



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 09:17 PM EDT

PDB ID : 3SHF / pdb_00003shf
Title : Crystal structure of the R265S mutant of full-length murine Apaf-1
Authors : Eschenburg, S.; Reubold, T.F.
Deposited on : 2011-06-16
Resolution : 3.55 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

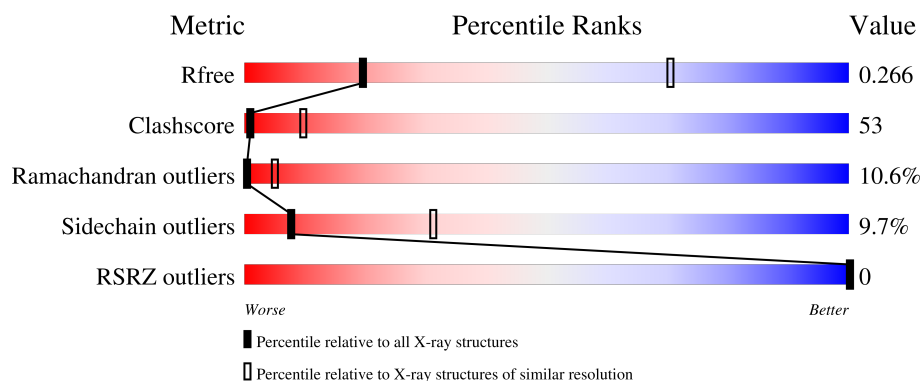
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

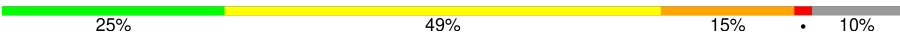
The reported resolution of this entry is 3.55 Å.

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	1410 (3.62-3.50)
Clashscore	190562	1480 (3.62-3.50)
Ramachandran outliers	187476	1440 (3.62-3.50)
Sidechain outliers	187428	1441 (3.62-3.50)
RSRZ outliers	180081	1409 (3.62-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	1256	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9122 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.

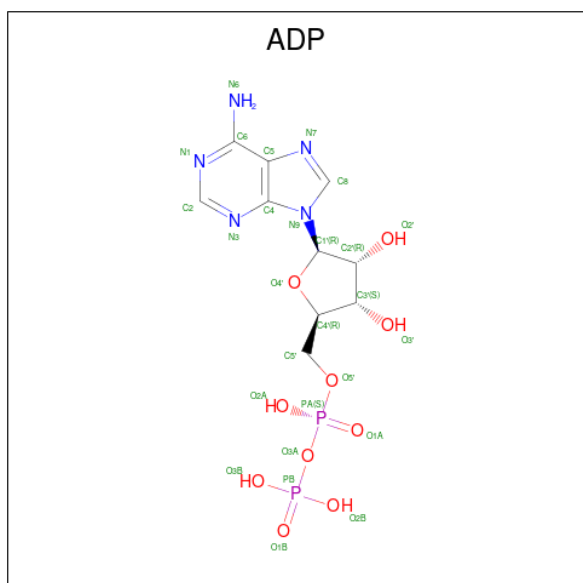
- Molecule 1 is a protein called Apoptotic peptidase activating factor 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1133	9010	5712	1551	1692	55	0	0	0

There are 8 discrepancies between the modelled and reference sequences:

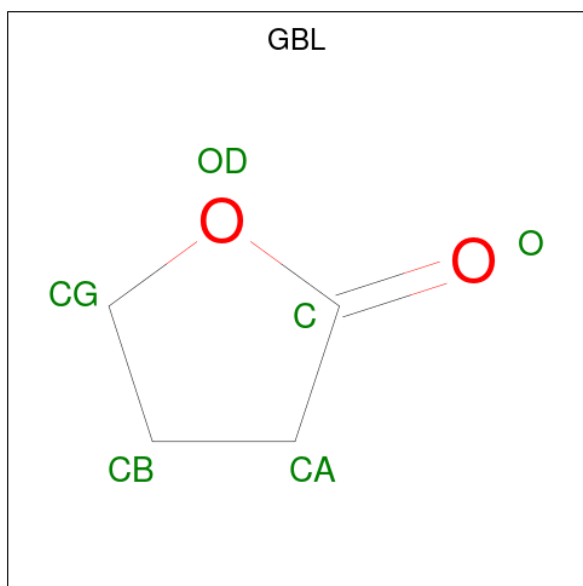
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	GLY	-	expression tag	UNP A2RRK8
A	-5	ALA	-	expression tag	UNP A2RRK8
A	-4	MET	-	expression tag	UNP A2RRK8
A	-3	ASP	-	expression tag	UNP A2RRK8
A	-2	PRO	-	expression tag	UNP A2RRK8
A	-1	GLU	-	expression tag	UNP A2RRK8
A	0	PHE	-	expression tag	UNP A2RRK8
A	265	SER	ARG	engineered mutation	UNP A2RRK8

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is GAMMA-BUTYROLACTONE (CCD ID: GBL) (formula: $C_4H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	4	2		
3	A	1	Total	C	O	0	0
			6	4	2		

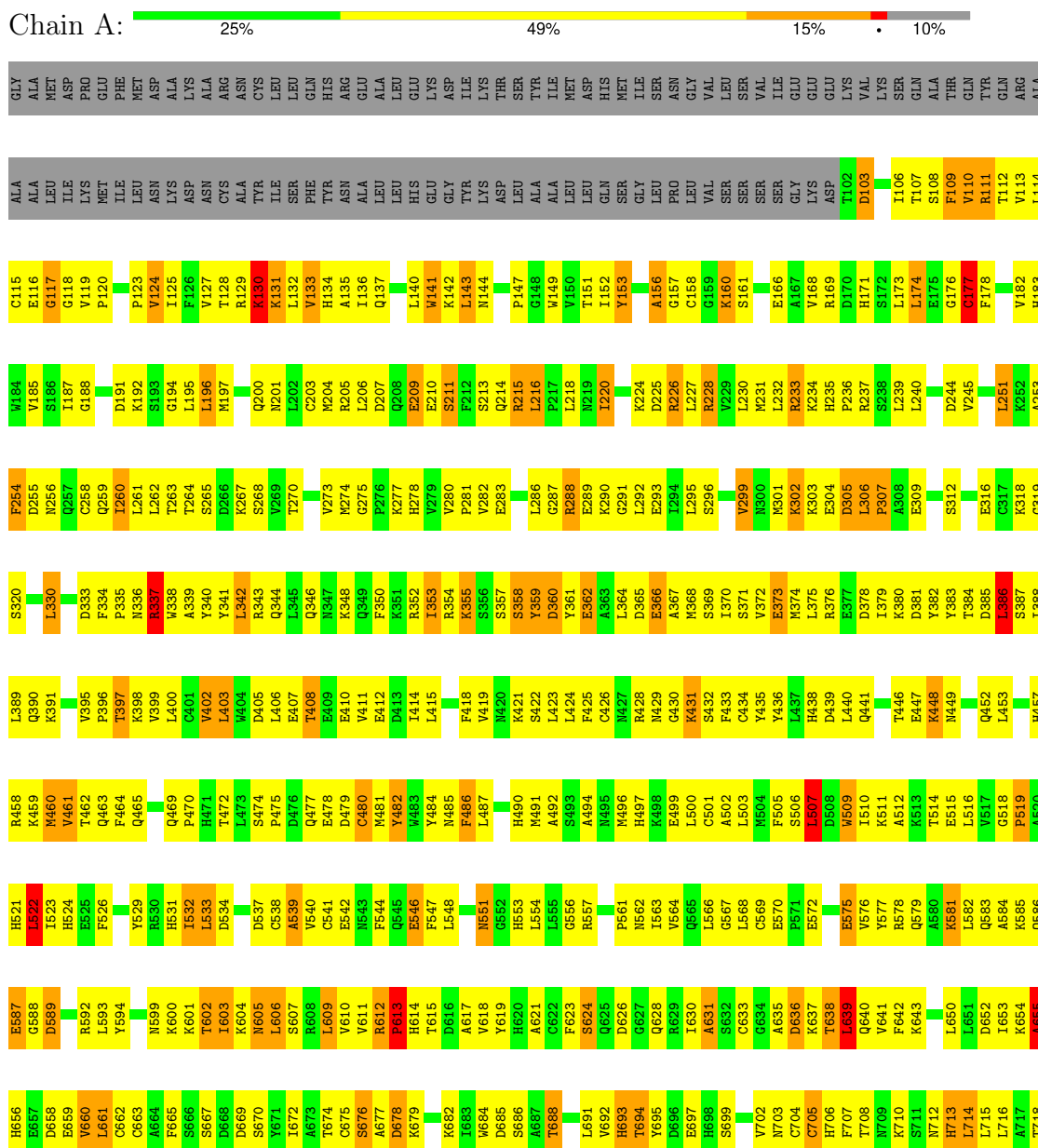
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	73	Total O 73 73	0	0

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: Apoptotic peptidase activating factor 1



L1242	L1243	L1244	L1245	Q1246	Q1247	L1248	E1249	ALA	THR	H1177	G1178	G1179	W1180	W1181	T1182	D1183	V1184	C1185	F1186	S1187	P1188	D1189	S1190	K1191	T1192	L1193	V1194	K1201	W1202	W1203	M1204	V1205	A1206	T1207	S1210	S1211	Q1212	T1213	F1214	M1217	G1218	T1219	N1220	L1221	K1222	K1223	I1224	H1225	V1226	S1227	P1228	D1229	F1230	R1231	T1232	Y1233	V1234	T1235	V1236	D1237	N1238	L1239	G1240	I1241	G1719	S720	N721	D722	F786	F787	LEU	SER	SER	GLU	ASP	PRO	PRO	GLU	L730	L731	Q732	K733	E734	C735	R736	L737	T738	M739	F740	G741	H742	T743	N744	S745	V746	L747	H748	C749	R750	F751	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T776	Q777	Y845	C846	D847	K784	R785	F786	F787	LEU	SER	SER	GLU	ASP	PRO	PRO	GLU	D796	V797	E798	V799	E799	I800	C801	R802	C803	C804	S805	W806	D809	G810	D811	K812	L813	I814	V815	K818	S752	V821	L822	L823	P824	D825	L826	H827	T828	S829	G830	L831	L832	I835	H836	T837	Q838	H839	H840	S841	T842	T843	Q844	Y845	C846	D847	F848	S849	P850	V856	L857	A858	L859	S860	Q861	Y862	C863	F930	Q931	E932	N933	E934	L938	A939	V940	D941	N942	I943	R944	G945	L946	Q947	L948	L949	A950	S951	K952	T953	Q954	Q955	I956	P957	Y958	L959	P960	E961	A962	L963	V964	C967	C968	D969	S970	I966	R967	H972	L973	Y974	Y975	V976	A977	F978	G979	D980	R1051	D982	G983	A984	I985	K986	I987	T988	E989	L990	P991	N992	N993	R994	V995	S998	G1001	H1002	K1003	V1006	R1007	H1008	I1009	Q1010	F1011	T1012	A1013	D1014	G1015	K1016	T1017	L1018	I1019	E1023	D1024	S1025	V1026	I1027	Q1028	V1029	W1030	M1031	W1032	Q1033	T1034	Q1041	A1042	H1043	Q1044	E1045	T1046	V1047	K1048	D1049	F1050	R1051	L1052	L1053	Q1054	R1057	L1058	L1059	S1060	W1061	F1062	S1063	D1064	L1065	T1066	V1067	K1068	V1069	W1070	M1071	V1072	I1073	G1075	R1076	I1077	E1078	R1079	D1080	F1081	T1082	G1083	H1084	T1087	V1088	L1089	S1090	C1091	A1092	I1093	S1094	S1095	D1096	A1097	T1098	S1101	S1102	T1103	S1104	A1105	D1106	K1107	T1108	A1109	K1110	I1111	W1112	S1113	F1114	D1115	L1116	L1117	S1118	P1119	L1120	H1121	E1122	L1123	K1124	G1125	H1126	N1127	G1128	C1129	V1130	R1131	C1132	S1133	A1134	F1135	S1136	L1137	D1138	G1139	I1140	L1141	A1143	T1144	G1145	D1146	D1147	N1148	G1149	E1150	I1151	R1152	I1153	W1154	N1155	V1156	S1157	D1158	G1159	Q1160	L1161	H1162	S1163	C1165	A1166	P1167	I1168	S1169	VAL	GLU	GLU	GLY	THR	L1242	Y1243	L1244	L1245	Q1246	Q1247	L1248	E1249	ALA	THR	H1177	G1178	G1179	W1180	W1181	T1182	D1183	V1184	C1185	F1186	S1187	P1188	D1189	S1190	K1191	T1192	L1193	V1194	K1201	W1202	W1203	M1204	V1205	A1206	T1207	S1210	S1211	Q1212	T1213	F1214	M1217	G1218	T1219	N1220	L1221	K1222	K1223	I1224	H1225	V1226	S1227	P1228	D1229	F1230	R1231	T1232	Y1233	V1234	T1235	V1236	D1237	N1238	L1239	G1240	I1241	G1719	S720	N721	D722	F786	F787	LEU	SER	SER	GLU	ASP	PRO	PRO	GLU	L730	L731	Q732	K733	E734	C735	R736	L737	T738	M739	F740	G741	H742	T743	N744	S745	V746	L747	H748	C749	R750	F751	S752	P753	D754	D755	E756	L757	L758	A759	S760	C761	S762	A763	D764	L767	R768	L769	W770	D771	V772	R773	S774	A775	T776	Q777	Y845	C846	D847	K784	R785	F786	F787	LEU	SER	SER	GLU	ASP	PRO	PRO	GLU	D796	V797	E798	V799	E799	I800	C801	R802	C803	C804	S805	W806	D809	G810	D811	K812	L813	I814	V815	K818	S752	V821	L822	L823	P824	D825	L826	H827	T828	S829	G830	L831	L832	I835	H836	T837	Q838	H839	H840	S841	T842	T843	Q844	Y845	C846	D847	F848	S849	P850	V856	L857	A858	L859	S860	Q861	Y862	C863	F930	Q931	E932	N933	E934	L938	A939	V940	D941	N942	I943	R944	G945	L946	Q947	L948	L949	A950	S951	K952	T953	Q954	Q955	I956	P957	Y958	L959	P960	E961	A962	L963	V964	C967	C968	D969	S970	I966	R967	H972	L973	Y974	Y975	V976	A977	F978	G979	D980	R1051	D982	G983	A984	I985	K986	I987	T988	E989	L990	P991	N992	N993	R994	V995	S998	G1001	H1002	K1003	V1006	R1007	H1008	I1009	Q1010	F1011	T1012	A1013	D1014	G1015	K1016	T1017	L1018	I1019	E1023	D1024	S1025	V1026	I1027	Q1028	V1029	W1030	M1031	W1032	Q1033	T1034	Q1041	A1042	H1043	Q1044	E1045	T1046	V1047	K1048	D1049	F1050	R1051	L1052	L1053	Q1054	R1057	L1058	L1059	S1060	W1061	F1062	S1063	D1064	L1065	T1066	V1067	K1068	V1069	W1070	M1071	V1072	I1073	G1075	R1076	I1077	E1078	R1079	D1080	F1081	T1082	G1083	H1084	T1087	V1088	L1089	S1090	C1091	A1092	I1093	S1094	S1095	D1096	A1097	T1098	S1101	S1102	T1103	S1104	A1105	D1106	K1107	T1108	A1109	K1110	I1111	W1112	S1113	F1114	D1115	L1116	L1117	S1118	P1119	L1120	H1121	E1122	L1123	K1124	G1125	H1126	N1127	G1128	C1129	V1130	R1131	C1132	S1133	A1134	F1135	S1136	L1137	D1138	G1139	I1140	L1141	A1143	T1144	G1145	D1146	D1147	N1148	G1149	E1150	I1151	R1152	I1153	W1154	N1155	V1156	S1157	D1158	G1159	Q1160	L1161	H1162	S1163	C1165	A1166	P1167	I1168	S1169	VAL	GLU	GLU	GLY	THR
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4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	72.88Å 111.82Å 244.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.55 20.00 – 3.55	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-3.55) 98.9 (20.00-3.55)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.83 (at 3.57Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.305 0.212 , 0.266	Depositor DCC
R_{free} test set	8050 reflections (3.99%)	wwPDB-VP
Wilson B-factor (Å ²)	98.8	Xtriage
Anisotropy	0.646	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 64.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9122	wwPDB-VP
Average B, all atoms (Å ²)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: GBL, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	0/9206	1.05	69/12465 (0.6%)

There are no bond length outliers.

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	460	MET	N-CA-C	-10.61	95.71	110.35
1	A	871	SER	N-CA-C	-9.33	101.91	113.38
1	A	1113	SER	N-CA-C	8.99	124.16	111.30
1	A	109	PHE	N-CA-C	-7.91	101.30	112.13
1	A	429	ASN	N-CA-C	-7.73	103.18	114.39
1	A	1163	HIS	N-CA-C	7.66	121.04	110.24
1	A	509	TRP	N-CA-C	-7.42	103.12	111.14
1	A	636	ASP	N-CA-C	-7.42	104.32	113.15
1	A	821	VAL	N-CA-C	-7.32	97.57	108.85
1	A	110	VAL	N-CA-C	-7.29	102.30	110.62
1	A	1034	THR	N-CA-C	-7.29	102.51	111.40
1	A	143	LEU	N-CA-C	-7.26	104.95	113.88
1	A	141	TRP	N-CA-C	-7.25	103.38	111.28
1	A	639	LEU	N-CA-C	-7.20	98.50	109.95
1	A	133	VAL	N-CA-C	-7.11	102.17	111.05
1	A	722	ASP	N-CA-C	-7.04	103.87	113.30
1	A	767	LEU	N-CA-C	-7.04	97.74	109.07
1	A	678	ASP	N-CA-C	-7.01	104.72	113.20
1	A	1062	SER	N-CA-C	6.31	116.61	108.34
1	A	474	SER	CA-C-N	6.31	127.73	119.84
1	A	474	SER	C-N-CA	6.31	127.73	119.84
1	A	676	SER	N-CA-C	6.23	116.67	108.07
1	A	1083	CYS	N-CA-C	6.22	119.90	112.93
1	A	1006	VAL	N-CA-C	6.15	116.68	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	661	LEU	N-CA-C	6.09	120.32	113.01
1	A	389	LEU	N-CA-C	-6.09	98.15	108.26
1	A	624	SER	N-CA-C	-6.07	102.36	110.55
1	A	998	SER	N-CA-C	6.04	118.77	108.02
1	A	390	GLN	N-CA-C	6.03	118.69	110.55
1	A	260	ILE	N-CA-C	5.99	116.56	108.17
1	A	1026	VAL	N-CA-C	5.87	117.03	108.58
1	A	903	ASP	N-CA-C	-5.79	105.38	113.37
1	A	655	ALA	N-CA-C	5.68	122.89	110.80
1	A	762	SER	N-CA-C	5.68	118.12	109.95
1	A	1057	ARG	N-CA-C	-5.67	101.31	110.32
1	A	849	SER	CA-C-N	5.66	125.19	119.19
1	A	849	SER	C-N-CA	5.66	125.19	119.19
1	A	265	SER	N-CA-C	-5.60	105.76	112.59
1	A	1219	THR	N-CA-C	5.58	115.38	108.19
1	A	891	SER	N-CA-C	-5.57	102.18	110.20
1	A	1065	GLY	N-CA-C	-5.57	108.17	115.47
1	A	342	LEU	N-CA-C	-5.57	104.63	111.75
1	A	1027	ILE	N-CA-C	-5.54	100.64	109.17
1	A	1082	THR	N-CA-C	-5.50	101.29	109.11
1	A	151	THR	N-CA-C	5.41	117.55	108.73
1	A	379	ILE	N-CA-C	-5.40	107.49	112.83
1	A	539	ALA	N-CA-C	-5.36	104.32	111.87
1	A	357	SER	N-CA-C	5.35	116.71	109.11
1	A	254	PHE	N-CA-C	-5.34	106.15	113.30
1	A	906	ILE	N-CA-C	-5.33	100.65	108.11
1	A	734	GLU	N-CA-C	5.30	117.32	109.69
1	A	862	TYR	N-CA-C	5.29	122.06	110.80
1	A	191	ASP	N-CA-C	-5.28	101.68	109.86
1	A	660	VAL	N-CA-C	5.28	114.34	106.85
1	A	459	LYS	N-CA-C	-5.27	105.71	111.82
1	A	805	SER	N-CA-C	5.27	118.32	110.52
1	A	537	ASP	N-CA-C	-5.25	106.81	113.43
1	A	631	ALA	N-CA-C	-5.21	101.67	109.95
1	A	1010	GLN	N-CA-C	5.19	116.97	108.76
1	A	761	CYS	CA-CB-SG	-5.15	102.55	114.40
1	A	144	ASN	CB-CA-C	-5.11	110.28	117.23
1	A	1214	PHE	N-CA-C	5.10	121.67	110.80
1	A	879	ARG	N-CA-C	-5.09	101.45	109.25
1	A	800	ILE	N-CA-C	5.08	115.41	107.99
1	A	740	PHE	N-CA-C	-5.07	102.36	109.96
1	A	115	CYS	N-CA-C	-5.06	106.61	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	306	LEU	CA-C-N	5.05	126.16	119.84
1	A	306	LEU	C-N-CA	5.05	126.16	119.84
1	A	507	LEU	N-CA-C	-5.00	105.91	111.36

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	9010	0	8875	954	0
2	A	27	0	12	3	0
3	A	12	0	12	1	0
4	A	73	0	0	3	0
All	All	9122	0	8899	954	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 53.

All (954) 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)
1:A:216:LEU:HD12	1:A:216:LEU:H	1.13	1.08
1:A:182:VAL:HG12	1:A:239:LEU:HB3	1.36	1.06
1:A:1108:THR:HG21	1:A:1124:LYS:HA	1.35	1.05
1:A:288:ARG:HE	1:A:288:ARG:N	1.58	1.00
1:A:785:ARG:HG3	1:A:785:ARG:HH11	1.28	0.97
1:A:992:ASN:HD21	1:A:995:VAL:N	1.63	0.96
1:A:342:LEU:O	1:A:346:GLN:HG2	1.64	0.96
1:A:288:ARG:H	1:A:288:ARG:NE	1.62	0.96
1:A:1002:HIS:HA	1:A:1003:LYS:HZ3	1.27	0.96
1:A:1150:GLU:HA	1:A:1166:ALA:HB1	1.45	0.96
1:A:575:GLU:HG2	1:A:578:ARG:HH11	1.29	0.94
1:A:785:ARG:H	1:A:785:ARG:HD2	1.29	0.94
1:A:612:ARG:HG3	1:A:905:THR:HG22	1.49	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:856:VAL:HG12	1:A:866:LEU:HB3	1.49	0.92
1:A:1029:VAL:HG11	1:A:1072:VAL:HG13	1.52	0.91
1:A:1084:HIS:ND1	1:A:1107:LYS:HE2	1.85	0.91
1:A:896:SER:HB2	1:A:909:TRP:O	1.69	0.91
1:A:204:MET:HE1	1:A:481:MET:HE2	1.53	0.91
1:A:1107:LYS:HD2	1:A:1108:THR:H	1.34	0.90
1:A:603:ILE:HG22	1:A:604:LYS:H	1.34	0.90
1:A:675:CYS:HB2	1:A:702:VAL:HG11	1.54	0.89
1:A:767:LEU:HD11	1:A:813:ILE:HD13	1.53	0.89
1:A:659:GLU:O	1:A:676:SER:HB2	1.71	0.89
1:A:1167:PRO:HD2	1:A:1203:TRP:HH2	1.39	0.88
1:A:682:LYS:HG2	1:A:694:THR:HG22	1.54	0.87
1:A:618:VAL:HG11	1:A:906:ILE:HD11	1.54	0.87
1:A:760:SER:HB3	1:A:770:TRP:HZ3	1.38	0.87
1:A:658:ASP:OD2	1:A:677:ALA:HB3	1.73	0.86
1:A:1016:LYS:HG2	1:A:1033:GLN:OE1	1.76	0.86
1:A:1112:TRP:HA	1:A:1120:LEU:HG	1.55	0.86
1:A:1139:GLY:O	1:A:1140:ILE:HG22	1.75	0.86
1:A:448:LYS:HZ2	1:A:449:ASN:HD21	1.23	0.86
1:A:732:GLN:HG2	1:A:734:GLU:H	1.36	0.86
1:A:785:ARG:HD2	1:A:785:ARG:N	1.92	0.84
1:A:1012:THR:HA	1:A:1052:LEU:HD21	1.59	0.84
1:A:1053:LEU:HB3	1:A:1057:ARG:HG3	1.58	0.84
1:A:1140:ILE:HG13	1:A:1156:VAL:HB	1.58	0.84
1:A:1151:ILE:H	1:A:1166:ALA:HB2	1.43	0.84
1:A:529:TYR:O	1:A:533:LEU:HB2	1.78	0.83
1:A:1125:GLY:HA3	1:A:1152:ARG:HH12	1.44	0.82
1:A:1167:PRO:HD2	1:A:1203:TRP:CH2	2.14	0.82
1:A:1112:TRP:HB3	1:A:1119:PRO:HA	1.61	0.82
1:A:714:LEU:HD23	1:A:714:LEU:O	1.80	0.81
1:A:920:ILE:HG23	1:A:921:VAL:HG23	1.61	0.81
1:A:448:LYS:NZ	1:A:449:ASN:HD21	1.78	0.81
1:A:491:MET:HE3	1:A:500:LEU:HD12	1.61	0.81
1:A:971:PRO:O	1:A:972:HIS:HB2	1.78	0.81
1:A:1151:ILE:HD11	1:A:1193:LEU:HD21	1.61	0.80
1:A:153:TYR:HE2	1:A:281:PRO:HG3	1.46	0.80
1:A:826:ILE:HG12	1:A:826:ILE:O	1.80	0.80
1:A:1071:ASN:HD21	1:A:1074:THR:HB	1.48	0.79
1:A:1138:ASP:O	1:A:1140:ILE:N	2.13	0.79
1:A:1074:THR:O	1:A:1076:ARG:N	2.16	0.79
1:A:1091:CYS:HB2	1:A:1102:SER:O	1.83	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:HD13	1:A:282:VAL:HG22	1.64	0.79
1:A:1106:ASP:O	1:A:1107:LYS:HB3	1.83	0.79
1:A:538:CYS:HB2	1:A:540:VAL:HG23	1.65	0.78
1:A:910:GLU:HG3	1:A:913:LYS:HB3	1.65	0.78
1:A:1136:SER:O	1:A:1138:ASP:N	2.14	0.78
1:A:546:GLU:HG2	1:A:612:ARG:HH22	1.46	0.78
1:A:1146:ASP:HB3	1:A:1150:GLU:O	1.83	0.78
1:A:1003:LYS:CE	1:A:1003:LYS:H	1.97	0.78
1:A:893:ASP:OD2	1:A:895:SER:HB3	1.85	0.77
1:A:1053:LEU:HD23	1:A:1059:LEU:HB2	1.66	0.77
1:A:309:GLU:HG2	1:A:339:ALA:HA	1.66	0.77
1:A:220:ILE:HD12	1:A:220:ILE:H	1.49	0.77
1:A:1091:CYS:HB3	1:A:1103:THR:HA	1.66	0.77
1:A:946:LEU:HD23	1:A:964:VAL:HG11	1.65	0.77
1:A:1112:TRP:HD1	1:A:1119:PRO:HB3	1.49	0.76
1:A:692:VAL:O	1:A:693:HIS:HB2	1.85	0.76
1:A:107:THR:C	1:A:109:PHE:H	1.93	0.76
1:A:663:CYS:HB3	1:A:674:THR:HG22	1.66	0.76
1:A:228:ARG:HG3	1:A:256:ASN:HB3	1.67	0.76
1:A:619:TYR:HE2	1:A:635:ALA:HB2	1.51	0.76
1:A:364:LEU:CD2	1:A:440:LEU:HB3	2.16	0.75
1:A:1003:LYS:H	1:A:1003:LYS:HE2	1.48	0.75
1:A:364:LEU:HD22	1:A:440:LEU:HB3	1.68	0.75
1:A:531:HIS:CD2	1:A:532:ILE:HG22	2.22	0.75
1:A:288:ARG:HE	1:A:288:ARG:H	0.82	0.75
1:A:930:PHE:CD2	1:A:1227:SER:HA	2.22	0.75
1:A:940:VAL:HG13	1:A:964:VAL:CG2	2.16	0.75
1:A:228:ARG:HB3	1:A:228:ARG:NH1	2.02	0.74
1:A:785:ARG:H	1:A:785:ARG:CD	2.00	0.74
1:A:382:TYR:CE2	1:A:414:ILE:HD13	2.23	0.74
1:A:129:ARG:HB3	1:A:131:LYS:HZ3	1.51	0.74
1:A:760:SER:CB	1:A:770:TRP:HZ3	2.01	0.73
1:A:992:ASN:HD21	1:A:995:VAL:H	1.35	0.73
1:A:785:ARG:HG3	1:A:785:ARG:NH1	1.98	0.73
1:A:305:ASP:O	1:A:307:PRO:HD3	1.88	0.73
1:A:864:VAL:O	1:A:878:CYS:HB3	1.88	0.73
1:A:214:GLN:HG2	1:A:215:ARG:H	1.51	0.73
1:A:204:MET:CE	1:A:481:MET:HE2	2.19	0.73
1:A:1141:LEU:HD11	1:A:1162:LEU:HD22	1.71	0.73
1:A:804:CYS:HB2	1:A:815:VAL:HG12	1.70	0.72
1:A:153:TYR:CE2	1:A:281:PRO:HG3	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1212:GLN:HE21	1:A:1212:GLN:C	1.96	0.72
1:A:408:THR:HG22	1:A:412:GLU:OE1	1.89	0.72
1:A:130:LYS:HD2	1:A:131:LYS:H	1.53	0.72
1:A:382:TYR:HD2	1:A:414:ILE:HG21	1.54	0.71
1:A:1029:VAL:HG11	1:A:1072:VAL:CG1	2.19	0.71
1:A:1107:LYS:HB3	1:A:1107:LYS:HZ2	1.54	0.71
1:A:426:CYS:HB3	1:A:435:TYR:CD1	2.26	0.71
1:A:460:MET:O	1:A:461:VAL:HG22	1.90	0.71
1:A:382:TYR:HE2	1:A:414:ILE:HD13	1.55	0.71
1:A:396:PRO:HG2	1:A:399:VAL:HG23	1.72	0.71
1:A:762:SER:O	1:A:801:VAL:HG22	1.90	0.71
1:A:539:ALA:C	1:A:541:CYS:H	1.98	0.71
1:A:714:LEU:HD21	1:A:730:LEU:HB2	1.71	0.71
1:A:178:PHE:CD1	1:A:239:LEU:HB2	2.26	0.71
1:A:446:THR:HG23	1:A:453:LEU:HD11	1.70	0.71
1:A:1042:ALA:HB1	1:A:1044:GLN:HG3	1.72	0.71
1:A:623:PHE:CD2	1:A:891:SER:HA	2.26	0.71
1:A:718:THR:O	1:A:725:LEU:HD23	1.90	0.71
1:A:841:SER:HB2	1:A:860:SER:OG	1.90	0.71
1:A:744:ASN:CG	1:A:745:SER:H	1.99	0.71
1:A:938:LEU:HD23	1:A:947:GLN:O	1.91	0.71
1:A:974:GLU:HG2	1:A:975:TYR:N	2.04	0.70
1:A:233:ARG:O	1:A:234:LYS:HB3	1.92	0.70
1:A:656:HIS:HE1	1:A:674:THR:OG1	1.74	0.70
1:A:656:HIS:HB3	1:A:678:ASP:OD2	1.90	0.70
1:A:675:CYS:HB2	1:A:702:VAL:CG1	2.21	0.70
1:A:1211:SER:C	1:A:1213:THR:H	1.97	0.70
1:A:618:VAL:HG23	1:A:904:GLN:HA	1.73	0.70
1:A:196:LEU:O	1:A:200:GLN:HG3	1.90	0.69
1:A:1160:GLN:C	1:A:1161:LEU:HD12	2.16	0.69
1:A:561:PRO:HB2	1:A:566:LEU:HD11	1.75	0.69
1:A:902:ASP:C	1:A:904:GLN:H	1.99	0.69
1:A:949:ILE:HG23	1:A:956:ILE:HD11	1.75	0.69
1:A:960:PRO:O	1:A:961:GLU:HB2	1.91	0.69
1:A:107:THR:OG1	1:A:110:VAL:HG23	1.93	0.69
1:A:532:ILE:O	1:A:532:ILE:HD12	1.92	0.69
1:A:568:LEU:HD23	1:A:577:TYR:HE2	1.56	0.69
1:A:1107:LYS:CD	1:A:1108:THR:H	2.06	0.69
1:A:395:VAL:O	1:A:434:CYS:HA	1.93	0.69
1:A:713:HIS:H	1:A:713:HIS:CD2	2.08	0.69
1:A:742:HIS:CE1	1:A:768:ARG:HG3	2.28	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:MET:HE3	1:A:275:GLY:H	1.57	0.68
1:A:898:LEU:HD12	1:A:898:LEU:C	2.18	0.68
1:A:614:HIS:CE1	1:A:640:GLN:HG3	2.28	0.68
1:A:986:LYS:HG2	1:A:998:SER:HB3	1.74	0.68
1:A:879:ARG:HH12	1:A:882:LEU:HG	1.57	0.68
1:A:1042:ALA:C	1:A:1044:GLN:H	1.98	0.68
1:A:1151:ILE:H	1:A:1166:ALA:CB	2.05	0.68
1:A:216:LEU:HD12	1:A:216:LEU:N	1.98	0.68
1:A:400:LEU:HD13	1:A:415:LEU:HD11	1.75	0.68
1:A:334:PHE:HB3	1:A:337:ARG:HD3	1.74	0.68
1:A:131:LYS:H	1:A:131:LYS:HD3	1.58	0.68
1:A:661:LEU:HD12	1:A:702:VAL:O	1.94	0.68
1:A:1008:HIS:HB2	1:A:1049:ASP:OD1	1.94	0.67
1:A:507:LEU:HD12	1:A:579:GLN:HB3	1.75	0.67
1:A:448:LYS:HG2	1:A:449:ASN:ND2	2.09	0.67
1:A:464:PHE:CE1	1:A:487:LEU:HD22	2.29	0.67
1:A:396:PRO:HD2	1:A:399:VAL:HG21	1.74	0.67
1:A:938:LEU:HD12	1:A:969:LEU:HG	1.76	0.67
1:A:1091:CYS:CB	1:A:1103:THR:HA	2.24	0.67
1:A:920:ILE:HG23	1:A:921:VAL:N	2.09	0.67
1:A:722:ASP:C	1:A:723:PHE:HD1	2.03	0.66
1:A:1116:LEU:H	1:A:1116:LEU:HD12	1.59	0.66
1:A:723:PHE:HD1	1:A:723:PHE:N	1.93	0.66
1:A:149:TRP:CZ2	1:A:273:VAL:HG21	2.31	0.66
1:A:176:GLY:O	1:A:177:CYS:HB2	1.94	0.66
1:A:849:SER:OG	1:A:850:PRO:HD2	1.95	0.66
1:A:270:THR:O	1:A:277:LYS:HE2	1.94	0.66
1:A:245:VAL:HG11	1:A:251:LEU:HD13	1.77	0.66
1:A:522:LEU:HD22	1:A:526:PHE:HE2	1.61	0.66
1:A:638:THR:HB	1:A:653:ILE:O	1.95	0.66
1:A:255:ASP:OD2	1:A:273:VAL:HG23	1.94	0.66
1:A:942:ASN:H	1:A:942:ASN:ND2	1.93	0.66
1:A:723:PHE:N	1:A:723:PHE:CD1	2.62	0.66
1:A:1248:LEU:HD22	1:A:1249:GLU:HG2	1.78	0.66
1:A:1019:ILE:N	1:A:1019:ILE:HD12	2.11	0.65
1:A:129:ARG:HB3	1:A:131:LYS:NZ	2.11	0.65
1:A:1211:SER:O	1:A:1213:THR:N	2.29	0.65
1:A:665:PHE:CE1	1:A:672:ILE:HD11	2.32	0.65
1:A:458:ARG:HG3	1:A:496:MET:CE	2.27	0.65
1:A:1064:ASP:HB2	1:A:1066:THR:OG1	1.97	0.65
1:A:1141:LEU:HD11	1:A:1162:LEU:CD2	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:THR:OG1	1:A:109:PHE:HB3	1.97	0.65
1:A:685:ASP:OD2	1:A:688:THR:HG23	1.97	0.65
1:A:532:ILE:HD12	1:A:532:ILE:C	2.22	0.64
1:A:802:LYS:O	1:A:803:CYS:O	2.16	0.64
1:A:1059:LEU:HD11	1:A:1067:VAL:CG1	2.27	0.64
1:A:218:LEU:HD22	1:A:518:GLY:CA	2.27	0.64
1:A:274:MET:HE3	1:A:275:GLY:N	2.12	0.64
1:A:1053:LEU:HD12	1:A:1054:GLN:H	1.61	0.64
1:A:1248:LEU:CD2	1:A:1249:GLU:HG2	2.27	0.64
1:A:1054:GLN:HB2	1:A:1057:ARG:HD3	1.78	0.64
1:A:514:THR:HA	1:A:518:GLY:O	1.98	0.64
1:A:924:GLN:HG2	1:A:1236:VAL:HG12	1.79	0.64
1:A:942:ASN:H	1:A:942:ASN:HD22	1.45	0.64
1:A:1074:THR:HG22	1:A:1076:ARG:HB2	1.80	0.64
1:A:713:HIS:H	1:A:713:HIS:HD2	1.46	0.63
1:A:742:HIS:HE1	1:A:768:ARG:HG3	1.61	0.63
1:A:1107:LYS:CG	1:A:1108:THR:N	2.61	0.63
1:A:1001:GLY:O	1:A:1002:HIS:HB2	1.99	0.63
1:A:676:SER:O	1:A:702:VAL:HG12	1.98	0.63
1:A:1071:ASN:ND2	1:A:1074:THR:HB	2.13	0.63
1:A:376:ARG:HH11	1:A:376:ARG:HB2	1.63	0.63
1:A:946:LEU:CD2	1:A:964:VAL:HG11	2.28	0.63
1:A:1110:LYS:HE2	1:A:1122:GLU:OE2	1.97	0.63
1:A:599:ASN:HB2	1:A:602:THR:OG1	1.99	0.63
1:A:1125:GLY:HA3	1:A:1152:ARG:NH1	2.14	0.63
1:A:1237:ASP:O	1:A:1239:LEU:N	2.32	0.63
1:A:697:GLU:HB3	1:A:726:LYS:HE3	1.81	0.63
1:A:114:LEU:HD11	1:A:169:ARG:HA	1.81	0.62
1:A:481:MET:O	1:A:482:TYR:C	2.42	0.62
1:A:971:PRO:O	1:A:972:HIS:CB	2.47	0.62
1:A:1111:ILE:HD13	1:A:1111:ILE:C	2.25	0.62
1:A:399:VAL:O	1:A:402:VAL:HG23	1.97	0.62
1:A:942:ASN:HD22	1:A:942:ASN:N	1.96	0.62
1:A:337:ARG:HG3	1:A:341:TYR:CE2	2.35	0.62
1:A:1116:LEU:C	1:A:1118:SER:H	2.08	0.62
1:A:1140:ILE:HG23	1:A:1140:ILE:O	1.99	0.62
1:A:237:ARG:HG2	1:A:237:ARG:HH11	1.65	0.62
1:A:919:ALA:HB2	1:A:947:GLN:OE1	2.00	0.62
1:A:337:ARG:HH21	1:A:374:MET:CE	2.13	0.62
1:A:402:VAL:O	1:A:463:GLN:HB3	2.00	0.62
1:A:1227:SER:HB3	1:A:1232:THR:HB	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:PHE:CE1	1:A:1142:LEU:HG	2.35	0.61
1:A:1236:VAL:HG23	1:A:1242:LEU:HD23	1.81	0.61
1:A:430:GLY:C	1:A:432:SER:H	2.07	0.61
1:A:1236:VAL:CG2	1:A:1242:LEU:HD23	2.29	0.61
1:A:1248:LEU:HD23	1:A:1249:GLU:H	1.64	0.61
1:A:303:LYS:H	1:A:306:LEU:HG	1.66	0.61
1:A:881:HIS:HE1	1:A:907:ARG:HG3	1.65	0.61
1:A:1108:THR:CG2	1:A:1124:LYS:HA	2.21	0.61
1:A:1237:ASP:C	1:A:1239:LEU:H	2.08	0.61
1:A:1065:GLY:HA3	1:A:1084:HIS:O	2.01	0.61
1:A:1097:ALA:O	1:A:1098:THR:HB	2.01	0.61
1:A:1135:PHE:CD1	1:A:1142:LEU:HB2	2.36	0.61
1:A:210:GLU:HG2	1:A:214:GLN:HG3	1.82	0.61
1:A:804:CYS:CB	1:A:815:VAL:HG12	2.29	0.61
1:A:251:LEU:HD11	1:A:262:LEU:HD13	1.81	0.61
1:A:1153:ILE:O	1:A:1162:LEU:HB3	2.01	0.60
1:A:215:ARG:HH12	1:A:557:ARG:HD3	1.65	0.60
1:A:974:GLU:HA	1:A:991:PRO:HD3	1.82	0.60
1:A:491:MET:HE1	1:A:503:LEU:HB3	1.83	0.60
1:A:879:ARG:NH1	1:A:882:LEU:HG	2.16	0.60
1:A:1135:PHE:HD1	1:A:1142:LEU:HB2	1.64	0.60
1:A:194:GLY:HA2	1:A:197:MET:HE3	1.84	0.60
1:A:239:LEU:HD12	1:A:240:LEU:H	1.66	0.60
1:A:499:GLU:O	1:A:502:ALA:HB3	2.02	0.60
1:A:803:CYS:SG	1:A:846:CYS:C	2.84	0.60
1:A:341:TYR:HA	1:A:344:GLN:HG2	1.81	0.60
1:A:484:TYR:CE2	1:A:516:LEU:HD12	2.36	0.60
1:A:551:ASN:HD22	1:A:566:LEU:HD22	1.66	0.60
1:A:1107:LYS:HG2	1:A:1108:THR:N	2.17	0.60
1:A:1113:SER:C	1:A:1115:ASP:H	2.09	0.60
1:A:470:PRO:HB3	1:A:503:LEU:CD1	2.31	0.60
1:A:821:VAL:O	1:A:822:LEU:HD13	2.02	0.60
1:A:563:ILE:O	1:A:563:ILE:HG13	2.02	0.59
1:A:547:PHE:CD1	1:A:576:VAL:HG11	2.38	0.59
1:A:636:ASP:O	1:A:638:THR:HG23	2.03	0.59
1:A:918:SER:OG	1:A:920:ILE:HG22	2.02	0.59
1:A:970:SER:HB3	1:A:1011:PHE:CE2	2.38	0.59
1:A:1165:CYS:C	1:A:1167:PRO:HD3	2.27	0.59
1:A:302:LYS:HE2	1:A:304:GLU:HG3	1.83	0.59
1:A:376:ARG:HB2	1:A:376:ARG:NH1	2.17	0.59
1:A:1003:LYS:HE3	1:A:1024:ASP:OD1	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1058:LEU:HD23	1:A:1058:LEU:O	2.03	0.59
1:A:1084:HIS:CE1	1:A:1107:LYS:HE2	2.37	0.59
1:A:117:GLY:HA3	1:A:182:VAL:O	2.02	0.59
1:A:366:GLU:O	1:A:367:ALA:C	2.46	0.59
1:A:539:ALA:C	1:A:541:CYS:N	2.59	0.59
1:A:1059:LEU:HD12	1:A:1068:LYS:O	2.02	0.59
1:A:1126:HIS:ND1	1:A:1146:ASP:HB2	2.17	0.59
1:A:1131:ARG:O	1:A:1132:CYS:HB3	2.03	0.59
1:A:1121:HIS:HB3	1:A:1158:ASP:O	2.03	0.59
1:A:1191:LYS:HA	1:A:1205:VAL:HG21	1.85	0.59
1:A:215:ARG:HD2	1:A:556:GLY:O	2.02	0.59
1:A:603:ILE:HG22	1:A:604:LYS:N	2.14	0.59
1:A:161:SER:HB2	2:A:1250:ADP:O2A	2.03	0.59
1:A:977:ALA:HB2	1:A:987:ILE:HG12	1.84	0.59
1:A:361:TYR:O	1:A:362:GLU:C	2.46	0.59
1:A:802:LYS:O	1:A:803:CYS:C	2.45	0.59
1:A:1093:ILE:HG13	1:A:1095:SER:H	1.68	0.59
1:A:225:ASP:O	1:A:226:ARG:C	2.46	0.58
1:A:534:ASP:HB2	1:A:541:CYS:HB2	1.84	0.58
1:A:926:ILE:HG22	1:A:939:ALA:CB	2.32	0.58
1:A:360:ASP:OD1	1:A:440:LEU:HD21	2.03	0.58
1:A:448:LYS:HG2	1:A:449:ASN:HD22	1.67	0.58
1:A:1194:VAL:HG23	1:A:1202:TRP:CD1	2.37	0.58
1:A:262:LEU:HD23	1:A:262:LEU:H	1.68	0.58
1:A:568:LEU:HD23	1:A:577:TYR:CE2	2.37	0.58
1:A:722:ASP:C	1:A:723:PHE:CD1	2.81	0.58
1:A:1131:ARG:O	1:A:1131:ARG:HG2	2.02	0.58
1:A:113:VAL:HG11	1:A:174:LEU:HD21	1.84	0.58
1:A:353:ILE:HG12	1:A:354:ARG:H	1.68	0.58
1:A:522:LEU:HD22	1:A:526:PHE:CE2	2.37	0.58
1:A:639:LEU:O	1:A:640:GLN:HG2	2.03	0.58
1:A:921:VAL:HB	1:A:942:ASN:OD1	2.03	0.58
1:A:1116:LEU:HD12	1:A:1116:LEU:N	2.19	0.58
1:A:1146:ASP:CB	1:A:1150:GLU:HB3	2.34	0.58
1:A:714:LEU:CD2	1:A:730:LEU:HB2	2.34	0.58
1:A:846:CYS:HB2	1:A:857:ILE:HG22	1.84	0.58
1:A:938:LEU:HD11	1:A:976:VAL:CG2	2.34	0.58
1:A:1042:ALA:C	1:A:1044:GLN:N	2.62	0.58
1:A:1059:LEU:HD11	1:A:1067:VAL:HG12	1.84	0.58
1:A:570:GLU:O	1:A:600:LYS:HE2	2.04	0.58
1:A:760:SER:CB	1:A:770:TRP:CZ3	2.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1003:LYS:HE2	1:A:1003:LYS:N	2.17	0.58
1:A:1042:ALA:HB1	1:A:1044:GLN:CG	2.33	0.58
1:A:604:LYS:HD3	1:A:606:LEU:HD21	1.85	0.58
1:A:938:LEU:HD13	1:A:967:CYS:SG	2.44	0.58
1:A:953:THR:O	1:A:954:GLY:C	2.46	0.58
1:A:1177:HIS:CD2	1:A:1178:GLY:H	2.20	0.58
1:A:953:THR:O	1:A:953:THR:HG22	2.02	0.58
1:A:382:TYR:CD2	1:A:414:ILE:HG21	2.38	0.58
1:A:130:LYS:HD2	1:A:131:LYS:HD3	1.85	0.57
1:A:1107:LYS:HB3	1:A:1107:LYS:NZ	2.17	0.57
1:A:619:TYR:CE2	1:A:635:ALA:HB2	2.36	0.57
1:A:811:ASP:HA	1:A:826:ILE:HG21	1.84	0.57
1:A:938:LEU:HG	1:A:948:LEU:HD22	1.85	0.57
1:A:1116:LEU:H	1:A:1116:LEU:CD1	2.18	0.57
1:A:1129:CYS:SG	1:A:1147:ASP:HB2	2.44	0.57
1:A:630:ILE:HD12	1:A:642:PHE:HE2	1.69	0.57
1:A:705:CYS:HB3	1:A:718:THR:HG22	1.87	0.57
1:A:225:ASP:O	1:A:227:LEU:N	2.38	0.57
1:A:107:THR:C	1:A:109:PHE:N	2.60	0.57
1:A:1027:ILE:HG13	1:A:1047:VAL:HG21	1.86	0.57
1:A:330:LEU:HD22	1:A:341:TYR:CE2	2.40	0.57
1:A:511:LYS:HE3	1:A:515:GLU:OE2	2.05	0.57
1:A:767:LEU:HD23	1:A:768:ARG:N	2.20	0.57
1:A:783:VAL:HG12	1:A:786:PHE:HE2	1.69	0.57
1:A:1222:LYS:O	1:A:1223:LYS:O	2.23	0.57
1:A:224:LYS:O	1:A:227:LEU:HB3	2.05	0.57
1:A:130:LYS:HA	1:A:133:VAL:HG23	1.86	0.57
1:A:192:LYS:HE3	4:A:1266:HOH:O	2.04	0.57
1:A:605:ASN:O	1:A:606:LEU:C	2.48	0.57
1:A:752:SER:O	1:A:753:PRO:C	2.47	0.57
1:A:1211:SER:C	1:A:1213:THR:N	2.62	0.57
1:A:697:GLU:CB	1:A:726:LYS:HE3	2.35	0.56
1:A:1183:ASP:OD1	1:A:1223:LYS:HE3	2.04	0.56
1:A:938:LEU:HD11	1:A:976:VAL:HG23	1.87	0.56
1:A:123:PRO:O	1:A:124:VAL:C	2.49	0.56
1:A:337:ARG:HH21	1:A:374:MET:HE1	1.71	0.56
1:A:410:GLU:O	1:A:414:ILE:HG13	2.05	0.56
1:A:682:LYS:HG2	1:A:694:THR:CG2	2.30	0.56
1:A:768:ARG:HB2	1:A:770:TRP:CZ3	2.40	0.56
1:A:842:THR:HG22	1:A:842:THR:O	2.05	0.56
1:A:987:ILE:HD11	1:A:1018:LEU:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1210:SER:OG	1:A:1211:SER:N	2.37	0.56
1:A:358:SER:HB3	1:A:361:TYR:HB2	1.87	0.56
1:A:532:ILE:HG13	1:A:533:LEU:N	2.19	0.56
1:A:980:ASP:CG	1:A:981:GLU:N	2.63	0.56
1:A:639:LEU:HD23	1:A:640:GLN:H	1.70	0.56
1:A:856:VAL:HG13	1:A:890:PHE:CZ	2.41	0.56
1:A:626:ASP:OD1	1:A:628:GLN:HB2	2.06	0.56
1:A:968:CYS:HB2	1:A:1009:ILE:HG23	1.86	0.56
1:A:970:SER:O	1:A:971:PRO:C	2.49	0.56
1:A:1151:ILE:HD11	1:A:1193:LEU:CD2	2.34	0.56
1:A:201:ASN:HA	1:A:204:MET:HE3	1.86	0.56
1:A:228:ARG:HB3	1:A:228:ARG:HH11	1.71	0.56
1:A:384:THR:HG23	1:A:449:ASN:OD1	2.05	0.56
1:A:1187:SER:OG	1:A:1188:PRO:HD2	2.06	0.56
1:A:128:THR:O	1:A:130:LYS:HE3	2.06	0.56
1:A:519:PRO:O	1:A:523:ILE:HG13	2.05	0.56
1:A:588:GLY:O	1:A:589:ASP:HB2	2.06	0.56
1:A:1113:SER:O	1:A:1115:ASP:N	2.38	0.56
1:A:1066:THR:HA	1:A:1081:PHE:O	2.06	0.55
1:A:1167:PRO:O	1:A:1168:ILE:HB	2.05	0.55
1:A:1072:VAL:C	1:A:1073:ILE:HG13	2.31	0.55
1:A:448:LYS:NZ	1:A:449:ASN:ND2	2.52	0.55
1:A:1177:HIS:CG	1:A:1178:GLY:H	2.25	0.55
1:A:237:ARG:O	1:A:237:ARG:HG3	2.06	0.55
1:A:458:ARG:NH1	1:A:496:MET:HE2	2.21	0.55
1:A:1102:SER:HB2	1:A:1111:ILE:CG1	2.37	0.55
1:A:1136:SER:O	1:A:1137:LEU:C	2.49	0.55
1:A:449:ASN:HD22	1:A:449:ASN:N	2.05	0.55
1:A:951:GLY:O	1:A:952:LYS:HB3	2.06	0.55
1:A:1121:HIS:CB	1:A:1158:ASP:O	2.55	0.55
1:A:926:ILE:HG22	1:A:939:ALA:HB2	1.88	0.55
1:A:946:LEU:HD12	1:A:959:LEU:HD12	1.88	0.55
1:A:1152:ARG:HG2	1:A:1164:SER:OG	2.06	0.55
1:A:1155:ASN:OD1	1:A:1160:GLN:HB2	2.06	0.55
1:A:1202:TRP:C	1:A:1203:TRP:CD1	2.83	0.55
1:A:395:VAL:O	1:A:434:CYS:CA	2.55	0.55
1:A:762:SER:OG	1:A:763:ALA:N	2.38	0.55
1:A:814:ILE:HG22	1:A:823:LEU:HD13	1.89	0.55
1:A:1029:VAL:HG12	1:A:1029:VAL:O	2.07	0.55
1:A:286:LEU:HG	1:A:287:GLY:H	1.71	0.55
1:A:302:LYS:O	1:A:303:LYS:HB2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:CYS:SG	1:A:663:CYS:N	2.80	0.55
1:A:917:ASN:HD21	1:A:947:GLN:HE22	1.55	0.55
1:A:921:VAL:HG13	1:A:1240:GLY:HA3	1.88	0.55
1:A:940:VAL:HG13	1:A:964:VAL:HG23	1.89	0.55
1:A:141:TRP:C	1:A:143:LEU:H	2.14	0.54
1:A:233:ARG:O	1:A:234:LYS:CB	2.55	0.54
1:A:479:ASP:O	1:A:480:CYS:C	2.49	0.54
1:A:902:ASP:C	1:A:904:GLN:N	2.63	0.54
1:A:1217:ASN:N	1:A:1217:ASN:HD22	2.04	0.54
1:A:604:LYS:C	1:A:606:LEU:H	2.15	0.54
1:A:831:LEU:HD23	1:A:831:LEU:C	2.32	0.54
1:A:1102:SER:HB2	1:A:1111:ILE:HG12	1.89	0.54
1:A:406:LEU:HB2	1:A:411:VAL:CG2	2.37	0.54
1:A:400:LEU:CD1	1:A:415:LEU:HD11	2.38	0.54
1:A:426:CYS:HB3	1:A:435:TYR:HD1	1.70	0.54
1:A:415:LEU:HA	1:A:418:PHE:HD2	1.71	0.54
1:A:774:SER:O	1:A:775:ALA:HB3	2.08	0.54
1:A:1237:ASP:OD1	1:A:1241:ILE:HB	2.08	0.54
1:A:470:PRO:HB3	1:A:503:LEU:HD12	1.90	0.53
1:A:784:LYS:C	1:A:786:PHE:H	2.15	0.53
1:A:1053:LEU:CD2	1:A:1059:LEU:HB2	2.36	0.53
1:A:1063:PHE:HA	1:A:1087:THR:HA	1.90	0.53
1:A:835:ILE:HD12	1:A:867:TRP:CE3	2.43	0.53
1:A:951:GLY:O	1:A:952:LYS:CB	2.56	0.53
1:A:1072:VAL:HG12	1:A:1073:ILE:N	2.22	0.53
1:A:1231:ARG:HB2	1:A:1231:ARG:CZ	2.37	0.53
1:A:511:LYS:O	1:A:515:GLU:HG3	2.07	0.53
1:A:302:LYS:HE2	1:A:304:GLU:CG	2.38	0.53
1:A:1046:THR:O	1:A:1047:VAL:C	2.49	0.53
1:A:497:HIS:HA	1:A:532:ILE:HD11	1.90	0.53
1:A:1152:ARG:HG2	1:A:1164:SER:CB	2.39	0.53
1:A:226:ARG:O	1:A:230:LEU:HG	2.09	0.53
1:A:1128:GLY:O	1:A:1129:CYS:HB3	2.09	0.53
1:A:1155:ASN:HD21	1:A:1160:GLN:CG	2.21	0.53
1:A:720:SER:OG	1:A:721:ASN:N	2.41	0.53
1:A:811:ASP:C	1:A:826:ILE:HG22	2.34	0.53
1:A:653:ILE:HG21	1:A:684:TRP:CZ3	2.44	0.53
1:A:196:LEU:O	1:A:196:LEU:HD12	2.09	0.53
1:A:364:LEU:O	1:A:365:ASP:C	2.51	0.53
1:A:385:ASP:C	1:A:387:SER:H	2.17	0.53
1:A:978:PHE:C	1:A:978:PHE:CD2	2.87	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:ARG:O	1:A:995:VAL:C	2.52	0.52
1:A:1204:ASN:ND2	1:A:1207:THR:O	2.42	0.52
1:A:1012:THR:HG22	1:A:1013:ALA:N	2.24	0.52
1:A:388:ILE:HB	1:A:457:HIS:CE1	2.44	0.52
1:A:739:MET:HG2	1:A:770:TRP:CD1	2.44	0.52
1:A:920:ILE:HG23	1:A:921:VAL:H	1.73	0.52
1:A:1140:ILE:CG1	1:A:1156:VAL:HB	2.34	0.52
1:A:143:LEU:HD13	1:A:259:GLN:HB3	1.92	0.52
1:A:438:HIS:HB3	1:A:441:GLN:HE21	1.74	0.52
1:A:960:PRO:O	1:A:961:GLU:CB	2.58	0.52
1:A:592:ARG:O	1:A:593:LEU:HB2	2.09	0.52
1:A:760:SER:HB3	1:A:770:TRP:CZ3	2.31	0.52
1:A:534:ASP:CG	1:A:541:CYS:HB2	2.35	0.52
1:A:1048:LYS:HB3	1:A:1061:TRP:CZ3	2.45	0.52
1:A:209:GLU:HB3	1:A:211:SER:OG	2.10	0.52
1:A:541:CYS:O	1:A:542:GLU:C	2.52	0.52
1:A:660:VAL:HA	1:A:676:SER:HB2	1.92	0.52
1:A:1062:SER:OG	1:A:1063:PHE:N	2.43	0.52
1:A:1163:HIS:CD2	1:A:1207:THR:HA	2.44	0.52
1:A:352:ARG:HB2	1:A:447:GLU:HG2	1.91	0.52
1:A:381:ASP:O	1:A:384:THR:HB	2.10	0.52
1:A:635:ALA:C	1:A:637:LYS:H	2.16	0.52
1:A:1019:ILE:HG21	1:A:1058:LEU:HD11	1.91	0.52
1:A:225:ASP:C	1:A:227:LEU:N	2.64	0.52
1:A:704:CYS:HB2	1:A:747:ASN:O	2.10	0.52
1:A:1062:SER:C	1:A:1064:ASP:H	2.18	0.52
1:A:109:PHE:O	1:A:110:VAL:C	2.53	0.51
1:A:207:ASP:OD2	1:A:230:LEU:HD11	2.10	0.51
1:A:846:CYS:HA	1:A:856:VAL:O	2.10	0.51
1:A:992:ASN:ND2	1:A:995:VAL:HB	2.26	0.51
1:A:1012:THR:O	1:A:1013:ALA:C	2.53	0.51
1:A:119:VAL:HG13	1:A:120:PRO:HD2	1.93	0.51
1:A:182:VAL:HA	1:A:239:LEU:O	2.10	0.51
1:A:196:LEU:HD12	1:A:200:GLN:HG3	1.91	0.51
1:A:309:GLU:HG3	1:A:342:LEU:HD22	1.91	0.51
1:A:838:GLY:O	1:A:839:HIS:C	2.52	0.51
1:A:980:ASP:OD1	1:A:982:ASP:N	2.41	0.51
1:A:207:ASP:C	1:A:209:GLU:H	2.17	0.51
1:A:448:LYS:HZ2	1:A:449:ASN:ND2	2.01	0.51
1:A:469:GLN:HB3	1:A:472:THR:OG1	2.10	0.51
1:A:708:THR:CG2	1:A:715:LEU:HB2	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:LEU:HG	1:A:860:SER:H	1.76	0.51
1:A:903:ASP:O	1:A:905:THR:HG23	2.10	0.51
1:A:183:HIS:HB2	1:A:240:LEU:HD12	1.93	0.51
1:A:771:ASP:HB2	1:A:778:ARG:HH11	1.75	0.51
1:A:1191:LYS:HA	1:A:1205:VAL:CG2	2.41	0.51
1:A:215:ARG:NH1	1:A:557:ARG:HA	2.24	0.51
1:A:336:ASN:C	1:A:338:TRP:H	2.18	0.51
1:A:477:GLN:HB3	1:A:479:ASP:OD1	2.10	0.51
1:A:704:CYS:SG	1:A:749:CYS:N	2.84	0.51
1:A:879:ARG:HD3	1:A:1239:LEU:HD13	1.93	0.51
1:A:1087:THR:O	1:A:1105:ALA:HB1	2.10	0.51
1:A:245:VAL:HG21	1:A:262:LEU:HD12	1.92	0.51
1:A:340:TYR:O	1:A:343:ARG:HB3	2.11	0.51
1:A:919:ALA:HB3	1:A:956:ILE:HG12	1.93	0.51
1:A:1194:VAL:HG13	1:A:1194:VAL:O	2.11	0.51
1:A:227:LEU:HD23	1:A:256:ASN:HD22	1.75	0.51
1:A:336:ASN:O	1:A:338:TRP:N	2.42	0.51
1:A:529:TYR:O	1:A:533:LEU:CB	2.54	0.51
1:A:924:GLN:OE1	1:A:1222:LYS:HD2	2.10	0.51
1:A:160:LYS:HB2	2:A:1250:ADP:O1B	2.11	0.51
1:A:492:ALA:C	1:A:494:ALA:H	2.18	0.51
1:A:980:ASP:HB3	1:A:984:ALA:O	2.11	0.51
1:A:736:ARG:O	1:A:737:ASN:ND2	2.44	0.51
1:A:1083:CYS:O	1:A:1084:HIS:CG	2.64	0.51
1:A:337:ARG:NH2	1:A:374:MET:HE1	2.26	0.50
1:A:841:SER:HB2	1:A:860:SER:CB	2.40	0.50
1:A:130:LYS:HD2	1:A:131:LYS:N	2.21	0.50
1:A:1097:ALA:O	1:A:1098:THR:CB	2.59	0.50
1:A:1157:SER:HB2	1:A:1160:GLN:NE2	2.26	0.50
1:A:239:LEU:HD12	1:A:240:LEU:N	2.25	0.50
1:A:343:ARG:HH21	1:A:343:ARG:HG3	1.76	0.50
1:A:485:ASN:O	1:A:486:PHE:CG	2.65	0.50
1:A:1146:ASP:CB	1:A:1150:GLU:O	2.58	0.50
1:A:704:CYS:O	1:A:718:THR:HA	2.12	0.50
1:A:920:ILE:CG2	1:A:921:VAL:N	2.74	0.50
1:A:534:ASP:CB	1:A:541:CYS:HB2	2.42	0.50
1:A:722:ASP:OD2	1:A:724:PHE:HD2	1.95	0.50
1:A:107:THR:HG21	1:A:171:HIS:HB2	1.94	0.50
1:A:396:PRO:HD2	1:A:399:VAL:CG2	2.40	0.50
1:A:461:VAL:CG2	1:A:462:THR:N	2.75	0.50
1:A:814:ILE:CD1	1:A:848:PHE:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:861:GLN:O	1:A:863:CYS:N	2.35	0.50
1:A:130:LYS:HA	1:A:133:VAL:CG2	2.42	0.50
1:A:185:VAL:HG12	1:A:187:ILE:HG13	1.92	0.50
1:A:108:SER:HA	1:A:111:ARG:CD	2.42	0.49
1:A:133:VAL:HG21	4:A:1259:HOH:O	2.12	0.49
1:A:584:ALA:C	1:A:586:GLN:H	2.19	0.49
1:A:133:VAL:HG13	1:A:166:GLU:HB3	1.94	0.49
1:A:723:PHE:CE2	1:A:744:ASN:HA	2.46	0.49
1:A:866:LEU:H	1:A:866:LEU:HD23	1.77	0.49
1:A:1017:THR:HA	1:A:1031:ASN:HA	1.94	0.49
1:A:1227:SER:HB2	1:A:1228:PRO:CD	2.41	0.49
1:A:835:ILE:HG22	1:A:872:ARG:HG2	1.95	0.49
1:A:1017:THR:HA	1:A:1030:TRP:O	2.12	0.49
1:A:612:ARG:CG	1:A:905:THR:HG22	2.34	0.49
1:A:756:GLU:O	1:A:772:VAL:HG23	2.13	0.49
1:A:942:ASN:ND2	1:A:942:ASN:N	2.55	0.49
1:A:458:ARG:HG3	1:A:496:MET:HE3	1.92	0.49
1:A:744:ASN:CG	1:A:745:SER:N	2.67	0.49
1:A:1107:LYS:CD	1:A:1108:THR:N	2.74	0.49
1:A:1191:LYS:O	1:A:1205:VAL:HG13	2.12	0.49
1:A:1120:LEU:HD13	1:A:1158:ASP:OD1	2.13	0.49
1:A:743:THR:HB	1:A:764:ASP:CB	2.43	0.49
1:A:1141:LEU:HD13	1:A:1155:ASN:HA	1.94	0.49
1:A:869:ILE:HG22	1:A:870:ASP:N	2.28	0.49
1:A:130:LYS:NZ	1:A:131:LYS:HD2	2.28	0.49
1:A:295:LEU:O	1:A:299:VAL:HG22	2.13	0.49
1:A:735:CYS:SG	1:A:737:ASN:O	2.71	0.49
1:A:756:GLU:C	1:A:772:VAL:HG23	2.37	0.49
1:A:302:LYS:C	1:A:304:GLU:H	2.21	0.49
1:A:531:HIS:NE2	1:A:532:ILE:HG22	2.28	0.49
1:A:1094:SER:O	1:A:1096:ASP:N	2.45	0.49
1:A:1107:LYS:HD2	1:A:1108:THR:N	2.15	0.49
1:A:480:CYS:O	1:A:481:MET:C	2.56	0.48
1:A:785:ARG:NH2	1:A:831:LEU:HD12	2.28	0.48
1:A:1047:VAL:HA	1:A:1062:SER:HB2	1.94	0.48
1:A:398:LYS:O	1:A:402:VAL:HG22	2.14	0.48
1:A:609:LEU:HD12	1:A:610:VAL:N	2.28	0.48
1:A:796:ASP:O	1:A:797:VAL:O	2.31	0.48
1:A:931:GLN:HG3	1:A:934:GLU:O	2.13	0.48
1:A:1161:LEU:O	1:A:1162:LEU:O	2.31	0.48
1:A:245:VAL:HG11	1:A:251:LEU:CD1	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:LEU:HD11	1:A:262:LEU:CD1	2.43	0.48
1:A:361:TYR:O	1:A:364:LEU:N	2.47	0.48
1:A:449:ASN:ND2	1:A:449:ASN:N	2.60	0.48
1:A:482:TYR:O	1:A:486:PHE:HB2	2.13	0.48
1:A:1024:ASP:OD1	1:A:1026:VAL:HG12	2.13	0.48
1:A:1191:LYS:C	1:A:1205:VAL:HG13	2.39	0.48
1:A:1231:ARG:HG2	1:A:1231:ARG:O	2.13	0.48
1:A:228:ARG:HG2	1:A:232:LEU:HD12	1.95	0.48
1:A:348:LYS:HD2	1:A:348:LYS:N	2.29	0.48
1:A:987:ILE:HD11	1:A:1018:LEU:CD1	2.43	0.48
1:A:119:VAL:HG12	1:A:120:PRO:O	2.14	0.48
1:A:614:HIS:HE1	1:A:640:GLN:HG3	1.76	0.48
1:A:1179:GLY:O	1:A:1180:TRP:HB2	2.12	0.48
1:A:214:GLN:HG2	1:A:215:ARG:N	2.24	0.48
1:A:216:LEU:H	1:A:216:LEU:CD1	1.90	0.48
1:A:758:LEU:HD23	1:A:759:ALA:N	2.28	0.48
1:A:944:ARG:HG2	1:A:961:GLU:O	2.14	0.48
1:A:130:LYS:HZ3	1:A:131:LYS:HD2	1.78	0.48
1:A:752:SER:HB2	1:A:806:TRP:CZ2	2.49	0.48
1:A:908:VAL:HG12	1:A:909:TRP:N	2.29	0.48
1:A:1019:ILE:N	1:A:1019:ILE:CD1	2.77	0.48
1:A:1146:ASP:HB3	1:A:1150:GLU:HB3	1.95	0.48
1:A:1221:LEU:C	1:A:1222:LYS:HG3	2.39	0.48
1:A:736:ARG:O	1:A:737:ASN:CG	2.57	0.48
1:A:835:ILE:O	1:A:835:ILE:HG13	2.14	0.48
1:A:1224:ILE:HD13	1:A:1235:THR:HB	1.96	0.48
1:A:239:LEU:HD12	1:A:259:GLN:O	2.14	0.47
1:A:714:LEU:HD23	1:A:714:LEU:C	2.37	0.47
1:A:809:ASP:OD2	1:A:809:ASP:N	2.47	0.47
1:A:932:GLU:C	1:A:934:GLU:H	2.22	0.47
1:A:152:ILE:HB	1:A:263:THR:HG22	1.96	0.47
1:A:415:LEU:HA	1:A:418:PHE:CD2	2.48	0.47
1:A:487:LEU:O	1:A:491:MET:HG3	2.13	0.47
1:A:624:SER:HB2	1:A:669:ASP:OD1	2.14	0.47
1:A:707:PHE:CZ	1:A:716:LEU:HD12	2.48	0.47
1:A:814:ILE:HA	1:A:822:LEU:O	2.13	0.47
1:A:1023:GLU:C	1:A:1046:THR:HG23	2.39	0.47
1:A:1131:ARG:HG3	1:A:1131:ARG:HH11	1.78	0.47
1:A:137:GLN:HG2	1:A:173:LEU:HD22	1.96	0.47
1:A:237:ARG:HG2	1:A:237:ARG:NH1	2.29	0.47
1:A:630:ILE:HB	1:A:642:PHE:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:682:LYS:HE2	1:A:694:THR:CG2	2.45	0.47
1:A:1053:LEU:CD1	1:A:1054:GLN:H	2.27	0.47
1:A:1189:ASP:OD1	1:A:1191:LYS:HB2	2.14	0.47
1:A:309:GLU:CD	1:A:309:GLU:H	2.21	0.47
1:A:406:LEU:HB2	1:A:411:VAL:HG22	1.94	0.47
1:A:899:THR:O	1:A:906:ILE:HA	2.15	0.47
1:A:980:ASP:O	1:A:1006:VAL:HG23	2.13	0.47
1:A:1006:VAL:C	1:A:1007:ARG:HE	2.21	0.47
1:A:1027:ILE:CG1	1:A:1047:VAL:HG21	2.44	0.47
1:A:1093:ILE:C	1:A:1095:SER:H	2.21	0.47
1:A:692:VAL:O	1:A:693:HIS:CB	2.59	0.47
1:A:207:ASP:C	1:A:209:GLU:N	2.73	0.47
1:A:340:TYR:CZ	1:A:344:GLN:NE2	2.83	0.47
1:A:801:VAL:HG23	1:A:801:VAL:O	2.15	0.47
1:A:127:VAL:HG22	2:A:1250:ADP:N1	2.30	0.47
1:A:231:MET:O	1:A:236:PRO:HA	2.15	0.47
1:A:375:LEU:HD21	1:A:423:LEU:CD1	2.44	0.47
1:A:431:LYS:NZ	1:A:431:LYS:HA	2.30	0.47
1:A:587:GLU:OE1	1:A:592:ARG:HD2	2.15	0.47
1:A:604:LYS:O	1:A:606:LEU:HD22	2.14	0.47
1:A:744:ASN:ND2	1:A:763:ALA:HB3	2.30	0.47
1:A:832:LEU:N	1:A:832:LEU:CD1	2.78	0.47
1:A:870:ASP:OD1	1:A:871:SER:N	2.48	0.47
1:A:1101:SER:O	1:A:1112:TRP:CZ3	2.68	0.47
1:A:1212:GLN:O	1:A:1213:THR:O	2.33	0.47
1:A:218:LEU:HD12	1:A:557:ARG:CZ	2.45	0.47
1:A:293:GLU:O	1:A:296:SER:HB3	2.15	0.47
1:A:1106:ASP:O	1:A:1107:LYS:CB	2.60	0.47
1:A:1184:VAL:HB	1:A:1193:LEU:HD11	1.97	0.47
1:A:1229:ASP:OD2	1:A:1229:ASP:N	2.45	0.47
1:A:230:LEU:O	1:A:235:HIS:HB2	2.15	0.47
1:A:453:LEU:HD13	3:A:1251:GBL:HBC1	1.96	0.47
1:A:507:LEU:O	1:A:510:ILE:HB	2.14	0.47
1:A:603:ILE:CG2	1:A:604:LYS:H	2.17	0.47
1:A:383:TYR:CE1	1:A:423:LEU:HB3	2.50	0.47
1:A:438:HIS:O	1:A:439:ASP:C	2.57	0.47
1:A:799:VAL:HG22	1:A:818:LYS:HD3	1.96	0.47
1:A:1182:THR:O	1:A:1183:ASP:HB2	2.15	0.47
1:A:112:THR:O	1:A:116:GLU:HG2	2.15	0.46
1:A:309:GLU:HG3	1:A:342:LEU:CD2	2.44	0.46
1:A:954:GLY:O	1:A:956:ILE:HD13	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:SER:O	1:A:316:GLU:HG2	2.15	0.46
1:A:337:ARG:CB	1:A:340:TYR:HB3	2.45	0.46
1:A:492:ALA:C	1:A:494:ALA:N	2.73	0.46
1:A:754:ASP:O	1:A:756:GLU:N	2.45	0.46
1:A:941:ASP:CG	1:A:942:ASN:N	2.74	0.46
1:A:990:LEU:O	1:A:991:PRO:C	2.58	0.46
1:A:1042:ALA:HB1	1:A:1044:GLN:OE1	2.14	0.46
1:A:1148:ASN:O	1:A:1168:ILE:HD12	2.15	0.46
1:A:496:MET:HB3	1:A:499:GLU:OE1	2.16	0.46
1:A:953:THR:O	1:A:955:GLN:N	2.48	0.46
1:A:1146:ASP:CG	1:A:1147:ASP:N	2.73	0.46
1:A:309:GLU:O	1:A:312:SER:N	2.47	0.46
1:A:706:HIS:CD2	1:A:707:PHE:N	2.83	0.46
1:A:106:ILE:HG22	1:A:107:THR:N	2.30	0.46
1:A:846:CYS:O	1:A:847:ASP:HB2	2.16	0.46
1:A:1140:ILE:HA	1:A:1156:VAL:HB	1.98	0.46
1:A:130:LYS:HD2	1:A:131:LYS:CD	2.45	0.46
1:A:227:LEU:HD23	1:A:256:ASN:ND2	2.30	0.46
1:A:562:ASN:OD1	1:A:564:VAL:HG23	2.16	0.46
1:A:938:LEU:CD1	1:A:976:VAL:HG23	2.46	0.46
1:A:1191:LYS:O	1:A:1205:VAL:HG22	2.16	0.46
1:A:866:LEU:HD23	1:A:866:LEU:N	2.31	0.46
1:A:923:LYS:HD2	1:A:940:VAL:HG11	1.98	0.46
1:A:542:GLU:O	1:A:546:GLU:N	2.26	0.46
1:A:868:ASN:C	1:A:868:ASN:ND2	2.73	0.46
1:A:941:ASP:OD2	1:A:943:ILE:N	2.45	0.46
1:A:946:LEU:CD1	1:A:959:LEU:HD12	2.46	0.46
1:A:1072:VAL:CG1	1:A:1073:ILE:N	2.79	0.46
1:A:1126:HIS:CE1	1:A:1146:ASP:HB2	2.51	0.46
1:A:113:VAL:HG11	1:A:174:LEU:CD2	2.45	0.45
1:A:353:ILE:O	1:A:354:ARG:C	2.59	0.45
1:A:430:GLY:C	1:A:432:SER:N	2.73	0.45
1:A:563:ILE:HA	1:A:566:LEU:HD12	1.98	0.45
1:A:677:ALA:C	1:A:679:LYS:H	2.23	0.45
1:A:708:THR:HG23	1:A:715:LEU:HB2	1.97	0.45
1:A:862:TYR:HB2	1:A:881:HIS:O	2.15	0.45
1:A:1140:ILE:HD11	1:A:1156:VAL:O	2.16	0.45
1:A:149:TRP:O	1:A:278:HIS:N	2.50	0.45
1:A:319:GLY:O	1:A:320:SER:C	2.60	0.45
1:A:352:ARG:C	1:A:353:ILE:O	2.58	0.45
1:A:353:ILE:HG23	1:A:354:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:LYS:CD	1:A:699:SER:O	2.65	0.45
1:A:847:ASP:OD2	1:A:889:MET:HB2	2.16	0.45
1:A:1201:LYS:HG3	1:A:1212:GLN:HA	1.98	0.45
1:A:187:ILE:HG22	1:A:188:GLY:N	2.31	0.45
1:A:1103:THR:HG23	1:A:1112:TRP:CZ2	2.51	0.45
1:A:337:ARG:O	1:A:338:TRP:C	2.59	0.45
1:A:482:TYR:C	1:A:482:TYR:CD1	2.94	0.45
1:A:604:LYS:CG	1:A:606:LEU:HD22	2.47	0.45
1:A:679:LYS:HD2	1:A:699:SER:O	2.15	0.45
1:A:1014:ASP:OD2	1:A:1016:LYS:HE3	2.17	0.45
1:A:1123:LEU:HB3	1:A:1154:TRP:CE3	2.52	0.45
1:A:123:PRO:O	1:A:125:ILE:N	2.50	0.45
1:A:218:LEU:HD22	1:A:518:GLY:HA3	1.97	0.45
1:A:354:ARG:O	1:A:355:LYS:C	2.59	0.45
1:A:491:MET:HE2	1:A:503:LEU:HD22	1.99	0.45
1:A:917:ASN:ND2	1:A:947:GLN:HE22	2.14	0.45
1:A:1146:ASP:CG	1:A:1147:ASP:H	2.25	0.45
1:A:1229:ASP:OD1	1:A:1231:ARG:HB3	2.17	0.45
1:A:288:ARG:N	1:A:288:ARG:NE	2.36	0.45
1:A:411:VAL:O	1:A:415:LEU:HG	2.15	0.45
1:A:491:MET:HE1	1:A:503:LEU:CB	2.46	0.45
1:A:624:SER:HA	1:A:665:PHE:CD2	2.52	0.45
1:A:693:HIS:CD2	1:A:694:THR:H	2.35	0.45
1:A:756:GLU:O	1:A:757:LEU:HD23	2.16	0.45
1:A:1101:SER:OG	1:A:1114:PHE:CE1	2.70	0.45
1:A:1237:ASP:OD2	1:A:1243:TYR:HE2	1.99	0.45
1:A:147:PRO:HA	1:A:259:GLN:HG2	1.98	0.45
1:A:376:ARG:NH1	1:A:376:ARG:CB	2.80	0.45
1:A:695:TYR:HD1	1:A:728:TRP:CE3	2.34	0.45
1:A:1122:GLU:OE1	1:A:1124:LYS:HD2	2.16	0.45
1:A:1137:LEU:O	1:A:1138:ASP:CB	2.65	0.45
1:A:405:ASP:O	1:A:406:LEU:HD23	2.16	0.45
1:A:491:MET:CE	1:A:503:LEU:HD22	2.46	0.45
1:A:584:ALA:C	1:A:586:GLN:N	2.75	0.45
1:A:1218:GLY:HA3	1:A:1239:LEU:HG	1.98	0.45
1:A:136:ILE:HD13	1:A:152:ILE:CD1	2.47	0.45
1:A:203:CYS:C	1:A:205:ARG:N	2.75	0.45
1:A:582:LEU:O	1:A:583:GLN:C	2.59	0.45
1:A:633:CYS:SG	1:A:662:CYS:C	3.00	0.45
1:A:928:VAL:HG12	1:A:929:VAL:N	2.31	0.45
1:A:604:LYS:HD3	1:A:606:LEU:CD2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:667:SER:HB3	1:A:708:THR:O	2.17	0.45
1:A:695:TYR:CD1	1:A:728:TRP:CE3	3.05	0.45
1:A:251:LEU:HD21	1:A:262:LEU:CD1	2.48	0.44
1:A:974:GLU:O	1:A:990:LEU:N	2.49	0.44
1:A:254:PHE:HB3	1:A:260:ILE:CD1	2.47	0.44
1:A:368:MET:O	1:A:369:SER:C	2.59	0.44
1:A:391:LYS:HD3	1:A:439:ASP:CB	2.47	0.44
1:A:586:GLN:O	1:A:587:GLU:HB3	2.17	0.44
1:A:724:PHE:HE1	1:A:740:PHE:HD2	1.65	0.44
1:A:920:ILE:CG2	1:A:921:VAL:H	2.29	0.44
1:A:421:LYS:O	1:A:422:SER:HB2	2.18	0.44
1:A:618:VAL:CG1	1:A:906:ILE:HD11	2.36	0.44
1:A:639:LEU:HD23	1:A:640:GLN:N	2.32	0.44
1:A:961:GLU:HG2	1:A:978:PHE:CZ	2.53	0.44
1:A:1102:SER:HB2	1:A:1111:ILE:CB	2.47	0.44
1:A:1153:ILE:HD13	1:A:1153:ILE:N	2.32	0.44
1:A:500:LEU:O	1:A:501:CYS:C	2.59	0.44
1:A:708:THR:HA	1:A:751:PHE:CD2	2.52	0.44
1:A:804:CYS:O	1:A:804:CYS:SG	2.76	0.44
1:A:1012:THR:OG1	1:A:1017:THR:HB	2.18	0.44
1:A:1143:ALA:HB2	1:A:1186:PHE:CZ	2.52	0.44
1:A:1212:GLN:C	1:A:1212:GLN:NE2	2.72	0.44
1:A:383:TYR:HB2	1:A:418:PHE:CE1	2.52	0.44
1:A:540:VAL:HG12	1:A:540:VAL:O	2.17	0.44
1:A:785:ARG:NH1	1:A:785:ARG:CG	2.67	0.44
1:A:923:LYS:HG3	1:A:941:ASP:O	2.18	0.44
1:A:232:LEU:O	1:A:233:ARG:HB2	2.17	0.44
1:A:316:GLU:C	1:A:318:LYS:H	2.24	0.44
1:A:358:SER:O	1:A:359:TYR:O	2.36	0.44
1:A:553:HIS:ND1	1:A:554:LEU:HG	2.32	0.44
1:A:604:LYS:HG2	1:A:606:LEU:HD22	1.99	0.44
1:A:615:THR:O	1:A:904:GLN:NE2	2.50	0.44
1:A:952:LYS:O	1:A:953:THR:OG1	2.23	0.44
1:A:1156:VAL:O	1:A:1156:VAL:HG12	2.16	0.44
1:A:903:ASP:C	1:A:904:GLN:HG3	2.43	0.44
1:A:116:GLU:O	1:A:118:GLY:N	2.50	0.44
1:A:137:GLN:O	1:A:140:LEU:HB2	2.18	0.44
1:A:448:LYS:CG	1:A:449:ASN:ND2	2.79	0.44
1:A:501:CYS:O	1:A:505:PHE:HB2	2.18	0.44
1:A:228:ARG:HB3	1:A:228:ARG:CZ	2.46	0.44
1:A:511:LYS:O	1:A:512:ALA:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:LYS:HG3	1:A:650:LEU:HD11	2.00	0.44
1:A:721:ASN:HA	1:A:745:SER:OG	2.17	0.44
1:A:803:CYS:SG	1:A:846:CYS:O	2.76	0.44
1:A:1132:CYS:O	1:A:1133:SER:HB3	2.18	0.44
1:A:1133:SER:HB3	1:A:1144:THR:HA	2.00	0.44
1:A:127:VAL:HG23	1:A:127:VAL:O	2.18	0.43
1:A:136:ILE:HD13	1:A:152:ILE:HD13	2.00	0.43
1:A:292:LEU:O	1:A:293:GLU:C	2.61	0.43
1:A:337:ARG:HH21	1:A:374:MET:HE3	1.81	0.43
1:A:373:GLU:OE1	1:A:380:LYS:NZ	2.50	0.43
1:A:672:ILE:O	1:A:684:TRP:HD1	2.00	0.43
1:A:692:VAL:O	1:A:692:VAL:HG12	2.17	0.43
1:A:888:VAL:O	1:A:888:VAL:HG13	2.17	0.43
1:A:1027:ILE:HG22	1:A:1028:GLN:N	2.33	0.43
1:A:1151:ILE:O	1:A:1151:ILE:HG12	2.17	0.43
1:A:415:LEU:O	1:A:419:VAL:HG23	2.18	0.43
1:A:706:HIS:ND1	1:A:750:ARG:HD3	2.33	0.43
1:A:727:LEU:HD21	1:A:758:LEU:HD12	2.00	0.43
1:A:837:THR:O	1:A:838:GLY:C	2.61	0.43
1:A:869:ILE:O	1:A:870:ASP:OD1	2.35	0.43
1:A:883:SER:O	1:A:884:TRP:C	2.61	0.43
1:A:1152:ARG:C	1:A:1153:ILE:HD13	2.43	0.43
1:A:1242:LEU:HD13	1:A:1244:ILE:HG13	2.00	0.43
1:A:290:LYS:O	1:A:291:GLY:C	2.59	0.43
1:A:562:ASN:HD21	1:A:564:VAL:HB	1.82	0.43
1:A:428:ARG:HG2	1:A:433:PHE:HE2	1.83	0.43
1:A:827:HIS:C	1:A:829:SER:N	2.73	0.43
1:A:954:GLY:O	1:A:955:GLN:C	2.59	0.43
1:A:158:CYS:SG	1:A:160:LYS:HD3	2.59	0.43
1:A:1226:VAL:O	1:A:1226:VAL:HG23	2.17	0.43
1:A:604:LYS:HE2	1:A:606:LEU:HD13	2.00	0.43
1:A:986:LYS:HG2	1:A:998:SER:CB	2.46	0.43
1:A:1072:VAL:O	1:A:1073:ILE:CB	2.67	0.43
1:A:1113:SER:C	1:A:1115:ASP:N	2.69	0.43
1:A:214:GLN:O	1:A:215:ARG:HB3	2.19	0.43
1:A:280:VAL:HG12	1:A:280:VAL:O	2.19	0.43
1:A:350:PHE:O	4:A:1255:HOH:O	2.21	0.43
1:A:641:VAL:HG21	1:A:672:ILE:CD1	2.48	0.43
1:A:652:ASP:OD1	1:A:652:ASP:O	2.36	0.43
1:A:903:ASP:O	1:A:904:GLN:HG3	2.18	0.43
1:A:989:GLU:HG3	1:A:992:ASN:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1007:ARG:N	1:A:1007:ARG:NE	2.66	0.43
1:A:1110:LYS:HG2	1:A:1122:GLU:HG3	2.01	0.43
1:A:1183:ASP:O	1:A:1184:VAL:HG13	2.18	0.43
1:A:114:LEU:HD21	1:A:168:VAL:O	2.18	0.43
1:A:370:ILE:O	1:A:371:SER:C	2.61	0.43
1:A:522:LEU:O	1:A:526:PHE:HD2	2.02	0.43
1:A:621:ALA:HA	1:A:631:ALA:O	2.18	0.43
1:A:658:ASP:CG	1:A:659:GLU:N	2.77	0.43
1:A:695:TYR:HB3	1:A:728:TRP:CZ3	2.54	0.43
1:A:835:ILE:HD12	1:A:867:TRP:CD2	2.54	0.43
1:A:1140:ILE:C	1:A:1156:VAL:HG23	2.44	0.43
1:A:1227:SER:CB	1:A:1232:THR:HB	2.47	0.43
1:A:147:PRO:HB3	1:A:258:CYS:O	2.18	0.43
1:A:1061:TRP:CD1	1:A:1061:TRP:N	2.87	0.43
1:A:1083:CYS:O	1:A:1084:HIS:CD2	2.72	0.43
1:A:587:GLU:O	1:A:588:GLY:C	2.62	0.43
1:A:706:HIS:ND1	1:A:750:ARG:HA	2.33	0.43
1:A:743:THR:HB	1:A:764:ASP:HB2	2.00	0.43
1:A:1064:ASP:C	1:A:1066:THR:H	2.26	0.43
1:A:553:HIS:CE1	1:A:554:LEU:HG	2.54	0.42
1:A:653:ILE:HG22	1:A:654:LYS:N	2.33	0.42
1:A:710:LYS:C	1:A:712:ASN:H	2.26	0.42
1:A:739:MET:HG2	1:A:770:TRP:NE1	2.34	0.42
1:A:1202:TRP:CD1	1:A:1202:TRP:N	2.87	0.42
1:A:131:LYS:HB2	1:A:131:LYS:HE2	1.83	0.42
1:A:137:GLN:HG2	1:A:173:LEU:CD2	2.49	0.42
1:A:187:ILE:HG22	1:A:188:GLY:O	2.19	0.42
1:A:541:CYS:O	1:A:544:PHE:N	2.52	0.42
1:A:581:LYS:HE2	1:A:1248:LEU:HD21	2.01	0.42
1:A:903:ASP:C	1:A:903:ASP:OD2	2.61	0.42
1:A:1113:SER:OG	1:A:1116:LEU:HD13	2.19	0.42
1:A:378:ASP:OD2	1:A:378:ASP:N	2.50	0.42
1:A:407:GLU:O	1:A:408:THR:C	2.62	0.42
1:A:868:ASN:C	1:A:868:ASN:HD22	2.26	0.42
1:A:896:SER:CB	1:A:909:TRP:O	2.54	0.42
1:A:107:THR:O	1:A:109:PHE:N	2.51	0.42
1:A:149:TRP:CE2	1:A:273:VAL:HG21	2.54	0.42
1:A:153:TYR:CD1	1:A:267:LYS:HB3	2.54	0.42
1:A:228:ARG:CG	1:A:256:ASN:HB3	2.44	0.42
1:A:333:ASP:O	1:A:334:PHE:CD1	2.72	0.42
1:A:630:ILE:HD12	1:A:642:PHE:CE2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:865:GLU:OE1	1:A:874:LYS:HE2	2.20	0.42
1:A:924:GLN:NE2	1:A:1236:VAL:O	2.51	0.42
1:A:953:THR:O	1:A:955:GLN:HB2	2.20	0.42
1:A:983:GLY:HA2	1:A:1006:VAL:CG2	2.50	0.42
1:A:1107:LYS:C	1:A:1108:THR:HG23	2.44	0.42
1:A:156:ALA:O	1:A:157:GLY:C	2.62	0.42
1:A:290:LYS:O	1:A:293:GLU:HB3	2.20	0.42
1:A:301:MET:C	1:A:302:LYS:HG2	2.44	0.42
1:A:465:GLN:HE21	1:A:465:GLN:HB2	1.71	0.42
1:A:713:HIS:CD2	1:A:713:HIS:N	2.80	0.42
1:A:290:LYS:O	1:A:293:GLU:N	2.52	0.42
1:A:391:LYS:HD3	1:A:439:ASP:CG	2.44	0.42
1:A:496:MET:O	1:A:497:HIS:C	2.63	0.42
1:A:509:TRP:O	1:A:510:ILE:C	2.62	0.42
1:A:628:GLN:OE1	1:A:628:GLN:HA	2.19	0.42
1:A:978:PHE:CD2	1:A:978:PHE:O	2.72	0.42
1:A:1029:VAL:HG21	1:A:1072:VAL:HG22	2.01	0.42
1:A:594:TYR:O	1:A:1248:LEU:HB2	2.20	0.42
1:A:603:ILE:HA	1:A:920:ILE:HG13	2.01	0.42
1:A:658:ASP:CG	1:A:659:GLU:H	2.28	0.42
1:A:670:SER:O	1:A:686:SER:HB3	2.20	0.42
1:A:682:LYS:HE2	1:A:694:THR:HG21	2.01	0.42
1:A:785:ARG:CZ	1:A:831:LEU:HD12	2.50	0.42
1:A:894:GLY:O	1:A:895:SER:C	2.61	0.42
1:A:1009:ILE:HG23	1:A:1009:ILE:O	2.19	0.42
1:A:1032:TRP:O	1:A:1033:GLN:CB	2.68	0.42
1:A:1044:GLN:HG2	1:A:1068:LYS:HZ3	1.83	0.42
1:A:1123:LEU:HB3	1:A:1154:TRP:CZ3	2.55	0.42
1:A:1233:TYR:HB2	1:A:1245:LEU:HB2	2.01	0.42
1:A:183:HIS:NE2	1:A:206:LEU:HD21	2.35	0.42
1:A:396:PRO:O	1:A:397:THR:C	2.62	0.42
1:A:572:GLU:HA	1:A:577:TYR:CD1	2.54	0.42
1:A:888:VAL:HA	1:A:898:LEU:O	2.19	0.42
1:A:1007:ARG:N	1:A:1007:ARG:CD	2.83	0.42
1:A:196:LEU:HD12	1:A:196:LEU:C	2.44	0.42
1:A:215:ARG:NH1	1:A:557:ARG:HD3	2.34	0.42
1:A:386:LEU:N	1:A:386:LEU:HD23	2.35	0.42
1:A:586:GLN:O	1:A:587:GLU:CB	2.68	0.42
1:A:835:ILE:HG22	1:A:872:ARG:CG	2.49	0.42
1:A:1090:SER:HB2	1:A:1132:CYS:HA	2.02	0.42
1:A:1140:ILE:CA	1:A:1156:VAL:HB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:388:ILE:O	1:A:388:ILE:HG13	2.18	0.42
1:A:482:TYR:OH	1:A:490:HIS:NE2	2.34	0.42
1:A:506:SER:O	1:A:510:ILE:HG12	2.20	0.41
1:A:607:SER:HB3	1:A:909:TRP:CZ3	2.55	0.41
1:A:911:THR:O	1:A:912:LYS:C	2.63	0.41
1:A:1131:ARG:HG3	1:A:1131:ARG:NH1	2.35	0.41
1:A:228:ARG:HG2	1:A:232:LEU:CD1	2.49	0.41
1:A:289:GLU:OE1	1:A:303:LYS:HE2	2.20	0.41
1:A:316:GLU:C	1:A:318:LYS:N	2.77	0.41
1:A:464:PHE:CD1	1:A:487:LEU:HD13	2.54	0.41
1:A:972:HIS:O	1:A:973:LEU:HB2	2.20	0.41
1:A:1071:ASN:OD1	1:A:1072:VAL:O	2.38	0.41
1:A:1089:LEU:O	1:A:1104:SER:O	2.38	0.41
1:A:1116:LEU:C	1:A:1118:SER:N	2.74	0.41
1:A:158:CYS:SG	1:A:160:LYS:CD	3.08	0.41
1:A:655:ALA:HA	1:A:684:TRP:CH2	2.55	0.41
1:A:945:GLY:N	1:A:958:TYR:OH	2.47	0.41
1:A:1191:LYS:HA	1:A:1205:VAL:HG11	2.00	0.41
1:A:424:LEU:O	1:A:425:PHE:CD2	2.73	0.41
1:A:786:PHE:CD2	1:A:786:PHE:N	2.87	0.41
1:A:1003:LYS:H	1:A:1003:LYS:NZ	2.16	0.41
1:A:1042:ALA:HA	1:A:1070:TRP:HH2	1.85	0.41
1:A:130:LYS:HD3	1:A:131:LYS:HG3	2.02	0.41
1:A:352:ARG:CZ	1:A:361:TYR:CE2	3.04	0.41
1:A:510:ILE:O	1:A:514:THR:HG23	2.20	0.41
1:A:582:LEU:O	1:A:584:ALA:N	2.54	0.41
1:A:918:SER:OG	1:A:920:ILE:CG2	2.66	0.41
1:A:1044:GLN:CG	1:A:1068:LYS:HZ3	2.33	0.41
1:A:1129:CYS:SG	1:A:1129:CYS:O	2.78	0.41
1:A:1132:CYS:O	1:A:1133:SER:CB	2.69	0.41
1:A:152:ILE:HD11	1:A:261:LEU:HD11	2.01	0.41
1:A:546:GLU:HA	1:A:612:ARG:HH12	1.85	0.41
1:A:567:GLY:C	1:A:569:CYS:N	2.77	0.41
1:A:849:SER:HB2	1:A:890:PHE:CE2	2.56	0.41
1:A:857:ILE:O	1:A:857:ILE:HG13	2.21	0.41
1:A:1016:LYS:O	1:A:1017:THR:CB	2.68	0.41
1:A:1116:LEU:O	1:A:1118:SER:N	2.47	0.41
1:A:706:HIS:HD2	1:A:707:PHE:H	1.68	0.41
1:A:1089:LEU:O	1:A:1090:SER:O	2.39	0.41
1:A:134:HIS:O	1:A:135:ALA:C	2.63	0.41
1:A:341:TYR:C	1:A:343:ARG:N	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:MET:O	1:A:372:VAL:HG23	2.21	0.41
1:A:396:PRO:O	1:A:398:LYS:N	2.54	0.41
1:A:460:MET:C	1:A:461:VAL:HG13	2.44	0.41
1:A:477:GLN:O	1:A:478:GLU:C	2.63	0.41
1:A:521:HIS:O	1:A:524:HIS:N	2.53	0.41
1:A:825:ASP:OD1	1:A:828:THR:HG23	2.21	0.41
1:A:844:GLN:H	1:A:844:GLN:HG2	1.58	0.41
1:A:945:GLY:HA3	1:A:959:LEU:O	2.20	0.41
1:A:970:SER:O	1:A:973:LEU:N	2.53	0.41
1:A:1131:ARG:O	1:A:1131:ARG:CG	2.69	0.41
1:A:231:MET:HE2	1:A:231:MET:HA	2.02	0.41
1:A:403:LEU:HG	1:A:460:MET:SD	2.61	0.41
1:A:601:LYS:HB2	1:A:601:LYS:HE3	1.81	0.41
1:A:611:VAL:HG12	1:A:613:PRO:HD3	2.03	0.41
1:A:1231:ARG:HG3	1:A:1247:VAL:HB	2.03	0.41
1:A:846:CYS:HA	1:A:857:ILE:HA	2.03	0.40
1:A:881:HIS:CE1	1:A:907:ARG:HG3	2.52	0.40
1:A:1223:LYS:HD3	1:A:1225:HIS:CE1	2.56	0.40
1:A:209:GLU:C	1:A:211:SER:N	2.76	0.40
1:A:302:LYS:O	1:A:303:LYS:CB	2.69	0.40
1:A:827:HIS:C	1:A:829:SER:H	2.29	0.40
1:A:1064:ASP:C	1:A:1066:THR:N	2.78	0.40
1:A:726:LYS:HD3	1:A:728:TRP:CH2	2.56	0.40
1:A:869:ILE:CG2	1:A:870:ASP:N	2.85	0.40
1:A:1061:TRP:HA	1:A:1066:THR:O	2.22	0.40
1:A:194:GLY:O	1:A:195:LEU:C	2.63	0.40
1:A:218:LEU:HD22	1:A:518:GLY:HA2	2.04	0.40
1:A:286:LEU:HG	1:A:287:GLY:N	2.36	0.40
1:A:601:LYS:O	1:A:603:ILE:O	2.40	0.40
1:A:930:PHE:CE2	1:A:1227:SER:HA	2.56	0.40
1:A:1090:SER:CB	1:A:1132:CYS:HA	2.51	0.40
1:A:1155:ASN:HD21	1:A:1160:GLN:CD	2.30	0.40
1:A:127:VAL:HB	1:A:290:LYS:HD2	2.02	0.40
1:A:153:TYR:HA	1:A:264:THR:O	2.21	0.40
1:A:585:LYS:HD2	1:A:1249:GLU:OE1	2.22	0.40
1:A:635:ALA:C	1:A:637:LYS:N	2.80	0.40
1:A:1060:SER:C	1:A:1061:TRP:CD1	3.00	0.40
1:A:1069:VAL:CG2	1:A:1079:ARG:HB2	2.52	0.40
1:A:1076:ARG:NH1	1:A:1078:GLU:HG2	2.36	0.40

There are no symmetry-related clashes.

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	A	1127/1256 (90%)	765 (68%)	242 (22%)	120 (11%)	0 5

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	124	VAL
1	A	174	LEU
1	A	177	CYS
1	A	253	ALA
1	A	337	ARG
1	A	359	TYR
1	A	362	GLU
1	A	397	THR
1	A	408	THR
1	A	533	LEU
1	A	587	GLU
1	A	655	ALA
1	A	693	HIS
1	A	755	ASP
1	A	797	VAL
1	A	803	CYS
1	A	839	HIS
1	A	862	TYR
1	A	953	THR
1	A	954	GLY
1	A	972	HIS
1	A	1032	TRP
1	A	1044	GLN
1	A	1054	GLN
1	A	1073	ILE
1	A	1087	THR
1	A	1095	SER
1	A	1098	THR

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Mol	Chain	Res	Type
1	A	1107	LYS
1	A	1129	CYS
1	A	1137	LEU
1	A	1139	GLY
1	A	1162	LEU
1	A	1168	ILE
1	A	1212	GLN
1	A	1213	THR
1	A	1214	PHE
1	A	1223	LYS
1	A	1238	ASN
1	A	117	GLY
1	A	130	LYS
1	A	142	LYS
1	A	244	ASP
1	A	302	LYS
1	A	355	LYS
1	A	386	LEU
1	A	480	CYS
1	A	603	ILE
1	A	606	LEU
1	A	880	GLY
1	A	884	TRP
1	A	933	ASN
1	A	952	LYS
1	A	1075	GLY
1	A	1090	SER
1	A	1114	PHE
1	A	1120	LEU
1	A	1133	SER
1	A	1247	VAL
1	A	156	ALA
1	A	160	LYS
1	A	211	SER
1	A	226	ARG
1	A	228	ARG
1	A	233	ARG
1	A	283	GLU
1	A	307	PRO
1	A	448	LYS
1	A	605	ASN
1	A	617	ALA

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Mol	Chain	Res	Type
1	A	785	ARG
1	A	842	THR
1	A	861	GLN
1	A	962	ALA
1	A	995	VAL
1	A	1015	GLY
1	A	1025	SER
1	A	1053	LEU
1	A	1063	PHE
1	A	1101	SER
1	A	1132	CYS
1	A	1182	THR
1	A	103	ASP
1	A	111	ARG
1	A	220	ILE
1	A	335	PRO
1	A	475	PRO
1	A	486	PHE
1	A	589	ASP
1	A	749	CYS
1	A	818	LYS
1	A	841	SER
1	A	847	ASP
1	A	955	GLN
1	A	961	GLU
1	A	1117	LEU
1	A	1180	TRP
1	A	1207	THR
1	A	213	SER
1	A	215	ARG
1	A	268	SER
1	A	353	ILE
1	A	360	ASP
1	A	482	TYR
1	A	522	LEU
1	A	609	LEU
1	A	613	PRO
1	A	741	GLY
1	A	838	GLY
1	A	1007	ARG
1	A	1017	THR
1	A	1167	PRO

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Mol	Chain	Res	Type
1	A	753	PRO
1	A	963	GLN
1	A	1047	VAL
1	A	1140	ILE
1	A	1185	CYS
1	A	519	PRO
1	A	964	VAL
1	A	945	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	A	1005/1109 (91%)	908 (90%)	97 (10%)	8 31

All (97) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ASP
1	A	130	LYS
1	A	131	LYS
1	A	153	TYR
1	A	177	CYS
1	A	196	LEU
1	A	209	GLU
1	A	216	LEU
1	A	251	LEU
1	A	288	ARG
1	A	299	VAL
1	A	305	ASP
1	A	330	LEU
1	A	337	ARG
1	A	358	SER
1	A	366	GLU
1	A	373	GLU
1	A	386	LEU

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Mol	Chain	Res	Type
1	A	402	VAL
1	A	403	LEU
1	A	431	LYS
1	A	436	TYR
1	A	452	GLN
1	A	461	VAL
1	A	507	LEU
1	A	522	LEU
1	A	532	ILE
1	A	546	GLU
1	A	548	LEU
1	A	551	ASN
1	A	575	GLU
1	A	581	LYS
1	A	602	THR
1	A	612	ARG
1	A	613	PRO
1	A	638	THR
1	A	639	LEU
1	A	688	THR
1	A	691	LEU
1	A	694	THR
1	A	703	ASN
1	A	705	CYS
1	A	713	HIS
1	A	714	LEU
1	A	723	PHE
1	A	725	LEU
1	A	752	SER
1	A	767	LEU
1	A	785	ARG
1	A	799	VAL
1	A	812	LYS
1	A	822	LEU
1	A	826	ILE
1	A	832	LEU
1	A	842	THR
1	A	844	GLN
1	A	863	CYS
1	A	866	LEU
1	A	870	ASP
1	A	871	SER

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Mol	Chain	Res	Type
1	A	902	ASP
1	A	904	GLN
1	A	922	LEU
1	A	938	LEU
1	A	942	ASN
1	A	946	LEU
1	A	948	LEU
1	A	956	ILE
1	A	963	GLN
1	A	967	CYS
1	A	974	GLU
1	A	992	ASN
1	A	1003	LYS
1	A	1007	ARG
1	A	1016	LYS
1	A	1019	ILE
1	A	1024	ASP
1	A	1031	ASN
1	A	1041	GLN
1	A	1043	HIS
1	A	1051	ARG
1	A	1052	LEU
1	A	1053	LEU
1	A	1064	ASP
1	A	1071	ASN
1	A	1107	LYS
1	A	1111	ILE
1	A	1112	TRP
1	A	1137	LEU
1	A	1142	LEU
1	A	1151	ILE
1	A	1153	ILE
1	A	1160	GLN
1	A	1212	GLN
1	A	1223	LYS
1	A	1242	LEU
1	A	1248	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	134	HIS

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Mol	Chain	Res	Type
1	A	137	GLN
1	A	138	GLN
1	A	208	GLN
1	A	300	ASN
1	A	390	GLN
1	A	429	ASN
1	A	441	GLN
1	A	449	ASN
1	A	465	GLN
1	A	477	GLN
1	A	495	ASN
1	A	543	ASN
1	A	551	ASN
1	A	586	GLN
1	A	625	GLN
1	A	656	HIS
1	A	709	ASN
1	A	713	HIS
1	A	737	ASN
1	A	747	ASN
1	A	782	ASN
1	A	836	HIS
1	A	844	GLN
1	A	868	ASN
1	A	917	ASN
1	A	924	GLN
1	A	933	ASN
1	A	942	ASN
1	A	955	GLN
1	A	963	GLN
1	A	992	ASN
1	A	993	ASN
1	A	1002	HIS
1	A	1008	HIS
1	A	1031	ASN
1	A	1041	GLN
1	A	1127	ASN
1	A	1160	GLN
1	A	1163	HIS
1	A	1177	HIS
1	A	1212	GLN
1	A	1217	ASN

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Mol	Chain	Res	Type
1	A	1225	HIS

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 ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
2	ADP	A	1250	-	28,29,29	1.85	6 (21%)	43,45,45	1.94	10 (23%)
3	GBL	A	1252	-	6,6,6	0.73	0	7,7,7	0.78	0
3	GBL	A	1251	-	6,6,6	1.03	0	7,7,7	0.79	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
2	ADP	A	1250	-	-	0/16/32/32	0/3/3/3
3	GBL	A	1252	-	-	-	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GBL	A	1251	-	-	-	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1250	ADP	PA-O3A	6.73	1.66	1.59
2	A	1250	ADP	C6-N6	2.84	1.41	1.34
2	A	1250	ADP	C5-C4	2.60	1.43	1.39
2	A	1250	ADP	PB-O3B	2.47	1.64	1.54
2	A	1250	ADP	O4'-C1'	2.13	1.46	1.42
2	A	1250	ADP	C5-C6	2.01	1.46	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1250	ADP	C5-C4-N3	-5.38	119.31	126.72
2	A	1250	ADP	N3-C2-N1	-4.56	121.67	128.58
2	A	1250	ADP	N3-C4-N9	4.47	134.77	127.17
2	A	1250	ADP	C2-N3-C4	4.04	121.69	111.83
2	A	1250	ADP	C5-N7-C8	3.69	109.25	103.45
2	A	1250	ADP	C4-C5-N7	-3.18	106.95	110.58
2	A	1250	ADP	O4'-C1'-N9	2.42	112.75	108.09
2	A	1250	ADP	C3'-C2'-C1'	2.37	105.95	101.46
2	A	1250	ADP	N9-C8-N7	-2.29	110.69	113.94
2	A	1250	ADP	C2'-C1'-N9	-2.16	107.93	113.30

There are no chirality outliers.

There are no torsion outliers.

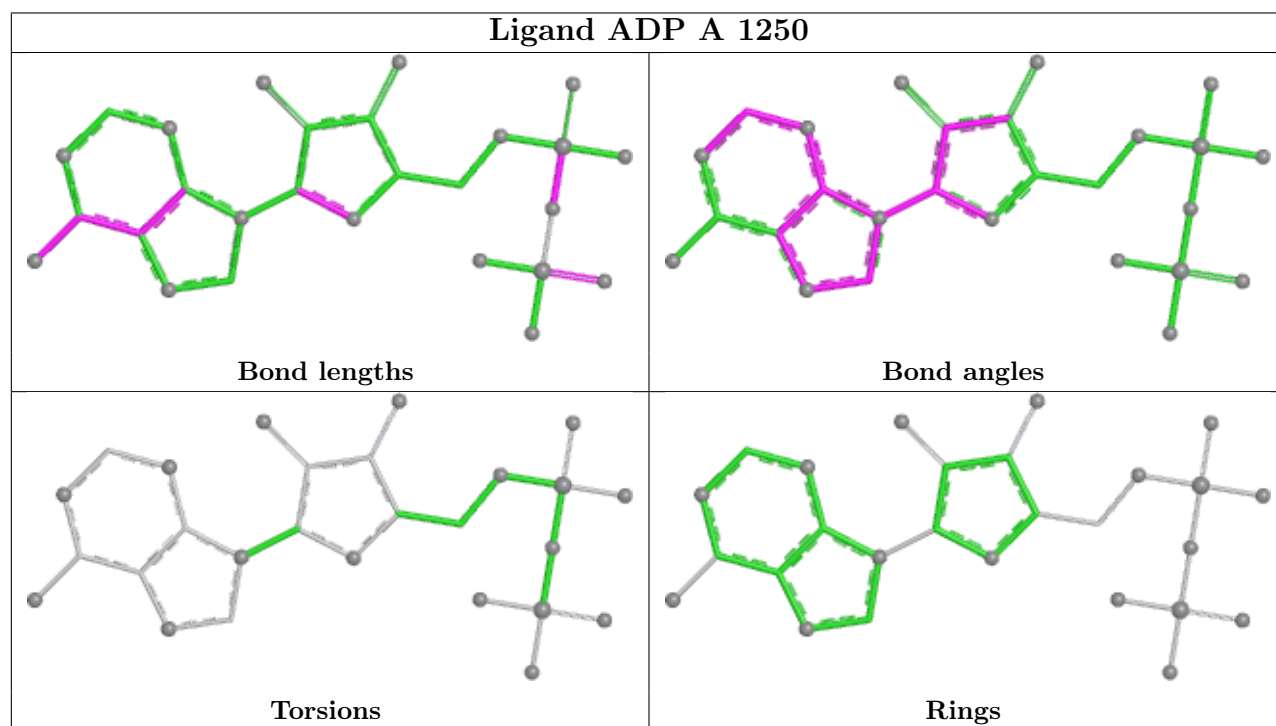
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1250	ADP	3	0
3	A	1251	GBL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1133/1256 (90%)	-0.41	0 100 100	74, 106, 140, 175	0

There are no RSRZ outliers to report.

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](#)

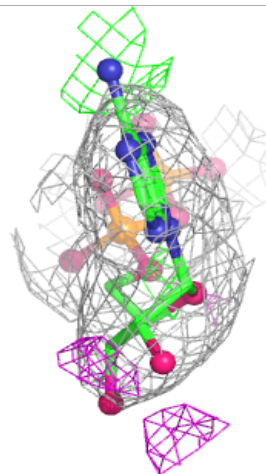
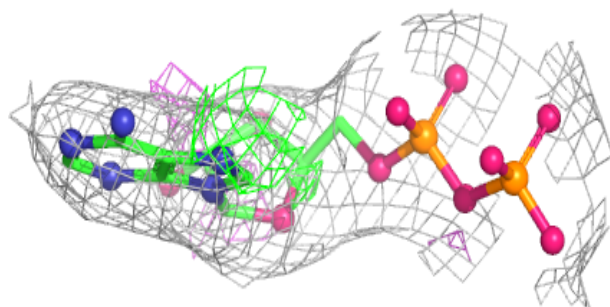
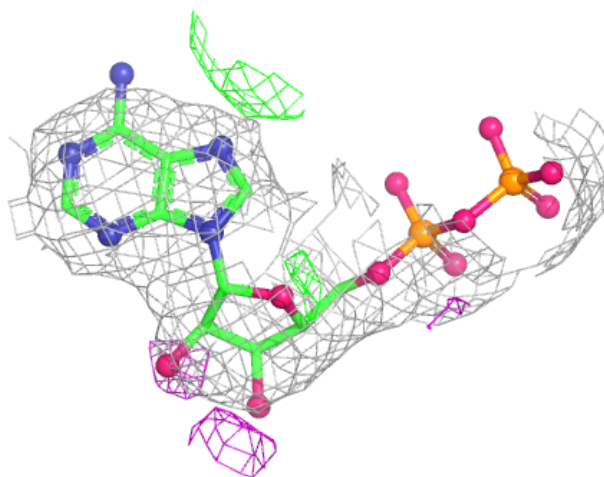
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q < 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ADP	A	1250	27/27	0.95	0.08	81,86,90,90	0
3	GBL	A	1251	6/6	0.95	0.10	91,92,92,93	0
3	GBL	A	1252	6/6	0.96	0.12	100,101,102,103	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ADP A 1250:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.