



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 12:38 PM UTC

PDB ID : 5UI8 / pdb_00005ui8
Title : structure of sigmaN-holoenzyme
Authors : Darst, S.A.; Campbell, E.A.
Deposited on : 2017-01-13
Resolution : 3.76 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

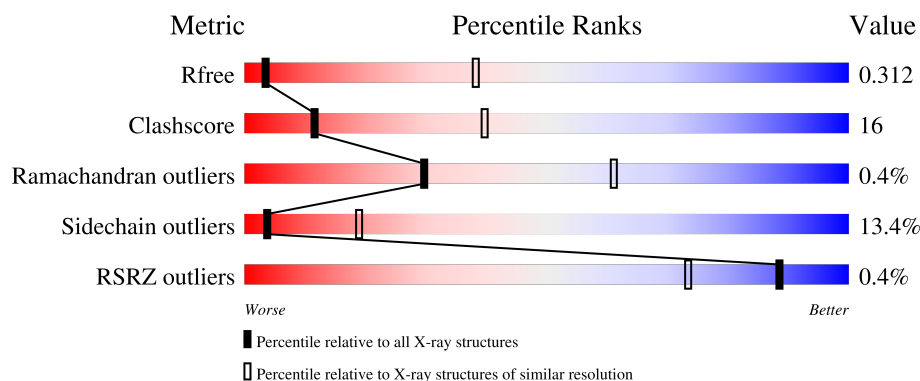
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.76 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	1029 (3.90-3.62)
Clashscore	190562	1061 (3.90-3.62)
Ramachandran outliers	187476	1014 (3.90-3.62)
Sidechain outliers	187428	1009 (3.90-3.62)
RSRZ outliers	180081	1028 (3.90-3.62)

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	G	329	59% 30% 5% 6%
1	H	329	41% 21% 35%
2	I	1342	54% 32% 5% 9%
3	J	1407	58% 32% 5% 5%
4	K	91	52% 29% 7% 13%

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Mol	Chain	Length	Quality of chain
5	M	477	 A horizontal bar chart showing the quality of chain M. The bar is divided into four segments: green (46%), yellow (29%), orange (5%), and grey (20%). The percentages are labeled below the bar.

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 27004 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	G	309	Total	C	N	O	S	0	0	0
			2337	1463	408	459	7			
1	H	215	Total	C	N	O	S	0	0	0
			1619	1013	279	321	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	I	1217	Total	C	N	O	S	0	0	0
			9382	5883	1632	1827	40			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	516	VAL	ASP	conflict	UNP B7MIX3

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	J	1336	Total	C	N	O	S	0	0	0
			10148	6364	1812	1923	49			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	79	Total	C	N	O	S	0	0	0
			620	377	118	124	1			

- Molecule 5 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	380	Total	C	N	O	S	0	0	0
			2895	1825	499	561	10			

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		

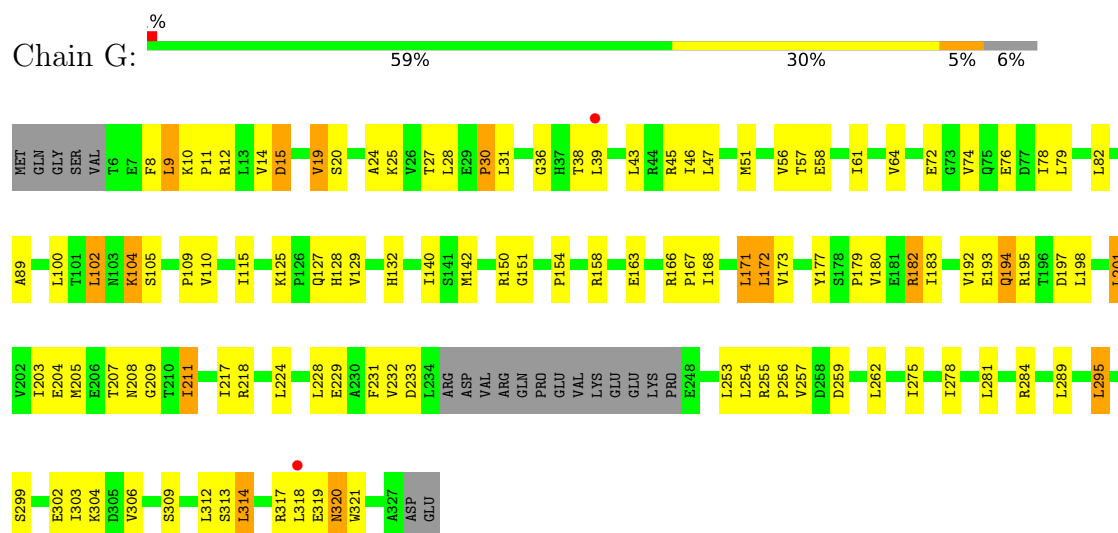
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	2	Total	Zn	0	0
			2	2		

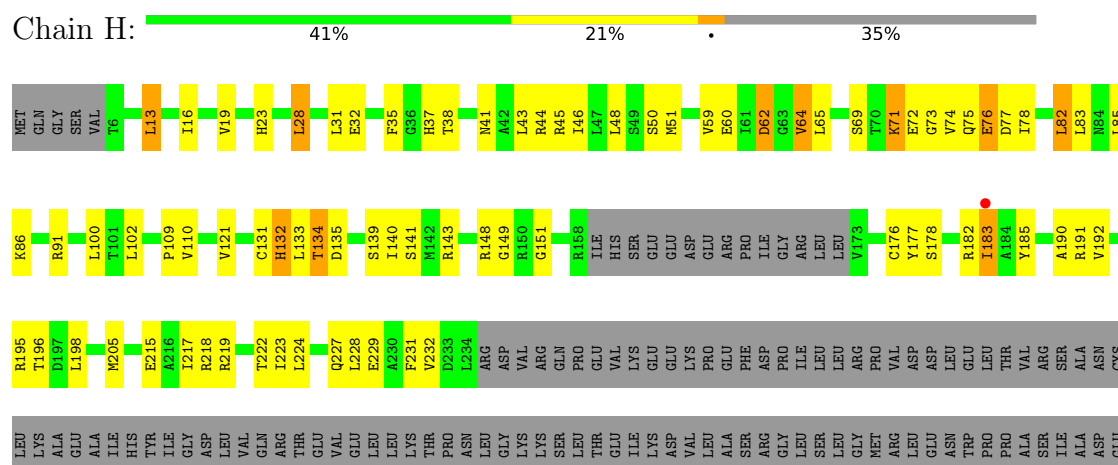
3 Residue-property plots

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



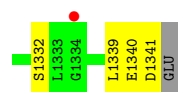
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 2: DNA-directed RNA polymerase subunit beta

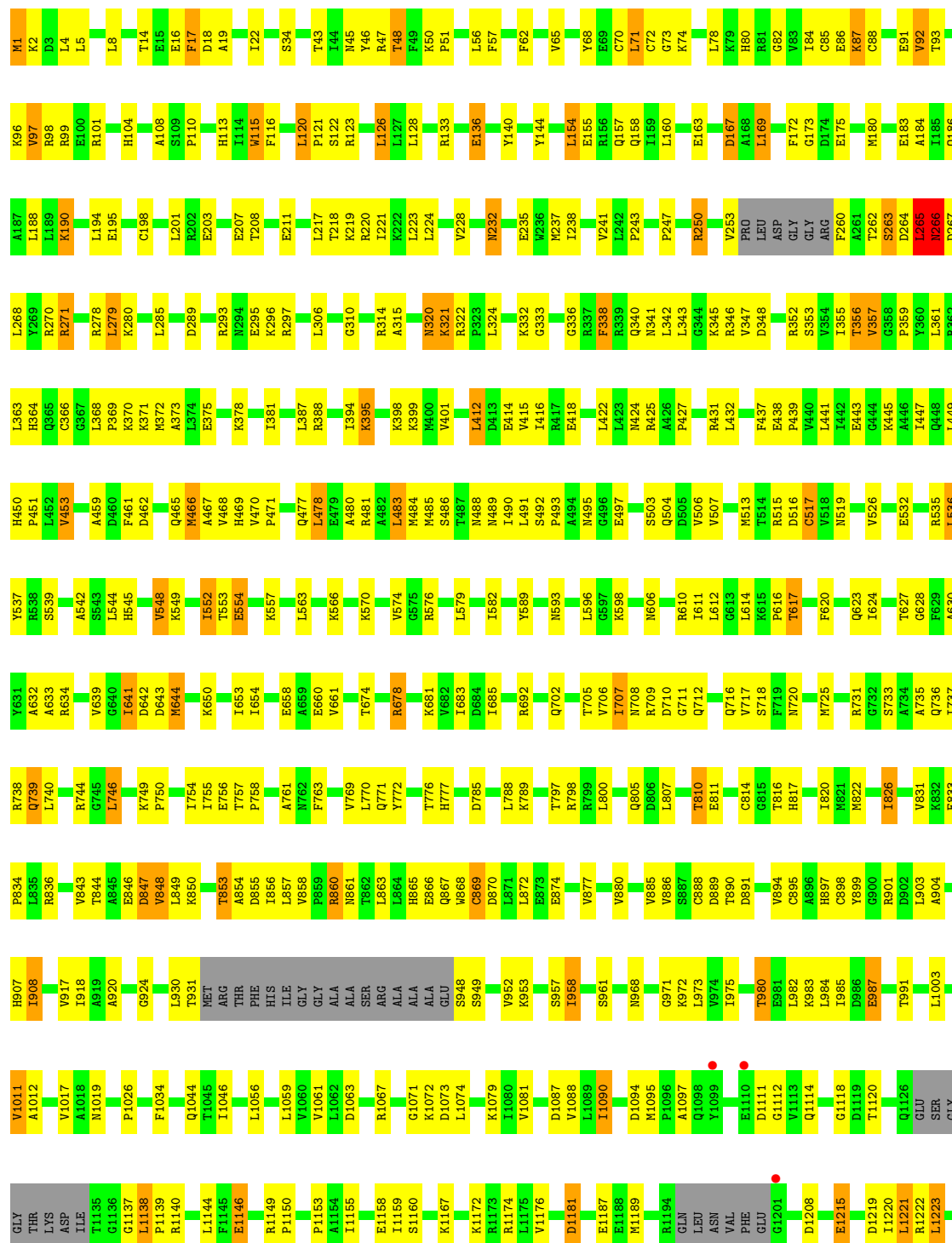


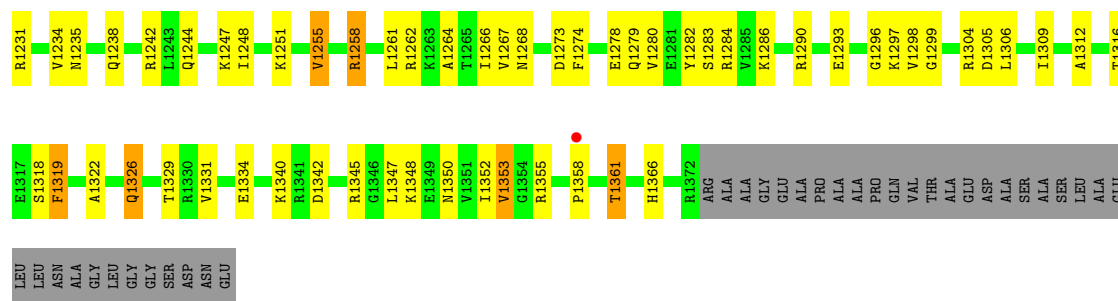
Y1229	R1156	V1075	R976	G885	R801	W685	T589	Q490	D393	LYS	ASN	S166	L75	MET
M1230	Q1157	I1076	L979	K886	M805	Q686	PS50	D491	D393	VAL	LYS	S167	F80	V2
M1231	V1159	I1079	V980	T888	P806	R687	V594	M492	R394	ALA	GLN	V170	Q83	Y3
L1233	D1160	M1080	P889	P889	W807	P691	V599	I493	Y395	LYS	MET		Y83	S4
V1239	L1161	P1081	V984	L895	W808	T692	T600	S499	S398	ASP	GLU	N173	R88	Y5
K1242	F1164	E1082	E985	L895	L693	L693	T600	V502	A399	TYR	LEU	A174	G89	E7
A1245	S1165	E1083	A966	E899	Y810	R694	D601	K503	V400	ILE	VAL	R175	G89	K8
R1246	D1166	M1085	K988	E899	N811	A695	E602	V502	G401	PRO	PRO	I176	G90	R9
S1247	E1167	P1086	L989	L902	F812	D696	H604	F505	M403	GLU	GLU	P177	T91	I11
S1250	E1168	Y1087	R894	I905	D814	T702	L606	Q510	K404	THR	ARG	Y179	A94	I11
L1253	M1170	M1080	D995	F906	S815	G703	L606	Q510	F405	GLY	LEU	R180	P95	K13
L1254	R1171	I1096	R996	F907	I816	G703	I609	M515	L409	GLU	GLY		R101	D14
T1255	L1172	V1097	R996	E908	L817	M704	I609	V516	L409	LEU	GLU	L184	R101	F15
Q1256	M1175	L1098	TRP	E908	W818	E705	E611	V516	L409	ILE	THR	D185	Y105	G16
Q1257	R1177	N1099	GLU	E908	S819	E705	E611	Q517	L420	CYS	ALA	F186	Y105	K17
P1258	P1180	P1100	LEU	E908	E820	V708	Y614	N518	K422	ALA	SER	E187	A109	Q20
L1259	M1181	F1104	GLY	E908	R821	A709	V615	P520	D423	ASN	PHE	F188	F110	V21
G1260	P1185	S1105	LYS	E908	V822	V710	V615	P520	D423	MET	ILE	D189	E111	
K1262	V1186	Q1010	ASN	E908	R827	V714	Q618	S522	I426	GLU	GLU	N193	I117	D83
F1263	F1187	Q1010	ASN	E908	R827	V714	Q618	S522	I426	THR	THR	L194	K118	K37
Q1264	D1188	Q1010	ASN	E908	R827	V714	Q618	S522	I426	LEU	LEU	D427	E119	Y26
F1265	K1191	Q1010	ASN	E908	R827	V714	Q618	S522	I426	SER	ALA	F195	T113	L27
G1266	E1192	Q1010	ASN	E908	R827	V714	Q618	S522	I426	GLY	GLY	F195	T113	L28
Q1267	A1193	Q1010	ASN	E908	R827	V714	Q618	S522	I426	LEU	LEU	F195	T113	L28
Q1268	R1269	Q1010	ASN	E908	R827	V714	Q618	S522	I426	ASP	LYS	R197	K118	
G1270	E1271	Q1010	ASN	E908	R827	V714	Q618	S522	I426	VAL	VAL	I198	E119	
E1272	L1198	Q1010	ASN	E908	R827	V714	Q618	S522	I426	THR	THR	D199	K118	
Y1281	L1199	Q1010	ASN	E908	R827	V714	Q618	S522	I426	LYS	LYS	F199	E119	
Q1288	K1200	Q1010	ASN	E908	R827	V714	Q618	S522	I426	ALA	ALA	R200	E121	
L1291	L1201	Q1010	ASN	E908	R827	V714	Q618	S522	I426	THR	THR	R201	Y123	
T1292	D1202	Q1010	ASN	E908	R827	V714	Q618	S522	I426	ARG	ARG	L204	L129	
V1293	L1203	Q1010	ASN	E908	R827	V714	Q618	S522	I426	GLY	GLY	P205	M130	
K1294	P1205	Q1010	ASN	E908	R827	V714	Q618	S522	I426	THR	THR	A206	D132	
S1295	T1206	Q1010	ASN	E908	R827	V714	Q618	S522	I426	LYS	LYS	T207	T131	
V1298	I1210	Q1010	ASN	E908	R827	V714	Q618	S522	I426	ALA	ALA	I208	M133	
R1301	R1211	Q1010	ASN	E908	R827	V714	Q618	S522	I426	ARG	ARG	L210	F136	
T1302	L1212	Q1010	ASN	E908	R827	V714	Q618	S522	I426	ILE	ILE	R211	V137	
D1310	G1215	Q1010	ASN	E908	R827	V714	Q618	S522	I426	THR	THR	L213	I138	
H1313	T1217	Q1010	ASN	E908	R827	V714	Q618	S522	I426	LEU	LEU	T216	R143	
H1313	Q1220	Q1010	ASN	E908	R827	V714	Q618	S522	I426	GLU	GLU	Q219	V144	
E1321	F1221	Q1010	ASN	E908	R827	V714	Q618	S522	I426	ASP	ASP	F220	I145	
S1322	E1222	Q1010	ASN	E908	R827	V714	Q618	S522	I426	VAL	VAL	L221	Q148	
L1327	V1225	Q1010	ASN	E908	R827	V714	Q618	S522	I426	LYS	LYS	D222	L149	
	G1228	Q1010	ASN	E908	R827	V714	Q618	S522	I426	LEU	LEU	F224	H150	
		Q1010	ASN	E908	R827	V714	Q618	S522	I426	ILE	ILE	E225	P153	
		Q1010	ASN	E908	R827	V714	Q618	S522	I426	GLU	GLU	F225	G154	
		Q1010	ASN	E908	R827	V714	Q618	S522	I426	VAL	VAL	LYS	V155	
		Q1010	ASN	E908	R827	V714	Q618	S522	I426	PRO	PRO	VAL	S66	
		Q1010	ASN	E908	R827	V714	Q618	S522	I426	VAL	VAL	ILE	E67	
		Q1010	ASN	E908	R827	V714	Q618	S522	I426	GLU	GLU	PHE	D158	
		Q1010	ASN	E908	R827	V714	Q618	S522	I426	THR	THR	GLU	K161	
		Q1010	ASN	E908	R827	V714	Q618	S522	I426	ILE	ILE	ILE	T164	
		Q1010	ASN	E908	R827	V714	Q618	S522	I426	ALA	ALA	ARG	T164	
		Q1010	ASN	E908	R827	V714	Q618	S522	I426	ASP	ASP	ASP	H165	



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

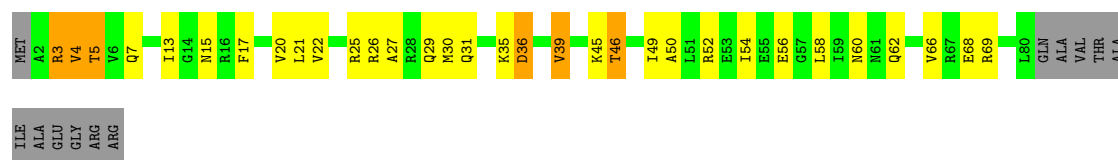
Chain J: 58% 32% 5% 5%





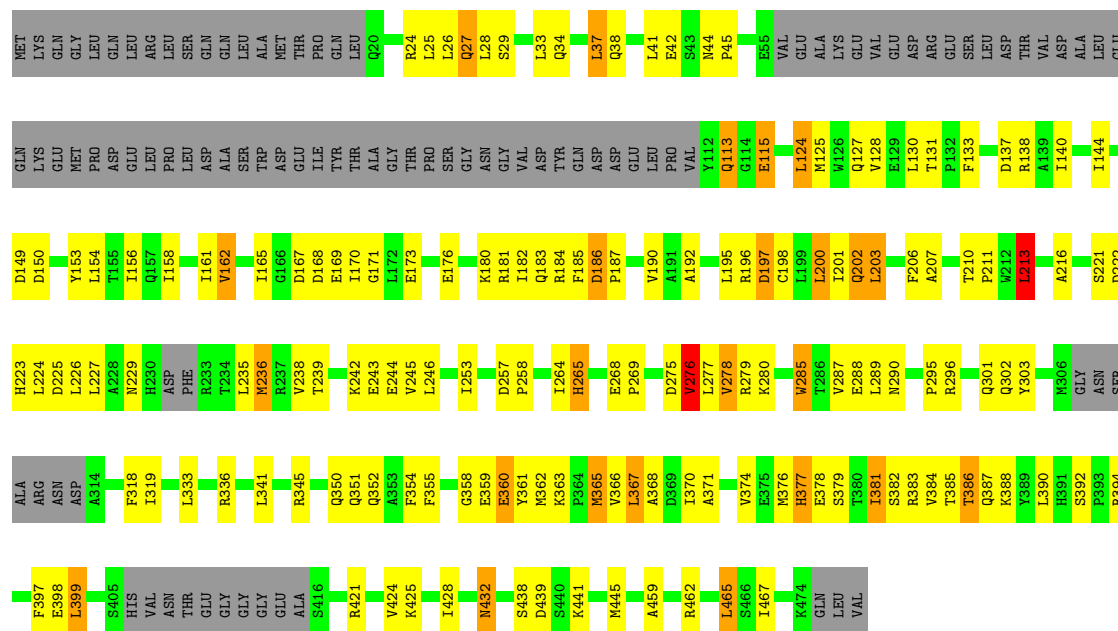
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 52% 29% 7% 13%



- Molecule 5: RNA polymerase sigma-54 factor

Chain M: 46% 29% 5% 20%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	208.48Å 151.52Å 195.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.64 – 3.76 29.64 – 3.76	Depositor EDS
% Data completeness (in resolution range)	98.4 (29.64-3.76) 98.1 (29.64-3.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 3.75Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.262 , 0.312 0.262 , 0.312	Depositor DCC
R_{free} test set	3078 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	143.4	Xtriage
Anisotropy	0.735	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 110.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27004	wwPDB-VP
Average B, all atoms (Å ²)	178.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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: MG, ZN

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	G	0.17	0/2366	0.52	2/3215 (0.1%)
1	H	0.15	0/1637	0.41	2/2224 (0.1%)
2	I	0.18	1/9533 (0.0%)	0.47	4/12893 (0.0%)
3	J	0.17	1/10294 (0.0%)	0.42	1/13920 (0.0%)
4	K	0.13	0/622	0.40	0/838
5	M	0.22	0/2935	0.58	4/3989 (0.1%)
All	All	0.18	2/27387 (0.0%)	0.47	13/37079 (0.0%)

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	G	0	1
2	I	0	5
3	J	0	4
5	M	0	1
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	109	ALA	C-N	9.59	1.56	1.33
3	J	120	LEU	C-N	5.63	1.47	1.33

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	909	LYS	N-CA-C	8.54	120.59	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	1154	ASP	N-CA-C	7.66	119.34	108.00
3	J	265	LEU	N-CA-C	-6.48	97.00	110.80
2	I	398	SER	CB-CA-C	-6.44	107.33	116.34
2	I	1154	ASP	CB-CA-C	-6.26	107.58	116.34
5	M	268	GLU	CA-C-N	5.64	140.54	127.00
5	M	268	GLU	C-N-CA	5.64	140.54	127.00
1	G	163	GLU	CA-C-N	5.63	132.30	121.54
1	G	163	GLU	C-N-CA	5.63	132.30	121.54
5	M	213	LEU	CA-CB-CG	5.19	134.47	116.30
1	H	71	LYS	CA-C-N	5.10	130.89	121.70
1	H	71	LYS	C-N-CA	5.10	130.89	121.70
5	M	268	GLU	C-N-CD	-5.08	109.43	120.60

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	194	GLN	Peptide
2	I	1040	ASP	Peptide
2	I	1154	ASP	Peptide
2	I	1202	GLY	Peptide
2	I	1259	LEU	Peptide
2	I	889	PRO	Peptide
3	J	1296	GLY	Peptide
3	J	263	SER	Peptide
3	J	264	ASP	Peptide
3	J	320	ASN	Peptide
5	M	210	THR	Peptide

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	G	2337	0	2343	80	0
1	H	1619	0	1619	56	0
2	I	9382	0	9211	327	0
3	J	10148	0	10169	336	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	620	0	621	21	0
5	M	2895	0	2828	115	1
6	J	1	0	0	0	0
7	J	2	0	0	0	0
All	All	27004	0	26791	858	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 16.

All (858) 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:I:49:LEU:O	2:I:53:PHE:HB2	1.68	0.93
1:G:43:LEU:O	1:G:47:LEU:HB2	1.74	0.88
5:M:216:ALA:HB1	5:M:253:ILE:HD11	1.56	0.87
3:J:289:ASP:O	3:J:293:ARG:HB2	1.77	0.84
5:M:127:GLN:HE22	5:M:182:ILE:HA	1.45	0.82
2:I:1154:ASP:HB3	2:I:1155:VAL:HG22	1.60	0.81
2:I:1245:ALA:HB2	3:J:372:MET:HG3	1.62	0.81
5:M:26:LEU:O	5:M:388:LYS:NZ	2.14	0.81
3:J:265:LEU:O	3:J:268:LEU:N	2.14	0.80
5:M:425:LYS:HB2	5:M:465:LEU:HD11	1.63	0.80
5:M:158:ILE:HD11	5:M:176:GLU:HG2	1.64	0.80
2:I:101:ARG:HG3	2:I:118:LYS:HB2	1.65	0.79
5:M:45:PRO:O	5:M:301:GLN:NE2	2.16	0.79
1:H:50:SER:HA	1:H:151:GLY:HA2	1.64	0.79
1:H:71:LYS:HA	1:H:72:GLU:HB2	1.65	0.78
2:I:8:LYS:HE3	2:I:1171:ARG:HH22	1.46	0.78
5:M:351:GLN:NE2	5:M:363:LYS:O	2.17	0.78
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.48	0.78
2:I:1262:LYS:HG2	2:I:1268:GLN:HE22	1.47	0.77
2:I:1254:VAL:O	3:J:99:ARG:NH2	2.18	0.76
5:M:285:TRP:HZ3	5:M:352:GLN:HG3	1.49	0.76
1:G:309:SER:O	5:M:184:ARG:NH1	2.19	0.76
1:H:109:PRO:HA	1:H:133:LEU:H	1.51	0.76
5:M:439:ASP:OD2	5:M:462:ARG:NH2	2.19	0.76
1:H:60:GLU:HG2	1:H:143:ARG:H	1.52	0.75
2:I:1268:GLN:HG3	3:J:352:ARG:HG3	1.67	0.75
2:I:211:ARG:HH21	2:I:351:LEU:HD21	1.52	0.75
5:M:127:GLN:HB2	5:M:185:PHE:CD2	2.22	0.74
2:I:886:LYS:HB3	2:I:917:SER:HA	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:971:LEU:HD11	2:I:1014:LEU:HD11	1.70	0.74
2:I:499:SER:O	2:I:503:LYS:HB2	1.88	0.74
2:I:176:ILE:HB	2:I:184:LEU:HB3	1.71	0.73
3:J:154:LEU:HD12	3:J:154:LEU:H	1.53	0.73
2:I:907:GLY:O	2:I:910:ALA:HA	1.88	0.73
2:I:1268:GLN:HE21	3:J:352:ARG:HE	1.37	0.72
1:G:47:LEU:HB3	1:G:183:ILE:HD13	1.71	0.72
2:I:1191:LYS:HD3	2:I:1192:GLU:H	1.55	0.72
3:J:1345:ARG:O	3:J:1350:ASN:ND2	2.24	0.71
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.72	0.71
3:J:425:ARG:HG2	3:J:427:PRO:HD2	1.73	0.70
3:J:4:LEU:O	3:J:8:LEU:CB	2.39	0.70
5:M:37:LEU:O	5:M:41:LEU:N	2.22	0.70
3:J:341:ASN:HB3	3:J:1352:ILE:HG23	1.73	0.70
3:J:797:THR:HB	3:J:924:GLY:HA3	1.74	0.69
2:I:17:LYS:HA	2:I:1155:VAL:HG23	1.73	0.69
3:J:56:LEU:HB3	3:J:250:ARG:HH12	1.58	0.69
5:M:128:VAL:O	5:M:138:ARG:NH1	2.26	0.69
3:J:1:MET:SD	3:J:1:MET:N	2.60	0.69
3:J:108:ALA:HB2	3:J:280:LYS:HG2	1.73	0.69
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.75	0.69
5:M:222:ASP:HB3	5:M:224:LEU:HG	1.75	0.69
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.73	0.69
2:I:3:TYR:HB3	2:I:7:GLU:HB2	1.75	0.69
3:J:262:THR:HG21	3:J:270:ARG:HE	1.57	0.69
2:I:1262:LYS:HD3	3:J:352:ARG:HB2	1.75	0.68
5:M:185:PHE:HD1	5:M:186:ASP:N	1.91	0.68
5:M:227:LEU:HA	5:M:229:ASN:H	1.57	0.68
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.75	0.68
3:J:278:ARG:NH1	3:J:295:GLU:OE1	2.24	0.68
3:J:253:VAL:O	3:J:260:PHE:N	2.26	0.68
3:J:369:PRO:HD2	3:J:372:MET:HE2	1.73	0.68
5:M:360:GLU:OE2	5:M:361:TYR:N	2.27	0.68
2:I:1258:PRO:HB2	3:J:346:ARG:HB2	1.75	0.68
2:I:1105:SER:HB2	3:J:731:ARG:HG3	1.74	0.68
3:J:886:VAL:HA	3:J:1258:ARG:HG3	1.75	0.67
3:J:816:THR:HB	3:J:889:ASP:HB2	1.77	0.67
2:I:702:THR:HG23	2:I:704:MET:H	1.60	0.67
3:J:863:LEU:HD11	3:J:901:ARG:HD3	1.76	0.66
2:I:816:ILE:HG12	2:I:1098:LEU:HD21	1.78	0.66
1:H:109:PRO:HB3	1:H:132:HIS:HA	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:576:SER:HB2	2:I:579:ALA:HB2	1.77	0.66
2:I:132:ASP:OD1	2:I:132:ASP:N	2.28	0.66
3:J:431:ARG:HG2	3:J:493:PRO:HG3	1.78	0.66
5:M:165:ILE:HG21	5:M:170:ILE:HG21	1.77	0.66
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.60	0.65
5:M:367:LEU:HD23	5:M:367:LEU:H	1.62	0.65
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.79	0.65
1:G:25:LYS:HG2	1:G:204:GLU:HA	1.78	0.65
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.78	0.65
1:G:253:LEU:HD21	1:G:278:ILE:HD12	1.78	0.65
2:I:165:HIS:O	2:I:167:SER:N	2.30	0.65
4:K:49:ILE:HA	4:K:52:ARG:HD3	1.78	0.65
2:I:980:VAL:HG13	2:I:984:VAL:HB	1.79	0.65
1:G:224:LEU:HD22	1:H:228:LEU:HD11	1.79	0.65
3:J:361:LEU:HD13	3:J:366:CYS:HA	1.78	0.64
3:J:1261:LEU:HB3	3:J:1304:ARG:HD3	1.78	0.64
3:J:1266:ILE:HG22	3:J:1268:ASN:H	1.62	0.64
2:I:1261:GLY:HA2	3:J:346:ARG:HH12	1.62	0.64
3:J:885:VAL:HG21	3:J:1255:VAL:HG12	1.79	0.64
1:G:46:ILE:HD11	1:H:38:THR:HG21	1.79	0.64
3:J:930:LEU:HD23	3:J:1138:LEU:HB2	1.78	0.64
1:H:195:ARG:HB3	1:H:198:LEU:HD21	1.80	0.64
5:M:462:ARG:HG3	5:M:467:ILE:HG23	1.80	0.64
2:I:138:ILE:HD13	2:I:143:ARG:HD2	1.80	0.63
2:I:386:GLU:HA	2:I:390:PHE:HD2	1.62	0.63
3:J:1286:LYS:O	3:J:1290:ARG:HB2	1.99	0.63
3:J:582:ILE:HD13	3:J:627:THR:HG21	1.81	0.63
1:H:73:GLY:O	1:H:133:LEU:HA	1.99	0.63
3:J:844:THR:OG1	3:J:860:ARG:O	2.16	0.63
5:M:38:GLN:O	5:M:42:GLU:HG2	1.98	0.63
1:G:38:THR:OG1	1:H:45:ARG:NH1	2.31	0.63
4:K:3:ARG:NH1	4:K:5:THR:O	2.32	0.63
3:J:746:LEU:HD22	3:J:754:ILE:HD11	1.80	0.63
3:J:1231:ARG:O	3:J:1235:ASN:HB2	1.99	0.62
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.81	0.62
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.81	0.62
2:I:40:GLU:O	2:I:73:TYR:OH	2.18	0.62
3:J:388:ARG:NH2	3:J:414:GLU:OE1	2.30	0.62
1:G:205:MET:HE1	1:G:217:ILE:HB	1.80	0.62
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.80	0.62
3:J:857:LEU:HD23	3:J:857:LEU:H	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.82	0.62
1:G:109:PRO:HA	1:G:132:HIS:HA	1.82	0.62
3:J:901:ARG:HB2	3:J:908:ILE:HA	1.81	0.62
3:J:968:ASN:HB3	3:J:1118:GLY:HA3	1.82	0.61
2:I:691:PRO:HD2	2:I:763:THR:HG21	1.81	0.61
2:I:533:LEU:HD21	2:I:571:LEU:HD13	1.82	0.61
5:M:242:LYS:O	5:M:245:VAL:HG12	2.00	0.61
3:J:338:PHE:HA	3:J:342:LEU:HB3	1.83	0.61
5:M:200:LEU:HD21	5:M:221:SER:HB3	1.82	0.61
2:I:929:ILE:HG13	2:I:930:ASP:H	1.65	0.61
3:J:478:LEU:HD22	4:K:20:VAL:HA	1.81	0.61
4:K:29:GLN:HB3	4:K:35:LYS:HD3	1.82	0.61
2:I:606:LEU:HD23	2:I:611:GLU:HA	1.83	0.61
2:I:158:ASP:HB3	2:I:173:ASN:HD21	1.64	0.61
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.65	0.61
2:I:1253:LEU:HB3	5:M:115:GLU:HB2	1.81	0.61
2:I:821:ARG:HH21	2:I:1082:ILE:HG21	1.64	0.60
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.82	0.60
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.84	0.60
1:G:304:LYS:HG2	1:G:314:LEU:HD11	1.84	0.60
2:I:401:GLY:O	2:I:405:PHE:HB2	2.01	0.60
3:J:826:ILE:H	3:J:831:VAL:HG23	1.65	0.60
3:J:85:CYS:SG	3:J:87:LYS:N	2.74	0.60
3:J:123:ARG:HH12	3:J:223:LEU:HD11	1.66	0.60
3:J:371:LYS:HZ2	3:J:371:LYS:HB2	1.66	0.60
1:H:44:ARG:HG3	1:H:183:ILE:HB	1.84	0.60
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.65	0.60
2:I:557:ARG:HB3	2:I:587:LEU:HD13	1.84	0.59
2:I:808:ASN:ND2	3:J:630:ALA:HA	2.17	0.59
3:J:203:GLU:O	3:J:207:GLU:HG2	2.02	0.59
5:M:285:TRP:CH2	5:M:355:PHE:HB3	2.38	0.59
2:I:848:GLU:OE1	2:I:886:LYS:NZ	2.35	0.59
2:I:758:ARG:NH2	2:I:762:ASN:OD1	2.36	0.59
2:I:338:THR:HG23	2:I:345:PRO:HG3	1.84	0.59
2:I:670:PHE:HB3	2:I:673:HIS:HD2	1.67	0.59
2:I:968:GLU:O	2:I:972:PHE:HB2	2.03	0.59
2:I:161:LYS:HA	2:I:170:VAL:HA	1.84	0.59
2:I:1164:PHE:O	2:I:1168:GLU:HB3	2.03	0.59
5:M:278:VAL:HG12	5:M:287:VAL:HG23	1.84	0.59
2:I:483:ASP:OD1	2:I:486:THR:OG1	2.20	0.59
2:I:980:VAL:HA	2:I:984:VAL:HA	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1105:SER:O	3:J:736:GLN:NE2	2.36	0.59
3:J:755:ILE:HG22	3:J:757:THR:H	1.66	0.59
3:J:1322:ALA:HA	3:J:1326:GLN:HE22	1.67	0.59
3:J:1347:LEU:H	3:J:1347:LEU:HD12	1.66	0.59
5:M:192:ALA:HB1	5:M:197:ASP:HB3	1.84	0.59
1:G:192:VAL:O	1:G:194:GLN:HB2	2.03	0.58
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.84	0.58
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.85	0.58
2:I:895:LEU:O	2:I:899:GLU:HB2	2.03	0.58
2:I:423:ASP:O	2:I:427:ASP:HB2	2.03	0.58
2:I:807:TRP:O	2:I:808:ASN:HB2	2.04	0.58
2:I:1261:GLY:HA2	3:J:346:ARG:NH1	2.18	0.58
3:J:576:ARG:HD3	3:J:593:ASN:HA	1.84	0.58
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.86	0.58
2:I:1262:LYS:HG2	2:I:1268:GLN:NE2	2.18	0.58
3:J:232:ASN:OD1	3:J:232:ASN:N	2.36	0.58
3:J:310:GLY:HA2	3:J:314:ARG:HG2	1.85	0.58
5:M:128:VAL:HA	5:M:133:PHE:HE2	1.67	0.58
3:J:1361:THR:HG23	4:K:21:LEU:HD11	1.85	0.58
2:I:882:ILE:HG13	2:I:919:ARG:HG2	1.85	0.58
2:I:1099:ASN:OD1	2:I:1101:LEU:N	2.36	0.58
3:J:1181:ASP:OD1	3:J:1181:ASP:N	2.37	0.58
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.86	0.58
3:J:116:PHE:HB3	3:J:123:ARG:HB2	1.85	0.58
3:J:418:GLU:O	3:J:481:ARG:NH2	2.36	0.58
4:K:4:VAL:HG22	4:K:5:THR:HG22	1.86	0.58
1:H:215:GLU:HA	1:H:218:ARG:HG3	1.87	0.57
2:I:206:ALA:O	2:I:209:ILE:HG22	2.05	0.57
3:J:120:LEU:HB3	3:J:121:PRO:HD3	1.87	0.57
1:H:19:VAL:HB	1:H:23:HIS:HB3	1.86	0.57
3:J:606:ASN:OD1	3:J:610:ARG:NH1	2.38	0.57
3:J:1238:GLN:O	3:J:1242:ARG:HB3	2.04	0.57
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.04	0.57
2:I:144:VAL:HG23	2:I:515:MET:HB2	1.87	0.57
3:J:1158:GLU:HA	3:J:1223:LEU:HD11	1.87	0.57
2:I:886:LYS:HE3	2:I:916:SER:HB3	1.85	0.57
5:M:115:GLU:OE1	5:M:115:GLU:N	2.34	0.57
3:J:198:CYS:HA	3:J:221:ILE:HD11	1.87	0.57
3:J:639:VAL:HB	3:J:725:MET:HE1	1.87	0.57
5:M:358:GLY:O	5:M:394:ARG:NH1	2.38	0.57
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1142:ARG:HH22	2:I:1166:ASP:CG	2.13	0.56
5:M:213:LEU:HA	5:M:216:ALA:HB3	1.87	0.56
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.70	0.56
3:J:1262:ARG:O	3:J:1280:VAL:HG23	2.05	0.56
3:J:416:ILE:HG21	3:J:441:LEU:HD21	1.88	0.56
3:J:398:LYS:HA	3:J:401:VAL:HG22	1.88	0.56
3:J:1319:PHE:HD2	3:J:1342:ASP:HB2	1.71	0.56
1:G:172:LEU:HD12	1:G:172:LEU:H	1.70	0.56
3:J:1264:ALA:HB2	3:J:1280:VAL:HG22	1.87	0.56
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.87	0.56
2:I:696:ASP:N	2:I:696:ASP:OD1	2.38	0.56
1:G:15:ASP:OD1	1:G:15:ASP:N	2.35	0.56
2:I:91:THR:HG23	2:I:138:ILE:HA	1.88	0.56
2:I:193:ASN:HB3	2:I:350:THR:HG23	1.87	0.56
5:M:235:LEU:O	5:M:239:THR:N	2.28	0.56
1:G:125:LYS:HE2	1:G:128:HIS:CG	2.40	0.56
3:J:84:ILE:HG13	3:J:85:CYS:H	1.69	0.56
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.87	0.56
2:I:926:GLY:HA2	2:I:1056:VAL:HG13	1.87	0.56
2:I:1085:MET:HA	2:I:1085:MET:HE2	1.88	0.56
3:J:424:ASN:O	3:J:466:MET:HG3	2.06	0.56
5:M:170:ILE:HD12	5:M:171:GLY:N	2.21	0.56
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.72	0.55
2:I:1073:LYS:HD3	3:J:462:ASP:HB2	1.88	0.55
3:J:218:THR:HA	3:J:221:ILE:HG22	1.88	0.55
3:J:1358:PRO:HB3	3:J:1366:HIS:CG	2.41	0.55
5:M:366:VAL:HG12	5:M:368:ALA:H	1.71	0.55
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.88	0.55
2:I:684:ASN:OD1	2:I:687:ARG:NH2	2.39	0.55
2:I:976:ARG:HG3	2:I:989:LEU:HD23	1.88	0.55
5:M:149:ASP:OD1	5:M:150:ASP:N	2.39	0.55
5:M:428:ILE:O	5:M:432:ASN:ND2	2.40	0.55
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.87	0.55
2:I:703:GLY:N	2:I:705:GLU:OE2	2.40	0.55
5:M:127:GLN:NE2	5:M:182:ILE:HA	2.19	0.55
5:M:153:TYR:OH	5:M:258:PRO:O	2.23	0.55
3:J:548:VAL:HG21	3:J:574:VAL:HG23	1.89	0.55
3:J:1067:ARG:HB2	3:J:1072:LYS:HG3	1.89	0.55
2:I:60:GLN:HA	2:I:67:GLU:HA	1.89	0.55
2:I:510:GLN:HG3	2:I:535:PRO:HD3	1.89	0.55
2:I:974:ARG:HG2	2:I:1014:LEU:HD21	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1026:PRO:HB3	3:J:1120:THR:HG22	1.89	0.55
5:M:341:LEU:O	5:M:345:ARG:HG3	2.07	0.55
2:I:686:GLN:HE21	2:I:796:LEU:HD13	1.72	0.55
2:I:942:ASP:OD1	2:I:942:ASP:N	2.40	0.55
3:J:952:VAL:HG21	3:J:984:LEU:HD13	1.89	0.55
2:I:889:PRO:HA	2:I:913:VAL:HG12	1.89	0.54
3:J:418:GLU:H	4:K:45:LYS:HZ3	1.54	0.54
1:G:56:VAL:HG13	1:G:173:VAL:HG21	1.88	0.54
2:I:16:GLY:HA3	2:I:1188:ASP:O	2.07	0.54
3:J:372:MET:HE1	3:J:447:ILE:HD11	1.89	0.54
1:G:51:MET:HB3	1:G:179:PRO:HD2	1.89	0.54
1:H:134:THR:HG22	1:H:135:ASP:H	1.73	0.54
2:I:225:PHE:HE1	2:I:345:PRO:HA	1.71	0.54
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.43	0.54
3:J:352:ARG:HG2	3:J:467:ALA:HA	1.89	0.54
5:M:27:GLN:HB3	5:M:383:ARG:HB3	1.89	0.54
2:I:1322:SER:OG	3:J:341:ASN:ND2	2.41	0.54
3:J:848:VAL:HG11	3:J:880:VAL:HG22	1.90	0.54
3:J:1138:LEU:HG	3:J:1139:PRO:HD3	1.89	0.54
2:I:725:GLN:N	2:I:733:VAL:O	2.38	0.54
3:J:17:PHE:HZ	3:J:1353:VAL:HG21	1.72	0.54
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.89	0.54
5:M:374:VAL:HG13	5:M:376:MET:HG2	1.90	0.54
2:I:223:LEU:HD13	2:I:426:ILE:HG21	1.89	0.54
2:I:518:ASN:OD1	2:I:518:ASN:N	2.41	0.54
2:I:524:ILE:HD12	2:I:708:VAL:HG13	1.90	0.54
2:I:800:MET:O	2:I:1229:TYR:HA	2.06	0.54
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.08	0.54
3:J:356:THR:OG1	3:J:357:VAL:N	2.41	0.54
1:G:27:THR:HA	1:G:201:LEU:O	2.08	0.53
2:I:985:GLU:O	2:I:989:LEU:HB2	2.08	0.53
3:J:422:LEU:HB2	3:J:469:HIS:HB2	1.90	0.53
5:M:186:ASP:HA	5:M:187:PRO:C	2.31	0.53
2:I:499:SER:HA	2:I:502:VAL:HG12	1.90	0.53
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.56	0.53
2:I:515:MET:HE3	2:I:517:GLN:HB2	1.91	0.53
3:J:194:LEU:HD21	3:J:224:LEU:HD22	1.90	0.53
3:J:395:LYS:HD2	5:M:186:ASP:H	1.74	0.53
5:M:167:ASP:OD2	5:M:168:ASP:N	2.42	0.53
5:M:276:VAL:HG13	5:M:277:LEU:N	2.23	0.53
1:G:275:ILE:HG21	1:G:281:LEU:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.88	0.53
4:K:39:VAL:HG21	4:K:56:GLU:HG3	1.91	0.53
3:J:70:CYS:HB3	3:J:73:GLY:H	1.73	0.53
3:J:357:VAL:HG13	3:J:461:PHE:HE1	1.73	0.53
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.89	0.53
1:G:207:THR:HG22	1:G:209:GLY:H	1.72	0.53
2:I:619:ALA:HB2	2:I:654:ASP:HB2	1.90	0.53
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.90	0.53
5:M:236:MET:SD	5:M:243:GLU:HA	2.48	0.53
1:G:312:LEU:HA	5:M:181:ARG:HH21	1.74	0.53
2:I:117:ILE:HG21	2:I:488:MET:HG2	1.89	0.53
2:I:153:PRO:HA	2:I:177:ILE:O	2.09	0.53
2:I:850:ILE:HD11	2:I:1048:LYS:HD2	1.91	0.53
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.42	0.53
2:I:1142:ARG:CZ	2:I:1165:SER:HB2	2.39	0.53
3:J:96:LYS:O	3:J:99:ARG:HG2	2.08	0.53
2:I:133:ASN:OD1	2:I:527:LYS:NZ	2.41	0.53
2:I:1129:ASN:O	2:I:1133:LYS:N	2.38	0.53
2:I:1257:GLN:HE22	3:J:340:GLN:HB3	1.73	0.53
3:J:948:SER:OG	3:J:949:SER:N	2.42	0.53
2:I:8:LYS:HE3	2:I:1171:ARG:NH2	2.20	0.53
2:I:841:ARG:HA	2:I:848:GLU:HB2	1.91	0.53
1:G:82:LEU:HD11	1:G:171:LEU:HG	1.91	0.53
1:G:228:LEU:O	1:G:232:VAL:HG23	2.09	0.53
3:J:519:ASN:CG	3:J:709:ARG:HD3	2.34	0.53
5:M:187:PRO:HG2	5:M:190:VAL:HB	1.91	0.52
2:I:1211:ARG:HE	2:I:1220:GLN:HE22	1.57	0.52
2:I:88:ARG:NE	2:I:1039:GLY:O	2.38	0.52
5:M:198:CYS:O	5:M:202:GLN:HB2	2.09	0.52
5:M:381:ILE:HA	5:M:384:VAL:HG12	1.90	0.52
3:J:930:LEU:HA	3:J:1244:GLN:HE22	1.74	0.52
2:I:886:LYS:CE	2:I:916:SER:HB3	2.40	0.52
3:J:85:CYS:SG	3:J:86:GLU:N	2.82	0.52
1:H:41:ASN:ND2	2:I:1217:THR:O	2.42	0.52
1:H:149:GLY:HA2	1:H:177:TYR:CG	2.45	0.52
2:I:409:LEU:HD11	2:I:428:VAL:HG22	1.92	0.52
2:I:629:PHE:HE2	2:I:650:VAL:HG21	1.74	0.52
2:I:947:GLU:O	2:I:951:MET:HB2	2.10	0.52
3:J:68:TYR:CD2	3:J:78:LEU:HB3	2.45	0.52
1:G:100:LEU:HD23	1:G:115:ILE:HG21	1.92	0.52
2:I:667:LEU:HA	2:I:702:THR:HG21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:916:SER:HA	5:M:264:ILE:HG21	1.92	0.52
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.92	0.52
1:G:314:LEU:H	1:G:314:LEU:HD12	1.74	0.52
2:I:1268:GLN:NE2	3:J:352:ARG:HE	2.05	0.52
3:J:616:PRO:O	3:J:620:PHE:CB	2.58	0.52
3:J:903:LEU:HG	3:J:904:ALA:H	1.75	0.52
1:H:48:LEU:HD11	3:J:539:SER:HB3	1.91	0.52
2:I:758:ARG:HG2	2:I:759:SER:H	1.75	0.52
2:I:820:GLU:N	2:I:1080:ASN:O	2.42	0.52
3:J:526:VAL:HA	3:J:549:LYS:O	2.10	0.52
3:J:1172:LYS:HB3	3:J:1189:MET:HB3	1.92	0.52
2:I:808:ASN:N	3:J:633:ALA:HB2	2.25	0.51
5:M:113:GLN:NE2	5:M:113:GLN:O	2.43	0.51
5:M:227:LEU:HA	5:M:229:ASN:N	2.24	0.51
2:I:180:ARG:NH2	2:I:393:ASP:O	2.35	0.51
2:I:1160:ASP:OD1	2:I:1160:ASP:N	2.30	0.51
3:J:471:PRO:O	3:J:477:GLN:HG2	2.11	0.51
5:M:336:ARG:HH21	5:M:388:LYS:HE2	1.74	0.51
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.93	0.51
2:I:734:ILE:HB	2:I:749:ASP:HB2	1.93	0.51
3:J:355:ILE:CG2	3:J:466:MET:HB2	2.40	0.51
5:M:124:LEU:O	5:M:127:GLN:HB3	2.10	0.51
5:M:288:GLU:OE1	5:M:289:LEU:N	2.43	0.51
1:G:61:ILE:HB	1:G:64:VAL:HB	1.92	0.51
1:H:73:GLY:O	1:H:134:THR:N	2.40	0.51
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.46	0.51
2:I:851:THR:C	2:I:853:ASP:H	2.19	0.51
2:I:810:TYR:HB3	2:I:817:LEU:HD23	1.91	0.51
3:J:113:HIS:CE1	3:J:115:TRP:HB2	2.46	0.51
3:J:154:LEU:HD23	3:J:160:LEU:HD21	1.93	0.51
5:M:367:LEU:HB2	5:M:381:ILE:HD11	1.92	0.51
1:G:151:GLY:O	1:G:177:TYR:HB2	2.09	0.51
2:I:886:LYS:HE3	2:I:916:SER:O	2.10	0.51
3:J:144:TYR:HA	3:J:180:MET:HB3	1.93	0.51
3:J:557:LYS:HA	3:J:563:LEU:HA	1.92	0.51
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.92	0.51
3:J:761:ALA:H	3:J:771:GLN:HE22	1.59	0.51
5:M:354:PHE:HB2	5:M:362:MET:HG2	1.91	0.51
3:J:97:VAL:HG12	3:J:101:ARG:HG3	1.92	0.51
3:J:110:PRO:HD2	3:J:183:GLU:HG2	1.92	0.51
5:M:113:GLN:HB2	5:M:115:GLU:OE1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:100:LEU:HD23	1:G:115:ILE:HD13	1.93	0.51
1:H:149:GLY:HA2	1:H:177:TYR:CD1	2.46	0.51
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.93	0.51
2:I:705:GLU:HB2	2:I:794:LEU:H	1.76	0.51
2:I:1262:LYS:NZ	3:J:352:ARG:HD2	2.26	0.51
5:M:381:ILE:O	5:M:385:THR:OG1	2.19	0.51
2:I:136:PHE:CZ	2:I:456:VAL:HG11	2.46	0.50
2:I:1262:LYS:HZ3	3:J:352:ARG:HD2	1.75	0.50
3:J:826:ILE:HA	3:J:831:VAL:HA	1.92	0.50
3:J:643:ASP:O	3:J:720:ASN:ND2	2.45	0.50
3:J:1034:PHE:HA	3:J:1114:GLN:HA	1.93	0.50
1:G:89:ALA:H	1:G:125:LYS:HD3	1.76	0.50
2:I:458:GLU:O	2:I:462:ASN:ND2	2.44	0.50
1:G:218:ARG:NH1	1:H:231:PHE:O	2.44	0.50
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.77	0.50
3:J:1176:VAL:HG13	3:J:1187:GLU:HG2	1.92	0.50
5:M:278:VAL:HG22	5:M:392:SER:HA	1.92	0.50
1:G:182:ARG:HG2	1:G:183:ILE:N	2.26	0.50
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.93	0.50
2:I:225:PHE:CE1	2:I:345:PRO:HA	2.47	0.50
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.94	0.50
2:I:972:PHE:HZ	2:I:994:ARG:O	1.94	0.50
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.77	0.50
3:J:674:THR:O	3:J:678:ARG:HB3	2.12	0.50
5:M:275:ASP:O	5:M:276:VAL:HG12	2.12	0.50
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.94	0.50
2:I:594:VAL:HG22	2:I:599:VAL:HG13	1.94	0.50
2:I:839:VAL:HG21	2:I:1046:VAL:HG13	1.94	0.50
3:J:320:ASN:CB	3:J:321:LYS:HA	2.42	0.50
3:J:357:VAL:C	3:J:359:PRO:HD3	2.36	0.50
4:K:60:ASN:ND2	4:K:62:GLN:H	2.09	0.50
5:M:432:ASN:OD1	5:M:432:ASN:N	2.44	0.50
2:I:487:LEU:HD23	2:I:487:LEU:H	1.76	0.49
2:I:1211:ARG:HE	2:I:1220:GLN:NE2	2.09	0.49
3:J:957:SER:N	3:J:985:ILE:O	2.45	0.49
3:J:1159:ILE:HG12	3:J:1160:SER:H	1.77	0.49
5:M:154:LEU:HD23	5:M:156:ILE:HD11	1.94	0.49
5:M:171:GLY:C	5:M:173:GLU:H	2.20	0.49
2:I:843:THR:OG1	2:I:846:GLY:O	2.24	0.49
1:G:166:ARG:N	1:G:167:PRO:HD2	2.26	0.49
2:I:1191:LYS:HD3	2:I:1192:GLU:HG2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:38:GLN:NE2	5:M:42:GLU:OE2	2.45	0.49
3:J:480:ALA:HA	3:J:484:MET:HB2	1.93	0.49
1:G:8:PHE:C	1:G:9:LEU:HG	2.38	0.49
1:H:60:GLU:HG2	1:H:143:ARG:N	2.24	0.49
5:M:196:ARG:O	5:M:200:LEU:N	2.29	0.49
2:I:817:LEU:HD12	2:I:1085:MET:HE1	1.94	0.49
2:I:839:VAL:HB	2:I:1049:ILE:HA	1.94	0.49
3:J:478:LEU:HB3	4:K:20:VAL:HG13	1.95	0.49
5:M:223:HIS:C	5:M:225:ASP:H	2.20	0.49
2:I:557:ARG:HD3	2:I:587:LEU:HB3	1.94	0.49
1:G:19:VAL:HG13	1:G:20:SER:H	1.78	0.49
2:I:75:LEU:HD12	2:I:94:ALA:HB3	1.95	0.49
2:I:204:LEU:HD11	2:I:369:MET:HG3	1.95	0.49
3:J:1140:ARG:O	3:J:1144:LEU:HG	2.13	0.49
1:G:203:ILE:HG22	1:G:205:MET:H	1.78	0.49
3:J:710:ASP:CG	3:J:711:GLY:H	2.18	0.49
2:I:440:GLY:HA3	2:I:441:GLU:CD	2.38	0.48
2:I:1258:PRO:HD3	2:I:1295:SER:HB2	1.93	0.48
3:J:34:SER:HB2	3:J:104:HIS:HB3	1.95	0.48
3:J:338:PHE:HB3	3:J:342:LEU:HD23	1.94	0.48
3:J:338:PHE:N	3:J:338:PHE:CD1	2.79	0.48
3:J:865:HIS:CE1	3:J:867:GLN:HB2	2.47	0.48
2:I:905:ILE:HG13	2:I:906:PHE:N	2.28	0.48
2:I:1193:ALA:O	2:I:1197:GLU:HB2	2.14	0.48
2:I:1246:ARG:HD2	2:I:1266:GLY:C	2.38	0.48
2:I:1281:TYR:HB3	3:J:483:LEU:HD12	1.96	0.48
3:J:1221:LEU:HD11	3:J:1304:ARG:O	2.12	0.48
2:I:65:ASN:HB3	2:I:105:TYR:HB2	1.96	0.48
2:I:459:MET:HA	2:I:462:ASN:HD22	1.77	0.48
2:I:1171:ARG:O	2:I:1175:ASN:ND2	2.47	0.48
3:J:425:ARG:NH1	3:J:459:ALA:HA	2.28	0.48
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.94	0.48
2:I:158:ASP:HB3	2:I:173:ASN:ND2	2.28	0.48
3:J:186:GLN:HA	3:J:238:ILE:HG13	1.95	0.48
3:J:848:VAL:HG22	3:J:858:VAL:HG22	1.96	0.48
4:K:15:ASN:C	4:K:17:PHE:H	2.22	0.48
1:G:19:VAL:HG12	1:G:24:ALA:HA	1.95	0.48
2:I:818:VAL:HG22	2:I:1096:ILE:HG12	1.95	0.48
2:I:1112:ILE:HG22	2:I:1113:LEU:HD12	1.95	0.48
5:M:280:LYS:HB3	5:M:285:TRP:CD1	2.49	0.48
1:G:10:LYS:O	1:G:30:PRO:HB2	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:399:ALA:O	2:I:403:MET:HB2	2.13	0.48
1:H:76:GLU:CD	1:H:76:GLU:H	2.22	0.48
2:I:1129:ASN:HB2	2:I:1177:ARG:HB2	1.95	0.48
3:J:1279:GLN:HB2	3:J:1282:TYR:HB2	1.96	0.48
5:M:128:VAL:HA	5:M:133:PHE:CE2	2.47	0.48
1:G:102:LEU:HD23	1:G:115:ILE:HG12	1.95	0.48
2:I:492:MET:H	2:I:492:MET:HG3	1.50	0.48
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.79	0.48
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.94	0.48
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.95	0.48
3:J:1081:VAL:HG12	3:J:1087:ASP:HA	1.96	0.48
1:G:284:ARG:HB3	1:G:289:LEU:CD2	2.43	0.48
2:I:38:PHE:HB2	2:I:457:GLY:CA	2.43	0.48
2:I:53:PHE:HD1	2:I:70:TYR:CE1	2.31	0.48
2:I:118:LYS:HB3	2:I:118:LYS:HE2	1.71	0.48
2:I:801:ARG:HD2	2:I:1229:TYR:CE1	2.48	0.48
2:I:985:GLU:HB3	2:I:988:LYS:HG3	1.95	0.48
2:I:1164:PHE:O	2:I:1169:VAL:HG23	2.14	0.48
3:J:72:CYS:N	3:J:88:CYS:SG	2.87	0.48
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.14	0.48
4:K:22:VAL:HG11	4:K:60:ASN:HA	1.95	0.48
2:I:95:PRO:HB3	2:I:123:TYR:HE1	1.79	0.47
2:I:708:VAL:HG11	2:I:794:LEU:HD22	1.94	0.47
3:J:678:ARG:NH1	3:J:756:GLU:OE2	2.47	0.47
1:G:10:LYS:NZ	1:H:229:GLU:OE1	2.36	0.47
1:H:182:ARG:O	1:H:205:MET:HG3	2.14	0.47
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.48	0.47
3:J:355:ILE:HG21	3:J:466:MET:HE2	1.96	0.47
5:M:140:ILE:O	5:M:144:ILE:HG13	2.14	0.47
5:M:287:VAL:HG11	5:M:345:ARG:HA	1.95	0.47
1:G:57:THR:HG22	1:G:58:GLU:HG3	1.96	0.47
1:G:284:ARG:O	1:G:314:LEU:HB3	2.14	0.47
2:I:1242:LYS:HD3	3:J:465:GLN:NE2	2.29	0.47
3:J:163:GLU:O	3:J:167:ASP:HB3	2.13	0.47
3:J:395:LYS:HB2	5:M:185:PHE:CE1	2.49	0.47
1:G:182:ARG:NH1	2:I:1090:ASN:OD1	2.47	0.47
1:H:51:MET:HB3	1:H:178:SER:HA	1.95	0.47
2:I:637:ARG:HG2	2:I:642:SER:HB3	1.96	0.47
2:I:670:PHE:HB3	2:I:673:HIS:CD2	2.48	0.47
2:I:1339:LEU:HB3	3:J:17:PHE:HD1	1.79	0.47
3:J:579:LEU:HA	3:J:582:ILE:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:650:LYS:HE3	3:J:654:ILE:HD11	1.95	0.47
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.47	0.47
5:M:203:LEU:HA	5:M:206:PHE:HB3	1.96	0.47
5:M:351:GLN:CD	5:M:362:MET:HB3	2.39	0.47
1:G:284:ARG:HB3	1:G:289:LEU:HD21	1.96	0.47
1:G:295:LEU:HD23	1:G:295:LEU:HA	1.77	0.47
2:I:1083:GLU:O	2:I:1215:GLY:HA3	2.14	0.47
2:I:1247:SER:HB3	3:J:375:GLU:O	2.14	0.47
3:J:437:PHE:CZ	3:J:453:VAL:HG21	2.50	0.47
4:K:4:VAL:HG13	4:K:5:THR:H	1.80	0.47
3:J:789:LYS:HD2	3:J:1138:LEU:CD2	2.44	0.47
3:J:870:ASP:O	3:J:874:GLU:HG2	2.14	0.47
5:M:381:ILE:HG13	5:M:382:SER:N	2.29	0.47
5:M:390:LEU:N	5:M:397:PHE:O	2.43	0.47
2:I:90:VAL:HG12	2:I:91:THR:H	1.80	0.47
2:I:198:ILE:HD13	2:I:388:LEU:HD13	1.96	0.47
2:I:817:LEU:HD11	2:I:1080:ASN:HB2	1.96	0.47
3:J:62:PHE:O	3:J:101:ARG:HD2	2.15	0.47
3:J:122:SER:O	3:J:126:LEU:HB3	2.15	0.47
3:J:271:ARG:HH22	3:J:315:ALA:HB1	1.79	0.47
3:J:321:LYS:HE3	3:J:321:LYS:H	1.77	0.47
3:J:958:ILE:HG12	3:J:1011:VAL:HG21	1.96	0.47
3:J:971:GLY:C	3:J:972:LYS:HG2	2.40	0.47
5:M:399:LEU:O	5:M:399:LEU:HD12	2.15	0.47
2:I:388:LEU:O	2:I:395:TYR:HB2	2.15	0.47
3:J:735:ALA:HA	3:J:738:ARG:NH1	2.30	0.47
3:J:485:MET:HB3	3:J:488:ASN:HD22	1.80	0.47
3:J:973:LEU:HB3	3:J:1003:LEU:HB2	1.97	0.47
1:G:74:VAL:HG22	1:G:76:GLU:H	1.80	0.47
2:I:173:ASN:HA	2:I:186:PHE:O	2.15	0.47
5:M:180:LYS:O	5:M:184:ARG:HG2	2.14	0.47
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.96	0.46
1:G:180:VAL:HG11	1:G:183:ILE:HD11	1.96	0.46
3:J:47:ARG:O	3:J:47:ARG:NE	2.41	0.46
3:J:513:MET:SD	3:J:544:LEU:HD11	2.55	0.46
5:M:377:HIS:O	5:M:381:ILE:HG23	2.15	0.46
1:G:158:ARG:CZ	1:G:172:LEU:HD23	2.46	0.46
1:G:179:PRO:HA	1:G:208:ASN:ND2	2.31	0.46
3:J:620:PHE:CZ	3:J:624:ILE:HD11	2.49	0.46
3:J:1090:ILE:HG13	3:J:1097:ALA:HB2	1.98	0.46
3:J:536:LEU:HD12	3:J:542:ALA:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:628:GLY:O	3:J:632:ALA:HB2	2.15	0.46
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.49	0.46
1:H:102:LEU:HD11	1:H:110:VAL:HG11	1.97	0.46
2:I:522:SER:O	2:I:526:HIS:HB2	2.16	0.46
2:I:739:ASP:OD1	2:I:739:ASP:N	2.40	0.46
2:I:922:ASN:OD1	2:I:922:ASN:N	2.47	0.46
3:J:123:ARG:HH21	3:J:1334:GLU:HG2	1.80	0.46
3:J:485:MET:HG3	3:J:486:SER:H	1.80	0.46
3:J:709:ARG:HD2	3:J:710:ASP:N	2.30	0.46
2:I:945:ALA:HA	2:I:948:ILE:HD12	1.97	0.46
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	1.97	0.46
3:J:194:LEU:HD13	3:J:224:LEU:HB3	1.96	0.46
3:J:888:CYS:SG	3:J:890:THR:HG22	2.56	0.46
3:J:1011:VAL:HG12	3:J:1012:ALA:H	1.81	0.46
3:J:19:ALA:HA	3:J:1342:ASP:O	2.16	0.46
3:J:84:ILE:HA	3:J:91:GLU:HA	1.97	0.46
1:H:13:LEU:HB2	1:H:28:LEU:HD12	1.97	0.46
1:H:102:LEU:HD22	1:H:140:ILE:HG12	1.98	0.46
2:I:138:ILE:HB	2:I:143:ARG:CZ	2.46	0.46
3:J:490:ILE:HG13	3:J:491:LEU:HG	1.97	0.46
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.97	0.46
1:G:150:ARG:NH2	1:H:32:GLU:OE1	2.49	0.46
3:J:733:SER:O	3:J:737:ILE:HG12	2.16	0.46
3:J:810:THR:HG23	3:J:811:GLU:H	1.81	0.46
3:J:847:ASP:HB3	3:J:856:ILE:HG23	1.98	0.46
5:M:296:ARG:HA	5:M:296:ARG:HD2	1.73	0.46
1:G:255:ARG:NE	1:G:259:ASP:OD2	2.44	0.46
2:I:221:LEU:HD12	2:I:221:LEU:H	1.79	0.46
2:I:842:ASP:HB2	2:I:1045:GLY:O	2.16	0.46
1:G:320:ASN:O	1:G:321:TRP:CD2	2.69	0.45
2:I:805:MET:O	2:I:811:ASN:ND2	2.49	0.45
3:J:381:ILE:HD11	3:J:412:LEU:HD12	1.98	0.45
3:J:395:LYS:HG3	5:M:186:ASP:HB3	1.99	0.45
3:J:422:LEU:O	3:J:468:VAL:HA	2.16	0.45
1:G:28:LEU:HD21	1:H:231:PHE:HE1	1.80	0.45
1:H:46:ILE:HD12	1:H:224:LEU:HB2	1.97	0.45
2:I:806:PRO:O	3:J:633:ALA:HA	2.16	0.45
2:I:822:VAL:HG13	2:I:827:ARG:HD3	1.99	0.45
5:M:382:SER:O	5:M:386:THR:HG23	2.17	0.45
5:M:441:LYS:HG3	5:M:445:MET:HE3	1.98	0.45
2:I:38:PHE:HB2	2:I:457:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1142:ARG:NH1	2:I:1165:SER:HB2	2.32	0.45
2:I:1341:ASP:HB3	3:J:18:ASP:HB3	1.98	0.45
3:J:266:ASN:O	3:J:270:ARG:HB2	2.17	0.45
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.97	0.45
3:J:961:SER:OG	3:J:983:LYS:HD2	2.16	0.45
1:G:14:VAL:HG22	1:G:15:ASP:H	1.81	0.45
2:I:1124:ILE:HD11	2:I:1201:LEU:HB3	1.97	0.45
3:J:616:PRO:O	3:J:620:PHE:HB2	2.17	0.45
3:J:789:LYS:HE3	3:J:931:THR:O	2.15	0.45
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	1.98	0.45
1:H:72:GLU:OE2	1:H:72:GLU:HA	2.16	0.45
2:I:2:VAL:HG11	2:I:1158:LYS:NZ	2.31	0.45
3:J:183:GLU:OE1	3:J:296:LYS:NZ	2.48	0.45
5:M:341:LEU:HD21	5:M:345:ARG:HH21	1.82	0.45
5:M:459:ALA:HA	5:M:462:ARG:NH2	2.31	0.45
3:J:22:ILE:HG22	3:J:1340:LYS:O	2.17	0.45
3:J:265:LEU:C	3:J:267:ASP:N	2.72	0.45
3:J:347:VAL:HG12	3:J:348:ASP:O	2.17	0.45
4:K:50:ALA:O	4:K:54:ILE:HG12	2.16	0.45
2:I:1258:PRO:CB	3:J:346:ARG:HB2	2.46	0.45
3:J:515:ARG:HH21	3:J:717:VAL:HG23	1.81	0.45
3:J:614:LEU:O	3:J:617:THR:HG22	2.17	0.45
3:J:449:LEU:HD13	3:J:466:MET:HE3	1.99	0.45
3:J:860:ARG:NH1	3:J:861:ASN:HD22	2.15	0.45
3:J:1150:PRO:HG2	3:J:1153:PRO:HB3	1.98	0.45
3:J:1297:LYS:HZ1	3:J:1299:GLY:HA3	1.82	0.45
1:G:28:LEU:HD13	1:G:201:LEU:HD22	1.98	0.45
3:J:332:LYS:O	3:J:336:GLY:HA2	2.16	0.45
3:J:495:ASN:HD22	3:J:497:GLU:HB2	1.81	0.45
2:I:710:VAL:HA	2:I:715:THR:HG21	1.98	0.45
2:I:801:ARG:HA	2:I:1228:GLY:O	2.16	0.45
2:I:808:ASN:HD21	3:J:630:ALA:HA	1.81	0.45
2:I:1288:GLN:HE21	2:I:1288:GLN:HB2	1.57	0.45
2:I:1321:GLU:OE2	3:J:99:ARG:NH1	2.50	0.45
3:J:1:MET:HG2	3:J:2:LYS:H	1.81	0.45
3:J:116:PHE:CD2	3:J:237:MET:HG2	2.52	0.45
2:I:807:TRP:N	2:I:811:ASN:HD21	2.14	0.44
2:I:1069:ARG:HG3	2:I:1233:LEU:HD21	1.99	0.44
3:J:709:ARG:HG3	3:J:710:ASP:OD2	2.16	0.44
5:M:279:ARG:O	5:M:285:TRP:HD1	2.00	0.44
2:I:522:SER:HA	2:I:525:THR:HG22	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1203:ASP:O	2:I:1204:LEU:HG	2.17	0.44
3:J:370:LYS:HG3	3:J:441:LEU:HD12	1.99	0.44
3:J:388:ARG:HH21	3:J:414:GLU:CD	2.21	0.44
2:I:814:ASP:O	2:I:1074:GLY:HA2	2.17	0.44
2:I:1109:ILE:HG12	3:J:644:MET:HE1	1.98	0.44
2:I:1111:GLN:HB2	2:I:1230:MET:HE3	1.99	0.44
3:J:958:ILE:HD12	3:J:982:LEU:HG	1.98	0.44
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.99	0.44
2:I:13:LYS:HE2	2:I:15:PHE:CE2	2.52	0.44
2:I:489:PRO:O	2:I:490:GLN:HB3	2.17	0.44
3:J:201:LEU:O	3:J:217:LEU:HD11	2.17	0.44
3:J:1146:GLU:HA	3:J:1309:ILE:HG12	1.97	0.44
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.99	0.44
2:I:12:ARG:NE	2:I:793:GLU:OE1	2.44	0.44
3:J:184:ALA:O	3:J:188:LEU:HB2	2.17	0.44
1:G:11:PRO:HG2	1:H:227:GLN:O	2.18	0.44
2:I:187:GLU:O	2:I:195:PHE:HB2	2.18	0.44
2:I:1142:ARG:HE	2:I:1142:ARG:HB2	1.42	0.44
5:M:398:GLU:O	5:M:399:LEU:HB3	2.15	0.44
2:I:1264:GLN:N	2:I:1264:GLN:OE1	2.50	0.44
3:J:128:LEU:HB3	3:J:157:GLN:NE2	2.33	0.44
3:J:333:GLY:HA3	3:J:336:GLY:C	2.43	0.44
3:J:707:ILE:HD11	3:J:716:GLN:HG2	2.00	0.44
5:M:197:ASP:O	5:M:201:ILE:N	2.28	0.44
5:M:424:VAL:O	5:M:428:ILE:HG22	2.17	0.44
1:H:31:LEU:HD12	1:H:35:PHE:HB3	1.99	0.44
2:I:692:THR:OG1	2:I:693:LEU:N	2.51	0.44
2:I:929:ILE:HG13	2:I:930:ASP:N	2.31	0.44
2:I:559:CYS:HB2	2:I:662:SER:HB3	2.00	0.44
2:I:697:LYS:H	2:I:697:LYS:HD3	1.83	0.44
2:I:818:VAL:HG21	2:I:1066:MET:HE1	2.00	0.44
2:I:1262:LYS:HZ1	3:J:465:GLN:CD	2.26	0.44
2:I:1269:ARG:HA	3:J:346:ARG:HA	1.98	0.44
3:J:50:LYS:HB3	3:J:71:LEU:HD21	1.98	0.44
3:J:836:ARG:HG3	3:J:869:CYS:SG	2.58	0.44
3:J:1262:ARG:NH2	3:J:1312:ALA:O	2.51	0.44
5:M:26:LEU:HD12	5:M:27:GLN:N	2.33	0.44
2:I:20:GLN:H	2:I:20:GLN:HG2	1.63	0.43
3:J:785:ASP:O	3:J:789:LYS:HG2	2.17	0.43
3:J:872:LEU:HD22	3:J:877:VAL:HG11	2.00	0.43
3:J:885:VAL:HG12	3:J:899:TYR:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:256:PRO:O	1:G:259:ASP:HB2	2.17	0.43
1:H:62:ASP:HB3	1:H:141:SER:O	2.17	0.43
2:I:827:ARG:HG3	2:I:828:PHE:HD1	1.84	0.43
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.53	0.43
3:J:850:LYS:HG3	3:J:857:LEU:HD22	2.00	0.43
3:J:1215:GLU:HB2	3:J:1220:ILE:HD11	2.00	0.43
5:M:183:GLN:CD	5:M:201:ILE:HD13	2.43	0.43
1:H:73:GLY:O	1:H:133:LEU:HD12	2.18	0.43
1:H:192:VAL:O	1:H:195:ARG:HB2	2.18	0.43
2:I:1120:ALA:HB1	2:I:1198:LEU:HD12	2.00	0.43
3:J:190:LYS:HA	3:J:235:GLU:HG3	2.00	0.43
3:J:432:LEU:HD11	3:J:492:SER:HA	2.01	0.43
3:J:1149:ARG:CZ	3:J:1153:PRO:HG2	2.48	0.43
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.83	0.43
2:I:1272:GLU:OE1	3:J:798:ARG:NH2	2.51	0.43
2:I:1313:HIS:CD2	3:J:477:GLN:HE22	2.36	0.43
3:J:57:PHE:CD1	3:J:247:PRO:HB3	2.53	0.43
2:I:33:ASP:O	2:I:37:LYS:HG2	2.19	0.43
2:I:62:TYR:C	2:I:64:GLY:H	2.27	0.43
2:I:979:LEU:HD11	2:I:989:LEU:HD22	1.98	0.43
2:I:1122:LYS:NZ	2:I:1126:ASP:OD1	2.46	0.43
2:I:1247:SER:O	3:J:348:ASP:HB3	2.18	0.43
2:I:1339:LEU:HD23	3:J:17:PHE:CD1	2.53	0.43
4:K:31:GLN:HE21	4:K:46:THR:HG21	1.84	0.43
5:M:25:LEU:O	5:M:33:LEU:HD12	2.17	0.43
1:G:320:ASN:C	1:G:321:TRP:CG	2.97	0.43
2:I:760:ASN:OD1	2:I:760:ASN:N	2.51	0.43
3:J:186:GLN:HB2	3:J:238:ILE:HG21	2.01	0.43
3:J:1355:ARG:HE	3:J:1355:ARG:HB3	1.59	0.43
1:H:190:ALA:HB3	1:H:198:LEU:HB2	2.00	0.43
2:I:519:ASN:ND2	2:I:796:LEU:HD23	2.25	0.43
3:J:1111:ASP:OD1	3:J:1112:GLY:N	2.52	0.43
2:I:145:ILE:HB	2:I:456:VAL:HG22	2.00	0.43
2:I:695:ALA:HB1	2:I:795:ALA:HB3	2.01	0.43
2:I:940:GLU:H	2:I:940:GLU:CD	2.16	0.43
2:I:1268:GLN:CG	3:J:352:ARG:HG3	2.41	0.43
3:J:47:ARG:HE	3:J:47:ARG:C	2.26	0.43
3:J:807:LEU:HD11	3:J:1258:ARG:NH1	2.34	0.43
5:M:368:ALA:HA	5:M:371:ALA:HB3	2.00	0.43
1:G:302:GLU:O	1:G:306:VAL:HG23	2.19	0.43
2:I:840:SER:CB	2:I:886:LYS:HZ3	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:554:GLU:HB3	3:J:589:TYR:HB2	2.01	0.43
3:J:746:LEU:HD23	3:J:758:PRO:HG3	2.00	0.43
3:J:1234:VAL:O	3:J:1238:GLN:HB2	2.19	0.43
5:M:170:ILE:H	5:M:170:ILE:HG13	1.60	0.43
5:M:235:LEU:O	5:M:239:THR:HG22	2.18	0.43
1:H:219:ARG:O	1:H:223:ILE:HG13	2.19	0.43
2:I:1250:SER:O	2:I:1259:LEU:HD13	2.19	0.43
3:J:220:ARG:O	3:J:224:LEU:HG	2.19	0.43
3:J:224:LEU:O	3:J:228:VAL:HG23	2.19	0.43
2:I:629:PHE:CE2	2:I:650:VAL:HG21	2.53	0.42
2:I:808:ASN:HD22	2:I:808:ASN:HA	1.66	0.42
2:I:884:VAL:HG22	2:I:918:LEU:HD23	2.00	0.42
3:J:858:VAL:HG12	3:J:868:TRP:CE3	2.54	0.42
5:M:127:GLN:HB2	5:M:185:PHE:HD2	1.78	0.42
2:I:189:ASP:OD1	2:I:189:ASP:N	2.52	0.42
3:J:1316:THR:HG22	3:J:1318:SER:H	1.84	0.42
1:G:125:LYS:HB2	1:G:128:HIS:HB2	2.00	0.42
2:I:1212:LEU:HB2	2:I:1225:VAL:HG21	2.01	0.42
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.83	0.42
2:I:1332:SER:HA	3:J:243:PRO:HB2	2.02	0.42
3:J:532:GLU:HG2	3:J:536:LEU:HD23	2.02	0.42
3:J:853:THR:HG22	3:J:854:ALA:H	1.82	0.42
2:I:216:THR:H	2:I:219:GLN:NE2	2.18	0.42
2:I:661:VAL:HB	2:I:665:ALA:HB3	2.00	0.42
2:I:972:PHE:CZ	2:I:994:ARG:HB3	2.54	0.42
2:I:979:LEU:HD21	2:I:989:LEU:HD21	2.01	0.42
2:I:1270:PHE:O	3:J:343:LEU:O	2.37	0.42
3:J:623:GLN:O	3:J:627:THR:HG22	2.20	0.42
3:J:634:ARG:HB3	3:J:634:ARG:NH1	2.35	0.42
5:M:24:ARG:O	5:M:28:LEU:HG	2.20	0.42
1:G:102:LEU:HB3	1:G:142:MET:HG2	2.00	0.42
1:G:317:ARG:HG3	3:J:387:LEU:HD11	2.02	0.42
2:I:557:ARG:NH2	2:I:611:GLU:OE1	2.53	0.42
2:I:860:ALA:O	2:I:863:SER:OG	2.29	0.42
2:I:866:ASP:HA	2:I:872:TYR:CZ	2.54	0.42
3:J:449:LEU:HD22	3:J:466:MET:HE1	2.02	0.42
3:J:553:THR:HG23	3:J:566:LYS:O	2.20	0.42
2:I:615:VAL:HG13	2:I:651:ASP:HB2	2.00	0.42
2:I:753:LEU:HB3	2:I:767:GLN:HB2	2.01	0.42
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.52	0.42
5:M:130:LEU:HD12	5:M:131:THR:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:264:ILE:HG13	5:M:265:HIS:O	2.20	0.42
3:J:833:GLU:HA	3:J:834:PRO:HD3	1.84	0.42
5:M:34:GLN:HA	5:M:37:LEU:HG	2.01	0.42
1:G:45:ARG:HH22	1:H:37:HIS:C	2.28	0.42
2:I:207:THR:HG21	2:I:354:ASP:HB2	2.02	0.42
2:I:1046:VAL:HG11	2:I:1049:ILE:HD11	2.01	0.42
2:I:1136:GLN:HE21	2:I:1136:GLN:HB3	1.52	0.42
3:J:844:THR:HG22	3:J:880:VAL:HG11	2.02	0.42
2:I:435:ILE:HA	2:I:439:LYS:O	2.20	0.42
3:J:814:CYS:HB3	3:J:890:THR:HB	2.01	0.42
3:J:1297:LYS:NZ	3:J:1299:GLY:HA3	2.35	0.42
5:M:295:PRO:HG2	5:M:333:LEU:HD21	2.01	0.42
1:G:12:ARG:H	1:G:30:PRO:HD2	1.85	0.42
1:G:25:LYS:HA	1:G:203:ILE:O	2.20	0.42
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.85	0.42
1:H:82:LEU:O	1:H:86:LYS:HG3	2.20	0.42
2:I:529:ARG:HH21	2:I:687:ARG:NH1	2.18	0.42
3:J:169:LEU:HD23	3:J:173:GLY:HA2	2.02	0.42
3:J:987:GLU:H	3:J:987:GLU:HG3	1.52	0.42
3:J:1251:LYS:O	3:J:1255:VAL:HG13	2.19	0.42
4:K:27:ALA:HA	4:K:30:MET:HE3	2.01	0.42
5:M:167:ASP:OD2	5:M:169:GLU:N	2.41	0.42
2:I:47:TYR:HA	2:I:51:ALA:HB2	2.02	0.41
2:I:542:ARG:HE	2:I:542:ARG:HB3	1.73	0.41
2:I:865:LEU:HD21	2:I:882:ILE:O	2.20	0.41
2:I:1098:LEU:HA	2:I:1098:LEU:HD23	1.65	0.41
2:I:1103:VAL:HB	2:I:1104:PRO:HD3	2.02	0.41
2:I:1254:VAL:HG22	2:I:1255:THR:HG23	2.01	0.41
3:J:853:THR:C	3:J:855:ASP:H	2.27	0.41
3:J:1081:VAL:HA	3:J:1088:VAL:HG23	2.01	0.41
3:J:1219:ASP:OD1	3:J:1222:ARG:NH2	2.52	0.41
1:H:78:ILE:O	1:H:82:LEU:HB2	2.20	0.41
2:I:401:GLY:O	2:I:405:PHE:CB	2.68	0.41
2:I:471:VAL:O	2:I:475:VAL:HG23	2.20	0.41
2:I:873:ILE:HG13	2:I:944:ARG:NH2	2.34	0.41
3:J:353:SER:HB3	3:J:447:ILE:HG13	2.02	0.41
1:G:38:THR:HG1	1:H:45:ARG:NH1	2.18	0.41
1:G:154:PRO:HB2	2:I:1059:ARG:HH22	1.84	0.41
2:I:56:VAL:HG13	2:I:57:PHE:CD2	2.55	0.41
2:I:148:GLN:O	2:I:453:ILE:HA	2.20	0.41
2:I:452:ARG:HG3	2:I:585:GLY:HA3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:489:PRO:HA	2:I:492:MET:HE2	2.03	0.41
3:J:123:ARG:HA	3:J:123:ARG:HD3	1.91	0.41
4:K:26:ARG:HG3	4:K:30:MET:HE2	2.02	0.41
2:I:548:ARG:NH2	2:I:567:PRO:O	2.54	0.41
3:J:265:LEU:O	3:J:267:ASP:N	2.54	0.41
5:M:162:VAL:HG22	5:M:170:ILE:HD13	2.01	0.41
1:G:299:SER:O	1:G:303:ILE:HG22	2.21	0.41
2:I:42:ASP:OD2	2:I:44:GLU:HG2	2.19	0.41
2:I:179:TYR:HE1	2:I:454:ARG:HH11	1.68	0.41
2:I:817:LEU:HD11	2:I:1080:ASN:HD22	1.85	0.41
2:I:817:LEU:HD22	2:I:817:LEU:HA	1.90	0.41
2:I:841:ARG:HA	2:I:848:GLU:CB	2.51	0.41
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.86	0.41
3:J:45:ASN:HB3	3:J:48:THR:O	2.21	0.41
3:J:833:GLU:OE2	3:J:1247:LYS:NZ	2.53	0.41
5:M:127:GLN:HB2	5:M:185:PHE:CE2	2.54	0.41
1:G:14:VAL:HG22	1:G:15:ASP:OD1	2.20	0.41
1:G:104:LYS:HG3	1:G:105:SER:N	2.34	0.41
1:H:44:ARG:HD3	1:H:185:TYR:HE2	1.85	0.41
1:H:74:VAL:HG11	1:H:131:CYS:HB2	2.03	0.41
2:I:101:ARG:HA	2:I:118:LYS:HA	2.03	0.41
2:I:175:ARG:HG3	2:I:184:LEU:O	2.20	0.41
2:I:528:ARG:NH2	2:I:575:LEU:HB3	2.36	0.41
2:I:843:THR:HG22	5:M:269:PRO:HD2	2.02	0.41
5:M:133:PHE:HB3	5:M:137:ASP:HB2	2.03	0.41
1:G:182:ARG:O	1:G:183:ILE:HG13	2.20	0.41
1:H:151:GLY:O	1:H:177:TYR:HB2	2.21	0.41
2:I:66:SER:HB3	2:I:479:LEU:HD22	2.02	0.41
2:I:204:LEU:HD13	2:I:208:ILE:HD13	2.01	0.41
2:I:403:MET:HE3	2:I:403:MET:HB3	1.97	0.41
3:J:71:LEU:HD22	3:J:71:LEU:HA	1.94	0.41
3:J:364:HIS:NE2	3:J:438:GLU:OE1	2.44	0.41
3:J:418:GLU:HB2	4:K:45:LYS:HG3	2.02	0.41
3:J:740:LEU:HD12	3:J:763:PHE:HB2	2.01	0.41
1:G:211:ILE:HD13	1:G:211:ILE:HA	1.83	0.41
1:H:64:VAL:HG21	1:H:69:SER:CB	2.51	0.41
2:I:575:LEU:HG	2:I:576:SER:H	1.86	0.41
2:I:1086:PRO:HB2	2:I:1212:LEU:HD23	2.03	0.41
2:I:1340:GLU:HB2	3:J:19:ALA:O	2.21	0.41
3:J:51:PRO:HB2	3:J:57:PHE:O	2.20	0.41
3:J:98:ARG:O	3:J:247:PRO:HD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:620:PHE:O	3:J:624:ILE:HG13	2.20	0.41
3:J:820:ILE:HD11	3:J:822:MET:HE2	2.03	0.41
4:K:26:ARG:NH2	4:K:36:ASP:O	2.54	0.41
5:M:354:PHE:CD1	5:M:359:GLU:HA	2.56	0.41
2:I:748:ILE:HD12	2:I:966:ILE:HD12	2.03	0.41
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.96	0.41
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.95	0.41
3:J:660:GLU:HB2	3:J:685:ILE:HD12	2.02	0.41
3:J:702:GLN:O	3:J:718:SER:N	2.51	0.41
3:J:739:GLN:NE2	3:J:744:ARG:HB2	2.36	0.41
3:J:1067:ARG:NH1	3:J:1074:LEU:O	2.54	0.41
5:M:203:LEU:O	5:M:207:ALA:N	2.54	0.41
5:M:289:LEU:CB	5:M:290:ASN:HA	2.51	0.41
5:M:365:MET:HE2	5:M:365:MET:HB3	1.84	0.41
1:G:14:VAL:HG12	1:G:27:THR:O	2.20	0.41
2:I:150:HIS:HE1	2:I:153:PRO:HD3	1.86	0.41
2:I:207:THR:OG1	2:I:354:ASP:OD1	2.39	0.41
2:I:606:LEU:HD21	2:I:614:TYR:HD1	1.86	0.41
3:J:45:ASN:O	3:J:46:TYR:HB2	2.20	0.41
3:J:263:SER:O	3:J:265:LEU:N	2.54	0.41
3:J:371:LYS:NZ	3:J:445:LYS:HE2	2.36	0.41
3:J:537:TYR:CE2	3:J:544:LEU:HD13	2.55	0.41
3:J:653:ILE:HG12	3:J:692:ARG:NH2	2.36	0.41
3:J:654:ILE:O	3:J:658:GLU:HB2	2.21	0.41
5:M:367:LEU:CB	5:M:381:ILE:HD11	2.50	0.41
1:G:231:PHE:HE2	1:H:217:ILE:HG22	1.86	0.40
2:I:13:LYS:HE2	2:I:15:PHE:CZ	2.56	0.40
2:I:209:ILE:HG23	2:I:210:LEU:N	2.37	0.40
3:J:394:ILE:HG21	5:M:130:LEU:HD21	2.03	0.40
3:J:416:ILE:HG21	3:J:441:LEU:CD2	2.50	0.40
2:I:6:THR:OG1	2:I:781:ASP:OD2	2.30	0.40
2:I:560:PRO:HB3	3:J:776:THR:HG21	2.03	0.40
2:I:629:PHE:O	2:I:647:ARG:NH2	2.53	0.40
3:J:133:ARG:NH1	3:J:136:GLU:OE1	2.54	0.40
3:J:805:GLN:HA	3:J:917:VAL:HG13	2.02	0.40
2:I:80:PHE:HZ	2:I:1038:GLN:HE22	1.69	0.40
2:I:404:LYS:HD3	2:I:586:PHE:HZ	1.86	0.40
2:I:841:ARG:HA	2:I:848:GLU:H	1.86	0.40
3:J:133:ARG:HA	3:J:133:ARG:HD2	1.77	0.40
3:J:441:LEU:HD13	3:J:441:LEU:HA	1.92	0.40
3:J:552:ILE:HD11	3:J:570:LYS:HG3	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	2.04	0.40
3:J:1264:ALA:N	3:J:1278:GLU:O	2.50	0.40
1:G:193:GLU:HA	1:G:194:GLN:HB2	2.03	0.40
1:H:148:ARG:HA	1:H:148:ARG:HD3	1.81	0.40
2:I:1063:GLY:HA3	2:I:1239:VAL:HG11	2.03	0.40
2:I:1264:GLN:HA	2:I:1265:PHE:HA	1.84	0.40
3:J:983:LYS:HD3	3:J:991:THR:HG21	2.02	0.40
5:M:192:ALA:HB3	5:M:198:CYS:HB2	2.04	0.40
5:M:285:TRP:CZ3	5:M:352:GLN:HG3	2.40	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:J:82:GLY:O	5:M:438:SER:OG[3_745]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	305/329 (93%)	270 (88%)	33 (11%)	2 (1%)	18	50
1	H	211/329 (64%)	191 (90%)	20 (10%)	0	100	100
2	I	1211/1342 (90%)	1094 (90%)	110 (9%)	7 (1%)	21	52
3	J	1326/1407 (94%)	1198 (90%)	125 (9%)	3 (0%)	43	72
4	K	77/91 (85%)	71 (92%)	6 (8%)	0	100	100
5	M	370/477 (78%)	345 (93%)	22 (6%)	3 (1%)	16	47
All	All	3500/3975 (88%)	3169 (90%)	316 (9%)	15 (0%)	30	61

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	166	SER
3	J	266	ASN
5	M	276	VAL
2	I	170	VAL
2	I	437	ASN
3	J	265	LEU
2	I	808	ASN
5	M	211	PRO
2	I	164	THR
1	G	313	SER
5	M	386	THR
2	I	201	ARG
2	I	1186	VAL
1	G	30	PRO
3	J	826	ILE

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	G	252/286 (88%)	222 (88%)	30 (12%)	5	22
1	H	175/286 (61%)	155 (89%)	20 (11%)	5	23
2	I	999/1157 (86%)	865 (87%)	134 (13%)	4	19
3	J	1058/1168 (91%)	915 (86%)	143 (14%)	4	18
4	K	65/75 (87%)	55 (85%)	10 (15%)	2	15
5	M	306/423 (72%)	261 (85%)	45 (15%)	3	17
All	All	2855/3395 (84%)	2473 (87%)	382 (13%)	4	19

All (382) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	9	LEU
1	G	15	ASP
1	G	19	VAL
1	G	39	LEU

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Mol	Chain	Res	Type
1	G	72	GLU
1	G	79	LEU
1	G	102	LEU
1	G	104	LYS
1	G	127	GLN
1	G	129	VAL
1	G	140	ILE
1	G	168	ILE
1	G	171	LEU
1	G	172	LEU
1	G	182	ARG
1	G	195	ARG
1	G	197	ASP
1	G	198	LEU
1	G	201	LEU
1	G	211	ILE
1	G	229	GLU
1	G	233	ASP
1	G	254	LEU
1	G	257	VAL
1	G	262	LEU
1	G	295	LEU
1	G	314	LEU
1	G	318	LEU
1	G	319	GLU
1	G	320	ASN
1	H	13	LEU
1	H	16	ILE
1	H	28	LEU
1	H	43	LEU
1	H	62	ASP
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	76	GLU
1	H	77	ASP
1	H	82	LEU
1	H	91	ARG
1	H	132	HIS
1	H	134	THR
1	H	139	SER
1	H	176	CYS

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Mol	Chain	Res	Type
1	H	183	ILE
1	H	191	ARG
1	H	222	THR
1	H	232	VAL
2	I	4	SER
2	I	6	THR
2	I	7	GLU
2	I	11	ILE
2	I	13	LYS
2	I	20	GLN
2	I	21	VAL
2	I	39	ILE
2	I	44	GLU
2	I	53	PHE
2	I	62	TYR
2	I	83	GLN
2	I	90	VAL
2	I	111	GLU
2	I	113	THR
2	I	119	GLU
2	I	121	GLU
2	I	131	THR
2	I	132	ASP
2	I	155	VAL
2	I	185	ASP
2	I	194	LEU
2	I	199	ASP
2	I	216	THR
2	I	219	GLN
2	I	349	GLU
2	I	351	LEU
2	I	354	ASP
2	I	400	VAL
2	I	402	ARG
2	I	470	ARG
2	I	481	LEU
2	I	483	ASP
2	I	486	THR
2	I	487	LEU
2	I	492	MET
2	I	493	ILE
2	I	510	GLN

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Mol	Chain	Res	Type
2	I	518	ASN
2	I	538	LEU
2	I	561	ILE
2	I	589	THR
2	I	600	THR
2	I	602	GLU
2	I	604	HIS
2	I	609	ILE
2	I	615	VAL
2	I	618	GLN
2	I	623	LEU
2	I	624	ASP
2	I	633	LEU
2	I	650	VAL
2	I	651	ASP
2	I	672	GLU
2	I	692	THR
2	I	693	LEU
2	I	696	ASP
2	I	697	LYS
2	I	705	GLU
2	I	711	ASP
2	I	748	ILE
2	I	757	THR
2	I	760	ASN
2	I	761	GLN
2	I	763	THR
2	I	768	MET
2	I	773	LEU
2	I	791	LEU
2	I	800	MET
2	I	805	MET
2	I	817	LEU
2	I	830	THR
2	I	836	LEU
2	I	839	VAL
2	I	840	SER
2	I	842	ASP
2	I	850	ILE
2	I	854	ILE
2	I	862	LEU
2	I	868	SER

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Mol	Chain	Res	Type
2	I	887	VAL
2	I	895	LEU
2	I	902	LEU
2	I	914	LYS
2	I	917	SER
2	I	922	ASN
2	I	928	VAL
2	I	935	THR
2	I	940	GLU
2	I	948	ILE
2	I	959	ASP
2	I	972	PHE
2	I	980	VAL
2	I	984	VAL
2	I	987	GLU
2	I	995	ASP
2	I	1019	ASP
2	I	1030	GLU
2	I	1036	ILE
2	I	1049	ILE
2	I	1056	VAL
2	I	1076	ILE
2	I	1082	ILE
2	I	1083	GLU
2	I	1112	ILE
2	I	1114	GLU
2	I	1136	GLN
2	I	1141	LEU
2	I	1146	GLN
2	I	1151	LEU
2	I	1156	ARG
2	I	1160	ASP
2	I	1161	LEU
2	I	1164	PHE
2	I	1165	SER
2	I	1170	MET
2	I	1172	LEU
2	I	1180	MET
2	I	1198	LEU
2	I	1203	ASP
2	I	1210	ILE
2	I	1212	LEU

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Mol	Chain	Res	Type
2	I	1217	THR
2	I	1222	GLU
2	I	1232	MET
2	I	1254	VAL
2	I	1265	PHE
2	I	1288	GLN
2	I	1291	LEU
2	I	1293	VAL
2	I	1298	VAL
2	I	1302	THR
2	I	1310	ASP
2	I	1327	LEU
3	J	1	MET
3	J	5	LEU
3	J	14	THR
3	J	16	GLU
3	J	17	PHE
3	J	43	THR
3	J	48	THR
3	J	65	VAL
3	J	71	LEU
3	J	74	LYS
3	J	80	HIS
3	J	87	LYS
3	J	92	VAL
3	J	93	THR
3	J	97	VAL
3	J	115	TRP
3	J	126	LEU
3	J	136	GLU
3	J	140	TYR
3	J	154	LEU
3	J	167	ASP
3	J	169	LEU
3	J	172	PHE
3	J	175	GLU
3	J	190	LYS
3	J	195	GLU
3	J	208	THR
3	J	211	GLU
3	J	219	LYS
3	J	232	ASN

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Mol	Chain	Res	Type
3	J	241	VAL
3	J	250	ARG
3	J	265	LEU
3	J	266	ASN
3	J	271	ARG
3	J	279	LEU
3	J	285	LEU
3	J	297	ARG
3	J	306	LEU
3	J	321	LYS
3	J	322	ARG
3	J	324	LEU
3	J	338	PHE
3	J	345	LYS
3	J	356	THR
3	J	357	VAL
3	J	363	LEU
3	J	378	LYS
3	J	395	LYS
3	J	399	LYS
3	J	412	LEU
3	J	415	VAL
3	J	453	VAL
3	J	466	MET
3	J	470	VAL
3	J	478	LEU
3	J	483	LEU
3	J	504	GLN
3	J	506	VAL
3	J	516	ASP
3	J	517	CYS
3	J	536	LEU
3	J	545	HIS
3	J	548	VAL
3	J	552	ILE
3	J	554	GLU
3	J	596	LEU
3	J	617	THR
3	J	641	ILE
3	J	642	ASP
3	J	644	MET
3	J	661	VAL

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Mol	Chain	Res	Type
3	J	678	ARG
3	J	681	LYS
3	J	683	ILE
3	J	705	THR
3	J	706	VAL
3	J	707	ILE
3	J	708	ASN
3	J	712	GLN
3	J	739	GLN
3	J	746	LEU
3	J	749	LYS
3	J	769	VAL
3	J	772	TYR
3	J	788	LEU
3	J	810	THR
3	J	817	HIS
3	J	843	VAL
3	J	846	GLU
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	860	ARG
3	J	866	GLU
3	J	869	CYS
3	J	891	ASP
3	J	894	VAL
3	J	895	CYS
3	J	897	HIS
3	J	898	CYS
3	J	907	HIS
3	J	908	ILE
3	J	918	ILE
3	J	953	LYS
3	J	958	ILE
3	J	980	THR
3	J	987	GLU
3	J	1011	VAL
3	J	1017	VAL
3	J	1019	ASN
3	J	1056	LEU
3	J	1061	VAL

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Mol	Chain	Res	Type
3	J	1063	ASP
3	J	1073	ASP
3	J	1079	LYS
3	J	1090	ILE
3	J	1094	ASP
3	J	1095	MET
3	J	1138	LEU
3	J	1146	GLU
3	J	1155	ILE
3	J	1167	LYS
3	J	1181	ASP
3	J	1208	ASP
3	J	1215	GLU
3	J	1221	LEU
3	J	1223	LEU
3	J	1255	VAL
3	J	1258	ARG
3	J	1267	VAL
3	J	1283	SER
3	J	1293	GLU
3	J	1298	VAL
3	J	1305	ASP
3	J	1306	LEU
3	J	1319	PHE
3	J	1326	GLN
3	J	1331	VAL
3	J	1348	LYS
3	J	1353	VAL
3	J	1361	THR
4	K	3	ARG
4	K	4	VAL
4	K	5	THR
4	K	13	ILE
4	K	25	ARG
4	K	36	ASP
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
4	K	68	GLU
5	M	27	GLN
5	M	29	SER
5	M	37	LEU

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Mol	Chain	Res	Type
5	M	44	ASN
5	M	113	GLN
5	M	115	GLU
5	M	124	LEU
5	M	125	MET
5	M	161	ILE
5	M	162	VAL
5	M	186	ASP
5	M	195	LEU
5	M	197	ASP
5	M	200	LEU
5	M	202	GLN
5	M	203	LEU
5	M	213	LEU
5	M	226	LEU
5	M	236	MET
5	M	238	VAL
5	M	244	GLU
5	M	246	LEU
5	M	257	ASP
5	M	265	HIS
5	M	276	VAL
5	M	278	VAL
5	M	285	TRP
5	M	302	GLN
5	M	303	TYR
5	M	318	PHE
5	M	319	ILE
5	M	350	GLN
5	M	360	GLU
5	M	365	MET
5	M	367	LEU
5	M	370	ILE
5	M	377	HIS
5	M	378	GLU
5	M	379	SER
5	M	381	ILE
5	M	387	GLN
5	M	399	LEU
5	M	421	ARG
5	M	432	ASN
5	M	465	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	18	GLN
1	G	23	HIS
1	G	75	GLN
1	G	84	ASN
1	G	103	ASN
1	G	132	HIS
1	G	194	GLN
1	G	320	ASN
1	H	23	HIS
1	H	147	GLN
2	I	20	GLN
2	I	173	ASN
2	I	214	ASN
2	I	219	GLN
2	I	450	ASN
2	I	462	ASN
2	I	463	GLN
2	I	510	GLN
2	I	513	GLN
2	I	613	ASN
2	I	686	GLN
2	I	808	ASN
2	I	811	ASN
2	I	832	HIS
2	I	834	GLN
2	I	1013	GLN
2	I	1038	GLN
2	I	1061	GLN
2	I	1080	ASN
2	I	1116	HIS
2	I	1134	GLN
2	I	1136	GLN
2	I	1175	ASN
2	I	1220	GLN
2	I	1268	GLN
2	I	1288	GLN
2	I	1299	ASN
2	I	1313	HIS
3	J	186	GLN
3	J	200	GLN
3	J	277	ASN

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Mol	Chain	Res	Type
3	J	341	ASN
3	J	488	ASN
3	J	495	ASN
3	J	594	GLN
3	J	680	ASN
3	J	690	ASN
3	J	702	GLN
3	J	739	GLN
3	J	817	HIS
3	J	861	ASN
3	J	867	GLN
3	J	1218	HIS
3	J	1268	ASN
3	J	1366	HIS
4	K	60	ASN
4	K	61	ASN
5	M	27	GLN
5	M	113	GLN
5	M	127	GLN
5	M	202	GLN
5	M	254	GLN
5	M	302	GLN
5	M	322	ASN
5	M	350	GLN
5	M	352	GLN
5	M	449	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	G	309/329 (93%)	-0.32	2 (0%) 85 67	115, 174, 216, 248	0
1	H	215/329 (65%)	-0.26	1 (0%) 87 70	144, 209, 239, 261	0
2	I	1217/1342 (90%)	-0.29	6 (0%) 87 70	97, 179, 242, 273	0
3	J	1336/1407 (94%)	-0.31	4 (0%) 90 77	88, 182, 243, 270	0
4	K	79/91 (86%)	-0.51	0 100 100	131, 168, 207, 230	0
5	M	380/477 (79%)	-0.23	0 100 100	103, 150, 191, 226	0
All	All	3536/3975 (88%)	-0.30	13 (0%) 88 73	88, 177, 239, 273	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	1334	GLY	3.3
3	J	1099	TYR	2.5
2	I	224	PHE	2.4
3	J	1110	GLU	2.4
1	G	39	LEU	2.4
2	I	905	ILE	2.4
3	J	1358	PRO	2.3
2	I	197	ARG	2.1
2	I	1148	ALA	2.1
1	H	183	ILE	2.1
3	J	1201	GLY	2.0
2	I	1066	MET	2.0
1	G	318	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	J	1501	1/1	0.78	0.06	192,192,192,192	0
7	ZN	J	1502	1/1	0.98	0.10	225,225,225,225	0
7	ZN	J	1503	1/1	0.98	0.07	179,179,179,179	0

6.5 Other polymers [i](#)

There are no such residues in this entry.