



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2020 – 02:06 PM BST

PDB ID : 6UU5
Title : E. coli sigma-S transcription initiation complex with a 6-nt RNA ("Old" crystal soaked with GTP, UTP, CTP, and dinucleotide GpA for 30 minutes)
Authors : Zuo, Y.; De, S.; Steitz, T.A.
Deposited on : 2019-10-30
Resolution : 5.40 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13

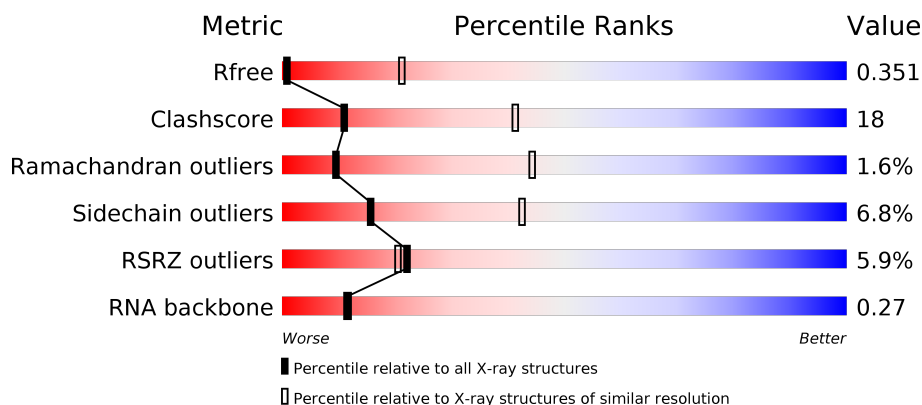
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 5.40 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}	130704	1207 (7.00-3.80)
Clashscore	141614	1016 (6.92-3.86)
Ramachandran outliers	138981	1210 (7.00-3.80)
Sidechain outliers	138945	1181 (7.00-3.80)
RSRZ outliers	127900	1021 (7.04-3.76)
RNA backbone	3102	1074 (7.80-3.00)

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 on 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	AAA	242	
1	BBB	242	
2	CCC	1342	
3	DDD	1407	

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Mol	Chain	Length	Quality of chain
4	EEE	90	
5	FFF	336	
6	111	50	
7	222	50	
8	333	6	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	DPO	DDD	1504	-	-	X	-
9	ZN	DDD	1502	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 29050 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	AAA	230	Total	C	N	O	S	0	0	0
			1787	1112	317	352	6			
1	BBB	228	Total	C	N	O	S	0	0	0
			1767	1100	312	349	6			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
AAA	-6	ALA	-	expression tag	UNP P0A7Z4
AAA	-5	HIS	-	expression tag	UNP P0A7Z4
AAA	-4	HIS	-	expression tag	UNP P0A7Z4
AAA	-3	HIS	-	expression tag	UNP P0A7Z4
AAA	-2	HIS	-	expression tag	UNP P0A7Z4
AAA	-1	HIS	-	expression tag	UNP P0A7Z4
AAA	0	HIS	-	expression tag	UNP P0A7Z4
BBB	-6	ALA	-	expression tag	UNP P0A7Z4
BBB	-5	HIS	-	expression tag	UNP P0A7Z4
BBB	-4	HIS	-	expression tag	UNP P0A7Z4
BBB	-3	HIS	-	expression tag	UNP P0A7Z4
BBB	-2	HIS	-	expression tag	UNP P0A7Z4
BBB	-1	HIS	-	expression tag	UNP P0A7Z4
BBB	0	HIS	-	expression tag	UNP P0A7Z4

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	CCC	1341	Total	C	N	O	S	0	0	0
			10576	6636	1842	2055	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	DDD	1362	Total	C	N	O	S	0	0	0
			10568	6633	1887	1998	50			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	EEE	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	FFF	277	Total	C	N	O	S	0	0	0
			2253	1411	415	423	4			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
FFF	2	GLY	SER	conflict	UNP P13445
FFF	33	GLU	GLN	conflict	UNP P13445
FFF	329	LEU	-	expression tag	UNP P13445
FFF	330	GLU	-	expression tag	UNP P13445
FFF	331	HIS	-	expression tag	UNP P13445
FFF	332	HIS	-	expression tag	UNP P13445
FFF	333	HIS	-	expression tag	UNP P13445
FFF	334	HIS	-	expression tag	UNP P13445
FFF	335	HIS	-	expression tag	UNP P13445
FFF	336	HIS	-	expression tag	UNP P13445

- Molecule 6 is a DNA chain called Synthetic DNA 50-MER (promoter non-template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	111	30	Total	C	N	O	P	0	0	0
			618	294	111	183	30			

- Molecule 7 is a DNA chain called Synthetic DNA 50-MER (promoter template strand).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	222	35	Total	C	N	O	P	0	0	0
			716	342	132	208	34			

- Molecule 8 is a RNA chain called RNA 6-mer (dinucleotide GpA primed synthesis).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	333	6	Total	C	N	O	P	0	0	0
			125	57	22	41	5			

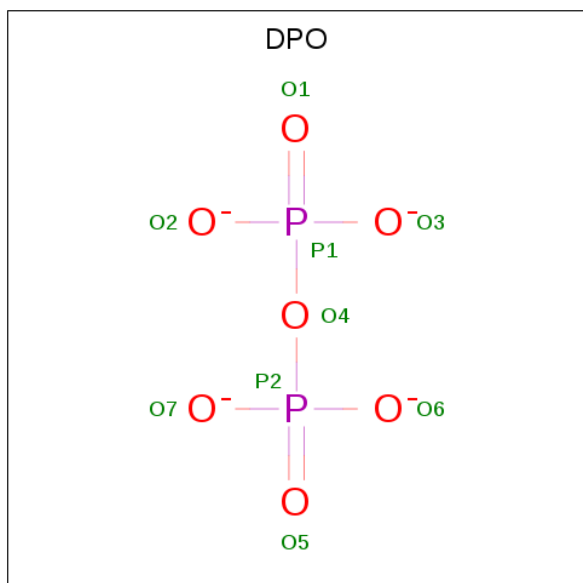
- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	333	1	Total	Mg	0	0
			1	1		
10	DDD	1	Total	Mg	0	0
			1	1		

- Molecule 11 is DIPHOSPHATE (three-letter code: DPO) (formula: O₇P₂).

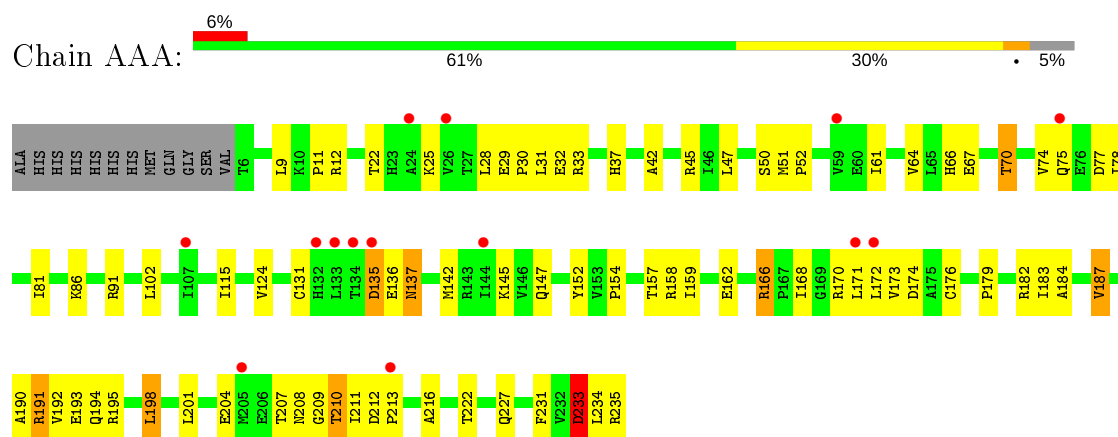


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	DDD	1	Total	O	P	0	0
			9	7	2		

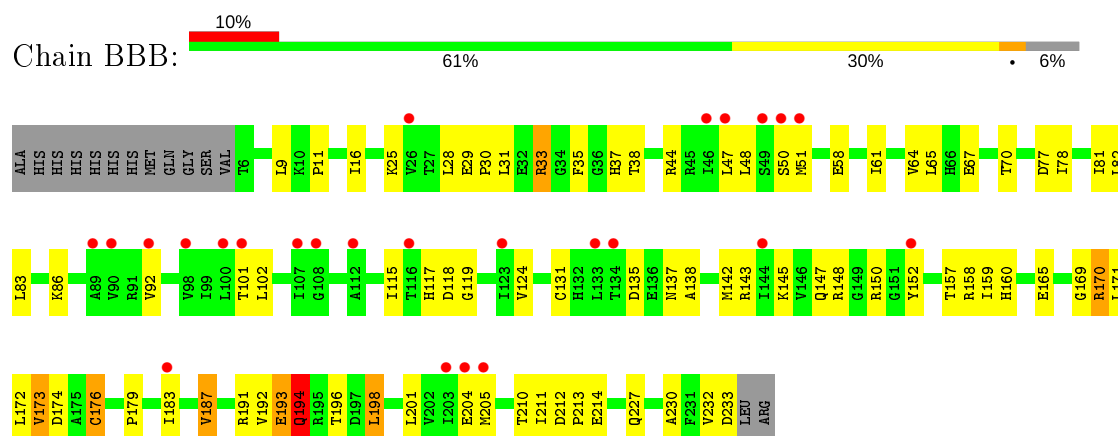
3 Residue-property plots [i](#)

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.

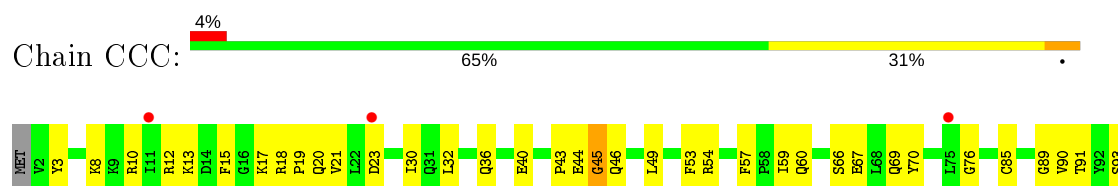
- Molecule 1: DNA-directed RNA polymerase subunit alpha



- Molecule 1: DNA-directed RNA polymerase subunit alpha

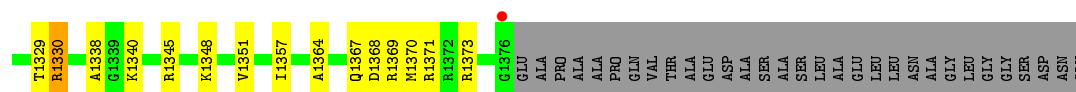


- Molecule 2: DNA-directed RNA polymerase subunit beta

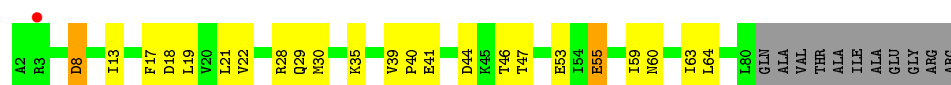




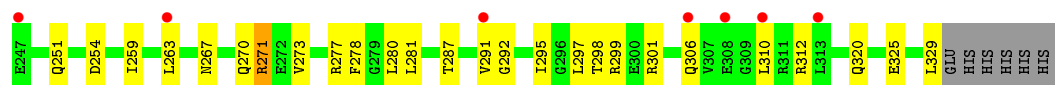
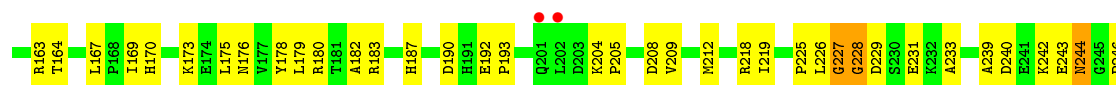
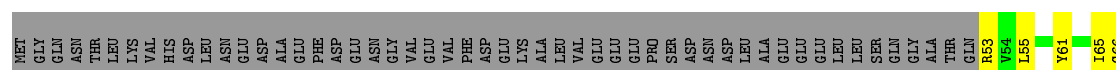
Q1238	G1129	Q1044	V963	S884	E811	G742	G628	L536	E443	R346	L223	A108	MET
R1242	G1130	T1047	K964	V885	D812	M743	F629	T637	G444	V347	L224	A109	LYS
L1243	K1131	T1047	S965	V886	D812	R744	G629	R538	K445	D348	L224	T111	ASP
Q1244	D1133	D1051	V966	S887	T816	G745	S638	S543	Q448	T356	P234	T111	LEU
G1245	L1134	E1052	S969	C888	E817	M746	V639	L544	Q448	T356	P234	H113	LEU
V1246	T1135	L1053	S970	D889	C819	R747	M644	E546	Q448	T356	P234	I114	PHE
N1249	L1138	T1054	L973	T890	I820	A748	V645	V548	Q448	T356	P234	W115	LEU
D1250	E1146	S1058	S974	F892	M821	R749	V645	E548	Q448	T356	P234	L115	LEU
E1254	L1059	V1060	V974	C893	M821	R749	V645	E548	Q448	T356	P234	L115	LEU
V1255	K1151	V1061	V975	C894	M821	R749	V645	E548	Q448	T356	P234	L115	LEU
L1256	L1155	L1062	S976	C895	M821	R749	V645	E548	Q448	T356	P234	L115	LEU
V1257	L1156	L1063	S977	C896	M821	R749	V645	E548	Q448	T356	P234	L115	LEU
R1258	L1156	L1063	S977	C896	M821	R749	V645	E548	Q448	T356	P234	L115	LEU
Q1259	G1161	A1065	L984	K911	G829	R758	E663	E555	L472	R370	R278	L127	E16
M1260	V1162	A1065	L985	K911	G829	R758	E663	E555	L472	R370	R278	L127	E16
L1261	V1163	A1066	D886	K912	G829	R758	E663	E555	L472	R370	R278	L127	E16
R1262	F1164	R1067	G989	K913	G829	R758	E663	E555	L472	R370	R278	L127	E16
K1263	F1165	T1068	R990	K914	G829	R758	E663	E555	L472	R370	R278	L127	E16
I1266	E1168	D1073	K991	K915	G829	R758	E663	E555	L472	R370	R278	L127	E16
G1270	T1169	A1077	K992	K916	G829	R758	E663	E555	L472	R370	R278	L127	E16
S1271	K1170	L1078	S994	K917	G829	R758	E663	E555	L472	R370	R278	L127	E16
S1272	R1173	T1080	S995	K918	G829	R758	E663	E555	L472	R370	R278	L127	E16
L1275	R1174	V1081	K996	K919	G829	R758	E663	E555	L472	R370	R278	L127	E16
E1276	L1175	D1082	P997	K920	G829	R758	E663	E555	L472	R370	R278	L127	E16
V1282	V1176	A1083	G999	K921	G829	R758	E663	E555	L472	R370	R278	L127	E16
S1283	P1179	Q1084	G1000	K922	G829	R758	E663	E555	L472	R370	R278	L127	E16
E1291	D1180	D1087	L1003	K923	G829	R758	E663	E555	L472	R370	R278	L127	E16
V1285	D1181	P1091	V1011	K924	G829	R758	E663	E555	L472	R370	R278	L127	E16
K1286	G1182	S1091	V1011	K925	G829	R758	E663	E555	L472	R370	R278	L127	E16
I1287	S1183	A1097	A1018	K926	G829	R758	E663	E555	L472	R370	R278	L127	E16
R1290	Y1186	Q1098	M1019	K927	G829	R758	E663	E555	L472	R370	R278	L127	E16
E1291	E1187	Y1099	M1020	K928	G829	R758	E663	E555	L472	R370	R278	L127	E16
L1292	E1188	D1021	A940	K929	G829	R758	E663	E555	L472	R370	R278	L127	E16
G1296	L1196	G1103	P1022	K930	G829	R758	E663	E555	L472	R370	R278	L127	E16
K1297	R1197	A1105	H1023	K931	G829	R758	E663	E555	L472	R370	R278	L127	E16
V1298	V1198	T1106	M1025	K932	G829	R758	E663	E555	L472	R370	R278	L127	E16
S1303	F1199	V1107	M1026	K933	G829	R758	E663	E555	L472	R370	R278	L127	E16
L1307	G1207	E1110	V1027	K934	G829	R758	E663	E555	L472	R370	R278	L127	E16
G1308	D1208	D1111	T1028	K935	G829	R758	E663	E555	L472	R370	R278	L127	E16
V1309	V1209	G1112	T1029	K936	G829	R758	E663	E555	L472	R370	R278	L127	E16
T1310	S1211	V1113	E1030	K937	G829	R758	E663	E555	L472	R370	R278	L127	E16
S1313	D1212	Q1114	V1031	K938	G829	R758	E663	E555	L472	R370	R278	L127	E16
T1316	G1118	I1115	S1032	K939	G829	R758	E663	E555	L472	R370	R278	L127	E16
T1319	D1119	G1119	V1035	K940	G829	R758	E663	E555	L472	R370	R278	L127	E16
F1319	H1227	T1120	F1037	K941	G829	R758	E663	E555	L472	R370	R278	L127	E16
S1324	T1230	A1122	I1041	K942	G829	R758	E663	E555	L472	R370	R278	L127	E16
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				K1008	G829	R758	E663	E555	L472	R370	R278	L127	E16
				K1009	G829	R758	E663	E555	L472	R370	R278	L127	E16
				K1010	G829	R758	E663	E555	L472	R370	R278	L127	E16
				K1011	G829	R758							



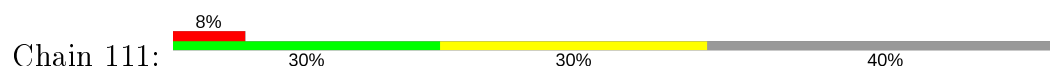
- Molecule 4: DNA-directed RNA polymerase subunit omega



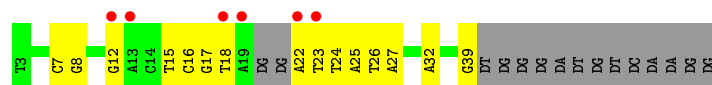
- Molecule 5: RNA polymerase sigma factor RpoS



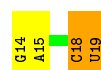
- Molecule 6: Synthetic DNA 50-MER (promoter non-template strand)



- Molecule 7: Synthetic DNA 50-MER (promoter template strand)



- Molecule 8: RNA 6-mer (dinucleotide GpA primed synthesis)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	132.36Å 153.77Å 231.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 5.40 49.02 – 5.40	Depositor EDS
% Data completeness (in resolution range)	98.2 (49.00-5.40) 98.4 (49.02-5.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 5.39Å)	Xtriage
Refinement program	REFMAC 5.8.0257	Depositor
R, R_{free}	0.295 , 0.362 0.282 , 0.351	Depositor DCC
R_{free} test set	770 reflections (4.67%)	wwPDB-VP
Wilson B-factor (Å ²)	225.3	Xtriage
Anisotropy	0.447	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 293.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.33$, $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	29050	wwPDB-VP
Average B, all atoms (Å ²)	345.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: DPO, 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	AAA	0.64	0/1809	0.73	0/2450
1	BBB	0.65	0/1789	0.73	0/2425
2	CCC	0.63	0/10745	0.78	2/14499 (0.0%)
3	DDD	0.64	0/10729	0.77	0/14487
4	EEE	0.62	0/629	0.76	0/847
5	FFF	0.65	0/2282	0.67	1/3076 (0.0%)
6	111	0.24	0/691	0.63	0/1063
7	222	0.28	0/802	0.64	0/1234
8	333	0.17	0/139	0.59	0/215
All	All	0.62	0/29615	0.75	3/40296 (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
2	CCC	0	1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	CCC	1088	ASP	CB-CA-C	-5.93	98.54	110.40
5	FFF	67	TYR	CB-CA-C	5.60	121.59	110.40
2	CCC	454	ARG	CB-CA-C	-5.19	100.01	110.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	CCC	1282	GLY	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	AAA	1787	0	1813	77	1
1	BBB	1767	0	1789	75	0
2	CCC	10576	0	10591	406	0
3	DDD	10568	0	10781	470	5
4	EEE	627	0	634	14	0
5	FFF	2253	0	2298	114	7
6	111	618	0	341	30	3
7	222	716	0	397	29	1
8	333	125	0	66	7	0
9	DDD	2	0	0	2	0
10	333	1	0	0	0	0
10	DDD	1	0	0	0	0
11	DDD	9	0	0	3	0
All	All	29050	0	28710	1042	12

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 (1042) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:843:VAL:HG11	3:DDD:883:ARG:CB	1.46	1.46
3:DDD:843:VAL:CG1	3:DDD:883:ARG:CB	1.99	1.40
3:DDD:843:VAL:CG1	3:DDD:883:ARG:HB2	1.49	1.40
6:111:54:DA:H2"	6:111:55:DC:C5	1.64	1.30
3:DDD:392:THR:HG21	5:FFF:320:GLN:O	1.27	1.27
3:DDD:392:THR:CG2	5:FFF:320:GLN:O	1.91	1.17
3:DDD:843:VAL:CG1	3:DDD:883:ARG:HB3	1.77	1.10
6:111:54:DA:H2"	6:111:55:DC:C6	1.87	1.09
3:DDD:843:VAL:HG12	3:DDD:883:ARG:CB	1.83	1.09
3:DDD:839:VAL:HG12	3:DDD:864:LEU:HD12	1.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:525:THR:HG21	2:CCC:687:ARG:HD3	1.35	1.05
5:FFF:109:TYR:OH	5:FFF:155:GLU:HG3	1.59	1.03
1:BBB:67:GLU:HB3	1:BBB:171:LEU:HD22	1.39	1.01
5:FFF:183:ARG:NH2	7:222:26:DT:OP2	1.96	0.97
2:CCC:196:VAL:HG23	2:CCC:206:ALA:HA	1.44	0.96
3:DDD:750:PRO:HA	3:DDD:781:LYS:HG2	1.46	0.96
3:DDD:888:CYS:SG	9:DDD:1502:ZN:ZN	1.55	0.95
3:DDD:843:VAL:HG12	3:DDD:883:ARG:H	1.32	0.95
6:111:54:DA:C2'	6:111:55:DC:C5	2.50	0.94
2:CCC:901:LEU:HD13	5:FFF:278:PHE:CE2	2.04	0.93
3:DDD:843:VAL:HG11	3:DDD:883:ARG:HB2	1.02	0.92
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:HD13	1.50	0.92
5:FFF:109:TYR:OH	5:FFF:155:GLU:CG	2.17	0.92
2:CCC:251:ALA:CB	2:CCC:263:VAL:HG11	2.00	0.92
5:FFF:273:VAL:HG13	5:FFF:291:VAL:HG11	1.50	0.91
3:DDD:388:ARG:NH2	3:DDD:414:GLU:OE1	2.03	0.90
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB2	1.71	0.90
1:BBB:179:PRO:HG3	1:BBB:211:ILE:HD12	1.54	0.90
2:CCC:32:LEU:HA	2:CCC:130:MET:HE1	1.52	0.89
1:BBB:25:LYS:HG2	1:BBB:204:GLU:HG2	1.55	0.88
1:BBB:193:GLU:O	1:BBB:194:GLN:HB2	1.71	0.88
2:CCC:1281:TYR:OH	3:DDD:434:ILE:O	1.91	0.87
7:222:17:DG:C2'	7:222:18:DT:O4'	2.21	0.87
2:CCC:804:PHE:O	3:DDD:638:SER:HB2	1.75	0.86
1:AAA:227:GLN:OE1	1:BBB:11:PRO:HD3	1.73	0.86
1:BBB:124:VAL:HG21	1:BBB:210:THR:HG22	1.58	0.86
1:BBB:176:CYS:HB3	3:DDD:535:ARG:HH22	1.42	0.84
2:CCC:901:LEU:CD1	5:FFF:310:LEU:HD21	2.06	0.84
2:CCC:681:MET:O	2:CCC:685:MET:HG2	1.75	0.84
3:DDD:843:VAL:HG12	3:DDD:883:ARG:N	1.93	0.83
3:DDD:395:LYS:HG2	5:FFF:329:LEU:HD13	1.59	0.83
5:FFF:227:GLY:HA2	7:222:17:DG:H22	1.41	0.83
3:DDD:121:PRO:O	3:DDD:122:SER:HB3	1.79	0.83
2:CCC:1259:LEU:HD11	5:FFF:239:ALA:HB2	1.60	0.83
2:CCC:1333:LEU:O	3:DDD:113:HIS:CE1	2.32	0.82
3:DDD:793:SER:OG	3:DDD:928:THR:OG1	1.95	0.82
1:AAA:222:THR:OG1	1:BBB:233:ASP:CB	2.28	0.82
2:CCC:1291:LEU:HD11	3:DDD:1351:VAL:HG13	1.62	0.82
2:CCC:726:TYR:HB3	2:CCC:733:VAL:CG2	2.09	0.82
3:DDD:836:ARG:HG3	3:DDD:869:CYS:HB3	1.61	0.81
3:DDD:22:ILE:HD11	3:DDD:1319:PHE:CE1	2.15	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:673:VAL:CG1	3:DDD:678:ARG:HB2	2.11	0.81
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:HD11	1.61	0.81
2:CCC:901:LEU:HD11	5:FFF:310:LEU:HD21	1.63	0.81
2:CCC:555:TYR:CD1	2:CCC:637:ARG:NH2	2.50	0.80
3:DDD:843:VAL:HG11	3:DDD:883:ARG:HB3	1.39	0.80
5:FFF:170:HIS:HE1	6:111:32:DA:N7	1.80	0.80
2:CCC:1077:SER:HA	3:DDD:356:THR:CG2	2.13	0.79
3:DDD:644:MET:O	3:DDD:764:ARG:NH1	2.14	0.79
2:CCC:255:ILE:HD12	2:CCC:263:VAL:HG21	1.65	0.78
3:DDD:888:CYS:HG	9:DDD:1502:ZN:ZN	0.90	0.78
2:CCC:1304:MET:HE1	3:DDD:472:LEU:HD13	1.65	0.78
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:HD12	1.65	0.78
5:FFF:163:ARG:HD3	5:FFF:167:LEU:HD12	1.66	0.78
3:DDD:475:GLU:O	3:DDD:479:GLU:HG2	1.84	0.77
2:CCC:186:PHE:CE1	2:CCC:196:VAL:HG22	2.18	0.77
2:CCC:165:HIS:CE1	2:CCC:190:PRO:HG3	2.19	0.77
3:DDD:26:SER:OG	3:DDD:28:ASP:OD1	2.00	0.77
2:CCC:1295:SER:OG	3:DDD:346:ARG:O	2.02	0.77
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HG3	1.67	0.77
2:CCC:790:ASP:O	2:CCC:792:GLY:N	2.17	0.77
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:NH1	2.00	0.76
2:CCC:237:LEU:HD12	2:CCC:289:VAL:HA	1.66	0.76
3:DDD:932:MET:SD	8:333:19:U:H2'	2.26	0.76
6:111:27:DC:H2''	6:111:28:DA:C8	2.21	0.76
2:CCC:525:THR:HG21	2:CCC:687:ARG:CD	2.13	0.76
2:CCC:1333:LEU:O	3:DDD:113:HIS:HE1	1.68	0.75
3:DDD:858:VAL:HG13	3:DDD:868:TRP:CZ3	2.21	0.75
3:DDD:895:CYS:SG	3:DDD:898:CYS:HB2	2.25	0.75
5:FFF:163:ARG:NH2	7:222:26:DT:O4	2.17	0.75
1:AAA:227:GLN:OE1	1:BBB:11:PRO:CD	2.35	0.75
5:FFF:226:LEU:O	5:FFF:228:GLY:N	2.20	0.75
3:DDD:823:THR:HB	3:DDD:824:PRO:HD2	1.67	0.74
3:DDD:1029:THR:HG23	3:DDD:1121:LEU:HG	1.70	0.74
3:DDD:843:VAL:O	3:DDD:882:VAL:HB	1.86	0.74
2:CCC:648:ASP:N	2:CCC:648:ASP:OD1	2.19	0.74
2:CCC:244:GLU:HG2	2:CCC:245:ARG:N	2.02	0.74
2:CCC:94:ALA:HB2	2:CCC:129:LEU:HD11	1.69	0.73
2:CCC:251:ALA:HB2	2:CCC:263:VAL:HG11	1.67	0.73
2:CCC:342:ASP:O	2:CCC:437:ASN:CG	2.26	0.73
7:222:17:DG:H2'	7:222:18:DT:O4'	1.89	0.73
2:CCC:10:ARG:NH2	2:CCC:790:ASP:OD1	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:3:TYR:O	2:CCC:8:LYS:HE3	1.87	0.73
3:DDD:845:ALA:O	3:DDD:881:LYS:CG	2.37	0.73
3:DDD:392:THR:HG22	5:FFF:320:GLN:O	1.88	0.72
1:AAA:9:LEU:HD21	1:AAA:198:LEU:HD11	1.69	0.72
5:FFF:170:HIS:CE1	6:111:32:DA:N7	2.56	0.72
3:DDD:1133:ASP:OD2	3:DDD:1134:ILE:N	2.23	0.72
2:CCC:1077:SER:HA	3:DDD:356:THR:HG23	1.71	0.72
3:DDD:829:GLY:HA2	3:DDD:993:GLU:HB3	1.72	0.72
2:CCC:555:TYR:CE1	2:CCC:637:ARG:NH2	2.58	0.72
2:CCC:855:PRO:HB3	2:CCC:910:ALA:HB1	1.72	0.72
3:DDD:134:ASP:CG	3:DDD:159:ILE:HD11	2.09	0.72
3:DDD:703:THR:OG1	3:DDD:704:GLU:N	2.22	0.72
3:DDD:845:ALA:O	3:DDD:881:LYS:HD3	1.89	0.72
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:CG2	2.18	0.72
3:DDD:698:MET:O	3:DDD:702:GLN:HB3	1.89	0.71
3:DDD:895:CYS:SG	3:DDD:898:CYS:CB	2.78	0.71
3:DDD:931:THR:O	3:DDD:935:PHE:CD2	2.44	0.71
1:AAA:182:ARG:NH1	2:CCC:1090:ASN:O	2.23	0.71
1:BBB:193:GLU:O	1:BBB:194:GLN:CB	2.39	0.71
1:BBB:9:LEU:HD21	1:BBB:198:LEU:HD11	1.71	0.71
2:CCC:18:ARG:NH2	2:CCC:620:ASN:O	2.23	0.71
5:FFF:182:ALA:HB1	5:FFF:193:PRO:HG3	1.70	0.71
3:DDD:173:GLY:O	3:DDD:175:GLU:N	2.23	0.71
3:DDD:395:LYS:CG	5:FFF:329:LEU:HD13	2.20	0.71
1:BBB:82:LEU:HB3	1:BBB:173:VAL:HG11	1.72	0.71
2:CCC:163:LYS:HG2	2:CCC:164:THR:N	2.05	0.71
2:CCC:496:LYS:HB3	7:222:24:DT:OP1	1.91	0.70
1:BBB:83:LEU:HG	3:DDD:526:VAL:HG11	1.74	0.70
1:BBB:82:LEU:HD22	1:BBB:173:VAL:HG21	1.73	0.70
3:DDD:528:THR:O	3:DDD:528:THR:OG1	2.02	0.70
5:FFF:192:GLU:HG3	5:FFF:193:PRO:HD2	1.74	0.69
2:CCC:93:SER:OG	2:CCC:126:GLU:OE1	2.09	0.69
2:CCC:700:VAL:O	2:CCC:1069:ARG:NH2	2.20	0.69
1:AAA:158:ARG:HH11	1:AAA:158:ARG:HG3	1.58	0.69
2:CCC:1245:ALA:HB2	3:DDD:372:MET:HG3	1.73	0.69
3:DDD:519:ASN:OD1	3:DDD:520:ALA:N	2.21	0.69
3:DDD:843:VAL:HG12	3:DDD:883:ARG:CA	2.23	0.69
1:AAA:184:ALA:HB2	2:CCC:1091:GLY:HA3	1.74	0.69
2:CCC:230:PHE:CD1	2:CCC:292:ILE:HD11	2.28	0.69
3:DDD:800:LEU:HD22	3:DDD:1256:ILE:CD1	2.22	0.69
1:BBB:47:LEU:HA	1:BBB:51:MET:HG2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:83:LEU:HG	3:DDD:526:VAL:CG1	2.23	0.68
1:BBB:83:LEU:HD21	3:DDD:526:VAL:HB	1.76	0.68
6:111:27:DC:H2''	6:111:28:DA:H8	1.56	0.68
2:CCC:1304:MET:CE	3:DDD:472:LEU:HD13	2.23	0.68
3:DDD:849:LEU:HD11	3:DDD:853:THR:HA	1.76	0.68
2:CCC:183:TRP:CZ3	6:111:51:DC:H2'	2.29	0.68
2:CCC:221:LEU:HD11	2:CCC:314:ASN:HB2	1.75	0.68
1:AAA:45:ARG:NE	1:BBB:38:THR:OG1	2.21	0.68
3:DDD:845:ALA:O	3:DDD:881:LYS:HB3	1.93	0.68
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD11	1.76	0.68
2:CCC:257:ALA:HB3	2:CCC:262:TYR:CE2	2.29	0.68
2:CCC:32:LEU:HD23	2:CCC:130:MET:CE	2.24	0.68
5:FFF:144:THR:HG22	6:111:39:DA:H8	1.57	0.67
2:CCC:804:PHE:O	3:DDD:638:SER:CB	2.41	0.67
2:CCC:1088:ASP:HB3	2:CCC:1090:ASN:H	1.58	0.67
3:DDD:839:VAL:HG12	3:DDD:839:VAL:O	1.95	0.67
2:CCC:696:ASP:O	2:CCC:795:ALA:HB1	1.95	0.67
3:DDD:312:ARG:O	3:DDD:312:ARG:HG2	1.94	0.67
3:DDD:958:ILE:HG23	3:DDD:982:LEU:CD1	2.25	0.67
5:FFF:170:HIS:CE1	6:111:31:DT:C6	2.82	0.66
5:FFF:164:THR:HB	5:FFF:219:ILE:HD12	1.78	0.66
2:CCC:560:PRO:HB2	3:DDD:776:THR:HG21	1.76	0.66
2:CCC:663:VAL:O	2:CCC:666:SER:OG	2.13	0.66
5:FFF:259:ILE:HG21	5:FFF:280:LEU:HD21	1.77	0.66
5:FFF:143:SER:HB3	6:111:41:DT:H73	1.77	0.66
2:CCC:43:PRO:O	2:CCC:54:ARG:NH1	2.28	0.66
3:DDD:320:ASN:O	3:DDD:321:LYS:CB	2.44	0.66
2:CCC:201:ARG:HB2	2:CCC:369:MET:CE	2.27	0.65
7:222:17:DG:H2'	7:222:18:DT:C6	2.32	0.65
3:DDD:1023:HIS:O	3:DDD:1024:THR:HB	1.95	0.65
2:CCC:223:LEU:HD13	2:CCC:426:ILE:HD13	1.77	0.65
2:CCC:541:GLU:HG3	2:CCC:542:ARG:N	2.11	0.65
3:DDD:378:LYS:N	3:DDD:379:PRO:HD2	2.11	0.65
3:DDD:839:VAL:HG12	3:DDD:864:LEU:CD1	2.19	0.65
2:CCC:1284:ALA:HA	3:DDD:1357:ILE:CD1	2.26	0.65
2:CCC:1281:TYR:OH	3:DDD:431:ARG:O	2.15	0.65
3:DDD:1134:ILE:HG23	3:DDD:1138:LEU:HG	1.79	0.65
4:EEE:8:ASP:OD1	4:EEE:8:ASP:N	2.29	0.65
3:DDD:295:GLU:OE1	5:FFF:121:GLU:HG2	1.96	0.65
3:DDD:58:CYS:SG	3:DDD:60:ARG:HB3	2.37	0.65
2:CCC:263:VAL:CG1	2:CCC:269:ILE:HD11	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:12:ARG:NH2	2:CCC:793:GLU:OE1	2.29	0.64
1:BBB:86:LYS:HE2	1:BBB:174:ASP:H	1.62	0.64
2:CCC:263:VAL:HG13	2:CCC:269:ILE:HD11	1.80	0.64
3:DDD:792:ASN:N	3:DDD:792:ASN:OD1	2.28	0.64
6:111:50:DT:H2"	6:111:51:DC:H5"	1.79	0.64
2:CCC:262:TYR:OH	2:CCC:280:ASP:OD2	2.15	0.64
2:CCC:1294:LYS:HB3	3:DDD:347:VAL:HG13	1.78	0.64
2:CCC:1237:HIS:HB3	2:CCC:1242:LYS:NZ	2.13	0.64
5:FFF:180:ARG:NH2	7:222:27:DA:H5"	2.12	0.64
3:DDD:929:GLN:O	3:DDD:933:ARG:HB2	1.98	0.64
3:DDD:807:LEU:CD2	3:DDD:1255:VAL:HG13	2.27	0.64
1:AAA:211:ILE:CG2	1:AAA:216:ALA:HB2	2.27	0.64
3:DDD:975:ILE:CD1	3:DDD:997:VAL:HG11	2.28	0.64
5:FFF:228:GLY:HA3	8:333:14:G:C8	2.33	0.64
3:DDD:114:ILE:HG12	3:DDD:311:ARG:HD2	1.79	0.63
1:AAA:37:HIS:NE2	1:AAA:187:VAL:HG21	2.14	0.63
3:DDD:525:MET:H	3:DDD:548:VAL:HG22	1.64	0.63
3:DDD:48:THR:O	3:DDD:50:LYS:N	2.30	0.63
2:CCC:342:ASP:O	2:CCC:437:ASN:ND2	2.32	0.63
3:DDD:392:THR:HG21	5:FFF:320:GLN:C	2.17	0.63
3:DDD:839:VAL:CG1	3:DDD:864:LEU:HD12	2.20	0.63
1:AAA:32:GLU:OE2	1:BBB:150:ARG:NH2	2.32	0.62
3:DDD:97:VAL:HG12	3:DDD:101:ARG:HG3	1.81	0.62
3:DDD:1161:GLY:HA3	3:DDD:1179:PRO:HA	1.81	0.62
2:CCC:529:ARG:NH2	8:333:15:A:O3'	2.32	0.62
1:BBB:58:GLU:OE1	1:BBB:170:ARG:NE	2.26	0.62
2:CCC:1291:LEU:HA	3:DDD:345:LYS:HD2	1.81	0.62
3:DDD:836:ARG:HD3	3:DDD:873:GLU:OE2	1.99	0.62
3:DDD:886:VAL:HG21	3:DDD:1230:THR:HG21	1.80	0.62
5:FFF:66:GLY:HA3	6:111:42:DG:C5	2.34	0.62
2:CCC:898:GLU:HG3	5:FFF:259:ILE:CD1	2.29	0.62
1:BBB:67:GLU:CB	1:BBB:171:LEU:HD22	2.23	0.62
2:CCC:524:ILE:O	2:CCC:528:ARG:HG2	1.99	0.62
3:DDD:1338:ALA:HB3	3:DDD:1340:LYS:HG3	1.81	0.62
3:DDD:510:LEU:HD11	3:DDD:624:ILE:HG23	1.81	0.62
1:BBB:30:PRO:HB2	1:BBB:198:LEU:HD12	1.80	0.62
3:DDD:845:ALA:O	3:DDD:881:LYS:CD	2.47	0.62
3:DDD:975:ILE:HD12	3:DDD:997:VAL:HG11	1.80	0.62
3:DDD:395:LYS:HG2	5:FFF:329:LEU:CD1	2.28	0.62
2:CCC:184:LEU:HG	2:CCC:389:PHE:CE2	2.35	0.62
3:DDD:139:LEU:HD22	3:DDD:300:GLN:HE22	1.63	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:822:MET:HE3	3:DDD:839:VAL:HG22	1.80	0.62
3:DDD:320:ASN:O	3:DDD:321:LYS:HB2	1.99	0.62
2:CCC:577:VAL:HG23	2:CCC:661:VAL:O	1.99	0.61
3:DDD:97:VAL:HG11	3:DDD:101:ARG:HE	1.65	0.61
2:CCC:157:PHE:O	2:CCC:442:VAL:HG13	2.00	0.61
2:CCC:901:LEU:HD12	5:FFF:310:LEU:HD21	1.81	0.61
3:DDD:22:ILE:CD1	3:DDD:1319:PHE:CE1	2.83	0.61
3:DDD:936:HIS:CE1	11:DDD:1504:DPO:O2	2.52	0.61
3:DDD:458:ASN:OD1	3:DDD:933:ARG:NH2	2.31	0.61
1:AAA:67:GLU:HB3	1:AAA:171:LEU:HD13	1.82	0.61
2:CCC:1129:ASN:HA	2:CCC:1177:ARG:HG3	1.81	0.61
2:CCC:241:LEU:HD13	2:CCC:285:ILE:HD12	1.82	0.61
3:DDD:43:THR:OG1	3:DDD:44:ILE:N	2.33	0.61
1:AAA:212:ASP:OD1	1:AAA:213:PRO:HD2	2.01	0.61
2:CCC:559:CYS:HB2	2:CCC:662:SER:HB3	1.83	0.61
2:CCC:1101:LEU:HD22	3:DDD:731:ARG:HB2	1.82	0.61
2:CCC:1073:LYS:NZ	8:333:18:C:OP1	2.32	0.61
5:FFF:227:GLY:O	5:FFF:229:ASP:N	2.33	0.61
3:DDD:845:ALA:O	3:DDD:881:LYS:CB	2.48	0.61
1:BBB:37:HIS:NE2	1:BBB:187:VAL:HG21	2.15	0.61
3:DDD:334:LYS:O	3:DDD:339:ARG:HB2	2.01	0.61
3:DDD:843:VAL:HG11	3:DDD:883:ARG:CD	2.29	0.61
3:DDD:291:ILE:HD11	5:FFF:99:LEU:HD21	1.82	0.61
2:CCC:19:PRO:HA	2:CCC:1156:ARG:HD2	1.83	0.61
2:CCC:389:PHE:HB3	2:CCC:420:LEU:HD12	1.83	0.61
3:DDD:1275:LEU:HG	3:DDD:1276:GLU:H	1.66	0.61
1:AAA:86:LYS:NZ	2:CCC:826:ASP:OD2	2.34	0.60
2:CCC:642:SER:CB	3:DDD:770:LEU:HD21	2.31	0.60
1:BBB:82:LEU:HD22	1:BBB:173:VAL:CG2	2.31	0.60
4:EEE:30:MET:HG2	4:EEE:35:LYS:O	2.01	0.60
2:CCC:201:ARG:HB2	2:CCC:369:MET:HE2	1.82	0.60
3:DDD:800:LEU:HD23	3:DDD:1309:ILE:CD1	2.31	0.60
2:CCC:447:HIS:CD2	2:CCC:449:GLY:H	2.20	0.60
2:CCC:118:LYS:HD3	2:CCC:488:MET:HG2	1.83	0.60
3:DDD:816:THR:HG22	3:DDD:818:GLU:H	1.65	0.60
3:DDD:824:PRO:HG3	3:DDD:878:ASP:OD1	2.02	0.60
1:AAA:11:PRO:O	1:BBB:230:ALA:HB2	2.02	0.60
1:BBB:157:THR:HG22	1:BBB:157:THR:O	2.02	0.60
3:DDD:362:ARG:N	3:DDD:365:GLN:OE1	2.24	0.60
3:DDD:609:TYR:HA	3:DDD:617:THR:HG21	1.84	0.60
2:CCC:414:ILE:HG13	2:CCC:415:GLU:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:548:ARG:HD3	2:CCC:569:ILE:O	2.01	0.60
3:DDD:750:PRO:HB3	3:DDD:781:LYS:HB2	1.83	0.60
2:CCC:3:TYR:O	2:CCC:8:LYS:CE	2.49	0.60
1:BBB:48:LEU:HD22	3:DDD:535:ARG:HG3	1.83	0.60
3:DDD:839:VAL:HG13	3:DDD:882:VAL:HG11	1.84	0.60
2:CCC:289:VAL:HG12	2:CCC:319:LEU:HD23	1.83	0.60
3:DDD:1003:LEU:HD23	3:DDD:1018:ALA:HB2	1.84	0.60
2:CCC:1210:ILE:HD12	2:CCC:1227:VAL:HB	1.83	0.59
3:DDD:519:ASN:HA	3:DDD:523:GLU:CD	2.22	0.59
3:DDD:826:ILE:HG22	3:DDD:831:VAL:HA	1.84	0.59
6:111:31:DT:H1'	6:111:32:DA:H5'	1.84	0.59
2:CCC:369:MET:HG3	2:CCC:370:MET:N	2.16	0.59
3:DDD:849:LEU:HA	3:DDD:857:LEU:HB3	1.83	0.59
2:CCC:734:ILE:HD11	2:CCC:777:VAL:HG23	1.85	0.59
2:CCC:292:ILE:CG2	2:CCC:322:LEU:HD11	2.32	0.59
3:DDD:245:LEU:HD12	3:DDD:246:PRO:HD2	1.83	0.59
3:DDD:825:VAL:HG11	3:DDD:1242:ARG:HH12	1.65	0.59
1:AAA:45:ARG:NH2	1:BBB:37:HIS:HB2	2.17	0.59
1:BBB:82:LEU:HB3	1:BBB:173:VAL:CG1	2.32	0.59
3:DDD:1330:ARG:NH2	7:222:7:DC:O3'	2.34	0.59
3:DDD:385:LEU:CD2	3:DDD:411:ILE:HD13	2.31	0.59
3:DDD:1282:TYR:CE1	3:DDD:1286:LYS:HD2	2.38	0.59
1:AAA:30:PRO:HB2	1:AAA:198:LEU:HD12	1.84	0.59
2:CCC:244:GLU:HG2	2:CCC:245:ARG:H	1.66	0.59
2:CCC:49:LEU:CD2	2:CCC:464:PHE:CE2	2.86	0.59
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:HG	2.32	0.59
5:FFF:98:ASN:HA	6:111:41:DT:O2	2.02	0.58
2:CCC:297:VAL:HG13	2:CCC:317:LEU:HG	1.85	0.58
3:DDD:843:VAL:HG12	3:DDD:883:ARG:HB3	1.60	0.58
5:FFF:292:GLY:HA2	5:FFF:297:LEU:H	1.68	0.58
2:CCC:582:ASN:OD1	2:CCC:586:PHE:N	2.35	0.58
3:DDD:1000:GLY:HA2	3:DDD:1028:ILE:HD12	1.84	0.58
3:DDD:514:THR:OG1	3:DDD:595:ALA:HA	2.03	0.58
1:BBB:135:ASP:OD1	1:BBB:138:ALA:HB2	2.03	0.58
2:CCC:1214:ASP:OD2	2:CCC:1217:THR:HG23	2.03	0.58
2:CCC:1270:PHE:CE1	2:CCC:1290:MET:CE	2.87	0.58
3:DDD:1134:ILE:HD11	3:DDD:1244:GLN:HG3	1.86	0.58
3:DDD:68:TYR:CD2	3:DDD:78:LEU:HD23	2.38	0.58
2:CCC:672:GLU:HG2	2:CCC:1187:PHE:HA	1.85	0.58
3:DDD:1309:ILE:HG22	3:DDD:1310:THR:N	2.19	0.58
2:CCC:993:PRO:HG2	2:CCC:996:ARG:CZ	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:183:TRP:CZ3	6:111:52:DT:H71	2.39	0.58
4:EEE:53:GLU:HB3	4:EEE:59:ILE:HG12	1.86	0.58
3:DDD:1330:ARG:NH2	7:222:8:DG:OP1	2.37	0.58
1:BBB:176:CYS:HB3	3:DDD:535:ARG:NH2	2.16	0.58
1:BBB:47:LEU:HD13	1:BBB:205:MET:HE2	1.86	0.58
3:DDD:609:TYR:HA	3:DDD:617:THR:CG2	2.34	0.58
5:FFF:170:HIS:CE1	6:111:31:DT:C5	2.92	0.58
2:CCC:748:ILE:HD11	2:CCC:970:GLY:HA3	1.85	0.57
5:FFF:109:TYR:CD2	5:FFF:154:ILE:HG21	2.39	0.57
1:AAA:86:LYS:HD3	1:AAA:174:ASP:HB2	1.86	0.57
3:DDD:211:GLU:HG2	3:DDD:212:THR:HG23	1.86	0.57
3:DDD:843:VAL:HG11	3:DDD:883:ARG:HD3	1.85	0.57
5:FFF:144:THR:HG22	6:111:39:DA:C8	2.39	0.57
2:CCC:1077:SER:HA	3:DDD:356:THR:HG21	1.85	0.57
2:CCC:36:GLN:O	2:CCC:40:GLU:HB2	2.04	0.57
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:HD11	1.86	0.57
2:CCC:599:VAL:HG21	2:CCC:623:LEU:HD21	1.86	0.57
2:CCC:666:SER:HA	2:CCC:1186:VAL:HG21	1.86	0.57
3:DDD:176:PHE:O	3:DDD:176:PHE:CD2	2.57	0.57
3:DDD:797:THR:O	3:DDD:801:VAL:HG23	2.05	0.57
2:CCC:901:LEU:HD11	5:FFF:310:LEU:CD2	2.33	0.57
5:FFF:61:TYR:CZ	5:FFF:65:ILE:HD11	2.39	0.57
2:CCC:734:ILE:CG2	2:CCC:749:ASP:HB2	2.34	0.57
5:FFF:244:ASN:N	5:FFF:244:ASN:OD1	2.37	0.57
3:DDD:16:GLU:OE2	3:DDD:1369:ARG:NH2	2.38	0.57
3:DDD:527:LEU:HB2	3:DDD:550:VAL:HG13	1.87	0.57
5:FFF:82:ARG:HG2	5:FFF:87:ASP:HB2	1.86	0.57
3:DDD:1042:ASP:OD1	3:DDD:1043:GLY:N	2.37	0.57
3:DDD:1134:ILE:CD1	3:DDD:1244:GLN:HG3	2.35	0.57
3:DDD:803:VAL:CG2	3:DDD:1313:SER:OG	2.53	0.57
5:FFF:271:ARG:O	5:FFF:271:ARG:HG2	2.04	0.57
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:CD	2.35	0.57
2:CCC:1161:LEU:HD12	2:CCC:1164:PHE:CD2	2.40	0.57
3:DDD:673:VAL:HG11	3:DDD:678:ARG:HB2	1.84	0.57
3:DDD:1110:GLU:O	3:DDD:1113:VAL:HG23	2.04	0.57
2:CCC:263:VAL:HG22	2:CCC:269:ILE:HD12	1.87	0.56
2:CCC:736:VAL:HB	2:CCC:741:MET:HE2	1.87	0.56
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:HD11	1.86	0.56
1:AAA:135:ASP:OD1	1:AAA:137:ASN:N	2.37	0.56
1:AAA:145:LYS:HD3	1:AAA:147:GLN:HE21	1.70	0.56
5:FFF:227:GLY:O	8:333:14:G:N7	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:302:ILE:HG22	2:CCC:309:LEU:HD23	1.86	0.56
3:DDD:385:LEU:HD23	3:DDD:411:ILE:HD13	1.87	0.56
3:DDD:707:ILE:HD12	3:DDD:716:GLN:HE21	1.70	0.56
5:FFF:53:ARG:O	5:FFF:55:LEU:HG	2.05	0.56
1:BBB:86:LYS:HG2	1:BBB:174:ASP:O	2.06	0.56
3:DDD:820:ILE:HG12	3:DDD:1227:HIS:HD2	1.70	0.56
3:DDD:1257:VAL:HG22	3:DDD:1260:MET:CE	2.36	0.56
3:DDD:343:LEU:HD11	3:DDD:1324:SER:HB2	1.88	0.56
1:BBB:158:ARG:HD2	1:BBB:172:LEU:HD21	1.88	0.56
2:CCC:1105:SER:HB3	3:DDD:731:ARG:HG3	1.88	0.56
2:CCC:150:HIS:CE1	2:CCC:454:ARG:HG3	2.41	0.56
2:CCC:685:MET:HE2	2:CCC:1235:LEU:HD11	1.87	0.56
3:DDD:843:VAL:CG1	3:DDD:883:ARG:H	2.12	0.56
7:222:17:DG:H2''	7:222:18:DT:O4'	2.03	0.56
2:CCC:340:ASP:HB3	2:CCC:341:LEU:HG	1.88	0.56
2:CCC:528:ARG:HD2	2:CCC:663:VAL:HG21	1.88	0.56
3:DDD:850:LYS:HB2	3:DDD:851:PRO:HD2	1.87	0.56
5:FFF:61:TYR:CE2	5:FFF:65:ILE:HD11	2.41	0.56
5:FFF:170:HIS:NE2	6:111:31:DT:H2'	2.21	0.56
1:AAA:11:PRO:HD3	1:BBB:227:GLN:NE2	2.21	0.56
1:AAA:42:ALA:HA	1:BBB:38:THR:HG23	1.88	0.56
2:CCC:292:ILE:HB	2:CCC:322:LEU:HD11	1.88	0.56
2:CCC:516:ASP:O	2:CCC:522:SER:OG	2.18	0.55
3:DDD:112:ALA:H	3:DDD:300:GLN:HE21	1.54	0.55
3:DDD:399:LYS:HE3	5:FFF:329:LEU:HD11	1.89	0.55
2:CCC:1283:ALA:HB1	2:CCC:1286:THR:OG1	2.07	0.55
3:DDD:950:ILE:HD13	3:DDD:995:TYR:HB3	1.89	0.55
1:AAA:22:THR:OG1	1:AAA:207:THR:O	2.21	0.55
2:CCC:731:ARG:NH2	2:CCC:962:GLU:OE1	2.39	0.55
1:AAA:209:GLY:O	1:AAA:210:THR:C	2.44	0.55
1:AAA:179:PRO:HG3	1:AAA:211:ILE:CD1	2.37	0.55
3:DDD:1156:LEU:HB3	3:DDD:1207:GLY:HA2	1.86	0.55
3:DDD:608:CYS:SG	3:DDD:612:LEU:HD12	2.46	0.55
3:DDD:750:PRO:CA	3:DDD:781:LYS:HG2	2.28	0.55
4:EEE:29:GLN:HB3	4:EEE:35:LYS:HG3	1.88	0.55
1:AAA:135:ASP:OD1	1:AAA:136:GLU:N	2.39	0.55
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CZ	2.42	0.55
3:DDD:367:GLY:HA3	3:DDD:448:GLN:HB2	1.87	0.55
1:BBB:44:ARG:HH12	3:DDD:538:ARG:HB3	1.72	0.55
5:FFF:122:GLU:HG2	5:FFF:157:ALA:HB2	1.88	0.55
5:FFF:298:THR:HG21	5:FFF:301:ARG:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:124:VAL:HG21	1:AAA:210:THR:H	1.72	0.55
2:CCC:726:TYR:HB3	2:CCC:733:VAL:HG23	1.87	0.55
1:BBB:145:LYS:HD3	1:BBB:147:GLN:HE21	1.70	0.55
3:DDD:295:GLU:CD	5:FFF:121:GLU:HG2	2.27	0.55
1:BBB:92:VAL:O	1:BBB:148:ARG:NH2	2.40	0.55
2:CCC:369:MET:CG	2:CCC:370:MET:N	2.69	0.55
2:CCC:1287:LEU:HD23	3:DDD:1357:ILE:CD1	2.36	0.55
3:DDD:709:ARG:O	3:DDD:709:ARG:CG	2.55	0.55
5:FFF:145:TYR:HE1	6:111:36:DT:OP2	1.90	0.55
2:CCC:1160:ASP:O	2:CCC:1161:LEU:C	2.45	0.55
2:CCC:582:ASN:ND2	2:CCC:586:PHE:HB2	2.21	0.55
3:DDD:334:LYS:NZ	7:222:12:DG:OP2	2.36	0.55
1:AAA:211:ILE:HG21	1:AAA:216:ALA:HB2	1.87	0.54
2:CCC:532:ALA:HB1	2:CCC:538:LEU:HD12	1.90	0.54
3:DDD:68:TYR:C	3:DDD:92:VAL:HG13	2.28	0.54
1:BBB:86:LYS:CE	1:BBB:174:ASP:HB2	2.37	0.54
2:CCC:253:PHE:CE1	2:CCC:287:VAL:HG12	2.42	0.54
3:DDD:709:ARG:O	3:DDD:710:ASP:C	2.45	0.54
3:DDD:800:LEU:CD2	3:DDD:1309:ILE:HD11	2.36	0.54
3:DDD:620:PHE:O	3:DDD:624:ILE:HG13	2.08	0.54
3:DDD:1163:VAL:HG13	3:DDD:1176:VAL:O	2.06	0.54
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:HD11	2.38	0.54
2:CCC:240:GLU:HA	2:CCC:283:LYS:O	2.08	0.54
1:AAA:86:LYS:HE2	1:AAA:174:ASP:H	1.73	0.54
3:DDD:1133:ASP:CG	3:DDD:1134:ILE:H	2.10	0.54
2:CCC:545:PHE:CE1	3:DDD:788:LEU:HD12	2.42	0.54
3:DDD:807:LEU:HD23	3:DDD:1255:VAL:HG13	1.90	0.54
3:DDD:335:GLN:O	3:DDD:336:GLY:O	2.26	0.54
3:DDD:609:TYR:CA	3:DDD:617:THR:HG21	2.37	0.54
4:EEE:29:GLN:HE22	4:EEE:64:LEU:HD22	1.72	0.54
1:AAA:11:PRO:O	1:BBB:230:ALA:CB	2.56	0.53
2:CCC:739:ASP:N	2:CCC:739:ASP:OD1	2.41	0.53
2:CCC:549:ASP:CG	3:DDD:750:PRO:HG3	2.29	0.53
2:CCC:661:VAL:HG13	2:CCC:665:ALA:HB3	1.89	0.53
3:DDD:574:VAL:O	3:DDD:578:ILE:HG13	2.08	0.53
2:CCC:1255:THR:HG21	3:DDD:341:ASN:CG	2.28	0.53
2:CCC:1304:MET:HE1	3:DDD:472:LEU:CD1	2.35	0.53
2:CCC:257:ALA:O	2:CCC:258:ASN:HB3	2.09	0.53
2:CCC:820:GLU:O	2:CCC:824:GLN:HG3	2.08	0.53
3:DDD:923:ILE:HD12	3:DDD:1256:ILE:HD12	1.90	0.53
2:CCC:720:ARG:HD2	2:CCC:736:VAL:HG21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:974:VAL:HG11	3:DDD:1028:ILE:HD13	1.91	0.53
1:AAA:70:THR:HG21	2:CCC:755:LYS:HG3	1.90	0.53
3:DDD:965:SER:CB	3:DDD:975:ILE:HA	2.37	0.53
2:CCC:1186:VAL:HG12	2:CCC:1187:PHE:CD2	2.42	0.53
2:CCC:123:TYR:CE1	5:FFF:190:ASP:O	2.61	0.53
2:CCC:726:TYR:HB3	2:CCC:733:VAL:HG22	1.89	0.53
3:DDD:795:TYR:CZ	3:DDD:799:ARG:HD3	2.43	0.53
1:AAA:179:PRO:HG3	1:AAA:211:ILE:HD12	1.91	0.53
1:AAA:31:LEU:CD1	1:AAA:201:LEU:HB2	2.38	0.53
2:CCC:216:THR:HG23	2:CCC:219:GLN:OE1	2.08	0.53
3:DDD:886:VAL:HG21	3:DDD:1230:THR:CG2	2.39	0.53
3:DDD:888:CYS:CB	3:DDD:898:CYS:SG	2.97	0.53
2:CCC:444:ASP:O	2:CCC:450:ASN:ND2	2.40	0.53
2:CCC:478:ARG:NH1	2:CCC:491:ASP:O	2.42	0.53
2:CCC:734:ILE:HD11	2:CCC:777:VAL:CG2	2.38	0.53
3:DDD:476:ALA:HA	3:DDD:479:GLU:HG3	1.90	0.53
3:DDD:686:TRP:CD2	3:DDD:758:PRO:HG3	2.43	0.53
2:CCC:1101:LEU:O	3:DDD:731:ARG:HG2	2.08	0.53
3:DDD:97:VAL:HG11	3:DDD:101:ARG:NE	2.23	0.53
5:FFF:80:ALA:O	5:FFF:84:LEU:HG	2.09	0.53
3:DDD:1257:VAL:HG22	3:DDD:1260:MET:HE3	1.91	0.53
5:FFF:231:GLU:OE2	7:222:16:DC:N4	2.42	0.53
1:AAA:47:LEU:HD13	1:AAA:183:ILE:HD12	1.92	0.52
3:DDD:1270:GLY:HA2	3:DDD:1298:VAL:O	2.09	0.52
3:DDD:209:ASN:HB2	3:DDD:214:ARG:HG3	1.91	0.52
3:DDD:812:ASP:N	3:DDD:812:ASP:OD1	2.40	0.52
3:DDD:63:GLY:O	3:DDD:98:ARG:HD2	2.09	0.52
3:DDD:829:GLY:HA2	3:DDD:993:GLU:CB	2.37	0.52
2:CCC:1243:MET:SD	3:DDD:445:LYS:HG2	2.50	0.52
5:FFF:119:LEU:CD2	5:FFF:158:ILE:HD11	2.38	0.52
1:AAA:29:GLU:HB2	1:AAA:30:PRO:HA	1.91	0.52
3:DDD:478:LEU:HG	4:EEE:47:THR:HG23	1.91	0.52
3:DDD:807:LEU:HD11	3:DDD:894:VAL:HG13	1.91	0.52
3:DDD:936:HIS:CE1	3:DDD:937:ILE:HG13	2.44	0.52
2:CCC:277:LEU:HD12	2:CCC:282:VAL:HG21	1.91	0.52
2:CCC:898:GLU:HG3	5:FFF:259:ILE:HD11	1.90	0.52
3:DDD:333:GLY:O	3:DDD:336:GLY:N	2.35	0.52
3:DDD:750:PRO:HA	3:DDD:781:LYS:CG	2.31	0.52
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD11	1.92	0.52
3:DDD:427:PRO:HG2	3:DDD:429:LEU:HD21	1.89	0.52
2:CCC:155:VAL:CG2	2:CCC:405:PHE:CD2	2.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:464:ASP:OD1	3:DDD:464:ASP:N	2.42	0.52
3:DDD:933:ARG:NH1	11:DDD:1504:DPO:O1	2.43	0.52
4:EEE:18:ASP:O	4:EEE:22:VAL:HG23	2.10	0.52
5:FFF:240:ASP:OD1	5:FFF:242:LYS:HG2	2.10	0.52
1:BBB:64:VAL:HG13	1:BBB:78:ILE:HD13	1.92	0.52
3:DDD:294:ASN:HB2	5:FFF:61:TYR:CD1	2.45	0.52
3:DDD:51:PRO:HB3	3:DDD:57:PHE:O	2.10	0.52
1:AAA:70:THR:OG1	2:CCC:729:ALA:O	2.17	0.52
2:CCC:808:ASN:N	2:CCC:808:ASN:HD22	2.06	0.52
3:DDD:1292:LEU:O	3:DDD:1296:GLY:N	2.36	0.52
3:DDD:278:ARG:HB3	3:DDD:295:GLU:OE2	2.10	0.52
3:DDD:821:MET:CE	3:DDD:879:ALA:HB1	2.40	0.52
2:CCC:1214:ASP:C	2:CCC:1214:ASP:OD1	2.49	0.52
2:CCC:89:GLY:HA2	2:CCC:140:GLY:HA3	1.92	0.52
3:DDD:707:ILE:HD12	3:DDD:716:GLN:NE2	2.25	0.52
2:CCC:366:ILE:O	2:CCC:369:MET:HG2	2.09	0.51
3:DDD:279:LEU:HD13	3:DDD:295:GLU:HB3	1.91	0.51
3:DDD:622:ASP:HB3	3:DDD:626:TYR:HE2	1.75	0.51
3:DDD:786:THR:HB	3:DDD:932:MET:HA	1.92	0.51
3:DDD:115:TRP:CZ2	3:DDD:1329:THR:HG22	2.45	0.51
3:DDD:889:ASP:OD1	3:DDD:1290:ARG:NH2	2.43	0.51
3:DDD:111:THR:HG21	3:DDD:303:VAL:HG11	1.92	0.51
3:DDD:1249:ASN:OD1	3:DDD:1250:ASP:N	2.43	0.51
3:DDD:97:VAL:CG1	3:DDD:101:ARG:HE	2.23	0.51
2:CCC:166:SER:OG	3:DDD:1151:LYS:NZ	2.38	0.51
2:CCC:661:VAL:HG12	2:CCC:662:SER:O	2.10	0.51
3:DDD:97:VAL:CG1	3:DDD:101:ARG:HG3	2.41	0.51
3:DDD:134:ASP:CB	3:DDD:159:ILE:HD11	2.41	0.51
2:CCC:555:TYR:CE1	2:CCC:637:ARG:CZ	2.94	0.51
3:DDD:121:PRO:O	3:DDD:122:SER:CB	2.51	0.51
3:DDD:517:CYS:HB3	3:DDD:545:HIS:HB2	1.91	0.51
2:CCC:477:GLU:HG3	2:CCC:478:ARG:N	2.24	0.51
2:CCC:496:LYS:CB	7:222:24:DT:OP1	2.58	0.51
2:CCC:521:LEU:HD13	2:CCC:667:LEU:HD11	1.93	0.51
3:DDD:1146:GLU:OE2	3:DDD:1309:ILE:CG2	2.58	0.51
2:CCC:799:ASN:HA	2:CCC:1231:TYR:HA	1.92	0.51
3:DDD:1155:ILE:HG22	3:DDD:1210:ILE:HD12	1.93	0.51
3:DDD:803:VAL:HG23	3:DDD:1313:SER:OG	2.11	0.51
3:DDD:395:LYS:HE3	5:FFF:251:GLN:OE1	2.11	0.51
3:DDD:809:VAL:CG2	3:DDD:915:ILE:HD11	2.41	0.51
3:DDD:974:VAL:CG1	3:DDD:1028:ILE:HD13	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:421:VAL:CG1	3:DDD:468:VAL:HG13	2.41	0.51
5:FFF:102:VAL:HG11	5:FFF:124:ASN:OD1	2.11	0.51
5:FFF:107:ARG:HD2	6:111:44:DG:OP2	2.10	0.51
1:AAA:50:SER:HG	1:BBB:35:PHE:HZ	1.57	0.51
2:CCC:290:GLU:HG2	2:CCC:290:GLU:O	2.10	0.51
2:CCC:1276:TRP:CH2	3:DDD:798:ARG:HG3	2.46	0.51
1:BBB:165:GLU:O	1:BBB:165:GLU:HG3	2.10	0.51
2:CCC:551:HIS:H	2:CCC:554:HIS:CE1	2.28	0.51
2:CCC:590:PRO:HB2	2:CCC:655:VAL:HG21	1.91	0.51
2:CCC:797:GLY:O	2:CCC:1231:TYR:OH	2.29	0.51
2:CCC:1161:LEU:HD12	2:CCC:1164:PHE:CE2	2.46	0.50
2:CCC:302:ILE:CG2	2:CCC:309:LEU:HD23	2.41	0.50
2:CCC:521:LEU:HD13	2:CCC:667:LEU:CD1	2.41	0.50
3:DDD:1064:SER:HA	3:DDD:1067:ARG:HB3	1.93	0.50
3:DDD:1079:LYS:HE3	3:DDD:1087:ASP:OD1	2.10	0.50
2:CCC:1291:LEU:HD13	3:DDD:1351:VAL:O	2.11	0.50
3:DDD:785:ASP:HB3	3:DDD:935:PHE:CE2	2.45	0.50
3:DDD:395:LYS:HE2	5:FFF:329:LEU:HD13	1.93	0.50
2:CCC:1107:MET:HE3	3:DDD:739:GLN:HB2	1.93	0.50
2:CCC:700:VAL:HG13	2:CCC:1117:LEU:HD23	1.92	0.50
5:FFF:104:LYS:HE3	6:111:42:DG:OP1	2.11	0.50
2:CCC:842:ASP:HB3	2:CCC:1047:LEU:HD21	1.93	0.50
1:BBB:124:VAL:HG21	1:BBB:210:THR:CG2	2.37	0.50
3:DDD:845:ALA:O	3:DDD:881:LYS:HG2	2.11	0.50
5:FFF:259:ILE:CG2	5:FFF:280:LEU:HD21	2.41	0.50
3:DDD:1082:ASP:OD1	3:DDD:1084:GLN:N	2.44	0.50
3:DDD:279:LEU:O	3:DDD:283:LEU:HG	2.11	0.50
2:CCC:1161:LEU:O	2:CCC:1163:THR:N	2.45	0.50
2:CCC:1292:THR:CG2	2:CCC:1293:VAL:N	2.74	0.50
2:CCC:344:GLY:HA3	2:CCC:346:TYR:CE2	2.46	0.50
2:CCC:66:SER:HB2	2:CCC:479:LEU:HD22	1.94	0.50
3:DDD:97:VAL:CG1	3:DDD:101:ARG:NE	2.75	0.50
1:AAA:222:THR:CG2	1:BBB:233:ASP:HB3	2.42	0.50
1:BBB:29:GLU:HB2	1:BBB:30:PRO:HA	1.92	0.50
3:DDD:101:ARG:O	3:DDD:246:PRO:HG3	2.12	0.50
5:FFF:170:HIS:H	5:FFF:170:HIS:CD2	2.30	0.50
2:CCC:1286:THR:HG23	3:DDD:476:ALA:HB1	1.93	0.49
3:DDD:1133:ASP:CG	3:DDD:1134:ILE:N	2.66	0.49
3:DDD:1368:ASP:O	3:DDD:1371:ARG:HG2	2.12	0.49
3:DDD:68:TYR:CE1	3:DDD:93:THR:HA	2.47	0.49
2:CCC:183:TRP:CZ3	6:111:51:DC:C2'	2.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:211:ILE:HG22	1:AAA:216:ALA:HB2	1.93	0.49
2:CCC:1237:HIS:HB3	2:CCC:1242:LYS:CE	2.41	0.49
3:DDD:1052:GLU:HG2	3:DDD:1053:LEU:H	1.77	0.49
3:DDD:925:GLU:HB3	3:DDD:926:PRO:HD3	1.94	0.49
5:FFF:182:ALA:CB	5:FFF:193:PRO:HG3	2.40	0.49
5:FFF:79:PHE:O	5:FFF:90:SER:OG	2.27	0.49
1:BBB:212:ASP:OD1	1:BBB:213:PRO:HD2	2.10	0.49
2:CCC:1312:ASN:O	2:CCC:1312:ASN:OD1	2.29	0.49
3:DDD:1029:THR:HG22	3:DDD:1121:LEU:CD1	2.42	0.49
5:FFF:78:TYR:OH	5:FFF:82:ARG:NH1	2.45	0.49
2:CCC:1273:MET:HG3	7:222:12:DG:H4'	1.95	0.49
2:CCC:1210:ILE:HG22	2:CCC:1211:ARG:N	2.27	0.49
2:CCC:555:TYR:CD1	2:CCC:637:ARG:CZ	2.96	0.49
1:BBB:179:PRO:HG3	1:BBB:211:ILE:CD1	2.35	0.49
1:BBB:192:VAL:O	1:BBB:194:GLN:N	2.46	0.49
1:AAA:222:THR:OG1	1:BBB:233:ASP:HB3	2.08	0.49
2:CCC:296:VAL:HB	2:CCC:336:LEU:HD12	1.93	0.49
2:CCC:661:VAL:CG1	2:CCC:665:ALA:HB3	2.42	0.49
2:CCC:228:VAL:HG22	2:CCC:245:ARG:NH1	2.27	0.49
5:FFF:175:LEU:O	5:FFF:179:LEU:HG	2.13	0.49
1:AAA:154:PRO:HG2	1:AAA:157:THR:HB	1.94	0.49
2:CCC:13:LYS:NZ	2:CCC:1151:LEU:HB3	2.28	0.49
2:CCC:799:ASN:C	2:CCC:800:MET:HG2	2.32	0.49
2:CCC:993:PRO:HG2	2:CCC:996:ARG:NH1	2.28	0.49
3:DDD:807:LEU:HD22	3:DDD:1255:VAL:HG13	1.95	0.49
1:BBB:196:THR:HG21	3:DDD:370:LYS:NZ	2.27	0.49
5:FFF:176:ASN:HD22	7:222:27:DA:P	2.35	0.49
2:CCC:173:ASN:C	2:CCC:173:ASN:OD1	2.50	0.49
2:CCC:206:ALA:O	2:CCC:209:ILE:HG22	2.13	0.49
3:DDD:885:VAL:O	3:DDD:1258:ARG:HD2	2.12	0.49
1:AAA:124:VAL:HG11	1:AAA:209:GLY:CA	2.43	0.49
2:CCC:1001:GLY:HA2	2:CCC:1011:LEU:CD2	2.43	0.49
2:CCC:1099:ASN:OD1	2:CCC:1100:PRO:HD2	2.13	0.49
2:CCC:20:GLN:O	2:CCC:20:GLN:HG3	2.13	0.49
2:CCC:244:GLU:O	2:CCC:245:ARG:C	2.51	0.49
2:CCC:871:VAL:CG2	2:CCC:883:LEU:HA	2.43	0.49
3:DDD:1163:VAL:HG11	3:DDD:1175:LEU:HD11	1.94	0.49
1:BBB:29:GLU:CB	1:BBB:30:PRO:HA	2.43	0.48
2:CCC:1103:VAL:HB	2:CCC:1104:PRO:HD3	1.94	0.48
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:CD1	2.91	0.48
2:CCC:1101:LEU:HD13	3:DDD:504:GLN:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:943:ARG:HG2	3:DDD:944:ALA:N	2.28	0.48
4:EEE:17:PHE:O	4:EEE:21:LEU:HG	2.12	0.48
2:CCC:1274:GLU:HG2	3:DDD:424:ASN:ND2	2.28	0.48
2:CCC:155:VAL:HG23	2:CCC:405:PHE:CD2	2.48	0.48
3:DDD:1146:GLU:OE2	3:DDD:1309:ILE:HG22	2.12	0.48
5:FFF:169:ILE:O	5:FFF:173:LYS:HG2	2.13	0.48
5:FFF:287:THR:O	5:FFF:291:VAL:HG23	2.13	0.48
2:CCC:297:VAL:HG22	2:CCC:315:MET:O	2.13	0.48
2:CCC:685:MET:HE2	2:CCC:1235:LEU:CD1	2.42	0.48
3:DDD:803:VAL:HG21	3:DDD:1309:ILE:HA	1.94	0.48
3:DDD:572:THR:HG21	3:DDD:589:TYR:OH	2.13	0.48
5:FFF:292:GLY:HA2	5:FFF:297:LEU:N	2.28	0.48
2:CCC:32:LEU:HD23	2:CCC:130:MET:HE1	1.94	0.48
3:DDD:1041:ILE:CG2	3:DDD:1044:GLN:HG3	2.44	0.48
3:DDD:1238:GLN:O	3:DDD:1242:ARG:HB2	2.13	0.48
1:AAA:45:ARG:NH1	2:CCC:1216:ARG:HA	2.28	0.48
2:CCC:1291:LEU:CD1	3:DDD:1351:VAL:HG13	2.37	0.48
3:DDD:378:LYS:N	3:DDD:379:PRO:CD	2.77	0.48
3:DDD:364:HIS:HB3	3:DDD:487:THR:CG2	2.43	0.48
5:FFF:170:HIS:NE2	6:111:31:DT:C2'	2.77	0.48
7:222:22:DA:H3'	7:222:22:DA:OP1	2.14	0.48
2:CCC:44:GLU:HG3	2:CCC:45:GLY:H	1.78	0.48
2:CCC:473:ARG:O	2:CCC:477:GLU:HB3	2.13	0.48
3:DDD:1029:THR:CG2	3:DDD:1121:LEU:CG	2.91	0.48
3:DDD:500:ILE:HG22	3:DDD:500:ILE:O	2.13	0.48
3:DDD:883:ARG:HG2	3:DDD:898:CYS:HA	1.95	0.48
3:DDD:821:MET:HE3	3:DDD:879:ALA:HB1	1.93	0.48
3:DDD:1308:GLY:O	3:DDD:1310:THR:N	2.47	0.48
3:DDD:582:ILE:HG23	3:DDD:623:GLN:HB3	1.95	0.48
1:AAA:158:ARG:HD2	1:AAA:172:LEU:HD21	1.95	0.48
2:CCC:1099:ASN:ND2	3:DDD:504:GLN:HE21	2.11	0.48
3:DDD:108:ALA:HB3	3:DDD:279:LEU:HD23	1.96	0.48
3:DDD:120:LEU:HA	3:DDD:121:PRO:C	2.33	0.48
3:DDD:518:VAL:O	3:DDD:520:ALA:N	2.47	0.48
1:AAA:86:LYS:CE	1:AAA:174:ASP:HB2	2.43	0.48
1:BBB:47:LEU:HD13	1:BBB:183:ILE:HD12	1.96	0.48
2:CCC:1028:LYS:O	2:CCC:1032:LYS:HG2	2.13	0.48
2:CCC:839:VAL:HG13	2:CCC:1046:VAL:HG13	1.95	0.48
2:CCC:1083:GLU:H	2:CCC:1083:GLU:CD	2.17	0.48
3:DDD:1174:ARG:O	3:DDD:1176:VAL:HG23	2.14	0.48
5:FFF:178:TYR:CE1	5:FFF:209:VAL:HG22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:AAA:78:ILE:HG21	1:AAA:171:LEU:CD1	2.44	0.47
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CE1	2.49	0.47
2:CCC:1327:LEU:O	2:CCC:1331:ARG:HG3	2.14	0.47
2:CCC:201:ARG:HB2	2:CCC:369:MET:HE1	1.94	0.47
3:DDD:382:TYR:OH	3:DDD:398:LYS:HG2	2.14	0.47
1:AAA:190:ALA:O	1:AAA:192:VAL:N	2.47	0.47
2:CCC:615:VAL:HA	2:CCC:638:SER:HB3	1.97	0.47
3:DDD:487:THR:O	3:DDD:490:ILE:HG13	2.14	0.47
1:AAA:52:PRO:O	1:AAA:211:ILE:HD11	2.12	0.47
2:CCC:205:PRO:O	2:CCC:208:ILE:HG22	2.15	0.47
1:AAA:66:HIS:CE1	2:CCC:929:ILE:HG13	2.48	0.47
1:AAA:102:LEU:HB2	1:AAA:115:ILE:HG12	1.97	0.47
1:AAA:25:LYS:HG2	1:AAA:204:GLU:HG2	1.95	0.47
3:DDD:1037:PHE:CZ	3:DDD:1059:LEU:CD1	2.98	0.47
3:DDD:930:LEU:HD11	3:DDD:1246:VAL:HG21	1.92	0.47
3:DDD:490:ILE:HA	3:DDD:500:ILE:HD12	1.95	0.47
3:DDD:822:MET:HE1	3:DDD:882:VAL:HG21	1.95	0.47
1:AAA:32:GLU:CD	1:BBB:150:ARG:HH21	2.17	0.47
2:CCC:1081:PRO:HB2	2:CCC:1083:GLU:OE2	2.14	0.47
2:CCC:1111:GLN:HB2	2:CCC:1230:MET:HE1	1.96	0.47
2:CCC:854:ILE:HD11	2:CCC:885:GLY:HA3	1.96	0.47
3:DDD:965:SER:HB2	3:DDD:975:ILE:HA	1.97	0.47
5:FFF:144:THR:O	5:FFF:147:THR:OG1	2.32	0.47
2:CCC:201:ARG:CB	2:CCC:369:MET:HE2	2.45	0.47
2:CCC:453:ILE:HD11	2:CCC:530:ILE:HD13	1.96	0.47
3:DDD:115:TRP:O	3:DDD:119:SER:HB3	2.14	0.47
3:DDD:584:PRO:HD3	3:DDD:620:PHE:CD1	2.50	0.47
3:DDD:709:ARG:O	3:DDD:709:ARG:HG3	2.15	0.47
5:FFF:267:ASN:HB2	5:FFF:270:GLN:HB2	1.96	0.47
5:FFF:263:LEU:HD22	5:FFF:271:ARG:HB2	1.96	0.47
1:AAA:29:GLU:CB	1:AAA:30:PRO:HA	2.43	0.47
1:AAA:75:GLN:O	2:CCC:729:ALA:HB2	2.14	0.47
2:CCC:1100:PRO:HB3	3:DDD:639:VAL:HG23	1.97	0.47
2:CCC:150:HIS:HE1	2:CCC:452:ARG:HH11	1.62	0.47
1:AAA:152:TYR:CE2	2:CCC:824:GLN:HA	2.49	0.47
3:DDD:570:LYS:HE3	3:DDD:589:TYR:CD2	2.50	0.47
3:DDD:886:VAL:CG1	3:DDD:1226:VAL:CG1	2.93	0.47
5:FFF:119:LEU:HD21	5:FFF:158:ILE:HD11	1.96	0.47
5:FFF:170:HIS:CD2	6:111:31:DT:H2'	2.49	0.47
2:CCC:369:MET:HG2	2:CCC:370:MET:HG2	1.97	0.47
2:CCC:49:LEU:HD23	2:CCC:464:PHE:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1107:MET:CE	3:DDD:739:GLN:HB2	2.45	0.47
3:DDD:835:LEU:HD13	3:DDD:878:ASP:O	2.15	0.47
3:DDD:1111:ASP:OD1	3:DDD:1112:GLY:N	2.47	0.47
3:DDD:1263:LYS:CG	3:DDD:1307:LEU:HD11	2.45	0.47
3:DDD:519:ASN:HA	3:DDD:523:GLU:CG	2.45	0.47
2:CCC:676:ALA:HA	3:DDD:772:TYR:OH	2.15	0.47
2:CCC:677:ASN:OD1	3:DDD:779:ALA:HB1	2.14	0.47
2:CCC:1214:ASP:OD1	2:CCC:1215:GLY:N	2.47	0.47
2:CCC:263:VAL:HG12	2:CCC:264:GLU:O	2.15	0.47
2:CCC:848:GLU:OE1	2:CCC:886:LYS:HD3	2.15	0.47
5:FFF:109:TYR:OH	5:FFF:155:GLU:HG2	2.10	0.47
2:CCC:898:GLU:OE2	5:FFF:259:ILE:HD13	2.15	0.47
2:CCC:263:VAL:HG22	2:CCC:269:ILE:CD1	2.44	0.47
2:CCC:452:ARG:NH1	2:CCC:458:GLU:OE2	2.42	0.47
2:CCC:660:VAL:HG21	3:DDD:769:VAL:CG1	2.45	0.46
1:BBB:33:ARG:NH1	2:CCC:1081:PRO:HB3	2.30	0.46
2:CCC:1301:ARG:HG3	5:FFF:246:PRO:HG3	1.96	0.46
2:CCC:277:LEU:CD1	2:CCC:282:VAL:HG21	2.45	0.46
2:CCC:150:HIS:CE1	2:CCC:452:ARG:HD3	2.51	0.46
2:CCC:887:VAL:HB	2:CCC:913:VAL:HG12	1.97	0.46
3:DDD:1060:VAL:HG22	3:DDD:1106:ILE:HG12	1.97	0.46
3:DDD:1156:LEU:HD23	3:DDD:1209:VAL:HA	1.97	0.46
3:DDD:44:ILE:HG22	3:DDD:51:PRO:HA	1.96	0.46
3:DDD:552:ILE:CG2	3:DDD:580:TRP:CD1	2.98	0.46
3:DDD:795:TYR:CE2	3:DDD:799:ARG:NE	2.83	0.46
3:DDD:795:TYR:CE2	3:DDD:799:ARG:CZ	2.98	0.46
5:FFF:93:ARG:O	5:FFF:97:SER:OG	2.28	0.46
2:CCC:594:VAL:HG22	2:CCC:599:VAL:HG22	1.96	0.46
2:CCC:674:ASP:O	3:DDD:772:TYR:HE1	1.98	0.46
2:CCC:1272:GLU:OE1	3:DDD:339:ARG:HD3	2.14	0.46
3:DDD:645:VAL:O	3:DDD:645:VAL:HG23	2.16	0.46
3:DDD:844:THR:O	3:DDD:844:THR:OG1	2.33	0.46
3:DDD:925:GLU:OE1	3:DDD:926:PRO:N	2.48	0.46
1:BBB:152:TYR:CE2	3:DDD:536:LEU:HD21	2.50	0.46
2:CCC:1312:ASN:C	2:CCC:1312:ASN:OD1	2.54	0.46
2:CCC:144:VAL:HB	2:CCC:526:HIS:CE1	2.50	0.46
2:CCC:479:LEU:HD21	2:CCC:492:MET:HE1	1.98	0.46
2:CCC:49:LEU:HD22	2:CCC:464:PHE:CE2	2.50	0.46
3:DDD:114:ILE:HG23	3:DDD:115:TRP:N	2.29	0.46
3:DDD:1330:ARG:NH2	7:222:8:DG:P	2.89	0.46
3:DDD:1212:ASP:N	3:DDD:1212:ASP:OD1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:174:ASP:OD1	3:DDD:174:ASP:N	2.48	0.46
5:FFF:208:ASP:O	5:FFF:212:MET:HG2	2.15	0.46
2:CCC:207:THR:CG2	2:CCC:354:ASP:HB2	2.45	0.46
3:DDD:1169:THR:OG1	3:DDD:1174:ARG:NH2	2.49	0.46
3:DDD:664:ILE:HG21	3:DDD:681:LYS:HD3	1.98	0.46
3:DDD:739:GLN:HG2	3:DDD:744:ARG:HA	1.98	0.46
5:FFF:270:GLN:OE1	5:FFF:312:ARG:HD2	2.16	0.46
1:AAA:152:TYR:CZ	2:CCC:824:GLN:HA	2.50	0.46
2:CCC:543:ALA:HB3	2:CCC:548:ARG:HH21	1.81	0.46
2:CCC:598:VAL:HG13	2:CCC:627:GLY:HA2	1.97	0.46
1:BBB:50:SER:HA	1:BBB:150:ARG:HD2	1.97	0.46
2:CCC:244:GLU:O	2:CCC:247:ARG:HB2	2.16	0.46
2:CCC:524:ILE:HD12	2:CCC:708:VAL:HG13	1.98	0.46
3:DDD:161:THR:N	3:DDD:164:GLN:HB2	2.31	0.46
1:AAA:233:ASP:O	1:AAA:235:ARG:N	2.47	0.46
1:BBB:31:LEU:CD1	1:BBB:201:LEU:HB2	2.46	0.46
3:DDD:519:ASN:HA	3:DDD:523:GLU:OE2	2.15	0.46
3:DDD:622:ASP:HB3	3:DDD:626:TYR:CE2	2.50	0.46
3:DDD:622:ASP:O	3:DDD:626:TYR:CD2	2.69	0.46
3:DDD:960:LEU:HB3	3:DDD:963:VAL:HG11	1.98	0.46
2:CCC:850:ILE:O	2:CCC:850:ILE:HG22	2.16	0.46
3:DDD:198:CYS:SG	3:DDD:224:LEU:HB3	2.56	0.46
3:DDD:552:ILE:HG23	3:DDD:580:TRP:CD1	2.51	0.46
3:DDD:809:VAL:HG22	3:DDD:915:ILE:HD11	1.97	0.46
7:222:17:DG:H2'	7:222:18:DT:C1'	2.46	0.45
1:BBB:64:VAL:CG1	1:BBB:78:ILE:HD13	2.46	0.45
2:CCC:292:ILE:CB	2:CCC:322:LEU:HD11	2.46	0.45
2:CCC:53:PHE:HB3	2:CCC:70:TYR:CD2	2.51	0.45
2:CCC:720:ARG:HD3	2:CCC:736:VAL:HG11	1.98	0.45
2:CCC:736:VAL:O	2:CCC:741:MET:HE3	2.16	0.45
3:DDD:1262:ARG:CZ	3:DDD:1316:THR:HG22	2.46	0.45
3:DDD:325:LYS:HE2	3:DDD:330:MET:CG	2.46	0.45
5:FFF:176:ASN:OD1	7:222:26:DT:H73	2.16	0.45
5:FFF:180:ARG:HH22	7:222:27:DA:H5''	1.79	0.45
2:CCC:734:ILE:HG22	2:CCC:749:ASP:HB2	1.98	0.45
3:DDD:118:LYS:NZ	3:DDD:136:GLU:OE2	2.47	0.45
3:DDD:697:MET:SD	3:DDD:741:ALA:HB3	2.57	0.45
2:CCC:561:ILE:HG21	3:DDD:772:TYR:HE2	1.81	0.45
4:EEE:41:GLU:O	4:EEE:44:ASP:HB2	2.16	0.45
5:FFF:204:LYS:HB3	5:FFF:205:PRO:CD	2.47	0.45
2:CCC:183:TRP:CH2	6:111:52:DT:C7	2.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BBB:61:ILE:HG12	1:BBB:142:MET:HB3	1.99	0.45
2:CCC:870:ILE:HD12	2:CCC:1050:VAL:HG11	1.99	0.45
2:CCC:1117:LEU:HD13	2:CCC:1195:ILE:HG12	1.98	0.45
2:CCC:15:PHE:O	2:CCC:17:LYS:HE3	2.16	0.45
2:CCC:569:ILE:O	2:CCC:569:ILE:HG23	2.16	0.45
2:CCC:660:VAL:HG21	3:DDD:769:VAL:HG12	1.98	0.45
3:DDD:347:VAL:HG12	3:DDD:348:ASP:O	2.17	0.45
2:CCC:244:GLU:CG	2:CCC:245:ARG:N	2.78	0.45
2:CCC:510:GLN:HG3	8:333:14:G:H4'	1.98	0.45
2:CCC:901:LEU:CD1	5:FFF:310:LEU:CD2	2.88	0.45
3:DDD:151:MET:SD	3:DDD:151:MET:N	2.90	0.45
3:DDD:517:CYS:SG	3:DDD:518:VAL:N	2.90	0.45
3:DDD:731:ARG:HA	3:DDD:731:ARG:HD3	1.73	0.45
3:DDD:845:ALA:HA	3:DDD:846:GLU:HA	1.75	0.45
2:CCC:1251:TYR:HE2	5:FFF:246:PRO:HD3	1.82	0.45
3:DDD:1168:GLU:OE2	3:DDD:1173:ARG:NH1	2.50	0.45
3:DDD:234:PRO:O	3:DDD:237:MET:HG3	2.17	0.45
5:FFF:158:ILE:CG2	7:222:26:DT:O2	2.64	0.45
1:AAA:135:ASP:OD1	1:AAA:135:ASP:C	2.55	0.45
2:CCC:400:VAL:HG13	2:CCC:584:TYR:HB3	1.98	0.45
2:CCC:1308:ILE:HG23	3:DDD:380:PHE:CD1	2.52	0.45
3:DDD:665:GLN:O	3:DDD:668:PHE:HB3	2.17	0.45
2:CCC:1251:TYR:HE2	5:FFF:246:PRO:CD	2.30	0.45
1:BBB:86:LYS:HE2	1:BBB:174:ASP:N	2.30	0.45
2:CCC:421:SER:OG	2:CCC:424:ASP:OD2	2.34	0.45
3:DDD:423:LEU:HB3	3:DDD:466:MET:CE	2.46	0.45
5:FFF:87:ASP:OD1	5:FFF:88:VAL:N	2.50	0.45
2:CCC:1088:ASP:HB3	2:CCC:1090:ASN:N	2.28	0.45
2:CCC:1109:ILE:HG22	2:CCC:1113:LEU:HD12	1.99	0.45
2:CCC:1119:MET:HB2	2:CCC:1228:GLY:HA2	1.98	0.45
2:CCC:57:PHE:CE1	2:CCC:59:ILE:HD12	2.52	0.45
2:CCC:76:GLY:O	2:CCC:94:ALA:HB1	2.16	0.45
3:DDD:839:VAL:CG1	3:DDD:839:VAL:O	2.64	0.45
2:CCC:1296:ASP:CB	2:CCC:1321:GLU:H	2.30	0.45
2:CCC:720:ARG:HB2	2:CCC:749:ASP:OD2	2.17	0.45
2:CCC:871:VAL:HG23	2:CCC:883:LEU:HA	1.99	0.45
2:CCC:887:VAL:HB	2:CCC:913:VAL:CG1	2.46	0.45
3:DDD:555:TYR:O	3:DDD:586:GLY:HA2	2.17	0.45
3:DDD:58:CYS:SG	3:DDD:61:ILE:N	2.90	0.45
3:DDD:872:LEU:CD2	3:DDD:877:VAL:HG21	2.47	0.45
2:CCC:1081:PRO:CB	2:CCC:1083:GLU:OE2	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:1160:ASP:O	2:CCC:1161:LEU:O	2.35	0.44
2:CCC:668:ILE:HG12	2:CCC:1069:ARG:O	2.18	0.44
2:CCC:840:SER:HB3	2:CCC:850:ILE:HD11	2.00	0.44
2:CCC:847:PRO:HB3	2:CCC:1047:LEU:HD11	1.97	0.44
3:DDD:248:ASP:OD1	3:DDD:248:ASP:N	2.49	0.44
3:DDD:530:PRO:HD3	3:DDD:552:ILE:CD1	2.47	0.44
5:FFF:122:GLU:HG2	5:FFF:157:ALA:CB	2.48	0.44
2:CCC:832:HIS:CD2	2:CCC:1058:ARG:HD2	2.53	0.44
2:CCC:165:HIS:HB3	2:CCC:167:SER:HB3	1.99	0.44
2:CCC:196:VAL:CG2	2:CCC:206:ALA:HA	2.31	0.44
3:DDD:1041:ILE:HG21	3:DDD:1044:GLN:HG3	2.00	0.44
3:DDD:820:ILE:HG12	3:DDD:1227:HIS:CD2	2.51	0.44
3:DDD:948:SER:OG	3:DDD:1019:ASN:ND2	2.51	0.44
2:CCC:670:PHE:CD2	2:CCC:1113:LEU:HB3	2.52	0.44
2:CCC:447:HIS:HD2	2:CCC:449:GLY:H	1.61	0.44
3:DDD:332:LYS:O	3:DDD:333:GLY:O	2.36	0.44
3:DDD:667:GLN:O	3:DDD:670:SER:OG	2.22	0.44
2:CCC:1061:GLN:NE2	2:CCC:1240:ASP:OD1	2.50	0.44
2:CCC:1280:ALA:HB1	3:DDD:918:ILE:HG12	1.99	0.44
2:CCC:292:ILE:HG21	2:CCC:322:LEU:HD21	2.00	0.44
2:CCC:1276:TRP:HH2	3:DDD:798:ARG:HG3	1.81	0.44
2:CCC:1293:VAL:HG12	2:CCC:1300:GLY:C	2.38	0.44
4:EEE:60:ASN:HB3	4:EEE:63:ILE:HD12	2.00	0.44
2:CCC:1030:GLU:HG3	2:CCC:1034:ARG:CZ	2.47	0.44
2:CCC:1087:TYR:HD2	2:CCC:1091:GLY:HA2	1.82	0.44
2:CCC:152:SER:O	2:CCC:156:PHE:CZ	2.70	0.44
2:CCC:189:ASP:OD1	2:CCC:190:PRO:N	2.51	0.44
2:CCC:297:VAL:HG13	2:CCC:317:LEU:CG	2.48	0.44
2:CCC:403:MET:HB3	2:CCC:403:MET:HE2	1.81	0.44
2:CCC:933:VAL:HG11	2:CCC:945:ALA:HB2	2.00	0.44
2:CCC:93:SER:OG	2:CCC:126:GLU:HB3	2.17	0.44
3:DDD:360:TYR:OH	3:DDD:448:GLN:OE1	2.28	0.44
7:222:15:DT:H2'	7:222:16:DC:C6	2.53	0.44
3:DDD:58:CYS:SG	3:DDD:60:ARG:N	2.91	0.44
3:DDD:733:SER:H	3:DDD:736:GLN:HG3	1.83	0.44
3:DDD:829:GLY:HA2	3:DDD:993:GLU:CG	2.47	0.44
3:DDD:850:LYS:HB2	3:DDD:851:PRO:CD	2.47	0.44
3:DDD:932:MET:SD	8:333:19:U:C2'	3.03	0.44
7:222:22:DA:H1'	7:222:23:DT:H5'	1.99	0.44
1:AAA:64:VAL:HG13	1:AAA:78:ILE:HD13	1.99	0.44
2:CCC:1129:ASN:CA	2:CCC:1177:ARG:HG3	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:127:LEU:HA	3:DDD:127:LEU:HD23	1.85	0.44
3:DDD:548:VAL:HG12	3:DDD:550:VAL:HG22	2.00	0.44
3:DDD:780:ARG:HB2	3:DDD:780:ARG:HE	1.65	0.44
3:DDD:930:LEU:CD1	3:DDD:1246:VAL:HG21	2.48	0.44
2:CCC:32:LEU:CD2	2:CCC:130:MET:CE	2.95	0.43
2:CCC:801:ARG:HG3	2:CCC:1229:TYR:CE1	2.53	0.43
2:CCC:838:CYS:SG	2:CCC:886:LYS:HE2	2.58	0.43
3:DDD:1364:ALA:O	3:DDD:1367:GLN:HG2	2.17	0.43
4:EEE:39:VAL:HG13	4:EEE:40:PRO:HD2	2.00	0.43
2:CCC:816:ILE:HD11	2:CCC:1074:GLY:HA3	1.99	0.43
2:CCC:978:VAL:O	2:CCC:981:ALA:HB3	2.18	0.43
3:DDD:886:VAL:HG12	3:DDD:1226:VAL:CG1	2.48	0.43
3:DDD:197:GLU:OE1	3:DDD:220:ARG:NH2	2.49	0.43
2:CCC:720:ARG:HB3	2:CCC:736:VAL:HG13	1.99	0.43
3:DDD:305:ALA:CB	3:DDD:316:ILE:HD12	2.48	0.43
3:DDD:502:PRO:HB3	3:DDD:506:VAL:CG1	2.48	0.43
1:BBB:176:CYS:CB	3:DDD:535:ARG:HH22	2.23	0.43
3:DDD:805:GLN:HG2	3:DDD:806:ASP:N	2.32	0.43
4:EEE:13:ILE:HD12	4:EEE:19:LEU:HA	2.00	0.43
5:FFF:183:ARG:O	5:FFF:187:HIS:ND1	2.51	0.43
7:222:17:DG:C2'	7:222:18:DT:C1'	2.96	0.43
2:CCC:963:GLU:O	2:CCC:967:LEU:HB2	2.19	0.43
3:DDD:528:THR:HG23	3:DDD:532:GLU:OE1	2.18	0.43
3:DDD:62:PHE:CD1	3:DDD:247:PRO:HD3	2.53	0.43
3:DDD:703:THR:O	3:DDD:704:GLU:C	2.56	0.43
3:DDD:747:MET:SD	3:DDD:759:ILE:HD12	2.58	0.43
5:FFF:263:LEU:HD13	5:FFF:281:LEU:CD1	2.49	0.43
2:CCC:496:LYS:N	2:CCC:497:PRO:CD	2.81	0.43
2:CCC:871:VAL:HG23	2:CCC:883:LEU:O	2.18	0.43
3:DDD:161:THR:H	3:DDD:164:GLN:HB2	1.83	0.43
3:DDD:45:ASN:HB2	3:DDD:52:GLU:OE1	2.18	0.43
3:DDD:824:PRO:HD3	3:DDD:878:ASP:O	2.19	0.43
1:AAA:158:ARG:HG3	1:AAA:158:ARG:NH1	2.30	0.43
1:AAA:61:ILE:HG12	1:AAA:142:MET:HB3	2.01	0.43
1:BBB:102:LEU:HB2	1:BBB:115:ILE:HG12	2.00	0.43
1:BBB:65:LEU:O	1:BBB:169:GLY:HA2	2.18	0.43
2:CCC:1257:GLN:NE2	3:DDD:341:ASN:O	2.51	0.43
2:CCC:409:LEU:HD13	2:CCC:427:ASP:HB3	2.00	0.43
2:CCC:1131:MET:HG2	2:CCC:1136:GLN:OE1	2.19	0.43
2:CCC:1212:LEU:HD23	2:CCC:1212:LEU:HA	1.87	0.43
2:CCC:751:TYR:N	2:CCC:751:TYR:CD2	2.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:119:SER:O	3:DDD:122:SER:N	2.51	0.43
3:DDD:884:SER:OG	3:DDD:1254:GLU:OE1	2.33	0.43
3:DDD:492:SER:HB2	3:DDD:499:ILE:CD1	2.49	0.43
2:CCC:208:ILE:HD11	2:CCC:365:GLU:HB3	2.01	0.43
2:CCC:898:GLU:OE2	5:FFF:280:LEU:CD1	2.67	0.43
3:DDD:803:VAL:HG22	3:DDD:1313:SER:OG	2.19	0.43
7:222:25:DA:H2''	7:222:26:DT:H5''	2.00	0.43
1:AAA:67:GLU:HB3	1:AAA:171:LEU:HD22	2.00	0.43
1:AAA:91:ARG:HG3	1:AAA:210:THR:HA	2.00	0.43
1:AAA:64:VAL:CG1	1:AAA:78:ILE:HD13	2.49	0.43
2:CCC:1285:TYR:HB2	3:DDD:479:GLU:OE2	2.19	0.43
2:CCC:512:SER:OG	2:CCC:512:SER:O	2.34	0.43
3:DDD:1186:TYR:CZ	3:DDD:1188:GLU:OE2	2.72	0.43
3:DDD:579:LEU:HB3	3:DDD:592:VAL:HG21	2.01	0.43
3:DDD:849:LEU:CD1	3:DDD:853:THR:HA	2.47	0.43
3:DDD:925:GLU:HB3	3:DDD:926:PRO:CD	2.49	0.43
5:FFF:158:ILE:HG22	7:222:26:DT:O2	2.19	0.43
5:FFF:277:ARG:CD	5:FFF:306:GLN:HE21	2.30	0.43
2:CCC:118:LYS:NZ	2:CCC:485:ASP:O	2.30	0.42
2:CCC:592:ARG:NH1	2:CCC:653:MET:HE1	2.33	0.42
3:DDD:750:PRO:O	3:DDD:781:LYS:HE3	2.18	0.42
3:DDD:823:THR:HB	3:DDD:824:PRO:CD	2.45	0.42
5:FFF:65:ILE:HG12	5:FFF:99:LEU:HD13	2.01	0.42
2:CCC:1134:GLN:O	2:CCC:1136:GLN:N	2.51	0.42
3:DDD:1165:PHE:HZ	3:DDD:1196:LEU:HD12	1.84	0.42
3:DDD:1357:ILE:HG13	3:DDD:1357:ILE:H	1.54	0.42
3:DDD:555:TYR:O	3:DDD:586:GLY:CA	2.67	0.42
3:DDD:872:LEU:HD23	3:DDD:877:VAL:HG21	2.01	0.42
5:FFF:263:LEU:HD13	5:FFF:281:LEU:HD11	2.00	0.42
2:CCC:183:TRP:CH2	6:111:51:DC:H2'	2.54	0.42
1:AAA:47:LEU:HA	1:AAA:51:MET:HG2	2.01	0.42
2:CCC:146:VAL:O	2:CCC:511:LEU:HD13	2.18	0.42
2:CCC:599:VAL:HG21	2:CCC:623:LEU:CD2	2.49	0.42
2:CCC:555:TYR:OH	2:CCC:654:ASP:OD2	2.20	0.42
2:CCC:726:TYR:CZ	2:CCC:728:ASP:HB2	2.54	0.42
3:DDD:130:MET:SD	3:DDD:157:GLN:HB3	2.59	0.42
3:DDD:205:LEU:HD22	3:DDD:214:ARG:HG2	2.01	0.42
3:DDD:490:ILE:HG12	3:DDD:500:ILE:HD12	2.01	0.42
3:DDD:58:CYS:SG	3:DDD:61:ILE:HG13	2.60	0.42
2:CCC:160:ASP:HB3	2:CCC:163:LYS:HD3	2.00	0.42
2:CCC:216:THR:N	2:CCC:219:GLN:OE1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:667:LEU:HD23	2:CCC:704:MET:HB2	2.00	0.42
3:DDD:599:LYS:H	3:DDD:599:LYS:HG3	1.53	0.42
3:DDD:846:GLU:HB3	3:DDD:860:ARG:NE	2.34	0.42
5:FFF:182:ALA:HB1	5:FFF:193:PRO:CG	2.45	0.42
3:DDD:1106:ILE:O	3:DDD:1106:ILE:HG22	2.19	0.42
3:DDD:810:THR:OG1	3:DDD:893:GLY:HA3	2.19	0.42
3:DDD:1196:LEU:HD22	3:DDD:1210:ILE:HG22	2.02	0.42
3:DDD:502:PRO:HB3	3:DDD:506:VAL:HG11	2.02	0.42
1:AAA:159:ILE:O	1:AAA:159:ILE:HG23	2.18	0.42
2:CCC:1128:ILE:HD11	2:CCC:1145:ILE:HG12	2.01	0.42
2:CCC:801:ARG:HG3	2:CCC:1229:TYR:CZ	2.54	0.42
2:CCC:90:VAL:HG12	2:CCC:91:THR:N	2.34	0.42
3:DDD:664:ILE:HD13	3:DDD:681:LYS:HG2	2.01	0.42
5:FFF:225:PRO:HA	5:FFF:233:ALA:HA	2.02	0.42
6:111:32:DA:N3	7:222:32:DA:C2	2.87	0.42
5:FFF:143:SER:CB	6:111:41:DT:H73	2.48	0.42
3:DDD:421:VAL:HG11	3:DDD:468:VAL:HG13	2.02	0.42
3:DDD:659:ALA:O	3:DDD:663:GLU:HG3	2.20	0.42
3:DDD:802:ASP:OD1	3:DDD:1348:LYS:HE3	2.20	0.42
1:AAA:78:ILE:HA	1:AAA:81:ILE:HD12	2.02	0.42
1:AAA:12:ARG:HA	1:BBB:230:ALA:HB1	2.01	0.42
2:CCC:104:ILE:HD13	2:CCC:484:LEU:HB3	2.01	0.42
2:CCC:515:MET:HG2	2:CCC:517:GLN:HG3	2.02	0.42
2:CCC:583:GLU:HG3	2:CCC:584:TYR:CD2	2.55	0.42
3:DDD:290:ILE:HD12	3:DDD:290:ILE:H	1.83	0.42
1:BBB:78:ILE:HA	1:BBB:81:ILE:HD12	2.01	0.42
2:CCC:32:LEU:CD2	2:CCC:130:MET:HE3	2.50	0.42
3:DDD:805:GLN:CG	3:DDD:806:ASP:N	2.82	0.42
5:FFF:145:TYR:CZ	5:FFF:149:TRP:NE1	2.86	0.42
1:BBB:16:ILE:HD13	1:BBB:214:GLU:OE2	2.20	0.41
2:CCC:1296:ASP:HB3	2:CCC:1321:GLU:H	1.84	0.41
2:CCC:49:LEU:HD23	2:CCC:464:PHE:CE2	2.54	0.41
2:CCC:538:LEU:HD23	2:CCC:542:ARG:NH2	2.35	0.41
2:CCC:898:GLU:N	2:CCC:898:GLU:OE1	2.51	0.41
2:CCC:936:ARG:CG	2:CCC:937:ASP:N	2.82	0.41
3:DDD:1180:VAL:HG23	3:DDD:1181:ASP:H	1.85	0.41
3:DDD:625:MET:HG2	3:DDD:629:PHE:CE2	2.55	0.41
3:DDD:746:LEU:HD23	3:DDD:758:PRO:HB3	2.02	0.41
3:DDD:849:LEU:HB3	3:DDD:856:ILE:HA	2.01	0.41
3:DDD:994:SER:O	3:DDD:995:TYR:CG	2.73	0.41
4:EEE:8:ASP:HB2	4:EEE:55:GLU:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:170:HIS:NE2	6:111:31:DT:C6	2.87	0.41
2:CCC:1286:THR:O	2:CCC:1289:GLU:HB2	2.21	0.41
2:CCC:799:ASN:ND2	2:CCC:799:ASN:H	2.18	0.41
3:DDD:680:ASN:HB3	3:DDD:1023:HIS:CE1	2.55	0.41
3:DDD:1061:VAL:O	3:DDD:1104:LYS:N	2.41	0.41
2:CCC:1290:MET:SD	3:DDD:347:VAL:HG11	2.60	0.41
3:DDD:829:GLY:O	3:DDD:993:GLU:HG2	2.20	0.41
2:CCC:251:ALA:CB	2:CCC:263:VAL:CG1	2.85	0.41
2:CCC:944:ARG:O	2:CCC:947:GLU:HG2	2.20	0.41
2:CCC:985:GLU:HB2	2:CCC:989:LEU:HG	2.01	0.41
3:DDD:1082:ASP:C	3:DDD:1082:ASP:OD1	2.59	0.41
1:BBB:160:HIS:C	1:BBB:160:HIS:CD2	2.93	0.41
2:CCC:1328:LYS:HA	2:CCC:1328:LYS:HD3	1.92	0.41
3:DDD:1054:THR:OG1	3:DDD:1055:GLY:N	2.53	0.41
3:DDD:784:ALA:O	3:DDD:788:LEU:HG	2.20	0.41
2:CCC:1269:ARG:HH21	2:CCC:1271:GLY:HA2	1.86	0.41
2:CCC:237:LEU:HD11	2:CCC:292:ILE:HD12	2.03	0.41
2:CCC:32:LEU:HD23	2:CCC:130:MET:HE3	2.02	0.41
5:FFF:68:SER:HB2	5:FFF:69:PRO:HD2	2.02	0.41
2:CCC:800:MET:O	2:CCC:1229:TYR:HA	2.21	0.41
2:CCC:1000:LEU:O	2:CCC:1011:LEU:HD21	2.20	0.41
2:CCC:967:LEU:HD12	2:CCC:967:LEU:HA	1.85	0.41
3:DDD:380:PHE:HB3	3:DDD:415:VAL:HG11	2.03	0.41
3:DDD:424:ASN:OD1	3:DDD:425:ARG:N	2.54	0.41
3:DDD:836:ARG:CD	3:DDD:873:GLU:CD	2.89	0.41
1:BBB:86:LYS:HD3	1:BBB:174:ASP:HB2	2.03	0.41
2:CCC:1262:LYS:HG2	2:CCC:1263:ALA:N	2.35	0.41
2:CCC:149:LEU:HB2	2:CCC:530:ILE:CG2	2.50	0.41
2:CCC:21:VAL:HG21	2:CCC:592:ARG:CZ	2.51	0.41
3:DDD:525:MET:N	3:DDD:548:VAL:HG22	2.34	0.41
1:AAA:124:VAL:HG11	1:AAA:209:GLY:HA2	2.02	0.41
1:AAA:195:ARG:HD2	1:AAA:198:LEU:HD23	2.02	0.41
1:BBB:101:THR:HG22	1:BBB:143:ARG:HG2	2.02	0.41
2:CCC:670:PHE:CE2	2:CCC:1113:LEU:HB3	2.56	0.41
2:CCC:479:LEU:HA	2:CCC:479:LEU:HD23	1.94	0.41
2:CCC:135:THR:HG22	2:CCC:527:LYS:HE2	2.03	0.41
1:AAA:74:VAL:O	2:CCC:729:ALA:CB	2.69	0.41
2:CCC:898:GLU:OE2	5:FFF:280:LEU:HD13	2.21	0.41
2:CCC:1281:TYR:CE1	3:DDD:431:ARG:HG3	2.55	0.41
2:CCC:1223:ARG:NH2	3:DDD:719:PHE:O	2.54	0.41
2:CCC:1081:PRO:HB2	2:CCC:1083:GLU:CD	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CCC:759:SER:OG	2:CCC:760:ASN:N	2.52	0.41
2:CCC:1284:ALA:CA	3:DDD:1357:ILE:HD12	2.45	0.41
3:DDD:1370:MET:O	3:DDD:1373:ARG:HB2	2.21	0.41
3:DDD:298:MET:HE3	5:FFF:117:LEU:HB3	2.03	0.41
7:222:17:DG:O3'	7:222:18:DT:C4'	2.68	0.41
1:AAA:30:PRO:HB2	1:AAA:198:LEU:CD1	2.50	0.41
2:CCC:1296:ASP:O	2:CCC:1297:ASP:C	2.59	0.41
2:CCC:44:GLU:HG3	2:CCC:45:GLY:N	2.36	0.41
2:CCC:975:ILE:HG23	2:CCC:1011:LEU:CD1	2.50	0.41
3:DDD:916:GLY:HA2	3:DDD:1255:VAL:HG11	2.02	0.41
3:DDD:809:VAL:CG2	3:DDD:915:ILE:CD1	2.99	0.41
3:DDD:822:MET:CE	3:DDD:882:VAL:HG21	2.50	0.41
1:AAA:231:PHE:O	1:AAA:235:ARG:OXT	2.39	0.40
2:CCC:60:GLN:HG2	2:CCC:67:GLU:CB	2.51	0.40
3:DDD:1047:THR:HB	3:DDD:1062:LEU:HD11	2.03	0.40
3:DDD:923:ILE:CD1	3:DDD:1256:ILE:HD12	2.51	0.40
3:DDD:661:VAL:HG23	3:DDD:685:ILE:HG21	2.03	0.40
3:DDD:679:TYR:HE1	3:DDD:754:ILE:O	2.05	0.40
3:DDD:819:GLY:N	3:DDD:881:LYS:HE2	2.36	0.40
3:DDD:933:ARG:NH1	11:DDD:1504:DPO:O5	2.54	0.40
1:AAA:222:THR:HG23	1:BBB:233:ASP:HB3	2.02	0.40
2:CCC:1234:LYS:HE3	2:CCC:1238:LEU:HD22	2.04	0.40
2:CCC:163:LYS:CG	2:CCC:164:THR:N	2.75	0.40
2:CCC:267:ARG:HD3	2:CCC:268:ARG:H	1.86	0.40
3:DDD:427:PRO:CG	3:DDD:429:LEU:HD21	2.51	0.40
3:DDD:783:LEU:HD12	3:DDD:783:LEU:HA	1.79	0.40
3:DDD:843:VAL:O	3:DDD:882:VAL:CB	2.65	0.40
3:DDD:958:ILE:HG23	3:DDD:982:LEU:HD13	2.03	0.40
1:AAA:166:ARG:NH2	2:CCC:863:SER:OG	2.55	0.40
1:AAA:45:ARG:HD3	1:BBB:38:THR:HG23	2.02	0.40
2:CCC:1246:ARG:NH2	2:CCC:1258:PRO:HB3	2.36	0.40
2:CCC:1292:THR:HG23	2:CCC:1293:VAL:N	2.36	0.40
2:CCC:160:ASP:N	2:CCC:160:ASP:OD1	2.54	0.40
2:CCC:99:LYS:HG2	2:CCC:121:GLU:HG3	2.02	0.40
3:DDD:742:GLY:O	3:DDD:762:ASN:HB3	2.22	0.40
3:DDD:935:PHE:HZ	3:DDD:1135:THR:OG1	2.04	0.40
3:DDD:955:LYS:HG2	3:DDD:1011:VAL:O	2.21	0.40
2:CCC:102:LEU:HD23	2:CCC:118:LYS:HD2	2.03	0.40
2:CCC:216:THR:O	2:CCC:220:ILE:HG13	2.21	0.40
2:CCC:582:ASN:OD1	2:CCC:585:GLY:N	2.52	0.40
2:CCC:1293:VAL:O	2:CCC:1301:ARG:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:DDD:1199:PHE:CD1	3:DDD:1200:GLU:N	2.90	0.40
3:DDD:397:ALA:O	3:DDD:401:VAL:HG23	2.21	0.40
3:DDD:509:GLY:O	3:DDD:513:MET:HG3	2.21	0.40
3:DDD:703:THR:C	3:DDD:705:THR:N	2.74	0.40
2:CCC:549:ASP:OD2	3:DDD:750:PRO:CG	2.70	0.40
3:DDD:809:VAL:HG22	3:DDD:915:ILE:CD1	2.52	0.40
2:CCC:1314:GLN:HA	4:EEE:28:ARG:NH2	2.37	0.40

All (12) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:FFF:67:TYR:CE1	5:FFF:299:ARG:NH2[3_644]	0.94	1.26
5:FFF:67:TYR:CZ	5:FFF:299:ARG:NH2[3_644]	1.07	1.13
5:FFF:67:TYR:CD1	5:FFF:299:ARG:NH2[3_644]	1.75	0.45
5:FFF:67:TYR:CE2	5:FFF:299:ARG:NH2[3_644]	1.89	0.31
5:FFF:67:TYR:CZ	5:FFF:299:ARG:CZ[3_644]	1.98	0.22
3:DDD:212:THR:OG1	6:111:26:DT:O3'[3_644]	1.99	0.21
3:DDD:129:ASP:OD1	7:222:39:DG:OP1[3_644]	2.02	0.18
1:AAA:193:GLU:OE1	3:DDD:174:ASP:OD2[2_555]	2.12	0.08
5:FFF:67:TYR:CE1	5:FFF:299:ARG:CZ[3_644]	2.15	0.05
5:FFF:67:TYR:OH	5:FFF:299:ARG:NH2[3_644]	2.15	0.05
3:DDD:212:THR:OG1	6:111:27:DC:OP1[3_644]	2.16	0.04
3:DDD:212:THR:OG1	6:111:27:DC:C5'[3_644]	2.19	0.01

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	AAA	228/242 (94%)	214 (94%)	8 (4%)	6 (3%)	5	33
1	BBB	226/242 (93%)	206 (91%)	14 (6%)	6 (3%)	5	33

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	CCC	1339/1342 (100%)	1237 (92%)	77 (6%)	25 (2%)	8	39
3	DDD	1360/1407 (97%)	1253 (92%)	91 (7%)	16 (1%)	13	50
4	EEE	77/90 (86%)	73 (95%)	4 (5%)	0	100	100
5	FFF	275/336 (82%)	256 (93%)	15 (6%)	4 (2%)	10	46
All	All	3505/3659 (96%)	3239 (92%)	209 (6%)	57 (2%)	9	44

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	BBB	117	HIS
1	BBB	193	GLU
1	BBB	194	GLN
2	CCC	46	GLN
2	CCC	247	ARG
2	CCC	791	LEU
2	CCC	892	GLU
2	CCC	1161	LEU
2	CCC	1162	SER
2	CCC	1281	TYR
3	DDD	53	ARG
3	DDD	174	ASP
3	DDD	336	GLY
3	DDD	519	ASN
5	FFF	227	GLY
5	FFF	228	GLY
1	AAA	234	LEU
1	BBB	119	GLY
1	BBB	232	VAL
2	CCC	258	ASN
2	CCC	625	GLU
2	CCC	730	SER
2	CCC	756	TYR
3	DDD	122	SER
3	DDD	321	LYS
3	DDD	1309	ILE
1	AAA	162	GLU
1	AAA	168	ILE
1	AAA	191	ARG
2	CCC	455	SER
2	CCC	867	GLU
2	CCC	981	ALA

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Mol	Chain	Res	Type
2	CCC	1103	VAL
2	CCC	1135	GLN
3	DDD	1053	LEU
3	DDD	1200	GLU
5	FFF	113	GLY
1	AAA	210	THR
2	CCC	45	GLY
2	CCC	163	LYS
2	CCC	669	PRO
2	CCC	729	ALA
3	DDD	1024	THR
2	CCC	234	ASP
2	CCC	986	ALA
2	CCC	1297	ASP
3	DDD	986	ASP
3	DDD	1091	PRO
3	DDD	1170	LYS
1	AAA	233	ASP
1	BBB	118	ASP
2	CCC	341	LEU
3	DDD	153	ASN
2	CCC	983	GLY
5	FFF	295	ILE
3	DDD	1103	GLY
3	DDD	829	GLY

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	AAA	198/208 (95%)	181 (91%)	17 (9%)	10	35
1	BBB	196/208 (94%)	182 (93%)	14 (7%)	14	41
2	CCC	1156/1157 (100%)	1069 (92%)	87 (8%)	13	40
3	DDD	1135/1168 (97%)	1064 (94%)	71 (6%)	18	44
4	EEE	67/74 (90%)	64 (96%)	3 (4%)	27	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	FFF	240/292 (82%)	230 (96%)	10 (4%)	30	54
All	All	2992/3107 (96%)	2790 (93%)	202 (7%)	16	42

All (202) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AAA	28	LEU
1	AAA	33	ARG
1	AAA	70	THR
1	AAA	77	ASP
1	AAA	131	CYS
1	AAA	135	ASP
1	AAA	137	ASN
1	AAA	166	ARG
1	AAA	170	ARG
1	AAA	173	VAL
1	AAA	176	CYS
1	AAA	187	VAL
1	AAA	191	ARG
1	AAA	194	GLN
1	AAA	198	LEU
1	AAA	208	ASN
1	AAA	233	ASP
1	BBB	28	LEU
1	BBB	33	ARG
1	BBB	70	THR
1	BBB	77	ASP
1	BBB	131	CYS
1	BBB	137	ASN
1	BBB	159	ILE
1	BBB	170	ARG
1	BBB	173	VAL
1	BBB	176	CYS
1	BBB	187	VAL
1	BBB	191	ARG
1	BBB	194	GLN
1	BBB	198	LEU
2	CCC	23	ASP
2	CCC	30	ILE
2	CCC	69	GLN
2	CCC	85	CYS
2	CCC	116	ASP

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Mol	Chain	Res	Type
2	CCC	120	GLN
2	CCC	121	GLU
2	CCC	160	ASP
2	CCC	166	SER
2	CCC	167	SER
2	CCC	173	ASN
2	CCC	184	LEU
2	CCC	185	ASP
2	CCC	189	ASP
2	CCC	209	ILE
2	CCC	237	LEU
2	CCC	241	LEU
2	CCC	244	GLU
2	CCC	256	GLU
2	CCC	264	GLU
2	CCC	275	ARG
2	CCC	290	GLU
2	CCC	304	GLU
2	CCC	316	GLU
2	CCC	332	ARG
2	CCC	335	THR
2	CCC	393	ASP
2	CCC	398	SER
2	CCC	403	MET
2	CCC	404	LYS
2	CCC	413	GLU
2	CCC	470	ARG
2	CCC	472	GLU
2	CCC	477	GLU
2	CCC	502	VAL
2	CCC	525	THR
2	CCC	529	ARG
2	CCC	539	THR
2	CCC	574	SER
2	CCC	576	SER
2	CCC	592	ARG
2	CCC	601	ASP
2	CCC	618	GLN
2	CCC	620	ASN
2	CCC	622	ASN
2	CCC	635	THR
2	CCC	648	ASP

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Mol	Chain	Res	Type
2	CCC	678	ARG
2	CCC	685	MET
2	CCC	694	ARG
2	CCC	730	SER
2	CCC	739	ASP
2	CCC	757	THR
2	CCC	758	ARG
2	CCC	759	SER
2	CCC	777	VAL
2	CCC	788	SER
2	CCC	789	THR
2	CCC	799	ASN
2	CCC	800	MET
2	CCC	801	ARG
2	CCC	802	VAL
2	CCC	808	ASN
2	CCC	815	SER
2	CCC	817	LEU
2	CCC	831	ILE
2	CCC	866	ASP
2	CCC	876	GLU
2	CCC	935	THR
2	CCC	942	ASP
2	CCC	995	ASP
2	CCC	1073	LYS
2	CCC	1088	ASP
2	CCC	1113	LEU
2	CCC	1143	GLU
2	CCC	1150	ASP
2	CCC	1154	ASP
2	CCC	1174	GLU
2	CCC	1223	ARG
2	CCC	1240	ASP
2	CCC	1248	THR
2	CCC	1262	LYS
2	CCC	1269	ARG
2	CCC	1286	THR
2	CCC	1292	THR
2	CCC	1293	VAL
2	CCC	1296	ASP
3	DDD	34	SER
3	DDD	52	GLU

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Mol	Chain	Res	Type
3	DDD	60	ARG
3	DDD	67	ASP
3	DDD	70	CYS
3	DDD	143	SER
3	DDD	167	ASP
3	DDD	176	PHE
3	DDD	210	SER
3	DDD	223	LEU
3	DDD	237	MET
3	DDD	256	ASP
3	DDD	319	SER
3	DDD	345	LYS
3	DDD	443	GLU
3	DDD	464	ASP
3	DDD	479	GLU
3	DDD	492	SER
3	DDD	499	ILE
3	DDD	503	SER
3	DDD	543	SER
3	DDD	548	VAL
3	DDD	570	LYS
3	DDD	590	SER
3	DDD	591	ILE
3	DDD	599	LYS
3	DDD	604	MET
3	DDD	610	ARG
3	DDD	619	ILE
3	DDD	627	THR
3	DDD	704	GLU
3	DDD	705	THR
3	DDD	717	VAL
3	DDD	731	ARG
3	DDD	736	GLN
3	DDD	747	MET
3	DDD	751	ASP
3	DDD	769	VAL
3	DDD	786	THR
3	DDD	790	THR
3	DDD	792	ASN
3	DDD	812	ASP
3	DDD	826	ILE
3	DDD	830	ASP

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Mol	Chain	Res	Type
3	DDD	835	LEU
3	DDD	842	ARG
3	DDD	843	VAL
3	DDD	846	GLU
3	DDD	849	LEU
3	DDD	860	ARG
3	DDD	863	LEU
3	DDD	889	ASP
3	DDD	911	LYS
3	DDD	957	SER
3	DDD	961	SER
3	DDD	969	SER
3	DDD	970	SER
3	DDD	1021	ASP
3	DDD	1025	MET
3	DDD	1032	SER
3	DDD	1051	ASP
3	DDD	1058	SER
3	DDD	1064	SER
3	DDD	1073	ASP
3	DDD	1183	SER
3	DDD	1200	GLU
3	DDD	1283	SER
3	DDD	1303	SER
3	DDD	1309	ILE
3	DDD	1330	ARG
3	DDD	1345	ARG
4	EEE	8	ASP
4	EEE	46	THR
4	EEE	55	GLU
5	FFF	107	ARG
5	FFF	109	TYR
5	FFF	122	GLU
5	FFF	127	LEU
5	FFF	218	ARG
5	FFF	243	GLU
5	FFF	244	ASN
5	FFF	254	ASP
5	FFF	271	ARG
5	FFF	325	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
8	333	5/6 (83%)	2 (40%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
8	333	18	C
8	333	19	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	DPO	DDD	1504	10	6,8,8	0.73	0	13,13,13	0.77	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	DPO	DDD	1504	10	-	0/6/6/6	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	DDD	1504	DPO	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	AAA	230/242 (95%)	0.24	14 (6%) 21 19	259, 372, 468, 533	0
1	BBB	228/242 (94%)	0.32	25 (10%) 5 8	220, 350, 469, 536	0
2	CCC	1341/1342 (99%)	0.06	52 (3%) 39 33	149, 303, 471, 650	0
3	DDD	1362/1407 (96%)	0.18	97 (7%) 16 15	154, 328, 517, 647	0
4	EEE	79/90 (87%)	-0.17	1 (1%) 77 68	269, 375, 517, 678	0
5	FFF	277/336 (82%)	0.29	13 (4%) 31 28	237, 384, 529, 633	0
6	111	30/50 (60%)	0.62	4 (13%) 3 5	310, 413, 536, 678	0
7	222	35/50 (70%)	0.87	6 (17%) 1 3	271, 388, 687, 743	0
8	333	6/6 (100%)	1.58	0 100 100	331, 366, 398, 405	0
All	All	3588/3765 (95%)	0.16	212 (5%) 22 20	149, 332, 504, 743	0

All (212) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	DDD	941	ALA	9.0
6	111	49	DG	8.3
2	CCC	230	PHE	7.9
3	DDD	1065	ALA	7.2
3	DDD	1098	GLN	6.1
7	222	19	DA	6.1
3	DDD	1129	GLY	6.0
3	DDD	748	ALA	5.9
3	DDD	1028	ILE	5.9
3	DDD	1111	ASP	5.7
7	222	22	DA	5.7
2	CCC	169	LYS	5.7
3	DDD	1107	VAL	5.5
3	DDD	1130	GLY	5.4
3	DDD	976	THR	5.3

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Mol	Chain	Res	Type	RSRZ
2	CCC	229	ILE	5.2
3	DDD	1029	THR	5.1
3	DDD	1099	TYR	5.1
3	DDD	878	ASP	5.0
3	DDD	983	LYS	5.0
2	CCC	231	GLU	4.9
3	DDD	750	PRO	4.8
2	CCC	240	GLU	4.7
3	DDD	1121	LEU	4.7
2	CCC	333	ILE	4.6
3	DDD	940	ALA	4.6
3	DDD	943	ARG	4.6
3	DDD	1066	GLU	4.5
6	111	44	DG	4.4
3	DDD	1266	ILE	4.4
5	FFF	310	LEU	4.3
1	BBB	98	VAL	4.3
6	111	50	DT	4.3
3	DDD	1122	ALA	4.3
3	DDD	752	GLY	4.2
3	DDD	982	LEU	4.2
3	DDD	880	VAL	4.2
3	DDD	991	THR	4.2
3	DDD	958	ILE	4.2
2	CCC	1004	ASP	4.1
1	AAA	59	VAL	4.0
3	DDD	1030	GLU	4.0
4	EEE	3	ARG	4.0
1	BBB	50	SER	3.9
3	DDD	854	ALA	3.9
1	AAA	134	THR	3.9
2	CCC	1001	GLY	3.9
3	DDD	1097	ALA	3.8
3	DDD	993	GLU	3.8
3	DDD	1078	LEU	3.8
5	FFF	131	VAL	3.8
3	DDD	992	LYS	3.7
3	DDD	392	THR	3.7
3	DDD	848	VAL	3.7
3	DDD	1118	GLY	3.6
5	FFF	306	GLN	3.5
1	BBB	204	GLU	3.5

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Mol	Chain	Res	Type	RSRZ
2	CCC	336	LEU	3.4
1	BBB	123	ILE	3.4
2	CCC	124	MET	3.3
2	CCC	153	PRO	3.3
3	DDD	1087	ASP	3.3
2	CCC	532	ALA	3.3
3	DDD	959	LYS	3.3
1	AAA	213	PRO	3.3
3	DDD	1079	LYS	3.3
3	DDD	747	MET	3.3
3	DDD	1120	THR	3.2
2	CCC	239	MET	3.2
3	DDD	997	VAL	3.2
3	DDD	856	ILE	3.2
3	DDD	1000	GLY	3.1
3	DDD	879	ALA	3.1
3	DDD	1003	LEU	3.1
2	CCC	152	SER	3.1
1	BBB	133	LEU	3.1
3	DDD	995	TYR	3.1
3	DDD	1035	VAL	3.0
2	CCC	261	VAL	3.0
1	BBB	90	VAL	3.0
2	CCC	164	THR	3.0
2	CCC	190	PRO	3.0
3	DDD	1196	LEU	3.0
1	BBB	49	SER	3.0
7	222	23	DT	2.9
1	AAA	205	MET	2.9
1	AAA	135	ASP	2.9
3	DDD	746	LEU	2.9
2	CCC	332	ARG	2.9
3	DDD	985	ILE	2.9
2	CCC	1159	VAL	2.9
3	DDD	1283	SER	2.9
1	BBB	205	MET	2.9
3	DDD	1115	ILE	2.9
5	FFF	263	LEU	2.8
2	CCC	771	VAL	2.8
1	BBB	47	LEU	2.8
2	CCC	1003	THR	2.8
3	DDD	391	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
3	DDD	855	ASP	2.8
3	DDD	1286	LYS	2.8
5	FFF	247	GLU	2.8
3	DDD	1198	VAL	2.8
3	DDD	939	GLY	2.8
3	DDD	984	LEU	2.8
1	BBB	107	ILE	2.7
5	FFF	202	LEU	2.7
3	DDD	1027	VAL	2.7
2	CCC	170	VAL	2.7
1	BBB	100	LEU	2.7
2	CCC	1002	LEU	2.7
3	DDD	1287	ILE	2.7
5	FFF	201	GLN	2.7
3	DDD	942	SER	2.7
3	DDD	847	ASP	2.7
3	DDD	953	LYS	2.7
2	CCC	531	SER	2.6
3	DDD	1271	SER	2.6
1	BBB	134	THR	2.6
2	CCC	911	SER	2.6
3	DDD	749	LYS	2.6
1	AAA	144	ILE	2.6
2	CCC	75	LEU	2.5
3	DDD	1036	ARG	2.5
3	DDD	1131	THR	2.5
2	CCC	855	PRO	2.5
3	DDD	1119	ASP	2.5
1	AAA	171	LEU	2.5
2	CCC	224	PHE	2.5
3	DDD	1068	THR	2.5
1	BBB	116	THR	2.5
1	AAA	133	LEU	2.5
1	BBB	26	VAL	2.4
2	CCC	743	PRO	2.4
1	BBB	92	VAL	2.4
2	CCC	228	VAL	2.4
1	BBB	101	THR	2.4
3	DDD	1110	GLU	2.4
2	CCC	188	PHE	2.4
7	222	12	DG	2.4
3	DDD	1080	ILE	2.4

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Mol	Chain	Res	Type	RSRZ
3	DDD	966	VAL	2.4
3	DDD	393	THR	2.4
3	DDD	989	GLY	2.4
7	222	18	DT	2.4
3	DDD	950	ILE	2.4
3	DDD	1064	SER	2.4
3	DDD	1285	VAL	2.4
3	DDD	951	GLN	2.4
3	DDD	960	LEU	2.4
3	DDD	1376	GLY	2.4
1	AAA	132	HIS	2.4
3	DDD	671	GLY	2.4
3	DDD	999	TYR	2.4
7	222	13	DA	2.3
2	CCC	241	LEU	2.3
2	CCC	378	ARG	2.3
1	BBB	144	ILE	2.3
1	BBB	89	ALA	2.3
3	DDD	965	SER	2.3
2	CCC	151	ARG	2.3
1	BBB	108	GLY	2.3
2	CCC	11	ILE	2.3
3	DDD	1026	PRO	2.3
2	CCC	96	LEU	2.3
2	CCC	422	LYS	2.3
3	DDD	1077	ALA	2.3
3	DDD	891	ASP	2.3
3	DDD	977	SER	2.3
2	CCC	533	LEU	2.3
3	DDD	1272	SER	2.2
2	CCC	94	ALA	2.2
2	CCC	171	LEU	2.2
5	FFF	313	LEU	2.2
5	FFF	308	GLU	2.2
3	DDD	754	ILE	2.2
5	FFF	69	PRO	2.2
1	BBB	183	ILE	2.2
3	DDD	639	VAL	2.2
6	111	43	DT	2.2
3	DDD	1063	ASP	2.2
2	CCC	870	ILE	2.2
2	CCC	1211	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	BBB	203	ILE	2.2
3	DDD	1227	HIS	2.2
2	CCC	232	ILE	2.2
3	DDD	944	ALA	2.2
2	CCC	1248	THR	2.1
5	FFF	124	ASN	2.1
1	BBB	152	TYR	2.1
3	DDD	973	LEU	2.1
1	AAA	24	ALA	2.1
3	DDD	753	SER	2.1
1	BBB	46	ILE	2.1
3	DDD	1055	GLY	2.1
1	AAA	75	GLN	2.1
2	CCC	977	ALA	2.1
2	CCC	23	ASP	2.1
5	FFF	94	MET	2.1
2	CCC	335	THR	2.1
2	CCC	1160	ASP	2.1
1	AAA	107	ILE	2.1
1	AAA	172	LEU	2.1
2	CCC	168	GLY	2.1
3	DDD	24	LEU	2.0
2	CCC	259	GLY	2.0
1	BBB	112	ALA	2.0
1	BBB	51	MET	2.0
2	CCC	1338	GLU	2.0
2	CCC	557	ARG	2.0
1	AAA	26	VAL	2.0
5	FFF	291	VAL	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 monosaccharides 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(\AA^2)	Q<0.9
10	MG	333	101	1/1	0.65	0.31	316,316,316,316	0
11	DPO	DDD	1504	9/9	0.93	0.69	265,283,350,352	0
9	ZN	DDD	1501	1/1	0.96	0.07	509,509,509,509	0
9	ZN	DDD	1502	1/1	0.97	0.14	376,376,376,376	0
10	MG	DDD	1503	1/1	0.97	0.63	477,477,477,477	0

6.5 Other polymers [i](#)

There are no such residues in this entry.