0.53
4:B:63:PHE:HE2	6:D:604:LYS:H	1.55	0.53
5:C:103:PHE:CZ	5:C:124:LEU:HG	2.44	0.53
5:C:509:LYS:O	5:C:516:THR:OG1	2.12	0.53
5:C:1139:ARG:HA	5:C:1139:ARG:NE	2.23	0.53
6:D:894:ARG:HB3	6:D:966:THR:HB	1.91	0.53
4:B:78:LEU:HD13	6:D:636:ARG:HE	1.74	0.53
5:C:721:ASN:HB3	5:C:727:ILE:HG13	1.91	0.53
2:P:48:DG:H2''	2:P:49:DC:OP2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:881:GLN:OE1	6:D:1250:LYS:HE2	2.09	0.53
6:D:1150:ILE:HG22	6:D:1151:HIS:H	1.73	0.53
6:D:1165:ARG:HG2	6:D:1181:LEU:HB3	1.90	0.53
4:A:30:PHE:HE1	4:B:44:SER:HB3	1.74	0.52
6:D:130:TYR:CZ	6:D:387:ARG:NH1	2.77	0.52
6:D:457:MET:O	6:D:461:VAL:HG23	2.08	0.52
6:D:599:TYR:HB3	6:D:633:ILE:HA	1.91	0.52
4:A:70:LYS:HG3	5:C:679:PRO:HG2	1.90	0.52
5:C:696:GLY:N	5:C:699:THR:OG1	2.42	0.52
6:D:1044:LYS:HG2	6:D:1045:ALA:H	1.74	0.52
8:F:207:LYS:O	8:F:209:GLU:HG3	2.09	0.52
5:C:432:ASP:OD2	5:C:438:SER:HB2	2.09	0.52
5:C:1116:LEU:O	5:C:1120:GLN:HG3	2.09	0.52
6:D:1101:SER:N	6:D:1104:ASP:OD2	2.32	0.52
6:D:1222:LEU:HD23	6:D:1244:ASP:OD2	2.08	0.52
8:F:406:SER:HB3	8:F:409:GLU:CG	2.39	0.52
5:C:325:THR:HG23	5:C:326:GLU:H	1.74	0.52
5:C:494:TYR:HB3	5:C:506:PRO:HG3	1.90	0.52
8:F:164:ASP:OD1	8:F:166:VAL:HG13	2.10	0.52
4:A:212:GLY:O	4:A:215:LEU:HD12	2.09	0.52
8:F:171:LYS:O	8:F:175:LYS:HG3	2.10	0.52
8:F:204:LEU:O	8:F:208:GLY:N	2.43	0.52
5:C:534:GLN:NE2	5:C:536:ASN:H	1.98	0.52
5:C:728:LEU:HD23	5:C:906:ILE:HG22	1.90	0.52
6:D:130:TYR:OH	6:D:379:ASP:OD2	2.27	0.52
8:F:440:ARG:NH1	8:F:443:GLN:OE1	2.38	0.52
1:O:39:DG:OP1	1:O:39:DG:H3'	2.10	0.52
4:A:14:VAL:HG13	4:A:18:ARG:HG3	1.90	0.52
4:A:46:ILE:CG2	4:A:170:PRO:HG2	2.39	0.52
5:C:1003:ASP:OD2	5:C:1005:ARG:N	2.43	0.52
5:C:1021:ILE:HD13	5:C:1021:ILE:N	2.25	0.52
6:D:912:ASP:HB3	6:D:915:VAL:HG13	1.90	0.52
8:F:399:GLN:O	8:F:403:GLU:HB2	2.10	0.52
4:B:97:LEU:HD13	4:B:110:ILE:HG22	1.92	0.52
5:C:56:VAL:O	5:C:58:SER:N	2.42	0.52
5:C:102:ARG:NH2	5:C:126:VAL:O	2.42	0.52
5:C:1021:ILE:HD13	5:C:1021:ILE:H	1.75	0.52
1:O:31:DT:H2''	8:F:239:ARG:HD2	1.90	0.51
1:O:34:DG:H4'	1:O:35:DA:H5'	1.92	0.51
1:O:38:DC:H2''	1:O:39:DG:C5'	2.39	0.51
2:P:16:DG:H8	2:P:16:DG:OP2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:B:76:ILE:HD11	4:B:126:ALA:HB2	1.92	0.51
5:C:403:ILE:HB	5:C:407:THR:CB	2.40	0.51
5:C:728:LEU:CD1	5:C:886:ILE:HD13	2.39	0.51
5:C:921:GLN:O	5:C:925:THR:OG1	2.26	0.51
6:D:967:CYS:SG	6:D:969:SER:OG	2.65	0.51
5:C:346:MET:HE2	5:C:348:VAL:HG22	1.92	0.51
1:O:19:DA:H2'	1:O:20:DT:C6	2.46	0.51
4:A:14:VAL:HG13	4:A:15:ALA:H	1.75	0.51
5:C:178:PHE:O	5:C:358:VAL:HG22	2.10	0.51
5:C:1031:LYS:HB3	6:D:540:GLN:NE2	2.25	0.51
6:D:226:PHE:CE1	6:D:248:TYR:HB3	2.45	0.51
1:O:41:DC:H2''	1:O:42:DA:OP2	2.11	0.51
6:D:586:TYR:O	6:D:590:THR:HG23	2.11	0.51
5:C:811:LEU:HD23	5:C:811:LEU:O	2.11	0.51
5:C:853:PRO:HD2	5:C:856:VAL:HG21	1.92	0.51
6:D:127:LYS:HA	6:D:132:ALA:HB3	1.93	0.51
6:D:667:LEU:O	6:D:671:MET:HG3	2.10	0.51
4:A:18:ARG:HB3	4:A:197:GLU:HB2	1.92	0.51
5:C:156:THR:HG21	5:C:163:GLU:OE2	2.10	0.51
5:C:1087:THR:HA	5:C:1090:ARG:HE	1.74	0.51
6:D:269:ASP:HB3	6:D:272:ALA:HB3	1.93	0.51
1:O:45:DG:H2''	1:O:46:DA:H8	1.75	0.51
4:A:49:ALA:HB1	4:A:85:VAL:O	2.10	0.51
5:C:535:ALA:HB2	5:C:571:ASP:CB	2.38	0.51
5:C:584:MET:HE3	5:C:622:GLU:HG3	1.93	0.51
6:D:693:ALA:O	6:D:697:ASN:HB2	2.11	0.51
4:A:2:LEU:HD22	4:A:2:LEU:O	2.11	0.51
5:C:427:LEU:HD21	5:C:451:PRO:HD2	1.93	0.51
5:C:1078:GLU:HG3	5:C:1082:ILE:HD11	1.93	0.51
6:D:140:ASP:OD2	6:D:143:MET:HB2	2.10	0.51
1:O:6:DA:C2'	1:O:7:DC:H5'	2.40	0.51
1:O:30:DC:OP2	8:F:282:SER:OG	2.27	0.51
5:C:102:ARG:HH22	5:C:142:THR:HG23	1.75	0.51
5:C:439:GLY:O	5:C:443:LYS:HG3	2.11	0.51
6:D:46:LEU:HB3	6:D:325:ARG:HH12	1.75	0.51
6:D:144:ARG:NH2	6:D:229:LEU:O	2.30	0.51
7:E:28:THR:HG23	7:E:28:THR:O	2.10	0.51
7:E:99:ASP:OD2	7:E:99:ASP:N	2.44	0.51
4:A:199:LYS:O	4:A:200:ASN:HB2	2.12	0.50
6:D:190:LYS:HD2	6:D:192:ASP:H	1.76	0.50
5:C:173:SER:O	5:C:177:TYR:OH	2.19	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:203:LEU:HA	5:C:217:ILE:HA	1.93	0.50
5:C:736:ASP:OD1	5:C:869:LYS:HE2	2.11	0.50
5:C:749:ASP:HB3	5:C:859:LEU:HD23	1.93	0.50
6:D:573:PRO:HG2	6:D:576:MET:CE	2.39	0.50
6:D:965:LEU:HD22	6:D:1132:GLN:OE1	2.11	0.50
6:D:1085:GLN:HB2	6:D:1113:MET:CE	2.41	0.50
1:O:23:DT:H71	8:F:308:VAL:HG21	1.92	0.50
5:C:112:GLU:HG2	5:C:116:LYS:HD2	1.94	0.50
5:C:518:GLN:C	5:C:519:ILE:HD12	2.35	0.50
6:D:888:HIS:N	10:D:2004:SO4:O2	2.42	0.50
4:B:28:PRO:HA	4:B:190:ASP:OD2	2.11	0.50
4:B:68:GLY:O	4:B:128:LEU:HD12	2.11	0.50
4:B:143:GLY:HA3	4:B:168:TYR:CD1	2.45	0.50
6:D:230:ALA:N	6:D:233:GLN:OE1	2.44	0.50
6:D:340:LEU:HD22	6:D:340:LEU:H	1.75	0.50
7:E:86:GLU:OE1	7:E:91:ILE:HG12	2.12	0.50
2:P:31:DT:H2"	2:P:32:DT:C6	2.46	0.50
5:C:685:GLN:HG2	5:C:686:ARG:N	2.26	0.50
5:C:1036:SER:O	6:D:423:ASP:HB3	2.10	0.50
6:D:901:ALA:HA	6:D:911:ARG:O	2.10	0.50
6:D:938:GLU:N	6:D:938:GLU:OE1	2.45	0.50
5:C:935:TRP:CZ2	5:C:954:LEU:HD23	2.41	0.50
6:D:557:ILE:HG22	6:D:558:LEU:HD12	1.94	0.50
6:D:1152:ASP:O	6:D:1156:GLU:HG3	2.12	0.50
6:D:1267:ARG:HG3	6:D:1268:TYR:H	1.77	0.50
5:C:176:VAL:HG22	5:C:307:VAL:HG12	1.93	0.50
5:C:435:ASN:HB2	5:C:436:PRO:HD2	1.93	0.50
5:C:762:ARG:NH1	5:C:775:LEU:O	2.40	0.50
8:F:273:PHE:O	9:J:88:ARG:NH2	2.44	0.50
5:C:711:LEU:HD23	5:C:904:VAL:HA	1.94	0.50
6:D:568:PRO:HB3	6:D:983:ALA:HB2	1.93	0.50
6:D:578:ARG:HA	6:D:582:VAL:HG23	1.91	0.50
6:D:748:HIS:O	6:D:752:ALA:N	2.29	0.50
1:O:14:DG:H2"	1:O:15:DT:OP2	2.12	0.50
1:O:30:DC:OP2	8:F:280:LYS:HG2	2.11	0.50
4:B:120:ASN:ND2	4:B:123:MET:SD	2.85	0.50
5:C:102:ARG:HB2	5:C:125:PHE:CB	2.41	0.50
8:F:338:ALA:HB1	8:F:343:ILE:O	2.11	0.50
4:A:159:ILE:HD12	4:A:159:ILE:N	2.27	0.49
6:D:736:LEU:N	6:D:792:TYR:OH	2.39	0.49
6:D:1140:GLN:O	6:D:1144:ARG:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:156:ASP:O	8:F:160:THR:HG23	2.12	0.49
4:B:73:VAL:O	4:B:77:ILE:HG12	2.12	0.49
5:C:229:LEU:H	5:C:229:LEU:HD22	1.77	0.49
6:D:102:THR:HG21	6:D:129:ILE:HG21	1.93	0.49
4:A:21:PHE:O	4:A:193:ILE:HD12	2.13	0.49
5:C:422:PHE:O	5:C:428:SER:OG	2.27	0.49
5:C:534:GLN:NE2	5:C:535:ALA:N	2.60	0.49
6:D:633:ILE:HD12	6:D:635:VAL:HG22	1.94	0.49
6:D:1151:HIS:ND1	6:D:1153:LYS:HG2	2.27	0.49
8:F:211:LEU:H	8:F:211:LEU:CD2	2.21	0.49
1:O:5:DG:H2''	1:O:6:DA:OP2	2.12	0.49
4:B:47:PRO:HA	4:B:144:ARG:HG3	1.93	0.49
9:J:85:LEU:HD13	9:J:88:ARG:NH1	2.27	0.49
4:A:2:LEU:HD13	4:A:2:LEU:N	2.28	0.49
4:A:40:ARG:HD3	4:B:33:THR:HG22	1.94	0.49
5:C:765:PRO:HB3	5:C:821:ARG:HD2	1.93	0.49
5:C:1075:THR:O	5:C:1079:LEU:HG	2.12	0.49
6:D:1062:PHE:CE1	6:D:1080:LYS:HB3	2.46	0.49
2:P:17:DG:H8	2:P:17:DG:OP2	1.96	0.49
5:C:277:PRO:HB3	8:F:154:ARG:HA	1.95	0.49
5:C:809:GLU:O	5:C:810:ARG:CB	2.60	0.49
6:D:507:LEU:CD2	6:D:574:LEU:HD23	2.41	0.49
6:D:1172:GLY:HA3	6:D:1176:PHE:HB2	1.95	0.49
9:J:88:ARG:O	9:J:89:ARG:NH1	2.38	0.49
4:B:106:THR:OG1	4:B:107:ALA:N	2.45	0.49
4:B:228:ASP:OD2	4:B:228:ASP:N	2.43	0.49
5:C:466:VAL:HG12	6:D:856:ARG:CZ	2.42	0.49
5:C:334:GLU:O	5:C:338:ARG:HB2	2.13	0.49
6:D:26:GLY:HA3	6:D:51:ILE:HG21	1.95	0.49
6:D:214:ARG:O	6:D:218:ARG:HG3	2.12	0.49
1:O:47:DT:H2''	1:O:48:DG:C8	2.48	0.49
5:C:34:LYS:HD3	5:C:34:LYS:N	2.27	0.49
5:C:264:ALA:O	5:C:268:ILE:HG22	2.12	0.49
5:C:1019:MET:HG2	5:C:1020:TYR:N	2.27	0.49
7:E:26:TYR:CZ	7:E:36:PRO:HG2	2.48	0.49
5:C:437:LEU:O	5:C:441:THR:OG1	2.30	0.49
5:C:641:ILE:HD12	5:C:641:ILE:H	1.77	0.49
6:D:64:LYS:HB3	6:D:64:LYS:HZ2	1.77	0.49
8:F:211:LEU:HG	8:F:216:ARG:HB2	1.94	0.49
1:O:25:DC:OP1	9:J:79:ARG:NH2	2.46	0.48
5:C:975:GLU:O	5:C:979:LEU:HG	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:218:ARG:O	6:D:222:ILE:HG13	2.13	0.48
4:A:107:ALA:HB2	4:A:123:MET:HB3	1.94	0.48
5:C:540:ASP:OD2	5:C:543:GLY:N	2.44	0.48
6:D:130:TYR:HE1	6:D:376:GLU:HG2	1.78	0.48
6:D:527:LEU:HD13	6:D:712:VAL:HG12	1.95	0.48
6:D:589:THR:OG1	6:D:686:GLN:HA	2.12	0.48
6:D:819:MET:HB2	6:D:835:ILE:O	2.13	0.48
6:D:901:ALA:CB	6:D:911:ARG:HA	2.43	0.48
7:E:26:TYR:O	7:E:27:ASP:HB2	2.13	0.48
1:O:32:DG:H5'	8:F:239:ARG:CD	2.42	0.48
4:A:197:GLU:OE1	5:C:987:ARG:NH1	2.45	0.48
5:C:178:PHE:CG	5:C:193:VAL:HG22	2.48	0.48
5:C:1069:ALA:HB3	6:D:506:ARG:HB3	1.94	0.48
4:B:74:THR:OG1	6:D:608:GLU:OE1	2.22	0.48
5:C:33:ALA:HB2	5:C:966:PRO:HG2	1.95	0.48
5:C:271:LYS:O	5:C:274:PRO:HD3	2.13	0.48
5:C:437:LEU:HD12	5:C:706:LEU:HD11	1.95	0.48
5:C:464:ARG:O	6:D:856:ARG:NH1	2.45	0.48
5:C:722:TYR:H	5:C:725:ALA:HB3	1.78	0.48
5:C:984:LEU:CB	5:C:991:VAL:HG23	2.43	0.48
8:F:198:THR:OG1	8:F:223:CYS:SG	2.69	0.48
4:A:84:VAL:HG22	4:A:120:ASN:ND2	2.29	0.48
4:B:55:ARG:HE	4:B:56:ILE:N	2.11	0.48
6:D:111:PRO:HD2	6:D:1232:ARG:HH12	1.79	0.48
6:D:746:GLU:O	6:D:750:ALA:HB3	2.13	0.48
6:D:1044:LYS:O	6:D:1085:GLN:NE2	2.40	0.48
7:E:79:LEU:HB2	7:E:95:GLU:HG2	1.95	0.48
4:A:216:VAL:HG13	4:B:216:VAL:HG23	1.96	0.48
5:C:609:LEU:HD13	5:C:708:LYS:HE3	1.96	0.48
5:C:768:SER:O	5:C:771:VAL:HG22	2.13	0.48
5:C:930:VAL:HG11	5:C:979:LEU:HB3	1.96	0.48
6:D:737:VAL:HG13	6:D:840:ARG:HD3	1.96	0.48
4:A:177:LYS:HG3	4:A:193:ILE:CG2	2.39	0.48
4:B:69:VAL:HG12	4:B:128:LEU:HA	1.94	0.48
5:C:125:PHE:CE1	5:C:144:PHE:HB2	2.48	0.48
5:C:534:GLN:HE21	5:C:536:ASN:N	2.00	0.48
6:D:898:VAL:HG11	6:D:919:ALA:HB2	1.96	0.48
5:C:79:GLU:O	5:C:83:GLU:HG3	2.14	0.48
5:C:178:PHE:CD1	5:C:193:VAL:HG22	2.49	0.48
6:D:114:LEU:HB3	6:D:125:LEU:HD21	1.95	0.48
6:D:372:ARG:HG3	6:D:373:MET:N	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:193:VAL:CG2	5:C:336:LEU:HG	2.44	0.48
5:C:231:ALA:HA	5:C:265:LEU:CD2	2.43	0.48
5:C:822:GLU:CD	5:C:822:GLU:H	2.21	0.48
6:D:925:ALA:HB3	6:D:960:LYS:HG2	1.95	0.48
6:D:661:TRP:CZ3	6:D:663:GLU:HB2	2.49	0.48
1:O:6:DA:H1'	1:O:7:DC:H5'	1.96	0.47
4:A:84:VAL:HG22	4:A:120:ASN:CG	2.39	0.47
5:C:780:ILE:HD12	5:C:841:ILE:HG21	1.97	0.47
1:O:40:DT:H5''	1:O:40:DT:C6	2.43	0.47
2:P:15:DA:P	5:C:1050:GLY:HA2	2.54	0.47
5:C:609:LEU:CD1	5:C:708:LYS:HE3	2.44	0.47
6:D:592:VAL:HG11	12:D:2006:EDO:H11	1.95	0.47
6:D:815:THR:HA	6:D:820:LYS:HA	1.96	0.47
6:D:1278:GLU:H	6:D:1278:GLU:HG3	1.40	0.47
4:B:55:ARG:HH11	4:B:160:GLY:CA	2.27	0.47
5:C:204:GLU:O	5:C:216:ARG:N	2.47	0.47
5:C:498:ASN:HB2	5:C:502:PHE:O	2.14	0.47
5:C:556:GLY:N	5:C:557:GLY:HA2	2.28	0.47
6:D:687:MET:HE3	6:D:687:MET:HA	1.96	0.47
6:D:822:LEU:HB2	6:D:830:PHE:CE1	2.50	0.47
6:D:916:GLU:HA	6:D:920:PHE:HB2	1.95	0.47
1:O:38:DC:H1'	1:O:39:DG:C5'	2.39	0.47
4:A:100:GLN:HG3	4:A:101:GLY:N	2.29	0.47
5:C:1126:VAL:HG12	6:D:12:ILE:HG13	1.95	0.47
6:D:51:ILE:HG13	6:D:52:PHE:H	1.79	0.47
6:D:473:LYS:HD2	8:F:386:VAL:HG21	1.97	0.47
6:D:655:TRP:C	6:D:657:PRO:HD3	2.39	0.47
4:B:40:ARG:HH22	6:D:623:ASP:HB3	1.79	0.47
4:B:170:PRO:HB2	4:B:202:ILE:CD1	2.44	0.47
5:C:365:GLY:HA3	5:C:525:ASP:OD1	2.15	0.47
5:C:766:ASN:HD22	8:F:466:ASP:CG	2.23	0.47
5:C:786:GLU:O	5:C:787:VAL:HG13	2.15	0.47
5:C:935:TRP:HA	5:C:983:THR:HG23	1.96	0.47
5:C:1086:ASP:O	5:C:1090:ARG:HG2	2.15	0.47
6:D:12:ILE:HG12	6:D:13:GLY:N	2.29	0.47
6:D:87:VAL:O	6:D:91:ARG:HG3	2.14	0.47
6:D:392:THR:OG1	6:D:396:ASN:HA	2.13	0.47
1:O:38:DC:N4	5:C:202:TRP:CB	2.78	0.47
1:O:38:DC:N4	5:C:202:TRP:HB2	2.30	0.47
5:C:52:PHE:CZ	5:C:150:MET:HE2	2.49	0.47
5:C:589:GLU:OE1	5:C:589:GLU:N	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:939:VAL:HA	5:C:944:PRO:HD3	1.96	0.47
6:D:550:GLU:O	6:D:554:GLU:HG3	2.15	0.47
4:A:94:THR:HG22	4:A:139:VAL:HG22	1.97	0.47
5:C:986:ASN:O	5:C:988:ASP:N	2.45	0.47
5:C:175:GLY:O	5:C:196:ILE:HG22	2.14	0.47
5:C:335:TYR:CE1	5:C:356:VAL:HG13	2.49	0.47
5:C:882:ASN:ND2	5:C:1019:MET:HE1	2.28	0.47
6:D:334:ARG:HD3	8:F:356:ARG:NH2	2.30	0.47
6:D:513:GLU:OE1	7:E:32:ILE:HB	2.15	0.47
6:D:580:ASP:OD1	6:D:580:ASP:N	2.48	0.47
6:D:735:VAL:O	6:D:840:ARG:NH1	2.48	0.47
6:D:930:ASP:OD2	6:D:934:ASN:N	2.31	0.47
8:F:465:LEU:O	8:F:466:ASP:HB2	2.14	0.47
1:O:45:DG:OP2	1:O:45:DG:H8	1.98	0.46
2:P:17:DG:H2"	5:C:430:PHE:CE2	2.50	0.46
4:A:147:VAL:CG1	4:A:166:SER:HB2	2.45	0.46
5:C:597:LEU:HD23	5:C:598:MET:N	2.30	0.46
6:D:503:THR:HG23	6:D:508:GLY:HA3	1.97	0.46
6:D:661:TRP:HZ3	6:D:663:GLU:HB2	1.80	0.46
1:O:46:DA:N6	2:P:4:DT:H3	2.08	0.46
4:A:38:LEU:HD13	4:A:208:LEU:HD11	1.97	0.46
4:B:55:ARG:O	4:B:137:GLU:N	2.34	0.46
4:B:76:ILE:HA	4:B:79:ASN:HB2	1.97	0.46
5:C:534:GLN:NE2	5:C:535:ALA:H	2.13	0.46
5:C:873:GLY:HA3	5:C:1028:VAL:HG11	1.96	0.46
6:D:515:GLN:O	6:D:517:VAL:HG23	2.15	0.46
6:D:948:ILE:O	6:D:952:LEU:HD13	2.15	0.46
4:B:101:GLY:O	4:B:128:LEU:HD23	2.14	0.46
5:C:932:LYS:HD3	5:C:932:LYS:C	2.40	0.46
6:D:17:ALA:O	6:D:21:ARG:HG3	2.15	0.46
6:D:350:ARG:HD3	6:D:373:MET:HB3	1.97	0.46
6:D:622:MET:CE	6:D:629:VAL:HG22	2.45	0.46
6:D:624:ARG:HE	6:D:624:ARG:HB3	1.52	0.46
4:B:28:PRO:HA	4:B:29:GLY:HA2	1.47	0.46
5:C:718:GLU:H	6:D:724:THR:HG21	1.80	0.46
5:C:951:PRO:CB	5:C:954:LEU:HD13	2.45	0.46
6:D:58:TRP:CD2	6:D:68:VAL:HG12	2.51	0.46
6:D:557:ILE:O	6:D:563:ASN:ND2	2.42	0.46
6:D:1062:PHE:H	6:D:1083:LYS:HE3	1.79	0.46
6:D:1168:ILE:O	6:D:1178:PRO:HA	2.16	0.46
4:A:113:PRO:HD2	4:A:116:VAL:HG21	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:751:ARG:CG	5:C:856:VAL:HG12	2.37	0.46
6:D:929:VAL:HG12	6:D:935:VAL:HG22	1.96	0.46
4:B:180:ALA:HB1	4:B:188:ASP:HA	1.97	0.46
5:C:80:VAL:HG12	5:C:384:LEU:HD12	1.98	0.46
6:D:432:VAL:HG13	6:D:434:PRO:HD3	1.97	0.46
8:F:408:ARG:HH21	8:F:444:ILE:HD11	1.80	0.46
8:F:439:GLU:OE1	8:F:442:ARG:NH2	2.47	0.46
8:F:454:HIS:CD2	8:F:456:SER:HG	2.22	0.46
4:A:19:SER:OG	4:A:204:PRO:HB2	2.16	0.46
4:B:55:ARG:HD3	4:B:160:GLY:HA3	1.98	0.46
4:B:124:HIS:HD1	4:B:124:HIS:C	2.23	0.46
5:C:154:LYS:HB3	5:C:154:LYS:HZ3	1.79	0.46
6:D:1088:ARG:HD3	6:D:1111:GLN:HB3	1.97	0.46
5:C:986:ASN:C	5:C:988:ASP:N	2.74	0.46
6:D:478:ARG:HH11	6:D:480:ARG:HG2	1.80	0.46
6:D:1153:LYS:O	6:D:1157:VAL:HG23	2.16	0.46
4:A:40:ARG:HD2	5:C:1004:GLY:O	2.16	0.46
4:B:205:ARG:NH2	4:B:205:ARG:HB2	2.32	0.46
5:C:1079:LEU:HA	5:C:1083:LYS:HG3	1.97	0.46
6:D:413:PHE:HA	6:D:417:LEU:HB2	1.97	0.46
4:B:89:ASP:C	4:B:91:GLU:H	2.24	0.45
5:C:505:THR:HG22	5:C:506:PRO:HD2	1.97	0.45
5:C:884:GLY:HA2	6:D:537:ASP:HA	1.98	0.45
2:P:15:DA:OP2	5:C:1050:GLY:HA2	2.15	0.45
4:A:84:VAL:HG23	4:A:84:VAL:O	2.16	0.45
5:C:37:GLU:OE1	5:C:494:TYR:OH	2.33	0.45
5:C:159:ILE:HB	5:C:164:ARG:HD2	1.99	0.45
5:C:954:LEU:O	5:C:955:TYR:C	2.59	0.45
6:D:469:ILE:HG12	6:D:469:ILE:O	2.16	0.45
6:D:739:PRO:HD3	6:D:791:PHE:HE2	1.81	0.45
6:D:831:ILE:O	6:D:831:ILE:HG13	2.14	0.45
6:D:877:VAL:HG13	6:D:996:ILE:HG23	1.99	0.45
5:C:357:GLU:HG2	5:C:358:VAL:O	2.16	0.45
5:C:601:ASN:O	5:C:604:ARG:HG2	2.16	0.45
6:D:50:LYS:O	6:D:50:LYS:HG2	2.16	0.45
6:D:823:VAL:O	6:D:831:ILE:HG12	2.17	0.45
6:D:837:SER:HB3	6:D:842:GLY:O	2.17	0.45
6:D:962:ARG:HH21	6:D:976:MET:CB	2.29	0.45
4:B:8:THR:O	4:B:23:ILE:HA	2.15	0.45
5:C:301:ARG:HD2	5:C:302:VAL:N	2.32	0.45
5:C:587:PHE:HZ	5:C:927:LEU:HD12	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:104:ILE:HG13	6:D:379:ASP:OD2	2.16	0.45
6:D:1252:ASN:OD1	6:D:1257:LYS:HD3	2.17	0.45
7:E:89:LEU:HD23	7:E:89:LEU:O	2.16	0.45
5:C:754:LYS:HD3	6:D:39:LEU:HD12	1.98	0.45
6:D:60:CYS:SG	6:D:64:LYS:N	2.90	0.45
6:D:1081:LEU:HD22	6:D:1113:MET:SD	2.56	0.45
8:F:197:ALA:O	8:F:201:LEU:HG	2.16	0.45
5:C:449:LEU:HD12	5:C:449:LEU:O	2.16	0.45
6:D:271:ASP:O	6:D:275:GLU:HG3	2.16	0.45
6:D:663:GLU:HG2	6:D:664:GLU:N	2.30	0.45
5:C:641:ILE:HD12	5:C:641:ILE:N	2.32	0.45
6:D:282:ARG:HD3	6:D:282:ARG:HA	1.86	0.45
4:B:105:VAL:C	4:B:125:ILE:HG23	2.42	0.45
4:B:203:SER:HB2	4:B:204:PRO:HD2	1.98	0.45
5:C:87:ILE:HB	5:C:96:LEU:HB3	1.99	0.45
5:C:106:VAL:HG11	5:C:120:TYR:CZ	2.51	0.45
5:C:216:ARG:NE	5:C:221:ARG:HA	2.32	0.45
6:D:54:PRO:HG3	6:D:81:GLU:O	2.17	0.45
6:D:1114:GLU:HA	6:D:1114:GLU:OE1	2.17	0.45
4:A:109:ASP:OD2	4:A:109:ASP:N	2.49	0.45
5:C:102:ARG:N	5:C:125:PHE:O	2.38	0.45
5:C:1077:GLN:O	5:C:1081:THR:OG1	2.33	0.45
6:D:129:ILE:HA	6:D:257:GLY:HA2	1.98	0.45
8:F:447:LYS:HA	8:F:447:LYS:HD3	1.71	0.45
2:P:2:DC:H2''	2:P:3:DA:C8	2.52	0.45
2:P:6:DC:H2''	2:P:7:DG:C8	2.52	0.45
5:C:753:THR:HG23	5:C:756:GLY:O	2.16	0.45
6:D:129:ILE:HG22	6:D:261:ILE:HG13	1.99	0.45
4:A:4:SER:O	4:A:5:GLN:HG3	2.17	0.44
5:C:126:VAL:HG21	5:C:145:MET:HE2	1.99	0.44
5:C:368:ARG:HB3	5:C:502:PHE:CE1	2.51	0.44
5:C:397:THR:O	5:C:397:THR:OG1	2.34	0.44
5:C:610:VAL:HG23	5:C:611:ARG:H	1.82	0.44
5:C:635:ALA:HB2	5:C:693:ILE:HD11	1.99	0.44
5:C:859:LEU:C	5:C:859:LEU:HD13	2.42	0.44
6:D:459:ARG:NH2	6:D:489:GLU:OE2	2.50	0.44
6:D:738:PRO:HA	6:D:739:PRO:HD3	1.91	0.44
4:A:152:ASN:HB3	4:A:157:ALA:HB3	1.99	0.44
5:C:751:ARG:HA	5:C:856:VAL:HA	2.00	0.44
5:C:1065:TRP:HB3	6:D:1000:GLN:HE21	1.82	0.44
6:D:76:GLU:CD	9:J:48:ALA:HB1	2.41	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:171:VAL:HG21	5:C:370:ARG:NE	2.33	0.44
6:D:1132:GLN:HG2	6:D:1163:LEU:CD1	2.47	0.44
6:D:1132:GLN:HG2	6:D:1163:LEU:HD13	1.99	0.44
6:D:1258:LEU:HD12	6:D:1258:LEU:HA	1.74	0.44
1:O:39:DG:O5'	1:O:39:DG:C8	2.68	0.44
5:C:798:THR:HG23	5:C:826:THR:HG21	1.99	0.44
6:D:527:LEU:CD1	6:D:712:VAL:HG12	2.48	0.44
7:E:31:GLY:C	7:E:33:THR:N	2.75	0.44
7:E:98:GLY:O	7:E:100:LEU:HD12	2.17	0.44
8:F:310:MET:O	8:F:313:VAL:HG22	2.18	0.44
1:O:32:DG:H5''	8:F:239:ARG:HG2	1.99	0.44
4:B:77:ILE:O	4:B:81:LYS:HG3	2.17	0.44
5:C:917:MET:HE2	5:C:917:MET:HA	1.97	0.44
5:C:942:GLY:O	5:C:943:VAL:HB	2.18	0.44
5:C:1138:MET:H	5:C:1138:MET:HG2	1.50	0.44
6:D:27:GLU:OE2	6:D:96:GLU:HB2	2.17	0.44
6:D:57:ASP:HB3	6:D:58:TRP:CE3	2.53	0.44
6:D:234:LEU:CD2	6:D:236:VAL:HG22	2.48	0.44
8:F:191:ILE:O	8:F:195:LEU:HD13	2.17	0.44
4:B:55:ARG:NH2	4:B:59:VAL:HB	2.32	0.44
5:C:1075:THR:OG1	6:D:554:GLU:OE2	2.24	0.44
6:D:120:LEU:HD13	6:D:120:LEU:HA	1.81	0.44
6:D:1221:TRP:NE1	6:D:1244:ASP:HB2	2.32	0.44
6:D:846:LEU:O	6:D:850:ILE:HG12	2.17	0.44
9:J:32:TYR:O	9:J:39:GLU:HA	2.17	0.44
4:B:110:ILE:HD12	4:B:111:VAL:N	2.32	0.44
5:C:1064:CYS:O	5:C:1068:GLN:HG3	2.17	0.44
6:D:103:HIS:C	6:D:105:TRP:H	2.26	0.44
8:F:317:LEU:HD23	8:F:317:LEU:HA	1.85	0.44
1:O:33:DG:C5'	8:F:246:LYS:HE2	2.46	0.44
4:A:172:LEU:HB3	4:A:197:GLU:HG2	1.99	0.44
5:C:751:ARG:HD2	6:D:332:GLY:CA	2.39	0.44
6:D:614:SER:HB2	6:D:615:PRO:HD2	1.98	0.44
6:D:1041:PRO:HB3	6:D:1116:ALA:HB3	1.99	0.44
6:D:1062:PHE:N	6:D:1083:LYS:HE3	2.32	0.44
8:F:372:GLN:H	8:F:372:GLN:HG2	1.51	0.44
1:O:29:DA:H8	8:F:283:THR:OG1	2.01	0.43
4:B:85:VAL:HG23	4:B:117:THR:O	2.18	0.43
6:D:64:LYS:HZ2	6:D:64:LYS:CB	2.30	0.43
6:D:987:LEU:HG	6:D:988:VAL:H	1.82	0.43
8:F:187:LEU:O	8:F:191:ILE:HG13	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:F:214:GLN:OE1	9:J:109:ARG:NH2	2.49	0.43
1:O:5:DG:H2"	1:O:6:DA:C8	2.53	0.43
2:P:43:DG:P	8:F:426:THR:HG1	2.40	0.43
5:C:710:LEU:HB2	5:C:1021:ILE:HD11	2.00	0.43
6:D:589:THR:CB	6:D:686:GLN:HA	2.48	0.43
8:F:394:LEU:HD13	8:F:394:LEU:C	2.43	0.43
5:C:753:THR:OG1	5:C:754:LYS:N	2.50	0.43
6:D:478:ARG:O	6:D:478:ARG:HG2	2.18	0.43
6:D:650:LEU:HD13	6:D:661:TRP:HB2	1.99	0.43
6:D:1044:LYS:HE3	6:D:1118:ASP:HB2	2.01	0.43
6:D:1100:LEU:HD23	6:D:1100:LEU:HA	1.81	0.43
6:D:1169:ILE:HG13	6:D:1204:GLY:HA2	2.00	0.43
8:F:196:TYR:OH	9:J:95:GLU:OE2	2.32	0.43
8:F:324:LEU:HB2	8:F:332:PRO:HG3	1.99	0.43
4:B:32:TYR:HB3	5:C:1005:ARG:HG3	2.00	0.43
4:B:54:ILE:HD11	4:B:77:ILE:HD13	1.99	0.43
5:C:85:SER:HA	5:C:86:PRO:HA	1.66	0.43
5:C:545:PHE:CE1	5:C:550:VAL:HG11	2.53	0.43
5:C:622:GLU:HB3	5:C:704:MET:H	1.84	0.43
6:D:739:PRO:HD3	6:D:791:PHE:CE2	2.53	0.43
6:D:885:VAL:HG21	6:D:988:VAL:HG11	1.99	0.43
1:O:14:DG:H1	2:P:36:DC:H42	1.66	0.43
5:C:276:GLU:O	5:C:277:PRO:C	2.60	0.43
5:C:313:LEU:HD11	5:C:348:VAL:HG11	1.99	0.43
5:C:926:HIS:O	5:C:930:VAL:HG23	2.18	0.43
6:D:430:ILE:HG21	6:D:541:MET:SD	2.59	0.43
6:D:655:TRP:O	6:D:657:PRO:HD3	2.17	0.43
6:D:757:ARG:CZ	6:D:757:ARG:HB3	2.48	0.43
4:A:9:LEU:HD12	4:A:10:SER:N	2.34	0.43
1:O:48:DG:P	6:D:123:LYS:HG2	2.59	0.43
4:A:111:VAL:O	4:A:111:VAL:HG22	2.17	0.43
5:C:196:ILE:O	5:C:196:ILE:CG2	2.67	0.43
5:C:306:LYS:HE3	5:C:306:LYS:HB3	1.93	0.43
5:C:841:ILE:HD12	5:C:862:VAL:HG22	2.01	0.43
5:C:973:GLU:OE2	6:D:841:GLU:HA	2.19	0.43
6:D:877:VAL:O	6:D:881:GLN:HB3	2.18	0.43
7:E:37:ILE:N	7:E:37:ILE:HD12	2.33	0.43
7:E:81:GLU:O	7:E:94:ARG:NH2	2.51	0.43
4:B:25:PRO:HG3	4:B:183:VAL:CG2	2.49	0.43
5:C:240:VAL:HG22	5:C:250:MET:HE1	2.00	0.43
5:C:591:ASP:OD2	5:C:880:HIS:ND1	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:715:MET:HA	5:C:910:THR:HG23	2.00	0.43
6:D:61:TYR:HB3	6:D:78:CYS:HB2	2.01	0.43
6:D:525:HIS:O	6:D:528:VAL:HG22	2.19	0.43
6:D:589:THR:HB	6:D:686:GLN:HA	2.01	0.43
6:D:592:VAL:HG21	12:D:2006:EDO:C1	2.49	0.43
6:D:636:ARG:CG	6:D:662:THR:HG22	2.49	0.43
6:D:889:ASP:OD2	6:D:890:CYS:N	2.52	0.43
6:D:900:LEU:HD12	6:D:959:VAL:HG22	2.01	0.43
6:D:996:ILE:H	6:D:996:ILE:HG13	1.62	0.43
4:A:173:LYS:HD3	5:C:900:ASP:O	2.19	0.43
4:A:212:GLY:O	4:A:216:VAL:HG23	2.18	0.43
5:C:156:THR:OG1	5:C:157:PHE:N	2.51	0.43
5:C:237:GLU:H	5:C:237:GLU:CD	2.26	0.43
5:C:531:VAL:HG22	5:C:552:VAL:HB	1.99	0.43
5:C:932:LYS:HG3	5:C:1018:TYR:CE2	2.54	0.43
5:C:938:ASP:O	5:C:939:VAL:HB	2.19	0.43
5:C:1098:VAL:HG11	6:D:469:ILE:HD12	2.01	0.43
5:C:1129:LEU:CA	5:C:1135:ALA:HA	2.47	0.43
6:D:822:LEU:H	6:D:822:LEU:CD1	2.25	0.43
4:A:214:THR:HG23	4:B:231:HIS:CB	2.49	0.43
6:D:124:ASP:O	6:D:128:ILE:HG12	2.19	0.43
6:D:591:LEU:HD12	6:D:666:THR:HG22	2.00	0.43
6:D:924:LEU:HD12	6:D:937:ILE:HG22	2.00	0.43
6:D:1192:ARG:O	6:D:1193:ARG:C	2.62	0.43
6:D:1257:LYS:HG2	6:D:1258:LEU:N	2.34	0.43
8:F:255:PHE:O	8:F:259:ILE:HG13	2.18	0.43
4:B:162:ILE:HG23	6:D:607:PRO:HG2	2.00	0.42
5:C:177:TYR:CE1	5:C:366:ASN:HB3	2.54	0.42
5:C:826:THR:O	5:C:826:THR:HG23	2.19	0.42
6:D:278:ARG:O	6:D:281:ILE:HG22	2.19	0.42
6:D:665:THR:HG22	6:D:684:ASN:OD1	2.19	0.42
7:E:31:GLY:O	7:E:33:THR:HG22	2.19	0.42
5:C:261:THR:O	5:C:265:LEU:HD23	2.19	0.42
5:C:714:ILE:HG22	5:C:910:THR:CG2	2.45	0.42
5:C:950:LEU:CB	5:C:951:PRO:CD	2.96	0.42
6:D:320:ILE:HG12	6:D:321:PRO:HD2	2.00	0.42
6:D:980:ARG:HD3	6:D:985:GLY:HA2	2.01	0.42
8:F:167:ARG:O	8:F:170:LEU:N	2.51	0.42
8:F:328:LEU:HD23	8:F:330:ARG:NH2	2.33	0.42
5:C:574:PRO:O	5:C:575:ARG:CG	2.67	0.42
5:C:776:ASP:CG	5:C:778:ARG:HG3	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:788:ARG:HG2	5:C:789:ASP:N	2.35	0.42
6:D:565:ILE:HG22	6:D:565:ILE:O	2.19	0.42
6:D:737:VAL:HG13	6:D:840:ARG:HD2	2.01	0.42
7:E:57:ARG:NE	7:E:95:GLU:OE1	2.40	0.42
8:F:192:GLU:OE2	9:J:88:ARG:NH2	2.52	0.42
8:F:195:LEU:HD21	9:J:81:HIS:CG	2.54	0.42
8:F:242:VAL:O	8:F:246:LYS:HG3	2.18	0.42
8:F:430:ILE:HB	8:F:441:ILE:HD13	2.00	0.42
4:B:192:LEU:HD12	4:B:193:ILE:N	2.33	0.42
5:C:301:ARG:HD2	5:C:302:VAL:HG23	2.02	0.42
5:C:800:LYS:HD2	5:C:824:ARG:HB2	2.01	0.42
6:D:173:ARG:NH2	6:D:201:GLY:HA2	2.35	0.42
6:D:581:MET:HG2	6:D:716:LYS:HA	2.00	0.42
7:E:31:GLY:O	7:E:32:ILE:HG22	2.19	0.42
4:A:100:GLN:CG	4:A:101:GLY:N	2.83	0.42
4:B:25:PRO:HG3	4:B:183:VAL:HG21	2.00	0.42
6:D:262:LYS:O	6:D:266:GLU:HG3	2.19	0.42
6:D:579:LEU:HD23	6:D:579:LEU:HA	1.95	0.42
6:D:735:VAL:HA	6:D:792:TYR:OH	2.19	0.42
5:C:431:MET:HE3	5:C:443:LYS:CE	2.50	0.42
5:C:534:GLN:HG3	5:C:536:ASN:H	1.85	0.42
6:D:171:GLU:O	6:D:175:GLN:HG3	2.19	0.42
6:D:1151:HIS:CE1	6:D:1153:LYS:HE3	2.55	0.42
4:A:59:VAL:HG11	4:A:73:VAL:HG21	2.00	0.42
4:A:107:ALA:O	4:A:110:ILE:HG12	2.19	0.42
5:C:427:LEU:HD22	5:C:427:LEU:H	1.85	0.42
5:C:809:GLU:O	5:C:810:ARG:HB3	2.20	0.42
6:D:237:ASP:OD1	6:D:240:LEU:N	2.46	0.42
6:D:449:LEU:HD22	6:D:449:LEU:O	2.20	0.42
7:E:40:LEU:CB	7:E:50:LEU:HD11	2.47	0.42
8:F:276:THR:HG23	9:J:89:ARG:NH2	2.34	0.42
4:A:146:TYR:CD2	4:A:167:ILE:HG12	2.49	0.42
5:C:562:VAL:HG22	5:C:563:SER:N	2.30	0.42
5:C:715:MET:HE2	5:C:896:PRO:HG3	2.02	0.42
5:C:808:GLU:OE1	5:C:808:GLU:N	2.37	0.42
1:O:14:DG:H1	2:P:36:DC:N4	2.18	0.42
4:A:97:LEU:HD21	4:A:105:VAL:HG11	2.02	0.42
4:B:59:VAL:O	4:B:60:LEU:HD23	2.20	0.42
4:B:97:LEU:HD21	4:B:105:VAL:HG11	2.02	0.42
4:B:223:ARG:O	4:B:223:ARG:HG2	2.20	0.42
5:C:38:PRO:CG	5:C:508:ARG:HD2	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:52:PHE:CE2	5:C:150:MET:HE2	2.55	0.42
5:C:94:MET:HB3	5:C:132:ASN:ND2	2.34	0.42
5:C:412:ARG:N	5:C:413:PRO:HD2	2.35	0.42
6:D:177:LEU:O	6:D:181:LEU:HB2	2.20	0.42
1:O:40:DT:P	5:C:458:ARG:HD3	2.60	0.42
5:C:77:LEU:O	5:C:81:LEU:HD22	2.20	0.42
5:C:288:GLU:O	5:C:293:LYS:N	2.48	0.42
5:C:1039:PRO:C	5:C:1040:TYR:HD1	2.28	0.42
5:C:1043:ILE:H	5:C:1043:ILE:HG13	1.57	0.42
6:D:633:ILE:CD1	6:D:635:VAL:HG22	2.50	0.42
8:F:409:GLU:HB3	8:F:448:THR:CG2	2.50	0.42
4:A:40:ARG:CD	4:B:33:THR:HG22	2.49	0.41
4:B:18:ARG:HA	4:B:196:VAL:O	2.20	0.41
5:C:433:GLN:HG3	5:C:669:SER:OG	2.19	0.41
6:D:394:PRO:O	6:D:397:ARG:HG2	2.20	0.41
1:O:34:DG:C4'	1:O:35:DA:H5'	2.50	0.41
4:B:74:THR:O	4:B:78:LEU:HG	2.19	0.41
5:C:235:THR:HB	5:C:237:GLU:CD	2.45	0.41
5:C:270:ARG:O	5:C:274:PRO:HD3	2.20	0.41
5:C:548:ASP:OD1	5:C:549:ARG:N	2.54	0.41
5:C:577:MET:HE2	6:D:845:VAL:HG13	2.01	0.41
5:C:786:GLU:HG2	5:C:787:VAL:H	1.85	0.41
6:D:1187:PHE:O	6:D:1191:ASN:HB2	2.20	0.41
8:F:254:ALA:HA	10:F:501:SO4:O4	2.20	0.41
1:O:38:DC:O2	1:O:38:DC:H5'	2.20	0.41
4:A:50:ALA:HB3	4:A:168:TYR:CE1	2.55	0.41
5:C:303:GLY:O	5:C:307:VAL:HG22	2.19	0.41
5:C:510:VAL:HG23	5:C:514:VAL:C	2.45	0.41
5:C:761:THR:OG1	5:C:762:ARG:N	2.53	0.41
5:C:1087:THR:HG22	5:C:1090:ARG:HH21	1.85	0.41
6:D:26:GLY:HA3	6:D:51:ILE:CG2	2.49	0.41
6:D:51:ILE:HG13	6:D:52:PHE:N	2.35	0.41
6:D:79:GLY:HA2	9:J:54:TRP:CH2	2.55	0.41
6:D:636:ARG:HG3	6:D:662:THR:HG22	2.02	0.41
6:D:980:ARG:HD3	6:D:985:GLY:C	2.45	0.41
1:O:43:DC:H2''	1:O:44:DG:C8	2.55	0.41
4:A:57:ASP:N	4:A:57:ASP:OD1	2.53	0.41
4:B:98:ARG:HE	4:B:98:ARG:HB3	1.65	0.41
4:B:226:ASN:O	4:B:227:ALA:HB3	2.21	0.41
5:C:228:LEU:HD12	5:C:228:LEU:HA	1.94	0.41
5:C:811:LEU:O	5:C:815:ILE:HG22	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:831:PRO:HD2	5:C:834:GLU:OE2	2.20	0.41
5:C:840:GLY:O	5:C:841:ILE:HD13	2.20	0.41
5:C:998:LYS:NZ	6:D:734:ASP:OD1	2.48	0.41
6:D:250:GLU:H	6:D:250:GLU:HG2	1.66	0.41
4:A:46:ILE:HA	4:A:47:PRO:HD3	1.91	0.41
5:C:477:ILE:HD12	5:C:477:ILE:N	2.34	0.41
6:D:726:SER:HB3	6:D:728:VAL:HG12	2.02	0.41
6:D:989:ASP:OD2	7:E:47:LYS:HE2	2.21	0.41
1:O:31:DT:O3'	8:F:239:ARG:HD2	2.19	0.41
4:A:26:LEU:HD21	4:B:218:LEU:HD21	2.02	0.41
5:C:24:PRO:HG3	5:C:689:ALA:O	2.21	0.41
5:C:237:GLU:OE1	5:C:237:GLU:N	2.37	0.41
5:C:919:ILE:O	5:C:919:ILE:HG13	2.21	0.41
6:D:367:VAL:HG12	6:D:371:LYS:HE3	2.03	0.41
6:D:541:MET:HE2	6:D:541:MET:HB3	1.98	0.41
6:D:822:LEU:HD23	6:D:831:ILE:O	2.20	0.41
6:D:886:ARG:HD2	6:D:886:ARG:HA	1.54	0.41
6:D:1056:LEU:HD11	6:D:1063:PHE:HE1	1.86	0.41
6:D:1126:GLN:OE1	6:D:1130:GLU:HG2	2.20	0.41
8:F:317:LEU:HG	8:F:341:MET:SD	2.61	0.41
9:J:102:LEU:O	9:J:105:ILE:HG23	2.19	0.41
1:O:17:DA:H1'	1:O:18:DA:H5'	2.01	0.41
4:A:52:THR:HA	4:A:166:SER:OG	2.21	0.41
4:B:144:ARG:HH11	4:B:144:ARG:HB2	1.86	0.41
5:C:205:PHE:CE1	5:C:215:VAL:HG13	2.56	0.41
5:C:387:MET:O	5:C:391:VAL:HG23	2.20	0.41
5:C:434:ASN:O	5:C:608:PRO:HD3	2.20	0.41
5:C:753:THR:HG23	5:C:756:GLY:C	2.45	0.41
6:D:17:ALA:HB1	6:D:21:ARG:NH1	2.36	0.41
6:D:52:PHE:CD2	6:D:322:PRO:HD3	2.55	0.41
8:F:291:GLN:HG3	8:F:292:ALA:N	2.35	0.41
1:O:12:DG:N2	2:P:39:DT:O2	2.54	0.41
4:B:105:VAL:HG12	4:B:125:ILE:HG21	2.01	0.41
5:C:524:ALA:O	5:C:527:GLU:N	2.52	0.41
5:C:722:TYR:O	6:D:536:PHE:HD1	2.04	0.41
5:C:907:ILE:HD12	5:C:907:ILE:N	2.35	0.41
5:C:935:TRP:HB3	5:C:982:SER:HB2	2.03	0.41
5:C:947:ALA:O	5:C:950:LEU:CB	2.69	0.41
5:C:1040:TYR:CE2	5:C:1090:ARG:NH1	2.88	0.41
6:D:666:THR:HG23	6:D:669:ARG:CD	2.49	0.41
8:F:200:LYS:O	8:F:204:LEU:HD23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:3:DA:H2"	2:P:4:DT:C7	2.50	0.41
4:A:83:LEU:HG	4:A:123:MET:HE1	2.03	0.41
4:A:110:ILE:HG12	4:A:110:ILE:H	1.58	0.41
4:A:146:TYR:CD2	5:C:734:GLU:HG2	2.55	0.41
4:B:24:GLU:HA	4:B:25:PRO:HA	1.75	0.41
4:B:56:ILE:HA	4:B:136:VAL:HA	2.03	0.41
4:B:146:TYR:O	6:D:624:ARG:HD3	2.21	0.41
4:B:161:ARG:HA	4:B:161:ARG:HD3	1.65	0.41
5:C:479:THR:HG22	5:C:597:LEU:HD12	2.03	0.41
5:C:723:GLU:O	6:D:536:PHE:HB2	2.21	0.41
6:D:129:ILE:HG13	6:D:130:TYR:CD2	2.56	0.41
6:D:339:ASP:OD2	6:D:397:ARG:NH2	2.53	0.41
6:D:791:PHE:HD1	6:D:791:PHE:O	2.04	0.41
6:D:1160:ARG:O	6:D:1164:ARG:HG3	2.20	0.41
7:E:84:LEU:H	7:E:84:LEU:CD1	2.29	0.41
8:F:178:LEU:HG	8:F:239:ARG:NH2	2.36	0.41
8:F:199:GLN:HG2	9:J:82:TRP:CE2	2.56	0.41
8:F:411:GLY:O	8:F:415:LEU:HG	2.21	0.41
1:O:40:DT:OP2	5:C:458:ARG:HD3	2.21	0.41
4:A:72:ASP:O	4:A:76:ILE:HG13	2.21	0.41
4:A:104:VAL:HG13	4:A:127:THR:HG22	2.03	0.41
5:C:763:ASP:O	5:C:764:ILE:C	2.63	0.41
5:C:938:ASP:C	5:C:940:ALA:H	2.29	0.41
6:D:479:GLN:O	6:D:480:ARG:C	2.64	0.41
6:D:745:LEU:O	6:D:749:GLU:HB3	2.21	0.41
6:D:990:ILE:O	6:D:990:ILE:HG22	2.21	0.41
6:D:1168:ILE:HD13	6:D:1176:PHE:HB3	2.03	0.41
6:D:1274:GLN:O	7:E:102:GLU:HG2	2.21	0.41
4:A:11:GLU:HB2	4:A:21:PHE:CE2	2.56	0.40
5:C:154:LYS:HD2	5:C:630:GLY:HA3	2.03	0.40
5:C:193:VAL:HG23	5:C:336:LEU:HG	2.03	0.40
5:C:335:TYR:OH	5:C:356:VAL:HA	2.21	0.40
5:C:403:ILE:HG13	5:C:404:THR:H	1.85	0.40
5:C:951:PRO:O	5:C:951:PRO:HG2	2.21	0.40
5:C:638:THR:HG23	5:C:688:GLU:HA	2.03	0.40
5:C:935:TRP:HA	5:C:982:SER:HB2	2.03	0.40
5:C:1100:GLY:CA	6:D:458:LYS:HE3	2.51	0.40
5:C:1122:LEU:O	5:C:1123:CYS:HB2	2.21	0.40
8:F:293:ILE:O	8:F:297:MET:HG3	2.21	0.40
1:O:44:DG:H2"	1:O:45:DG:C8	2.56	0.40
5:C:431:MET:HE3	5:C:443:LYS:HE3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:D:890:CYS:SG	6:D:892:THR:HG22	2.61	0.40
1:O:43:DC:H2''	1:O:44:DG:H8	1.85	0.40
2:P:32:DT:H2''	2:P:33:DT:OP2	2.18	0.40
4:A:14:VAL:CG1	4:A:18:ARG:HG3	2.51	0.40
4:B:147:VAL:O	4:B:147:VAL:HG22	2.21	0.40
5:C:348:VAL:CG1	5:C:349:PRO:HD2	2.50	0.40
6:D:240:LEU:HD23	6:D:240:LEU:C	2.46	0.40
6:D:596:THR:HG22	6:D:626:ALA:O	2.22	0.40
2:P:8:DT:H4'	6:D:1229:GLU:HG3	2.04	0.40
5:C:35:LEU:N	5:C:35:LEU:HD12	2.37	0.40
5:C:632:VAL:HG22	5:C:694:ALA:O	2.21	0.40
6:D:517:VAL:HG12	6:D:518:GLU:O	2.21	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)
5:C:782:ARG:NH1	6:D:171:GLU:OE2[2_356]	1.98	0.22

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	
4	A	218/350 (62%)	203 (93%)	13 (6%)	2 (1%)	14	47
4	B	231/350 (66%)	217 (94%)	13 (6%)	1 (0%)	30	62
5	C	1109/1169 (95%)	1031 (93%)	66 (6%)	12 (1%)	11	43
6	D	1224/1317 (93%)	1165 (95%)	53 (4%)	6 (0%)	24	59
7	E	72/107 (67%)	64 (89%)	5 (7%)	3 (4%)	2	16
8	F	310/466 (66%)	303 (98%)	5 (2%)	2 (1%)	21	56
9	J	84/114 (74%)	81 (96%)	3 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	3248/3873 (84%)	3064 (94%)	158 (5%)	26 (1%)	16	50

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	C	57	GLY
5	C	274	PRO
5	C	939	VAL
6	D	104	ILE
6	D	802	VAL
7	E	32	ILE
7	E	77	GLY
8	F	162	SER
4	A	49	ALA
5	C	248	ILE
5	C	544	ARG
6	D	969	SER
4	B	65	THR
7	E	76	VAL
5	C	202	TRP
5	C	810	ARG
5	C	967	VAL
5	C	987	ARG
6	D	1192	ARG
8	F	419	LEU
5	C	276	GLU
4	A	183	VAL
5	C	273	ARG
5	C	404	THR
6	D	1108	VAL
6	D	935	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	
4	A	174/297 (59%)	151 (87%)	23 (13%)	4	19
4	B	170/297 (57%)	138 (81%)	32 (19%)	1	9
5	C	812/984 (82%)	709 (87%)	103 (13%)	4	20
6	D	953/1096 (87%)	851 (89%)	102 (11%)	6	27
7	E	62/86 (72%)	55 (89%)	7 (11%)	5	24
8	F	255/379 (67%)	229 (90%)	26 (10%)	7	29
9	J	65/98 (66%)	56 (86%)	9 (14%)	3	18
All	All	2491/3237 (77%)	2189 (88%)	302 (12%)	5	22

All (302) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	2	LEU
4	A	6	ARG
4	A	9	LEU
4	A	11	GLU
4	A	14	VAL
4	A	24	GLU
4	A	51	VAL
4	A	60	LEU
4	A	62	GLU
4	A	69	VAL
4	A	72	ASP
4	A	110	ILE
4	A	111	VAL
4	A	116	VAL
4	A	117	THR
4	A	128	LEU
4	A	130	ASP
4	A	138	LEU
4	A	150	VAL
4	A	152	ASN
4	A	171	VAL
4	A	193	ILE
4	A	215	LEU
4	B	3	ILE
4	B	17	ASN
4	B	38	LEU
4	B	66	VAL
4	B	76	ILE
4	B	78	LEU

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Mol	Chain	Res	Type
4	B	83	LEU
4	B	85	VAL
4	B	88	ASP
4	B	89	ASP
4	B	93	VAL
4	B	99	LYS
4	B	106	THR
4	B	110	ILE
4	B	116	VAL
4	B	123	MET
4	B	125	ILE
4	B	136	VAL
4	B	141	GLU
4	B	144	ARG
4	B	147	VAL
4	B	161	ARG
4	B	176	TYR
4	B	189	PHE
4	B	192	LEU
4	B	196	VAL
4	B	200	ASN
4	B	202	ILE
4	B	218	LEU
4	B	221	LEU
4	B	223	ARG
4	B	228	ASP
5	C	30	VAL
5	C	34	LYS
5	C	46	ASP
5	C	56	VAL
5	C	61	TRP
5	C	66	ILE
5	C	81	LEU
5	C	96	LEU
5	C	105	GLU
5	C	106	VAL
5	C	110	VAL
5	C	119	THR
5	C	124	LEU
5	C	126	VAL
5	C	129	GLU
5	C	133	ASN

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Mol	Chain	Res	Type
5	C	141	GLN
5	C	150	MET
5	C	154	LYS
5	C	235	THR
5	C	236	ASN
5	C	313	LEU
5	C	325	THR
5	C	336	LEU
5	C	338	ARG
5	C	340	HIS
5	C	357	GLU
5	C	358	VAL
5	C	361	ILE
5	C	364	PHE
5	C	372	VAL
5	C	379	GLN
5	C	397	THR
5	C	410	ASN
5	C	428	SER
5	C	437	LEU
5	C	441	THR
5	C	449	LEU
5	C	458	ARG
5	C	463	VAL
5	C	466	VAL
5	C	481	GLU
5	C	505	THR
5	C	522	LEU
5	C	523	THR
5	C	525	ASP
5	C	531	VAL
5	C	545	PHE
5	C	550	VAL
5	C	552	VAL
5	C	568	ASP
5	C	575	ARG
5	C	578	VAL
5	C	597	LEU
5	C	611	ARG
5	C	616	LEU
5	C	617	VAL
5	C	623	LEU

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Mol	Chain	Res	Type
5	C	636	ASP
5	C	640	VAL
5	C	658	ARG
5	C	664	ARG
5	C	674	CYS
5	C	699	THR
5	C	701	ASN
5	C	737	VAL
5	C	753	THR
5	C	767	VAL
5	C	777	GLU
5	C	778	ARG
5	C	787	VAL
5	C	797	VAL
5	C	803	THR
5	C	804	GLU
5	C	809	GLU
5	C	815	ILE
5	C	830	VAL
5	C	839	ILE
5	C	848	ASP
5	C	890	LEU
5	C	917	MET
5	C	927	LEU
5	C	946	TRP
5	C	952	GLU
5	C	965	THR
5	C	973	GLU
5	C	980	LEU
5	C	983	THR
5	C	988	ASP
5	C	991	VAL
5	C	1014	VAL
5	C	1021	ILE
5	C	1043	ILE
5	C	1045	GLN
5	C	1048	LEU
5	C	1092	LYS
5	C	1108	ILE
5	C	1114	VAL
5	C	1128	VAL
5	C	1129	LEU

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Mol	Chain	Res	Type
5	C	1138	MET
5	C	1139	ARG
5	C	1140	ASP
6	D	7	PHE
6	D	9	GLU
6	D	10	LEU
6	D	40	LYS
6	D	49	GLU
6	D	64	LYS
6	D	70	PHE
6	D	104	ILE
6	D	105	TRP
6	D	120	LEU
6	D	144	ARG
6	D	165	GLN
6	D	177	LEU
6	D	195	ARG
6	D	208	LEU
6	D	211	ARG
6	D	236	VAL
6	D	239	VAL
6	D	243	GLU
6	D	245	GLN
6	D	250	GLU
6	D	256	MET
6	D	267	ASN
6	D	270	ILE
6	D	298	VAL
6	D	314	LEU
6	D	330	LEU
6	D	348	ILE
6	D	356	ARG
6	D	372	ARG
6	D	392	THR
6	D	397	ARG
6	D	406	LEU
6	D	417	LEU
6	D	429	VAL
6	D	449	LEU
6	D	456	VAL
6	D	458	LYS
6	D	467	GLN

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Mol	Chain	Res	Type
6	D	479	GLN
6	D	483	VAL
6	D	488	GLU
6	D	490	VAL
6	D	491	ILE
6	D	504	LEU
6	D	505	HIS
6	D	507	LEU
6	D	518	GLU
6	D	581	MET
6	D	599	TYR
6	D	600	GLN
6	D	627	LEU
6	D	629	VAL
6	D	633	ILE
6	D	635	VAL
6	D	638	THR
6	D	664	GLU
6	D	666	THR
6	D	667	LEU
6	D	675	LEU
6	D	687	MET
6	D	701	GLU
6	D	713	ASP
6	D	724	THR
6	D	736	LEU
6	D	737	VAL
6	D	781	THR
6	D	796	ASN
6	D	819	MET
6	D	822	LEU
6	D	850	ILE
6	D	864	LEU
6	D	868	ASP
6	D	886	ARG
6	D	894	ARG
6	D	900	LEU
6	D	923	THR
6	D	938	GLU
6	D	941	HIS
6	D	956	ILE
6	D	961	VAL

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Mol	Chain	Res	Type
6	D	962	ARG
6	D	964	VAL
6	D	984	THR
6	D	994	VAL
6	D	996	ILE
6	D	1009	LEU
6	D	1055	ARG
6	D	1089	VAL
6	D	1114	GLU
6	D	1122	VAL
6	D	1131	VAL
6	D	1165	ARG
6	D	1183	GLU
6	D	1207	VAL
6	D	1208	LEU
6	D	1213	LYS
6	D	1229	GLU
6	D	1234	LEU
6	D	1258	LEU
6	D	1263	THR
6	D	1278	GLU
7	E	32	ILE
7	E	34	ASN
7	E	50	LEU
7	E	62	ASN
7	E	85	GLN
7	E	99	ASP
7	E	103	HIS
8	F	166	VAL
8	F	172	GLN
8	F	204	LEU
8	F	211	LEU
8	F	213	VAL
8	F	219	MET
8	F	238	LEU
8	F	239	ARG
8	F	246	LYS
8	F	270	VAL
8	F	291	GLN
8	F	317	LEU
8	F	325	LEU
8	F	331	GLU

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Mol	Chain	Res	Type
8	F	333	THR
8	F	337	LEU
8	F	344	THR
8	F	348	VAL
8	F	349	LEU
8	F	372	GLN
8	F	383	VAL
8	F	386	VAL
8	F	421	ASP
8	F	448	THR
8	F	454	HIS
8	F	465	LEU
9	J	39	GLU
9	J	47	ASP
9	J	49	GLU
9	J	55	LEU
9	J	63	THR
9	J	76	LYS
9	J	79	ARG
9	J	86	LEU
9	J	105	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
4	B	36	ASN
5	C	48	GLN
5	C	132	ASN
5	C	141	GLN
5	C	236	ASN
5	C	534	GLN
5	C	576	GLN
5	C	720	HIS
5	C	921	GLN
6	D	165	GLN
6	D	523	GLN
6	D	564	ASN
6	D	934	ASN
6	D	1000	GLN
7	E	62	ASN
8	F	309	HIS
8	F	372	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	Q	3/4 (75%)	1 (33%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	Q	2	C

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 10 ligands modelled in this entry, 2 are monoatomic - leaving 8 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	SO4	D	2005	-	4,4,4	0.23	0	6,6,6	0.07	0
12	EDO	D	2006	-	3,3,3	0.42	0	2,2,2	0.34	0
10	SO4	D	2004	-	4,4,4	0.23	0	6,6,6	0.07	0
10	SO4	F	502	-	4,4,4	0.24	0	6,6,6	0.06	0
12	EDO	F	503	-	3,3,3	0.42	0	2,2,2	0.35	0
10	SO4	D	2003	-	4,4,4	0.23	0	6,6,6	0.08	0
10	SO4	F	501	-	4,4,4	0.24	0	6,6,6	0.06	0
10	SO4	C	1201	-	4,4,4	0.24	0	6,6,6	0.08	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
12	EDO	F	503	-	-	0/1/1/1	-
12	EDO	D	2006	-	-	0/1/1/1	-

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.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	D	2006	EDO	3	0
10	D	2004	SO4	1	0
10	F	502	SO4	2	0
10	F	501	SO4	1	0
10	C	1201	SO4	2	0

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	O	49/50 (98%)	-0.27	0	100	100	53, 109, 179, 196	0
2	P	44/50 (88%)	-0.13	0	100	100	75, 107, 177, 193	0
3	Q	4/4 (100%)	0.16	0	100	100	119, 123, 126, 143	0
4	A	220/350 (62%)	0.16	5 (2%)	61	41	56, 91, 125, 159	0
4	B	233/350 (66%)	0.27	2 (0%)	81	64	78, 111, 137, 145	0
5	C	1113/1169 (95%)	0.17	16 (1%)	73	54	33, 84, 146, 168	0
6	D	1238/1317 (94%)	0.05	13 (1%)	78	61	32, 76, 123, 152	0
7	E	76/107 (71%)	0.17	0	100	100	55, 86, 121, 132	0
8	F	314/466 (67%)	-0.00	3 (0%)	79	63	37, 80, 132, 154	0
9	J	86/114 (75%)	-0.01	2 (2%)	61	41	58, 101, 138, 169	0
All	All	3377/3977 (84%)	0.10	41 (1%)	76	58	32, 85, 138, 196	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	C	228	LEU	4.8
4	A	37	SER	4.1
6	D	609	GLN	3.8
8	F	365	ILE	2.9
4	A	187	THR	2.9
9	J	26	PRO	2.8
4	A	26	LEU	2.8
6	D	991	GLY	2.7
8	F	337	LEU	2.6
6	D	5	ASN	2.6
5	C	979	LEU	2.6
4	A	41	THR	2.6
5	C	951	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
5	C	552	VAL	2.5
5	C	536	ASN	2.5
6	D	866	THR	2.4
5	C	225	VAL	2.4
5	C	455	SER	2.4
5	C	278	PRO	2.4
5	C	559	VAL	2.3
5	C	405	PRO	2.3
5	C	401	GLU	2.2
6	D	722	TRP	2.2
8	F	238	LEU	2.2
6	D	759	TYR	2.2
4	A	180	ALA	2.2
4	B	231	HIS	2.2
5	C	402	ALA	2.1
6	D	832	PRO	2.1
5	C	1019	MET	2.1
6	D	234	LEU	2.1
6	D	587	TYR	2.1
6	D	619	ILE	2.1
5	C	661	TYR	2.1
6	D	720	PHE	2.1
5	C	330	VAL	2.1
6	D	607	PRO	2.1
6	D	623	ASP	2.0
9	J	67	GLY	2.0
5	C	269	TYR	2.0
4	B	134	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 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
10	SO4	C	1201	5/5	0.53	0.13	120,128,134,230	0
12	EDO	F	503	4/4	0.68	0.14	76,91,105,111	0
12	EDO	D	2006	4/4	0.73	0.22	68,85,104,104	0
10	SO4	D	2003	5/5	0.78	0.12	91,97,128,130	0
10	SO4	F	501	5/5	0.83	0.10	72,80,89,163	0
10	SO4	F	502	5/5	0.88	0.09	73,78,115,167	0
10	SO4	D	2004	5/5	0.89	0.08	83,90,99,120	0
10	SO4	D	2005	5/5	0.95	0.08	85,92,116,121	0
11	ZN	D	2001	1/1	0.99	0.09	116,116,116,116	0
11	ZN	D	2002	1/1	0.99	0.04	100,100,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.