



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 10:04 PM UTC

PDB ID : 4GZY / pdb_00004gzy
Title : Crystal structures of bacterial RNA Polymerase paused elongation complexes
Authors : Weixlbaumer, A.; Leon, K.; Landick, R.; Darst, S.A.
Deposited on : 2012-09-06
Resolution : 3.51 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
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

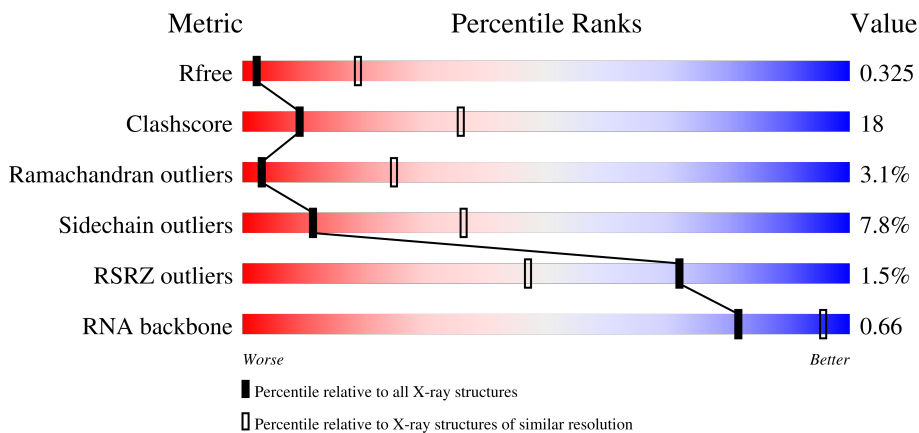
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.51 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	315	42% 25% • 29%
1	B	315	47% 22% • 29%
2	C	1119	2% 53% 38% 5% •
3	D	1534	% 50% 34% 5% 11%

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Mol	Chain	Length	Quality of chain
4	E	99	5% 55% 32% 6% 6%
5	N	13	69% 15% 15%
6	R	29	10% 17% 69%
7	T	22	5% 64% 36%

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 24400 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			
1	B	223	Total	C	N	O	S	0	0	0
			1759	1123	306	328	2			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1083	Total	C	N	O	S	0	0	0
			8548	5412	1524	1588	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1358	Total	C	N	O	S	0	0	0
			10714	6780	1900	2001	33			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1525	HIS	-	expression tag	UNP Q8RQE8
D	1526	HIS	-	expression tag	UNP Q8RQE8
D	1527	HIS	-	expression tag	UNP Q8RQE8
D	1528	HIS	-	expression tag	UNP Q8RQE8
D	1529	HIS	-	expression tag	UNP Q8RQE8
D	1530	HIS	-	expression tag	UNP Q8RQE8
D	1531	HIS	-	expression tag	UNP Q8RQE8
D	1532	HIS	-	expression tag	UNP Q8RQE8
D	1533	HIS	-	expression tag	UNP Q8RQE8
D	1534	HIS	-	expression tag	UNP Q8RQE8

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			754	481	131	138	4			

- Molecule 5 is a DNA chain called non-template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	N	11	Total	C	N	O	P	0	0	0
			225	107	43	64	11			

- Molecule 6 is a RNA chain called RNA transcript.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	R	9	Total	C	N	O	P	0	0	0
			191	85	31	66	9			

- Molecule 7 is a DNA chain called template DNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	T	22	Total	C	N	O	P	0	0	0
			447	213	81	131	22			

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

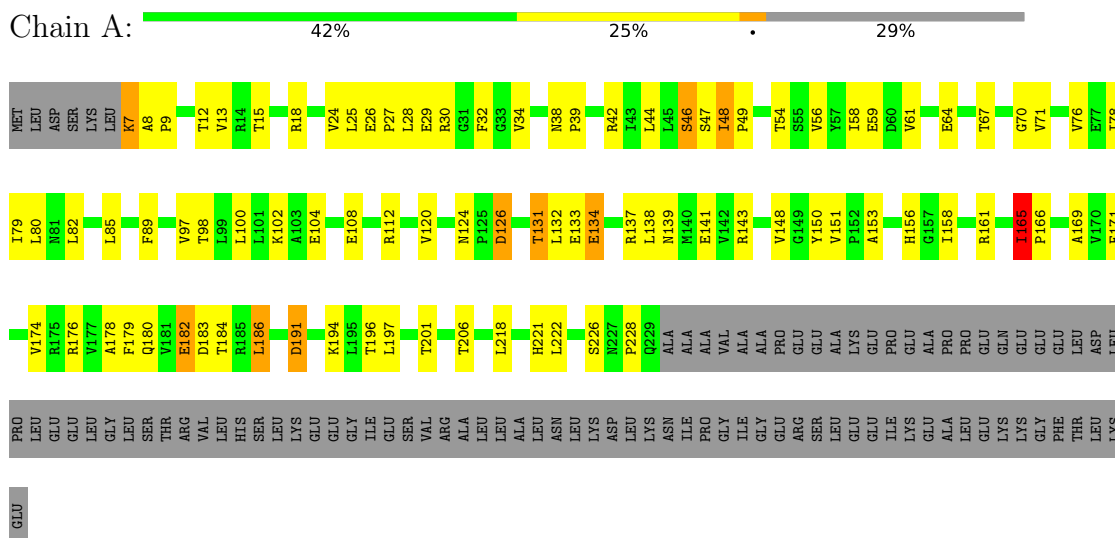
- Molecule 9 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

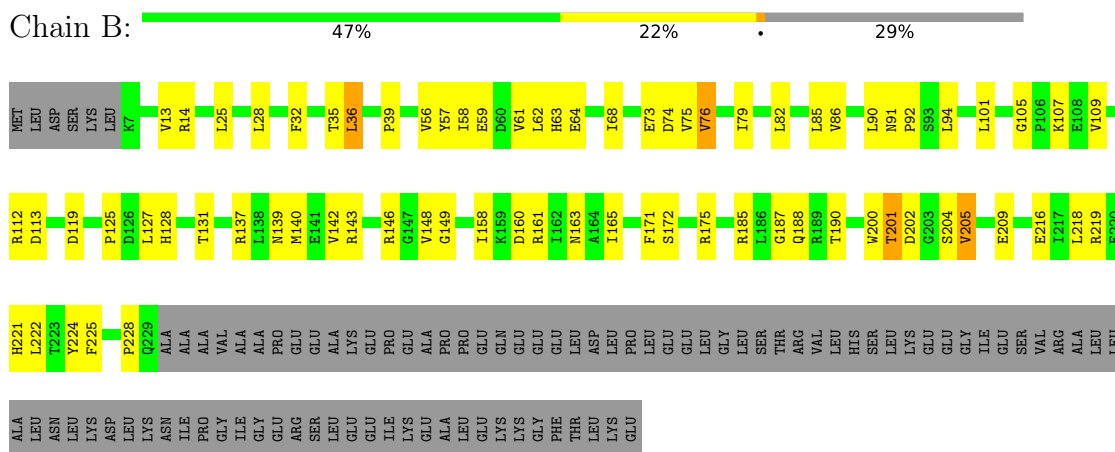
3 Residue-property plots

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

• Molecule 1: DNA-directed RNA polymerase subunit alpha

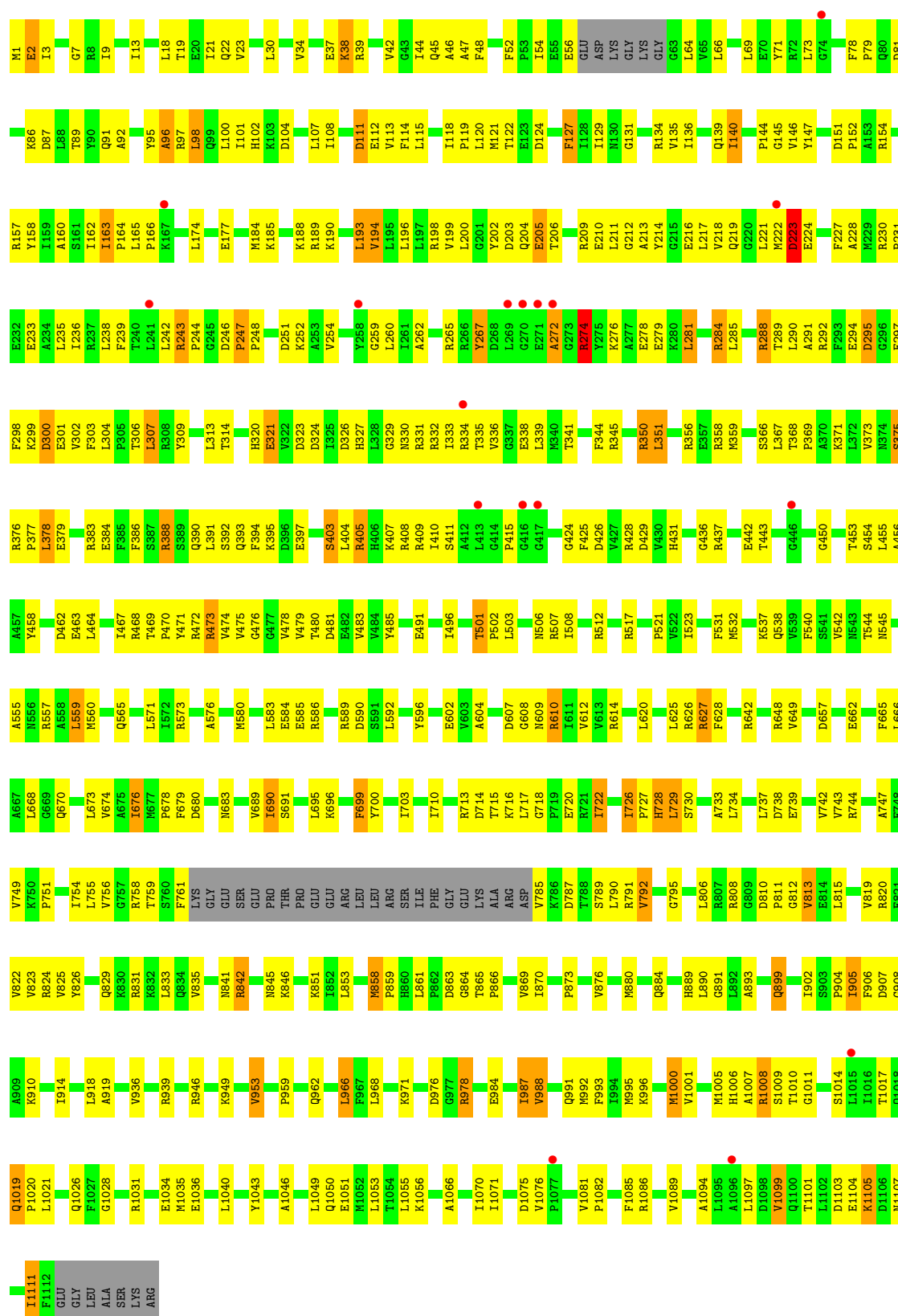


• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta

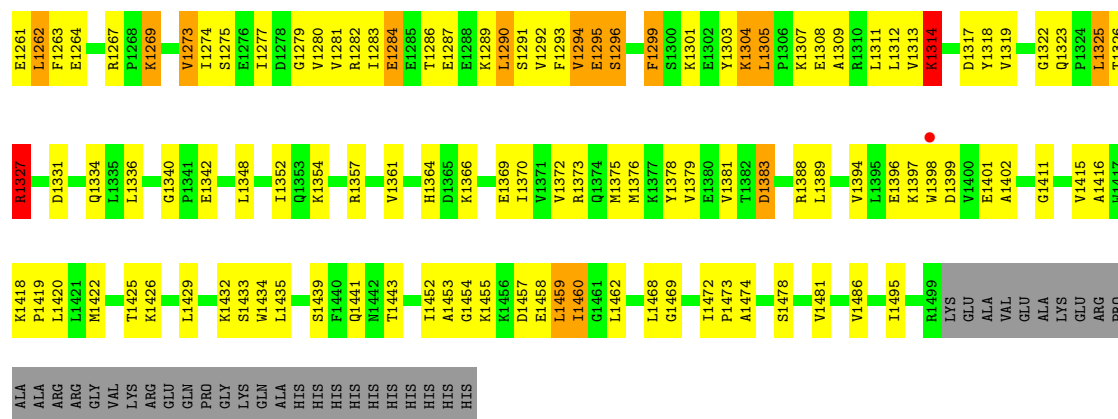




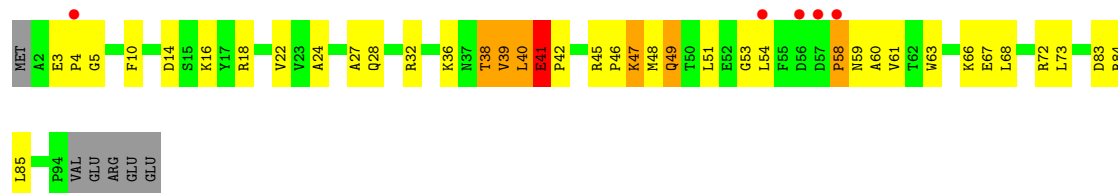
• Molecule 3: DNA-directed RNA polymerase subunit beta'



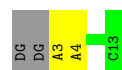
Y1185	S1074	L983	R872	R796	A715	D624	N541	R441	E362	GLU	TYR	T168	A96	MET
L1174	A1077	D985	L873	K797	F716	Y625	D642	V446	A363	ILE	LYS	Y169	A96	K2
I1183	K1078	R988	E874	K799	Q717		L543	V447	G364	VAL	PRO	P170	A100	K7
E1185	K1079	R988	P877	G801	V719	R628	Y548	Y450	D365	LYS	GLU	P172	I102	K17
	D1083	Q991		A802	L720	S629	N549	D451	K366	GLN	ILE	V175	W103	I18
V1188	L1086	L995	I880	G803	G723	V630	R653	I452	V368	PRO	ALA	D176	F104	G24
R1189	L1087	W996	L881	E805	G725		K555	D453	A369	LEU	GLU	A177		
Q1195	R1096	E1001	D892	F806	S726	H640	K555	A454	A370	ALA	LEU	V179	V108	K28
T1198	S1091	K1002	V895	A807	I726	Q641	K558	A458	I371	ALA	GLU	K180	S110	P29
R1197	R1096	V1003	L902	T808	Q727	C642	L557	T461	E374	LYS	PRO	D181	K111	E30
G1199	V1099	F1008	L908	E810	E734	G643	L558	L473	E376	GLY	TYR	G182	I112	T31
V1200			K908	E811	A735	L644	Q560	L473	V377	LEU	PHE	E183	T114	I32
C1204	V1106	F1011	Q917	L813	D739	K646	G561	L477	A379	MET	ALA	V185	L115	L37
Y1205	V1107	F1012	A918	A814	F740	M648	P563	E480	E382	ARG	GLU	K187	L116	K38
Y1207	R1108	E1012	F919	A815	D741	A649	E564			ARG	GLU	L191	S119	P39
D1208	E1109	E1013	R921	H816	G742	L850	L565	P484	V385	VAL	GLY	A192	L123	E40
L1209	G1112	Y1015	L922	E817	Q744	P655	L567			ARG	VAL	E124	E124	D42
S1210	T1115	N1018	T927	E820	M745	F656	N568	S485	H388	ALA	VAL	V195	L127	D46
M1211				A822	A746	L657	N569	B486	E389	ALA	GLU	R198	Y128	I49
A1212				R823	H748	L658	E570	A487	P390	GLN	LEU		F129	F50
R1213				N824	V749	K660	R572	R488	A391	VAL	LYS	L199	S130	G51
P1214	S1119	V1022	K935	E831	A759	I683	D583	R489	S392	GLU	GLU	D200	K131	P52
V1215		M1023	F939	A825	P750	M661	N573		I393	ALA	LEU	G201	Y132	I53
			P826	L574	L751	A673	N584	K494	L394	GLU	GLU	V202	I133	K54
G1218	F1123	G1027	T940	K827	Q756			B495	V395	GLU	GLY	A203	V134	D55
E1219	P1124	A1028	F941	K828	A757	L677	L581	V499	D405	GLY	ALA	L204	L135	Y56
A1220	P1125	R1029	S942	G829	F758		L582	R500	V407	GLU	PHE	Y205	D136	E57
	D1126	G1030	T943	A830	A759	I683	D583	A501	E408	THR	LEU	R209	P137	C58
P1232	V1128	P1031	T948	R832	R760	E686	N584	S505	D405	VAL	VAL	R210	K138	A59
Q1235	T1129	P1032	I949	E833	I761				D406	TYR	LEU	R211	G139	C60
L1236	R1130	Q1033	G950	T834	Q762	A690	P590		V407	LEU	ARG	R212		G61
THR	S1131	Q1034	I951	S835	L764	L691	N593		E408	THR	GLU	V213	L142	K62
MET	L1132	R1036	V955	V955	S765	E692	G595	M511	R414	PHE	ASP	V216	P146	Y63
ARG	R1133	Q1037	I956	K840	A766	E693	G595	M512	V415	LEU	GLU	LYS	V147	R65
THR	L1134	L1038	I956	Y841	H767	V694	L600	I513	A416	GLU	PRO	GLY	K149	E74
PHE	R1135	C1039	K960	V842	H768	H696	L601	V517	P417	VAL	ALA	ARG	R150	R75
HIS	K1136	G1040			L769		G602	P518		THR	ALA	ALA	Q151	V78
				D847	L770	V700	S602	V519	G418	TYR	THR	ALA	Q151	E79
THR	D1139	L1041	Y963	E848		L701	L603	L520	D419	PHE	LEU	GLY	L152	
GLY	I1140	R1042	E965	A849	E776	L702	T604	P521	V420	LEU	ARG	ARG	T154	
GLY	G1146	L1044	E966	L850	P777	N703	D605	P522	L421	PRO	LEU	LEU		
ALA	R1147		A967	L851		R704	L606		G425	VAL	PRO	PRO	E157	
GLY		V1055	D968	A852	K780	A705	L607	R525	K426	GLY	LEU	LEU		
ALA	R1151	P1056	R969	V853			S609	V528	V427	GLY	LEU	PRO	E160	
ALA	V1155	R1057	K970	V853	R783	L708	R613			GLY	GLY	GLY	L161	
ASP	L1156	R1058	L971	I857	D784	H709	F614	D531	Y431	THR	THR	ALA	L162	
ILE			E975		I785	R710	R615	G532	Y432	PRO	PRO	TRP	Y163	
	E1161	E1063		L860	I786	L711	R615	G533	G433	LEU	VAL	VAL	G164	
THR	E1162	E1069	Y978	Q861	I786	L711	R615	G533	G433	LEU	VAL	GLY	G164	
	G1163	Y1070	E979	V864	I792	I713	N617	D539	R434	VAL	VAL	LYS	K165	
	R1164			T865	I793	Q714	K621	L540	V435	HIS	GLY	ALA	E167	



- Molecule 4: DNA-directed RNA polymerase subunit omega



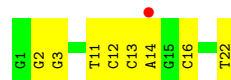
- Molecule 5: non-template DNA



- Molecule 6: RNA transcript



- Molecule 7: template DNA



4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	207.21Å 207.21Å 203.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.77 – 3.51 49.77 – 3.51	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.77-3.51) 87.9 (49.77-3.51)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.76 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.8_1069, CNS	Depositor
R, R_{free}	0.263 , 0.322 0.265 , 0.325	Depositor DCC
R_{free} test set	3199 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	95.9	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 83.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.038 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	24400	wwPDB-VP
Average B, all atoms (Å ²)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.40	0/1791	0.83	4/2436 (0.2%)
1	B	0.39	0/1791	0.84	1/2436 (0.0%)
2	C	0.39	0/8711	0.87	19/11784 (0.2%)
3	D	0.40	1/10897 (0.0%)	0.85	21/14726 (0.1%)
4	E	0.40	0/768	0.91	2/1035 (0.2%)
5	N	0.11	0/252	0.57	0/386
6	R	0.11	0/212	0.23	0/328
7	T	0.12	0/500	0.58	0/768
All	All	0.39	1/24922 (0.0%)	0.84	47/33899 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	101	HIS	CG-ND1	5.18	1.44	1.38

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	705	ALA	CA-C-N	-10.81	106.33	119.84
3	D	705	ALA	C-N-CA	-10.81	106.33	119.84
2	C	792	VAL	CA-C-N	8.76	129.40	120.38
2	C	792	VAL	C-N-CA	8.76	129.40	120.38
2	C	247	PRO	N-CA-C	8.16	120.65	110.70
2	C	726	ILE	CA-C-N	7.66	128.36	119.47
2	C	726	ILE	C-N-CA	7.66	128.36	119.47
3	D	80	VAL	N-CA-C	7.66	119.11	107.77
3	D	827	ILE	N-CA-C	7.49	117.46	110.42
3	D	1188	VAL	N-CA-C	7.17	117.81	108.35
4	E	41	GLU	CA-C-N	-6.99	111.10	119.84
4	E	41	GLU	C-N-CA	-6.99	111.10	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	729	LEU	N-CA-C	6.84	121.42	111.02
2	C	728	HIS	N-CA-C	6.08	120.76	112.68
1	B	68	ILE	N-CA-C	5.94	113.43	107.55
2	C	151	ASP	CA-C-N	5.82	127.12	119.84
2	C	151	ASP	C-N-CA	5.82	127.12	119.84
3	D	593	ASN	CA-C-N	5.62	126.87	119.84
3	D	593	ASN	C-N-CA	5.62	126.87	119.84
3	D	171	LEU	CA-C-N	5.59	123.69	119.66
3	D	171	LEU	C-N-CA	5.59	123.69	119.66
2	C	1019	GLN	CA-C-N	5.51	126.38	119.98
2	C	1019	GLN	C-N-CA	5.51	126.38	119.98
1	A	165	ILE	CA-C-N	5.46	125.38	119.76
1	A	165	ILE	C-N-CA	5.46	125.38	119.76
3	D	528	VAL	N-CA-C	5.40	115.67	108.11
2	C	177	GLU	CA-C-N	5.30	125.62	119.47
2	C	177	GLU	C-N-CA	5.30	125.62	119.47
1	A	8	ALA	CA-C-N	5.30	125.60	119.93
1	A	8	ALA	C-N-CA	5.30	125.60	119.93
3	D	1126	ASP	N-CA-C	5.24	116.72	109.54
2	C	1111	ILE	N-CA-C	-5.19	108.78	113.71
3	D	956	ILE	CA-C-N	5.19	125.19	119.90
3	D	956	ILE	C-N-CA	5.19	125.19	119.90
3	D	521	PRO	CA-C-N	5.18	126.31	119.84
3	D	521	PRO	C-N-CA	5.18	126.31	119.84
2	C	501	THR	CA-C-N	5.16	125.08	119.76
2	C	501	THR	C-N-CA	5.16	125.08	119.76
3	D	181	ASP	CB-CA-C	-5.15	110.62	116.54
2	C	247	PRO	CA-C-N	-5.10	113.46	119.84
2	C	247	PRO	C-N-CA	-5.10	113.46	119.84
2	C	730	SER	N-CA-C	5.08	117.53	109.50
3	D	1340	GLY	CA-C-N	5.08	124.69	119.05
3	D	1340	GLY	C-N-CA	5.08	124.69	119.05
3	D	1015	TYR	CA-C-N	5.06	124.23	118.97
3	D	1015	TYR	C-N-CA	5.06	124.23	118.97
3	D	183	GLU	N-CA-C	5.04	116.25	107.93

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1759	0	1805	59	0
1	B	1759	0	1805	54	0
2	C	8548	0	8650	386	0
3	D	10714	0	10936	415	0
4	E	754	0	769	25	0
5	N	225	0	124	1	0
6	R	191	0	95	7	0
7	T	447	0	248	6	0
8	D	2	0	0	0	0
9	D	1	0	0	0	0
All	All	24400	0	24432	880	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 18.

All (880) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:610:ARG:HG3	2:C:610:ARG:HH11	1.16	1.08
3:D:346:ARG:NH1	3:D:347:VAL:O	1.89	1.05
2:C:405:ARG:NH1	2:C:442:GLU:OE2	1.90	1.04
2:C:274:ARG:NH1	2:C:284:ARG:HH12	1.54	1.03
3:D:550:ARG:HH11	3:D:573:MET:HB3	1.25	0.98
4:E:39:VAL:O	4:E:72:ARG:NH1	1.98	0.96
2:C:194:VAL:HG21	2:C:224:GLU:HG3	1.49	0.94
2:C:714:ASP:OD1	2:C:820:ARG:NH1	2.02	0.92
2:C:978:ARG:HG3	2:C:978:ARG:HH11	1.34	0.91
2:C:274:ARG:HH12	2:C:284:ARG:NH1	1.66	0.91
2:C:1103:ASP:HB3	2:C:1105:LYS:HZ1	1.35	0.90
2:C:274:ARG:HH12	2:C:284:ARG:HH12	1.13	0.90
2:C:829:GLN:HE21	2:C:831:ARG:HH11	1.17	0.87
3:D:1198:TYR:OH	3:D:1432:LYS:NZ	2.09	0.86
3:D:1106:VAL:HG12	3:D:1220:ALA:HA	1.57	0.83
2:C:290:LEU:HD11	2:C:301:GLU:H	1.43	0.82
2:C:239:PHE:HB2	2:C:251:ASP:HB3	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:486:ARG:HH21	3:D:489:ARG:HH11	1.29	0.80
2:C:272:ALA:HB1	2:C:276:LYS:HZ1	1.46	0.80
1:B:56:VAL:HG21	1:B:82:LEU:HD13	1.63	0.80
1:B:91:ASN:ND2	1:B:119:ASP:OD2	2.14	0.80
2:C:512:ARG:HB3	2:C:523:ILE:HD11	1.64	0.80
2:C:288:ARG:H	2:C:288:ARG:HH11	1.30	0.79
3:D:1108:ARG:HH22	3:D:1460:ILE:HD11	1.47	0.79
1:B:188:GLN:O	3:D:646:LYS:NZ	2.14	0.78
2:C:738:ASP:HB2	2:C:744:ARG:HB3	1.66	0.78
3:D:770:LEU:HD12	3:D:1211:MET:HA	1.64	0.78
3:D:135:LEU:HD23	3:D:148:GLU:HB2	1.64	0.77
2:C:274:ARG:HH12	2:C:284:ARG:NH2	1.82	0.77
2:C:224:GLU:HB3	2:C:227:PHE:HB3	1.67	0.77
2:C:212:GLY:HA2	2:C:218:VAL:HG21	1.65	0.77
2:C:274:ARG:HH12	2:C:284:ARG:CZ	1.96	0.77
2:C:309:TYR:CZ	2:C:321:GLU:HB3	2.20	0.77
3:D:1486:VAL:HG11	4:E:22:VAL:HG13	1.67	0.76
2:C:1105:LYS:HZ2	2:C:1105:LYS:H	1.34	0.76
3:D:501:ALA:O	3:D:505:SER:OG	2.02	0.76
3:D:557:LEU:HD21	3:D:566:ILE:HG22	1.68	0.76
2:C:274:ARG:NH1	2:C:284:ARG:NH1	2.29	0.76
2:C:334:ARG:HH12	2:C:415:PRO:HG2	1.48	0.76
4:E:54:LEU:HG	4:E:58:PRO:HG2	1.66	0.75
2:C:1103:ASP:HB3	2:C:1105:LYS:NZ	2.01	0.75
2:C:274:ARG:HH21	2:C:278:GLU:HB2	1.51	0.74
2:C:437:ARG:NH1	2:C:491:GLU:OE1	2.14	0.74
3:D:700:VAL:HG12	3:D:749:VAL:HG12	1.70	0.74
3:D:960:LYS:NZ	3:D:1063:GLU:OE2	2.19	0.74
2:C:1008:ARG:HD2	2:C:1026:GLN:HB3	1.68	0.74
1:B:79:ILE:HA	1:B:82:LEU:HD12	1.68	0.74
2:C:584:GLU:HB3	2:C:666:LEU:H	1.52	0.74
2:C:274:ARG:HH12	2:C:284:ARG:HH22	1.35	0.74
3:D:983:LEU:HD13	3:D:988:ARG:HB2	1.69	0.74
2:C:185:LYS:HG2	2:C:190:LYS:HG2	1.67	0.73
2:C:462:ASP:OD2	2:C:468:ARG:NH1	2.17	0.73
2:C:205:GLU:HB2	2:C:209:ARG:HH12	1.54	0.73
3:D:213:VAL:HG11	3:D:385:VAL:HA	1.70	0.73
4:E:46:PRO:HG3	4:E:66:LYS:HD3	1.71	0.72
1:A:58:ILE:HB	1:A:61:VAL:HB	1.71	0.72
2:C:204:GLN:NE2	2:C:222:MET:O	2.22	0.72
3:D:1147:ARG:HD3	3:D:1188:VAL:HG21	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:ARG:NH2	1:A:126:ASP:OD1	2.23	0.72
1:B:90:LEU:HB2	1:B:119:ASP:HB3	1.72	0.71
1:A:80:LEU:HD21	2:C:573:ARG:HH11	1.55	0.71
2:C:224:GLU:O	2:C:228:ALA:N	2.24	0.71
2:C:710:ILE:HD11	2:C:758:ARG:HH21	1.55	0.71
2:C:755:LEU:HD11	2:C:825:VAL:HG11	1.73	0.71
1:A:182:GLU:HB2	1:A:194:LYS:HD3	1.72	0.70
3:D:1273:VAL:HG12	3:D:1274:ILE:H	1.56	0.70
2:C:332:ARG:NH2	2:C:338:GLU:OE1	2.25	0.70
2:C:1005:MET:HB2	3:D:724:GLN:HE22	1.56	0.70
2:C:734:LEU:HG	2:C:737:LEU:HD12	1.73	0.70
3:D:362:GLU:O	3:D:364:GLY:N	2.23	0.70
1:B:185:ARG:NH1	3:D:692:GLU:OE1	2.24	0.70
2:C:610:ARG:HG3	2:C:610:ARG:NH1	1.90	0.70
3:D:1161:GLU:HB2	3:D:1164:ARG:HB2	1.74	0.69
3:D:1418:LYS:HD3	3:D:1419:PRO:HD2	1.74	0.69
3:D:112:ILE:HD11	3:D:461:ILE:HG21	1.73	0.69
3:D:136:ASP:HB2	3:D:137:PRO:HD2	1.74	0.69
1:A:104:GLU:OE1	1:A:137:ARG:NH1	2.25	0.69
4:E:40:LEU:HD21	4:E:67:GLU:HA	1.74	0.69
3:D:550:ARG:NH1	3:D:573:MET:HB3	2.03	0.69
2:C:442:GLU:HG2	2:C:454:SER:HB2	1.75	0.69
3:D:111:LYS:HD2	3:D:1452:ILE:HD13	1.73	0.69
3:D:133:ILE:HG23	3:D:454:ALA:HB1	1.75	0.69
3:D:501:ALA:HB1	3:D:1453:ALA:HB2	1.75	0.69
2:C:302:VAL:O	2:C:306:THR:OG1	2.11	0.68
3:D:691:LEU:HD23	3:D:720:LEU:HD21	1.74	0.68
3:D:1267:ARG:NH2	3:D:1331:ASP:OD2	2.25	0.68
2:C:670:GLN:NE2	2:C:699:PHE:O	2.27	0.68
2:C:324:ASP:HB3	2:C:327:HIS:HB2	1.75	0.68
2:C:829:GLN:NE2	2:C:831:ARG:HH11	1.89	0.68
3:D:486:ARG:HE	3:D:489:ARG:HD2	1.58	0.68
3:D:154:THR:HG23	3:D:157:GLU:H	1.59	0.67
3:D:1283:ILE:HD11	3:D:1290:LEU:HD12	1.76	0.67
2:C:978:ARG:HH11	2:C:978:ARG:CG	2.06	0.67
2:C:726:ILE:HD13	2:C:754:ILE:HD13	1.76	0.67
3:D:525:ARG:NH1	3:D:541:ASN:OD1	2.26	0.67
3:D:798:GLU:HB2	3:D:828:LYS:HE3	1.75	0.67
2:C:89:THR:HG22	2:C:129:ILE:HA	1.76	0.67
2:C:292:ARG:HB3	2:C:299:LYS:HB3	1.76	0.67
2:C:260:LEU:HD22	2:C:288:ARG:HH22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:292:ARG:HG2	2:C:299:LYS:HE3	1.77	0.67
2:C:292:ARG:NH1	2:C:294:GLU:HB2	2.10	0.67
3:D:356:PRO:HB3	3:D:441:ARG:HA	1.77	0.67
1:A:54:THR:HG21	1:A:158:ILE:HD12	1.77	0.66
2:C:873:PRO:HB2	3:D:1023:MET:HE1	1.76	0.66
1:B:101:LEU:HD21	1:B:109:VAL:HG11	1.77	0.66
1:A:67:THR:HG21	2:C:609:ASN:HD21	1.60	0.66
2:C:274:ARG:NH1	2:C:284:ARG:HH22	1.93	0.66
3:D:1453:ALA:O	3:D:1455:LYS:N	2.29	0.66
3:D:114:THR:O	3:D:495:ARG:NH1	2.29	0.66
2:C:267:TYR:HB2	2:C:272:ALA:HB3	1.78	0.65
2:C:388:ARG:NH1	7:T:22:DT:OP1	2.29	0.65
2:C:829:GLN:HE21	2:C:831:ARG:NH1	1.91	0.65
2:C:808:ARG:HD3	2:C:820:ARG:HD2	1.78	0.65
2:C:56:GLU:HA	2:C:356:ARG:HH12	1.61	0.65
2:C:292:ARG:HG3	2:C:292:ARG:HH11	1.62	0.65
3:D:1495:ILE:HG23	4:E:84:ARG:HD3	1.78	0.65
2:C:1031:ARG:HB3	7:T:16:DC:OP1	1.97	0.65
2:C:144:PRO:HA	2:C:163:ILE:HG23	1.79	0.64
2:C:953:VAL:HG13	2:C:966:LEU:HD13	1.78	0.64
2:C:1008:ARG:HH12	2:C:1011:GLY:N	1.95	0.64
2:C:1008:ARG:NH2	3:D:624:ASP:OD1	2.30	0.64
2:C:230:ARG:HB3	2:C:233:GLU:HB2	1.79	0.64
2:C:720:GLU:O	2:C:820:ARG:NH2	2.31	0.64
3:D:165:LYS:HE3	3:D:200:ASP:HB2	1.80	0.64
2:C:48:PHE:HB3	2:C:52:PHE:HD2	1.63	0.64
2:C:23:VAL:HA	2:C:121:MET:HE1	1.77	0.64
2:C:428:ARG:NH1	3:D:1086:LEU:HD11	2.12	0.64
2:C:1008:ARG:HH12	2:C:1010:THR:C	2.05	0.64
3:D:18:ILE:HG23	3:D:518:PRO:HG3	1.78	0.64
3:D:808:THR:H	3:D:809:PRO:HD2	1.63	0.64
3:D:629:SER:HB3	3:D:726:ILE:HG12	1.79	0.63
2:C:292:ARG:HH12	2:C:294:GLU:HB2	1.63	0.63
3:D:100:ALA:HB2	3:D:513:ILE:HG13	1.81	0.63
3:D:813:LEU:HD12	3:D:814:ALA:H	1.64	0.63
2:C:205:GLU:HB2	2:C:209:ARG:NH1	2.14	0.63
1:A:39:PRO:HG3	1:B:39:PRO:HG3	1.81	0.63
2:C:680:ASP:H	3:D:943:THR:HG21	1.63	0.62
2:C:845:ASN:HD22	2:C:884:GLN:HE22	1.46	0.62
3:D:734:GLU:OE2	3:D:780:LYS:NZ	2.32	0.62
1:A:221:HIS:HB3	1:B:36:LEU:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:160:ALA:HB3	2:C:174:LEU:HB2	1.82	0.62
2:C:395:LYS:HD3	2:C:397:GLU:OE2	1.99	0.62
1:A:70:GLY:HA2	1:A:133:GLU:HB3	1.80	0.62
2:C:473:ARG:HA	2:C:531:PHE:HA	1.82	0.62
3:D:148:GLU:HB3	3:D:151:GLN:HB2	1.80	0.62
3:D:1296:SER:HB3	3:D:1299:PHE:HD2	1.64	0.62
3:D:368:VAL:HB	3:D:377:VAL:HG12	1.81	0.62
3:D:764:LEU:O	3:D:768:ASN:ND2	2.32	0.62
4:E:38:THR:HG23	4:E:41:GLU:HG2	1.80	0.62
1:A:85:LEU:HA	1:A:124:ASN:HD22	1.63	0.62
3:D:702:LEU:HB3	3:D:745:MET:HE2	1.80	0.61
2:C:146:VAL:HG22	2:C:162:ILE:HG12	1.82	0.61
2:C:290:LEU:HD21	2:C:300:ASP:HB2	1.83	0.61
1:B:216:GLU:OE2	1:B:219:ARG:NH2	2.32	0.61
2:C:336:VAL:HA	2:C:339:LEU:HD12	1.82	0.61
3:D:1273:VAL:HG21	3:D:1305:LEU:HD12	1.82	0.61
3:D:553:ARG:NH2	3:D:570:GLU:OE2	2.34	0.61
2:C:428:ARG:HB3	2:C:450:GLY:HA3	1.82	0.61
3:D:808:THR:H	3:D:809:PRO:CD	2.13	0.61
2:C:22:GLN:HG3	2:C:407:LYS:HB3	1.82	0.61
2:C:384:GLU:HA	2:C:388:ARG:HH21	1.66	0.61
3:D:477:LEU:HA	3:D:480:GLU:HB3	1.82	0.61
3:D:800:LYS:HZ3	3:D:804:LEU:HD13	1.66	0.61
3:D:1174:LEU:HD22	3:D:1183:ILE:HD11	1.83	0.61
1:B:175:ARG:N	1:B:200:TRP:O	2.33	0.61
3:D:1274:ILE:HG21	3:D:1334:GLN:HB3	1.83	0.61
2:C:326:ASP:HB2	2:C:331:ARG:NH1	2.16	0.61
3:D:643:GLY:HA3	3:D:727:GLN:HB2	1.82	0.61
3:D:1057:VAL:HG13	3:D:1069:GLU:HB3	1.83	0.60
1:A:176:ARG:NH2	2:C:863:ASP:OD1	2.34	0.60
2:C:185:LYS:NZ	2:C:190:LYS:HE2	2.16	0.60
2:C:437:ARG:HD3	2:C:467:ILE:HB	1.82	0.60
2:C:642:ARG:NE	2:C:657:ASP:OD2	2.35	0.60
3:D:1319:VAL:HG23	3:D:1323:GLN:HE21	1.67	0.60
3:D:852:ALA:HB1	3:D:857:ILE:HD11	1.83	0.60
2:C:292:ARG:NH1	2:C:292:ARG:HG3	2.17	0.60
1:A:108:GLU:HG2	1:A:131:THR:HG22	1.84	0.59
2:C:987:ILE:HA	3:D:948:THR:HG21	1.83	0.59
2:C:7:GLY:HA3	2:C:904:PRO:HG2	1.85	0.59
1:A:151:VAL:HB	1:A:169:ALA:HB3	1.85	0.59
2:C:540:PHE:O	2:C:545:ASN:ND2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:787:ASP:OD1	2:C:791:ARG:NH2	2.35	0.59
2:C:824:ARG:NH2	2:C:826:TYR:OH	2.35	0.59
3:D:164:GLY:HA3	3:D:397:LYS:HE3	1.85	0.59
3:D:629:SER:OG	3:D:630:VAL:N	2.34	0.59
3:D:1108:ARG:HH12	3:D:1460:ILE:CG1	2.16	0.59
2:C:744:ARG:HG3	2:C:747:ALA:HB2	1.84	0.59
2:C:971:LYS:HA	2:C:988:VAL:HA	1.85	0.58
3:D:1258:ARG:NH1	3:D:1262:LEU:HD11	2.17	0.58
2:C:101:ILE:HD12	2:C:107:LEU:HD22	1.86	0.58
3:D:820:GLU:HB2	3:D:836:VAL:HG21	1.86	0.58
1:A:71:VAL:HG11	1:A:78:ILE:HD11	1.84	0.58
3:D:135:LEU:HD22	3:D:153:LEU:HD23	1.85	0.58
2:C:115:LEU:HA	2:C:375:SER:HB2	1.85	0.58
2:C:674:VAL:HG22	2:C:869:VAL:HB	1.86	0.58
2:C:1009:SER:HA	3:D:625:TYR:HA	1.86	0.58
3:D:32:ILE:HG21	3:D:37:LEU:HD13	1.86	0.58
2:C:863:ASP:OD1	2:C:864:GLY:N	2.37	0.58
2:C:1105:LYS:HZ2	2:C:1105:LYS:N	2.00	0.58
1:A:7:LYS:HD3	1:A:186:LEU:HD22	1.86	0.57
2:C:324:ASP:O	2:C:330:ASN:ND2	2.32	0.57
6:R:22:U:H2'	6:R:23:G:C8	2.39	0.57
2:C:122:THR:HB	2:C:124:ASP:OD2	2.04	0.57
2:C:145:GLY:H	2:C:163:ILE:HG23	1.69	0.57
2:C:64:LEU:HD13	2:C:359:MET:SD	2.44	0.57
2:C:1082:PRO:HB2	2:C:1085:PHE:HB3	1.86	0.57
2:C:158:TYR:HD1	2:C:314:THR:HG22	1.69	0.57
2:C:193:LEU:HD21	2:C:307:LEU:HD21	1.87	0.57
3:D:210:ARG:HB3	3:D:388:HIS:HB2	1.85	0.57
2:C:246:ASP:OD1	2:C:246:ASP:N	2.38	0.57
2:C:576:ALA:N	2:C:662:GLU:OE1	2.37	0.57
3:D:860:LEU:HD23	3:D:877:PRO:HB2	1.87	0.57
4:E:27:ALA:HB1	4:E:60:ALA:HB1	1.87	0.57
2:C:243:ARG:HE	2:C:254:VAL:HG21	1.70	0.56
2:C:1008:ARG:HH21	2:C:1020:PRO:HB3	1.69	0.56
2:C:1008:ARG:HD3	2:C:1028:GLY:H	1.70	0.56
3:D:169:TYR:HB3	3:D:195:VAL:HG11	1.85	0.56
2:C:1050:GLN:HG3	3:D:1469:GLY:O	2.05	0.56
3:D:827:ILE:O	3:D:835:SER:OG	2.23	0.56
2:C:111:ASP:HB3	2:C:112:GLU:OE2	2.05	0.56
2:C:1051:GLU:HG3	2:C:1055:LEU:HD23	1.87	0.56
3:D:1458:GLU:O	3:D:1460:ILE:HG22	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:284:ARG:HG3	2:C:285:LEU:N	2.21	0.56
3:D:1283:ILE:HD13	3:D:1311:LEU:HD22	1.87	0.56
2:C:936:VAL:HG11	2:C:959:PRO:HB2	1.86	0.56
3:D:978:TYR:HB2	3:D:988:ARG:HD3	1.86	0.56
3:D:1289:LYS:HZ3	3:D:1304:LYS:HB2	1.70	0.56
1:A:59:GLU:HB2	1:A:139:ASN:HB3	1.88	0.56
3:D:1165:TYR:HB3	3:D:1207:TYR:HE1	1.70	0.55
3:D:1289:LYS:NZ	3:D:1304:LYS:HB2	2.21	0.55
2:C:194:VAL:HG12	2:C:221:LEU:HB2	1.86	0.55
1:A:132:LEU:HD21	1:A:138:LEU:HD23	1.89	0.55
3:D:96:ALA:HB2	3:D:555:LYS:HG3	1.86	0.55
3:D:1281:VAL:HG11	3:D:1313:VAL:HG22	1.89	0.55
2:C:54:ILE:HG22	2:C:66:LEU:HD23	1.89	0.55
2:C:537:LYS:HG2	2:C:905:ILE:HG12	1.89	0.55
2:C:846:LYS:NZ	6:R:29:U:OP1	2.35	0.55
3:D:827:ILE:HG23	3:D:828:LYS:HG3	1.89	0.55
1:A:64:GLU:HG2	1:A:76:VAL:HG22	1.87	0.55
1:A:25:LEU:HD23	1:A:28:LEU:HD11	1.88	0.55
3:D:53:ILE:HA	3:D:86:ARG:HD3	1.89	0.55
2:C:462:ASP:O	2:C:464:LEU:N	2.38	0.55
2:C:571:LEU:HD13	2:C:670:GLN:HE21	1.72	0.55
3:D:616:GLN:OE1	3:D:621:LYS:NZ	2.38	0.55
1:B:32:PHE:HA	1:B:35:THR:HB	1.89	0.55
2:C:140:ILE:HG12	2:C:333:ILE:HG12	1.89	0.55
2:C:468:ARG:HB3	2:C:485:TYR:HB3	1.88	0.55
3:D:119:SER:HB2	3:D:123:LEU:HB2	1.89	0.55
3:D:165:LYS:HG2	3:D:199:LEU:HB3	1.88	0.55
3:D:1379:VAL:HG12	3:D:1419:PRO:HA	1.89	0.55
3:D:660:LYS:HG3	3:D:694:VAL:HG12	1.89	0.55
3:D:770:LEU:HD23	3:D:777:PRO:HA	1.89	0.55
3:D:130:SER:OG	3:D:131:LYS:N	2.40	0.54
1:B:76:VAL:HG13	3:D:872:ARG:HH21	1.72	0.54
2:C:2:GLU:HG3	2:C:899:GLN:HB3	1.88	0.54
3:D:1128:VAL:HG12	3:D:1129:THR:H	1.72	0.54
3:D:187:LYS:HG3	3:D:199:LEU:HA	1.88	0.54
1:B:163:ASN:OD1	1:B:163:ASN:N	2.41	0.54
3:D:1282:ARG:HB2	3:D:1293:PHE:O	2.06	0.54
1:B:86:VAL:HG21	1:B:204:SER:HB2	1.90	0.54
1:B:149:GLY:HA2	1:B:172:SER:HB2	1.90	0.54
2:C:52:PHE:HE1	2:C:98:LEU:HD13	1.72	0.54
2:C:54:ILE:CG2	2:C:66:LEU:HD23	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:345:TYR:CZ	3:D:377:VAL:HB	2.43	0.54
3:D:1283:ILE:HG13	3:D:1292:VAL:HG22	1.90	0.54
6:R:26:U:H2'	6:R:27:G:C8	2.43	0.54
1:A:222:LEU:HD21	1:B:218:LEU:HD23	1.88	0.54
3:D:608:SER:HB3	3:D:1443:THR:HB	1.89	0.54
3:D:1018:ASN:HB3	3:D:1021:TYR:HB3	1.90	0.54
1:A:7:LYS:NZ	1:A:7:LYS:HB3	2.23	0.54
2:C:18:LEU:HD22	2:C:404:LEU:HD21	1.89	0.54
2:C:949:LYS:HD3	3:D:796:ARG:NH1	2.23	0.54
3:D:171:LEU:N	3:D:391:ALA:O	2.36	0.54
3:D:783:ARG:HD3	3:D:1029:ARG:HG2	1.90	0.54
3:D:955:VAL:HB	3:D:1011:PHE:HE1	1.72	0.54
3:D:1434:TRP:NE1	3:D:1457:ASP:HB2	2.23	0.54
2:C:390:GLN:HB3	6:R:25:G:H5'	1.90	0.53
3:D:24:GLY:HA3	3:D:49:ILE:HG12	1.90	0.53
3:D:100:ALA:HB3	3:D:128:TYR:CE1	2.42	0.53
3:D:1106:VAL:HG11	3:D:1474:ALA:HB2	1.90	0.53
2:C:351:LEU:HD11	2:C:373:VAL:HG13	1.88	0.53
2:C:1082:PRO:HB3	3:D:1469:GLY:HA3	1.89	0.53
2:C:1101:THR:HG21	2:C:1111:ILE:HD11	1.89	0.53
3:D:908:LYS:HB2	3:D:1027:GLY:HA3	1.89	0.53
2:C:1085:PHE:HD1	3:D:1468:LEU:HD22	1.74	0.53
3:D:52:PRO:HG2	3:D:80:VAL:HG13	1.88	0.53
3:D:568:ARG:NH1	3:D:571:LYS:HE3	2.22	0.53
3:D:1155:VAL:HG23	3:D:1156:LEU:H	1.73	0.53
3:D:1286:THR:OG1	3:D:1287:GLU:N	2.39	0.53
2:C:334:ARG:NH1	2:C:415:PRO:HG2	2.21	0.53
2:C:1034:GLU:CD	3:D:1096:ARG:HH12	2.17	0.53
3:D:1435:LEU:HD21	3:D:1468:LEU:HD21	1.91	0.53
1:A:133:GLU:HG2	1:A:134:GLU:H	1.73	0.53
3:D:172:PRO:HG2	3:D:175:VAL:HG21	1.89	0.53
3:D:458:ALA:HB2	3:D:575:GLN:HE22	1.73	0.53
2:C:185:LYS:HZ2	2:C:190:LYS:HE2	1.73	0.53
2:C:1034:GLU:OE2	3:D:1096:ARG:NH2	2.42	0.53
3:D:87:ARG:HD2	3:D:88:TYR:CE1	2.44	0.53
2:C:284:ARG:NH1	2:C:285:LEU:H	2.05	0.53
3:D:1232:PRO:HB3	3:D:1361:VAL:HG21	1.89	0.53
3:D:1275:SER:OG	3:D:1322:GLY:N	2.42	0.53
1:B:64:GLU:HA	1:B:165:ILE:HD13	1.90	0.53
2:C:1007:ALA:HB2	3:D:648:MET:HG2	1.90	0.53
3:D:614:PHE:HB3	3:D:1439:SER:HA	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:149:GLY:H	1:B:171:PHE:HB2	1.74	0.53
3:D:176:ASP:O	3:D:390:PRO:HD2	2.08	0.53
3:D:784:ASP:HB3	3:D:939:PHE:CE1	2.44	0.53
3:D:554:LEU:HD13	3:D:570:GLU:HB3	1.91	0.52
3:D:1372:VAL:HG23	3:D:1375:MET:HE2	1.90	0.52
2:C:300:ASP:OD2	2:C:303:PHE:HB2	2.10	0.52
3:D:165:LYS:H	3:D:199:LEU:HD13	1.74	0.52
1:B:205:VAL:HG13	1:B:209:GLU:HB2	1.90	0.52
2:C:91:GLN:HA	2:C:119:PRO:HA	1.90	0.52
2:C:184:MET:HB2	2:C:193:LEU:HB2	1.91	0.52
2:C:1034:GLU:OE2	3:D:1096:ARG:NH1	2.39	0.52
3:D:39:PRO:HD3	3:D:53:ILE:HG21	1.91	0.52
3:D:792:ILE:HG13	3:D:793:THR:HG23	1.92	0.52
3:D:802:ALA:HB3	3:D:824:ASN:HB3	1.92	0.52
3:D:964:LEU:HD13	3:D:1058:ARG:HH12	1.74	0.52
3:D:1128:VAL:HB	3:D:1131:SER:OG	2.10	0.52
2:C:236:ILE:HA	2:C:251:ASP:OD2	2.09	0.52
2:C:66:LEU:HD12	2:C:98:LEU:HD11	1.90	0.52
2:C:1043:TYR:CD2	3:D:763:MET:HE3	2.45	0.52
3:D:800:LYS:NZ	3:D:804:LEU:HD13	2.24	0.52
3:D:805:GLU:HG2	3:D:809:PRO:HG2	1.91	0.52
2:C:1:MET:O	2:C:899:GLN:HA	2.10	0.52
3:D:832:ARG:NE	3:D:833:GLU:OE2	2.43	0.52
3:D:1112:CYS:HB2	3:D:1195:GLN:HG2	1.91	0.52
2:C:408:ARG:NH2	2:C:456:ALA:O	2.43	0.52
2:C:437:ARG:HG2	2:C:469:THR:HG23	1.92	0.52
2:C:806:LEU:HB2	2:C:822:VAL:HG22	1.91	0.52
3:D:421:LEU:HB2	3:D:427:VAL:HG12	1.92	0.52
3:D:543:LEU:HD13	3:D:581:LEU:HA	1.91	0.52
1:A:80:LEU:HD21	2:C:573:ARG:HD2	1.92	0.52
2:C:165:LEU:HG	2:C:166:PRO:HA	1.91	0.52
2:C:756:VAL:O	2:C:789:SER:HB3	2.10	0.52
3:D:50:PHE:CD1	3:D:522:PRO:HD3	2.45	0.52
3:D:367:ILE:HG13	3:D:377:VAL:HG13	1.91	0.52
2:C:756:VAL:HB	2:C:790:LEU:HB3	1.91	0.52
2:C:841:ASN:HD21	2:C:884:GLN:HE21	1.56	0.52
2:C:842:ARG:HH11	2:C:842:ARG:HB3	1.75	0.52
2:C:1008:ARG:HH12	2:C:1010:THR:CA	2.23	0.52
3:D:806:PHE:CD1	3:D:812:ALA:HB3	2.45	0.52
1:B:73:GLU:OE2	1:B:128:HIS:NE2	2.40	0.51
2:C:205:GLU:CB	2:C:209:ARG:HH12	2.22	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:560:GLN:HG3	3:D:561:GLY:H	1.74	0.51
1:A:34:VAL:HG21	2:C:939:ARG:HE	1.75	0.51
2:C:288:ARG:H	2:C:288:ARG:NH1	2.04	0.51
2:C:425:PHE:H	2:C:428:ARG:HD2	1.75	0.51
2:C:458:TYR:HB3	2:C:470:PRO:HG3	1.92	0.51
2:C:733:ALA:HB1	2:C:754:ILE:HD12	1.91	0.51
3:D:522:PRO:O	3:D:525:ARG:N	2.30	0.51
3:D:988:ARG:HA	3:D:991:GLN:HB2	1.92	0.51
3:D:1108:ARG:NH2	3:D:1460:ILE:HD11	2.19	0.51
2:C:679:PHE:CE2	2:C:853:LEU:HD21	2.45	0.51
3:D:1107:VAL:O	3:D:1218:GLY:N	2.42	0.51
2:C:95:TYR:HD1	2:C:112:GLU:HB3	1.74	0.51
3:D:842:VAL:HG12	3:D:865:THR:HB	1.93	0.51
3:D:1396:GLU:HA	3:D:1399:ASP:OD2	2.11	0.51
1:A:44:LEU:HD23	1:A:48:ILE:HD11	1.90	0.51
1:B:56:VAL:HG22	1:B:142:VAL:HG22	1.92	0.51
1:B:185:ARG:NH2	1:B:187:GLY:HA2	2.26	0.51
3:D:100:ALA:HB3	3:D:128:TYR:HE1	1.76	0.51
3:D:1036:ARG:HH21	3:D:1042:ARG:HA	1.75	0.51
2:C:468:ARG:NE	2:C:485:TYR:O	2.41	0.51
1:B:185:ARG:HB3	1:B:190:THR:HG23	1.92	0.51
3:D:61:GLY:HA3	3:D:64:LYS:NZ	2.26	0.51
3:D:484:PRO:HB3	3:D:488:ARG:NE	2.25	0.51
3:D:1425:THR:O	3:D:1429:LEU:HB2	2.10	0.51
2:C:890:LEU:HB2	2:C:914:ILE:HD12	1.91	0.51
3:D:139:GLY:HA2	3:D:452:ILE:HG12	1.93	0.51
1:A:100:LEU:HD22	1:A:141:GLU:HG3	1.92	0.51
1:B:59:GLU:HB3	1:B:137:ARG:HH12	1.75	0.51
2:C:42:VAL:HA	2:C:46:ALA:HB2	1.92	0.51
4:E:48:MET:HB2	4:E:54:LEU:HB2	1.93	0.51
1:A:178:ALA:HB2	2:C:864:GLY:HA2	1.92	0.51
2:C:19:THR:HG21	2:C:124:ASP:O	2.11	0.51
2:C:140:ILE:HG13	2:C:410:ILE:HG21	1.93	0.51
3:D:54:LYS:HG3	3:D:55:ASP:H	1.76	0.51
3:D:996:TRP:CD2	3:D:1056:PRO:HG3	2.46	0.51
4:E:48:MET:HG2	4:E:49:GLN:H	1.75	0.51
1:A:24:VAL:HG22	1:A:196:THR:HG22	1.94	0.50
2:C:841:ASN:HD22	2:C:992:MET:HE1	1.76	0.50
3:D:101:HIS:ND1	3:D:582:LEU:HD13	2.25	0.50
3:D:584:ASN:OD1	3:D:590:PRO:HD2	2.11	0.50
6:R:22:U:H2'	6:R:23:G:H8	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:160:GLU:HA	3:D:163:TYR:CZ	2.46	0.50
3:D:414:ARG:HG3	3:D:433:GLY:H	1.75	0.50
3:D:800:LYS:NZ	3:D:804:LEU:HD22	2.27	0.50
3:D:1197:ARG:HB3	3:D:1396:GLU:CD	2.36	0.50
3:D:832:ARG:O	3:D:834:THR:N	2.42	0.50
3:D:1372:VAL:HA	3:D:1375:MET:HE2	1.93	0.50
1:A:9:PRO:HG2	1:B:224:TYR:CE2	2.47	0.50
2:C:327:HIS:C	2:C:329:GLY:H	2.20	0.50
3:D:52:PRO:HG3	3:D:78:VAL:HG13	1.94	0.50
3:D:637:LEU:HB2	3:D:641:GLN:HG3	1.94	0.50
3:D:917:GLN:HB3	3:D:921:ARG:NH1	2.26	0.50
3:D:1294:VAL:O	3:D:1295:GLU:HB2	2.11	0.50
1:B:59:GLU:HG3	1:B:139:ASN:HB3	1.94	0.50
3:D:191:LEU:HD11	3:D:395:VAL:HG13	1.94	0.50
3:D:483:HIS:HB2	3:D:484:PRO:HD3	1.93	0.50
7:T:13:DC:H2''	7:T:14:DA:OP2	2.12	0.50
2:C:210:GLU:HG2	2:C:304:LEU:HD21	1.94	0.50
2:C:471:TYR:CE2	2:C:496:ILE:HG21	2.46	0.50
3:D:584:ASN:HB2	3:D:602:SER:HB3	1.94	0.50
1:B:14:ARG:HG3	1:B:14:ARG:HH11	1.77	0.49
2:C:108:ILE:HG13	2:C:366:SER:HB2	1.94	0.49
6:R:26:U:H2'	6:R:27:G:H8	1.76	0.49
1:A:18:ARG:HG3	1:A:206:THR:HG22	1.94	0.49
2:C:251:ASP:OD1	2:C:252:LYS:N	2.45	0.49
2:C:442:GLU:HG2	2:C:454:SER:CB	2.41	0.49
2:C:1094:ALA:HB2	3:D:520:LEU:HD12	1.92	0.49
1:A:153:ALA:HA	1:A:156:HIS:CE1	2.47	0.49
3:D:119:SER:H	3:D:123:LEU:HD22	1.76	0.49
2:C:1046:ALA:HB2	3:D:1472:ILE:HG13	1.94	0.49
2:C:1103:ASP:H	2:C:1107:ASN:H	1.59	0.49
3:D:1261:GLU:OE2	3:D:1269:LYS:HG3	2.12	0.49
3:D:1383:ASP:HB2	3:D:1416:ALA:HB3	1.94	0.49
1:A:89:PHE:HE1	1:A:97:VAL:HB	1.78	0.49
2:C:44:ILE:HG23	2:C:344:PHE:CE2	2.47	0.49
2:C:272:ALA:C	2:C:276:LYS:NZ	2.71	0.49
2:C:338:GLU:HA	2:C:341:THR:HG22	1.94	0.49
3:D:1108:ARG:HH12	3:D:1460:ILE:HG13	1.76	0.49
3:D:1108:ARG:NH2	3:D:1198:TYR:O	2.45	0.49
3:D:1301:LYS:HD2	3:D:1303:TYR:CE1	2.48	0.49
1:B:128:HIS:CE1	1:B:131:THR:HG23	2.48	0.49
2:C:428:ARG:NH1	3:D:1086:LEU:HD21	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:31:THR:OG1	3:D:32:ILE:N	2.45	0.49
3:D:473:LEU:HD23	3:D:499:VAL:HG21	1.95	0.49
3:D:1074:SER:HA	3:D:1077:ALA:HB3	1.95	0.49
2:C:689:VAL:HB	2:C:870:ILE:HB	1.94	0.49
2:C:1105:LYS:HZ1	2:C:1107:ASN:HB2	1.77	0.49
2:C:604:ALA:HB3	2:C:612:VAL:HB	1.95	0.49
2:C:1006:HIS:HB2	3:D:628:ARG:HG2	1.95	0.49
2:C:474:VAL:HG12	2:C:479:VAL:HA	1.95	0.49
3:D:1258:ARG:NH1	3:D:1262:LEU:HD21	2.28	0.49
1:B:185:ARG:HD3	3:D:692:GLU:OE2	2.13	0.49
2:C:327:HIS:HA	2:C:431:HIS:NE2	2.28	0.48
2:C:739:GLU:HB2	2:C:742:VAL:HB	1.95	0.48
3:D:179:VAL:HG13	3:D:183:GLU:HB3	1.95	0.48
1:A:98:THR:HG22	1:A:143:ARG:HG3	1.94	0.48
1:A:228:PRO:HB3	1:B:13:VAL:HG23	1.95	0.48
1:B:85:LEU:HB3	1:B:127:LEU:HD23	1.95	0.48
2:C:858:MET:HG3	2:C:859:PRO:HD2	1.93	0.48
3:D:690:ALA:O	3:D:694:VAL:HG13	2.13	0.48
3:D:695:ILE:HG13	3:D:696:HIS:H	1.77	0.48
3:D:820:GLU:HB3	3:D:836:VAL:HG11	1.95	0.48
2:C:472:ARG:O	2:C:532:MET:N	2.46	0.48
2:C:1008:ARG:HD3	2:C:1028:GLY:N	2.29	0.48
3:D:7:LYS:HA	3:D:1459:LEU:HD13	1.94	0.48
3:D:539:ASP:HB3	3:D:600:LEU:HB3	1.94	0.48
3:D:1146:GLY:HA3	3:D:1207:TYR:HB2	1.96	0.48
2:C:97:ARG:HG2	2:C:112:GLU:OE2	2.13	0.48
2:C:424:GLY:O	2:C:426:ASP:N	2.41	0.48
3:D:353:VAL:HG22	3:D:368:VAL:HG22	1.94	0.48
3:D:153:LEU:HB2	3:D:157:GLU:HG2	1.95	0.48
3:D:739:ASP:OD1	3:D:739:ASP:N	2.47	0.48
3:D:820:GLU:OE2	3:D:840:LYS:NZ	2.37	0.48
3:D:850:LEU:HD22	3:D:881:LEU:HD12	1.95	0.48
2:C:540:PHE:HB3	2:C:544:THR:HB	1.95	0.48
2:C:810:ASP:HB2	2:C:813:VAL:HG13	1.96	0.48
3:D:101:HIS:HE1	3:D:582:LEU:HD22	1.77	0.48
3:D:1189:ARG:HD2	3:D:1204:CYS:SG	2.54	0.48
3:D:50:PHE:O	3:D:89:ARG:HD2	2.14	0.48
2:C:9:ILE:HG12	2:C:907:ASP:CG	2.38	0.48
2:C:680:ASP:N	3:D:943:THR:HG21	2.27	0.48
3:D:415:VAL:O	3:D:432:TYR:HA	2.14	0.48
2:C:272:ALA:CB	2:C:276:LYS:HZ1	2.23	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:702:LEU:HB3	3:D:745:MET:CE	2.44	0.48
3:D:1284:GLU:HB2	3:D:1291:SER:O	2.14	0.48
1:A:133:GLU:HG2	1:A:134:GLU:N	2.29	0.47
2:C:45:GLN:O	2:C:48:PHE:HB2	2.14	0.47
1:B:75:VAL:O	1:B:79:ILE:HG13	2.14	0.47
2:C:1056:LYS:O	3:D:624:ASP:HB2	2.14	0.47
2:C:198:ARG:NH1	2:C:202:TYR:O	2.39	0.47
2:C:919:ALA:HB2	2:C:968:LEU:HD21	1.95	0.47
3:D:123:LEU:HG	3:D:152:LEU:HD13	1.96	0.47
3:D:531:ASP:C	3:D:533:GLY:H	2.23	0.47
3:D:1031:ASN:HB3	3:D:1034:GLN:HB2	1.96	0.47
2:C:198:ARG:NH1	2:C:203:ASP:HA	2.30	0.47
2:C:713:ARG:HA	2:C:819:VAL:HA	1.97	0.47
2:C:1008:ARG:NH1	2:C:1011:GLY:N	2.61	0.47
3:D:365:ASP:O	3:D:379:ALA:HB2	2.13	0.47
3:D:1264:GLU:OE2	3:D:1425:THR:HG22	2.15	0.47
2:C:47:ALA:CB	2:C:345:ARG:HG2	2.43	0.47
2:C:602:GLU:H	2:C:614:ARG:HB3	1.80	0.47
2:C:865:THR:HA	2:C:866:PRO:HD3	1.78	0.47
3:D:165:LYS:O	3:D:167:GLU:N	2.48	0.47
3:D:829:VAL:O	3:D:831:GLY:N	2.43	0.47
3:D:1354:LYS:HA	3:D:1357:ARG:HD2	1.96	0.47
3:D:1394:VAL:HG21	3:D:1432:LYS:NZ	2.30	0.47
2:C:891:GLY:O	2:C:991:GLN:HG2	2.15	0.47
2:C:978:ARG:CG	2:C:978:ARG:NH1	2.73	0.47
3:D:348:GLN:HB3	3:D:350:HIS:CE1	2.50	0.47
3:D:565:ILE:O	3:D:569:ASN:HB2	2.15	0.47
5:N:3:DA:H2"	5:N:4:DA:C8	2.50	0.47
3:D:956:ILE:HA	3:D:1039:CYS:HB3	1.97	0.47
2:C:216:GLU:O	2:C:218:VAL:N	2.48	0.47
3:D:1401:GLU:CD	3:D:1415:VAL:HG22	2.40	0.47
1:A:150:TYR:CD1	2:C:696:LYS:HG2	2.50	0.46
2:C:295:ASP:C	2:C:297:GLU:H	2.23	0.46
2:C:976:ASP:OD2	2:C:978:ARG:NH1	2.48	0.46
1:A:165:ILE:HA	1:A:166:PRO:HD3	1.83	0.46
2:C:397:GLU:HG2	2:C:403:SER:OG	2.15	0.46
2:C:759:THR:HG22	2:C:787:ASP:HA	1.98	0.46
2:C:910:LYS:O	2:C:914:ILE:HG12	2.15	0.46
2:C:946:ARG:HH11	2:C:946:ARG:HG2	1.80	0.46
3:D:29:PRO:HB3	3:D:548:ILE:HB	1.97	0.46
3:D:607:LEU:HD23	3:D:614:PHE:CE1	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1051:GLU:OE2	3:D:751:LEU:HB2	2.16	0.46
3:D:786:ILE:HG21	3:D:1027:GLY:H	1.81	0.46
1:A:97:VAL:HG21	1:A:120:VAL:HG21	1.97	0.46
3:D:1107:VAL:HA	3:D:1200:VAL:O	2.16	0.46
1:B:58:ILE:HB	1:B:61:VAL:HB	1.98	0.46
3:D:1458:GLU:O	3:D:1460:ILE:N	2.49	0.46
2:C:98:LEU:HD21	2:C:373:VAL:HG21	1.98	0.46
2:C:290:LEU:HD13	2:C:302:VAL:HG12	1.97	0.46
2:C:904:PRO:HD2	2:C:908:GLY:HA2	1.97	0.46
3:D:1135:ARG:NH1	3:D:1139:ASP:HB3	2.31	0.46
1:A:169:ALA:HB1	1:A:171:PHE:CE2	2.51	0.46
2:C:100:LEU:HB3	2:C:368:THR:OG1	2.15	0.46
2:C:478:VAL:HG22	2:C:507:ARG:HG2	1.97	0.46
1:A:67:THR:HB	2:C:627:ARG:HD3	1.98	0.46
1:B:94:LEU:HD11	1:B:119:ASP:HB2	1.97	0.46
2:C:198:ARG:HH12	2:C:203:ASP:HA	1.81	0.46
2:C:851:LYS:HG3	2:C:853:LEU:HD12	1.98	0.46
3:D:28:LYS:C	3:D:548:ILE:HG21	2.40	0.46
3:D:1041:LEU:HD12	3:D:1058:ARG:HA	1.98	0.46
1:B:201:THR:HG22	1:B:202:ASP:H	1.81	0.46
2:C:184:MET:HB2	2:C:184:MET:HE2	1.82	0.46
2:C:288:ARG:HH11	2:C:288:ARG:N	2.07	0.46
2:C:861:LEU:HD12	2:C:865:THR:HG23	1.97	0.46
3:D:1044:LEU:HA	3:D:1056:PRO:HA	1.97	0.46
1:A:13:VAL:HG21	1:B:228:PRO:HB3	1.98	0.45
1:A:174:VAL:HA	1:A:201:THR:HG22	1.97	0.45
2:C:3:ILE:HD11	2:C:665:PHE:CE2	2.50	0.45
2:C:165:LEU:HD12	2:C:165:LEU:HA	1.87	0.45
2:C:966:LEU:HD12	2:C:966:LEU:HA	1.77	0.45
3:D:182:GLY:HA2	3:D:203:ALA:O	2.16	0.45
3:D:356:PRO:HG2	3:D:359:ALA:HB2	1.98	0.45
3:D:792:ILE:HD13	3:D:941:PHE:CD2	2.51	0.45
3:D:792:ILE:HD13	3:D:941:PHE:HD2	1.81	0.45
2:C:86:LYS:HD3	2:C:813:VAL:HG12	1.98	0.45
2:C:335:THR:O	2:C:339:LEU:HG	2.16	0.45
2:C:586:ARG:NH1	2:C:590:ASP:OD2	2.49	0.45
2:C:136:ILE:HB	2:C:336:VAL:HG13	1.98	0.45
2:C:146:VAL:HB	2:C:281:LEU:HD11	1.99	0.45
2:C:602:GLU:HA	2:C:648:ARG:HA	1.99	0.45
3:D:30:GLU:HB3	3:D:40:GLU:HB3	1.97	0.45
3:D:805:GLU:HA	3:D:832:ARG:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:908:LYS:HB2	3:D:1027:GLY:CA	2.47	0.45
3:D:1369:GLU:HA	3:D:1372:VAL:HG12	1.98	0.45
2:C:97:ARG:HG2	2:C:111:ASP:HB3	1.97	0.45
2:C:586:ARG:HH12	2:C:590:ASP:CG	2.25	0.45
2:C:1009:SER:HB2	3:D:625:TYR:CD1	2.51	0.45
2:C:1040:LEU:HD23	2:C:1049:LEU:HA	1.99	0.45
3:D:165:LYS:NZ	3:D:199:LEU:HD22	2.31	0.45
3:D:613:ARG:NH1	3:D:616:GLN:HG2	2.32	0.45
3:D:826:PRO:HD2	3:D:829:VAL:HG21	1.98	0.45
3:D:939:PHE:O	3:D:943:THR:HG23	2.17	0.45
4:E:72:ARG:HB2	4:E:73:LEU:HD12	1.97	0.45
1:B:109:VAL:HA	1:B:113:ASP:OD2	2.16	0.45
2:C:134:ARG:NH2	2:C:392:SER:O	2.50	0.45
2:C:976:ASP:OD1	2:C:978:ARG:NH1	2.50	0.45
1:A:30:ARG:HH21	1:A:191:ASP:HB3	1.82	0.45
1:A:85:LEU:HD12	1:A:124:ASN:HB3	1.98	0.45
2:C:290:LEU:HD12	2:C:290:LEU:HA	1.60	0.45
2:C:344:PHE:CE1	2:C:378:LEU:HD11	2.52	0.45
3:D:58:CYS:HA	3:D:78:VAL:HG11	1.98	0.45
3:D:1381:VAL:HB	3:D:1389:LEU:HA	1.98	0.45
4:E:47:LYS:HA	4:E:54:LEU:HB3	1.98	0.45
1:A:49:PRO:HA	1:A:148:VAL:HG22	1.99	0.45
2:C:92:ALA:HB2	2:C:120:LEU:HD11	1.97	0.45
2:C:235:LEU:HD11	2:C:298:PHE:HE2	1.81	0.45
2:C:503:LEU:HD23	2:C:508:ILE:HA	1.97	0.45
3:D:558:LEU:HD23	3:D:567:ILE:HD13	1.99	0.45
3:D:657:LEU:HG	3:D:661:MET:HE2	1.99	0.45
3:D:963:TYR:CE1	3:D:1002:LYS:HB3	2.51	0.45
1:A:56:VAL:HG21	1:A:82:LEU:HD13	1.99	0.45
2:C:288:ARG:H	2:C:288:ARG:HD3	1.81	0.45
2:C:1089:VAL:HA	2:C:1099:VAL:HG21	1.99	0.45
3:D:123:LEU:O	3:D:127:LEU:HG	2.16	0.45
3:D:805:GLU:OE2	3:D:816:HIS:NE2	2.49	0.45
3:D:209:ARG:HB2	3:D:389:GLU:HG3	1.99	0.45
3:D:346:ARG:HH22	3:D:349:PRO:HD3	1.82	0.45
3:D:553:ARG:O	3:D:557:LEU:HB2	2.17	0.45
3:D:721:VAL:HG12	3:D:722:GLU:O	2.17	0.45
3:D:784:ASP:HB3	3:D:939:PHE:HE1	1.82	0.45
3:D:1462:LEU:HG	3:D:1472:ILE:HB	1.99	0.45
1:A:183:ASP:OD1	1:A:183:ASP:N	2.50	0.45
1:B:143:ARG:HD2	1:B:160:ASP:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:139:GLN:HA	2:C:411:SER:O	2.17	0.45
2:C:716:LYS:HA	2:C:716:LYS:HD3	1.83	0.45
2:C:953:VAL:HB	2:C:962:GLN:OE1	2.17	0.45
2:C:996:LYS:HD3	2:C:1000:MET:HE1	1.99	0.45
3:D:179:VAL:HG11	3:D:203:ALA:HB3	1.99	0.45
3:D:800:LYS:HG2	3:D:804:LEU:HD22	1.99	0.45
1:B:74:ASP:HB2	3:D:872:ARG:HH22	1.83	0.44
2:C:428:ARG:HH11	3:D:1086:LEU:HD11	1.81	0.44
2:C:473:ARG:HG3	2:C:480:THR:HB	1.99	0.44
2:C:1053:LEU:HD13	3:D:617:ASN:HB3	1.99	0.44
3:D:701:LEU:O	3:D:747:VAL:HA	2.17	0.44
3:D:758:GLU:O	3:D:762:GLN:HG2	2.18	0.44
3:D:1481:VAL:HG13	4:E:18:ARG:HA	1.99	0.44
2:C:200:LEU:HA	2:C:298:PHE:HB2	1.99	0.44
2:C:223:ASP:HB2	2:C:224:GLU:H	1.36	0.44
2:C:341:THR:O	2:C:345:ARG:HG3	2.18	0.44
2:C:1043:TYR:CD1	3:D:763:MET:HG2	2.52	0.44
3:D:176:ASP:HB3	3:D:177:ALA:H	1.56	0.44
3:D:510:GLU:HG3	3:D:511:TRP:HD1	1.82	0.44
3:D:764:LEU:HD23	3:D:766:ALA:H	1.83	0.44
1:A:42:ARG:O	1:A:46:SER:HB3	2.18	0.44
2:C:557:ARG:NH1	2:C:560:MET:HE1	2.33	0.44
2:C:1036:GLU:OE1	2:C:1036:GLU:N	2.47	0.44
2:C:1055:LEU:HD11	2:C:1066:ALA:HB2	1.99	0.44
3:D:708:LEU:HD21	3:D:1091:SER:HB2	1.99	0.44
3:D:709:HIS:CD2	3:D:711:LEU:HB2	2.52	0.44
2:C:290:LEU:HD22	2:C:302:VAL:HG12	2.00	0.44
3:D:486:ARG:HH21	3:D:489:ARG:NH1	2.04	0.44
3:D:1433:SER:OG	3:D:1457:ASP:OD1	2.29	0.44
2:C:146:VAL:HB	2:C:281:LEU:HD21	1.99	0.44
3:D:101:HIS:HD2	3:D:104:PHE:CE2	2.35	0.44
3:D:602:SER:O	3:D:606:ILE:HG12	2.17	0.44
3:D:1136:LYS:HB3	3:D:1139:ASP:OD2	2.17	0.44
3:D:1213:ARG:NH2	4:E:10:PHE:O	2.51	0.44
2:C:673:LEU:HA	2:C:991:GLN:HA	1.99	0.44
2:C:710:ILE:HG22	2:C:823:VAL:HB	1.99	0.44
3:D:108:VAL:HB	3:D:109:PRO:HD3	1.99	0.44
3:D:714:GLN:HB2	3:D:716:PHE:CE2	2.53	0.44
2:C:78:PHE:HA	2:C:79:PRO:HD3	1.90	0.44
2:C:695:LEU:HD21	2:C:833:LEU:HB3	2.00	0.44
3:D:42:ASP:HA	3:D:46:ASP:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:165:LYS:HZ2	3:D:199:LEU:HD22	1.81	0.44
3:D:967:ALA:HB1	3:D:995:LEU:HD21	2.00	0.44
3:D:1294:VAL:HG12	3:D:1295:GLU:N	2.32	0.44
3:D:1307:LYS:HB3	3:D:1308:GLU:OE2	2.18	0.44
2:C:48:PHE:HB3	2:C:52:PHE:CD2	2.49	0.44
2:C:71:TYR:HA	2:C:96:ALA:HA	2.00	0.44
2:C:246:ASP:HA	2:C:247:PRO:HD3	1.72	0.44
2:C:1070:ILE:HD11	2:C:1076:VAL:HG22	2.00	0.44
3:D:1422:MET:HB2	3:D:1426:LYS:HD3	2.00	0.44
3:D:65:ARG:HD2	3:D:65:ARG:HA	1.69	0.44
3:D:355:VAL:HG11	3:D:385:VAL:HG11	2.00	0.44
3:D:661:MET:HE3	3:D:673:ALA:HB1	2.00	0.44
3:D:1311:LEU:HA	3:D:1325:LEU:O	2.18	0.44
1:B:57:TYR:CD2	1:B:161:ARG:HG3	2.53	0.43
2:C:136:ILE:HD11	2:C:386:PHE:CE1	2.53	0.43
2:C:358:ARG:HD3	2:C:371:LYS:O	2.17	0.43
3:D:136:ASP:CB	3:D:137:PRO:HD2	2.45	0.43
3:D:1364:HIS:CE1	3:D:1366:LYS:HG3	2.53	0.43
1:A:79:ILE:HA	1:A:82:LEU:HD12	2.00	0.43
2:C:585:GLU:O	2:C:589:ARG:HG2	2.19	0.43
3:D:408:GLU:H	3:D:408:GLU:HG2	1.59	0.43
3:D:650:LEU:HD21	3:D:677:LEU:HD23	2.00	0.43
3:D:1131:SER:OG	3:D:1133:ARG:NH2	2.51	0.43
1:B:62:LEU:HD23	1:B:163:ASN:HD22	1.83	0.43
2:C:121:MET:HB3	2:C:121:MET:HE2	1.74	0.43
2:C:124:ASP:HB3	2:C:592:LEU:HD12	2.01	0.43
2:C:184:MET:O	2:C:190:LYS:HA	2.18	0.43
2:C:666:LEU:HG	2:C:668:LEU:HG	2.00	0.43
2:C:858:MET:HB2	2:C:858:MET:HE3	1.62	0.43
3:D:710:ARG:C	3:D:712:GLY:H	2.26	0.43
3:D:1336:LEU:HD13	3:D:1376:MET:HE1	2.00	0.43
2:C:21:ILE:HD11	2:C:455:LEU:HD22	2.00	0.43
2:C:47:ALA:HB2	2:C:345:ARG:HG2	2.00	0.43
2:C:233:GLU:OE1	2:C:233:GLU:N	2.41	0.43
2:C:627:ARG:HG3	2:C:628:PHE:CD2	2.54	0.43
2:C:722:ILE:HD12	2:C:823:VAL:HG21	2.00	0.43
2:C:1103:ASP:CG	2:C:1104:GLU:H	2.26	0.43
3:D:798:GLU:HG2	3:D:799:LYS:H	1.83	0.43
3:D:919:PHE:HA	3:D:927:THR:OG1	2.19	0.43
3:D:1280:VAL:O	3:D:1294:VAL:HG13	2.17	0.43
3:D:1348:LEU:HD13	3:D:1375:MET:HE1	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LYS:HA	1:A:138:LEU:O	2.19	0.43
1:A:218:LEU:HD23	1:B:222:LEU:HD21	2.01	0.43
2:C:853:LEU:HB2	2:C:858:MET:CE	2.49	0.43
3:D:563:PRO:HG2	3:D:566:ILE:HG13	2.01	0.43
3:D:568:ARG:HH11	3:D:571:LYS:HE3	1.83	0.43
3:D:739:ASP:OD2	3:D:741:ASP:OD2	2.36	0.43
3:D:1118:ILE:HD12	3:D:1118:ILE:HA	1.84	0.43
1:B:221:HIS:HA	1:B:224:TYR:CD2	2.53	0.43
2:C:13:ILE:HD13	2:C:483:VAL:HG11	2.00	0.43
2:C:1075:ASP:OD1	2:C:1076:VAL:N	2.52	0.43
3:D:1123:PHE:HB3	3:D:1132:LEU:HG	2.00	0.43
2:C:18:LEU:HB3	2:C:408:ARG:HD2	2.00	0.43
2:C:147:TYR:HA	2:C:323:ASP:OD2	2.18	0.43
2:C:429:ASP:OD1	3:D:1079:LYS:HD3	2.19	0.43
2:C:715:THR:OG1	2:C:718:GLY:O	2.36	0.43
2:C:810:ASP:O	2:C:812:GLY:N	2.50	0.43
3:D:975:GLU:HG3	3:D:979:GLU:OE2	2.18	0.43
3:D:1135:ARG:HB3	3:D:1140:ILE:HD11	2.00	0.43
3:D:1274:ILE:HA	3:D:1325:LEU:HD21	2.00	0.43
2:C:501:THR:HA	2:C:502:PRO:HD3	1.88	0.43
2:C:759:THR:HB	2:C:785:VAL:HG22	2.01	0.43
1:A:38:ASN:O	1:A:42:ARG:HG2	2.18	0.43
1:B:14:ARG:HG3	1:B:14:ARG:NH1	2.34	0.43
2:C:219:GLN:O	2:C:223:ASP:OD2	2.37	0.43
2:C:334:ARG:HH22	2:C:415:PRO:HG2	1.84	0.43
3:D:165:LYS:HD2	3:D:397:LYS:HB2	2.00	0.43
3:D:486:ARG:HA	3:D:489:ARG:HB3	2.00	0.43
3:D:645:PRO:HA	3:D:721:VAL:O	2.19	0.43
3:D:1003:VAL:O	3:D:1007:VAL:HG23	2.19	0.43
4:E:45:ARG:HH21	4:E:63:TRP:HH2	1.66	0.43
2:C:238:LEU:HD21	2:C:242:LEU:HD13	2.01	0.43
2:C:676:ILE:HG23	2:C:988:VAL:HG13	1.99	0.43
2:C:749:VAL:HB	2:C:792:VAL:HG21	2.00	0.43
3:D:1314:LYS:HE3	3:D:1314:LYS:C	2.44	0.43
3:D:1366:LYS:O	3:D:1370:ILE:HG13	2.19	0.43
1:B:143:ARG:CZ	1:B:158:ILE:HG21	2.49	0.42
3:D:163:TYR:O	3:D:164:GLY:C	2.61	0.42
3:D:625:TYR:CD2	3:D:751:LEU:HD11	2.54	0.42
3:D:628:ARG:NH1	7:T:16:DC:H2"	2.34	0.42
2:C:87:ASP:HA	2:C:131:GLY:HA3	2.00	0.42
2:C:876:VAL:HG11	3:D:949:ILE:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:82:LYS:C	3:D:84:ILE:H	2.26	0.42
3:D:895:VAL:HG21	3:D:922:LEU:HD21	2.00	0.42
4:E:54:LEU:HG	4:E:58:PRO:CG	2.44	0.42
1:B:92:PRO:HA	1:B:146:ARG:HH12	1.85	0.42
2:C:37:GLU:OE2	2:C:38:LYS:HG2	2.20	0.42
2:C:52:PHE:CE1	2:C:98:LEU:HD13	2.53	0.42
2:C:274:ARG:HH22	2:C:284:ARG:HA	1.84	0.42
2:C:334:ARG:HE	2:C:339:LEU:HD23	1.85	0.42
2:C:512:ARG:HA	2:C:512:ARG:HD3	1.84	0.42
3:D:520:LEU:HG	3:D:521:PRO:HD2	2.01	0.42
3:D:630:VAL:O	3:D:725:SER:HB3	2.18	0.42
3:D:1018:ASN:O	3:D:1021:TYR:N	2.51	0.42
3:D:1037:GLN:HG2	3:D:1042:ARG:HG2	2.00	0.42
3:D:1124:GLN:HA	3:D:1125:PRO:HD3	1.85	0.42
3:D:1277:ILE:H	3:D:1277:ILE:HG13	1.68	0.42
3:D:1435:LEU:HB2	3:D:1457:ASP:OD1	2.20	0.42
2:C:379:GLU:O	2:C:383:ARG:HB3	2.19	0.42
2:C:893:ALA:HB2	2:C:918:LEU:HD23	2.00	0.42
3:D:205:TYR:CE1	3:D:390:PRO:HG3	2.54	0.42
3:D:374:GLU:C	3:D:376:GLU:H	2.27	0.42
3:D:500:ARG:HG2	3:D:1388:ARG:NH1	2.35	0.42
3:D:966:GLU:HA	3:D:969:ARG:HG2	2.01	0.42
3:D:1128:VAL:HG12	3:D:1129:THR:N	2.33	0.42
2:C:700:TYR:HB2	2:C:833:LEU:HB2	2.01	0.42
2:C:718:GLY:HA3	2:C:761:PHE:CG	2.54	0.42
3:D:93:ILE:HB	3:D:517:VAL:HB	2.01	0.42
3:D:864:VAL:HG22	3:D:877:PRO:HD3	2.01	0.42
3:D:1209:LEU:HD11	4:E:16:LYS:HD2	2.01	0.42
3:D:1296:SER:HB3	3:D:1299:PHE:CD2	2.49	0.42
2:C:202:TYR:CE1	2:C:304:LEU:HD22	2.55	0.42
2:C:211:LEU:HD13	2:C:221:LEU:HD21	2.01	0.42
2:C:880:MET:HE2	2:C:880:MET:HB2	1.87	0.42
2:C:889:HIS:CE1	3:D:951:ILE:H	2.37	0.42
2:C:1085:PHE:HB2	3:D:1468:LEU:HB3	2.01	0.42
3:D:212:ARG:HB3	3:D:388:HIS:CD2	2.54	0.42
3:D:1008:PHE:CZ	3:D:1032:PRO:HA	2.55	0.42
3:D:1312:LEU:HD21	3:D:1327:ARG:HH21	1.85	0.42
4:E:3:GLU:O	4:E:5:GLY:N	2.52	0.42
2:C:113:VAL:O	2:C:115:LEU:N	2.49	0.42
2:C:313:LEU:HD22	2:C:321:GLU:O	2.20	0.42
2:C:393:GLN:HG2	6:R:25:G:O2'	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:475:VAL:HG23	2:C:480:THR:OG1	2.19	0.42
2:C:678:PRO:HA	2:C:683:ASN:HD21	1.84	0.42
2:C:905:ILE:HG22	2:C:906:PHE:CD2	2.54	0.42
2:C:1019:GLN:HA	2:C:1020:PRO:HD3	1.70	0.42
3:D:167:GLU:OE1	3:D:198:ARG:NH2	2.53	0.42
3:D:171:LEU:HD23	3:D:171:LEU:HA	1.91	0.42
3:D:458:ALA:HB2	3:D:575:GLN:NE2	2.33	0.42
3:D:583:ASP:OD2	3:D:604:THR:HG21	2.19	0.42
4:E:24:ALA:O	4:E:28:GLN:HG3	2.20	0.42
1:A:180:GLN:HB2	1:A:196:THR:OG1	2.19	0.42
2:C:469:THR:O	2:C:485:TYR:HA	2.20	0.42
2:C:1014:SER:HB3	2:C:1017:THR:O	2.19	0.42
1:A:228:PRO:HB3	1:B:13:VAL:CG2	2.50	0.42
2:C:127:PHE:O	2:C:129:ILE:HD12	2.20	0.42
3:D:719:VAL:O	3:D:721:VAL:HG23	2.20	0.42
3:D:877:PRO:O	3:D:880:ILE:HG22	2.20	0.42
2:C:350:ARG:HB3	2:C:377:PRO:HB3	2.00	0.42
2:C:521:PRO:HB2	3:D:1055:VAL:HG21	2.02	0.42
3:D:352:ASN:HB2	3:D:369:ALA:O	2.20	0.42
3:D:1401:GLU:OE2	3:D:1402:ALA:N	2.53	0.42
2:C:127:PHE:HB2	2:C:129:ILE:HD11	2.01	0.41
2:C:906:PHE:HZ	3:D:1070:TYR:HD1	1.67	0.41
2:C:1071:ILE:HD13	2:C:1071:ILE:HA	1.91	0.41
3:D:212:ARG:H	3:D:388:HIS:HD2	1.68	0.41
3:D:494:LYS:HB2	3:D:494:LYS:NZ	2.35	0.41
3:D:1263:PHE:CZ	3:D:1352:ILE:HD13	2.55	0.41
1:B:101:LEU:HD23	1:B:140:MET:HG2	2.02	0.41
2:C:34:VAL:HB	2:C:38:LYS:HZ2	1.85	0.41
2:C:34:VAL:HG11	2:C:38:LYS:HZ1	1.84	0.41
2:C:48:PHE:O	2:C:52:PHE:HB2	2.20	0.41
2:C:205:GLU:H	2:C:205:GLU:HG3	1.43	0.41
2:C:223:ASP:OD1	2:C:224:GLU:HG2	2.20	0.41
2:C:993:PHE:CE2	2:C:995:MET:HE2	2.55	0.41
3:D:433:GLY:HA3	3:D:447:VAL:O	2.19	0.41
3:D:607:LEU:HD23	3:D:614:PHE:HE1	1.85	0.41
2:C:265:ARG:NH1	2:C:267:TYR:HD1	2.18	0.41
3:D:184:GLU:HA	3:D:202:VAL:HA	2.03	0.41
3:D:416:ALA:HB3	3:D:419:ASP:OD1	2.20	0.41
3:D:703:ASN:HB3	3:D:746:ALA:HB3	2.02	0.41
3:D:1378:TYR:O	3:D:1420:LEU:HB3	2.21	0.41
3:D:1394:VAL:HB	3:D:1397:LYS:HG2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:11:DT:H2''	7:T:12:DC:O5'	2.20	0.41
1:B:190:THR:HG21	3:D:720:LEU:O	2.20	0.41
2:C:18:LEU:HD21	2:C:542:VAL:HG11	2.02	0.41
2:C:710:ILE:HD11	2:C:758:ARG:NH2	2.28	0.41
3:D:1209:LEU:HD12	3:D:1213:ARG:HD3	2.01	0.41
1:A:25:LEU:HD22	1:B:225:PHE:CE1	2.55	0.41
2:C:384:GLU:HA	2:C:388:ARG:NH2	2.33	0.41
2:C:555:ALA:HB2	3:D:1070:TYR:HE2	1.86	0.41
2:C:580:MET:HG3	2:C:902:ILE:HG12	2.02	0.41
2:C:1005:MET:HB2	3:D:724:GLN:NE2	2.31	0.41
3:D:655:PRO:HA	3:D:658:LEU:HD12	2.01	0.41
3:D:717:GLN:HA	3:D:718:PRO:HD3	1.87	0.41
1:A:34:VAL:HG21	2:C:939:ARG:NE	2.36	0.41
2:C:726:ILE:HA	2:C:727:PRO:HD3	1.81	0.41
3:D:62:LYS:HD2	3:D:75:ARG:HD2	2.03	0.41
3:D:646:LYS:HE3	3:D:722:GLU:HG2	2.02	0.41
3:D:1309:ALA:HB1	3:D:1326:THR:HG23	2.03	0.41
2:C:409:ARG:HA	2:C:454:SER:HA	2.03	0.41
2:C:1097:LEU:HD11	3:D:103:TRP:CZ3	2.56	0.41
3:D:131:LYS:HB2	3:D:568:ARG:HG2	2.03	0.41
3:D:165:LYS:CG	3:D:199:LEU:HB3	2.49	0.41
3:D:826:PRO:HB2	3:D:829:VAL:HG23	2.01	0.41
3:D:880:ILE:HD12	3:D:880:ILE:HA	1.93	0.41
3:D:1279:GLY:O	3:D:1319:VAL:HG12	2.21	0.41
3:D:1398:TRP:HA	3:D:1398:TRP:CE3	2.56	0.41
3:D:1472:ILE:HA	3:D:1473:PRO:HD3	1.82	0.41
3:D:756:GLN:O	3:D:760:ARG:HG2	2.21	0.41
3:D:1284:GLU:HG2	3:D:1291:SER:HB2	2.02	0.41
3:D:1364:HIS:ND1	3:D:1366:LYS:HG3	2.35	0.41
4:E:59:ASN:OD1	4:E:60:ALA:N	2.53	0.41
1:B:105:GLY:C	1:B:107:LYS:H	2.29	0.41
2:C:196:LEU:HA	2:C:199:VAL:HG23	2.02	0.41
2:C:290:LEU:HD11	2:C:301:GLU:N	2.23	0.41
2:C:443:THR:HG22	2:C:453:THR:HG22	2.02	0.41
2:C:607:ASP:OD1	2:C:608:GLY:N	2.49	0.41
2:C:743:VAL:HG11	2:C:755:LEU:HD12	2.02	0.41
2:C:1081:VAL:HB	2:C:1086:ARG:NH1	2.36	0.41
3:D:111:LYS:HB2	3:D:111:LYS:HE2	1.88	0.41
3:D:832:ARG:HD2	3:D:832:ARG:HA	1.86	0.41
3:D:1295:GLU:HB3	3:D:1296:SER:H	1.53	0.41
4:E:51:LEU:HG	4:E:53:GLY:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:436:GLY:HA2	2:C:538:GLN:O	2.21	0.41
3:D:61:GLY:HA3	3:D:64:LYS:HZ2	1.85	0.41
3:D:352:ASN:CG	3:D:371:ILE:HG12	2.46	0.41
3:D:704:ARG:NH2	3:D:743:ASP:OD2	2.53	0.41
3:D:861:GLN:N	3:D:861:GLN:OE1	2.54	0.41
3:D:1108:ARG:NH1	3:D:1460:ILE:HG13	2.36	0.41
1:B:25:LEU:HD23	1:B:28:LEU:HD21	2.04	0.40
2:C:200:LEU:HD23	2:C:298:PHE:HB3	2.03	0.40
2:C:474:VAL:HG12	2:C:479:VAL:HG13	2.03	0.40
2:C:729:LEU:HD23	2:C:729:LEU:HA	1.93	0.40
2:C:1085:PHE:CD1	3:D:1468:LEU:HB3	2.55	0.40
3:D:807:ALA:HA	3:D:833:GLU:CD	2.46	0.40
3:D:1119:SER:HB2	3:D:1185:GLU:CB	2.51	0.40
3:D:1128:VAL:HG23	3:D:1133:ARG:HH22	1.85	0.40
7:T:2:DG:H2"	7:T:3:DG:C8	2.56	0.40
1:A:179:PHE:HB3	1:A:197:LEU:HD12	2.03	0.40
1:B:185:ARG:HB3	1:B:190:THR:HA	2.03	0.40
2:C:259:GLY:CA	2:C:291:ALA:HB2	2.51	0.40
2:C:559:LEU:HD12	2:C:559:LEU:O	2.21	0.40
2:C:589:ARG:HB3	2:C:596:TYR:CZ	2.56	0.40
3:D:367:ILE:HG13	3:D:368:VAL:H	1.85	0.40
4:E:22:VAL:CG1	4:E:68:LEU:HD21	2.51	0.40
4:E:36:LYS:C	4:E:38:THR:H	2.29	0.40
2:C:205:GLU:OE1	2:C:206:THR:HG23	2.20	0.40
2:C:350:ARG:CB	2:C:377:PRO:HB3	2.51	0.40
2:C:503:LEU:HD21	2:C:508:ILE:HD13	2.03	0.40
2:C:690:ILE:HG12	2:C:691:SER:N	2.37	0.40
3:D:549:ASN:O	3:D:553:ARG:HB2	2.21	0.40
2:C:831:ARG:HH21	2:C:1000:MET:HG3	1.86	0.40
3:D:164:GLY:C	3:D:166:GLN:H	2.29	0.40
3:D:192:ALA:HB2	3:D:393:ILE:HD12	2.04	0.40
3:D:760:ARG:HD3	4:E:61:VAL:HG11	2.04	0.40
3:D:830:ALA:C	3:D:832:ARG:H	2.29	0.40
3:D:1004:THR:HG23	3:D:1036:ARG:HB2	2.02	0.40
3:D:1211:MET:HE3	3:D:1211:MET:HB2	1.99	0.40
1:A:26:GLU:HA	1:A:27:PRO:HA	1.88	0.40
2:C:69:LEU:O	2:C:97:ARG:HB2	2.22	0.40
2:C:222:MET:O	2:C:222:MET:HG2	2.19	0.40
3:D:57:GLU:HG2	3:D:58:CYS:N	2.37	0.40
3:D:116:LEU:HA	3:D:116:LEU:HD23	1.85	0.40
3:D:800:LYS:HZ2	3:D:804:LEU:HD22	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:849:ALA:O	3:D:853:VAL:HG23	2.21	0.40
4:E:45:ARG:HA	4:E:46:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	221/315 (70%)	193 (87%)	19 (9%)	9 (4%)	2	19
1	B	221/315 (70%)	199 (90%)	21 (10%)	1 (0%)	24	57
2	C	1077/1119 (96%)	901 (84%)	149 (14%)	27 (2%)	4	28
3	D	1352/1534 (88%)	1112 (82%)	189 (14%)	51 (4%)	2	20
4	E	91/99 (92%)	74 (81%)	14 (15%)	3 (3%)	3	23
All	All	2962/3382 (88%)	2479 (84%)	392 (13%)	91 (3%)	3	25

All (91) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	184	THR
2	C	2	GLU
2	C	111	ASP
2	C	164	PRO
2	C	213	ALA
2	C	217	LEU
2	C	223	ASP
2	C	320	HIS
2	C	369	PRO
3	D	136	ASP
3	D	176	ASP
3	D	363	ALA

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Mol	Chain	Res	Type
3	D	806	PHE
3	D	808	THR
3	D	830	ALA
3	D	1273	VAL
3	D	1294	VAL
3	D	1295	GLU
3	D	1327	ARG
3	D	1454	GLY
1	A	47	SER
1	A	161	ARG
2	C	248	PRO
2	C	262	ALA
2	C	274	ARG
2	C	476	GLY
2	C	517	ARG
2	C	795	GLY
3	D	50	PHE
3	D	200	ASP
3	D	522	PRO
3	D	594	PRO
3	D	616	GLN
3	D	823	LEU
3	D	1411	GLY
3	D	1459	LEU
4	E	58	PRO
1	A	48	ILE
1	A	186	LEU
1	A	226	SER
2	C	96	ALA
2	C	188	LYS
2	C	272	ALA
2	C	815	LEU
2	C	984	GLU
3	D	166	GLN
3	D	345	TYR
3	D	417	PRO
3	D	735	ALA
3	D	822	ALA
3	D	832	ARG
3	D	1208	ASP
4	E	4	PRO
1	A	29	GLU

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Mol	Chain	Res	Type
1	A	191	ASP
2	C	114	PHE
3	D	82	LYS
3	D	109	PRO
3	D	132	TYR
3	D	146	PRO
3	D	374	GLU
3	D	406	ASP
3	D	425	GLY
3	D	595	GLY
3	D	696	HIS
3	D	711	LEU
3	D	750	PRO
3	D	1205	TYR
3	D	1269	LYS
3	D	1284	GLU
3	D	1317	ASP
4	E	42	PRO
1	A	134	GLU
2	C	751	PRO
2	C	905	ILE
3	D	560	GLN
3	D	621	LYS
3	D	1314	LYS
1	B	125	PRO
2	C	152	PRO
2	C	231	PRO
2	C	463	GLU
3	D	55	ASP
3	D	124	GLU
3	D	705	ALA
2	C	811	PRO
3	D	683	ILE
3	D	809	PRO
3	D	1032	PRO
3	D	1057	VAL
2	C	244	PRO

5.3.2 Protein sidechains ⓘ

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

resolution.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	196/273 (72%)	187 (95%)	9 (5%)	24	50
1	B	196/273 (72%)	189 (96%)	7 (4%)	31	57
2	C	912/941 (97%)	832 (91%)	80 (9%)	9	32
3	D	1147/1289 (89%)	1055 (92%)	92 (8%)	11	35
4	E	82/88 (93%)	72 (88%)	10 (12%)	5	22
All	All	2533/2864 (88%)	2335 (92%)	198 (8%)	11	36

All (198) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	12	THR
1	A	15	THR
1	A	32	PHE
1	A	46	SER
1	A	126	ASP
1	A	131	THR
1	A	165	ILE
1	A	182	GLU
1	B	36	LEU
1	B	63	HIS
1	B	76	VAL
1	B	112	ARG
1	B	148	VAL
1	B	201	THR
1	B	205	VAL
2	C	30	LEU
2	C	38	LYS
2	C	39	ARG
2	C	73	LEU
2	C	81	ASP
2	C	98	LEU
2	C	102	HIS
2	C	104	ASP
2	C	118	ILE
2	C	127	PHE
2	C	135	VAL

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Mol	Chain	Res	Type
2	C	140	ILE
2	C	154	ARG
2	C	157	ARG
2	C	163	ILE
2	C	189	ARG
2	C	193	LEU
2	C	194	VAL
2	C	205	GLU
2	C	214	TYR
2	C	223	ASP
2	C	243	ARG
2	C	267	TYR
2	C	274	ARG
2	C	279	GLU
2	C	281	LEU
2	C	284	ARG
2	C	288	ARG
2	C	289	THR
2	C	295	ASP
2	C	300	ASP
2	C	307	LEU
2	C	321	GLU
2	C	350	ARG
2	C	351	LEU
2	C	367	LEU
2	C	375	SER
2	C	376	ARG
2	C	378	LEU
2	C	388	ARG
2	C	391	LEU
2	C	394	PHE
2	C	403	SER
2	C	405	ARG
2	C	473	ARG
2	C	481	ASP
2	C	506	ASN
2	C	559	LEU
2	C	565	GLN
2	C	583	LEU
2	C	610	ARG
2	C	620	LEU
2	C	625	LEU

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Mol	Chain	Res	Type
2	C	626	ARG
2	C	627	ARG
2	C	649	VAL
2	C	676	ILE
2	C	690	ILE
2	C	699	PHE
2	C	703	ILE
2	C	717	LEU
2	C	722	ILE
2	C	728	HIS
2	C	813	VAL
2	C	835	VAL
2	C	842	ARG
2	C	858	MET
2	C	899	GLN
2	C	953	VAL
2	C	966	LEU
2	C	978	ARG
2	C	987	ILE
2	C	988	VAL
2	C	1000	MET
2	C	1001	VAL
2	C	1008	ARG
2	C	1021	LEU
2	C	1035	MET
2	C	1099	VAL
2	C	1105	LYS
3	D	17	LYS
3	D	41	ARG
3	D	57	GLU
3	D	60	CYS
3	D	74	GLU
3	D	75	ARG
3	D	79	GLU
3	D	80	VAL
3	D	82	LYS
3	D	87	ARG
3	D	124	GLU
3	D	142	LEU
3	D	149	LYS
3	D	166	GLN
3	D	176	ASP

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Mol	Chain	Res	Type
3	D	178	LEU
3	D	185	VAL
3	D	340	THR
3	D	347	VAL
3	D	371	ILE
3	D	378	ILE
3	D	382	GLU
3	D	392	SER
3	D	400	VAL
3	D	405	ASP
3	D	408	GLU
3	D	414	ARG
3	D	431	VAL
3	D	435	VAL
3	D	446	VAL
3	D	450	TYR
3	D	494	LYS
3	D	520	LEU
3	D	686	GLU
3	D	694	VAL
3	D	724	GLN
3	D	734	GLU
3	D	776	GLU
3	D	796	ARG
3	D	804	LEU
3	D	808	THR
3	D	813	LEU
3	D	817	GLU
3	D	823	LEU
3	D	828	LYS
3	D	833	GLU
3	D	874	GLU
3	D	892	ASP
3	D	902	LEU
3	D	935	LYS
3	D	943	THR
3	D	971	LEU
3	D	983	LEU
3	D	985	ASP
3	D	1001	GLU
3	D	1012	GLU
3	D	1013	GLU

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Mol	Chain	Res	Type
3	D	1033	GLN
3	D	1041	LEU
3	D	1044	LEU
3	D	1058	ARG
3	D	1079	LYS
3	D	1083	ASP
3	D	1099	VAL
3	D	1106	VAL
3	D	1109	GLU
3	D	1115	THR
3	D	1131	SER
3	D	1135	ARG
3	D	1151	ARG
3	D	1162	GLU
3	D	1197	ARG
3	D	1207	TYR
3	D	1209	LEU
3	D	1215	VAL
3	D	1235	GLN
3	D	1262	LEU
3	D	1290	LEU
3	D	1296	SER
3	D	1299	PHE
3	D	1304	LYS
3	D	1305	LEU
3	D	1314	LYS
3	D	1318	TYR
3	D	1325	LEU
3	D	1327	ARG
3	D	1342	GLU
3	D	1373	ARG
3	D	1383	ASP
3	D	1441	GLN
3	D	1460	ILE
3	D	1478	SER
4	E	14	ASP
4	E	32	ARG
4	E	38	THR
4	E	39	VAL
4	E	40	LEU
4	E	41	GLU
4	E	47	LYS

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Mol	Chain	Res	Type
4	E	49	GLN
4	E	83	ASP
4	E	85	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	ASN
1	A	124	ASN
1	B	16	GLN
1	B	95	GLN
2	C	99	GLN
2	C	141	HIS
2	C	343	GLN
2	C	431	HIS
2	C	543	ASN
2	C	609	ASN
2	C	670	GLN
2	C	829	GLN
2	C	884	GLN
2	C	991	GLN
2	C	1064	ASN
3	D	101	HIS
3	D	125	GLN
3	D	350	HIS
3	D	388	HIS
3	D	552	ASN
3	D	696	HIS
3	D	768	ASN
3	D	1010	ASN
3	D	1489	GLN
4	E	28	GLN
4	E	49	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
6	R	8/29 (27%)	1 (12%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	R	22	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	223/315 (70%)	-0.15	0 100 100	45, 90, 147, 194	0
1	B	223/315 (70%)	-0.21	0 100 100	40, 86, 139, 173	0
2	C	1083/1119 (96%)	0.03	17 (1%) 70 45	32, 101, 186, 255	0
3	D	1358/1534 (88%)	0.01	23 (1%) 69 43	34, 102, 194, 264	0
4	E	93/99 (93%)	0.15	5 (5%) 31 18	58, 107, 184, 204	0
5	N	11/13 (84%)	0.62	0 100 100	369, 412, 462, 465	0
6	R	9/29 (31%)	0.80	0 100 100	178, 188, 215, 227	0
7	T	22/22 (100%)	0.88	1 (4%) 38 20	202, 334, 453, 466	0
All	All	3022/3446 (87%)	0.00	46 (1%) 72 47	32, 100, 193, 466	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	802	ALA	5.3
4	E	56	ASP	4.5
2	C	417	GLY	4.0
4	E	57	ASP	3.6
3	D	1090	ASP	3.5
3	D	124	GLU	3.3
3	D	801	GLY	3.1
3	D	848	GLU	3.0
4	E	54	LEU	2.9
2	C	416	GLY	2.9
3	D	108	VAL	2.8
3	D	810	GLU	2.8
3	D	165	LYS	2.8
3	D	162	ARG	2.7
4	E	58	PRO	2.7
2	C	271	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
3	D	640	HIS	2.6
2	C	269	LEU	2.6
3	D	128	TYR	2.6
2	C	1096	ALA	2.6
3	D	1209	LEU	2.6
3	D	847	ASP	2.6
3	D	710	ARG	2.6
2	C	1077	PRO	2.5
3	D	139	GLY	2.5
2	C	222	MET	2.5
3	D	712	GLY	2.4
2	C	272	ALA	2.4
3	D	1087	ARG	2.4
3	D	191	LEU	2.4
3	D	1398	TRP	2.3
3	D	393	ILE	2.3
4	E	4	PRO	2.3
3	D	161	LEU	2.3
7	T	14	DA	2.2
2	C	413	LEU	2.2
3	D	532	GLY	2.2
2	C	270	GLY	2.1
2	C	167	LYS	2.1
2	C	334	ARG	2.1
2	C	74	GLY	2.1
2	C	258	TYR	2.1
2	C	446	GLY	2.0
2	C	241	LEU	2.0
2	C	1015	LEU	2.0
3	D	1254	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

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
8	ZN	D	1601	1/1	0.78	0.14	188,188,188,188	0
9	MG	D	1603	1/1	0.97	0.05	46,46,46,46	0
8	ZN	D	1602	1/1	0.99	0.04	80,80,80,80	0

6.5 Other polymers [i](#)

There are no such residues in this entry.