



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 01:54 AM EDT

PDB ID : 1RZR / pdb_00001rzs
Title : crystal structure of transcriptional regulator-phosphoprotein-DNA complex
Authors : Schumacher, M.A.; Allen, G.S.; Brennan, R.G.
Deposited on : 2003-12-27
Resolution : 2.80 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

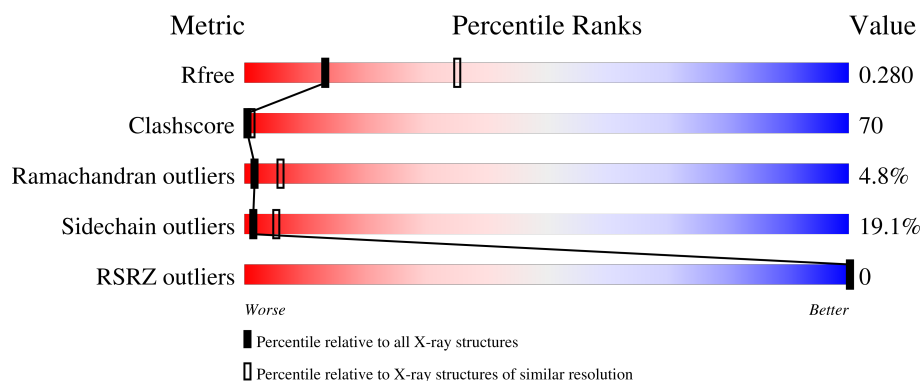
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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.



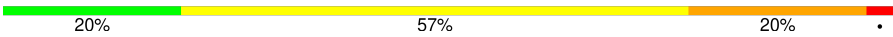
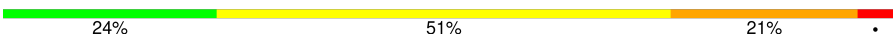
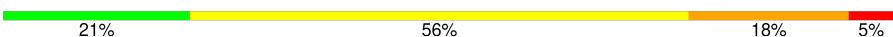
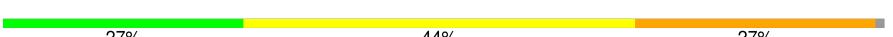
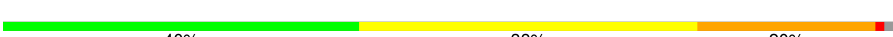
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	E	16	88%12%
1	H	16	94%6%
2	B	16	75%19%6%
2	R	16	6% 75%12%6%
3	A	332	19% 58%20%.

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Mol	Chain	Length	Quality of chain
3	C	332	 20% 57% 20% .
3	G	332	 24% 51% 21% .
4	D	332	 21% 56% 18% 5%
5	L	88	 27% 55% 17% .
5	S	88	 28% 55% 14% ..
5	T	88	 27% 44% 27% .
5	Y	88	 40% 38% 20% ..

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
5	SEP	Y	46	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 14194 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 DNA chain called 5'-D(*CP*TP*GP*AP*AP*AP*GP*CP*GP*CP*TP*AP*AP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	16	Total	C	N	O	P	0	0	0
			327	156	66	90	15			
1	E	16	Total	C	N	O	P	0	0	0
			327	156	66	90	15			

- Molecule 2 is a DNA chain called 5'-D(*CP*TP*GP*TP*TP*AP*GP*CP*GP*CP*TP*TP*TP*CP*AP*G)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	16	Total	C	N	O	P	0	0	0
			323	156	54	98	15			
2	B	16	Total	C	N	O	P	0	0	0
			323	156	54	98	15			

- Molecule 3 is a protein called Glucose-resistance amylase regulator.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	332	Total	C	N	O	Se	0	0	0
			2564	1610	438	506	10			
3	C	332	Total	C	N	O	Se	0	0	0
			2558	1606	437	505	10			
3	A	332	Total	C	N	O	Se	0	0	0
			2562	1608	437	507	10			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	modified residue	UNP P46828
A	16	MSE	MET	modified residue	UNP P46828
A	88	MSE	MET	modified residue	UNP P46828
A	112	MSE	MET	modified residue	UNP P46828

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Chain	Residue	Modelled	Actual	Comment	Reference
A	123	MSE	MET	modified residue	UNP P46828
A	250	MSE	MET	modified residue	UNP P46828
A	282	MSE	MET	modified residue	UNP P46828
A	294	MSE	MET	modified residue	UNP P46828
A	302	MSE	MET	modified residue	UNP P46828
A	309	MSE	MET	modified residue	UNP P46828
C	1	MSE	MET	modified residue	UNP P46828
C	16	MSE	MET	modified residue	UNP P46828
C	88	MSE	MET	modified residue	UNP P46828
C	112	MSE	MET	modified residue	UNP P46828
C	123	MSE	MET	modified residue	UNP P46828
C	250	MSE	MET	modified residue	UNP P46828
C	282	MSE	MET	modified residue	UNP P46828
C	294	MSE	MET	modified residue	UNP P46828
C	302	MSE	MET	modified residue	UNP P46828
C	309	MSE	MET	modified residue	UNP P46828
G	1	MSE	MET	modified residue	UNP P46828
G	16	MSE	MET	modified residue	UNP P46828
G	88	MSE	MET	modified residue	UNP P46828
G	112	MSE	MET	modified residue	UNP P46828
G	123	MSE	MET	modified residue	UNP P46828
G	250	MSE	MET	modified residue	UNP P46828
G	282	MSE	MET	modified residue	UNP P46828
G	294	MSE	MET	modified residue	UNP P46828
G	302	MSE	MET	modified residue	UNP P46828
G	309	MSE	MET	modified residue	UNP P46828

- Molecule 4 is a protein called Glucose-resistance amylase regulator.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	332	Total	C	N	O	S	Se	0	0	0
			2558	1606	437	505	1	9			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	16	MSE	MET	modified residue	UNP P46828
D	88	MSE	MET	modified residue	UNP P46828
D	112	MSE	MET	modified residue	UNP P46828
D	123	MSE	MET	modified residue	UNP P46828
D	250	MSE	MET	modified residue	UNP P46828
D	282	MSE	MET	modified residue	UNP P46828

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Chain	Residue	Modelled	Actual	Comment	Reference
D	294	MSE	MET	modified residue	UNP P46828
D	302	MSE	MET	modified residue	UNP P46828
D	309	MSE	MET	modified residue	UNP P46828

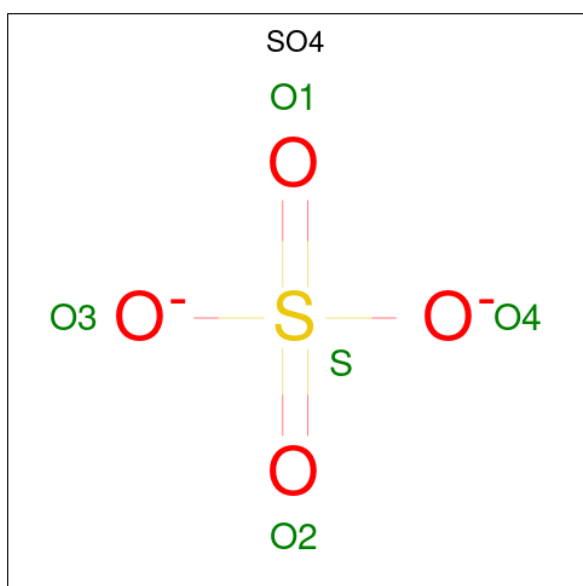
- Molecule 5 is a protein called Phosphocarrier protein HPr.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	T	87	Total	C	N	O	P	S	0	0	0
			632	386	104	138	1	3			
5	L	87	Total	C	N	O	P	S	0	0	0
			632	386	104	138	1	3			
5	Y	87	Total	C	N	O	P	S	0	0	0
			632	386	104	138	1	3			
5	S	87	Total	C	N	O	P	S	0	0	0
			632	386	104	138	1	3			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	46	SEP	SER	modified residue	UNP O69250
T	46	SEP	SER	modified residue	UNP O69250
L	46	SEP	SER	modified residue	UNP O69250
Y	46	SEP	SER	modified residue	UNP O69250

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total O S 5 4 1	0	0
6	G	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	C	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0
6	A	1	Total O S 5 4 1	0	0

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Mg 1 1	0	0
7	D	1	Total Mg 1 1	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	1	Total O 1 1	0	0
8	R	1	Total O 1 1	0	0
8	E	2	Total O 2 2	0	0
8	B	1	Total O 1 1	0	0
8	G	10	Total O 10 10	0	0
8	C	13	Total O 13 13	0	0
8	A	17	Total O 17 17	0	0
8	D	12	Total O 12 12	0	0
8	T	9	Total O 9 9	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	L	4	Total 4	O 4	0	0
8	Y	10	Total 10	O 10	0	0
8	S	7	Total 7	O 7	0	0

● Molecule 1: 5'-D(*CP*TP*GP*AP*AP*AP*GP*CP*GP*CP*TP*AP*AP*CP*AP*G)-3'

C700	T701	G702	A703	A704	A705	G706	C707	G708	C709	T710	A711	A712	C713	A714	G715
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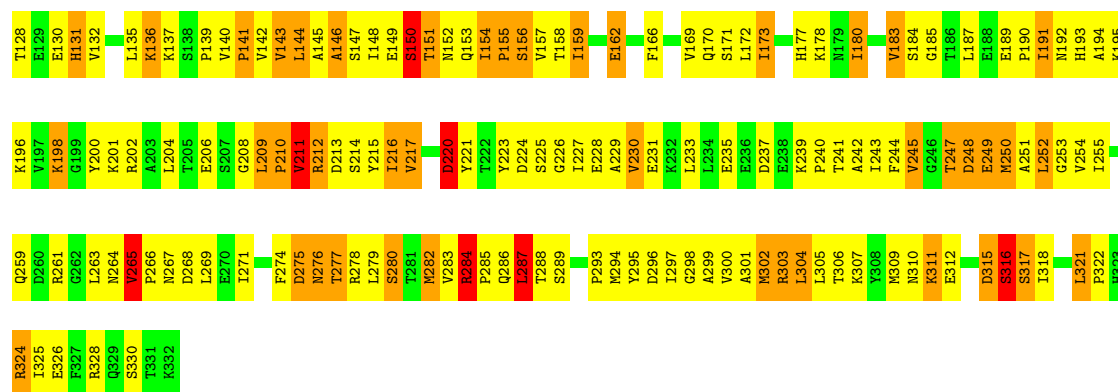
C700	T701	G702	A703	A704	A705	G706	C707	G708	C709	T710	A711	A712	C713	A714	G715
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C700	T701	G702	T703	T704	A705	G706	C707	G708	C709	T710	T711	T712	C713	A714	G715
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C700	T701	G702	T703	T704	A705	G706	C707	G708	C709	T710	T711	T712	C713	A714	G715
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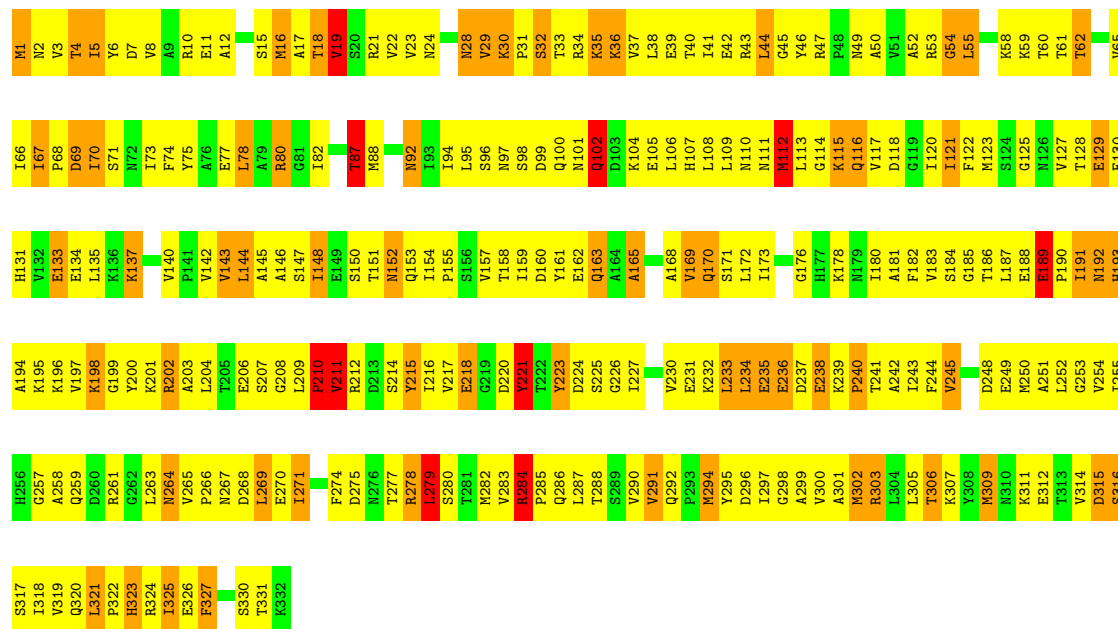
K1	K2	K3	K4	K5	K6	K7	K8	K9	K10	K11	K12	K13	K14	K15	K16	K17	K18	K19	K20	K21	K22	K23	K24	K25	K26	K27	K28	K29	K30	K31	K32	K33	K34	K35	K36	K37	K38	K39	K40	K41	K42	K43	K44	K45	K46	K47	K48	K49	K50	K51	K52	K53	K54	K55	K56	K57	K58	K59	K60	K61	K62	K63	K64	K65	K66	K67	K68	K69	K70	K71	K72	K73	K74	K75	K76	K77	K78	K79	K80	K81	K82	K83	K84	K85	K86	K87	K88	K89	K90	K91	K92	K93	K94	K95	K96	K97	K98	K99	K100	K101	K102	K103	K104	K105	K106	K107	K108	K109	K110	K111	K112	K113	K114	K115	K116	K117	K118	K119	K120	K121	K122	K123	K124	K125	K126	K127	K128	K129	K130	K131	K132	K133	K134	K135	K136	K137	K138	K139	K140	K141	K142	K143	K144	K145	K146	K147	K148	K149	K150	K151	K152	K153	K154	K155	K156	K157	K158	K159	K160	K161	K162	K163	K164	K165	K166	K167	K168	K169	K170	K171	K172	K173	K174	K175	K176	K177	K178	K179	K180	K181	K182	K183	K184	K185	K186	K187	K188	K189	K190	K191	K192	K193	K194	K195	K196	K197	K198	K199	K200	K201	K202	K203	K204	K205	K206	K207	K208	K209	K210	K211	K212	K213	K214	K215	K216	K217	K218	K219	K220	K221	K222	K223	K224	K225	K226	K227	K228	K229	K230	K231	K232	K233	K234	K235	K236	K237	K238	K239	K240	K241	K242	K243	K244	K245	K246	K247	K248	K249	K250	K251	K252	K253	K254	K255	K256	K257	K258	K259	K260	K261	K262	K263	K264	K265	K266	K267	K268	K269	K270	K271	K272	K273	K274	K275	K276	K277	K278	K279	K280	K281	K282	K283	K284	K285	K286	K287	K288	K289	K290	K291	K292	K293	K294	K295	K296	K297	K298	K299	K300	K301	K302	K303	K304	K305	K306	K307	K308	K309	K310	K311	K312	K313	K314	K315	K316	K317	K318	K319	K320	K321	K322	K323	K324	K325	K326	K327	K328	K329	K330	K331	K332	K333	K334	K335	K336	K337	K338	K339	K340	K341	K342	K343	K344	K345	K346	K347	K348	K349	K350	K351	K352	K353	K354	K355	K356	K357	K358	K359	K360	K361	K362	K363	K364	K365	K366	K367	K368	K369	K370	K371	K372	K373	K374	K375	K376	K377	K378	K379	K380	K381	K382	K383	K384	K385	K386	K387	K388	K389	K390	K391	K392	K393	K394	K395	K396	K397	K398	K399	K400	K401	K402	K403	K404	K405	K406	K407	K408	K409	K410	K411	K412	K413	K414	K415	K416	K417	K418	K419	K420	K421	K422	K423	K424	K425	K426	K427	K428	K429	K430	K431	K432	K433	K434	K435	K436	K437	K438	K439	K440	K441	K442	K443	K444	K445	K446	K447	K448	K449	K450	K451	K452	K453	K454	K455	K456	K457	K458	K459	K460	K461	K462	K463	K464	K465	K466	K467	K468	K469	K470	K471	K472	K473	K474	K475	K476	K477	K478	K479	K480	K481	K482	K483	K484	K485	K486	K487	K488	K489	K490	K491	K492	K493	K494	K495	K496	K497	K498	K499	K500	K501	K502	K503	K504	K505	K506	K507	K508	K509	K510	K511	K512	K513	K514	K515	K516	K517	K518	K519	K520	K521	K522	K523	K524	K5
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I66	I67	I68	D69	I70	S71	I72	I73	F74	F75	E76	I77	I78	A79	R80	G81	I82	E83	D84	I85	T86	M87	M88	Y89	K90	Y91	N92	I93	I94	L95	S96	N97	S98	D99	I100	X101	Q102	D103	K104	E105	E106	I107	L108	L109	N110	N111	M112	L113	G114	K115	Q116	V117	D118	G119	I120	I121	F122	M123	F124	V127
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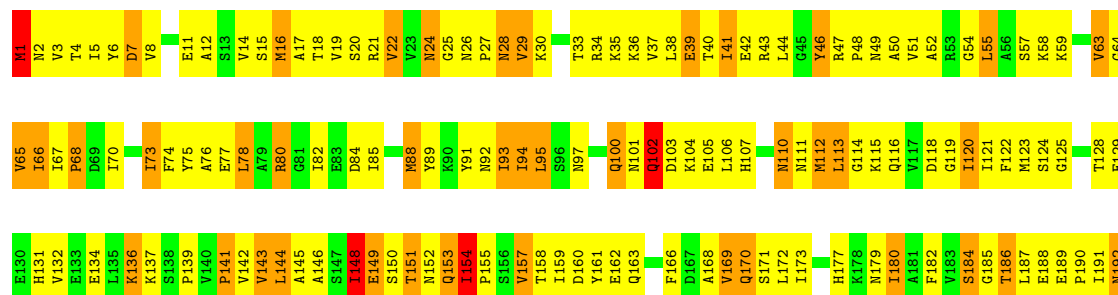
• Molecule 3: Glucose-resistance amylase regulator

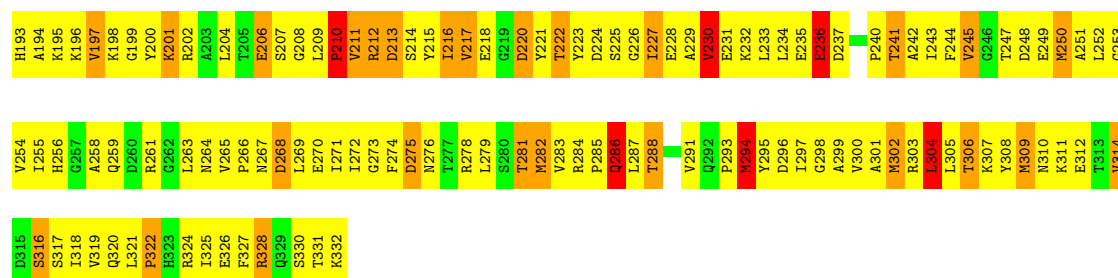
Chain C: 20% 57% 20%



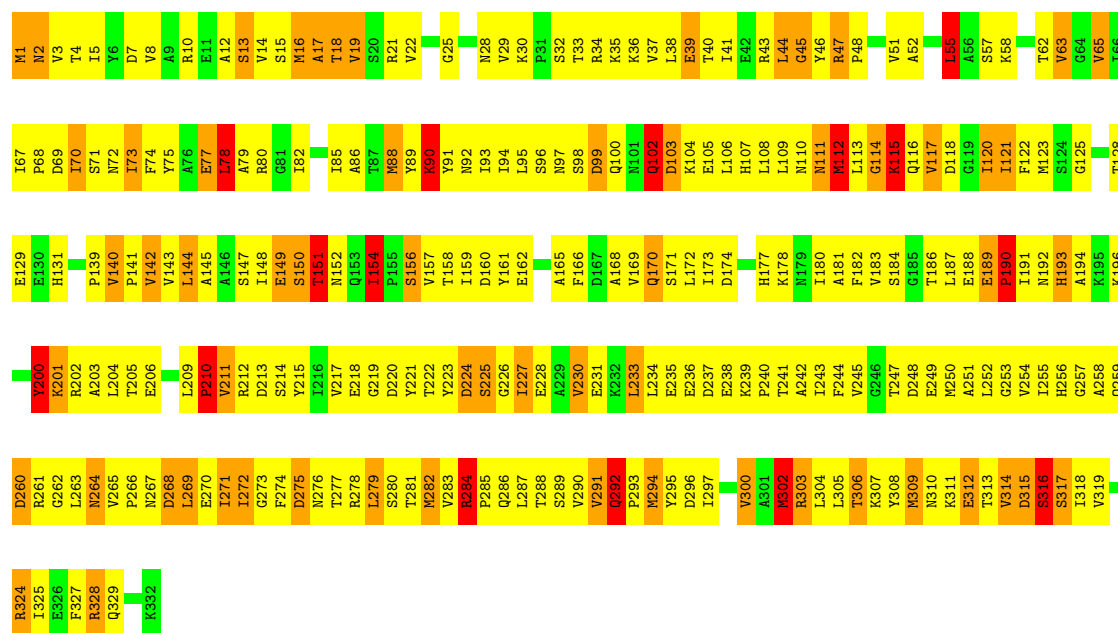
• Molecule 3: Glucose-resistance amylase regulator

Chain A: 19% 58% 20%

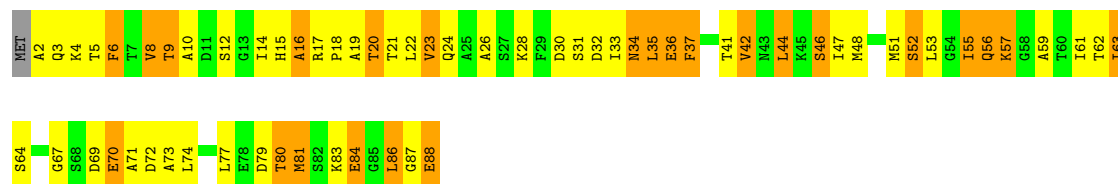




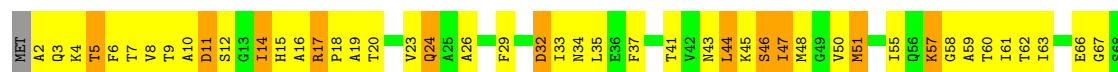
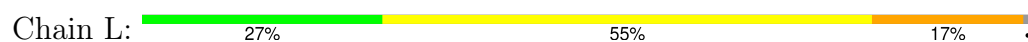
• Molecule 4: Glucose-resistance amylase regulator



• Molecule 5: Phosphocarrier protein HPr



• Molecule 5: Phosphocarrier protein HPr





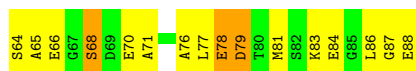
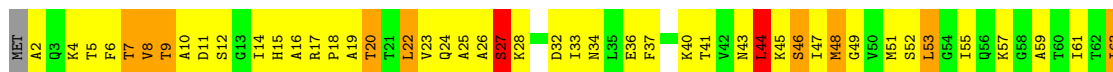
• Molecule 5: Phosphocarrier protein HPr

Chain Y: 40% 38% 20% ..



• Molecule 5: Phosphocarrier protein HPr

Chain S: 28% 55% 14% ..



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.71Å 109.24Å 117.81Å 90.00° 90.05° 90.00°	Depositor
Resolution (Å)	78.70 – 2.80 78.70 – 2.80	Depositor EDS
% Data completeness (in resolution range)	86.8 (78.70-2.80) 86.7 (78.70-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.82Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.242 , 0.288 0.234 , 0.280	Depositor DCC
R_{free} test set	5845 reflections (10.17%)	wwPDB-VP
Wilson B-factor (Å ²)	81.1	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 107.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.037 for -k,-h,-l 0.038 for k,h,-l 0.349 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14194	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.32% 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: SEP, SO4, 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	E	0.44	0/368	0.86	0/566
1	H	0.50	0/368	0.86	0/566
2	B	0.41	0/360	0.97	1/554 (0.2%)
2	R	0.42	0/360	1.08	2/554 (0.4%)
3	A	1.00	13/2590 (0.5%)	1.29	26/3492 (0.7%)
3	C	0.87	6/2586 (0.2%)	1.28	35/3486 (1.0%)
3	G	0.96	10/2593 (0.4%)	1.40	42/3498 (1.2%)
4	D	0.88	11/2586 (0.4%)	1.30	46/3486 (1.3%)
5	L	0.68	0/625	1.16	4/839 (0.5%)
5	S	0.71	0/625	1.08	4/839 (0.5%)
5	T	0.74	1/625 (0.2%)	1.12	3/839 (0.4%)
5	Y	0.79	3/625 (0.5%)	1.28	2/839 (0.2%)
All	All	0.86	44/14311 (0.3%)	1.25	165/19558 (0.8%)

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
1	E	0	2
1	H	0	1
2	B	0	4
2	R	0	2
4	D	0	1
5	Y	0	1
All	All	0	11

All (44) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1	MSE	SE-CE	22.48	2.62	1.95
4	D	1	MET	SD-CE	14.43	2.15	1.79
3	A	302	MSE	SE-CE	-10.82	1.62	1.95
3	G	302	MSE	SE-CE	-9.41	1.67	1.95
3	C	1	MSE	SE-CE	8.33	2.20	1.95
5	Y	7	THR	C-N	-8.18	1.23	1.33
4	D	112	MSE	SE-CE	-8.08	1.71	1.95
3	G	123	MSE	SE-CE	-7.71	1.72	1.95
3	A	309	MSE	SE-CE	-7.46	1.73	1.95
4	D	302	MSE	SE-CE	-7.15	1.74	1.95
3	G	2	ASN	CG-OD1	6.75	1.36	1.23
3	C	302	MSE	SE-CE	-6.75	1.75	1.95
3	G	2	ASN	C-O	6.67	1.32	1.24
3	A	88	MSE	SE-CE	-6.17	1.76	1.95
3	A	112	MSE	SE-CE	-6.10	1.77	1.95
3	G	16	MSE	SE-CE	-5.97	1.77	1.95
3	A	129	GLU	CD-OE1	5.86	1.36	1.25
3	A	250	MSE	SE-CE	-5.81	1.78	1.95
4	D	129	GLU	CD-OE1	5.72	1.36	1.25
3	A	112	MSE	CG-SE	-5.70	1.78	1.95
3	G	2	ASN	CB-CG	-5.70	1.37	1.52
4	D	309	MSE	SE-CE	-5.63	1.78	1.95
3	A	16	MSE	SE-CE	-5.52	1.78	1.95
4	D	282	MSE	CG-SE	-5.51	1.78	1.95
4	D	88	MSE	SE-CE	-5.46	1.79	1.95
3	A	2	ASN	CG-ND2	5.44	1.44	1.33
4	D	302	MSE	CG-SE	-5.43	1.79	1.95
3	G	88	MSE	SE-CE	-5.39	1.79	1.95
3	C	129	GLU	CD-OE1	5.30	1.35	1.25
5	Y	6	PHE	C-N	-5.28	1.25	1.33
3	A	286	GLN	CB-CG	5.26	1.68	1.52
3	C	309	MSE	SE-CE	-5.26	1.79	1.95
3	C	129	GLU	CD-OE2	5.22	1.35	1.25
3	C	1	MSE	CG-SE	-5.22	1.79	1.95
4	D	309	MSE	CG-SE	-5.18	1.79	1.95
3	G	1	MSE	C-N	5.17	1.41	1.33
4	D	282	MSE	SE-CE	-5.11	1.80	1.95
3	G	2	ASN	CA-CB	-5.09	1.44	1.53
3	A	294	MSE	CG-SE	-5.07	1.80	1.95
5	T	20	THR	CA-CB	5.06	1.61	1.53
3	G	250	MSE	CG-SE	-5.03	1.80	1.95
5	Y	20	THR	CA-CB	5.02	1.61	1.53
4	D	112	MSE	CG-SE	-5.00	1.80	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	286	GLN	CG-CD	5.00	1.64	1.52

All (165) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	236	GLU	N-CA-C	-15.08	91.49	110.19
3	G	3	VAL	N-CA-C	13.19	128.36	108.71
4	D	236	GLU	N-CA-C	11.39	124.92	111.02
3	A	237	ASP	N-CA-C	11.27	123.64	111.36
5	Y	7	THR	CA-C-O	-10.74	108.87	120.36
3	G	211	VAL	N-CA-C	10.72	123.55	108.12
3	G	209	LEU	CA-C-N	10.69	133.20	119.84
3	G	209	LEU	C-N-CA	10.69	133.20	119.84
3	G	4	THR	N-CA-C	10.27	125.72	110.52
4	D	47	ARG	CA-C-N	9.99	130.07	119.78
4	D	47	ARG	C-N-CA	9.99	130.07	119.78
3	G	41	ILE	N-CA-C	9.78	119.61	110.42
3	A	107	HIS	N-CA-C	-9.25	100.76	111.03
3	G	111	ASN	N-CA-C	-9.12	101.29	111.14
3	C	211	VAL	N-CA-C	9.08	121.55	108.48
4	D	284	ARG	CA-C-N	-9.04	109.03	120.79
4	D	284	ARG	C-N-CA	-9.04	109.03	120.79
3	C	323	HIS	N-CA-C	-8.61	97.55	109.95
3	G	156	SER	N-CA-C	8.52	121.61	108.07
3	G	284	ARG	CA-C-N	-8.26	110.06	120.79
3	G	284	ARG	C-N-CA	-8.26	110.06	120.79
2	R	715	DG	C4'-C3'-O3'	8.13	122.19	110.00
3	G	220	ASP	N-CA-C	-8.01	97.94	109.31
3	G	287	LEU	N-CA-C	7.92	120.56	109.15
3	A	197	VAL	N-CA-C	-7.84	102.70	110.30
3	A	94	ILE	N-CA-C	-7.74	96.87	108.17
3	A	120	ILE	N-CA-C	7.68	118.79	108.27
3	C	133	GLU	N-CA-C	-7.65	102.89	111.07
3	C	287	LEU	N-CA-C	7.64	120.16	109.15
3	G	178	LYS	N-CA-C	-7.57	104.65	114.04
3	C	16	MSE	N-CA-C	-7.56	104.29	113.97
4	D	315	ASP	N-CA-C	7.35	121.00	107.99
3	C	69	ASP	N-CA-C	7.33	119.48	107.23
3	G	277	THR	N-CA-C	-7.30	101.12	110.53
4	D	292	GLN	CA-C-N	7.21	128.86	119.84
4	D	292	GLN	C-N-CA	7.21	128.86	119.84
5	L	78	GLU	N-CA-C	-7.20	103.36	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	291	VAL	N-CA-C	7.19	118.64	108.93
3	A	214	SER	N-CA-C	-7.17	103.20	112.23
5	Y	57	LYS	N-CA-C	7.12	119.90	111.71
5	S	78	GLU	N-CA-C	-7.09	103.61	112.90
3	G	57	SER	N-CA-C	6.99	121.83	113.16
3	G	239	LYS	CA-C-N	6.98	128.02	120.13
3	G	239	LYS	C-N-CA	6.98	128.02	120.13
3	G	115	LYS	N-CA-C	-6.96	104.65	113.01
4	D	102	GLN	N-CA-C	6.96	119.75	111.33
3	C	284	ARG	CA-C-N	-6.95	111.15	119.84
3	C	284	ARG	C-N-CA	-6.95	111.15	119.84
4	D	189	GLU	CA-C-N	6.87	128.42	119.84
4	D	189	GLU	C-N-CA	6.87	128.42	119.84
3	G	29	VAL	N-CA-C	-6.78	95.23	109.34
3	C	30	LYS	CA-C-N	6.78	127.33	119.47
3	C	30	LYS	C-N-CA	6.78	127.33	119.47
3	C	87	THR	OG1-CB-CG2	-6.76	95.77	109.30
4	D	200	TYR	N-CA-C	-6.74	103.41	111.69
3	C	316	SER	N-CA-C	-6.72	103.04	110.91
4	D	90	LYS	N-CA-C	6.69	120.64	111.54
4	D	225	SER	N-CA-C	-6.69	105.23	113.19
3	A	211	VAL	N-CA-C	6.67	118.43	108.23
5	T	23	VAL	N-CA-C	-6.66	103.84	110.30
3	A	314	VAL	N-CA-C	-6.63	98.94	108.42
4	D	103	ASP	N-CA-C	6.63	118.16	111.07
3	G	93	ILE	N-CA-C	6.54	117.67	107.28
3	C	19	VAL	N-CA-C	-6.51	104.15	110.72
3	C	92	ASN	N-CA-C	-6.41	99.86	110.17
3	G	249	GLU	N-CA-C	-6.40	104.22	111.07
3	C	1	MSE	CB-CG-SE	-6.39	93.53	112.70
3	G	183	VAL	N-CA-C	-6.38	99.24	108.36
5	S	27	SER	N-CA-C	-6.36	105.01	112.89
3	C	176	GLY	CA-C-N	-6.35	114.04	123.00
3	C	176	GLY	C-N-CA	-6.35	114.04	123.00
4	D	77	GLU	N-CA-C	-6.31	104.33	111.14
3	G	317	SER	N-CA-C	-6.24	105.31	113.17
4	D	312	GLU	N-CA-C	-6.23	102.14	110.24
3	G	66	ILE	N-CA-C	-6.22	101.53	109.80
4	D	140	VAL	CA-C-N	6.18	126.20	119.90
4	D	140	VAL	C-N-CA	6.18	126.20	119.90
3	G	1	MSE	CA-C-N	-6.16	109.77	121.54
3	G	1	MSE	C-N-CA	-6.16	109.77	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	715	DG	C2'-C3'-O3'	-6.13	102.31	111.50
3	C	189	GLU	CA-C-N	6.07	127.43	119.84
3	C	189	GLU	C-N-CA	6.07	127.43	119.84
4	D	151	THR	N-CA-C	6.07	123.72	110.80
4	D	114	GLY	N-CA-C	-6.04	105.18	112.49
3	G	101	ASN	N-CA-C	6.04	118.57	108.96
3	G	28	ASN	N-CA-C	6.02	123.61	110.80
4	D	121	ILE	N-CA-C	-6.00	99.22	107.99
3	C	311	LYS	N-CA-C	5.99	120.39	113.38
3	A	169	VAL	N-CA-C	-5.98	105.89	111.45
4	D	111	ASN	N-CA-C	-5.96	103.95	111.11
3	G	87	THR	N-CA-C	-5.95	104.49	110.97
3	A	102	GLN	N-CA-C	5.91	119.31	111.75
3	A	6	TYR	N-CA-C	-5.90	105.18	112.90
5	T	84	GLU	N-CA-C	-5.89	105.86	113.16
5	T	81	MET	N-CA-C	-5.87	104.80	111.14
4	D	120	ILE	CB-CA-C	-5.84	103.76	110.41
3	C	221	TYR	N-CA-C	5.81	123.18	110.80
3	C	35	LYS	N-CA-C	-5.81	106.17	113.20
5	L	7	THR	CA-C-O	-5.79	114.89	120.92
3	C	121	ILE	N-CA-C	-5.76	99.44	107.80
4	D	291	VAL	N-CA-C	5.75	116.42	108.84
4	D	211	VAL	N-CA-C	5.74	118.18	109.12
3	A	46	TYR	N-CA-C	5.70	118.62	110.24
3	A	113	LEU	N-CA-C	-5.69	105.08	111.28
3	G	2	ASN	N-CA-C	-5.68	98.69	110.80
3	G	235	GLU	N-CA-C	-5.68	106.95	112.97
5	L	16	ALA	CB-CA-C	-5.65	109.06	115.79
3	C	78	LEU	N-CA-C	-5.64	105.03	111.07
3	C	223	TYR	N-CA-C	-5.61	105.69	112.54
3	G	47	ARG	N-CA-C	-5.58	97.49	109.81
3	C	80	ARG	N-CA-C	-5.54	104.46	111.11
3	C	140	VAL	CA-C-N	5.53	125.53	119.89
3	C	140	VAL	C-N-CA	5.53	125.53	119.89
3	A	222	THR	N-CA-C	5.52	118.24	109.24
4	D	316	SER	N-CA-C	-5.52	99.05	110.80
3	G	1	MSE	CB-CA-C	5.49	120.53	110.10
3	G	321	LEU	N-CA-C	-5.48	103.17	110.07
4	D	314	VAL	N-CA-C	-5.48	100.71	108.65
3	A	304	LEU	N-CA-C	-5.45	104.57	111.11
4	D	238	GLU	N-CA-C	-5.44	99.21	110.80
3	A	129	GLU	N-CA-C	-5.44	105.46	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	120	ILE	N-CA-C	5.44	116.58	107.18
3	A	148	ILE	N-CA-C	5.40	115.56	107.51
3	A	201	LYS	N-CA-C	5.40	117.61	111.02
4	D	328	ARG	N-CA-C	-5.40	99.30	110.80
4	D	52	ALA	N-CA-C	-5.40	105.56	111.82
3	A	278	ARG	N-CA-C	-5.38	106.22	112.89
3	G	54	GLY	N-CA-C	-5.38	105.98	112.49
3	A	110	ASN	N-CA-C	5.37	116.94	111.14
3	G	102	GLN	N-CA-C	5.35	122.19	110.80
3	C	116	GLN	N-CA-C	5.35	118.96	111.74
5	S	7	THR	CA-C-O	-5.34	115.07	120.84
3	A	319	VAL	N-CA-C	5.29	116.59	108.71
3	C	54	GLY	N-CA-C	-5.29	106.24	112.64
3	A	154	ILE	CA-C-N	5.27	126.09	119.98
3	A	154	ILE	C-N-CA	5.27	126.09	119.98
3	G	189	GLU	CA-C-N	5.25	125.31	119.32
3	G	189	GLU	C-N-CA	5.25	125.31	119.32
3	G	76	ALA	N-CA-C	-5.24	105.48	111.14
4	D	140	VAL	N-CA-C	5.21	114.71	108.45
4	D	300	VAL	N-CA-C	-5.21	105.42	110.42
4	D	314	VAL	CA-C-N	-5.20	115.73	123.11
4	D	314	VAL	C-N-CA	-5.20	115.73	123.11
3	G	316	SER	N-CA-C	-5.20	99.73	110.80
3	G	150	SER	N-CA-C	5.17	121.82	110.80
3	C	102	GLN	N-CA-C	5.17	121.80	110.80
4	D	154	ILE	N-CA-C	5.15	113.06	108.63
3	C	36	LYS	N-CA-C	-5.14	104.63	112.04
4	D	99	ASP	N-CA-C	-5.14	106.42	113.56
4	D	313	THR	N-CA-C	-5.12	100.35	109.06
3	C	66	ILE	N-CA-C	5.11	113.74	106.53
5	L	57	LYS	N-CA-C	-5.11	103.41	110.35
3	G	315	ASP	N-CA-C	5.10	117.05	108.73
3	C	165	ALA	N-CA-C	-5.10	105.37	111.03
4	D	171	SER	N-CA-C	-5.09	106.57	112.89
4	D	55	LEU	N-CA-C	-5.08	105.44	110.97
5	S	44	LEU	N-CA-C	-5.08	106.78	112.87
3	A	66	ILE	N-CA-C	-5.07	101.11	108.36
4	D	33	THR	N-CA-C	-5.05	105.47	110.97
2	R	709	DC	C4'-C3'-O3'	5.04	117.56	110.00
4	D	78	LEU	N-CA-C	-5.04	105.78	111.28
4	D	262	GLY	N-CA-C	-5.04	108.65	115.36
4	D	227	ILE	N-CA-C	-5.04	105.63	110.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	281	THR	N-CA-C	-5.02	107.00	113.23
4	D	317	SER	N-CA-C	-5.00	107.86	114.31

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	702	DG	Sidechain
2	B	703	DT	Sidechain
2	B	704	DT	Sidechain
2	B	715	DG	Sidechain
4	D	200	TYR	Sidechain
1	E	702	DG	Sidechain
1	E	703	DA	Sidechain
1	H	700	DC	Sidechain
2	R	712	DT	Sidechain
2	R	715	DG	Sidechain
5	Y	7	THR	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	327	0	180	51	0
1	H	327	0	180	56	0
2	B	323	0	184	44	0
2	R	323	0	184	57	0
3	A	2562	0	2587	407	0
3	C	2558	0	2584	399	1
3	G	2564	0	2594	392	1
4	D	2558	0	2584	393	0
5	L	632	0	624	75	0
5	S	632	0	624	71	0
5	T	632	0	624	88	0
5	Y	632	0	624	73	0
6	A	10	0	0	1	0
6	C	15	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	G	10	0	0	0	0
7	A	1	0	0	0	0
7	D	1	0	0	0	0
8	A	17	0	0	0	0
8	B	1	0	0	0	0
8	C	13	0	0	0	0
8	D	12	0	0	0	0
8	E	2	0	0	0	0
8	G	10	0	0	0	0
8	H	1	0	0	0	0
8	L	4	0	0	0	0
8	R	1	0	0	0	0
8	S	7	0	0	0	0
8	T	9	0	0	0	0
8	Y	10	0	0	0	0
All	All	14194	0	13573	1939	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 70.

All (1939) 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)
3:C:1:MSE:CE	3:C:1:MSE:SE	2.20	1.40
4:D:1:MET:CE	4:D:1:MET:SD	2.15	1.34
3:G:139:PRO:CG	3:C:1:MSE:HE2	1.66	1.26
3:G:73:ILE:CG2	3:C:278:ARG:HH22	1.53	1.22
3:G:73:ILE:HG22	3:C:278:ARG:NH2	1.54	1.21
3:C:305:LEU:HG	3:C:309:MSE:HE2	1.25	1.16
2:R:700:DC:H2"	2:R:701:DT:H5"	1.16	1.15
4:D:231:GLU:HA	4:D:261:ARG:HH22	1.10	1.14
3:A:284:ARG:HB2	3:A:285:PRO:HD3	1.24	1.14
4:D:41:ILE:HG23	4:D:46:TYR:HB3	1.27	1.13
5:T:36:GLU:HB2	5:T:41:THR:HG22	1.22	1.13
5:Y:18:PRO:HB3	5:Y:86:LEU:HD21	1.24	1.13
3:C:303:ARG:HH12	3:C:307:LYS:HE3	1.18	1.09
3:A:55:LEU:HD12	4:D:55:LEU:HD12	1.33	1.08
3:A:111:ASN:ND2	6:A:946:SO4:O3	1.86	1.08
5:S:26:ALA:HB2	5:S:77:LEU:HD21	1.14	1.08
3:C:231:GLU:HB2	3:C:261:ARG:HH21	1.07	1.08
3:C:255:ILE:HG23	3:C:265:VAL:HG21	1.30	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:212:ARG:H	3:C:212:ARG:HD2	1.14	1.07
4:D:149:GLU:HG2	4:D:154:ILE:HD11	1.36	1.07
3:G:49:ASN:HD21	3:G:52:ALA:HB3	1.20	1.06
3:C:232:LYS:O	3:C:236:GLU:HG2	1.55	1.06
5:S:9:THR:HG22	5:S:87:GLY:HA2	1.37	1.06
2:B:713:DC:H2''	2:B:714:DA:H5''	1.37	1.06
5:Y:14:ILE:HD13	5:Y:14:ILE:O	1.55	1.05
3:G:139:PRO:HG3	3:C:1:MSE:HE2	1.07	1.05
5:T:79:ASP:HB3	5:T:83:LYS:HE2	1.38	1.04
5:Y:9:THR:HG22	5:Y:87:GLY:HA2	1.39	1.04
3:G:284:ARG:HB2	3:G:285:PRO:HD3	1.38	1.03
3:G:139:PRO:CG	3:C:1:MSE:CE	2.37	1.01
3:C:22:VAL:HG11	3:C:37:VAL:HG11	1.39	1.01
4:D:82:ILE:HG23	4:D:302:MSE:HG2	1.39	1.01
4:D:304:LEU:HB2	5:Y:48:MET:HE1	1.43	1.01
5:T:26:ALA:HB2	5:T:77:LEU:HD21	1.42	1.00
3:A:12:ALA:HA	3:A:36:LYS:HE3	1.36	1.00
5:T:14:ILE:HD12	5:T:55:ILE:HG21	1.40	1.00
4:D:288:THR:HG23	4:D:327:PHE:HA	1.42	1.00
3:A:7:ASP:HB3	3:A:44:LEU:HD21	1.40	0.99
3:C:148:ILE:HG12	3:C:190:PRO:HB2	1.45	0.98
4:D:231:GLU:HA	4:D:261:ARG:NH2	1.77	0.98
3:A:212:ARG:H	3:A:212:ARG:HD2	1.27	0.98
3:A:1:MSE:CE	3:A:1:MSE:SE	2.62	0.97
4:D:69:ASP:OD2	4:D:71:SER:HB3	1.64	0.97
4:D:284:ARG:HB3	4:D:285:PRO:HD3	1.43	0.97
4:D:63:VAL:HG21	4:D:302:MSE:HE1	1.45	0.97
3:A:326:GLU:HB3	3:A:328:ARG:HH12	1.26	0.97
3:G:284:ARG:HH21	3:C:284:ARG:HA	1.29	0.96
4:D:204:LEU:HD23	4:D:211:VAL:HG12	1.48	0.96
2:R:700:DC:C2'	2:R:701:DT:H5''	1.95	0.96
1:E:712:DA:H2''	1:E:713:DC:H5''	1.44	0.95
3:G:47:ARG:HH22	3:C:113:LEU:HD12	1.29	0.95
3:G:90:LYS:HG2	3:G:90:LYS:O	1.66	0.95
3:G:139:PRO:HG3	3:C:1:MSE:CE	1.95	0.95
3:A:152:ASN:HD22	3:A:318:ILE:HG12	1.32	0.94
4:D:169:VAL:HG23	4:D:172:LEU:HD12	1.50	0.94
4:D:182:PHE:HE1	4:D:184:SER:HG	1.02	0.94
1:H:709:DC:H5'	1:H:709:DC:H6	1.30	0.93
5:S:70:GLU:HG3	5:S:71:ALA:H	1.30	0.93
2:R:702:DG:H2''	2:R:703:DT:H5'	1.48	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:180:ILE:HG22	4:D:242:ALA:HB3	1.49	0.93
3:C:74:PHE:HE2	3:C:294:MSE:HG2	1.32	0.93
3:C:191:ILE:HD11	3:C:196:LYS:NZ	1.84	0.93
3:A:1:MSE:HG2	3:A:47:ARG:HH11	1.33	0.92
3:G:49:ASN:HD21	3:G:52:ALA:CB	1.81	0.92
3:C:74:PHE:CE2	3:C:294:MSE:HG2	2.04	0.92
3:C:288:THR:HG23	3:C:327:PHE:HA	1.52	0.92
3:C:148:ILE:HG12	3:C:190:PRO:CB	2.00	0.92
3:A:11:GLU:HG2	3:A:40:THR:HG22	1.50	0.92
2:B:701:DT:H2''	2:B:702:DG:H5'	1.52	0.91
3:C:180:ILE:HD11	3:C:204:LEU:HD21	1.51	0.91
3:G:220:ASP:OD2	3:G:225:SER:HB3	1.69	0.91
3:A:63:VAL:HG21	3:A:302:MSE:HE1	1.53	0.91
3:G:73:ILE:HD11	3:G:277:THR:HG22	1.52	0.90
3:A:121:ILE:HD11	3:A:302:MSE:HE2	1.51	0.90
3:A:121:ILE:CD1	3:A:302:MSE:HE2	2.00	0.90
3:A:11:GLU:OE1	3:A:43:ARG:HD3	1.71	0.90
3:A:293:PRO:O	3:A:297:ILE:HG12	1.72	0.90
3:G:73:ILE:HG22	3:C:278:ARG:HH22	0.75	0.90
3:A:67:ILE:HD11	3:A:75:TYR:HB3	1.51	0.90
3:C:264:ASN:HD22	3:C:267:ASN:H	1.20	0.89
4:D:121:ILE:CD1	4:D:302:MSE:HE3	2.03	0.89
2:B:713:DC:C2'	2:B:714:DA:H5''	2.04	0.88
3:C:144:LEU:HD21	3:C:154:ILE:HG23	1.55	0.88
3:C:264:ASN:ND2	3:C:267:ASN:H	1.72	0.88
3:A:252:LEU:HD12	3:A:283:VAL:HG22	1.54	0.88
1:E:706:DG:OP1	1:E:706:DG:H4'	1.74	0.88
3:A:3:VAL:HG11	3:A:44:LEU:HG	1.55	0.88
3:G:293:PRO:HB2	3:G:296:ASP:HB2	1.56	0.87
4:D:264:ASN:HD21	4:D:267:ASN:HB2	1.37	0.87
3:G:73:ILE:HG13	3:G:74:PHE:N	1.89	0.87
5:L:11:ASP:HA	5:L:57:LYS:HE3	1.57	0.87
3:C:212:ARG:HD2	3:C:212:ARG:N	1.89	0.87
2:R:711:DT:H2''	2:R:712:DT:C6	2.09	0.86
4:D:154:ILE:HD12	4:D:154:ILE:O	1.76	0.86
2:R:705:DA:H2''	2:R:706:DG:O4'	1.74	0.85
3:A:1:MSE:HG2	3:A:47:ARG:NH1	1.90	0.85
3:G:65:VAL:HG12	3:G:121:ILE:HB	1.58	0.85
3:G:173:ILE:HD11	3:G:204:LEU:HD23	1.56	0.85
4:D:74:PHE:CE2	4:D:294:MSE:HG2	2.12	0.85
4:D:180:ILE:O	4:D:180:ILE:HD12	1.75	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:101:ASN:ND2	3:G:103:ASP:OD2	2.09	0.85
4:D:144:LEU:HB3	4:D:147:SER:OG	1.77	0.85
2:B:704:DT:H1'	2:B:705:DA:H5''	1.56	0.85
3:G:70:ILE:HG23	3:G:97:ASN:OD1	1.76	0.84
4:D:82:ILE:HG23	4:D:302:MSE:CG	2.06	0.84
1:E:700:DC:H5'	1:E:701:DT:H71	1.60	0.84
3:G:274:PHE:O	3:G:275:ASP:HB2	1.77	0.84
3:C:105:GLU:OE1	3:C:122:PHE:HZ	1.60	0.84
1:E:714:DA:H2''	1:E:715:DG:H5''	1.59	0.84
3:G:143:VAL:HG23	3:G:156:SER:HA	1.58	0.84
2:R:712:DT:H2'	2:R:713:DC:C6	2.12	0.84
3:G:43:ARG:HH21	3:G:44:LEU:HB2	1.41	0.84
5:S:26:ALA:HB2	5:S:77:LEU:CD2	2.04	0.83
3:G:42:GLU:HA	3:G:42:GLU:OE2	1.78	0.83
1:H:707:DC:H6	1:H:707:DC:H5''	1.42	0.83
4:D:62:THR:HA	4:D:92:ASN:O	1.78	0.83
3:G:139:PRO:HG2	3:C:1:MSE:CE	2.09	0.83
3:A:29:VAL:HB	3:A:34:ARG:NH2	1.94	0.83
3:G:154:ILE:H	3:G:154:ILE:HD12	1.44	0.83
3:A:51:VAL:HG13	4:D:51:VAL:HG13	1.60	0.83
4:D:202:ARG:O	4:D:206:GLU:HB2	1.78	0.83
3:C:212:ARG:H	3:C:212:ARG:CD	1.91	0.83
3:C:277:THR:HB	3:C:279:LEU:HD11	1.60	0.83
5:T:36:GLU:CB	5:T:41:THR:HG22	2.05	0.82
3:C:252:LEU:HG	3:C:283:VAL:CG1	2.09	0.82
2:R:712:DT:H2''	2:R:713:DC:O4'	1.79	0.82
4:D:106:LEU:HD11	4:D:131:HIS:CD2	2.15	0.82
4:D:284:ARG:HB3	4:D:285:PRO:CD	2.09	0.82
5:Y:11:ASP:HA	5:Y:57:LYS:HE2	1.59	0.82
3:A:326:GLU:HB3	3:A:328:ARG:NH1	1.95	0.82
5:T:19:ALA:O	5:T:23:VAL:HG23	1.80	0.82
2:B:713:DC:H2''	2:B:714:DA:C5'	2.10	0.82
5:L:9:THR:O	5:L:57:LYS:HE2	1.80	0.82
1:E:714:DA:H2''	1:E:715:DG:O4'	1.80	0.82
3:C:231:GLU:HB2	3:C:261:ARG:NH2	1.92	0.82
3:A:284:ARG:HB2	3:A:285:PRO:CD	2.08	0.82
3:G:47:ARG:NH2	3:C:113:LEU:HD12	1.94	0.82
4:D:302:MSE:HE2	4:D:302:MSE:HA	1.61	0.82
3:A:259:GLN:HG3	3:A:284:ARG:NH2	1.94	0.81
3:C:28:ASN:O	3:C:29:VAL:HG23	1.80	0.81
2:R:700:DC:H2'	2:R:701:DT:C5	2.16	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:177:HIS:ND1	3:A:241:THR:HB	1.96	0.81
3:G:49:ASN:ND2	3:G:52:ALA:HB3	1.95	0.81
4:D:182:PHE:HB2	4:D:200:TYR:CE2	2.15	0.81
3:G:47:ARG:HH22	3:C:113:LEU:CD1	1.93	0.81
3:G:296:ASP:CG	5:L:51:MET:HG2	2.05	0.81
3:G:284:ARG:HB2	3:G:285:PRO:CD	2.11	0.81
3:A:41:ILE:HG12	3:A:46:TYR:HB3	1.63	0.81
5:L:37:PHE:HE2	5:L:59:ALA:HB1	1.44	0.80
5:S:27:SER:HA	5:S:45:LYS:HD3	1.62	0.80
3:A:180:ILE:HG22	3:A:242:ALA:HB3	1.62	0.80
3:C:180:ILE:HG22	3:C:242:ALA:HB3	1.63	0.80
3:C:191:ILE:HD11	3:C:196:LYS:HZ1	1.46	0.80
2:B:701:DT:H2''	2:B:702:DG:C5'	2.11	0.80
3:A:217:VAL:HG11	3:A:233:LEU:HG	1.64	0.80
5:T:47:ILE:HG22	5:T:51:MET:HE2	1.63	0.80
2:B:712:DT:H2'	2:B:713:DC:C5	2.16	0.80
4:D:259:GLN:HB2	4:D:284:ARG:NH2	1.97	0.80
5:T:32:ASP:O	5:T:33:ILE:HG13	1.82	0.80
5:Y:44:LEU:HD13	5:Y:44:LEU:O	1.82	0.80
3:G:73:ILE:C	3:G:73:ILE:HD12	2.06	0.79
3:A:288:THR:HG23	3:A:330:SER:HB3	1.64	0.79
3:A:305:LEU:HG	3:A:309:MSE:HE3	1.62	0.79
2:B:705:DA:H2''	2:B:706:DG:O4'	1.82	0.79
3:C:2:ASN:OD1	3:C:2:ASN:O	1.99	0.79
4:D:44:LEU:HD12	4:D:44:LEU:O	1.82	0.79
4:D:144:LEU:H	4:D:144:LEU:HD22	1.47	0.79
3:C:29:VAL:HG12	3:C:34:ARG:HB2	1.63	0.79
3:G:73:ILE:HG12	3:G:277:THR:HG21	1.65	0.79
3:C:252:LEU:HG	3:C:283:VAL:HG11	1.63	0.79
3:G:43:ARG:HH21	3:G:44:LEU:CB	1.95	0.79
3:G:317:SER:C	3:G:318:ILE:HD12	2.07	0.79
5:T:79:ASP:O	5:T:83:LYS:HG2	1.83	0.79
3:G:73:ILE:HD11	3:G:277:THR:CG2	2.14	0.78
5:S:9:THR:HG22	5:S:87:GLY:CA	2.11	0.78
3:G:144:LEU:HD22	3:G:144:LEU:N	1.98	0.78
3:G:276:ASN:HD21	3:G:328:ARG:HH22	1.31	0.78
3:A:29:VAL:HB	3:A:34:ARG:HH21	1.49	0.78
5:S:47:ILE:HG23	5:S:51:MET:HE3	1.66	0.78
3:A:36:LYS:O	3:A:39:GLU:HG3	1.83	0.78
4:D:22:VAL:HG21	4:D:37:VAL:HG11	1.66	0.78
3:C:35:LYS:O	3:C:39:GLU:HB2	1.82	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:303:ARG:HH11	3:C:303:ARG:HG3	1.48	0.78
3:A:247:THR:HG22	3:A:249:GLU:N	1.98	0.78
3:C:105:GLU:OE1	3:C:122:PHE:CZ	2.37	0.78
5:S:19:ALA:O	5:S:23:VAL:HG23	1.83	0.78
3:G:247:THR:HG22	3:G:250:MSE:H	1.48	0.77
3:G:102:GLN:O	3:G:106:LEU:HD13	1.83	0.77
3:C:190:PRO:O	3:C:194:ALA:HB3	1.84	0.77
3:C:194:ALA:O	3:C:198:LYS:HG3	1.84	0.77
4:D:41:ILE:CG2	4:D:46:TYR:HB3	2.13	0.77
4:D:255:ILE:HG23	4:D:265:VAL:HG21	1.65	0.77
1:E:703:DA:N6	3:A:17:ALA:HB2	1.99	0.77
3:G:284:ARG:HE	3:C:284:ARG:HG2	1.50	0.77
4:D:184:SER:HB2	4:D:192:ASN:ND2	1.99	0.77
5:Y:37:PHE:HB2	5:Y:61:ILE:HG22	1.66	0.77
1:E:714:DA:C2'	1:E:715:DG:H5''	2.14	0.77
3:A:132:VAL:HG12	3:A:136:LYS:HE2	1.67	0.77
3:G:63:VAL:HG21	3:G:302:MSE:HE1	1.66	0.76
1:H:709:DC:H5'	1:H:709:DC:C6	2.18	0.76
4:D:303:ARG:HH21	4:D:306:THR:HB	1.49	0.76
4:D:201:LYS:HD3	4:D:202:ARG:H	1.50	0.76
3:C:243:ILE:HG22	3:C:244:PHE:N	1.99	0.76
4:D:168:ALA:HB1	4:D:272:ILE:HG21	1.66	0.76
4:D:73:ILE:HD13	4:D:73:ILE:N	2.01	0.76
2:B:706:DG:H2''	2:B:707:DC:C5	2.21	0.76
5:L:67:GLY:O	5:L:70:GLU:HG3	1.86	0.76
3:G:139:PRO:HG2	3:C:1:MSE:HE1	1.66	0.75
3:G:217:VAL:CG1	3:G:233:LEU:HD21	2.16	0.75
1:H:714:DA:H2'	1:H:715:DG:C8	2.21	0.75
3:G:284:ARG:NE	3:C:284:ARG:HG2	2.00	0.75
3:G:213:ASP:O	3:G:216:ILE:HG22	1.86	0.75
3:A:170:GLN:HE21	3:A:170:GLN:HA	1.51	0.75
4:D:144:LEU:HD23	4:D:154:ILE:HD13	1.65	0.75
4:D:263:LEU:HD12	4:D:268:ASP:OD1	1.86	0.75
4:D:302:MSE:HE1	4:D:305:LEU:HD23	1.69	0.75
1:H:707:DC:H2''	3:G:55:LEU:HD22	1.68	0.75
3:G:216:ILE:HG23	3:G:216:ILE:O	1.87	0.75
1:E:704:DA:H2''	1:E:705:DA:OP2	1.87	0.75
3:G:226:GLY:O	3:G:230:VAL:HG23	1.87	0.75
3:A:148:ILE:H	3:A:148:ILE:HD12	1.50	0.75
5:S:63:ILE:HD12	5:S:77:LEU:HD13	1.68	0.75
5:S:70:GLU:HG3	5:S:71:ALA:N	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:113:LEU:HD13	3:C:47:ARG:HH12	1.52	0.74
3:C:303:ARG:NH1	3:C:307:LYS:HE3	1.98	0.74
5:Y:14:ILE:HG23	5:Y:55:ILE:HB	1.69	0.74
5:Y:18:PRO:CB	5:Y:86:LEU:HD21	2.11	0.74
3:G:230:VAL:HG21	3:G:254:VAL:HA	1.69	0.74
1:H:708:DG:H2''	1:H:709:DC:C5'	2.17	0.74
3:G:230:VAL:CG2	3:G:254:VAL:HA	2.17	0.74
3:A:1:MSE:HG3	4:D:139:PRO:HG2	1.67	0.74
5:L:80:THR:HA	5:L:83:LYS:HG2	1.68	0.74
5:S:26:ALA:CB	5:S:77:LEU:HD21	2.07	0.74
5:S:33:ILE:HG21	5:S:44:LEU:HD12	1.69	0.74
4:D:82:ILE:HD11	4:D:123:MSE:CE	2.18	0.74
3:G:173:ILE:HD11	3:G:204:LEU:CD2	2.17	0.74
4:D:90:LYS:O	4:D:90:LYS:HG2	1.86	0.74
3:C:121:ILE:CD1	3:C:302:MSE:HE2	2.16	0.74
1:H:707:DC:H5''	1:H:707:DC:C6	2.23	0.74
3:G:88:MSE:HE2	5:L:24:GLN:CD	2.12	0.74
3:C:152:ASN:HD22	3:C:152:ASN:N	1.85	0.74
3:G:259:GLN:OE1	3:G:284:ARG:HD2	1.88	0.73
3:A:50:ALA:HB3	4:D:115:LYS:HA	1.68	0.73
3:A:143:VAL:HG11	3:A:305:LEU:HB2	1.69	0.73
3:A:324:ARG:NH1	3:A:324:ARG:HB3	2.03	0.73
4:D:67:ILE:HD11	4:D:75:TYR:HB3	1.70	0.73
3:G:150:SER:O	3:G:152:ASN:OD1	2.07	0.73
3:G:304:LEU:HD23	3:G:305:LEU:N	2.04	0.73
3:C:102:GLN:CA	3:C:102:GLN:HE21	1.99	0.73
4:D:287:LEU:HD12	4:D:288:THR:H	1.53	0.73
4:D:192:ASN:HA	4:D:196:LYS:HB2	1.68	0.73
2:B:712:DT:H2'	2:B:713:DC:C6	2.22	0.73
3:A:247:THR:HG22	3:A:249:GLU:H	1.53	0.73
5:Y:33:ILE:HG23	5:Y:65:ALA:HB2	1.69	0.73
3:G:43:ARG:NH2	3:G:44:LEU:HB2	2.03	0.73
3:C:121:ILE:HD11	3:C:302:MSE:HE2	1.70	0.73
3:A:88:MSE:HE1	5:S:20:THR:HG22	1.71	0.73
3:A:187:LEU:O	3:A:193:HIS:HB3	1.89	0.73
4:D:70:ILE:H	4:D:97:ASN:HD21	1.37	0.73
4:D:106:LEU:HD11	4:D:131:HIS:HD2	1.51	0.73
5:T:22:LEU:CD1	5:T:77:LEU:HD22	2.19	0.73
1:E:702:DG:H2'	3:A:15:SER:HB3	1.71	0.72
1:E:708:DG:H1'	1:E:709:DC:H5''	1.70	0.72
3:C:319:VAL:HG21	5:T:48:MET:HE1	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:102:GLN:OE1	4:D:103:ASP:N	2.20	0.72
3:A:11:GLU:HG2	3:A:40:THR:CG2	2.19	0.72
3:A:212:ARG:HD2	3:A:212:ARG:N	2.03	0.72
3:A:230:VAL:HG22	3:A:254:VAL:HA	1.70	0.72
3:A:38:LEU:HD23	3:A:38:LEU:O	1.89	0.72
4:D:172:LEU:HD22	4:D:242:ALA:HB1	1.72	0.72
2:R:706:DG:H2''	2:R:707:DC:C5	2.25	0.72
5:L:8:VAL:HG12	5:L:59:ALA:O	1.88	0.72
3:C:109:LEU:HD12	3:C:109:LEU:O	1.90	0.72
3:A:15:SER:O	3:A:19:VAL:HG23	1.90	0.72
3:A:259:GLN:HG3	3:A:284:ARG:CZ	2.20	0.72
3:A:305:LEU:HD12	3:A:305:LEU:O	1.89	0.72
5:T:32:ASP:C	5:T:33:ILE:HG13	2.12	0.72
4:D:47:ARG:HG3	4:D:47:ARG:O	1.90	0.72
5:Y:26:ALA:HB2	5:Y:44:LEU:HD12	1.71	0.72
3:G:143:VAL:HG12	3:G:305:LEU:HD13	1.71	0.72
3:C:322:PRO:HG2	5:T:52:SER:O	1.90	0.71
4:D:290:VAL:HA	4:D:325:ILE:HG22	1.70	0.71
5:Y:30:ASP:OD2	5:Y:69:ASP:OD2	2.07	0.71
3:G:193:HIS:CD2	3:G:194:ALA:N	2.58	0.71
3:C:233:LEU:HD22	3:C:240:PRO:HG2	1.72	0.71
4:D:300:VAL:HG13	5:Y:48:MET:HE3	1.71	0.71
3:A:282:MSE:HE3	4:D:279:LEU:HD22	1.72	0.71
4:D:191:ILE:HD11	4:D:196:LYS:HE3	1.72	0.71
1:H:706:DG:H2''	1:H:707:DC:C5	2.25	0.71
2:R:711:DT:H2'	2:R:712:DT:H72	1.72	0.71
3:A:274:PHE:O	3:A:275:ASP:HB2	1.90	0.71
3:C:150:SER:O	3:C:152:ASN:ND2	2.24	0.71
4:D:144:LEU:HD22	4:D:144:LEU:N	2.04	0.71
5:S:9:THR:CG2	5:S:87:GLY:HA2	2.19	0.71
5:T:42:VAL:HG11	5:T:53:LEU:HD21	1.73	0.71
1:H:712:DA:H2''	1:H:713:DC:H5''	1.72	0.71
3:A:191:ILE:C	3:A:192:ASN:HD22	1.98	0.71
3:A:230:VAL:CG2	3:A:254:VAL:HA	2.21	0.71
3:C:158:THR:OG1	3:C:161:TYR:HE1	1.74	0.71
3:A:231:GLU:OE1	3:A:261:ARG:HD3	1.90	0.71
4:D:121:ILE:HD11	4:D:302:MSE:HE3	1.71	0.71
3:A:197:VAL:HG12	3:A:201:LYS:HE2	1.73	0.70
3:G:115:LYS:HA	3:C:50:ALA:HB3	1.74	0.70
3:A:216:ILE:HG23	3:A:216:ILE:O	1.90	0.70
4:D:144:LEU:CD2	4:D:154:ILE:HD13	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:711:DA:H2	2:R:704:DT:H3	1.36	0.70
2:R:703:DT:H71	3:C:17:ALA:HB2	1.73	0.70
4:D:121:ILE:HD11	4:D:302:MSE:CE	2.21	0.70
3:C:185:GLY:HA3	3:C:221:TYR:CE1	2.26	0.70
4:D:154:ILE:O	4:D:154:ILE:CD1	2.40	0.70
5:T:37:PHE:HB2	5:T:61:ILE:HG22	1.74	0.70
3:A:46:TYR:HE1	3:A:48:PRO:HG3	1.56	0.70
4:D:304:LEU:HB2	5:Y:48:MET:CE	2.20	0.70
2:B:702:DG:H2''	2:B:703:DT:OP2	1.89	0.70
3:A:252:LEU:CD1	3:A:283:VAL:HG22	2.21	0.70
2:B:704:DT:C1'	2:B:705:DA:H5''	2.22	0.69
3:A:3:VAL:HG11	3:A:44:LEU:CG	2.22	0.69
1:H:711:DA:H2''	1:H:712:DA:C8	2.27	0.69
3:G:69:ASP:OD1	3:C:80:ARG:NH1	2.26	0.69
3:C:315:ASP:CG	3:C:316:SER:H	2.00	0.69
5:L:20:THR:HG23	5:L:47:ILE:HD11	1.73	0.69
3:C:288:THR:CG2	3:C:327:PHE:HA	2.22	0.69
3:C:295:TYR:CD1	5:T:16:ALA:HA	2.27	0.69
5:T:36:GLU:HB2	5:T:41:THR:CG2	2.12	0.69
5:T:30:ASP:HB2	5:T:69:ASP:OD1	1.91	0.69
3:A:102:GLN:OE1	3:A:103:ASP:N	2.24	0.69
4:D:69:ASP:CG	4:D:71:SER:HB3	2.17	0.69
3:G:26:ASN:OD1	3:G:27:PRO:HD2	1.93	0.69
4:D:264:ASN:ND2	4:D:267:ASN:HB2	2.07	0.69
3:G:217:VAL:HG12	3:G:233:LEU:HD21	1.74	0.69
3:C:82:ILE:HD11	3:C:123:MSE:HE1	1.75	0.69
3:A:180:ILE:HD11	3:A:204:LEU:HD21	1.75	0.69
4:D:304:LEU:CB	5:Y:48:MET:HE1	2.22	0.69
5:S:43:ASN:OD1	5:S:45:LYS:HB2	1.93	0.69
2:R:700:DC:H2''	2:R:701:DT:C5'	2.09	0.68
2:R:711:DT:H2''	2:R:712:DT:C5	2.29	0.68
3:G:149:GLU:CG	3:G:154:ILE:HD11	2.23	0.68
3:G:264:ASN:N	3:G:268:ASP:OD1	2.24	0.68
3:A:137:LYS:HE2	3:A:137:LYS:HA	1.75	0.68
5:T:2:ALA:N	5:T:74:LEU:HD11	2.07	0.68
5:Y:55:ILE:HD13	5:Y:61:ILE:HG21	1.74	0.68
3:A:3:VAL:CG1	3:A:44:LEU:HG	2.22	0.68
1:E:715:DG:H1	2:B:700:DC:H42	1.42	0.68
3:A:259:GLN:CG	3:A:284:ARG:HH22	2.06	0.68
4:D:57:SER:C	4:D:58:LYS:HD2	2.18	0.68
1:H:703:DA:N1	2:R:712:DT:O4	2.27	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:259:GLN:HB2	3:C:284:ARG:NH2	2.08	0.68
5:T:22:LEU:HD11	5:T:77:LEU:HD22	1.75	0.68
3:G:73:ILE:CD1	3:G:277:THR:CG2	2.71	0.68
5:S:10:ALA:HB2	5:S:86:LEU:HA	1.75	0.68
5:S:44:LEU:O	5:S:44:LEU:HD22	1.92	0.68
1:E:707:DC:H2''	3:A:55:LEU:CD2	2.24	0.68
3:C:108:LEU:O	3:C:112:MSE:HB2	1.92	0.68
3:A:38:LEU:HD23	3:A:38:LEU:C	2.18	0.68
1:E:707:DC:H2''	3:A:55:LEU:HD22	1.75	0.68
3:A:70:ILE:H	3:A:97:ASN:ND2	1.91	0.68
5:T:42:VAL:CG1	5:T:53:LEU:HD21	2.24	0.68
3:A:41:ILE:C	3:A:41:ILE:HD13	2.18	0.68
4:D:113:LEU:O	4:D:116:GLN:NE2	2.27	0.68
3:C:60:THR:OG1	3:C:62:THR:HG23	1.93	0.68
4:D:187:LEU:O	4:D:193:HIS:HB2	1.94	0.68
3:G:8:VAL:HG13	3:G:40:THR:HG22	1.76	0.67
3:A:226:GLY:O	3:A:230:VAL:HG23	1.95	0.67
3:A:192:ASN:HD22	3:A:192:ASN:N	1.93	0.67
4:D:239:LYS:N	4:D:239:LYS:HD3	2.09	0.67
4:D:274:PHE:O	4:D:275:ASP:HB2	1.92	0.67
5:L:37:PHE:CE2	5:L:59:ALA:HB1	2.29	0.67
4:D:3:VAL:CG1	4:D:7:ASP:HB2	2.24	0.67
3:C:137:LYS:HE3	3:C:137:LYS:HA	1.75	0.67
2:R:712:DT:H2'	2:R:713:DC:H6	1.60	0.67
3:G:3:VAL:HG13	3:G:7:ASP:OD2	1.94	0.67
3:G:317:SER:O	3:G:318:ILE:HD12	1.95	0.67
4:D:85:ILE:CG2	4:D:302:MSE:HB3	2.24	0.67
1:E:702:DG:H2'	3:A:15:SER:CB	2.25	0.67
3:G:43:ARG:NH2	3:G:44:LEU:HD22	2.09	0.67
3:A:208:GLY:O	3:A:210:PRO:HD3	1.94	0.67
4:D:74:PHE:CD2	4:D:294:MSE:HG2	2.28	0.67
3:G:303:ARG:O	3:G:306:THR:OG1	2.12	0.67
1:H:707:DC:C2'	3:G:55:LEU:HD22	2.25	0.67
2:B:704:DT:C2'	2:B:705:DA:H5''	2.25	0.66
3:C:165:ALA:HB3	3:C:199:GLY:HA3	1.75	0.66
3:G:231:GLU:HB2	3:G:261:ARG:NH2	2.09	0.66
4:D:63:VAL:HG21	4:D:302:MSE:CE	2.24	0.66
3:G:73:ILE:CG1	3:G:74:PHE:N	2.57	0.66
3:A:82:ILE:CG2	3:A:302:MSE:HE3	2.26	0.66
1:E:703:DA:H1'	1:E:704:DA:H5'	1.77	0.66
3:G:276:ASN:ND2	3:G:328:ARG:HH22	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:265:VAL:HB	3:C:266:PRO:HD3	1.76	0.66
4:D:201:LYS:HD3	4:D:202:ARG:N	2.11	0.66
3:G:55:LEU:HD12	3:C:55:LEU:HD12	1.77	0.66
3:C:22:VAL:HG11	3:C:37:VAL:CG1	2.19	0.66
3:A:251:ALA:O	3:A:255:ILE:HG13	1.94	0.66
1:H:701:DT:OP2	3:G:29:VAL:HA	1.96	0.66
3:A:121:ILE:HD12	3:A:302:MSE:HE2	1.77	0.66
4:D:34:ARG:O	4:D:38:LEU:HB2	1.95	0.66
5:T:80:THR:O	5:T:84:GLU:HB2	1.95	0.66
5:Y:37:PHE:HE2	5:Y:59:ALA:HB1	1.60	0.66
2:R:700:DC:H2'	2:R:701:DT:H72	1.77	0.66
3:G:88:MSE:HE2	5:L:24:GLN:OE1	1.96	0.66
3:C:102:GLN:HE21	3:C:102:GLN:HA	1.58	0.66
3:A:50:ALA:CB	4:D:115:LYS:HA	2.26	0.66
3:G:6:TYR:O	3:G:9:ALA:HB3	1.95	0.66
3:G:43:ARG:HE	3:G:44:LEU:N	1.93	0.66
3:G:85:ILE:HD11	5:L:47:ILE:CD1	2.25	0.66
4:D:186:THR:HG22	4:D:187:LEU:N	2.11	0.66
5:Y:35:LEU:HB2	5:Y:44:LEU:HD23	1.78	0.66
3:G:122:PHE:O	3:G:144:LEU:HA	1.96	0.66
3:A:159:ILE:HD12	3:A:321:LEU:O	1.95	0.66
4:D:73:ILE:HD13	4:D:73:ILE:H	1.60	0.66
3:G:187:LEU:HD21	3:G:216:ILE:HD11	1.78	0.66
2:R:700:DC:H2'	2:R:701:DT:C7	2.25	0.65
3:C:3:VAL:HG13	3:C:7:ASP:HB3	1.77	0.65
4:D:118:ASP:O	4:D:309:MSE:SE	2.64	0.65
4:D:304:LEU:HD13	5:Y:48:MET:HE1	1.79	0.65
1:E:700:DC:H2'	1:E:701:DT:C6	2.31	0.65
3:G:183:VAL:HG22	3:G:229:ALA:HB1	1.78	0.65
3:C:82:ILE:HG23	3:C:302:MSE:CE	2.26	0.65
3:A:213:ASP:O	3:A:216:ILE:HG22	1.95	0.65
3:G:282:MSE:HG2	3:C:252:LEU:HD22	1.77	0.65
3:A:186:THR:HA	3:A:218:GLU:OE1	1.96	0.65
3:A:192:ASN:O	3:A:197:VAL:HG23	1.96	0.65
3:A:305:LEU:HG	3:A:309:MSE:CE	2.27	0.65
5:S:33:ILE:CG2	5:S:44:LEU:HD12	2.27	0.65
3:C:3:VAL:HG13	3:C:7:ASP:CB	2.26	0.65
1:H:703:DA:OP2	1:H:703:DA:H2'	1.96	0.65
1:E:709:DC:H2'	1:E:710:DT:H72	1.79	0.65
3:C:144:LEU:HD21	3:C:154:ILE:CG2	2.27	0.65
3:A:307:LYS:HE2	5:S:48:MET:HE2	1.77	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:714:DA:H2''	1:E:715:DG:C5'	2.26	0.65
3:C:226:GLY:HA3	3:C:253:GLY:HA3	1.79	0.65
2:R:712:DT:H4'	2:R:712:DT:OP1	1.97	0.65
3:C:188:GLU:CD	3:C:188:GLU:H	2.05	0.65
3:A:265:VAL:HB	3:A:266:PRO:HD3	1.77	0.65
1:E:703:DA:H62	3:A:17:ALA:HB2	1.60	0.65
1:E:709:DC:H5'	1:E:709:DC:H6	1.62	0.65
3:C:292:GLN:O	3:C:294:MSE:HE2	1.95	0.65
3:A:149:GLU:HG2	3:A:154:ILE:CD1	2.26	0.65
3:G:298:GLY:O	3:G:299:ALA:C	2.36	0.64
3:C:144:LEU:N	3:C:144:LEU:HD22	2.12	0.64
4:D:3:VAL:HG12	4:D:7:ASP:HB2	1.78	0.64
2:B:708:DG:H1'	2:B:709:DC:H5''	1.80	0.64
4:D:265:VAL:HB	4:D:266:PRO:HD3	1.79	0.64
3:C:230:VAL:CG2	3:C:254:VAL:HA	2.27	0.64
4:D:248:ASP:O	4:D:251:ALA:HB3	1.96	0.64
3:G:180:ILE:HA	3:G:242:ALA:O	1.98	0.64
4:D:227:ILE:O	4:D:231:GLU:HG2	1.97	0.64
4:D:261:ARG:HG2	4:D:261:ARG:HH11	1.62	0.64
5:T:9:THR:HG21	5:T:88:GLU:HG3	1.80	0.64
1:E:715:DG:H1	2:B:700:DC:N4	1.96	0.64
3:C:148:ILE:HG12	3:C:190:PRO:HB3	1.80	0.64
3:A:12:ALA:HA	3:A:36:LYS:CE	2.22	0.64
3:A:49:ASN:OD1	3:A:52:ALA:N	2.27	0.64
3:A:324:ARG:HG2	3:A:325:ILE:N	2.11	0.64
4:D:317:SER:O	4:D:318:ILE:HD12	1.98	0.64
5:Y:14:ILE:O	5:Y:14:ILE:CD1	2.39	0.64
3:C:307:LYS:NZ	3:C:314:VAL:HG11	2.13	0.64
3:A:161:TYR:O	3:A:162:GLU:C	2.40	0.64
3:A:247:THR:HG21	3:A:249:GLU:HB3	1.80	0.64
3:G:169:VAL:HG21	3:G:200:TYR:HA	1.79	0.64
3:G:307:LYS:HZ2	5:L:48:MET:HE3	1.62	0.64
2:B:702:DG:H2'	2:B:703:DT:H72	1.79	0.64
3:G:64:GLY:HA3	3:G:112:MSE:HG2	1.80	0.64
3:G:149:GLU:HG3	3:G:154:ILE:HD11	1.77	0.64
3:A:151:THR:OG1	3:A:153:GLN:HB2	1.98	0.64
1:E:706:DG:H2''	1:E:707:DC:C6	2.33	0.64
3:C:232:LYS:O	3:C:236:GLU:CG	2.41	0.64
3:A:212:ARG:HD3	3:A:215:TYR:CD2	2.32	0.64
5:S:20:THR:O	5:S:24:GLN:HB2	1.98	0.64
2:B:701:DT:OP2	4:D:29:VAL:HA	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:247:THR:CG2	3:G:250:MSE:H	2.11	0.63
3:G:307:LYS:NZ	5:L:48:MET:HE3	2.13	0.63
3:A:279:LEU:HA	3:A:282:MSE:HB2	1.78	0.63
5:L:67:GLY:H	5:L:70:GLU:CG	2.09	0.63
5:S:47:ILE:HD12	5:S:51:MET:CE	2.28	0.63
4:D:317:SER:C	4:D:318:ILE:HD12	2.24	0.63
5:T:47:ILE:HG22	5:T:51:MET:CE	2.27	0.63
3:G:177:HIS:HE1	3:G:241:THR:HG22	1.64	0.63
5:L:73:ALA:O	5:L:76:ALA:HB3	1.99	0.63
5:Y:44:LEU:HG	5:Y:63:ILE:CD1	2.27	0.63
3:G:80:ARG:HD2	3:C:70:ILE:HD11	1.80	0.63
3:G:204:LEU:HB3	3:G:209:LEU:O	1.97	0.63
3:C:62:THR:HA	3:C:92:ASN:O	1.97	0.63
3:C:305:LEU:CG	3:C:309:MSE:HE2	2.16	0.63
4:D:78:LEU:HG	4:D:123:MSE:SE	2.49	0.63
4:D:182:PHE:CE1	4:D:184:SER:HB3	2.33	0.63
5:T:10:ALA:HB2	5:T:86:LEU:HA	1.80	0.63
5:Y:6:PHE:HD2	5:Y:88:GLU:HA	1.64	0.63
3:G:43:ARG:HH21	3:G:44:LEU:CG	2.11	0.63
3:C:243:ILE:CG2	3:C:244:PHE:N	2.61	0.63
3:A:179:ASN:HB3	3:A:215:TYR:HE2	1.64	0.63
3:A:252:LEU:HD13	4:D:282:MSE:HE2	1.80	0.63
4:D:166:PHE:CE2	4:D:202:ARG:CZ	2.81	0.63
5:T:14:ILE:HD12	5:T:55:ILE:CG2	2.25	0.63
3:G:204:LEU:HD12	3:G:211:VAL:CG1	2.28	0.63
3:A:261:ARG:HH11	3:A:261:ARG:HG3	1.63	0.63
3:G:80:ARG:O	3:G:84:ASP:HB2	1.99	0.62
3:A:206:GLU:C	3:A:208:GLY:H	2.05	0.62
4:D:296:ASP:OD1	5:Y:51:MET:SD	2.57	0.62
4:D:252:LEU:HA	4:D:255:ILE:HD12	1.81	0.62
5:T:2:ALA:N	5:T:74:LEU:CD1	2.62	0.62
3:G:80:ARG:CD	3:C:70:ILE:HD11	2.29	0.62
3:C:231:GLU:CB	3:C:261:ARG:HH21	1.98	0.62
3:C:277:THR:O	3:C:279:LEU:HD12	1.99	0.62
1:H:703:DA:H62	3:G:17:ALA:HB2	1.64	0.62
1:E:702:DG:N7	3:A:21:ARG:NH2	2.44	0.62
3:A:288:THR:HB	3:A:327:PHE:HA	1.82	0.62
5:T:6:PHE:N	5:T:6:PHE:CD1	2.67	0.62
5:T:67:GLY:O	5:T:70:GLU:HB2	1.99	0.62
3:G:47:ARG:NH2	3:C:113:LEU:HB2	2.13	0.62
3:A:1:MSE:CG	3:A:47:ARG:NH1	2.60	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:222:THR:OG1	3:A:225:SER:HB3	1.99	0.62
3:G:155:PRO:O	3:G:156:SER:HB3	1.99	0.62
3:C:144:LEU:HB3	3:C:147:SER:HB2	1.82	0.62
3:A:67:ILE:O	3:A:97:ASN:HA	1.99	0.62
4:D:103:ASP:OD2	4:D:104:LYS:HG3	2.00	0.62
5:S:14:ILE:HD12	5:S:55:ILE:HD13	1.80	0.62
3:C:94:ILE:CG2	3:C:112:MSE:HE1	2.29	0.62
3:C:109:LEU:O	3:C:113:LEU:HG	2.00	0.62
3:C:148:ILE:HG23	3:C:148:ILE:O	1.98	0.62
1:H:712:DA:C2'	1:H:713:DC:H5''	2.28	0.62
3:G:73:ILE:CG1	3:G:277:THR:HG21	2.29	0.62
4:D:275:ASP:HA	4:D:292:GLN:HB3	1.82	0.62
1:H:714:DA:H2'	1:H:715:DG:H8	1.65	0.62
3:G:284:ARG:CB	3:G:285:PRO:HD3	2.22	0.62
3:G:324:ARG:NH2	3:G:326:GLU:OE2	2.29	0.62
3:C:168:ALA:HB2	3:C:290:VAL:HG21	1.82	0.62
3:C:186:THR:HG23	3:C:189:GLU:HB2	1.82	0.62
3:C:303:ARG:HA	3:C:306:THR:OG1	2.00	0.62
3:A:54:GLY:HA2	3:A:59:LYS:O	2.00	0.62
4:D:122:PHE:HD1	4:D:144:LEU:HD12	1.64	0.62
3:G:64:GLY:N	3:G:117:VAL:HG11	2.14	0.62
3:G:154:ILE:CD1	3:G:154:ILE:O	2.48	0.62
3:A:103:ASP:OD1	3:A:104:LYS:N	2.33	0.62
4:D:264:ASN:HD21	4:D:268:ASP:H	1.48	0.61
1:H:705:DA:H2''	1:H:706:DG:O5'	2.00	0.61
1:H:714:DA:H4'	1:H:714:DA:OP1	1.98	0.61
3:A:152:ASN:HD22	3:A:318:ILE:CG1	2.10	0.61
4:D:43:ARG:HG2	4:D:43:ARG:HH11	1.64	0.61
2:R:700:DC:H2'	2:R:701:DT:C6	2.34	0.61
3:G:43:ARG:HE	3:G:44:LEU:CA	2.13	0.61
3:C:275:ASP:OD2	3:C:292:GLN:NE2	2.33	0.61
3:A:24:ASN:HD22	3:A:24:ASN:N	1.97	0.61
3:A:88:MSE:CE	5:S:20:THR:HG22	2.30	0.61
3:A:332:LYS:HD3	3:A:332:LYS:N	2.14	0.61
4:D:82:ILE:HD11	4:D:123:MSE:HE1	1.81	0.61
3:G:49:ASN:ND2	3:G:49:ASN:O	2.33	0.61
3:G:73:ILE:HD12	3:G:73:ILE:O	2.01	0.61
3:C:37:VAL:HG13	3:C:38:LEU:N	2.16	0.61
3:A:149:GLU:HG2	3:A:154:ILE:HD11	1.82	0.61
3:A:259:GLN:HG3	3:A:284:ARG:HH22	1.61	0.61
3:C:73:ILE:HD12	3:C:74:PHE:N	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:1:MSE:HG2	3:G:2:ASN:O	1.99	0.61
3:C:238:GLU:OE1	3:C:238:GLU:HA	2.00	0.61
4:D:187:LEU:C	4:D:189:GLU:H	2.09	0.61
5:L:8:VAL:HA	5:L:86:LEU:O	2.01	0.61
4:D:121:ILE:HD11	4:D:302:MSE:HA	1.82	0.61
1:E:703:DA:H2''	1:E:704:DA:OP2	1.99	0.61
2:B:702:DG:O6	4:D:21:ARG:NH2	2.34	0.61
3:C:32:SER:O	3:C:36:LYS:HB2	2.00	0.61
3:A:18:THR:O	3:A:22:VAL:HG13	2.00	0.61
3:A:122:PHE:O	3:A:144:LEU:HA	2.00	0.61
3:A:180:ILE:CG2	3:A:242:ALA:HB3	2.31	0.61
3:A:279:LEU:O	3:A:283:VAL:HG23	2.01	0.61
4:D:173:ILE:HD12	4:D:209:LEU:HD12	1.83	0.61
4:D:284:ARG:CB	4:D:285:PRO:HD3	2.26	0.61
3:G:83:GLU:HB2	3:G:93:ILE:HD11	1.82	0.61
3:G:287:LEU:HD22	3:G:288:THR:N	2.16	0.61
3:C:258:ALA:HB1	3:C:269:LEU:HD21	1.81	0.61
4:D:2:ASN:C	4:D:2:ASN:OD1	2.44	0.61
3:C:102:GLN:CD	3:C:102:GLN:H	2.09	0.60
3:C:284:ARG:HB2	3:C:285:PRO:CD	2.31	0.60
4:D:222:THR:OG1	4:D:225:SER:HB3	2.00	0.60
5:Y:17:ARG:HB2	5:Y:18:PRO:HD3	1.82	0.60
3:C:12:ALA:HB2	3:C:37:VAL:HG23	1.81	0.60
3:A:224:ASP:O	3:A:227:ILE:HG12	2.01	0.60
2:B:706:DG:H2''	2:B:707:DC:C6	2.36	0.60
3:G:247:THR:CG2	3:G:248:ASP:N	2.64	0.60
3:C:102:GLN:NE2	3:C:102:GLN:N	2.50	0.60
3:A:286:GLN:O	3:A:328:ARG:HB2	2.01	0.60
4:D:72:ASN:HD22	4:D:73:ILE:HD13	1.67	0.60
3:C:277:THR:O	3:C:278:ARG:C	2.44	0.60
4:D:3:VAL:HG13	4:D:7:ASP:OD2	2.02	0.60
4:D:191:ILE:HG23	4:D:192:ASN:OD1	2.02	0.60
3:G:318:ILE:O	3:G:318:ILE:HG22	2.01	0.60
3:C:263:LEU:N	3:C:263:LEU:HD12	2.16	0.60
1:H:709:DC:H2'	1:H:710:DT:H71	1.84	0.60
3:G:208:GLY:O	3:G:209:LEU:HD23	2.02	0.60
3:C:3:VAL:O	3:C:46:TYR:HD2	1.85	0.60
4:D:90:LYS:O	4:D:90:LYS:CG	2.50	0.60
3:A:114:GLY:O	3:A:116:GLN:HG2	2.02	0.60
3:A:288:THR:CG2	3:A:328:ARG:H	2.14	0.60
5:T:3:GLN:N	5:T:74:LEU:HD11	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:195:LYS:N	3:C:195:LYS:HD2	2.16	0.60
3:A:192:ASN:HA	3:A:196:LYS:HB2	1.83	0.60
5:T:67:GLY:H	5:T:70:GLU:HB2	1.67	0.60
1:E:706:DG:H2''	1:E:707:DC:C5	2.37	0.60
1:E:712:DA:C2'	1:E:713:DC:H5''	2.26	0.60
3:G:180:ILE:HG22	3:G:242:ALA:HB3	1.82	0.60
3:G:220:ASP:OD2	3:G:225:SER:CB	2.46	0.60
3:C:265:VAL:CG1	3:C:271:ILE:HD12	2.32	0.60
3:A:166:PHE:HE2	3:A:202:ARG:HG2	1.67	0.60
3:A:298:GLY:O	3:A:299:ALA:C	2.40	0.60
4:D:74:PHE:HE2	4:D:294:MSE:HG2	1.59	0.60
4:D:159:ILE:HG22	4:D:160:ASP:N	2.17	0.60
3:C:98:SER:O	3:C:99:ASP:HB2	2.02	0.60
4:D:121:ILE:HD12	4:D:302:MSE:HE3	1.81	0.60
4:D:144:LEU:O	4:D:157:VAL:HG12	2.02	0.60
3:G:60:THR:O	3:G:61:THR:OG1	2.18	0.59
3:C:263:LEU:HD23	3:C:269:LEU:HG	1.84	0.59
3:A:29:VAL:HB	3:A:34:ARG:CZ	2.32	0.59
3:A:235:GLU:C	3:A:236:GLU:O	2.35	0.59
3:A:284:ARG:HG2	4:D:256:HIS:CE1	2.37	0.59
4:D:183:VAL:CG1	4:D:250:MSE:HE2	2.31	0.59
1:H:708:DG:H2''	1:H:709:DC:H5'	1.83	0.59
3:G:83:GLU:HB2	3:G:93:ILE:CD1	2.32	0.59
4:D:191:ILE:O	4:D:196:LYS:HG3	2.03	0.59
1:H:708:DG:H2''	1:H:709:DC:H5''	1.83	0.59
3:C:100:GLN:HE22	3:C:125:GLY:H	1.49	0.59
3:C:192:ASN:HA	3:C:196:LYS:HB2	1.84	0.59
4:D:103:ASP:OD2	4:D:104:LYS:N	2.35	0.59
5:T:57:LYS:O	5:T:57:LYS:HD3	2.02	0.59
3:G:284:ARG:NH2	3:C:284:ARG:HA	2.11	0.59
3:G:229:ALA:O	3:G:233:LEU:HG	2.02	0.59
4:D:73:ILE:H	4:D:73:ILE:CD1	2.15	0.59
3:G:194:ALA:O	3:G:198:LYS:NZ	2.24	0.59
3:C:30:LYS:HB3	3:C:33:THR:OG1	2.01	0.59
5:T:20:THR:O	5:T:24:GLN:HG3	2.02	0.59
3:C:82:ILE:HG23	3:C:302:MSE:HE3	1.83	0.59
3:C:200:TYR:O	3:C:203:ALA:HB3	2.02	0.59
4:D:70:ILE:H	4:D:97:ASN:ND2	1.99	0.59
3:G:162:GLU:OE1	3:G:202:ARG:NH2	2.31	0.59
3:C:255:ILE:HG22	3:C:284:ARG:NH2	2.17	0.59
3:C:271:ILE:H	3:C:271:ILE:HD13	1.67	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:2:ALA:N	5:L:74:LEU:HD22	2.17	0.59
3:C:235:GLU:H	3:C:235:GLU:CD	2.10	0.59
3:A:82:ILE:HG23	3:A:302:MSE:HE3	1.85	0.59
2:B:704:DT:H2''	2:B:705:DA:C5'	2.33	0.59
3:G:276:ASN:HD21	3:G:328:ARG:NH2	1.98	0.59
4:D:38:LEU:HD23	4:D:38:LEU:O	2.02	0.59
1:H:707:DC:H2''	3:G:55:LEU:CD2	2.32	0.58
3:C:109:LEU:HD22	3:C:135:LEU:HD12	1.84	0.58
4:D:145:ALA:HA	4:D:157:VAL:HG13	1.85	0.58
4:D:166:PHE:HE2	4:D:202:ARG:HG2	1.68	0.58
3:G:325:ILE:HG22	3:G:326:GLU:N	2.18	0.58
3:C:106:LEU:HD23	3:C:134:GLU:OE2	2.02	0.58
3:C:307:LYS:HG2	3:C:312:GLU:OE2	2.03	0.58
3:A:128:THR:O	3:A:131:HIS:HB2	2.03	0.58
3:A:180:ILE:HA	3:A:242:ALA:O	2.03	0.58
4:D:85:ILE:HG22	4:D:302:MSE:HB3	1.85	0.58
5:S:8:VAL:CG1	5:S:59:ALA:HB3	2.33	0.58
5:S:25:ALA:HA	5:S:28:LYS:HE2	1.84	0.58
3:G:220:ASP:O	3:G:250:MSE:SE	2.71	0.58
4:D:273:GLY:O	4:D:290:VAL:HG23	2.03	0.58
5:S:4:LYS:HD2	5:S:6:PHE:CZ	2.38	0.58
3:G:113:LEU:O	3:G:116:GLN:NE2	2.35	0.58
3:G:193:HIS:HD2	3:G:194:ALA:N	2.00	0.58
3:G:208:GLY:C	3:G:210:PRO:HD3	2.28	0.58
3:C:221:TYR:HD1	3:C:250:MSE:HE2	1.68	0.58
3:C:307:LYS:HB3	3:C:312:GLU:HG3	1.84	0.58
4:D:247:THR:O	4:D:251:ALA:HB2	2.04	0.58
4:D:288:THR:CG2	4:D:327:PHE:HA	2.25	0.58
3:C:37:VAL:HG13	3:C:38:LEU:H	1.69	0.58
3:C:96:SER:OG	3:C:108:LEU:HD22	2.03	0.58
3:C:204:LEU:HD12	3:C:211:VAL:HG21	1.84	0.58
3:C:209:LEU:O	3:C:210:PRO:C	2.47	0.58
2:R:706:DG:H4'	2:R:706:DG:OP1	2.02	0.58
3:G:127:VAL:HG21	3:G:149:GLU:HB3	1.86	0.58
3:G:202:ARG:O	3:G:206:GLU:HB2	2.04	0.58
4:D:191:ILE:CD1	4:D:196:LYS:HE3	2.34	0.58
5:T:8:VAL:HA	5:T:86:LEU:O	2.02	0.58
5:Y:9:THR:CG2	5:Y:87:GLY:HA2	2.25	0.58
3:G:74:PHE:CE2	3:G:294:MSE:HG2	2.38	0.58
3:G:141:PRO:O	3:G:142:VAL:HG23	2.04	0.58
3:C:212:ARG:O	3:C:215:TYR:HB2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:247:THR:CG2	3:A:249:GLU:HB3	2.33	0.58
4:D:86:ALA:HB2	4:D:302:MSE:SE	2.54	0.58
4:D:88:MSE:HE2	5:Y:24:GLN:HG3	1.85	0.58
4:D:212:ARG:HD3	4:D:215:TYR:CD2	2.38	0.58
1:H:710:DT:H5''	3:C:53:ARG:NH2	2.19	0.58
2:R:711:DT:C2'	2:R:712:DT:C5	2.86	0.58
5:T:48:MET:O	5:T:52:SER:OG	2.22	0.58
3:G:252:LEU:HD21	3:G:283:VAL:HG22	1.85	0.58
3:G:254:VAL:HG12	3:G:271:ILE:CD1	2.33	0.58
3:A:187:LEU:H	3:A:218:GLU:CD	2.12	0.58
3:C:197:VAL:HG12	3:C:201:LYS:HD3	1.85	0.57
3:C:202:ARG:O	3:C:206:GLU:HB2	2.03	0.57
5:T:26:ALA:HB2	5:T:77:LEU:CD2	2.27	0.57
1:H:702:DG:H5''	3:G:15:SER:OG	2.04	0.57
3:G:99:ASP:O	3:G:101:ASN:N	2.37	0.57
3:G:103:ASP:OD2	3:G:104:LYS:N	2.37	0.57
3:A:259:GLN:HG3	3:A:284:ARG:NH1	2.18	0.57
1:H:702:DG:H2''	1:H:703:DA:C8	2.40	0.57
3:C:187:LEU:HD11	3:C:218:GLU:HG2	1.85	0.57
4:D:85:ILE:HG13	5:Y:47:ILE:HD12	1.84	0.57
4:D:158:THR:OG1	4:D:159:ILE:N	2.37	0.57
5:Y:37:PHE:CE2	5:Y:59:ALA:HB1	2.38	0.57
2:B:700:DC:H2''	2:B:701:DT:O5'	2.04	0.57
3:G:113:LEU:CD2	3:G:139:PRO:HD2	2.34	0.57
3:C:112:MSE:HA	3:C:112:MSE:HE3	1.86	0.57
3:C:288:THR:HG23	3:C:327:PHE:CA	2.31	0.57
3:A:173:ILE:HD11	3:A:204:LEU:HD23	1.87	0.57
3:G:43:ARG:NH2	3:G:44:LEU:HD13	2.19	0.57
3:A:68:PRO:HD3	3:A:123:MSE:O	2.04	0.57
3:A:304:LEU:HD22	3:A:308:TYR:CE2	2.39	0.57
4:D:73:ILE:N	4:D:73:ILE:CD1	2.67	0.57
4:D:180:ILE:HD12	4:D:180:ILE:C	2.29	0.57
5:Y:14:ILE:HD11	5:Y:50:VAL:HG12	1.86	0.57
3:G:113:LEU:HD22	3:G:139:PRO:HD2	1.86	0.57
4:D:41:ILE:HG23	4:D:46:TYR:CB	2.17	0.57
4:D:114:GLY:C	4:D:116:GLN:H	2.12	0.57
5:Y:56:GLN:H	5:Y:56:GLN:CD	2.12	0.57
1:E:703:DA:H2''	1:E:704:DA:H5'	1.87	0.57
3:G:65:VAL:HG22	3:G:94:ILE:O	2.05	0.57
3:G:113:LEU:HD13	3:C:47:ARG:NH1	2.20	0.57
3:C:160:ASP:OD1	3:C:163:GLN:HG2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:1:MET:O	4:D:3:VAL:HG23	2.03	0.57
5:T:87:GLY:C	5:T:88:GLU:HG2	2.29	0.57
5:S:79:ASP:O	5:S:83:LYS:HB2	2.05	0.57
1:H:710:DT:H5''	3:C:53:ARG:CZ	2.34	0.57
3:G:151:THR:OG1	3:G:153:GLN:HG3	2.05	0.57
3:C:61:THR:N	3:C:118:ASP:OD2	2.35	0.57
3:C:188:GLU:CD	3:C:188:GLU:N	2.62	0.57
3:C:300:VAL:O	3:C:301:ALA:C	2.48	0.57
3:A:36:LYS:O	3:A:40:THR:HG23	2.05	0.57
3:A:208:GLY:C	3:A:210:PRO:HD3	2.30	0.57
4:D:258:ALA:HB2	4:D:269:LEU:HD21	1.87	0.57
5:T:22:LEU:HD12	5:T:77:LEU:HD22	1.87	0.57
5:S:27:SER:HA	5:S:45:LYS:CD	2.35	0.57
3:G:255:ILE:HG23	3:G:265:VAL:HG11	1.87	0.57
3:C:12:ALA:CB	3:C:37:VAL:HG23	2.34	0.57
3:C:303:ARG:HD2	3:C:303:ARG:O	2.04	0.57
4:D:142:VAL:HG23	4:D:143:VAL:N	2.19	0.57
5:L:18:PRO:HA	5:L:84:GLU:CD	2.30	0.57
3:C:182:PHE:CZ	3:C:184:SER:HB3	2.39	0.57
3:A:169:VAL:HG12	3:A:173:ILE:HG12	1.87	0.57
4:D:264:ASN:HD22	4:D:264:ASN:C	2.09	0.57
4:D:293:PRO:O	4:D:294:MSE:C	2.48	0.57
1:H:706:DG:OP1	1:H:706:DG:H4'	2.04	0.56
3:C:102:GLN:O	3:C:106:LEU:HD13	2.05	0.56
3:C:123:MSE:HA	3:C:147:SER:OG	2.05	0.56
3:C:162:GLU:OE2	3:C:199:GLY:HA2	2.04	0.56
3:C:235:GLU:O	3:C:236:GLU:C	2.47	0.56
4:D:230:VAL:HG21	4:D:257:GLY:HA3	1.86	0.56
1:E:714:DA:H2''	1:E:715:DG:C4'	2.36	0.56
3:G:145:ALA:O	3:G:146:ALA:C	2.49	0.56
3:G:177:HIS:CE1	3:G:241:THR:HG22	2.39	0.56
3:G:204:LEU:HD12	3:G:211:VAL:HG11	1.87	0.56
3:C:67:ILE:HG22	3:C:123:MSE:SE	2.55	0.56
3:C:155:PRO:HG3	3:C:317:SER:HB2	1.87	0.56
3:C:194:ALA:C	3:C:195:LYS:HD2	2.30	0.56
3:C:274:PHE:O	3:C:275:ASP:HB2	2.04	0.56
3:A:3:VAL:CG1	3:A:44:LEU:CD2	2.84	0.56
3:A:182:PHE:HB2	3:A:200:TYR:CD2	2.41	0.56
3:G:208:GLY:C	3:G:209:LEU:HD23	2.30	0.56
3:C:148:ILE:O	3:C:148:ILE:CG2	2.54	0.56
3:G:254:VAL:HG12	3:G:271:ILE:HD13	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:285:PRO:O	3:G:286:GLN:C	2.49	0.56
3:C:1:MSE:SE	3:C:47:ARG:NH2	2.89	0.56
3:C:295:TYR:CD1	3:C:295:TYR:C	2.83	0.56
4:D:144:LEU:HB3	4:D:147:SER:HG	1.68	0.56
4:D:149:GLU:CG	4:D:154:ILE:HD11	2.24	0.56
3:A:193:HIS:HA	3:A:197:VAL:CG2	2.35	0.56
4:D:100:GLN:NE2	4:D:125:GLY:HA3	2.20	0.56
5:Y:11:ASP:HA	5:Y:57:LYS:CE	2.31	0.56
3:G:70:ILE:HG21	3:G:95:LEU:HD21	1.87	0.56
3:G:265:VAL:HB	3:G:285:PRO:HG2	1.88	0.56
3:A:63:VAL:HG22	3:A:93:ILE:HD12	1.86	0.56
3:A:259:GLN:CG	3:A:284:ARG:NH2	2.65	0.56
3:C:102:GLN:CA	3:C:102:GLN:NE2	2.65	0.56
4:D:290:VAL:HG22	4:D:325:ILE:CG2	2.36	0.56
2:R:701:DT:H2''	2:R:702:DG:H8	1.70	0.56
2:B:703:DT:O4	4:D:17:ALA:HB2	2.05	0.56
3:A:80:ARG:NH1	5:S:17:ARG:HD2	2.20	0.56
3:A:157:VAL:HG11	3:A:301:ALA:HA	1.88	0.56
4:D:184:SER:HB2	4:D:192:ASN:HD22	1.68	0.56
1:H:712:DA:H2'	1:H:713:DC:C6	2.40	0.56
2:B:701:DT:H3'	4:D:18:THR:HG21	1.87	0.56
3:C:38:LEU:HA	3:C:41:ILE:HD12	1.88	0.56
4:D:259:GLN:C	4:D:261:ARG:H	2.14	0.56
5:L:4:LYS:HG2	5:L:5:THR:N	2.20	0.56
1:H:708:DG:C2'	1:H:709:DC:H5''	2.36	0.55
3:G:64:GLY:HA3	3:G:112:MSE:CG	2.36	0.55
3:G:82:ILE:HD11	3:G:121:ILE:HG21	1.87	0.55
3:G:247:THR:HG22	3:G:250:MSE:N	2.19	0.55
3:C:160:ASP:C	3:C:162:GLU:H	2.14	0.55
3:A:65:VAL:HG22	3:A:95:LEU:HB2	1.88	0.55
4:D:108:LEU:O	4:D:112:MSE:HB2	2.06	0.55
5:L:6:PHE:CB	5:L:81:MET:HE2	2.36	0.55
5:S:8:VAL:HG13	5:S:59:ALA:HB3	1.88	0.55
3:C:271:ILE:HD13	3:C:330:SER:OG	2.06	0.55
4:D:244:PHE:HD1	4:D:272:ILE:HG22	1.71	0.55
5:Y:8:VAL:O	5:Y:57:LYS:O	2.23	0.55
1:H:702:DG:H2''	1:H:703:DA:OP2	2.05	0.55
1:H:714:DA:H2''	1:H:715:DG:O4'	2.06	0.55
3:G:92:ASN:HD21	3:C:111:ASN:ND2	2.04	0.55
3:G:139:PRO:CB	3:C:1:MSE:HE2	2.34	0.55
3:G:297:ILE:O	3:G:301:ALA:N	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:25:GLY:O	3:A:26:ASN:C	2.49	0.55
3:A:324:ARG:HB3	3:A:324:ARG:HH11	1.71	0.55
4:D:186:THR:HA	4:D:218:GLU:OE1	2.06	0.55
4:D:245:VAL:CG1	4:D:250:MSE:HG3	2.36	0.55
4:D:275:ASP:OD1	4:D:292:GLN:HG2	2.06	0.55
5:T:2:ALA:O	5:T:64:SER:HA	2.07	0.55
5:Y:33:ILE:HG12	5:Y:65:ALA:HB1	1.87	0.55
3:A:318:ILE:HD12	3:A:318:ILE:N	2.21	0.55
5:Y:67:GLY:O	5:Y:68:SER:C	2.48	0.55
3:G:83:GLU:O	3:G:84:ASP:C	2.48	0.55
3:G:99:ASP:C	3:G:101:ASN:H	2.14	0.55
3:C:204:LEU:HD13	3:C:211:VAL:HG13	1.89	0.55
3:A:302:MSE:O	3:A:305:LEU:HB3	2.07	0.55
1:E:709:DC:OP1	4:D:48:PRO:HA	2.06	0.55
3:A:3:VAL:HG11	3:A:44:LEU:CD2	2.37	0.55
4:D:37:VAL:HA	4:D:40:THR:HB	1.88	0.55
4:D:264:ASN:OD1	4:D:267:ASN:ND2	2.38	0.55
1:E:700:DC:H2''	1:E:701:DT:H5'	1.88	0.55
3:G:5:ILE:HG23	3:G:6:TYR:N	2.21	0.55
3:G:230:VAL:HG22	3:G:254:VAL:HG13	1.89	0.55
3:C:73:ILE:HD13	3:C:277:THR:HG21	1.87	0.55
5:L:18:PRO:HA	5:L:84:GLU:OE2	2.07	0.55
1:H:711:DA:N1	2:R:704:DT:O4	2.40	0.55
3:C:263:LEU:HG	3:C:268:ASP:OD1	2.06	0.55
3:A:131:HIS:O	3:A:134:GLU:HB3	2.07	0.55
3:A:177:HIS:CE1	3:A:241:THR:HB	2.41	0.55
4:D:182:PHE:HE1	4:D:184:SER:OG	1.80	0.55
4:D:290:VAL:HG22	4:D:325:ILE:HG22	1.89	0.55
2:R:700:DC:C2'	2:R:701:DT:C6	2.90	0.55
3:A:82:ILE:HD11	3:A:123:MSE:HE1	1.89	0.55
3:G:80:ARG:HH12	5:L:17:ARG:NH1	2.05	0.54
3:G:265:VAL:O	3:G:269:LEU:O	2.25	0.54
3:A:288:THR:CG2	3:A:330:SER:HB3	2.35	0.54
4:D:241:THR:O	4:D:269:LEU:HA	2.07	0.54
3:G:73:ILE:CD1	3:G:77:GLU:OE2	2.56	0.54
3:G:166:PHE:CD1	3:G:166:PHE:C	2.85	0.54
3:G:255:ILE:HG23	3:G:265:VAL:HG21	1.87	0.54
3:C:107:HIS:O	3:C:110:ASN:HB2	2.07	0.54
3:A:221:TYR:O	3:A:249:GLU:HG2	2.07	0.54
5:L:15:HIS:O	5:L:18:PRO:HD2	2.07	0.54
3:G:180:ILE:HD11	3:G:204:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:243:ILE:CG2	3:C:244:PHE:H	2.20	0.54
4:D:243:ILE:HG22	4:D:244:PHE:H	1.73	0.54
4:D:271:ILE:HD13	4:D:271:ILE:H	1.71	0.54
3:G:310:ASN:O	3:G:312:GLU:N	2.40	0.54
3:A:177:HIS:NE2	3:A:270:GLU:OE2	2.38	0.54
4:D:277:THR:C	4:D:279:LEU:H	2.15	0.54
5:T:44:LEU:O	5:T:44:LEU:HD22	2.07	0.54
5:L:14:ILE:HG13	5:L:55:ILE:HG21	1.88	0.54
5:Y:6:PHE:HE1	5:Y:63:ILE:HG22	1.72	0.54
2:B:703:DT:H71	4:D:17:ALA:HB2	1.90	0.54
3:A:106:LEU:O	3:A:110:ASN:ND2	2.40	0.54
3:A:128:THR:H	3:A:131:HIS:CD2	2.26	0.54
4:D:249:GLU:C	4:D:251:ALA:H	2.15	0.54
1:E:700:DC:O5'	3:A:29:VAL:HA	2.08	0.54
3:G:216:ILE:O	3:G:216:ILE:CG2	2.54	0.54
3:C:17:ALA:O	3:C:21:ARG:HG3	2.07	0.54
3:C:98:SER:O	3:C:104:LYS:HD2	2.07	0.54
3:C:148:ILE:CG1	3:C:190:PRO:HB2	2.28	0.54
3:C:165:ALA:O	3:C:169:VAL:HG12	2.07	0.54
3:C:257:GLY:O	3:C:261:ARG:HG2	2.08	0.54
3:C:303:ARG:HH11	3:C:303:ARG:CG	2.19	0.54
3:A:11:GLU:OE2	3:A:43:ARG:NH1	2.40	0.54
3:A:245:VAL:HG11	3:A:251:ALA:N	2.21	0.54
4:D:58:LYS:HD2	4:D:58:LYS:N	2.23	0.54
4:D:245:VAL:HG11	4:D:251:ALA:HA	1.89	0.54
3:C:40:THR:O	3:C:44:LEU:HD23	2.08	0.54
3:C:144:LEU:CD2	3:C:154:ILE:HG23	2.34	0.54
3:A:170:GLN:O	3:A:171:SER:C	2.51	0.54
5:S:18:PRO:CB	5:S:86:LEU:HD21	2.37	0.54
3:G:73:ILE:HD12	3:G:77:GLU:OE2	2.06	0.54
3:G:274:PHE:O	3:G:275:ASP:CB	2.50	0.54
4:D:85:ILE:HG21	4:D:302:MSE:HB3	1.89	0.54
4:D:177:HIS:CD2	4:D:177:HIS:H	2.25	0.54
3:C:69:ASP:OD2	3:C:71:SER:HB3	2.07	0.54
3:C:94:ILE:HG21	3:C:112:MSE:HE1	1.89	0.54
3:C:230:VAL:HG23	3:C:254:VAL:HA	1.90	0.54
3:A:29:VAL:CB	3:A:34:ARG:HH21	2.18	0.54
4:D:98:SER:HB2	4:D:105:GLU:HG2	1.89	0.54
4:D:204:LEU:HG	4:D:209:LEU:O	2.08	0.54
4:D:275:ASP:O	4:D:276:ASN:HB3	2.08	0.54
2:R:714:DA:H2''	2:R:715:DG:C8	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:712:DT:C2'	2:B:713:DC:C6	2.90	0.54
3:G:315:ASP:O	3:G:316:SER:HB2	2.08	0.54
3:A:121:ILE:HG13	3:A:305:LEU:HD23	1.89	0.54
3:A:173:ILE:HD12	3:A:209:LEU:HD12	1.89	0.54
3:A:276:ASN:OD1	3:A:328:ARG:NH2	2.39	0.54
3:G:4:THR:HG23	3:G:7:ASP:CG	2.32	0.53
3:G:265:VAL:HB	3:G:266:PRO:HD3	1.90	0.53
3:A:166:PHE:CE2	3:A:202:ARG:HG2	2.42	0.53
3:A:184:SER:OG	3:A:185:GLY:N	2.41	0.53
3:A:270:GLU:HB3	3:A:331:THR:HB	1.89	0.53
3:A:299:ALA:HB1	5:S:51:MET:HE1	1.90	0.53
5:L:67:GLY:H	5:L:70:GLU:CD	2.15	0.53
2:B:701:DT:H1'	2:B:702:DG:H5''	1.90	0.53
3:G:73:ILE:HG13	3:G:74:PHE:H	1.72	0.53
3:G:144:LEU:N	3:G:144:LEU:CD2	2.68	0.53
3:G:192:ASN:HA	3:G:196:LYS:HB2	1.91	0.53
3:C:143:VAL:HG12	3:C:305:LEU:HD13	1.90	0.53
5:S:23:VAL:O	5:S:23:VAL:HG12	2.07	0.53
3:G:43:ARG:HH21	3:G:44:LEU:HD13	1.73	0.53
3:G:121:ILE:HD11	3:G:302:MSE:HA	1.89	0.53
3:G:180:ILE:HD11	3:G:204:LEU:HD21	1.91	0.53
3:C:307:LYS:HZ2	3:C:314:VAL:HG11	1.73	0.53
3:A:179:ASN:HB3	3:A:215:TYR:CE2	2.43	0.53
4:D:205:THR:HG22	4:D:210:PRO:HA	1.89	0.53
4:D:230:VAL:HG13	4:D:254:VAL:HG13	1.89	0.53
5:T:35:LEU:HD23	5:T:35:LEU:C	2.33	0.53
1:H:705:DA:H1'	1:H:706:DG:O4'	2.08	0.53
3:G:73:ILE:CD1	3:G:277:THR:HG22	2.29	0.53
3:C:67:ILE:HA	3:C:123:MSE:HG3	1.91	0.53
3:A:128:THR:H	3:A:131:HIS:HD2	1.55	0.53
4:D:88:MSE:HE2	5:Y:24:GLN:CG	2.37	0.53
4:D:324:ARG:HE	5:Y:56:GLN:HG2	1.74	0.53
5:T:32:ASP:O	5:T:33:ILE:CG1	2.56	0.53
5:S:18:PRO:HB2	5:S:86:LEU:HD21	1.90	0.53
5:S:36:GLU:HG2	5:S:41:THR:OG1	2.08	0.53
3:G:73:ILE:CD1	3:G:277:THR:HG21	2.38	0.53
3:A:92:ASN:ND2	4:D:111:ASN:OD1	2.40	0.53
4:D:98:SER:C	4:D:100:GLN:H	2.16	0.53
5:Y:6:PHE:N	5:Y:6:PHE:CD1	2.77	0.53
3:A:300:VAL:HG13	5:S:48:MET:HG2	1.89	0.53
5:Y:69:ASP:C	5:Y:69:ASP:OD1	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:140:VAL:O	3:G:141:PRO:O	2.26	0.53
4:D:4:THR:HG22	4:D:7:ASP:OD2	2.08	0.53
4:D:239:LYS:HD3	4:D:239:LYS:H	1.74	0.53
3:G:33:THR:O	3:G:34:ARG:C	2.52	0.53
3:C:127:VAL:O	3:C:127:VAL:HG12	2.09	0.53
3:C:152:ASN:N	3:C:152:ASN:ND2	2.56	0.53
3:C:243:ILE:HG22	3:C:244:PHE:H	1.74	0.53
3:C:279:LEU:HD12	3:C:280:SER:N	2.24	0.53
3:A:276:ASN:ND2	3:A:291:VAL:HG22	2.24	0.53
5:S:76:ALA:HA	5:S:79:ASP:HB3	1.89	0.53
3:G:22:VAL:HG23	3:G:23:VAL:N	2.23	0.53
3:G:69:ASP:OD1	5:T:17:ARG:NH2	2.42	0.53
3:C:53:ARG:O	3:C:54:GLY:C	2.52	0.53
3:A:22:VAL:HG21	3:A:37:VAL:CG1	2.39	0.53
4:D:212:ARG:HG3	4:D:212:ARG:HH11	1.72	0.53
1:E:701:DT:OP1	3:A:33:THR:HG21	2.09	0.53
3:A:50:ALA:HB1	4:D:115:LYS:HD2	1.91	0.53
4:D:62:THR:HG22	4:D:117:VAL:HG12	1.91	0.53
4:D:128:THR:O	4:D:131:HIS:HB2	2.08	0.53
5:T:12:SER:O	5:T:15:HIS:HD2	1.91	0.53
3:G:11:GLU:CB	3:G:40:THR:HG23	2.40	0.52
3:G:128:THR:O	3:G:131:HIS:HB2	2.09	0.52
3:C:146:ALA:HB2	3:C:297:ILE:HG21	1.91	0.52
3:C:300:VAL:CG1	5:T:48:MET:HE3	2.39	0.52
3:A:70:ILE:O	3:A:70:ILE:HG12	2.08	0.52
4:D:43:ARG:HG2	4:D:43:ARG:NH1	2.23	0.52
3:G:114:GLY:C	3:G:116:GLN:HE21	2.17	0.52
4:D:15:SER:O	4:D:19:VAL:HG23	2.10	0.52
4:D:69:ASP:HA	4:D:97:ASN:HD22	1.73	0.52
4:D:104:LYS:O	4:D:107:HIS:HB3	2.09	0.52
3:G:141:PRO:O	3:G:142:VAL:CG2	2.58	0.52
3:C:112:MSE:O	3:C:115:LYS:N	2.42	0.52
3:C:220:ASP:O	3:C:225:SER:CB	2.57	0.52
3:A:216:ILE:O	3:A:216:ILE:CG2	2.58	0.52
4:D:172:LEU:HD22	4:D:242:ALA:CB	2.40	0.52
5:T:34:ASN:HA	5:T:44:LEU:H	1.73	0.52
3:G:65:VAL:HG23	3:G:65:VAL:O	2.09	0.52
3:C:162:GLU:O	3:C:165:ALA:HB3	2.09	0.52
3:C:307:LYS:HD3	3:C:314:VAL:CB	2.39	0.52
3:A:291:VAL:CG2	3:A:326:GLU:HG2	2.39	0.52
4:D:261:ARG:HH11	4:D:261:ARG:CG	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:712:DA:H2''	1:H:713:DC:C5'	2.40	0.52
3:C:307:LYS:HE2	3:C:314:VAL:HG21	1.91	0.52
4:D:244:PHE:CD1	4:D:272:ILE:HG22	2.45	0.52
4:D:252:LEU:HD13	4:D:279:LEU:HD11	1.90	0.52
4:D:295:TYR:CD1	4:D:295:TYR:C	2.87	0.52
5:T:47:ILE:O	5:T:51:MET:HE2	2.10	0.52
5:Y:46:SEP:O3P	5:Y:48:MET:HB3	2.10	0.52
5:S:26:ALA:O	5:S:45:LYS:HD3	2.09	0.52
2:R:701:DT:H2''	2:R:702:DG:C8	2.44	0.52
3:G:85:ILE:HD11	5:L:47:ILE:HD13	1.91	0.52
3:C:151:THR:OG1	3:C:153:GLN:HB2	2.09	0.52
3:C:160:ASP:C	3:C:162:GLU:N	2.66	0.52
4:D:3:VAL:CG1	4:D:7:ASP:CB	2.88	0.52
4:D:280:SER:OG	4:D:287:LEU:HB3	2.10	0.52
5:Y:84:GLU:HA	5:Y:84:GLU:OE1	2.10	0.52
1:H:709:DC:OP2	3:C:5:ILE:HG22	2.09	0.52
3:G:185:GLY:HA3	3:G:221:TYR:CE1	2.45	0.52
3:C:104:LYS:O	3:C:108:LEU:HG	2.09	0.52
3:C:109:LEU:CD2	3:C:135:LEU:HD12	2.40	0.52
3:C:264:ASN:ND2	3:C:267:ASN:N	2.52	0.52
4:D:22:VAL:HG21	4:D:37:VAL:CG1	2.38	0.52
4:D:182:PHE:CE1	4:D:184:SER:CB	2.92	0.52
5:L:32:ASP:CB	5:L:66:GLU:HG3	2.39	0.52
3:G:80:ARG:HD3	3:C:70:ILE:CD1	2.39	0.52
3:C:296:ASP:O	3:C:300:VAL:HG23	2.10	0.52
3:A:180:ILE:HD13	3:A:180:ILE:H	1.74	0.52
4:D:277:THR:O	4:D:279:LEU:N	2.42	0.52
5:L:2:ALA:O	5:L:3:GLN:HB3	2.09	0.52
3:G:115:LYS:O	3:G:116:GLN:HB2	2.10	0.52
3:G:145:ALA:O	3:G:147:SER:N	2.43	0.52
3:C:68:PRO:HB2	3:C:75:TYR:CE2	2.45	0.52
3:A:294:MSE:O	3:A:297:ILE:HB	2.10	0.52
2:B:709:DC:H6	2:B:709:DC:H5'	1.75	0.52
3:A:38:LEU:O	3:A:41:ILE:HG23	2.10	0.52
3:A:191:ILE:HG22	3:A:192:ASN:ND2	2.25	0.52
3:A:223:TYR:CD2	4:D:282:MSE:HG2	2.45	0.52
3:A:288:THR:HG22	3:A:328:ARG:H	1.75	0.52
4:D:201:LYS:CD	4:D:202:ARG:N	2.73	0.52
3:G:296:ASP:O	3:G:300:VAL:HG23	2.10	0.51
3:C:82:ILE:HD11	3:C:123:MSE:CE	2.40	0.51
3:C:169:VAL:O	3:C:170:GLN:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:214:SER:C	3:C:216:ILE:H	2.19	0.51
3:C:265:VAL:HG13	3:C:271:ILE:HD12	1.91	0.51
3:A:22:VAL:HG12	3:A:29:VAL:HG11	1.92	0.51
3:A:89:TYR:CG	3:A:306:THR:HG21	2.45	0.51
3:A:222:THR:O	3:A:223:TYR:C	2.53	0.51
5:T:9:THR:CG2	5:T:88:GLU:HG3	2.40	0.51
5:L:69:ASP:O	5:L:70:GLU:C	2.52	0.51
5:Y:63:ILE:HG23	5:Y:63:ILE:O	2.11	0.51
5:S:43:ASN:HB3	5:S:46:SEP:HB2	1.91	0.51
1:H:704:DA:H61	2:R:711:DT:H3	1.58	0.51
3:G:83:GLU:HG3	3:G:84:ASP:N	2.25	0.51
3:G:245:VAL:HB	3:G:251:ALA:HB2	1.91	0.51
3:C:36:LYS:O	3:C:39:GLU:HB3	2.10	0.51
3:C:159:ILE:HG13	3:C:159:ILE:O	2.11	0.51
4:D:302:MSE:HA	4:D:302:MSE:CE	2.35	0.51
5:Y:9:THR:O	5:Y:10:ALA:C	2.52	0.51
3:C:295:TYR:CD1	3:C:295:TYR:O	2.63	0.51
3:A:49:ASN:HD21	4:D:116:GLN:HG3	1.75	0.51
3:A:121:ILE:HG13	3:A:305:LEU:CD2	2.40	0.51
3:A:220:ASP:O	3:A:250:MSE:SE	2.78	0.51
5:L:47:ILE:O	5:L:51:MET:HB2	2.11	0.51
3:G:53:ARG:O	3:G:53:ARG:HG2	2.11	0.51
3:G:324:ARG:HH21	3:G:326:GLU:CD	2.17	0.51
3:C:208:GLY:C	3:C:209:LEU:HD12	2.36	0.51
3:A:37:VAL:O	3:A:41:ILE:HG22	2.10	0.51
3:C:111:ASN:ND2	6:C:947:SO4:O1	2.44	0.51
3:C:173:ILE:HD13	3:C:207:SER:OG	2.11	0.51
3:A:64:GLY:HA3	3:A:112:MSE:SE	2.61	0.51
4:D:5:ILE:HD11	4:D:19:VAL:CG1	2.40	0.51
4:D:22:VAL:HG11	4:D:37:VAL:HG13	1.92	0.51
4:D:30:LYS:HG2	4:D:32:SER:H	1.74	0.51
4:D:287:LEU:HD12	4:D:288:THR:N	2.22	0.51
5:L:72:ASP:O	5:L:76:ALA:HB2	2.11	0.51
3:G:180:ILE:HD13	3:G:180:ILE:H	1.74	0.51
3:G:204:LEU:CD1	3:G:211:VAL:HG13	2.41	0.51
3:A:261:ARG:HG3	3:A:261:ARG:NH1	2.26	0.51
4:D:169:VAL:HG13	4:D:170:GLN:N	2.25	0.51
5:L:19:ALA:O	5:L:23:VAL:HG23	2.10	0.51
1:H:702:DG:H5"	3:G:15:SER:CB	2.39	0.51
3:G:159:ILE:CD1	3:G:321:LEU:O	2.58	0.51
3:C:37:VAL:C	3:C:39:GLU:N	2.68	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:LEU:HD12	3:C:211:VAL:CG2	2.41	0.51
3:C:300:VAL:HG13	5:T:48:MET:HE3	1.92	0.51
3:A:275:ASP:O	3:A:276:ASN:HB3	2.10	0.51
4:D:152:ASN:N	4:D:152:ASN:HD22	2.08	0.51
4:D:182:PHE:HB2	4:D:200:TYR:CD2	2.46	0.51
4:D:292:GLN:HG3	4:D:292:GLN:O	2.11	0.51
5:L:26:ALA:HB1	5:L:33:ILE:HD12	1.92	0.51
5:S:4:LYS:NZ	5:S:78:GLU:OE1	2.43	0.51
2:R:702:DG:H2'	2:R:703:DT:H72	1.91	0.51
3:C:191:ILE:HD11	3:C:196:LYS:HZ2	1.69	0.51
4:D:98:SER:O	4:D:99:ASP:HB2	2.10	0.51
4:D:187:LEU:C	4:D:189:GLU:N	2.68	0.51
4:D:259:GLN:NE2	4:D:260:ASP:HA	2.26	0.51
4:D:307:LYS:O	4:D:308:TYR:C	2.54	0.51
5:T:12:SER:O	5:T:15:HIS:CD2	2.63	0.51
5:L:10:ALA:HB2	5:L:85:GLY:O	2.10	0.51
3:C:168:ALA:CB	3:C:244:PHE:HE2	2.24	0.51
3:C:212:ARG:O	3:C:215:TYR:N	2.43	0.51
3:A:3:VAL:HG13	3:A:44:LEU:HD21	1.93	0.51
3:A:194:ALA:O	3:A:195:LYS:HD2	2.11	0.51
4:D:291:VAL:HB	4:D:324:ARG:O	2.11	0.51
1:H:714:DA:N1	2:R:701:DT:O2	2.44	0.51
3:G:67:ILE:HD11	3:G:75:TYR:HB3	1.92	0.51
3:A:73:ILE:HG22	3:A:74:PHE:N	2.24	0.51
5:Y:68:SER:OG	5:Y:69:ASP:N	2.43	0.51
3:G:116:GLN:HG3	3:C:49:ASN:HD21	1.76	0.50
3:A:224:ASP:C	3:A:226:GLY:N	2.69	0.50
3:A:247:THR:CG2	3:A:248:ASP:N	2.73	0.50
4:D:273:GLY:O	4:D:289:SER:HA	2.12	0.50
2:B:709:DC:OP2	3:A:5:ILE:HB	2.11	0.50
3:G:154:ILE:HD12	3:G:154:ILE:N	2.17	0.50
3:C:265:VAL:O	3:C:269:LEU:O	2.29	0.50
3:A:226:GLY:O	3:A:227:ILE:C	2.55	0.50
4:D:293:PRO:O	4:D:295:TYR:N	2.44	0.50
2:B:706:DG:C2'	2:B:707:DC:C5	2.94	0.50
3:C:285:PRO:O	3:C:286:GLN:C	2.54	0.50
5:S:4:LYS:HG2	5:S:5:THR:N	2.26	0.50
5:S:18:PRO:HA	5:S:84:GLU:OE2	2.12	0.50
2:R:710:DT:H2''	2:R:711:DT:C6	2.46	0.50
2:R:713:DC:H2'	2:R:714:DA:C8	2.46	0.50
3:C:283:VAL:HG23	3:C:286:GLN:HA	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:46:SEP:O	5:L:50:VAL:HG23	2.11	0.50
5:S:2:ALA:HA	5:S:65:ALA:O	2.11	0.50
3:G:61:THR:N	3:G:118:ASP:OD2	2.42	0.50
3:G:204:LEU:HD12	3:G:211:VAL:HG13	1.94	0.50
3:C:157:VAL:HG21	3:C:301:ALA:HA	1.92	0.50
3:A:4:THR:HG23	3:A:7:ASP:H	1.75	0.50
3:A:66:ILE:HG13	3:A:112:MSE:HE1	1.94	0.50
3:A:101:ASN:O	3:A:105:GLU:HG3	2.12	0.50
3:A:145:ALA:O	3:A:146:ALA:C	2.54	0.50
4:D:223:TYR:O	4:D:226:GLY:N	2.39	0.50
3:G:11:GLU:HB2	3:G:40:THR:HG23	1.94	0.50
3:G:39:GLU:C	3:G:41:ILE:N	2.67	0.50
3:G:142:VAL:HG12	3:G:143:VAL:N	2.26	0.50
3:A:267:ASN:O	3:A:268:ASP:C	2.54	0.50
4:D:2:ASN:OD1	4:D:2:ASN:O	2.29	0.50
4:D:310:ASN:C	4:D:312:GLU:H	2.19	0.50
3:G:1:MSE:C	3:G:2:ASN:O	2.54	0.50
3:G:215:TYR:CZ	3:G:240:PRO:HG3	2.46	0.50
3:C:134:GLU:OE1	3:C:134:GLU:HA	2.12	0.50
3:A:187:LEU:HB2	3:A:218:GLU:OE2	2.12	0.50
3:A:193:HIS:ND1	3:A:194:ALA:N	2.60	0.50
3:A:271:ILE:H	3:A:331:THR:HG22	1.76	0.50
4:D:107:HIS:O	4:D:110:ASN:N	2.41	0.50
4:D:187:LEU:HD21	4:D:193:HIS:HD2	1.77	0.50
4:D:209:LEU:O	4:D:210:PRO:C	2.55	0.50
4:D:259:GLN:HB2	4:D:284:ARG:HH22	1.76	0.50
4:D:269:LEU:HD12	4:D:269:LEU:O	2.12	0.50
4:D:303:ARG:HH21	4:D:306:THR:CB	2.22	0.50
1:H:700:DC:H3'	3:G:29:VAL:HA	1.92	0.50
2:R:701:DT:H2'	3:C:18:THR:HG23	1.94	0.50
3:G:37:VAL:O	3:G:41:ILE:HG13	2.12	0.50
3:G:47:ARG:HH22	3:C:113:LEU:HB2	1.76	0.50
3:G:154:ILE:O	3:G:154:ILE:HD13	2.11	0.50
3:G:252:LEU:HG	3:G:283:VAL:HG21	1.93	0.50
3:C:38:LEU:O	3:C:38:LEU:HD23	2.11	0.50
3:A:119:GLY:C	3:A:120:ILE:HG13	2.36	0.50
3:A:247:THR:HG22	3:A:248:ASP:N	2.26	0.50
5:L:32:ASP:HB2	5:L:66:GLU:HG3	1.94	0.50
3:G:85:ILE:HG22	3:G:302:MSE:HG3	1.94	0.49
3:C:11:GLU:HG3	3:C:44:LEU:HD21	1.94	0.49
3:C:22:VAL:HG23	3:C:23:VAL:N	2.26	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:106:LEU:O	3:C:107:HIS:C	2.54	0.49
3:C:170:GLN:O	3:C:171:SER:C	2.54	0.49
3:C:182:PHE:HD1	3:C:216:ILE:HG23	1.76	0.49
3:C:234:LEU:HB3	3:C:235:GLU:OE1	2.12	0.49
3:C:307:LYS:HD3	3:C:314:VAL:HB	1.94	0.49
3:A:193:HIS:CE1	3:A:194:ALA:HB2	2.46	0.49
2:R:706:DG:H2''	2:R:707:DC:C6	2.47	0.49
1:E:700:DC:O5'	3:A:28:ASN:O	2.25	0.49
3:G:43:ARG:HE	3:G:44:LEU:HB2	1.77	0.49
3:G:49:ASN:ND2	3:G:52:ALA:CB	2.62	0.49
3:G:204:LEU:CD1	3:G:211:VAL:CG1	2.90	0.49
3:C:29:VAL:CG1	3:C:34:ARG:HB2	2.38	0.49
3:C:248:ASP:OD1	3:C:275:ASP:HB2	2.12	0.49
3:C:315:ASP:CG	3:C:316:SER:N	2.66	0.49
3:A:43:ARG:HH11	3:A:43:ARG:HG3	1.77	0.49
3:A:200:TYR:CE1	3:A:204:LEU:HD12	2.47	0.49
3:A:252:LEU:HD21	3:A:256:HIS:CD2	2.47	0.49
4:D:249:GLU:C	4:D:251:ALA:N	2.68	0.49
5:L:43:ASN:C	5:L:45:LYS:H	2.19	0.49
5:S:63:ILE:CD1	5:S:77:LEU:HD13	2.39	0.49
1:H:702:DG:H5''	3:G:15:SER:HB3	1.94	0.49
1:E:700:DC:H5''	3:A:28:ASN:C	2.37	0.49
1:E:708:DG:C2'	1:E:709:DC:H5''	2.42	0.49
3:G:82:ILE:CD1	3:G:121:ILE:HG21	2.41	0.49
3:G:115:LYS:HZ1	3:C:92:ASN:CG	2.20	0.49
3:G:127:VAL:HG11	3:G:149:GLU:CB	2.43	0.49
3:C:259:GLN:HE22	3:C:284:ARG:HD2	1.77	0.49
3:C:277:THR:HG22	3:C:278:ARG:N	2.26	0.49
3:A:324:ARG:HH11	3:A:324:ARG:CB	2.26	0.49
5:T:23:VAL:O	5:T:26:ALA:N	2.43	0.49
5:Y:77:LEU:O	5:Y:81:MET:HG2	2.13	0.49
3:G:278:ARG:O	3:G:279:LEU:C	2.56	0.49
3:C:201:LYS:O	3:C:202:ARG:C	2.50	0.49
4:D:82:ILE:HD11	4:D:123:MSE:HE3	1.93	0.49
4:D:230:VAL:HG22	4:D:254:VAL:HA	1.94	0.49
1:H:708:DG:H1'	3:C:52:ALA:HB1	1.93	0.49
3:C:121:ILE:HD12	3:C:302:MSE:HE2	1.94	0.49
3:A:46:TYR:CE1	3:A:48:PRO:HG3	2.41	0.49
3:A:287:LEU:HD12	3:A:288:THR:N	2.26	0.49
4:D:310:ASN:O	4:D:311:LYS:HB2	2.12	0.49
5:S:4:LYS:HZ2	5:S:78:GLU:HG3	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:282:MSE:HG2	3:C:252:LEU:CD2	2.43	0.49
3:A:4:THR:OG1	3:A:5:ILE:N	2.46	0.49
4:D:149:GLU:O	4:D:149:GLU:HG3	2.13	0.49
5:S:49:GLY:O	5:S:53:LEU:HD22	2.13	0.49
2:R:712:DT:C2'	2:R:713:DC:O4'	2.58	0.49
3:G:151:THR:CB	3:G:153:GLN:HE21	2.25	0.49
3:G:157:VAL:HG21	3:G:301:ALA:HA	1.95	0.49
3:A:38:LEU:HA	3:A:41:ILE:CG2	2.42	0.49
3:A:291:VAL:HG21	3:A:326:GLU:HG2	1.93	0.49
4:D:75:TYR:O	4:D:79:ALA:N	2.40	0.49
4:D:144:LEU:N	4:D:144:LEU:CD2	2.75	0.49
4:D:255:ILE:CG2	4:D:265:VAL:HG21	2.41	0.49
2:R:711:DT:C2'	2:R:712:DT:C6	2.91	0.49
3:G:22:VAL:CG2	3:G:23:VAL:N	2.75	0.49
3:G:223:TYR:CE1	3:G:227:ILE:HD11	2.48	0.49
3:C:1:MSE:SE	3:C:47:ARG:HH21	2.46	0.49
3:C:82:ILE:CG2	3:C:302:MSE:HE3	2.42	0.49
3:A:193:HIS:HA	3:A:197:VAL:HG21	1.93	0.49
3:A:306:THR:O	3:A:310:ASN:ND2	2.46	0.49
4:D:109:LEU:O	4:D:113:LEU:HG	2.12	0.49
4:D:245:VAL:HG21	4:D:251:ALA:HA	1.94	0.49
2:B:711:DT:H2''	2:B:712:DT:O4'	2.13	0.49
3:G:141:PRO:C	3:G:142:VAL:HG23	2.37	0.49
3:G:144:LEU:HD22	3:G:144:LEU:H	1.76	0.49
3:G:251:ALA:O	3:G:255:ILE:HG13	2.13	0.49
3:C:2:ASN:OD1	3:C:2:ASN:C	2.55	0.49
3:A:180:ILE:HD13	3:A:180:ILE:N	2.27	0.49
4:D:157:VAL:O	4:D:158:THR:HB	2.12	0.49
5:S:77:LEU:O	5:S:81:MET:HG2	2.12	0.49
3:G:136:LYS:NZ	3:G:153:GLN:OE1	2.22	0.49
3:C:22:VAL:CG2	3:C:23:VAL:N	2.76	0.49
3:A:28:ASN:O	3:A:29:VAL:HG23	2.13	0.49
3:A:187:LEU:CD1	3:A:218:GLU:HB2	2.43	0.49
2:R:712:DT:OP1	2:R:712:DT:C4'	2.60	0.48
3:G:43:ARG:HH21	3:G:44:LEU:HD22	1.78	0.48
3:G:85:ILE:HD11	5:L:47:ILE:HD11	1.95	0.48
3:A:247:THR:CG2	3:A:249:GLU:H	2.23	0.48
3:A:284:ARG:CB	3:A:285:PRO:HD3	2.15	0.48
4:D:144:LEU:H	4:D:144:LEU:CD2	2.22	0.48
4:D:295:TYR:CD1	5:Y:16:ALA:HA	2.48	0.48
5:S:22:LEU:HD11	5:S:81:MET:HE2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:154:ILE:HD12	3:G:154:ILE:O	2.11	0.48
3:G:303:ARG:CG	5:L:47:ILE:HG22	2.42	0.48
3:A:14:VAL:HG21	3:A:37:VAL:HG22	1.95	0.48
3:A:270:GLU:OE1	3:A:331:THR:HB	2.13	0.48
3:A:303:ARG:O	3:A:306:THR:OG1	2.24	0.48
4:D:16:MSE:HE3	4:D:16:MSE:HB3	1.72	0.48
4:D:186:THR:CG2	4:D:187:LEU:N	2.75	0.48
4:D:311:LYS:O	4:D:312:GLU:C	2.56	0.48
5:T:56:GLN:CD	5:T:56:GLN:H	2.21	0.48
5:L:67:GLY:N	5:L:70:GLU:CG	2.74	0.48
1:H:709:DC:H2'	1:H:710:DT:C7	2.43	0.48
2:R:701:DT:H6	2:R:701:DT:H5'	1.79	0.48
3:G:5:ILE:CG2	3:G:6:TYR:N	2.76	0.48
3:G:39:GLU:O	3:G:40:THR:C	2.56	0.48
3:G:146:ALA:H	3:G:297:ILE:HG21	1.76	0.48
3:A:265:VAL:HG11	3:A:285:PRO:CB	2.44	0.48
3:A:271:ILE:N	3:A:331:THR:CG2	2.76	0.48
4:D:85:ILE:CG1	5:Y:47:ILE:HD12	2.43	0.48
4:D:228:GLU:HA	4:D:231:GLU:HG3	1.94	0.48
4:D:285:PRO:O	4:D:286:GLN:C	2.56	0.48
4:D:292:GLN:OE1	4:D:297:ILE:HD11	2.12	0.48
1:H:706:DG:H2''	1:H:707:DC:C6	2.47	0.48
2:R:711:DT:H2'	2:R:712:DT:C7	2.43	0.48
3:G:226:GLY:O	3:G:230:VAL:CG2	2.60	0.48
4:D:279:LEU:HD12	4:D:279:LEU:C	2.38	0.48
3:G:145:ALA:C	3:G:147:SER:N	2.71	0.48
3:C:130:GLU:OE2	3:C:133:GLU:OE1	2.31	0.48
3:A:17:ALA:O	3:A:21:ARG:N	2.30	0.48
4:D:67:ILE:O	4:D:97:ASN:HA	2.13	0.48
5:L:44:LEU:CD1	5:L:77:LEU:HD13	2.43	0.48
3:G:4:THR:CG2	3:G:7:ASP:CG	2.87	0.48
3:A:3:VAL:CG1	3:A:44:LEU:CG	2.89	0.48
4:D:5:ILE:CG2	4:D:16:MSE:HE1	2.44	0.48
4:D:159:ILE:CG2	4:D:160:ASP:N	2.76	0.48
4:D:243:ILE:HG22	4:D:244:PHE:N	2.29	0.48
4:D:277:THR:C	4:D:279:LEU:N	2.71	0.48
3:G:49:ASN:HB2	3:C:116:GLN:NE2	2.28	0.48
3:G:82:ILE:HG23	3:G:302:MSE:CE	2.44	0.48
3:C:151:THR:O	3:C:152:ASN:C	2.56	0.48
3:A:70:ILE:N	3:A:97:ASN:ND2	2.60	0.48
3:A:186:THR:HB	3:A:189:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:43:ARG:HH21	3:G:44:LEU:CD1	2.26	0.48
3:G:83:GLU:HG2	3:C:97:ASN:ND2	2.28	0.48
3:C:121:ILE:HG13	3:C:305:LEU:HD22	1.94	0.48
3:C:319:VAL:HG21	5:T:48:MET:CE	2.41	0.48
3:A:57:SER:C	3:A:59:LYS:H	2.22	0.48
3:A:113:LEU:O	3:A:116:GLN:NE2	2.46	0.48
3:A:271:ILE:N	3:A:271:ILE:HD12	2.29	0.48
5:T:8:VAL:CG2	5:T:57:LYS:HA	2.44	0.48
5:T:23:VAL:O	5:T:24:GLN:C	2.56	0.48
3:G:34:ARG:O	3:G:38:LEU:HD12	2.14	0.48
3:G:44:LEU:HD12	3:G:44:LEU:O	2.13	0.48
3:C:209:LEU:O	3:C:210:PRO:O	2.31	0.48
4:D:290:VAL:HG13	4:D:325:ILE:HG23	1.96	0.48
3:G:60:THR:O	3:G:62:THR:HG22	2.14	0.48
3:G:93:ILE:O	3:G:93:ILE:HG13	2.14	0.48
3:C:82:ILE:HG23	3:C:302:MSE:HE2	1.93	0.48
3:A:1:MSE:CE	3:A:1:MSE:HB3	2.44	0.48
3:A:17:ALA:O	3:A:20:SER:HB3	2.13	0.48
4:D:12:ALA:HB3	4:D:14:VAL:HG22	1.96	0.48
4:D:178:LYS:O	4:D:209:LEU:HD13	2.13	0.48
4:D:242:ALA:HA	4:D:270:GLU:H	1.79	0.48
5:L:34:ASN:ND2	5:L:41:THR:HG21	2.29	0.48
3:C:234:LEU:CD1	3:C:261:ARG:HG3	2.44	0.47
3:A:12:ALA:N	3:A:40:THR:HG21	2.29	0.47
4:D:264:ASN:ND2	4:D:264:ASN:C	2.72	0.47
4:D:276:ASN:CG	4:D:276:ASN:O	2.56	0.47
1:E:703:DA:C2'	1:E:704:DA:H5'	2.44	0.47
3:G:88:MSE:HG2	3:G:89:TYR:CD2	2.49	0.47
3:G:259:GLN:CD	3:G:284:ARG:HH11	2.22	0.47
3:C:24:ASN:HD21	3:C:53:ARG:NH2	2.11	0.47
3:C:324:ARG:CG	3:C:325:ILE:N	2.76	0.47
3:C:325:ILE:HD13	3:C:327:PHE:HE1	1.80	0.47
3:A:39:GLU:HG3	3:A:40:THR:H	1.79	0.47
3:A:75:TYR:O	3:A:76:ALA:C	2.57	0.47
5:L:43:ASN:C	5:L:45:LYS:N	2.71	0.47
3:G:241:THR:HG22	3:G:241:THR:O	2.13	0.47
3:G:263:LEU:HD12	3:G:263:LEU:N	2.28	0.47
3:C:2:ASN:O	3:C:4:THR:N	2.46	0.47
3:C:220:ASP:O	3:C:225:SER:HB3	2.14	0.47
3:C:237:ASP:C	3:C:239:LYS:H	2.22	0.47
3:A:234:LEU:HD12	3:A:261:ARG:HH12	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:328:ARG:HG2	3:A:328:ARG:HH11	1.78	0.47
4:D:224:ASP:C	4:D:226:GLY:N	2.72	0.47
4:D:252:LEU:HD21	4:D:283:VAL:HG22	1.96	0.47
5:T:35:LEU:C	5:T:35:LEU:CD2	2.87	0.47
5:T:46:SEP:O3P	5:T:48:MET:HB2	2.14	0.47
3:G:99:ASP:C	3:G:101:ASN:N	2.70	0.47
3:A:206:GLU:C	3:A:208:GLY:N	2.72	0.47
3:A:258:ALA:HB1	3:A:263:LEU:HB2	1.97	0.47
4:D:98:SER:C	4:D:100:GLN:N	2.69	0.47
4:D:261:ARG:CG	4:D:261:ARG:NH1	2.78	0.47
5:S:12:SER:O	5:S:15:HIS:HD2	1.97	0.47
1:E:704:DA:H2	2:B:711:DT:H3	1.60	0.47
3:G:282:MSE:HG3	3:C:223:TYR:CD2	2.49	0.47
3:G:309:MSE:C	3:G:311:LYS:H	2.21	0.47
3:C:106:LEU:HG	3:C:134:GLU:HG2	1.96	0.47
3:C:303:ARG:O	3:C:306:THR:OG1	2.33	0.47
4:D:209:LEU:O	4:D:210:PRO:O	2.31	0.47
3:C:87:THR:HG22	3:C:88:MSE:N	2.30	0.47
3:A:188:GLU:O	3:A:193:HIS:HD2	1.98	0.47
1:H:709:DC:C2'	1:H:710:DT:C6	2.98	0.47
2:R:702:DG:C5'	3:C:15:SER:HB2	2.45	0.47
3:G:116:GLN:CG	3:C:49:ASN:ND2	2.78	0.47
3:G:201:LYS:O	3:G:202:ARG:C	2.57	0.47
3:G:224:ASP:O	3:G:228:GLU:HG3	2.14	0.47
3:C:245:VAL:HG21	3:C:251:ALA:HA	1.96	0.47
3:C:284:ARG:CB	3:C:285:PRO:CD	2.93	0.47
3:A:168:ALA:HB1	3:A:272:ILE:CD1	2.44	0.47
3:A:192:ASN:N	3:A:192:ASN:ND2	2.54	0.47
3:A:318:ILE:N	3:A:318:ILE:CD1	2.78	0.47
4:D:209:LEU:N	4:D:210:PRO:CD	2.77	0.47
5:T:17:ARG:HB2	5:T:18:PRO:HD3	1.96	0.47
5:T:63:ILE:HD13	5:T:81:MET:HE1	1.96	0.47
5:Y:71:ALA:O	5:Y:74:LEU:N	2.47	0.47
3:C:248:ASP:OD1	3:C:274:PHE:O	2.33	0.47
3:G:62:THR:HA	3:G:92:ASN:O	2.15	0.47
3:G:73:ILE:CG2	3:C:278:ARG:NH2	2.38	0.47
3:C:160:ASP:HB3	3:C:163:GLN:HB2	1.96	0.47
3:A:41:ILE:HD13	3:A:41:ILE:O	2.15	0.47
3:A:77:GLU:HG3	3:A:294:MSE:HE2	1.97	0.47
3:A:231:GLU:O	3:A:232:LYS:C	2.58	0.47
3:A:264:ASN:OD1	3:A:266:PRO:HD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:304:LEU:CD2	3:A:308:TYR:CE2	2.97	0.47
4:D:193:HIS:ND1	4:D:193:HIS:C	2.73	0.47
5:Y:47:ILE:HG22	5:Y:51:MET:HE3	1.96	0.47
3:G:128:THR:H	3:G:131:HIS:CG	2.32	0.47
3:G:217:VAL:HG11	3:G:233:LEU:HD11	1.96	0.47
3:G:304:LEU:HA	5:L:48:MET:HE1	1.97	0.47
3:C:121:ILE:HG13	3:C:305:LEU:CD2	2.45	0.47
3:C:238:GLU:O	3:C:239:LYS:C	2.57	0.47
3:C:265:VAL:O	3:C:266:PRO:C	2.56	0.47
4:D:181:ALA:CB	4:D:233:LEU:HD11	2.45	0.47
4:D:255:ILE:HG12	4:D:271:ILE:CD1	2.44	0.47
4:D:265:VAL:HB	4:D:285:PRO:HG2	1.97	0.47
5:T:26:ALA:CB	5:T:77:LEU:HD21	2.29	0.47
3:G:33:THR:C	3:G:35:LYS:N	2.72	0.46
3:G:50:ALA:HB3	3:C:115:LYS:HD3	1.96	0.46
3:C:169:VAL:O	3:C:172:LEU:HB2	2.15	0.46
3:A:82:ILE:HG23	3:A:302:MSE:CE	2.44	0.46
4:D:187:LEU:O	4:D:189:GLU:N	2.48	0.46
5:T:79:ASP:HB3	5:T:83:LYS:CE	2.28	0.46
2:R:714:DA:C2'	2:R:715:DG:C8	2.99	0.46
3:G:108:LEU:O	3:G:112:MSE:HB2	2.14	0.46
3:G:132:VAL:O	3:G:132:VAL:HG12	2.15	0.46
3:C:154:ILE:HD12	3:C:155:PRO:CD	2.44	0.46
3:A:162:GLU:OE1	3:A:198:LYS:HE3	2.15	0.46
3:A:185:GLY:O	3:A:186:THR:C	2.59	0.46
3:A:299:ALA:CB	5:S:51:MET:HE1	2.46	0.46
5:T:17:ARG:N	5:T:18:PRO:CD	2.78	0.46
5:Y:31:SER:HA	5:Y:67:GLY:HA3	1.97	0.46
3:G:4:THR:N	3:G:7:ASP:OD2	2.41	0.46
3:G:83:GLU:HA	3:G:93:ILE:HD13	1.97	0.46
3:G:212:ARG:C	3:G:214:SER:N	2.73	0.46
3:C:288:THR:H	3:C:330:SER:HB3	1.80	0.46
3:A:194:ALA:C	3:A:195:LYS:HD2	2.41	0.46
3:A:241:THR:O	3:A:269:LEU:HA	2.16	0.46
3:A:248:ASP:OD1	3:A:274:PHE:O	2.33	0.46
4:D:102:GLN:N	4:D:102:GLN:CD	2.73	0.46
4:D:140:VAL:HB	4:D:141:PRO:HD2	1.96	0.46
5:T:36:GLU:HA	5:T:41:THR:HA	1.97	0.46
5:L:6:PHE:CG	5:L:81:MET:HE2	2.49	0.46
3:G:263:LEU:CD2	3:G:269:LEU:HD22	2.46	0.46
3:C:68:PRO:HG2	3:C:75:TYR:CZ	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:ILE:HG22	3:C:321:LEU:O	2.16	0.46
3:A:158:THR:HG23	3:A:159:ILE:N	2.31	0.46
3:A:234:LEU:HD12	3:A:261:ARG:NH1	2.31	0.46
4:D:122:PHE:O	4:D:144:LEU:HA	2.16	0.46
4:D:224:ASP:C	4:D:226:GLY:H	2.22	0.46
3:G:8:VAL:HG13	3:G:40:THR:CG2	2.43	0.46
3:G:156:SER:N	3:G:317:SER:O	2.43	0.46
3:G:287:LEU:HD22	3:G:287:LEU:C	2.40	0.46
3:A:169:VAL:O	3:A:170:GLN:C	2.58	0.46
4:D:258:ALA:O	4:D:263:LEU:HB3	2.16	0.46
5:S:65:ALA:O	5:S:70:GLU:HB2	2.16	0.46
1:E:708:DG:C1'	1:E:709:DC:H5''	2.40	0.46
2:B:701:DT:C2'	2:B:702:DG:C5'	2.88	0.46
3:G:113:LEU:CD1	3:C:47:ARG:HH12	2.25	0.46
3:G:180:ILE:HD11	3:G:204:LEU:CD1	2.45	0.46
3:C:143:VAL:CG1	3:C:305:LEU:HD13	2.45	0.46
3:A:124:SER:OG	3:A:125:GLY:N	2.49	0.46
3:A:245:VAL:HG11	3:A:251:ALA:CA	2.46	0.46
5:T:57:LYS:HD3	5:T:57:LYS:C	2.41	0.46
5:Y:6:PHE:HE1	5:Y:63:ILE:CG2	2.27	0.46
3:G:279:LEU:O	3:G:280:SER:C	2.58	0.46
3:A:305:LEU:HD11	3:A:309:MSE:HE2	1.97	0.46
3:A:324:ARG:CG	3:A:325:ILE:N	2.78	0.46
4:D:182:PHE:CD1	4:D:182:PHE:C	2.92	0.46
4:D:304:LEU:HG	4:D:308:TYR:CE2	2.51	0.46
1:H:703:DA:H62	3:G:17:ALA:CB	2.27	0.46
3:G:284:ARG:CB	3:G:285:PRO:CD	2.88	0.46
3:C:307:LYS:CD	3:C:314:VAL:HG21	2.46	0.46
3:A:57:SER:O	3:A:58:LYS:HB2	2.15	0.46
4:D:62:THR:CG2	4:D:94:ILE:HG13	2.46	0.46
4:D:234:LEU:HD21	4:D:269:LEU:HD23	1.97	0.46
5:T:22:LEU:HD13	5:T:80:THR:HG22	1.98	0.46
5:L:4:LYS:HD3	5:L:78:GLU:OE1	2.15	0.46
3:G:43:ARG:NE	3:G:44:LEU:HB2	2.31	0.46
3:G:193:HIS:CD2	3:G:193:HIS:C	2.93	0.46
3:A:114:GLY:C	3:A:116:GLN:N	2.74	0.46
3:A:115:LYS:O	3:A:116:GLN:HB2	2.15	0.46
3:A:295:TYR:CD1	3:A:295:TYR:C	2.94	0.46
4:D:18:THR:O	4:D:22:VAL:HG23	2.16	0.46
4:D:112:MSE:HE3	4:D:112:MSE:HA	1.98	0.46
3:C:67:ILE:HD12	3:C:95:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:183:VAL:HA	3:C:217:VAL:O	2.15	0.46
3:C:185:GLY:O	3:C:186:THR:C	2.59	0.46
3:A:170:GLN:HA	3:A:170:GLN:NE2	2.26	0.46
4:D:39:GLU:C	4:D:41:ILE:N	2.73	0.46
4:D:170:GLN:HE21	4:D:173:ILE:HG13	1.80	0.46
4:D:237:ASP:O	4:D:239:LYS:N	2.49	0.46
5:L:17:ARG:N	5:L:18:PRO:CD	2.79	0.46
1:H:709:DC:H2'	1:H:710:DT:C5	2.51	0.45
1:E:706:DG:OP1	1:E:706:DG:C4'	2.53	0.45
3:G:80:ARG:HD3	3:C:70:ILE:HD11	1.98	0.45
3:C:159:ILE:HD12	3:C:323:HIS:HB3	1.98	0.45
3:A:8:VAL:CG2	3:A:44:LEU:HD23	2.47	0.45
3:A:38:LEU:C	3:A:38:LEU:CD2	2.88	0.45
3:A:310:ASN:O	3:A:311:LYS:HB2	2.16	0.45
4:D:78:LEU:HD11	4:D:123:MSE:HE1	1.98	0.45
4:D:166:PHE:CD2	4:D:203:ALA:HB2	2.52	0.45
4:D:279:LEU:C	4:D:281:THR:N	2.73	0.45
5:L:61:ILE:HD11	5:L:81:MET:HE1	1.98	0.45
2:R:707:DC:C2	3:C:55:LEU:HD13	2.51	0.45
3:A:137:LYS:HE2	3:A:137:LYS:CA	2.44	0.45
2:R:713:DC:C2'	2:R:714:DA:C8	3.00	0.45
3:G:84:ASP:OD1	3:G:295:TYR:OH	2.34	0.45
3:C:190:PRO:O	3:C:191:ILE:C	2.58	0.45
3:A:148:ILE:HD13	3:A:190:PRO:HB2	1.98	0.45
3:A:160:ASP:HB2	3:A:320:GLN:OE1	2.16	0.45
3:A:224:ASP:O	3:A:226:GLY:N	2.49	0.45
3:A:285:PRO:O	3:A:286:GLN:C	2.59	0.45
5:S:9:THR:H	5:S:87:GLY:HA3	1.81	0.45
5:S:11:ASP:HA	5:S:57:LYS:HE2	1.98	0.45
2:B:705:DA:H2''	2:B:706:DG:O5'	2.17	0.45
3:G:128:THR:H	3:G:131:HIS:CD2	2.35	0.45
3:C:169:VAL:HG11	3:C:203:ALA:CB	2.46	0.45
3:C:324:ARG:HH12	3:C:326:GLU:CD	2.25	0.45
3:A:39:GLU:HG3	3:A:40:THR:N	2.31	0.45
3:A:154:ILE:HD12	3:A:154:ILE:O	2.17	0.45
3:A:271:ILE:N	3:A:331:THR:HG22	2.32	0.45
3:A:284:ARG:HG2	4:D:256:HIS:HE1	1.81	0.45
5:S:63:ILE:HG13	5:S:64:SER:N	2.28	0.45
1:H:700:DC:H42	2:R:715:DG:H1	1.63	0.45
3:G:247:THR:HG22	3:G:249:GLU:N	2.31	0.45
3:C:19:VAL:O	3:C:22:VAL:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:170:GLN:CA	3:C:170:GLN:HE21	2.30	0.45
3:C:204:LEU:HD13	3:C:211:VAL:CG1	2.46	0.45
3:C:285:PRO:O	3:C:285:PRO:HG2	2.17	0.45
3:A:29:VAL:HB	3:A:34:ARG:NE	2.31	0.45
3:A:304:LEU:HD22	3:A:308:TYR:HE2	1.80	0.45
4:D:166:PHE:O	4:D:170:GLN:HB2	2.17	0.45
5:S:76:ALA:O	5:S:79:ASP:HB3	2.17	0.45
3:G:116:GLN:HG3	3:C:49:ASN:ND2	2.32	0.45
3:C:6:TYR:HB2	3:C:16:MSE:SE	2.66	0.45
3:C:235:GLU:CD	3:C:235:GLU:N	2.74	0.45
3:A:12:ALA:HB2	3:A:40:THR:HG21	1.98	0.45
3:A:12:ALA:HB3	3:A:14:VAL:HG22	1.98	0.45
3:A:29:VAL:CG2	3:A:34:ARG:HH21	2.29	0.45
3:A:144:LEU:HD11	3:A:154:ILE:CD1	2.47	0.45
3:A:330:SER:OG	3:A:331:THR:HG23	2.15	0.45
4:D:15:SER:O	4:D:16:MSE:C	2.59	0.45
4:D:290:VAL:CA	4:D:325:ILE:HG22	2.44	0.45
1:E:714:DA:C3'	1:E:715:DG:H5''	2.46	0.45
5:Y:14:ILE:HG12	5:Y:19:ALA:HB2	1.99	0.45
2:R:709:DC:H6	2:R:709:DC:H5''	1.82	0.45
3:G:22:VAL:O	3:G:25:GLY:N	2.48	0.45
3:C:230:VAL:O	3:C:231:GLU:C	2.59	0.45
3:A:50:ALA:CB	4:D:115:LYS:HD2	2.47	0.45
3:A:193:HIS:ND1	3:A:193:HIS:C	2.75	0.45
3:A:230:VAL:HG21	3:A:254:VAL:HA	1.98	0.45
4:D:209:LEU:N	4:D:210:PRO:HD3	2.31	0.45
4:D:228:GLU:HA	4:D:231:GLU:CG	2.47	0.45
4:D:276:ASN:OD1	4:D:328:ARG:NH2	2.48	0.45
3:C:144:LEU:HD22	3:C:144:LEU:H	1.80	0.45
3:C:189:GLU:O	3:C:192:ASN:HB2	2.16	0.45
3:A:212:ARG:HD3	3:A:215:TYR:CG	2.52	0.45
4:D:180:ILE:HD11	4:D:204:LEU:HD13	1.98	0.45
4:D:253:GLY:O	4:D:254:VAL:C	2.59	0.45
5:L:44:LEU:HD23	5:L:44:LEU:HA	1.85	0.45
5:S:43:ASN:OD1	5:S:45:LYS:N	2.43	0.45
5:S:43:ASN:C	5:S:45:LYS:N	2.73	0.45
5:S:66:GLU:OE1	5:S:66:GLU:N	2.50	0.45
1:H:703:DA:H2	2:R:712:DT:H3	1.65	0.45
2:R:702:DG:C2'	2:R:703:DT:H5'	2.35	0.45
3:G:98:SER:O	3:G:99:ASP:HB2	2.17	0.45
3:C:159:ILE:O	3:C:161:TYR:CD1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:204:LEU:CD1	3:C:211:VAL:CG1	2.95	0.45
3:C:263:LEU:CD2	3:C:269:LEU:HG	2.47	0.45
3:C:303:ARG:NH1	3:C:303:ARG:CG	2.80	0.45
3:A:4:THR:HG22	3:A:7:ASP:OD2	2.17	0.45
4:D:181:ALA:HB1	4:D:233:LEU:HD11	1.99	0.45
4:D:269:LEU:HD12	4:D:269:LEU:C	2.42	0.45
4:D:319:VAL:HG21	5:Y:48:MET:HE2	1.99	0.45
3:G:102:GLN:CD	3:G:102:GLN:N	2.75	0.44
3:C:291:VAL:N	3:C:324:ARG:O	2.48	0.44
3:C:327:PHE:N	3:C:327:PHE:CD1	2.85	0.44
3:A:157:VAL:O	3:A:157:VAL:HG22	2.17	0.44
3:A:305:LEU:CG	3:A:309:MSE:HE3	2.41	0.44
4:D:72:ASN:ND2	4:D:73:ILE:HD13	2.31	0.44
4:D:219:GLY:O	4:D:220:ASP:C	2.60	0.44
4:D:252:LEU:HG	4:D:283:VAL:HG22	1.98	0.44
5:Y:46:SEP:O	5:Y:50:VAL:HG23	2.17	0.44
5:S:34:ASN:HD21	5:S:41:THR:CG2	2.30	0.44
3:C:30:LYS:HA	3:C:31:PRO:HD3	1.79	0.44
3:C:160:ASP:O	3:C:162:GLU:N	2.50	0.44
3:C:315:ASP:O	3:C:316:SER:HB3	2.17	0.44
3:A:121:ILE:HD12	3:A:302:MSE:CE	2.44	0.44
3:A:211:VAL:O	3:A:211:VAL:HG23	2.17	0.44
4:D:62:THR:O	4:D:117:VAL:HG12	2.17	0.44
4:D:109:LEU:HD12	4:D:120:ILE:HD13	1.99	0.44
5:L:8:VAL:HG11	5:L:55:ILE:HG23	1.99	0.44
5:S:37:PHE:HE2	5:S:59:ALA:HB1	1.83	0.44
2:R:710:DT:O4'	3:G:56:ALA:HB1	2.17	0.44
3:G:4:THR:OG1	3:G:5:ILE:N	2.50	0.44
3:G:22:VAL:HG21	3:G:37:VAL:CG1	2.47	0.44
3:G:82:ILE:HG23	3:G:302:MSE:HE2	1.99	0.44
4:D:327:PHE:N	4:D:327:PHE:CD1	2.84	0.44
3:G:287:LEU:HD11	3:G:289:SER:HB3	2.00	0.44
3:C:278:ARG:HB3	3:C:282:MSE:CE	2.48	0.44
3:A:149:GLU:HG2	3:A:154:ILE:HD12	1.98	0.44
3:A:172:LEU:O	3:A:173:ILE:C	2.61	0.44
3:A:228:GLU:O	3:A:229:ALA:C	2.61	0.44
5:T:72:ASP:O	5:T:73:ALA:C	2.61	0.44
3:G:43:ARG:HH21	3:G:44:LEU:CD2	2.30	0.44
3:G:66:ILE:HG23	3:G:108:LEU:HD12	1.99	0.44
3:G:263:LEU:HB3	3:G:268:ASP:HB2	1.99	0.44
3:G:303:ARG:O	3:G:304:LEU:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:158:THR:OG1	3:C:161:TYR:CE1	2.62	0.44
3:A:68:PRO:O	3:A:97:ASN:HB3	2.17	0.44
3:A:204:LEU:HD23	3:A:204:LEU:HA	1.79	0.44
4:D:89:TYR:O	4:D:91:TYR:HD1	2.00	0.44
4:D:315:ASP:O	4:D:316:SER:HB2	2.18	0.44
5:L:3:GLN:N	5:L:74:LEU:HD21	2.33	0.44
5:L:12:SER:O	5:L:15:HIS:HD2	2.01	0.44
3:G:276:ASN:HD22	3:G:276:ASN:C	2.26	0.44
3:C:265:VAL:HA	3:C:269:LEU:CD1	2.48	0.44
4:D:183:VAL:HG12	4:D:250:MSE:HE2	1.99	0.44
4:D:283:VAL:O	4:D:284:ARG:O	2.36	0.44
1:E:706:DG:C2'	1:E:707:DC:C5	3.01	0.44
3:G:33:THR:O	3:G:35:LYS:N	2.50	0.44
3:G:87:THR:O	3:G:88:MSE:C	2.59	0.44
3:C:67:ILE:H	3:C:67:ILE:HD13	1.82	0.44
3:C:181:ALA:HB1	3:C:233:LEU:HD11	1.99	0.44
3:A:22:VAL:HG21	3:A:37:VAL:HG11	1.99	0.44
3:A:70:ILE:O	3:A:70:ILE:CG1	2.65	0.44
3:A:295:TYR:CD1	5:S:16:ALA:HA	2.53	0.44
4:D:165:ALA:HA	4:D:244:PHE:CZ	2.53	0.44
5:T:79:ASP:C	5:T:83:LYS:HG2	2.43	0.44
5:L:18:PRO:HA	5:L:84:GLU:OE1	2.18	0.44
5:Y:46:SEP:O3P	5:Y:48:MET:CB	2.65	0.44
1:E:701:DT:P	3:A:30:LYS:HB2	2.58	0.44
2:B:709:DC:H2'	2:B:710:DT:H72	2.00	0.44
3:G:303:ARG:HD3	5:L:46:SEP:O3P	2.18	0.44
3:C:154:ILE:HD12	3:C:155:PRO:HD2	2.00	0.44
3:C:252:LEU:CG	3:C:283:VAL:CG1	2.90	0.44
3:A:29:VAL:CG1	3:A:34:ARG:HE	2.31	0.44
3:A:43:ARG:NH1	3:A:43:ARG:HG3	2.33	0.44
4:D:193:HIS:ND1	4:D:194:ALA:N	2.66	0.44
5:T:63:ILE:O	5:T:63:ILE:HG22	2.17	0.44
2:R:713:DC:H4'	2:R:713:DC:OP1	2.18	0.44
2:B:701:DT:H2'	4:D:18:THR:HG23	2.00	0.44
2:B:704:DT:H1'	2:B:705:DA:C5'	2.37	0.44
3:G:247:THR:HG23	3:G:248:ASP:N	2.33	0.44
3:C:58:LYS:O	3:C:59:LYS:HG2	2.18	0.44
3:C:182:PHE:CE1	3:C:184:SER:HB3	2.53	0.44
3:C:263:LEU:N	3:C:263:LEU:CD1	2.79	0.44
3:A:22:VAL:HG21	3:A:37:VAL:HG12	2.00	0.44
3:A:41:ILE:C	3:A:41:ILE:CD1	2.87	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:149:GLU:HG3	3:A:149:GLU:O	2.16	0.44
3:A:252:LEU:CD2	4:D:282:MSE:HB3	2.48	0.44
3:A:274:PHE:O	3:A:275:ASP:CB	2.62	0.44
4:D:201:LYS:HE3	4:D:202:ARG:HA	2.00	0.44
4:D:255:ILE:HG23	4:D:265:VAL:CG2	2.41	0.44
5:T:26:ALA:HB2	5:T:77:LEU:HD11	2.00	0.44
5:L:82:SER:C	5:L:85:GLY:H	2.25	0.44
3:G:43:ARG:CZ	3:G:44:LEU:HB2	2.46	0.43
3:G:113:LEU:CB	3:C:47:ARG:HH11	2.30	0.43
3:G:149:GLU:OE1	3:G:154:ILE:HD11	2.18	0.43
3:G:275:ASP:O	3:G:276:ASN:HB3	2.18	0.43
3:A:3:VAL:HG21	3:A:44:LEU:HG	2.00	0.43
3:A:39:GLU:O	3:A:42:GLU:HB3	2.17	0.43
4:D:150:SER:O	4:D:152:ASN:ND2	2.50	0.43
4:D:212:ARG:C	4:D:214:SER:H	2.26	0.43
5:T:37:PHE:CE2	5:T:59:ALA:HB1	2.53	0.43
3:G:159:ILE:HA	3:G:159:ILE:HD12	1.70	0.43
3:G:180:ILE:HD11	3:G:204:LEU:HD11	1.99	0.43
3:C:8:VAL:C	3:C:10:ARG:N	2.75	0.43
3:C:251:ALA:O	3:C:254:VAL:HB	2.18	0.43
3:C:307:LYS:HD3	3:C:314:VAL:HG21	2.00	0.43
3:A:85:ILE:O	3:A:89:TYR:HD2	2.01	0.43
3:A:158:THR:OG1	3:A:161:TYR:HE1	2.01	0.43
3:A:244:PHE:HA	3:A:272:ILE:HG23	1.99	0.43
4:D:35:LYS:HD3	4:D:38:LEU:HD13	2.00	0.43
4:D:212:ARG:HG3	4:D:212:ARG:NH1	2.33	0.43
4:D:220:ASP:O	4:D:225:SER:OG	2.28	0.43
5:T:84:GLU:OE1	5:T:84:GLU:HA	2.18	0.43
5:Y:33:ILE:HG12	5:Y:65:ALA:CB	2.48	0.43
3:G:89:TYR:O	3:G:90:LYS:HD3	2.18	0.43
3:C:125:GLY:O	3:C:189:GLU:OE2	2.35	0.43
3:C:190:PRO:O	3:C:194:ALA:CB	2.62	0.43
3:A:188:GLU:O	3:A:193:HIS:CD2	2.71	0.43
4:D:247:THR:HB	4:D:250:MSE:HG2	2.00	0.43
4:D:279:LEU:C	4:D:281:THR:H	2.27	0.43
5:T:15:HIS:O	5:T:18:PRO:HD2	2.18	0.43
1:H:702:DG:C5'	3:G:15:SER:HB3	2.48	0.43
2:R:700:DC:C3'	2:R:701:DT:H5''	2.42	0.43
3:G:286:GLN:HB3	3:G:328:ARG:HD3	2.00	0.43
3:A:12:ALA:CA	3:A:40:THR:HG21	2.48	0.43
3:A:199:GLY:O	3:A:200:TYR:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:212:ARG:HH11	3:A:212:ARG:HG3	1.83	0.43
3:A:272:ILE:HG23	3:A:272:ILE:O	2.18	0.43
4:D:169:VAL:CG2	4:D:172:LEU:HD12	2.35	0.43
4:D:204:LEU:HD23	4:D:211:VAL:CG1	2.33	0.43
4:D:258:ALA:CB	4:D:269:LEU:HD21	2.47	0.43
5:T:17:ARG:O	5:T:18:PRO:C	2.62	0.43
5:Y:20:THR:O	5:Y:24:GLN:HB2	2.18	0.43
5:S:7:THR:OG1	5:S:88:GLU:OXT	2.33	0.43
2:R:702:DG:H2'	2:R:703:DT:C7	2.49	0.43
1:E:703:DA:H1'	1:E:704:DA:C5'	2.48	0.43
3:C:227:ILE:HD13	3:C:253:GLY:O	2.19	0.43
3:A:245:VAL:O	3:A:273:GLY:HA2	2.19	0.43
4:D:173:ILE:CD1	4:D:209:LEU:HD12	2.46	0.43
4:D:182:PHE:CZ	4:D:184:SER:HB3	2.53	0.43
4:D:303:ARG:HG2	5:Y:48:MET:HB2	2.00	0.43
5:Y:4:LYS:O	5:Y:62:THR:HG23	2.18	0.43
3:G:80:ARG:CD	3:C:70:ILE:CD1	2.95	0.43
3:G:184:SER:C	3:G:250:MSE:HE1	2.44	0.43
3:G:212:ARG:C	3:G:214:SER:H	2.26	0.43
3:C:41:ILE:HG22	3:C:42:GLU:N	2.33	0.43
3:A:85:ILE:HD11	5:S:20:THR:CG2	2.48	0.43
3:A:204:LEU:O	3:A:209:LEU:N	2.42	0.43
3:A:253:GLY:O	3:A:254:VAL:C	2.62	0.43
3:A:296:ASP:O	3:A:297:ILE:C	2.59	0.43
4:D:41:ILE:O	4:D:45:GLY:N	2.50	0.43
4:D:114:GLY:C	4:D:116:GLN:N	2.76	0.43
4:D:190:PRO:O	4:D:194:ALA:HB3	2.19	0.43
2:R:712:DT:C5	2:R:713:DC:C4	3.07	0.43
3:C:37:VAL:C	3:C:39:GLU:H	2.26	0.43
3:C:145:ALA:O	3:C:146:ALA:C	2.62	0.43
3:A:143:VAL:CG1	3:A:305:LEU:HB2	2.43	0.43
4:D:70:ILE:O	4:D:70:ILE:HG23	2.18	0.43
4:D:115:LYS:NZ	4:D:115:LYS:HB3	2.34	0.43
4:D:243:ILE:N	4:D:270:GLU:O	2.52	0.43
5:T:2:ALA:HB2	5:T:70:GLU:OE2	2.19	0.43
5:L:80:THR:O	5:L:81:MET:C	2.62	0.43
5:Y:73:ALA:O	5:Y:77:LEU:HG	2.17	0.43
3:G:217:VAL:HG11	3:G:233:LEU:HD21	1.99	0.43
3:G:255:ILE:CG2	3:G:265:VAL:HG21	2.49	0.43
3:G:263:LEU:HD23	3:G:269:LEU:HD22	2.00	0.43
3:C:324:ARG:NE	5:T:56:GLN:HG2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:8:VAL:HG13	3:A:40:THR:OG1	2.19	0.43
3:A:26:ASN:O	3:A:27:PRO:C	2.60	0.43
3:A:212:ARG:HG3	3:A:212:ARG:NH1	2.33	0.43
4:D:156:SER:OG	4:D:157:VAL:N	2.52	0.43
5:T:46:SEP:P	5:T:48:MET:HB2	2.59	0.43
5:L:3:GLN:HA	5:L:74:LEU:HD11	2.00	0.43
5:L:61:ILE:HG13	5:L:63:ILE:CD1	2.49	0.43
3:G:22:VAL:O	3:G:23:VAL:C	2.61	0.43
3:G:80:ARG:NH1	5:L:17:ARG:NH1	2.66	0.43
3:G:298:GLY:O	3:G:299:ALA:O	2.37	0.43
3:C:264:ASN:HD22	3:C:267:ASN:N	2.02	0.43
3:C:317:SER:C	3:C:318:ILE:HD12	2.44	0.43
3:A:16:MSE:O	3:A:20:SER:N	2.45	0.43
3:A:265:VAL:HG21	3:A:285:PRO:HG2	2.00	0.43
4:D:259:GLN:C	4:D:261:ARG:N	2.75	0.43
1:E:709:DC:H2''	1:E:710:DT:O5'	2.19	0.43
3:G:104:LYS:O	3:G:105:GLU:C	2.60	0.43
3:G:190:PRO:O	3:G:191:ILE:C	2.61	0.43
3:G:325:ILE:HG22	3:G:326:GLU:H	1.83	0.43
3:C:2:ASN:O	3:C:4:THR:HG22	2.19	0.43
3:C:300:VAL:CG2	5:T:51:MET:HE3	2.48	0.43
3:A:193:HIS:HA	3:A:197:VAL:HG23	1.99	0.43
3:A:242:ALA:HB2	3:A:270:GLU:HB2	2.00	0.43
5:S:14:ILE:HD11	5:S:61:ILE:HD13	2.01	0.43
3:G:140:VAL:C	3:G:141:PRO:O	2.60	0.42
3:G:144:LEU:HD23	3:G:156:SER:HB3	2.00	0.42
3:C:169:VAL:O	3:C:172:LEU:N	2.50	0.42
3:C:178:LYS:HA	3:C:209:LEU:CD2	2.49	0.42
3:C:178:LYS:HG3	3:C:209:LEU:HD23	2.01	0.42
3:C:187:LEU:C	3:C:189:GLU:H	2.26	0.42
3:C:303:ARG:HG3	3:C:303:ARG:NH1	2.25	0.42
3:A:5:ILE:HD12	3:A:5:ILE:HA	1.85	0.42
3:A:93:ILE:HG23	3:A:94:ILE:N	2.33	0.42
3:A:100:GLN:OE1	3:A:125:GLY:N	2.51	0.42
5:Y:23:VAL:HG22	5:Y:50:VAL:HG21	2.01	0.42
5:Y:53:LEU:HD23	5:Y:53:LEU:HA	1.90	0.42
3:A:252:LEU:HD23	3:A:252:LEU:C	2.43	0.42
4:D:82:ILE:O	4:D:302:MSE:HG3	2.19	0.42
4:D:255:ILE:HD11	4:D:287:LEU:HD13	2.01	0.42
5:T:53:LEU:HB2	5:T:55:ILE:HG13	2.01	0.42
5:Y:31:SER:OG	5:Y:70:GLU:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:30:LYS:HG3	3:G:31:PRO:HD2	2.00	0.42
3:G:78:LEU:HD21	3:G:146:ALA:CB	2.49	0.42
3:G:127:VAL:HG11	3:G:149:GLU:HB2	2.01	0.42
3:G:143:VAL:CG2	3:G:144:LEU:N	2.82	0.42
3:G:224:ASP:O	3:G:227:ILE:N	2.53	0.42
3:C:162:GLU:OE2	3:C:199:GLY:CA	2.66	0.42
3:A:35:LYS:O	3:A:39:GLU:N	2.49	0.42
3:A:114:GLY:C	3:A:116:GLN:H	2.27	0.42
4:D:233:LEU:CD2	4:D:240:PRO:HG2	2.50	0.42
4:D:294:MSE:H	4:D:294:MSE:HG3	1.71	0.42
3:G:69:ASP:OD2	3:G:72:ASN:N	2.52	0.42
3:G:106:LEU:CD2	3:G:130:GLU:OE1	2.67	0.42
3:G:150:SER:O	3:G:152:ASN:N	2.53	0.42
3:G:183:VAL:CG2	3:G:229:ALA:HB1	2.49	0.42
3:C:182:PHE:HD2	3:C:244:PHE:HD1	1.68	0.42
3:C:270:GLU:OE2	3:C:331:THR:HG23	2.18	0.42
3:A:91:TYR:CE2	3:A:309:MSE:SE	3.23	0.42
3:A:173:ILE:HD11	3:A:204:LEU:CD2	2.49	0.42
4:D:252:LEU:CG	4:D:283:VAL:HG22	2.50	0.42
1:E:711:DA:N1	2:B:705:DA:C2	2.88	0.42
3:G:159:ILE:HD12	3:G:321:LEU:O	2.19	0.42
3:G:286:GLN:O	3:G:328:ARG:HB2	2.20	0.42
3:G:287:LEU:CD1	3:G:289:SER:HB3	2.48	0.42
3:C:131:HIS:O	3:C:135:LEU:N	2.41	0.42
3:C:144:LEU:CD2	3:C:155:PRO:O	2.68	0.42
3:C:158:THR:O	3:C:320:GLN:HA	2.19	0.42
3:A:144:LEU:HD11	3:A:154:ILE:HD11	2.01	0.42
4:D:186:THR:HG22	4:D:187:LEU:H	1.82	0.42
3:G:11:GLU:HB3	3:G:40:THR:HG23	2.02	0.42
3:G:296:ASP:HB3	3:G:321:LEU:HD23	2.01	0.42
3:G:325:ILE:CG2	3:G:326:GLU:N	2.82	0.42
3:A:159:ILE:CD1	3:A:321:LEU:O	2.65	0.42
3:A:212:ARG:O	3:A:215:TYR:HB2	2.20	0.42
3:A:304:LEU:HG	5:S:48:MET:HE1	2.01	0.42
5:L:8:VAL:HG11	5:L:59:ALA:HB3	2.02	0.42
5:Y:5:THR:HG23	5:Y:61:ILE:O	2.20	0.42
5:Y:44:LEU:HG	5:Y:63:ILE:HD13	2.00	0.42
2:B:710:DT:H2"	2:B:711:DT:H72	2.02	0.42
3:G:4:THR:HG22	3:G:7:ASP:OD2	2.19	0.42
3:G:172:LEU:O	3:G:173:ILE:C	2.62	0.42
3:A:33:THR:O	3:A:37:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:123:MSE:HB2	3:A:145:ALA:O	2.20	0.42
3:A:321:LEU:O	3:A:322:PRO:C	2.63	0.42
4:D:106:LEU:O	4:D:109:LEU:HB3	2.19	0.42
5:L:8:VAL:O	5:L:58:GLY:N	2.46	0.42
5:L:67:GLY:N	5:L:70:GLU:OE1	2.48	0.42
1:E:703:DA:C1'	1:E:704:DA:H5'	2.46	0.42
2:B:714:DA:H5'	2:B:714:DA:H8	1.85	0.42
3:C:165:ALA:CB	3:C:199:GLY:HA3	2.48	0.42
4:D:145:ALA:C	4:D:147:SER:N	2.78	0.42
5:L:6:PHE:HE1	5:L:63:ILE:HB	1.84	0.42
5:L:11:ASP:CA	5:L:57:LYS:HE3	2.38	0.42
5:L:73:ALA:O	5:L:76:ALA:N	2.51	0.42
5:L:81:MET:HE3	5:L:87:GLY:HA3	2.02	0.42
5:S:6:PHE:CD1	5:S:6:PHE:N	2.87	0.42
3:G:106:LEU:HD12	3:G:106:LEU:N	2.34	0.42
3:G:243:ILE:HG22	3:G:244:PHE:N	2.35	0.42
3:A:158:THR:O	3:A:159:ILE:HD13	2.19	0.42
3:A:252:LEU:CD2	3:A:256:HIS:CD2	3.02	0.42
4:D:245:VAL:HG11	4:D:251:ALA:CA	2.50	0.42
5:T:42:VAL:HG13	5:T:53:LEU:HD21	2.01	0.42
1:H:709:DC:H2'	1:H:710:DT:C6	2.54	0.41
3:G:267:ASN:O	3:G:268:ASP:C	2.62	0.41
3:G:279:LEU:O	3:G:282:MSE:N	2.53	0.41
3:C:318:ILE:HD12	3:C:318:ILE:N	2.34	0.41
3:A:141:PRO:C	3:A:142:VAL:HG23	2.45	0.41
3:A:265:VAL:HG11	3:A:285:PRO:HB2	2.02	0.41
3:A:304:LEU:CD2	3:A:308:TYR:HE2	2.32	0.41
5:T:4:LYS:HE3	5:T:5:THR:O	2.21	0.41
5:L:29:PHE:HB3	5:L:69:ASP:OD1	2.20	0.41
5:L:74:LEU:C	5:L:76:ALA:N	2.74	0.41
5:Y:6:PHE:HA	5:Y:88:GLU:O	2.20	0.41
5:S:22:LEU:HD23	5:S:44:LEU:HD21	2.01	0.41
5:S:43:ASN:C	5:S:45:LYS:H	2.27	0.41
2:R:709:DC:OP2	3:G:5:ILE:HB	2.20	0.41
1:E:707:DC:C2'	3:A:55:LEU:HD22	2.49	0.41
3:G:119:GLY:HA3	3:G:305:LEU:HD21	2.02	0.41
3:A:3:VAL:HG13	3:A:44:LEU:CD2	2.49	0.41
3:A:74:PHE:CD2	3:A:294:MSE:HG2	2.55	0.41
3:A:168:ALA:HB1	3:A:272:ILE:HD11	2.01	0.41
3:A:288:THR:HA	3:A:328:ARG:HG3	2.01	0.41
3:G:22:VAL:HG21	3:G:37:VAL:HG11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:223:TYR:O	3:G:253:GLY:HA3	2.20	0.41
3:C:82:ILE:CG2	3:C:302:MSE:CE	2.98	0.41
3:C:264:ASN:ND2	3:C:264:ASN:C	2.78	0.41
3:A:30:LYS:O	3:A:34:ARG:N	2.43	0.41
3:A:224:ASP:C	3:A:226:GLY:H	2.28	0.41
3:A:252:LEU:HD23	3:A:252:LEU:O	2.19	0.41
3:A:307:LYS:HZ2	3:A:314:VAL:HG21	1.84	0.41
4:D:35:LYS:O	4:D:36:LYS:C	2.61	0.41
4:D:187:LEU:C	4:D:187:LEU:HD23	2.46	0.41
2:B:701:DT:C2'	2:B:702:DG:H5''	2.51	0.41
3:C:15:SER:OG	3:C:16:MSE:N	2.52	0.41
3:C:114:GLY:C	3:C:116:GLN:H	2.27	0.41
3:C:191:ILE:HG13	3:C:192:ASN:N	2.34	0.41
3:C:204:LEU:CD1	3:C:211:VAL:HG11	2.49	0.41
3:C:283:VAL:O	3:C:284:ARG:O	2.38	0.41
3:C:324:ARG:NH1	3:C:326:GLU:OE1	2.52	0.41
3:A:154:ILE:HA	3:A:155:PRO:HD3	1.87	0.41
3:A:243:ILE:O	3:A:272:ILE:HG22	2.21	0.41
4:D:10:ARG:O	4:D:13:SER:N	2.50	0.41
4:D:187:LEU:O	4:D:193:HIS:CB	2.64	0.41
4:D:201:LYS:O	4:D:202:ARG:C	2.64	0.41
4:D:204:LEU:HD12	4:D:204:LEU:HA	1.90	0.41
4:D:247:THR:HG22	4:D:249:GLU:N	2.36	0.41
1:E:705:DA:OP2	1:E:705:DA:H8	2.04	0.41
3:G:47:ARG:HH22	3:C:113:LEU:CB	2.33	0.41
3:C:127:VAL:HA	3:C:131:HIS:ND1	2.36	0.41
3:C:158:THR:OG1	3:C:159:ILE:N	2.52	0.41
3:C:300:VAL:HG23	5:T:51:MET:HE3	2.03	0.41
3:C:312:GLU:HG3	3:C:314:VAL:HG23	2.01	0.41
4:D:143:VAL:HG12	4:D:305:LEU:HD13	2.02	0.41
4:D:166:PHE:CE2	4:D:202:ARG:HG2	2.54	0.41
4:D:201:LYS:CG	4:D:202:ARG:N	2.83	0.41
4:D:233:LEU:HD13	4:D:243:ILE:HD12	2.01	0.41
4:D:245:VAL:HG11	4:D:250:MSE:C	2.46	0.41
4:D:305:LEU:O	4:D:309:MSE:HG3	2.20	0.41
5:T:37:PHE:CD1	5:T:37:PHE:C	2.96	0.41
5:T:63:ILE:HD13	5:T:81:MET:CE	2.50	0.41
5:L:73:ALA:HA	5:L:76:ALA:HB3	2.01	0.41
5:Y:46:SEP:P	5:Y:48:MET:HB3	2.60	0.41
1:H:706:DG:C2'	1:H:707:DC:C5	3.00	0.41
2:B:714:DA:H2'	2:B:715:DG:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:108:LEU:HD23	3:G:108:LEU:HA	1.84	0.41
3:G:130:GLU:O	3:G:130:GLU:HG2	2.19	0.41
3:G:144:LEU:CD2	3:G:144:LEU:H	2.33	0.41
3:G:170:GLN:O	3:G:171:SER:C	2.64	0.41
3:C:5:ILE:HG23	3:C:6:TYR:N	2.35	0.41
3:A:163:GLN:O	3:A:166:PHE:N	2.53	0.41
4:D:201:LYS:O	4:D:204:LEU:N	2.47	0.41
4:D:302:MSE:CE	4:D:305:LEU:HD23	2.46	0.41
5:T:23:VAL:HG11	5:T:47:ILE:HD13	2.03	0.41
3:G:4:THR:O	3:G:7:ASP:HB2	2.20	0.41
3:G:6:TYR:C	3:G:6:TYR:CD1	2.98	0.41
3:G:307:LYS:HE3	5:L:46:SEP:O3P	2.20	0.41
3:C:100:GLN:NE2	3:C:125:GLY:H	2.14	0.41
3:C:192:ASN:O	3:C:193:HIS:C	2.63	0.41
3:A:1:MSE:HB3	3:A:1:MSE:HE3	2.03	0.41
4:D:69:ASP:C	4:D:71:SER:N	2.75	0.41
5:Y:47:ILE:H	5:Y:47:ILE:HG12	1.61	0.41
3:G:180:ILE:HD13	3:G:180:ILE:N	2.36	0.41
3:G:282:MSE:SE	3:C:249:GLU:HG3	2.70	0.41
3:C:258:ALA:CB	3:C:269:LEU:HD21	2.51	0.41
3:A:57:SER:C	3:A:59:LYS:N	2.78	0.41
3:A:317:SER:C	3:A:318:ILE:HD12	2.44	0.41
4:D:8:VAL:HG13	4:D:40:THR:HG22	2.03	0.41
4:D:174:ASP:OD2	4:D:174:ASP:O	2.38	0.41
5:L:73:ALA:O	5:L:77:LEU:N	2.47	0.41
5:Y:74:LEU:O	5:Y:78:GLU:HB2	2.21	0.41
2:R:703:DT:C7	3:C:15:SER:OG	2.69	0.41
2:R:712:DT:C6	2:R:713:DC:C5	3.09	0.41
1:E:709:DC:H5'	1:E:709:DC:C6	2.49	0.41
3:G:46:TYR:CE1	3:G:48:PRO:HB3	2.56	0.41
3:C:78:LEU:HD12	3:C:298:GLY:HA3	2.02	0.41
3:C:233:LEU:CD2	3:C:240:PRO:HG2	2.47	0.41
3:C:263:LEU:CD1	3:C:263:LEU:H	2.34	0.41
3:A:16:MSE:HA	3:A:19:VAL:HG23	2.03	0.41
3:A:38:LEU:O	3:A:41:ILE:CG2	2.69	0.41
3:A:78:LEU:O	3:A:82:ILE:HG13	2.20	0.41
3:A:80:ARG:HA	3:A:80:ARG:HD3	1.90	0.41
3:A:118:ASP:O	3:A:309:MSE:HG2	2.20	0.41
3:A:177:HIS:ND1	3:A:241:THR:CB	2.78	0.41
3:A:324:ARG:HG2	3:A:325:ILE:O	2.21	0.41
4:D:78:LEU:CD1	4:D:123:MSE:HE1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:80:ARG:O	4:D:80:ARG:HG3	2.20	0.41
4:D:223:TYR:OH	4:D:256:HIS:HD2	2.03	0.41
4:D:248:ASP:OD1	4:D:275:ASP:HB2	2.21	0.41
4:D:271:ILE:HG12	4:D:287:LEU:CD1	2.51	0.41
4:D:295:TYR:CE1	5:Y:16:ALA:HA	2.55	0.41
5:T:35:LEU:HD23	5:T:36:GLU:N	2.35	0.41
5:Y:17:ARG:O	5:Y:18:PRO:C	2.63	0.41
5:Y:69:ASP:OD1	5:Y:70:GLU:N	2.54	0.41
1:H:708:DG:H1'	1:H:709:DC:H5''	2.03	0.41
1:H:711:DA:N1	2:R:704:DT:C4	2.89	0.41
2:B:707:DC:O5'	2:B:707:DC:H6	2.04	0.41
3:G:1:MSE:O	3:G:2:ASN:C	2.59	0.41
3:G:157:VAL:O	3:G:158:THR:HB	2.20	0.41
3:C:11:GLU:OE2	3:C:40:THR:HG21	2.21	0.41
3:C:69:ASP:CG	3:C:71:SER:HB3	2.46	0.41
3:C:265:VAL:HB	3:C:285:PRO:HG3	2.02	0.41
3:A:46:TYR:CD1	3:A:46:TYR:C	2.99	0.41
3:A:74:PHE:CD2	3:A:294:MSE:CG	3.04	0.41
3:A:305:LEU:CG	3:A:309:MSE:CE	2.97	0.41
4:D:63:VAL:CG2	4:D:305:LEU:HD23	2.51	0.41
4:D:65:VAL:HG22	4:D:95:LEU:HD12	2.02	0.41
4:D:67:ILE:HG22	4:D:96:SER:O	2.20	0.41
4:D:69:ASP:C	4:D:71:SER:H	2.29	0.41
4:D:161:TYR:CD2	4:D:191:ILE:HG13	2.55	0.41
4:D:227:ILE:O	4:D:230:VAL:HG23	2.21	0.41
5:S:18:PRO:HB3	5:S:84:GLU:HG2	2.03	0.41
1:H:700:DC:N4	2:R:715:DG:H1	2.18	0.40
1:E:703:DA:C2'	1:E:704:DA:OP2	2.67	0.40
3:G:209:LEU:N	3:G:210:PRO:HD3	2.36	0.40
3:G:247:THR:HG22	3:G:248:ASP:N	2.36	0.40
3:A:7:ASP:HB3	3:A:44:LEU:CD2	2.30	0.40
3:A:187:LEU:HG	3:A:218:GLU:HB2	2.03	0.40
4:D:4:THR:HG23	4:D:7:ASP:H	1.86	0.40
4:D:252:LEU:CD2	4:D:283:VAL:HG22	2.51	0.40
5:L:20:THR:HG22	5:L:20:THR:O	2.21	0.40
2:B:708:DG:C1'	2:B:709:DC:H5''	2.50	0.40
3:G:15:SER:O	3:G:18:THR:N	2.48	0.40
3:G:166:PHE:CE2	3:G:202:ARG:HG2	2.56	0.40
4:D:180:ILE:HD11	4:D:204:LEU:CD1	2.51	0.40
4:D:303:ARG:C	4:D:306:THR:HG1	2.25	0.40
5:T:31:SER:HA	5:T:67:GLY:HA3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:Y:69:ASP:OD1	5:Y:73:ALA:HB2	2.21	0.40
1:E:709:DC:H2'	1:E:710:DT:C7	2.49	0.40
3:G:43:ARG:HE	3:G:44:LEU:CB	2.33	0.40
3:G:84:ASP:CG	3:G:295:TYR:HH	2.28	0.40
3:G:143:VAL:CG2	3:G:156:SER:HA	2.40	0.40
3:G:143:VAL:HG22	3:G:144:LEU:O	2.21	0.40
3:G:310:ASN:C	3:G:312:GLU:H	2.28	0.40
3:C:241:THR:O	3:C:269:LEU:HA	2.21	0.40
3:C:303:ARG:HD2	3:C:303:ARG:C	2.46	0.40
3:A:70:ILE:HG22	3:A:97:ASN:HD21	1.85	0.40
3:A:85:ILE:HD11	5:S:20:THR:HG23	2.02	0.40
3:A:113:LEU:HD22	3:A:139:PRO:HD2	2.02	0.40
4:D:39:GLU:O	4:D:41:ILE:N	2.55	0.40
4:D:217:VAL:O	4:D:217:VAL:HG13	2.21	0.40
4:D:303:ARG:HE	4:D:303:ARG:HA	1.86	0.40
5:L:18:PRO:HB3	5:L:86:LEU:HD21	2.02	0.40
5:L:80:THR:O	5:L:84:GLU:HB2	2.21	0.40
3:G:106:LEU:HD21	3:G:130:GLU:CD	2.46	0.40
3:G:142:VAL:CG1	3:G:143:VAL:N	2.85	0.40
3:G:212:ARG:H	3:G:212:ARG:HG2	1.62	0.40
3:C:120:ILE:HB	3:C:142:VAL:HG22	2.03	0.40
3:C:182:PHE:CD1	3:C:216:ILE:HG23	2.56	0.40
3:C:299:ALA:HB3	5:T:51:MET:HE1	2.03	0.40
4:D:35:LYS:HD3	4:D:35:LYS:HA	1.83	0.40
5:T:57:LYS:C	5:T:59:ALA:H	2.29	0.40
5:S:47:ILE:HD12	5:S:51:MET:HE2	2.04	0.40
3:G:112:MSE:O	3:G:115:LYS:HB3	2.22	0.40
3:C:42:GLU:O	3:C:43:ARG:C	2.64	0.40
3:C:168:ALA:HB3	3:C:244:PHE:HE2	1.85	0.40
3:A:173:ILE:CD1	3:A:209:LEU:HD12	2.52	0.40
3:A:182:PHE:CD2	3:A:244:PHE:O	2.75	0.40
3:A:230:VAL:O	3:A:231:GLU:C	2.64	0.40
3:A:330:SER:OG	3:A:331:THR:N	2.54	0.40
4:D:166:PHE:CD2	4:D:202:ARG:CZ	3.04	0.40
4:D:169:VAL:O	4:D:172:LEU:N	2.43	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:198:LYS:NZ	3:C:133:GLU:OE1[2_556]	2.17	0.03

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	
3	A	330/332 (99%)	259 (78%)	56 (17%)	15 (4%)	2	7
3	C	330/332 (99%)	251 (76%)	62 (19%)	17 (5%)	1	5
3	G	330/332 (99%)	271 (82%)	40 (12%)	19 (6%)	1	4
4	D	330/332 (99%)	246 (74%)	63 (19%)	21 (6%)	1	3
5	L	84/88 (96%)	71 (84%)	12 (14%)	1 (1%)	10	34
5	S	84/88 (96%)	76 (90%)	7 (8%)	1 (1%)	10	34
5	T	84/88 (96%)	72 (86%)	8 (10%)	4 (5%)	2	6
5	Y	84/88 (96%)	73 (87%)	10 (12%)	1 (1%)	10	34
All	All	1656/1680 (99%)	1319 (80%)	258 (16%)	79 (5%)	2	6

All (79) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	100	GLN
3	G	102	GLN
3	G	141	PRO
3	G	150	SER
3	G	151	THR
3	G	275	ASP
3	G	311	LYS
3	G	316	SER
3	C	44	LEU
3	C	221	TYR
3	C	236	GLU
3	C	284	ARG
3	A	286	GLN
3	A	316	SER
4	D	150	SER
4	D	151	THR
4	D	210	PRO

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Mol	Chain	Res	Type
4	D	275	ASP
4	D	284	ARG
4	D	316	SER
5	Y	70	GLU
3	G	28	ASN
3	G	29	VAL
3	G	146	ALA
3	G	210	PRO
3	G	284	ARG
3	G	330	SER
3	C	29	VAL
3	C	128	THR
3	C	192	ASN
3	A	210	PRO
3	A	230	VAL
4	D	25	GLY
4	D	45	GLY
4	D	213	ASP
4	D	221	TYR
4	D	268	ASP
4	D	278	ARG
4	D	294	MSE
5	T	70	GLU
5	T	71	ALA
5	S	68	SER
3	G	68	PRO
3	C	45	GLY
3	C	112	MSE
3	C	210	PRO
3	C	215	TYR
3	C	279	LEU
3	A	141	PRO
3	A	186	THR
3	A	213	ASP
3	A	268	ASP
3	A	275	ASP
4	D	17	ALA
4	D	68	PRO
4	D	115	LYS
4	D	190	PRO
3	G	237	ASP
3	G	265	VAL

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Mol	Chain	Res	Type
3	G	276	ASN
3	C	28	ASN
3	C	278	ARG
3	C	315	ASP
3	A	68	PRO
4	D	28	ASN
4	D	188	GLU
5	T	16	ALA
3	C	234	LEU
3	C	240	PRO
3	A	150	SER
4	D	260	ASP
5	L	70	GLU
3	A	28	ASN
4	D	16	MSE
3	G	173	ILE
5	T	55	ILE
3	A	73	ILE
3	A	322	PRO
3	A	29	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	
3	A	286/279 (102%)	235 (82%)	51 (18%)	2	6
3	C	285/279 (102%)	236 (83%)	49 (17%)	2	7
3	G	287/279 (103%)	229 (80%)	58 (20%)	1	4
4	D	285/280 (102%)	237 (83%)	48 (17%)	2	8
5	L	66/67 (98%)	51 (77%)	15 (23%)	1	3
5	S	66/67 (98%)	52 (79%)	14 (21%)	1	4
5	T	66/67 (98%)	47 (71%)	19 (29%)	0	1
5	Y	66/67 (98%)	51 (77%)	15 (23%)	1	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1407/1385 (102%)	1138 (81%)	269 (19%)	1 5

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	G	1	MSE
3	G	26	ASN
3	G	29	VAL
3	G	42	GLU
3	G	43	ARG
3	G	49	ASN
3	G	55	LEU
3	G	62	THR
3	G	63	VAL
3	G	68	PRO
3	G	73	ILE
3	G	77	GLU
3	G	78	LEU
3	G	83	GLU
3	G	84	ASP
3	G	87	THR
3	G	88	MSE
3	G	90	LYS
3	G	101	ASN
3	G	109	LEU
3	G	111	ASN
3	G	112	MSE
3	G	117	VAL
3	G	121	ILE
3	G	131	HIS
3	G	135	LEU
3	G	136	LYS
3	G	137	LYS
3	G	143	VAL
3	G	144	LEU
3	G	148	ILE
3	G	150	SER
3	G	154	ILE
3	G	155	PRO
3	G	159	ILE
3	G	162	GLU
3	G	180	ILE

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Mol	Chain	Res	Type
3	G	191	ILE
3	G	195	LYS
3	G	198	LYS
3	G	211	VAL
3	G	212	ARG
3	G	216	ILE
3	G	217	VAL
3	G	220	ASP
3	G	230	VAL
3	G	245	VAL
3	G	247	THR
3	G	248	ASP
3	G	252	LEU
3	G	265	VAL
3	G	280	SER
3	G	282	MSE
3	G	287	LEU
3	G	303	ARG
3	G	304	LEU
3	G	322	PRO
3	G	324	ARG
3	C	4	THR
3	C	5	ILE
3	C	18	THR
3	C	19	VAL
3	C	32	SER
3	C	55	LEU
3	C	62	THR
3	C	65	VAL
3	C	67	ILE
3	C	70	ILE
3	C	77	GLU
3	C	87	THR
3	C	101	ASN
3	C	102	GLN
3	C	112	MSE
3	C	115	LYS
3	C	117	VAL
3	C	129	GLU
3	C	137	LYS
3	C	143	VAL
3	C	144	LEU

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Mol	Chain	Res	Type
3	C	148	ILE
3	C	152	ASN
3	C	163	GLN
3	C	169	VAL
3	C	170	GLN
3	C	189	GLU
3	C	191	ILE
3	C	193	HIS
3	C	198	LYS
3	C	202	ARG
3	C	210	PRO
3	C	211	VAL
3	C	218	GLU
3	C	224	ASP
3	C	233	LEU
3	C	235	GLU
3	C	238	GLU
3	C	245	VAL
3	C	264	ASN
3	C	269	LEU
3	C	271	ILE
3	C	279	LEU
3	C	294	MSE
3	C	303	ARG
3	C	306	THR
3	C	321	LEU
3	C	325	ILE
3	C	327	PHE
3	A	1	MSE
3	A	7	ASP
3	A	22	VAL
3	A	24	ASN
3	A	39	GLU
3	A	41	ILE
3	A	55	LEU
3	A	63	VAL
3	A	65	VAL
3	A	78	LEU
3	A	80	ARG
3	A	84	ASP
3	A	93	ILE
3	A	95	LEU

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Mol	Chain	Res	Type
3	A	100	GLN
3	A	102	GLN
3	A	136	LYS
3	A	143	VAL
3	A	144	LEU
3	A	148	ILE
3	A	149	GLU
3	A	151	THR
3	A	153	GLN
3	A	154	ILE
3	A	157	VAL
3	A	170	GLN
3	A	180	ILE
3	A	184	SER
3	A	192	ASN
3	A	206	GLU
3	A	207	SER
3	A	210	PRO
3	A	212	ARG
3	A	216	ILE
3	A	217	VAL
3	A	220	ASP
3	A	227	ILE
3	A	230	VAL
3	A	236	GLU
3	A	240	PRO
3	A	241	THR
3	A	245	VAL
3	A	281	THR
3	A	282	MSE
3	A	288	THR
3	A	294	MSE
3	A	304	LEU
3	A	306	THR
3	A	312	GLU
3	A	316	SER
3	A	328	ARG
4	D	2	ASN
4	D	13	SER
4	D	18	THR
4	D	19	VAL
4	D	39	GLU

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Mol	Chain	Res	Type
4	D	44	LEU
4	D	55	LEU
4	D	63	VAL
4	D	65	VAL
4	D	70	ILE
4	D	73	ILE
4	D	77	GLU
4	D	78	LEU
4	D	90	LYS
4	D	93	ILE
4	D	102	GLN
4	D	112	MSE
4	D	115	LYS
4	D	117	VAL
4	D	142	VAL
4	D	144	LEU
4	D	148	ILE
4	D	149	GLU
4	D	151	THR
4	D	154	ILE
4	D	156	SER
4	D	162	GLU
4	D	170	GLN
4	D	190	PRO
4	D	193	HIS
4	D	201	LYS
4	D	210	PRO
4	D	224	ASP
4	D	230	VAL
4	D	233	LEU
4	D	235	GLU
4	D	264	ASN
4	D	269	LEU
4	D	271	ILE
4	D	272	ILE
4	D	279	LEU
4	D	292	GLN
4	D	302	MSE
4	D	303	ARG
4	D	306	THR
4	D	314	VAL
4	D	324	ARG

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Mol	Chain	Res	Type
4	D	329	GLN
5	T	6	PHE
5	T	8	VAL
5	T	9	THR
5	T	21	THR
5	T	28	LYS
5	T	34	ASN
5	T	35	LEU
5	T	36	GLU
5	T	37	PHE
5	T	42	VAL
5	T	44	LEU
5	T	52	SER
5	T	56	GLN
5	T	57	LYS
5	T	62	THR
5	T	63	ILE
5	T	80	THR
5	T	86	LEU
5	T	88	GLU
5	L	5	THR
5	L	11	ASP
5	L	14	ILE
5	L	17	ARG
5	L	24	GLN
5	L	32	ASP
5	L	35	LEU
5	L	44	LEU
5	L	47	ILE
5	L	51	MET
5	L	60	THR
5	L	62	THR
5	L	74	LEU
5	L	84	GLU
5	L	88	GLU
5	Y	6	PHE
5	Y	8	VAL
5	Y	9	THR
5	Y	11	ASP
5	Y	14	ILE
5	Y	18	PRO
5	Y	24	GLN

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Mol	Chain	Res	Type
5	Y	36	GLU
5	Y	44	LEU
5	Y	47	ILE
5	Y	56	GLN
5	Y	69	ASP
5	Y	74	LEU
5	Y	84	GLU
5	Y	88	GLU
5	S	8	VAL
5	S	9	THR
5	S	20	THR
5	S	22	LEU
5	S	27	SER
5	S	32	ASP
5	S	40	LYS
5	S	44	LEU
5	S	48	MET
5	S	52	SER
5	S	53	LEU
5	S	63	ILE
5	S	68	SER
5	S	79	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
3	G	49	ASN
3	G	92	ASN
3	G	116	GLN
3	G	163	GLN
3	G	177	HIS
3	G	192	ASN
3	G	193	HIS
3	G	276	ASN
3	G	329	GLN
3	C	2	ASN
3	C	24	ASN
3	C	100	GLN
3	C	102	GLN
3	C	111	ASN
3	C	152	ASN
3	C	163	GLN

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Mol	Chain	Res	Type
3	C	170	GLN
3	C	259	GLN
3	C	264	ASN
3	C	323	HIS
3	A	24	ASN
3	A	97	ASN
3	A	131	HIS
3	A	152	ASN
3	A	170	GLN
3	A	192	ASN
3	A	193	HIS
3	A	256	HIS
3	A	310	ASN
4	D	72	ASN
4	D	97	ASN
4	D	131	HIS
4	D	152	ASN
4	D	170	GLN
4	D	177	HIS
4	D	256	HIS
4	D	259	GLN
4	D	329	GLN
5	T	3	GLN
5	T	15	HIS
5	L	34	ASN
5	L	56	GLN
5	Y	56	GLN
5	S	3	GLN
5	S	34	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	$\# Z > 2$
5	SEP	T	46	5	8,9,10	1.20	1 (12%)	7,12,14	1.46	2 (28%)
5	SEP	Y	46	5	8,9,10	1.21	1 (12%)	7,12,14	1.26	1 (14%)
5	SEP	L	46	5	8,9,10	1.21	1 (12%)	7,12,14	1.32	1 (14%)
5	SEP	S	46	5	8,9,10	1.17	1 (12%)	7,12,14	1.67	2 (28%)

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
5	SEP	T	46	5	-	5/6/8/10	-
5	SEP	Y	46	5	-	3/6/8/10	-
5	SEP	L	46	5	-	4/6/8/10	-
5	SEP	S	46	5	-	6/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	S	46	SEP	P-O3P	-2.56	1.45	1.54
5	L	46	SEP	P-O3P	-2.49	1.45	1.54
5	Y	46	SEP	P-O3P	-2.43	1.45	1.54
5	T	46	SEP	P-O3P	-2.08	1.47	1.54

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	S	46	SEP	O3P-P-O1P	3.01	122.57	110.83
5	T	46	SEP	O3P-P-O1P	2.68	121.27	110.83
5	L	46	SEP	O3P-P-O1P	2.58	120.88	110.83
5	T	46	SEP	OG-CB-CA	-2.41	105.80	108.14
5	Y	46	SEP	O3P-P-O1P	2.36	120.02	110.83
5	S	46	SEP	OG-CB-CA	2.35	110.43	108.14

There are no chirality outliers.

All (18) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	T	46	SEP	C-CA-CB-OG
5	T	46	SEP	CB-OG-P-O1P
5	T	46	SEP	CB-OG-P-O2P
5	T	46	SEP	CB-OG-P-O3P
5	L	46	SEP	N-CA-CB-OG
5	L	46	SEP	CB-OG-P-O1P
5	L	46	SEP	CB-OG-P-O2P
5	L	46	SEP	CB-OG-P-O3P
5	Y	46	SEP	N-CA-CB-OG
5	S	46	SEP	C-CA-CB-OG
5	S	46	SEP	CB-OG-P-O1P
5	S	46	SEP	CB-OG-P-O2P
5	S	46	SEP	CB-OG-P-O3P
5	Y	46	SEP	CB-OG-P-O3P
5	S	46	SEP	CA-CB-OG-P
5	T	46	SEP	N-CA-CB-OG
5	S	46	SEP	N-CA-CB-OG
5	Y	46	SEP	CB-OG-P-O1P

There are no ring outliers.

4 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	T	46	SEP	2	0
5	Y	46	SEP	4	0
5	L	46	SEP	3	0
5	S	46	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 2 are monoatomic - leaving 7 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	$\# Z > 2$
6	SO4	A	946	-	4,4,4	0.38	0	6,6,6	0.71	0
6	SO4	G	646	-	4,4,4	0.39	0	6,6,6	0.11	0
6	SO4	C	346	-	4,4,4	0.41	0	6,6,6	0.08	0
6	SO4	C	947	-	4,4,4	0.33	0	6,6,6	0.23	0
6	SO4	G	647	-	4,4,4	0.36	0	6,6,6	0.20	0
6	SO4	A	599	-	4,4,4	0.41	0	6,6,6	0.14	0
6	SO4	C	846	-	4,4,4	0.36	0	6,6,6	0.29	0

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.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	946	SO4	1	0
6	C	947	SO4	1	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	E	16/16 (100%)	-1.38	0 100 100	49, 75, 90, 91	0
1	H	16/16 (100%)	-1.33	0 100 100	52, 78, 93, 111	0
2	B	16/16 (100%)	-1.35	0 100 100	54, 79, 95, 104	0
2	R	16/16 (100%)	-1.41	0 100 100	46, 77, 94, 94	0
3	A	322/332 (96%)	-1.22	0 100 100	34, 80, 119, 141	0
3	C	322/332 (96%)	-1.18	0 100 100	33, 86, 119, 135	0
3	G	322/332 (96%)	-1.27	0 100 100	28, 71, 107, 127	0
4	D	323/332 (97%)	-1.11	0 100 100	33, 90, 129, 148	0
5	L	86/88 (97%)	-1.15	0 100 100	43, 79, 102, 127	0
5	S	86/88 (97%)	-1.18	0 100 100	43, 74, 96, 109	0
5	T	86/88 (97%)	-1.12	0 100 100	54, 75, 96, 103	0
5	Y	86/88 (97%)	-1.25	0 100 100	54, 75, 89, 111	0
All	All	1697/1744 (97%)	-1.20	0 100 100	28, 79, 118, 148	0

There are no RSRZ outliers to report.

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	SEP	T	46	10/11	0.99	0.05	54,66,74,75	0
5	SEP	L	46	10/11	0.99	0.05	49,59,66,72	0
5	SEP	Y	46	10/11	0.99	0.04	61,66,80,84	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SEP	S	46	10/11	0.99	0.03	48,58,66,69	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
6	SO4	G	646	5/5	0.98	0.06	139,141,143,146	0
6	SO4	G	647	5/5	0.98	0.04	120,123,124,127	0
6	SO4	C	947	5/5	0.99	0.07	133,136,138,141	0
6	SO4	C	846	5/5	0.99	0.11	94,98,99,102	0
6	SO4	C	346	5/5	0.99	0.04	113,119,120,122	0
6	SO4	A	599	5/5	0.99	0.04	109,114,116,116	0
6	SO4	A	946	5/5	0.99	0.05	110,111,114,115	0
7	MG	D	754	1/1	0.99	0.06	74,74,74,74	0
7	MG	A	704	1/1	1.00	0.01	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.