



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:28 PM GMT

PDB ID : 1FOE
Title : CRYSTAL STRUCTURE OF RAC1 IN COMPLEX WITH THE GUANINE
NUCLEOTIDE EXCHANGE REGION OF TIAM1
Authors : Worthylake, D.K.; Rossman, K.L.; Sondek, J.
Deposited on : 2000-08-27
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

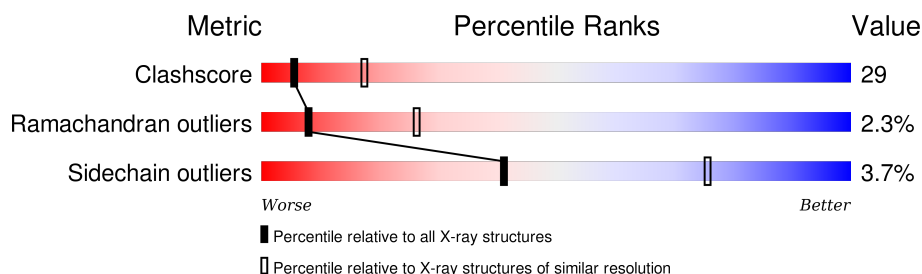
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)


The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	377	
1	C	377	
1	E	377	
1	G	377	
2	B	177	
2	D	177	
2	F	177	

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Mol	Chain	Length	Quality of chain
2	H	177	 A horizontal bar chart showing the quality of chain H. The bar is divided into three segments: a green segment on the left labeled '53%', a yellow segment in the middle labeled '44%', and a small orange segment on the right labeled with a single dot '•'.

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17570 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 T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	368	Total	C	N	O	S	Se	369	0	0
			2989	1918	509	550	6	6			
1	C	366	Total	C	N	O	S	Se	309	0	0
			2972	1907	506	547	6	6			
1	E	367	Total	C	N	O	S	Se	369	0	0
			2980	1913	507	548	6	6			
1	G	367	Total	C	N	O	S	Se	307	0	0
			2980	1913	507	548	6	6			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1031	MSE	THR	MODIFIED RESIDUE	UNP Q60610
A	1032	GLY	THR	CLONING ARTIFACT	UNP Q60610
A	1063	MSE	MET	MODIFIED RESIDUE	UNP Q60610
A	1091	MSE	MET	MODIFIED RESIDUE	UNP Q60610
A	1224	MSE	MET	MODIFIED RESIDUE	UNP Q60610
A	1234	MSE	MET	MODIFIED RESIDUE	UNP Q60610
A	1264	MSE	MET	MODIFIED RESIDUE	UNP Q60610
A	1334	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1031	MSE	THR	MODIFIED RESIDUE	UNP Q60610
C	1032	GLY	THR	CLONING ARTIFACT	UNP Q60610
C	1063	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1091	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1224	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1234	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1264	MSE	MET	MODIFIED RESIDUE	UNP Q60610
C	1334	MSE	MET	MODIFIED RESIDUE	UNP Q60610
E	1031	MSE	THR	MODIFIED RESIDUE	UNP Q60610
E	1032	GLY	THR	CLONING ARTIFACT	UNP Q60610
E	1063	MSE	MET	MODIFIED RESIDUE	UNP Q60610
E	1091	MSE	MET	MODIFIED RESIDUE	UNP Q60610

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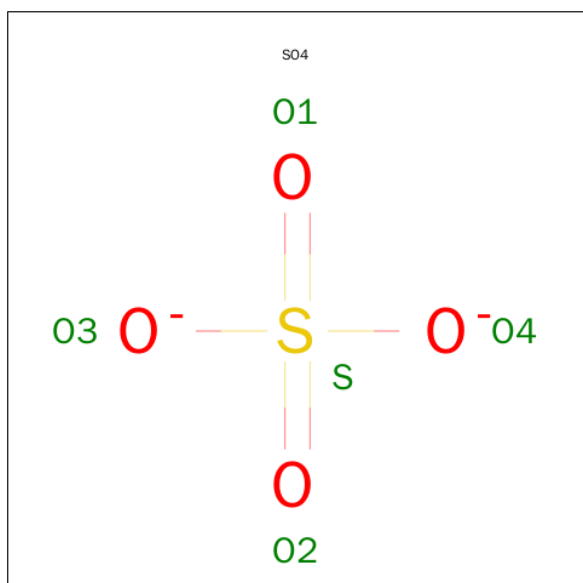
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Chain	Residue	Modelled	Actual	Comment	Reference
E	1224	MSE	MET	MODIFIED RESIDUE	UNP Q60610
E	1234	MSE	MET	MODIFIED RESIDUE	UNP Q60610
E	1264	MSE	MET	MODIFIED RESIDUE	UNP Q60610
E	1334	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1031	MSE	THR	MODIFIED RESIDUE	UNP Q60610
G	1032	GLY	THR	CLONING ARTIFACT	UNP Q60610
G	1063	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1091	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1224	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1234	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1264	MSE	MET	MODIFIED RESIDUE	UNP Q60610
G	1334	MSE	MET	MODIFIED RESIDUE	UNP Q60610

- Molecule 2 is a protein called RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	177	Total	C	N	O	S	14	0	0
			1384	889	228	259	8			
2	D	177	Total	C	N	O	S	14	0	0
			1384	889	228	259	8			
2	F	177	Total	C	N	O	S	14	0	0
			1384	889	228	259	8			
2	H	177	Total	C	N	O	S	14	0	0
			1384	889	228	259	8			

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total O S 5 4 1	0	0
3	D	1	Total O S 5 4 1	0	0
3	F	1	Total O S 5 4 1	0	0
3	H	1	Total O S 5 4 1	0	0

- Molecule 4 is water.

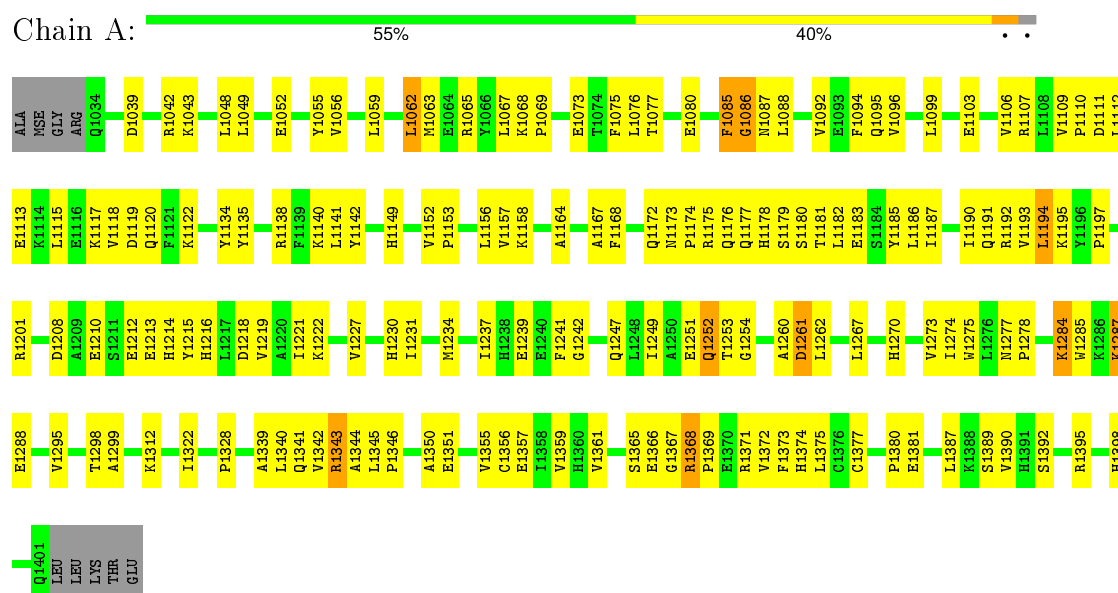
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	14	Total O 14 14	0	0
4	B	6	Total O 6 6	0	0
4	C	8	Total O 8 8	0	0
4	D	6	Total O 6 6	0	0
4	E	7	Total O 7 7	0	0
4	F	7	Total O 7 7	0	0
4	G	19	Total O 19 19	0	0
4	H	26	Total O 26 26	0	0

3 Residue-property plots

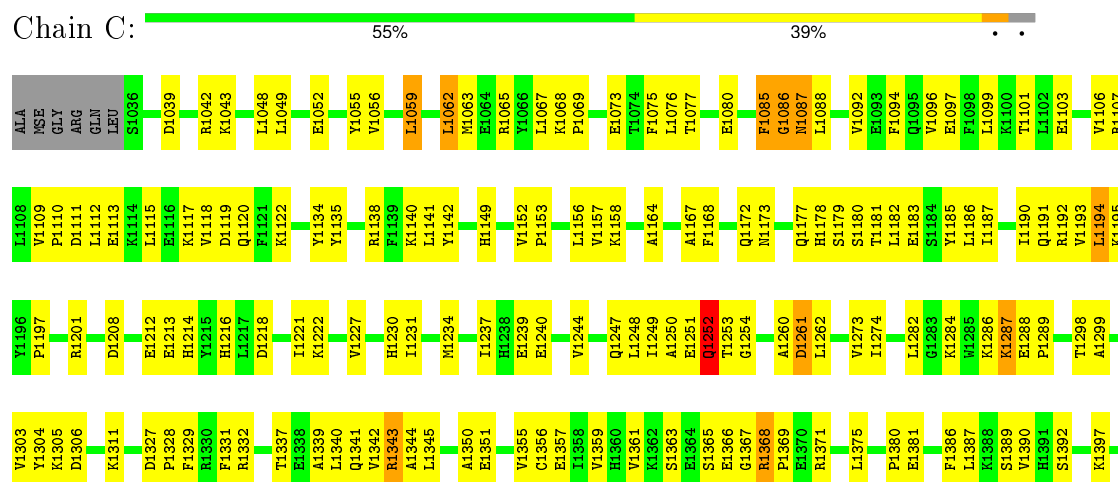
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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.

Note EDS was not executed.

• Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1



• Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1



Q1401	LEU
	LEU
	LYS
	THR
	GLU

- Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1

Chain E:  55% 38% 7%

LEU	Al299	Y196 P197	L108 V109	ALA
LEU	K1305	R1201	P110 D111	PSE GLY
THR	K4306	D1208	L112 E113	ARG GLN
GLU	K1313	E1213 H1214	K114 L115	L1035
	E1325	Y1215 H1216	E116 V118	D1039
	D1327	L1217 D1218	L119 Q120	R1042 K1043
	F1331	K1222	F1121 K122	E1047 L1048
	K1332	V1227	Y134 Y135	L1049
	H1333	H1230 I1231	R138 F139	E1050 T1051
	A1339	M1234	L141 Y142	E1052
	L1340	I1237 H1238	E1063 M1063	Y1055 V1056
	Q1341	E1239	H149	L1059
	V1342	Q1247 L1248	Y152 P153	L1062
	R1343	I1249 A1250	L156 V157	E1064
	A1344	E1251 Q1252	K158	R1065 Y1066
	L1345	T1253 G1254	A1164	L1067 K1068
	P1346			P1069
	A1350			E1073
	E1351			T1074
	V1355			F1075
	C1356			L1076
	E1357			T1077
	I1358			E1080
	V1359			F1085
	H1360			G1086
	V1361			M1087
	S1365			L1088
	E1366			L1092
	G1367			V1093
	R1368			F1094
	P1369			Q1095
	E1370			V1096
	R1371			E1097
	H1374			F1098
	L1375			L1099
	C1376			L1102
	C1377			E1103
	L1387			
	K1388			
	S1389			
	H1390			
	V1391			
	S1392			
	K1397			
	H1398			
	R1399			
	F1400			
	Q1401			

- Molecule 1: T-LYMPHOMA INVASION AND METASTASIS INDUCING PROTEIN 1

Chain G: 54% 41% .

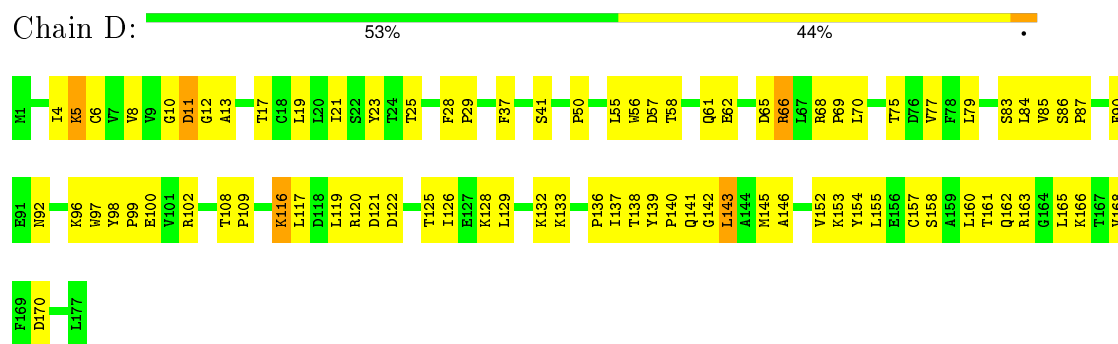
S1392 I1393 L1394	K1397 H1398 A1399 R1400	Q1401 LEU LYS THR GLU	V1303	P1197	P1110	ALA
			V1304	R1201	D1111	MSE
			K1305	E1213 H1214 Y1215	L1112	GLY
			D1306		E1113	ARG
			G1307		K1114	GLN
	S1308	K1311 K1312 K1313	E1116	L1035	S1036	
	E1324 E1325 Y1326 P1328 F1329		H1216	K1117	D1039	
			D1218	V1118	R1042	
			V1219	Q1120	K1043	
			A1220	F1121	L1048	
L1221		K1122	L1049			
A1339 Q1340 R1341 V1342 R1343 A1344 L1345	E1330 F1331 R1332	K1222	Y1134	E1052		
		V1227	Y1135	Y1055		
		H1230	R1138	V1056		
		I1231	F1139	L1059		
		M1234	Y1142	L1062		
	A1350 E1351	Q1237 H1238 E1239	H1149	M1063		
			L1248	E1064	R1065	
			L1249	P1152	Y1066	
			A1250	P1153	L1067	
			K1247	L1156	K1068	
V1355 C1356 E1357 L1358	Q1252 T1253 G1254	Y1157	P1069			
		K1158	E1073			
		A1164	T1074			
		A1167	F1075			
		F1168	L1076			
	V1359 H1360 V1361	Q1252 T1253 G1254	Q1172	T1077		
			N1173	E1080		
			Q1176	F1085		
			Q1177	G1086		
			H1178	M1087		
K1362 L1363 E1364	V1273 I1274	S1180	L1088			
		T1181	V1092			
		L1182	E1093			
		E1183	F1094			
		S1184	Q1095			
	S1365 E1366 G1367	K1284 W1285	Y1185	V1096		
			L1186	E1097		
			I1187	F1098		
			L1099	L1099		
			I1190	E1103		
R1370 R1371	K1287 E1288	Q1191	V1106			
		R1192	R1107			
		V1193	L1194			
		K1195	L1108			
		Y1196	V1109			
	L1375	K1287 E1288	A1299	L1105		
			P1289	K1195		
			E1381	V1196		
			V1295	L1197		
			L1387	V1106		
F1388 S1389 V1390	T1298 A1299	V1193	V1106			
		L1194	R1107			
		K1195	L1108			
H1391	E1293	V1196	V1109			
		K1195	L1105			
		V1196	V1106			

- Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE

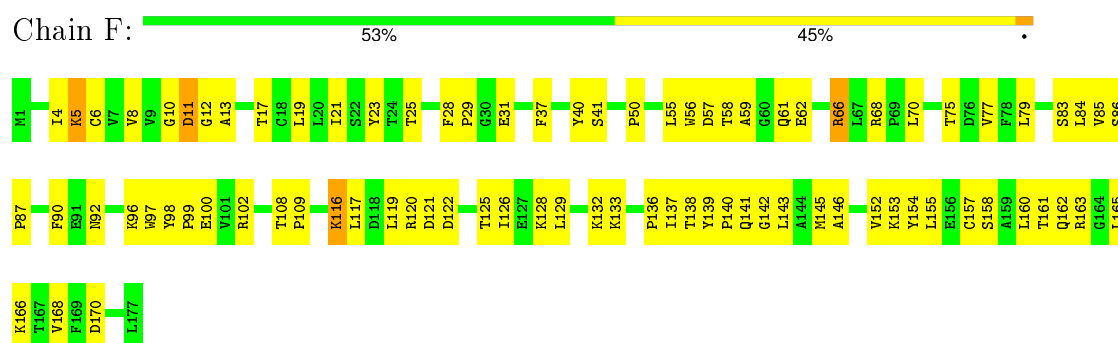
Chain B:  54% 44%

N92	N97	N98	N99	N100	N101	N102	T108	K116	L117	D118	L119	R120	D121	D122	I126	E127	K128	L129	K132	K133	P136	L137	T138	I139	P140	P141	P142	L143	L144	A144	M145	A146	V152	K153	V154	L155	E156	C157	S158	T161	Q162	R163	G164	L165	K166	L167	V168	F169	D170	L177
N91	I4	K5	O6	T7	V8	V9	G10	D11	G12	A13	T17	G18	L19	L20	L21	S22	Y23	T24	T25	F28	P29	Y40	S41	P50	L55	M56	D57	T58	Q61	E62	D65	R66	L67	R68	P69	L70	Q74	T75	D76	V77	F78	L79	S83	L84	V85	S86	P87	A88	S89	

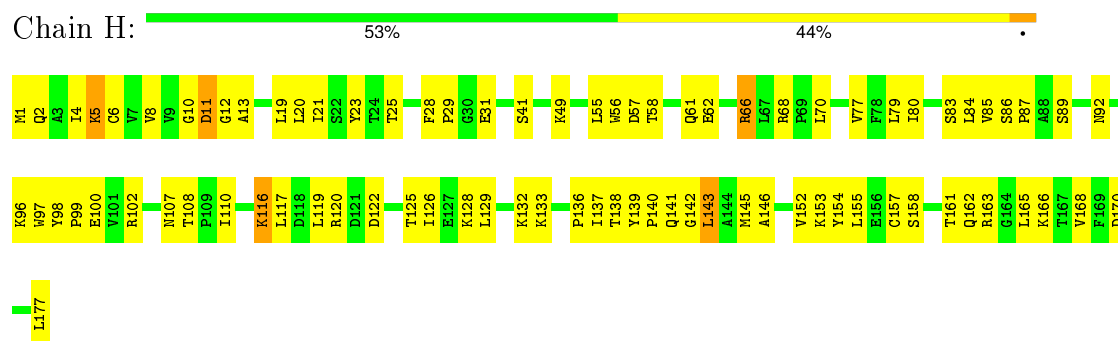
- Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE



- Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE



- Molecule 2: RAS-RELATED C3 BOTULINUM TOXIN SUBSTRATE



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	186.95Å 149.27Å 149.21Å 90.00° 121.00° 90.00°	Depositor
Resolution (Å)	15.00 – 2.80	Depositor
% Data completeness (in resolution range)	93.8 (15.00-2.80)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.3	Depositor
R, R_{free}	0.262 , 0.293	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	17570	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: SO4

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	0.42	0/3045	0.61	0/4095
1	C	0.41	0/3028	0.61	0/4072
1	E	0.41	0/3036	0.61	0/4083
1	G	0.45	1/3036 (0.0%)	0.62	0/4083
2	B	0.42	0/1414	0.79	3/1922 (0.2%)
2	D	0.40	0/1414	0.79	3/1922 (0.2%)
2	F	0.40	0/1414	0.79	3/1922 (0.2%)
2	H	0.51	0/1414	0.82	3/1922 (0.2%)
All	All	0.43	1/17801 (0.0%)	0.68	12/24021 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	1264	MSE	CG-SE	-5.10	1.78	1.95

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	5	LYS	N-CA-CB	-13.85	85.67	110.60
2	H	5	LYS	N-CA-CB	-13.35	86.58	110.60
2	D	5	LYS	N-CA-CB	-13.34	86.59	110.60
2	F	5	LYS	N-CA-CB	-13.23	86.79	110.60
2	D	4	ILE	CB-CA-C	-8.00	95.61	111.60
2	B	4	ILE	CB-CA-C	-7.96	95.69	111.60
2	H	4	ILE	CB-CA-C	-7.86	95.89	111.60
2	F	4	ILE	CB-CA-C	-7.81	95.99	111.60
2	F	4	ILE	N-CA-C	-6.73	92.82	111.00
2	H	4	ILE	N-CA-C	-6.55	93.32	111.00
2	D	4	ILE	N-CA-C	-6.53	93.36	111.00
2	B	4	ILE	N-CA-C	-6.33	93.92	111.00

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	2989	0	3035	170	0
1	C	2972	0	3016	175	0
1	E	2980	0	3027	173	0
1	G	2980	0	3027	171	0
2	B	1384	0	1405	84	0
2	D	1384	0	1405	84	0
2	F	1384	0	1405	82	1
2	H	1384	0	1405	86	1
3	B	5	0	0	0	0
3	D	5	0	0	0	0
3	F	5	0	0	0	0
3	H	5	0	0	0	0
4	A	14	0	0	0	0
4	B	6	0	0	0	0
4	C	8	0	0	0	0
4	D	6	0	0	0	0
4	E	7	0	0	0	0
4	F	7	0	0	0	0
4	G	19	0	0	0	0
4	H	26	0	0	0	0
All	All	17570	0	17725	949	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 29.

All (949) 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:1285:TRP:HH2	2:D:102:ARG:HG2	1.01	1.09
1:A:1285:TRP:CH2	2:D:102:ARG:HG2	1.88	1.08
2:B:138:THR:H	2:B:141:GLN:HE21	1.09	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1248:LEU:HD21	1:C:1332:ARG:HG3	1.46	0.97
1:E:1249:ILE:HD12	1:E:1261:ASP:H	1.29	0.96
2:H:138:THR:H	2:H:141:GLN:HE21	0.99	0.95
2:F:138:THR:H	2:F:141:GLN:HE21	1.07	0.94
2:D:138:THR:H	2:D:141:GLN:HE21	1.08	0.93
1:C:1249:ILE:HD11	1:C:1262:LEU:HG	1.52	0.91
1:A:1249:ILE:HD11	1:A:1262:LEU:HG	1.53	0.89
1:C:1056:VAL:HG21	1:C:1099:LEU:HD22	1.55	0.89
1:G:1287:LYS:HG2	1:G:1288:GLU:HG2	1.53	0.89
1:E:1343:ARG:HD3	1:E:1357:GLU:HG3	1.54	0.88
1:C:1287:LYS:HG2	1:C:1288:GLU:HG2	1.56	0.87
1:C:1193:VAL:HG23	1:C:1194:LEU:HD13	1.57	0.87
1:A:1343:ARG:HD3	1:A:1357:GLU:HG3	1.55	0.87
1:C:1343:ARG:HD3	1:C:1357:GLU:HG3	1.57	0.87
1:G:1190:ILE:HD13	2:H:70:LEU:HD13	1.55	0.86
1:E:1193:VAL:HG23	1:E:1194:LEU:HD13	1.57	0.86
1:E:1039:ASP:HA	1:E:1042:ARG:HH12	1.40	0.86
1:A:1190:ILE:HD13	2:B:70:LEU:HD13	1.55	0.86
1:E:1287:LYS:HG2	1:E:1288:GLU:HG2	1.57	0.85
1:G:1343:ARG:HD3	1:G:1357:GLU:HG3	1.56	0.85
1:A:1287:LYS:HG2	1:A:1288:GLU:HG2	1.58	0.85
1:A:1039:ASP:HA	1:A:1042:ARG:HH12	1.42	0.85
1:A:1239:GLU:OE2	2:B:66:ARG:HG3	1.77	0.84
1:G:1193:VAL:HG23	1:G:1194:LEU:HD13	1.59	0.84
2:B:138:THR:OG1	2:B:141:GLN:HG3	1.78	0.84
1:E:1190:ILE:HD13	2:F:70:LEU:HD13	1.59	0.83
1:A:1056:VAL:HG21	1:A:1099:LEU:HD22	1.58	0.83
1:E:1260:ALA:O	1:E:1261:ASP:HB2	1.75	0.83
2:H:138:THR:OG1	2:H:141:GLN:HG3	1.78	0.83
1:E:1062:LEU:HD11	1:E:1186:LEU:HD23	1.60	0.83
1:G:1035:LEU:HD12	2:H:31:GLU:HB2	1.61	0.83
1:C:1039:ASP:HA	1:C:1042:ARG:HH12	1.42	0.82
1:E:1248:LEU:HD21	1:E:1332:ARG:HG2	1.61	0.82
1:A:1039:ASP:O	1:A:1043:LYS:HG2	1.78	0.82
1:A:1284:LYS:HB3	2:D:99:PRO:HB3	1.62	0.82
1:E:1368:ARG:HG3	1:E:1368:ARG:HH11	1.44	0.82
1:E:1056:VAL:HG21	1:E:1099:LEU:HD22	1.60	0.82
1:G:1039:ASP:HA	1:G:1042:ARG:HH12	1.43	0.82
1:G:1249:ILE:HD11	1:G:1262:LEU:HG	1.61	0.82
1:E:1039:ASP:O	1:E:1043:LYS:HG2	1.80	0.81
1:G:1039:ASP:O	1:G:1043:LYS:HG2	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1193:VAL:HG23	1:A:1194:LEU:HD13	1.59	0.81
1:C:1039:ASP:O	1:C:1043:LYS:HG2	1.81	0.81
1:E:1234:MSE:HE2	1:E:1234:MSE:HA	1.62	0.81
1:G:1234:MSE:HA	1:G:1234:MSE:HE2	1.64	0.80
1:E:1249:ILE:HD11	1:E:1262:LEU:HG	1.62	0.79
1:C:1368:ARG:HH11	1:C:1368:ARG:HG3	1.47	0.79
1:A:1249:ILE:HD12	1:A:1261:ASP:H	1.47	0.79
1:G:1056:VAL:HG21	1:G:1099:LEU:HD22	1.65	0.79
1:A:1062:LEU:HD11	1:A:1186:LEU:HD23	1.63	0.78
1:G:1368:ARG:HG3	1:G:1368:ARG:HH11	1.47	0.78
2:D:138:THR:OG1	2:D:141:GLN:HG3	1.83	0.78
1:C:1234:MSE:HE2	1:C:1234:MSE:HA	1.64	0.78
1:G:1248:LEU:HD21	1:G:1332:ARG:HG3	1.67	0.77
1:A:1368:ARG:HH11	1:A:1368:ARG:HG3	1.50	0.77
1:C:1249:ILE:HD12	1:C:1261:ASP:H	1.49	0.77
1:G:1062:LEU:HD11	1:G:1186:LEU:HD23	1.67	0.76
2:F:138:THR:OG1	2:F:141:GLN:HG3	1.85	0.76
1:C:1062:LEU:HD11	1:C:1186:LEU:HD23	1.65	0.76
1:G:1304:TYR:HB3	1:G:1331:PHE:HB3	1.68	0.76
1:A:1234:MSE:HE2	1:A:1234:MSE:HA	1.66	0.76
1:E:1285:TRP:HZ2	2:H:98:TYR:CE2	2.05	0.74
1:C:1190:ILE:HD13	2:D:70:LEU:HD13	1.70	0.74
1:G:1249:ILE:HG23	1:G:1260:ALA:HA	1.70	0.73
1:C:1287:LYS:HD2	1:G:1306:ASP:OD2	1.89	0.73
1:E:1287:LYS:HD3	1:E:1287:LYS:N	2.03	0.73
1:C:1075:PHE:HE1	1:C:1168:PHE:HB2	1.53	0.73
1:E:1039:ASP:HA	1:E:1042:ARG:NH1	2.04	0.72
2:D:66:ARG:HH11	2:D:66:ARG:HG3	1.54	0.72
1:A:1287:LYS:N	1:A:1287:LYS:HD3	2.04	0.72
2:F:21:ILE:O	2:F:25:THR:HG22	1.90	0.71
1:A:1039:ASP:HA	1:A:1042:ARG:NH1	2.05	0.71
1:C:1039:ASP:HA	1:C:1042:ARG:NH1	2.05	0.71
1:C:1287:LYS:N	1:C:1287:LYS:HD3	2.06	0.71
1:A:1075:PHE:HE1	1:A:1168:PHE:HB2	1.55	0.70
1:E:1251:GLU:HG2	1:E:1251:GLU:O	1.90	0.70
1:A:1092:VAL:O	1:A:1096:VAL:HG23	1.91	0.70
1:G:1092:VAL:O	1:G:1096:VAL:HG23	1.91	0.70
1:E:1075:PHE:HE1	1:E:1168:PHE:HB2	1.55	0.70
1:C:1240:GLU:OE2	1:C:1305:LYS:NZ	2.24	0.70
1:G:1039:ASP:HA	1:G:1042:ARG:NH1	2.05	0.69
2:H:21:ILE:O	2:H:25:THR:HG22	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1249:ILE:HD12	1:G:1261:ASP:H	1.57	0.69
2:F:66:ARG:HG3	2:F:66:ARG:HH11	1.56	0.69
1:A:1251:GLU:HG2	1:A:1251:GLU:O	1.91	0.69
1:G:1273:VAL:HG21	1:G:1375:LEU:HB3	1.73	0.69
1:A:1249:ILE:HG23	1:A:1260:ALA:HA	1.73	0.69
1:A:1157:VAL:HG12	1:A:1157:VAL:O	1.92	0.69
2:H:122:ASP:O	2:H:126:ILE:HG13	1.93	0.69
1:E:1249:ILE:HG23	1:E:1260:ALA:HA	1.74	0.69
1:E:1092:VAL:O	1:E:1096:VAL:HG23	1.92	0.68
1:G:1062:LEU:HD13	1:G:1088:LEU:HD11	1.74	0.68
1:C:1249:ILE:HG23	1:C:1260:ALA:HA	1.74	0.68
1:E:1157:VAL:HG12	1:E:1157:VAL:O	1.93	0.68
1:A:1062:LEU:HD13	1:A:1088:LEU:HD11	1.74	0.68
1:A:1260:ALA:O	1:A:1261:ASP:HB2	1.93	0.68
1:G:1251:GLU:O	1:G:1251:GLU:HG2	1.93	0.68
1:G:1287:LYS:N	1:G:1287:LYS:HD3	2.08	0.67
1:C:1157:VAL:HG12	1:C:1157:VAL:O	1.94	0.67
1:G:1157:VAL:HG12	1:G:1157:VAL:O	1.94	0.67
1:E:1194:LEU:HD23	2:F:61:GLN:HB3	1.76	0.67
2:D:21:ILE:O	2:D:25:THR:HG22	1.95	0.67
1:C:1092:VAL:O	1:C:1096:VAL:HG23	1.95	0.67
1:G:1075:PHE:HE1	1:G:1168:PHE:HB2	1.59	0.67
2:H:66:ARG:HG3	2:H:66:ARG:HH11	1.59	0.66
1:A:1239:GLU:OE1	2:B:66:ARG:NH1	2.28	0.66
2:B:66:ARG:HH11	2:B:66:ARG:HG3	1.58	0.66
1:C:1156:LEU:HD13	1:C:1183:GLU:HG3	1.76	0.66
1:C:1251:GLU:O	1:C:1251:GLU:HG2	1.96	0.66
2:F:139:TYR:HE2	2:F:143:LEU:HD12	1.61	0.66
1:E:1156:LEU:HD13	1:E:1183:GLU:HG3	1.78	0.66
2:F:161:THR:HG21	2:F:163:ARG:HD2	1.78	0.66
1:A:1218:ASP:O	1:A:1222:LYS:HD3	1.96	0.66
1:E:1234:MSE:HE1	1:E:1267:LEU:HD23	1.77	0.66
2:B:21:ILE:O	2:B:25:THR:HG22	1.96	0.66
2:D:116:LYS:HG3	2:D:119:LEU:HD23	1.77	0.66
2:F:138:THR:H	2:F:141:GLN:NE2	1.89	0.65
2:B:116:LYS:HG3	2:B:119:LEU:HD23	1.77	0.65
2:B:128:LYS:HE2	2:B:132:LYS:HZ1	1.61	0.65
2:F:102:ARG:NH2	2:F:108:THR:O	2.28	0.65
2:F:6:CYS:HB3	2:F:55:LEU:HD23	1.78	0.65
2:D:102:ARG:NH2	2:D:108:THR:O	2.29	0.65
2:H:102:ARG:NH2	2:H:108:THR:O	2.28	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1260:ALA:O	1:C:1261:ASP:HB2	1.95	0.65
1:C:1156:LEU:CD1	1:C:1183:GLU:HG3	2.26	0.65
2:F:128:LYS:HE2	2:F:132:LYS:HZ1	1.62	0.65
2:D:120:ARG:NH2	2:D:139:TYR:N	2.45	0.64
2:F:116:LYS:HG3	2:F:119:LEU:HD23	1.78	0.64
2:B:120:ARG:NH2	2:B:139:TYR:N	2.45	0.64
1:C:1062:LEU:HD13	1:C:1088:LEU:HD11	1.77	0.64
2:F:120:ARG:NH2	2:F:139:TYR:N	2.45	0.64
1:E:1239:GLU:OE2	2:F:66:ARG:HG3	1.97	0.64
1:A:1346:PRO:HG3	1:E:1374:HIS:ND1	2.12	0.64
1:G:1156:LEU:HD13	1:G:1183:GLU:HG3	1.79	0.64
2:B:122:ASP:O	2:B:126:ILE:HG13	1.97	0.64
2:D:161:THR:HG21	2:D:163:ARG:HD2	1.79	0.64
1:G:1176:GLN:NE2	2:H:1:MET:N	2.45	0.64
1:C:1140:LYS:HD2	1:C:1230:HIS:CD2	2.33	0.64
2:B:157:CYS:HB2	2:B:165:LEU:HD12	1.80	0.64
1:E:1179:SER:H	2:F:41:SER:HB2	1.63	0.63
2:B:102:ARG:NH2	2:B:108:THR:O	2.31	0.63
1:C:1273:VAL:HG21	1:C:1375:LEU:HB3	1.81	0.63
2:D:138:THR:H	2:D:141:GLN:NE2	1.90	0.63
1:E:1248:LEU:HD21	1:E:1332:ARG:CG	2.28	0.63
1:E:1218:ASP:O	1:E:1222:LYS:HD3	1.98	0.63
1:C:1056:VAL:HG21	1:C:1099:LEU:CD2	2.27	0.63
1:E:1062:LEU:HD13	1:E:1088:LEU:HD11	1.79	0.63
1:G:1086:GLY:O	1:G:1088:LEU:N	2.32	0.63
2:F:84:LEU:HD12	2:F:117:LEU:HA	1.81	0.63
1:E:1331:PHE:CZ	1:E:1333:HIS:HB2	2.34	0.63
2:B:84:LEU:HD12	2:B:117:LEU:HA	1.81	0.63
2:B:161:THR:HG21	2:B:163:ARG:HD2	1.81	0.63
2:H:128:LYS:HE2	2:H:132:LYS:HZ1	1.63	0.63
1:E:1156:LEU:CD1	1:E:1183:GLU:HG3	2.28	0.62
1:E:1260:ALA:O	1:E:1261:ASP:CB	2.45	0.62
1:G:1218:ASP:O	1:G:1222:LYS:HD3	1.99	0.62
1:E:1088:LEU:O	1:E:1092:VAL:HG23	2.00	0.62
2:F:139:TYR:CE2	2:F:143:LEU:HD12	2.34	0.62
1:C:1287:LYS:HG2	1:C:1288:GLU:N	2.15	0.62
2:D:84:LEU:HD12	2:D:117:LEU:HA	1.82	0.62
1:G:1287:LYS:HG2	1:G:1288:GLU:N	2.14	0.62
1:G:1178:HIS:HA	1:G:1181:THR:HG23	1.82	0.62
2:H:116:LYS:HG3	2:H:119:LEU:HD23	1.80	0.62
1:A:1086:GLY:O	1:A:1088:LEU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1178:HIS:HA	1:C:1181:THR:HG23	1.82	0.61
1:G:1156:LEU:CD1	1:G:1183:GLU:HG3	2.29	0.61
2:D:122:ASP:O	2:D:126:ILE:HG13	1.99	0.61
1:C:1088:LEU:O	1:C:1092:VAL:HG23	1.99	0.61
1:C:1218:ASP:O	1:C:1222:LYS:HD3	2.00	0.61
2:D:139:TYR:HE2	2:D:143:LEU:HD12	1.65	0.61
1:G:1365:SER:O	1:G:1366:GLU:HB3	2.01	0.61
1:A:1178:HIS:HA	1:A:1181:THR:HG23	1.83	0.61
1:E:1140:LYS:HD2	1:E:1230:HIS:CD2	2.36	0.61
1:G:1112:LEU:HA	1:G:1115:LEU:HD13	1.83	0.61
1:C:1112:LEU:HA	1:C:1115:LEU:HD13	1.83	0.61
2:H:161:THR:HG21	2:H:163:ARG:HD2	1.82	0.60
1:C:1304:TYR:HB3	1:C:1331:PHE:HB3	1.81	0.60
2:F:122:ASP:O	2:F:126:ILE:HG13	2.00	0.60
1:G:1140:LYS:HD2	1:G:1230:HIS:CD2	2.36	0.60
1:C:1247:GLN:HB3	1:C:1332:ARG:NH1	2.16	0.60
2:D:157:CYS:HB2	2:D:165:LEU:HD12	1.83	0.60
2:H:6:CYS:HB3	2:H:55:LEU:HD23	1.83	0.60
2:B:138:THR:H	2:B:141:GLN:NE2	1.89	0.60
2:H:120:ARG:NH2	2:H:139:TYR:N	2.49	0.60
1:E:1365:SER:O	1:E:1366:GLU:HB3	2.02	0.60
2:B:6:CYS:HB3	2:B:55:LEU:HD23	1.83	0.60
1:G:1088:LEU:O	1:G:1092:VAL:HG23	2.02	0.60
1:E:1076:LEU:HB3	1:E:1080:GLU:HB2	1.84	0.60
2:H:138:THR:H	2:H:141:GLN:NE2	1.84	0.60
1:C:1075:PHE:HE1	1:C:1168:PHE:CB	2.15	0.60
1:A:1076:LEU:HB3	1:A:1080:GLU:HB2	1.82	0.60
1:C:1365:SER:O	1:C:1366:GLU:HB3	2.02	0.60
2:F:157:CYS:HB2	2:F:165:LEU:HD12	1.82	0.60
2:F:154:TYR:C	2:F:155:LEU:HD12	2.23	0.60
1:C:1179:SER:H	2:D:41:SER:HB2	1.67	0.60
1:E:1086:GLY:O	1:E:1088:LEU:N	2.35	0.59
1:E:1365:SER:C	1:E:1367:GLY:H	2.05	0.59
1:A:1194:LEU:HD23	2:B:61:GLN:HB3	1.84	0.59
1:A:1140:LYS:HD2	1:A:1230:HIS:CD2	2.37	0.59
1:G:1343:ARG:N	1:G:1343:ARG:HD2	2.17	0.59
1:C:1076:LEU:HB3	1:C:1080:GLU:HB2	1.83	0.59
1:E:1343:ARG:HD3	1:E:1357:GLU:CG	2.29	0.59
2:D:154:TYR:C	2:D:155:LEU:HD12	2.23	0.59
1:E:1042:ARG:HE	1:E:1113:GLU:HA	1.67	0.59
1:C:1103:GLU:O	1:C:1106:VAL:HG12	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1112:LEU:HA	1:E:1115:LEU:HD13	1.84	0.59
2:H:84:LEU:HD12	2:H:117:LEU:HA	1.83	0.59
1:G:1343:ARG:HD3	1:G:1357:GLU:CG	2.32	0.59
2:F:83:SER:HB3	2:F:86:SER:HB3	1.84	0.59
1:C:1343:ARG:HD2	1:C:1343:ARG:N	2.17	0.59
1:C:1042:ARG:HE	1:C:1113:GLU:HA	1.68	0.59
1:E:1274:ILE:HG21	1:E:1288:GLU:HB2	1.85	0.59
1:G:1076:LEU:HB3	1:G:1080:GLU:HB2	1.85	0.59
1:C:1149:HIS:HA	1:C:1152:VAL:HG23	1.85	0.58
1:E:1117:LYS:HB2	1:E:1120:GLN:HG3	1.84	0.58
2:H:157:CYS:HB2	2:H:165:LEU:HD12	1.85	0.58
1:A:1365:SER:O	1:A:1366:GLU:HB3	2.03	0.58
1:A:1274:ILE:HG21	1:A:1288:GLU:HB2	1.85	0.58
1:A:1212:GLU:CD	1:G:1097:GLU:HG2	2.23	0.58
2:D:139:TYR:CE2	2:D:143:LEU:HD12	2.39	0.58
1:E:1063:MSE:CE	1:E:1088:LEU:HD22	2.34	0.58
1:E:1178:HIS:HA	1:E:1181:THR:HG23	1.83	0.58
1:A:1042:ARG:HE	1:A:1113:GLU:HA	1.68	0.58
2:H:128:LYS:HE2	2:H:132:LYS:NZ	2.18	0.58
1:A:1343:ARG:CD	1:A:1357:GLU:HG3	2.32	0.58
1:C:1365:SER:C	1:C:1367:GLY:H	2.06	0.58
2:D:6:CYS:HB3	2:D:55:LEU:HD23	1.85	0.58
1:C:1075:PHE:CE1	1:C:1168:PHE:HB2	2.36	0.58
1:G:1365:SER:C	1:G:1367:GLY:H	2.07	0.58
1:A:1365:SER:C	1:A:1367:GLY:H	2.06	0.58
2:H:83:SER:HB3	2:H:86:SER:HB3	1.86	0.58
1:E:1343:ARG:HD2	1:E:1343:ARG:N	2.19	0.57
1:A:1149:HIS:HA	1:A:1152:VAL:HG23	1.84	0.57
2:F:128:LYS:HE2	2:F:132:LYS:NZ	2.18	0.57
1:A:1287:LYS:HG2	1:A:1288:GLU:N	2.19	0.57
1:G:1176:GLN:HE22	2:H:1:MET:N	2.02	0.57
1:A:1112:LEU:HA	1:A:1115:LEU:HD13	1.86	0.57
2:D:138:THR:N	2:D:141:GLN:HE21	1.91	0.57
1:E:1075:PHE:HE1	1:E:1168:PHE:CB	2.17	0.57
1:A:1117:LYS:HB2	1:A:1120:GLN:HG3	1.87	0.57
1:E:1287:LYS:HG2	1:E:1288:GLU:N	2.19	0.57
1:E:1149:HIS:HA	1:E:1152:VAL:HG23	1.86	0.57
1:A:1103:GLU:O	1:A:1106:VAL:HG12	2.04	0.57
1:C:1086:GLY:O	1:C:1088:LEU:N	2.38	0.57
1:C:1117:LYS:HB2	1:C:1120:GLN:HG3	1.87	0.57
1:C:1274:ILE:CG2	1:C:1288:GLU:HB2	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1274:ILE:CG2	1:E:1288:GLU:HB2	2.34	0.57
1:C:1274:ILE:HG21	1:C:1288:GLU:HB2	1.86	0.57
1:A:1343:ARG:N	1:A:1343:ARG:HD2	2.20	0.57
1:E:1287:LYS:HZ2	1:E:1288:GLU:H	1.53	0.57
1:A:1274:ILE:CG2	1:A:1288:GLU:HB2	2.35	0.57
1:A:1067:LEU:HB3	1:A:1085:PHE:CZ	2.40	0.57
1:A:1075:PHE:HE1	1:A:1168:PHE:CB	2.17	0.57
1:E:1343:ARG:CD	1:E:1357:GLU:HG3	2.31	0.57
1:A:1056:VAL:HG21	1:A:1099:LEU:CD2	2.32	0.57
1:G:1260:ALA:O	1:G:1261:ASP:HB2	2.05	0.57
2:B:154:TYR:C	2:B:155:LEU:HD12	2.25	0.57
1:C:1343:ARG:HD3	1:C:1357:GLU:CG	2.32	0.57
1:E:1177:GLN:HG3	2:F:41:SER:HB3	1.86	0.57
2:D:83:SER:HB3	2:D:86:SER:HB3	1.86	0.56
1:A:1287:LYS:HZ2	1:A:1288:GLU:H	1.53	0.56
1:A:1088:LEU:O	1:A:1092:VAL:HG23	2.05	0.56
2:H:87:PRO:HA	2:H:137:ILE:HD11	1.88	0.56
2:H:139:TYR:HE2	2:H:143:LEU:HD12	1.70	0.56
1:C:1056:VAL:CG2	1:C:1099:LEU:HD22	2.32	0.56
1:G:1042:ARG:HE	1:G:1113:GLU:HA	1.69	0.56
2:D:128:LYS:HE2	2:D:132:LYS:HZ1	1.70	0.56
2:D:128:LYS:HE2	2:D:132:LYS:NZ	2.20	0.56
2:D:87:PRO:HA	2:D:137:ILE:HD11	1.87	0.56
2:B:139:TYR:HE2	2:B:143:LEU:HD12	1.70	0.56
2:H:138:THR:N	2:H:141:GLN:HE21	1.84	0.56
1:C:1287:LYS:CD	1:G:1306:ASP:OD2	2.54	0.56
1:G:1063:MSE:CE	1:G:1088:LEU:HD22	2.35	0.56
1:C:1343:ARG:HD2	1:C:1343:ARG:H	1.71	0.56
1:E:1067:LEU:HB3	1:E:1085:PHE:CZ	2.41	0.56
1:G:1103:GLU:O	1:G:1106:VAL:HG12	2.06	0.56
1:A:1343:ARG:HD3	1:A:1357:GLU:CG	2.30	0.56
2:B:128:LYS:HE2	2:B:132:LYS:NZ	2.19	0.56
1:C:1247:GLN:O	1:C:1251:GLU:HB3	2.05	0.56
1:G:1345:LEU:HD12	1:G:1355:VAL:HG12	1.88	0.56
1:E:1075:PHE:CE1	1:E:1168:PHE:HB2	2.39	0.55
2:B:139:TYR:CE2	2:B:143:LEU:HD12	2.41	0.55
2:B:87:PRO:HA	2:B:137:ILE:HD11	1.87	0.55
1:A:1190:ILE:HD13	2:B:70:LEU:CD1	2.35	0.55
1:G:1343:ARG:H	1:G:1343:ARG:HD2	1.70	0.55
1:A:1295:VAL:HG11	1:A:1389:SER:OG	2.06	0.55
1:C:1248:LEU:HD21	1:C:1332:ARG:CG	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1111:ASP:OD2	1:G:1113:GLU:HB2	2.06	0.55
2:B:83:SER:HB3	2:B:86:SER:HB3	1.87	0.55
2:F:139:TYR:HB3	2:F:140:PRO:HD3	1.88	0.55
1:A:1173:ASN:HD21	1:A:1180:SER:HB2	1.72	0.55
1:C:1287:LYS:HD2	1:G:1306:ASP:CG	2.27	0.55
2:H:98:TYR:HB3	2:H:99:PRO:HD3	1.89	0.55
1:E:1109:VAL:HG13	1:E:1110:PRO:HD2	1.89	0.55
2:F:87:PRO:HA	2:F:137:ILE:HD11	1.88	0.55
1:C:1288:GLU:OE1	1:G:1308:SER:HB2	2.07	0.55
1:G:1067:LEU:HB3	1:G:1085:PHE:CZ	2.42	0.55
1:C:1063:MSE:CE	1:C:1088:LEU:HD22	2.37	0.55
2:B:98:TYR:OH	2:B:102:ARG:HD2	2.07	0.55
1:A:1215:TYR:OH	1:G:1138:ARG:HG3	2.07	0.55
1:C:1306:ASP:OD2	1:G:1287:LYS:N	2.31	0.55
1:C:1218:ASP:OD1	1:C:1222:LYS:HE3	2.06	0.55
1:A:1119:ASP:O	1:A:1122:LYS:HG3	2.07	0.55
2:H:139:TYR:CE2	2:H:143:LEU:HD12	2.42	0.54
1:E:1343:ARG:HD2	1:E:1343:ARG:H	1.72	0.54
1:E:1035:LEU:HB2	1:E:1039:ASP:HB2	1.88	0.54
1:C:1227:VAL:O	1:C:1231:ILE:HG12	2.06	0.54
1:C:1173:ASN:HD21	1:C:1180:SER:HB2	1.71	0.54
1:G:1179:SER:H	2:H:41:SER:HB2	1.71	0.54
1:A:1345:LEU:HD12	1:A:1355:VAL:HG12	1.89	0.54
2:B:138:THR:N	2:B:141:GLN:HE21	1.92	0.54
1:E:1247:GLN:O	1:E:1251:GLU:HB3	2.06	0.54
1:C:1216:HIS:HB3	1:E:1134:TYR:CE2	2.42	0.54
2:H:154:TYR:C	2:H:155:LEU:HD12	2.27	0.54
1:G:1176:GLN:NE2	2:H:1:MET:H3	2.03	0.54
1:E:1103:GLU:O	1:E:1106:VAL:HG12	2.07	0.54
2:B:139:TYR:HB3	2:B:140:PRO:HD3	1.89	0.54
1:G:1274:ILE:HG21	1:G:1288:GLU:HB2	1.88	0.54
1:G:1035:LEU:HD12	2:H:31:GLU:CB	2.35	0.54
1:C:1067:LEU:HB3	1:C:1085:PHE:CZ	2.41	0.54
1:G:1075:PHE:CE1	1:G:1168:PHE:HB2	2.43	0.54
1:E:1094:PHE:HE1	1:E:1135:TYR:HD2	1.55	0.54
1:A:1343:ARG:H	1:A:1343:ARG:HD2	1.72	0.54
1:A:1234:MSE:HE1	1:A:1267:LEU:HD23	1.90	0.54
1:C:1287:LYS:HZ2	1:C:1288:GLU:H	1.56	0.54
1:A:1247:GLN:O	1:A:1251:GLU:HB3	2.08	0.54
2:F:98:TYR:HB3	2:F:99:PRO:HD3	1.90	0.54
1:A:1075:PHE:CE1	1:A:1168:PHE:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1115:LEU:HD12	1:E:1115:LEU:N	2.23	0.54
1:A:1063:MSE:CE	1:A:1088:LEU:HD22	2.37	0.53
1:A:1218:ASP:OD1	1:A:1222:LYS:HE3	2.09	0.53
1:G:1117:LYS:HB2	1:G:1120:GLN:HG3	1.89	0.53
1:G:1343:ARG:CD	1:G:1357:GLU:HG3	2.33	0.53
1:G:1094:PHE:HE1	1:G:1135:TYR:HD2	1.56	0.53
1:A:1135:TYR:CE2	1:A:1138:ARG:NH2	2.75	0.53
2:H:138:THR:HG1	2:H:141:GLN:HG3	1.70	0.53
1:A:1135:TYR:HE2	1:A:1138:ARG:NH2	2.05	0.53
2:F:8:VAL:HG22	2:F:79:LEU:HD12	1.90	0.53
1:A:1395:ARG:O	1:A:1398:HIS:HB3	2.07	0.53
1:A:1260:ALA:O	1:A:1261:ASP:CB	2.55	0.53
1:G:1274:ILE:CG2	1:G:1288:GLU:HB2	2.38	0.53
1:A:1111:ASP:OD2	1:A:1113:GLU:HB2	2.09	0.53
1:C:1156:LEU:HD21	1:C:1182:LEU:HD23	1.91	0.53
1:A:1056:VAL:CG2	1:A:1099:LEU:HD22	2.36	0.53
1:E:1285:TRP:HH2	2:H:102:ARG:HG2	1.74	0.53
1:C:1368:ARG:CG	1:C:1368:ARG:HH11	2.19	0.53
1:E:1187:ILE:O	1:E:1191:GLN:HG3	2.09	0.53
1:A:1109:VAL:HG13	1:A:1110:PRO:HD2	1.89	0.53
1:G:1247:GLN:O	1:G:1251:GLU:HB3	2.09	0.53
1:E:1135:TYR:CE2	1:E:1138:ARG:NH2	2.77	0.53
1:C:1345:LEU:HD12	1:C:1355:VAL:HG12	1.90	0.53
1:G:1075:PHE:HE1	1:G:1168:PHE:CB	2.20	0.53
1:C:1140:LYS:HD2	1:C:1230:HIS:HD2	1.74	0.53
1:G:1140:LYS:HE2	1:G:1227:VAL:HA	1.89	0.53
1:C:1179:SER:H	2:D:41:SER:CB	2.22	0.53
2:D:139:TYR:HB3	2:D:140:PRO:HD3	1.90	0.52
1:E:1035:LEU:HB2	1:E:1039:ASP:CB	2.39	0.52
1:A:1239:GLU:CD	2:B:66:ARG:NH1	2.63	0.52
2:B:57:ASP:OD1	2:B:58:THR:N	2.41	0.52
1:G:1115:LEU:N	1:G:1115:LEU:HD12	2.23	0.52
1:C:1115:LEU:HD12	1:C:1115:LEU:N	2.23	0.52
1:A:1115:LEU:N	1:A:1115:LEU:HD12	2.24	0.52
1:A:1094:PHE:HE1	1:A:1135:TYR:HD2	1.58	0.52
2:H:155:LEU:CD2	2:H:168:VAL:HA	2.39	0.52
1:C:1282:LEU:HG	1:C:1289:PRO:HG2	1.91	0.52
1:A:1346:PRO:HG3	1:E:1374:HIS:CG	2.44	0.52
1:E:1298:THR:O	1:E:1299:ALA:HB2	2.08	0.52
2:F:12:GLY:O	2:F:13:ALA:HB3	2.10	0.52
1:E:1249:ILE:HD12	1:E:1261:ASP:N	2.12	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1306:ASP:OD2	1:G:1286:LYS:HA	2.10	0.52
1:G:1287:LYS:HG2	1:G:1288:GLU:H	1.72	0.52
1:C:1287:LYS:HG2	1:C:1288:GLU:H	1.74	0.52
1:G:1149:HIS:HA	1:G:1152:VAL:HG23	1.92	0.52
1:C:1345:LEU:HD12	1:C:1355:VAL:CG1	2.40	0.52
1:A:1177:GLN:HG3	2:B:41:SER:HB3	1.90	0.52
2:B:68:ARG:NH1	2:B:100:GLU:OE1	2.43	0.52
1:G:1287:LYS:HZ2	1:G:1288:GLU:H	1.55	0.52
1:C:1343:ARG:CD	1:C:1357:GLU:HG3	2.33	0.52
1:C:1140:LYS:HE2	1:C:1227:VAL:HA	1.92	0.52
1:E:1056:VAL:HG21	1:E:1099:LEU:CD2	2.35	0.52
1:C:1234:MSE:HE2	1:C:1237:ILE:HD12	1.91	0.52
1:C:1062:LEU:HG	1:C:1185:TYR:HB3	1.92	0.52
1:E:1285:TRP:CZ2	2:H:98:TYR:CE2	2.92	0.52
1:A:1346:PRO:HG3	1:E:1374:HIS:CE1	2.45	0.52
1:C:1109:VAL:HG13	1:C:1110:PRO:HD2	1.92	0.52
1:E:1273:VAL:HG21	1:E:1375:LEU:HB3	1.92	0.51
1:C:1094:PHE:HE1	1:C:1135:TYR:HD2	1.58	0.51
2:H:139:TYR:HB3	2:H:140:PRO:HD3	1.91	0.51
2:F:5:LYS:HE3	2:F:56:TRP:CE3	2.46	0.51
2:D:96:LYS:O	2:D:99:PRO:HD2	2.10	0.51
2:B:152:VAL:HG12	2:B:153:LYS:HG2	1.91	0.51
1:C:1260:ALA:O	1:C:1261:ASP:CB	2.57	0.51
1:C:1194:LEU:HD23	2:D:61:GLN:HB3	1.93	0.51
1:C:1191:GLN:O	1:C:1195:LYS:HG2	2.11	0.51
2:D:68:ARG:NH1	2:D:100:GLU:OE1	2.44	0.51
1:A:1187:ILE:O	1:A:1191:GLN:HG3	2.09	0.51
1:A:1183:GLU:CD	2:B:74:GLN:NE2	2.64	0.51
1:G:1109:VAL:HG13	1:G:1110:PRO:HD2	1.91	0.51
1:G:1398:HIS:C	1:G:1400:ARG:H	2.14	0.51
1:C:1111:ASP:OD2	1:C:1113:GLU:HB2	2.10	0.51
1:E:1140:LYS:HE2	1:E:1227:VAL:HA	1.91	0.51
1:A:1345:LEU:HD12	1:A:1355:VAL:CG1	2.40	0.51
1:G:1339:ALA:HB1	1:G:1361:VAL:HG22	1.92	0.51
1:E:1339:ALA:HB1	1:E:1361:VAL:HG22	1.93	0.51
1:A:1339:ALA:HB1	1:A:1361:VAL:HG22	1.92	0.51
1:G:1194:LEU:HD23	2:H:61:GLN:HB3	1.93	0.51
2:B:58:THR:O	2:B:61:GLN:HG2	2.11	0.51
1:E:1218:ASP:OD1	1:E:1222:LYS:HE3	2.10	0.51
2:B:8:VAL:HG22	2:B:79:LEU:HD12	1.93	0.51
1:C:1119:ASP:O	1:C:1122:LYS:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1368:ARG:HG3	1:E:1368:ARG:NH1	2.20	0.51
2:F:138:THR:OG1	2:F:140:PRO:HD2	2.12	0.50
1:A:1173:ASN:ND2	1:A:1180:SER:HB2	2.26	0.50
2:B:142:GLY:HA3	2:B:154:TYR:CZ	2.46	0.50
1:G:1282:LEU:HG	1:G:1289:PRO:HG2	1.93	0.50
1:A:1234:MSE:SE	1:A:1267:LEU:HD23	2.61	0.50
2:F:145:MET:HA	2:F:145:MET:CE	2.41	0.50
1:E:1345:LEU:HD12	1:E:1355:VAL:HG12	1.93	0.50
1:C:1341:GLN:HB3	1:C:1359:VAL:HB	1.93	0.50
1:C:1339:ALA:HB1	1:C:1361:VAL:HG22	1.93	0.50
1:G:1119:ASP:O	1:G:1122:LYS:HG3	2.11	0.50
1:G:1282:LEU:HD21	1:G:1289:PRO:HB3	1.94	0.50
1:C:1328:PRO:HG2	1:C:1329:PHE:CD1	2.46	0.50
2:B:138:THR:HG23	2:B:141:GLN:HE21	1.76	0.50
1:E:1142:TYR:CE2	1:E:1193:VAL:HG13	2.46	0.50
1:A:1239:GLU:CD	2:B:66:ARG:HH11	2.15	0.50
1:E:1135:TYR:HE2	1:E:1138:ARG:NH2	2.10	0.50
1:C:1282:LEU:HB2	1:G:1285:TRP:CE2	2.47	0.50
1:G:1187:ILE:O	1:G:1191:GLN:HG3	2.11	0.50
2:D:66:ARG:CG	2:D:66:ARG:HH11	2.23	0.50
1:A:1140:LYS:HE2	1:A:1227:VAL:HA	1.94	0.50
2:F:142:GLY:HA3	2:F:154:TYR:CZ	2.47	0.50
2:F:153:LYS:HB3	2:F:155:LEU:CD1	2.41	0.50
1:C:1177:GLN:HG3	2:D:41:SER:HB3	1.94	0.50
2:B:145:MET:HA	2:B:145:MET:CE	2.42	0.50
2:H:19:LEU:C	2:H:19:LEU:HD23	2.32	0.50
1:E:1062:LEU:HG	1:E:1185:TYR:HB3	1.94	0.50
1:E:1179:SER:H	2:F:41:SER:CB	2.24	0.50
1:G:1345:LEU:HD12	1:G:1355:VAL:CG1	2.40	0.50
2:H:10:GLY:HA2	2:H:97:TRP:CE2	2.47	0.50
1:E:1397:LYS:O	1:E:1401:GLN:HB2	2.12	0.50
2:D:138:THR:OG1	2:D:140:PRO:HD2	2.11	0.50
1:E:1368:ARG:CG	1:E:1368:ARG:HH11	2.17	0.50
1:G:1135:TYR:CE2	1:G:1138:ARG:NH2	2.79	0.50
2:H:152:VAL:HG12	2:H:153:LYS:HG2	1.94	0.50
2:H:28:PHE:CD1	2:H:29:PRO:HD2	2.46	0.50
1:C:1173:ASN:ND2	1:C:1180:SER:HB2	2.26	0.49
1:C:1306:ASP:OD2	1:G:1287:LYS:HD2	2.13	0.49
1:C:1287:LYS:CG	1:C:1288:GLU:N	2.75	0.49
2:F:153:LYS:HB3	2:F:155:LEU:HD11	1.94	0.49
2:D:155:LEU:CD2	2:D:168:VAL:HA	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1273:VAL:HG21	1:A:1375:LEU:HB3	1.94	0.49
2:F:19:LEU:HD23	2:F:19:LEU:C	2.33	0.49
1:A:1212:GLU:OE1	1:G:1138:ARG:NH2	2.45	0.49
2:H:146:ALA:CB	2:H:154:TYR:HB2	2.42	0.49
1:C:1049:LEU:HD11	1:C:1106:VAL:HB	1.94	0.49
2:F:155:LEU:N	2:F:155:LEU:HD12	2.27	0.49
1:E:1049:LEU:HD11	1:E:1106:VAL:HB	1.94	0.49
2:D:28:PHE:CD1	2:D:29:PRO:HD2	2.47	0.49
1:C:1350:ALA:O	1:C:1351:GLU:HB3	2.12	0.49
1:E:1153:PRO:O	1:E:1157:VAL:HG23	2.13	0.49
2:D:153:LYS:HB3	2:D:155:LEU:CD1	2.43	0.49
2:D:153:LYS:HB3	2:D:155:LEU:HD11	1.94	0.49
2:H:12:GLY:O	2:H:13:ALA:HB3	2.13	0.49
2:B:28:PHE:CD1	2:B:29:PRO:HD2	2.47	0.49
1:A:1134:TYR:CE2	1:G:1216:HIS:HB3	2.47	0.49
2:F:138:THR:N	2:F:141:GLN:HE21	1.91	0.49
1:E:1111:ASP:OD2	1:E:1113:GLU:HB2	2.11	0.49
2:B:98:TYR:HB3	2:B:99:PRO:HD3	1.94	0.49
2:H:153:LYS:HB3	2:H:155:LEU:CD1	2.42	0.49
2:B:145:MET:HA	2:B:145:MET:HE3	1.94	0.49
1:A:1062:LEU:HG	1:A:1185:TYR:HB3	1.95	0.49
2:F:155:LEU:CD2	2:F:168:VAL:HA	2.42	0.49
1:E:1195:LYS:NZ	2:F:59:ALA:HB3	2.28	0.49
1:A:1340:LEU:HD11	1:A:1390:VAL:CG1	2.42	0.49
2:D:145:MET:CE	2:D:145:MET:HA	2.43	0.49
1:G:1173:ASN:ND2	1:G:1180:SER:HB2	2.28	0.49
1:E:1227:VAL:O	1:E:1231:ILE:HG12	2.12	0.49
1:C:1282:LEU:HD21	1:C:1289:PRO:HB3	1.94	0.49
1:C:1340:LEU:HD11	1:C:1390:VAL:CG1	2.43	0.49
2:F:133:LYS:N	2:F:133:LYS:HD3	2.28	0.49
1:G:1287:LYS:CG	1:G:1288:GLU:N	2.76	0.49
1:A:1368:ARG:HH11	1:A:1368:ARG:CG	2.21	0.49
1:G:1173:ASN:HD21	1:G:1180:SER:HB2	1.77	0.49
2:F:146:ALA:CB	2:F:154:TYR:HB2	2.42	0.49
1:E:1273:VAL:HG23	1:E:1377:CYS:HA	1.95	0.49
1:G:1350:ALA:O	1:G:1351:GLU:HB3	2.13	0.49
1:G:1341:GLN:HB3	1:G:1359:VAL:HB	1.94	0.49
1:C:1149:HIS:CE1	1:C:1186:LEU:O	2.66	0.49
1:G:1049:LEU:HD11	1:G:1106:VAL:HB	1.93	0.49
1:G:1298:THR:O	1:G:1299:ALA:HB2	2.12	0.49
2:H:145:MET:CE	2:H:145:MET:HA	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1298:THR:O	1:C:1299:ALA:HB2	2.13	0.49
1:E:1156:LEU:HD21	1:E:1182:LEU:HD23	1.94	0.48
1:E:1191:GLN:O	1:E:1195:LYS:HG2	2.13	0.48
1:C:1248:LEU:CD2	1:C:1332:ARG:HG3	2.32	0.48
1:A:1368:ARG:NH1	1:A:1368:ARG:HG3	2.25	0.48
2:F:66:ARG:HH11	2:F:66:ARG:CG	2.25	0.48
2:D:8:VAL:HG22	2:D:79:LEU:HD12	1.94	0.48
2:D:142:GLY:HA3	2:D:154:TYR:CZ	2.47	0.48
1:G:1328:PRO:HG2	1:G:1329:PHE:CD1	2.49	0.48
1:G:1156:LEU:C	1:G:1158:LYS:H	2.16	0.48
2:D:161:THR:HB	2:D:163:ARG:HG2	1.94	0.48
2:B:155:LEU:CD2	2:B:168:VAL:HA	2.43	0.48
1:C:1156:LEU:CD2	1:C:1182:LEU:HD23	2.44	0.48
1:G:1218:ASP:OD1	1:G:1222:LYS:HE3	2.13	0.48
1:G:1135:TYR:HE2	1:G:1138:ARG:NH2	2.11	0.48
2:B:12:GLY:O	2:B:13:ALA:HB3	2.13	0.48
1:C:1287:LYS:CG	1:C:1288:GLU:H	2.27	0.48
1:E:1035:LEU:HG	2:F:31:GLU:OE1	2.14	0.48
2:H:142:GLY:HA3	2:H:154:TYR:CZ	2.48	0.48
2:H:153:LYS:HB3	2:H:155:LEU:HD11	1.96	0.48
2:F:28:PHE:CD1	2:F:29:PRO:HD2	2.49	0.48
1:E:1340:LEU:HD11	1:E:1390:VAL:CG1	2.44	0.48
2:F:68:ARG:NH1	2:F:100:GLU:OE1	2.46	0.48
1:A:1052:GLU:OE2	1:A:1095:GLN:NE2	2.43	0.48
1:G:1056:VAL:HG21	1:G:1099:LEU:CD2	2.40	0.48
2:D:152:VAL:HG12	2:D:153:LYS:HG2	1.94	0.48
2:B:153:LYS:HB3	2:B:155:LEU:HD11	1.96	0.48
1:C:1135:TYR:CE2	1:C:1138:ARG:NH2	2.81	0.48
1:E:1341:GLN:HB3	1:E:1359:VAL:HB	1.96	0.48
1:G:1176:GLN:HE22	2:H:1:MET:H3	1.61	0.48
2:D:146:ALA:CB	2:D:154:TYR:HB2	2.43	0.48
1:G:1164:ALA:O	1:G:1167:ALA:HB3	2.14	0.48
1:E:1119:ASP:O	1:E:1122:LYS:HG3	2.13	0.48
1:C:1134:TYR:CE2	1:E:1216:HIS:HB3	2.48	0.48
2:D:19:LEU:C	2:D:19:LEU:HD23	2.34	0.48
1:E:1350:ALA:O	1:E:1351:GLU:HB3	2.13	0.48
2:B:10:GLY:HA2	2:B:97:TRP:CE2	2.49	0.48
1:C:1368:ARG:NH1	1:C:1368:ARG:HG3	2.23	0.47
2:H:96:LYS:O	2:H:99:PRO:HD2	2.14	0.47
1:A:1227:VAL:O	1:A:1231:ILE:HG12	2.14	0.47
2:B:146:ALA:CB	2:B:154:TYR:HB2	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1179:SER:HB3	2:H:41:SER:HB2	1.96	0.47
1:A:1191:GLN:O	1:A:1195:LYS:HG2	2.14	0.47
1:A:1298:THR:O	1:A:1299:ALA:HB2	2.12	0.47
2:H:5:LYS:HE3	2:H:56:TRP:CE3	2.49	0.47
2:B:138:THR:HG23	2:B:141:GLN:NE2	2.29	0.47
1:A:1077:THR:OG1	1:A:1080:GLU:HG3	2.14	0.47
2:B:153:LYS:HB3	2:B:155:LEU:CD1	2.43	0.47
1:E:1055:TYR:CD2	1:E:1192:ARG:HG2	2.49	0.47
1:A:1350:ALA:O	1:A:1351:GLU:HB3	2.14	0.47
2:D:58:THR:O	2:D:61:GLN:HG2	2.14	0.47
2:B:161:THR:HB	2:B:163:ARG:HG2	1.96	0.47
2:H:6:CYS:HB3	2:H:55:LEU:CD2	2.45	0.47
1:A:1142:TYR:CE2	1:A:1193:VAL:HG13	2.49	0.47
1:G:1153:PRO:O	1:G:1157:VAL:HG23	2.14	0.47
1:G:1227:VAL:O	1:G:1231:ILE:HG12	2.14	0.47
2:H:68:ARG:HD2	2:H:100:GLU:OE2	2.14	0.47
2:H:133:LYS:HD3	2:H:133:LYS:N	2.30	0.47
1:A:1216:HIS:HB3	1:G:1134:TYR:CE2	2.49	0.47
2:D:98:TYR:HB3	2:D:99:PRO:HD3	1.97	0.47
2:B:138:THR:OG1	2:B:140:PRO:HD2	2.14	0.47
1:E:1287:LYS:N	1:E:1287:LYS:CD	2.76	0.47
1:E:1052:GLU:O	1:E:1056:VAL:HG23	2.15	0.47
1:C:1152:VAL:HB	1:C:1153:PRO:HD3	1.95	0.47
1:A:1055:TYR:CD2	1:A:1192:ARG:HG2	2.50	0.47
2:B:66:ARG:HH11	2:B:66:ARG:CG	2.27	0.47
2:F:152:VAL:HG12	2:F:153:LYS:HG2	1.96	0.47
1:A:1389:SER:O	1:A:1392:SER:HB3	2.14	0.47
2:D:10:GLY:HA2	2:D:97:TRP:CE2	2.49	0.47
2:B:133:LYS:N	2:B:133:LYS:HD3	2.30	0.47
1:G:1287:LYS:CG	1:G:1288:GLU:H	2.27	0.47
1:E:1287:LYS:HG2	1:E:1288:GLU:H	1.79	0.47
1:E:1067:LEU:CD1	1:E:1088:LEU:HD13	2.45	0.47
2:F:161:THR:HB	2:F:163:ARG:HG2	1.97	0.47
1:E:1345:LEU:HD12	1:E:1355:VAL:CG1	2.45	0.47
2:B:6:CYS:HB3	2:B:55:LEU:CD2	2.45	0.47
1:C:1077:THR:OG1	1:C:1080:GLU:HG3	2.14	0.47
2:D:155:LEU:N	2:D:155:LEU:HD12	2.30	0.47
1:A:1049:LEU:HD11	1:A:1106:VAL:HB	1.96	0.47
2:H:68:ARG:NH1	2:H:100:GLU:OE1	2.47	0.47
1:E:1164:ALA:O	1:E:1167:ALA:HB3	2.15	0.47
2:H:8:VAL:HG22	2:H:79:LEU:HD12	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:19:LEU:HD23	2:B:19:LEU:C	2.35	0.47
2:D:133:LYS:HD3	2:D:133:LYS:N	2.30	0.47
1:C:1287:LYS:CD	1:C:1287:LYS:N	2.77	0.47
1:G:1239:GLU:OE2	2:H:66:ARG:HG3	2.15	0.47
1:C:1337:THR:HG21	1:C:1397:LYS:HB2	1.97	0.47
2:F:10:GLY:HA2	2:F:97:TRP:CE2	2.49	0.47
1:G:1138:ARG:O	1:G:1141:LEU:HG	2.15	0.47
1:C:1055:TYR:CD2	1:C:1192:ARG:HG2	2.50	0.47
2:B:11:ASP:OD1	2:B:89:SER:HA	2.15	0.47
1:C:1156:LEU:C	1:C:1158:LYS:H	2.18	0.47
1:E:1197:PRO:HB2	1:E:1201:ARG:HH12	1.80	0.47
1:C:1368:ARG:NH1	1:C:1368:ARG:CG	2.78	0.46
1:C:1234:MSE:CE	1:C:1237:ILE:HD12	2.45	0.46
1:A:1273:VAL:HG23	1:A:1377:CYS:HA	1.97	0.46
1:E:1149:HIS:CE1	1:E:1186:LEU:O	2.68	0.46
1:A:1157:VAL:CG1	1:A:1157:VAL:O	2.63	0.46
2:B:128:LYS:HD3	2:B:128:LYS:C	2.36	0.46
2:D:158:SER:O	2:D:162:GLN:N	2.47	0.46
2:B:155:LEU:N	2:B:155:LEU:HD12	2.30	0.46
2:D:137:ILE:HD12	2:D:137:ILE:N	2.31	0.46
2:F:58:THR:O	2:F:61:GLN:HG2	2.15	0.46
1:A:1368:ARG:HD2	1:A:1369:PRO:O	2.15	0.46
1:A:1179:SER:H	2:B:41:SER:HB2	1.80	0.46
1:G:1303:VAL:HG11	1:G:1329:PHE:HD2	1.81	0.46
1:G:1340:LEU:HD11	1:G:1390:VAL:CG1	2.45	0.46
2:D:57:ASP:OD1	2:D:58:THR:N	2.48	0.46
1:E:1234:MSE:HE2	1:E:1237:ILE:HD12	1.97	0.46
2:H:11:ASP:OD1	2:H:89:SER:HA	2.16	0.46
2:F:137:ILE:N	2:F:137:ILE:HD12	2.31	0.46
1:C:1067:LEU:CD1	1:C:1088:LEU:HD13	2.44	0.46
2:F:128:LYS:C	2:F:128:LYS:HD3	2.36	0.46
2:D:155:LEU:N	2:D:155:LEU:CD1	2.79	0.46
2:B:158:SER:O	2:B:162:GLN:N	2.49	0.46
2:D:129:LEU:HD12	2:D:136:PRO:HG3	1.97	0.46
1:A:1042:ARG:NE	1:A:1113:GLU:HA	2.31	0.46
1:C:1115:LEU:HA	1:C:1120:GLN:NE2	2.30	0.46
1:E:1173:ASN:HD21	1:E:1180:SER:HB2	1.79	0.46
2:D:128:LYS:C	2:D:128:LYS:HD3	2.36	0.46
1:G:1179:SER:H	2:H:41:SER:CB	2.28	0.46
1:C:1135:TYR:HE2	1:C:1138:ARG:NH2	2.13	0.46
1:A:1164:ALA:O	1:A:1167:ALA:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:GLN:HB3	1:A:1359:VAL:HB	1.96	0.46
1:A:1067:LEU:CD1	1:A:1088:LEU:HD13	2.45	0.46
1:E:1168:PHE:O	1:E:1172:GLN:HG2	2.16	0.46
1:E:1287:LYS:CG	1:E:1288:GLU:N	2.79	0.46
1:E:1063:MSE:HE2	1:E:1088:LEU:HD22	1.98	0.46
1:C:1052:GLU:HG3	1:C:1099:LEU:HD13	1.97	0.46
1:A:1287:LYS:CG	1:A:1288:GLU:N	2.79	0.46
1:E:1056:VAL:CG2	1:E:1099:LEU:HD22	2.38	0.46
1:G:1152:VAL:HB	1:G:1153:PRO:HD3	1.97	0.46
1:C:1063:MSE:HE2	1:C:1088:LEU:HD22	1.97	0.46
1:E:1138:ARG:O	1:E:1141:LEU:HG	2.16	0.46
2:D:120:ARG:HH21	2:D:139:TYR:N	2.13	0.45
1:C:1306:ASP:OD2	1:G:1287:LYS:CD	2.64	0.45
1:A:1287:LYS:HG2	1:A:1288:GLU:H	1.81	0.45
1:E:1077:THR:OG1	1:E:1080:GLU:HG3	2.16	0.45
1:G:1062:LEU:HG	1:G:1185:TYR:HB3	1.98	0.45
2:B:121:ASP:HA	2:B:126:ILE:HD11	1.98	0.45
1:C:1164:ALA:O	1:C:1167:ALA:HB3	2.15	0.45
1:A:1052:GLU:O	1:A:1056:VAL:HG23	2.16	0.45
1:G:1248:LEU:HD21	1:G:1332:ARG:CG	2.42	0.45
2:F:121:ASP:HA	2:F:126:ILE:HD11	1.98	0.45
1:G:1191:GLN:O	1:G:1195:LYS:HG2	2.16	0.45
2:D:23:TYR:HE1	2:D:166:LYS:HD3	1.81	0.45
1:G:1190:ILE:HD13	2:H:70:LEU:CD1	2.38	0.45
1:E:1156:LEU:CD2	1:E:1182:LEU:HD23	2.47	0.45
2:B:155:LEU:CD1	2:B:155:LEU:N	2.80	0.45
1:C:1138:ARG:O	1:C:1141:LEU:HG	2.16	0.45
2:H:137:ILE:N	2:H:137:ILE:HD12	2.31	0.45
1:A:1340:LEU:HD11	1:A:1390:VAL:HG13	1.99	0.45
2:H:80:ILE:HD12	2:H:110:ILE:HG21	1.98	0.45
1:A:1190:ILE:CD1	2:B:70:LEU:HD13	2.38	0.45
1:A:1063:MSE:HE2	1:A:1088:LEU:HD22	1.98	0.45
1:A:1153:PRO:O	1:A:1157:VAL:HG23	2.17	0.45
1:G:1067:LEU:CD1	1:G:1088:LEU:HD13	2.46	0.45
1:C:1086:GLY:O	1:C:1087:ASN:OD1	2.35	0.45
1:A:1212:GLU:HG3	1:G:1097:GLU:HG3	1.99	0.45
2:B:23:TYR:HE1	2:B:166:LYS:HD3	1.81	0.45
1:E:1035:LEU:HD12	1:E:1035:LEU:O	2.17	0.45
1:G:1157:VAL:CG1	1:G:1157:VAL:O	2.64	0.45
2:D:66:ARG:NH1	2:D:66:ARG:HG3	2.29	0.45
1:E:1365:SER:O	1:E:1367:GLY:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:155:LEU:N	2:F:155:LEU:CD1	2.79	0.45
1:E:1173:ASN:ND2	1:E:1180:SER:HB2	2.32	0.45
1:C:1355:VAL:HG12	1:C:1356:CYS:N	2.32	0.45
1:A:1183:GLU:CD	2:B:74:GLN:HE21	2.21	0.45
2:F:11:ASP:OD1	2:F:92:ASN:ND2	2.45	0.45
1:A:1156:LEU:C	1:A:1158:LYS:H	2.19	0.45
2:F:138:THR:HG23	2:F:141:GLN:NE2	2.31	0.45
2:F:120:ARG:HH21	2:F:139:TYR:N	2.13	0.45
2:H:58:THR:O	2:H:61:GLN:HG2	2.16	0.45
2:F:6:CYS:HB3	2:F:55:LEU:CD2	2.43	0.45
2:D:121:ASP:HA	2:D:126:ILE:HD11	1.99	0.45
1:E:1115:LEU:HA	1:E:1120:GLN:NE2	2.31	0.45
1:C:1340:LEU:HD11	1:C:1390:VAL:HG13	1.99	0.45
2:B:137:ILE:HD12	2:B:137:ILE:N	2.32	0.45
1:C:1142:TYR:CE2	1:C:1193:VAL:HG13	2.51	0.45
1:G:1142:TYR:CE2	1:G:1193:VAL:HG13	2.52	0.45
1:G:1368:ARG:NH1	1:G:1368:ARG:HG3	2.23	0.45
1:G:1063:MSE:HE2	1:G:1088:LEU:HD22	1.98	0.45
1:C:1073:GLU:HG2	1:C:1075:PHE:CD1	2.52	0.45
1:G:1177:GLN:HG3	2:H:41:SER:HB3	1.98	0.45
1:A:1213:GLU:H	1:A:1213:GLU:CD	2.20	0.45
2:D:138:THR:HG23	2:D:141:GLN:NE2	2.32	0.44
1:E:1156:LEU:C	1:E:1158:LYS:H	2.19	0.44
2:F:158:SER:O	2:F:162:GLN:N	2.50	0.44
2:D:6:CYS:HB3	2:D:55:LEU:CD2	2.46	0.44
2:D:5:LYS:HE3	2:D:56:TRP:CE3	2.52	0.44
2:D:138:THR:HG23	2:D:141:GLN:HE21	1.82	0.44
1:G:1042:ARG:NE	1:G:1113:GLU:HA	2.32	0.44
1:C:1103:GLU:O	1:C:1107:ARG:HG3	2.17	0.44
1:C:1212:GLU:CD	1:E:1097:GLU:HG2	2.37	0.44
1:A:1344:ALA:HB2	1:A:1387:LEU:CD1	2.47	0.44
2:H:138:THR:OG1	2:H:140:PRO:HD2	2.18	0.44
1:C:1287:LYS:HE2	1:G:1307:GLY:O	2.17	0.44
1:E:1068:LYS:N	1:E:1069:PRO:HD2	2.33	0.44
1:E:1152:VAL:HB	1:E:1153:PRO:HD3	2.00	0.44
1:E:1340:LEU:HD11	1:E:1390:VAL:HG13	1.99	0.44
2:F:23:TYR:HE1	2:F:166:LYS:HD3	1.82	0.44
1:A:1285:TRP:HZ2	2:D:98:TYR:CE2	2.36	0.44
1:A:1052:GLU:HG3	1:A:1099:LEU:HD13	2.00	0.44
1:E:1368:ARG:HD2	1:E:1369:PRO:O	2.17	0.44
2:H:162:GLN:HG3	2:H:165:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:ARG:HD2	2:D:100:GLU:OE2	2.18	0.44
1:A:1374:HIS:ND1	1:E:1346:PRO:HG3	2.32	0.44
1:A:1368:ARG:NH1	1:A:1368:ARG:CG	2.80	0.44
1:E:1073:GLU:HG2	1:E:1075:PHE:CD1	2.52	0.44
2:H:1:MET:HG2	2:H:2:GLN:N	2.33	0.44
1:A:1215:TYR:O	1:A:1219:VAL:HG23	2.18	0.44
1:A:1115:LEU:HA	1:A:1120:GLN:NE2	2.33	0.44
2:H:155:LEU:HD12	2:H:155:LEU:N	2.32	0.44
1:A:1138:ARG:O	1:A:1141:LEU:HG	2.17	0.44
1:E:1234:MSE:CE	1:E:1237:ILE:HD12	2.47	0.44
1:G:1368:ARG:NH1	1:G:1368:ARG:CG	2.78	0.44
1:E:1140:LYS:HD2	1:E:1230:HIS:HD2	1.82	0.44
1:E:1389:SER:O	1:E:1392:SER:HB3	2.17	0.44
1:G:1149:HIS:CE1	1:G:1186:LEU:O	2.71	0.44
2:D:66:ARG:NH1	2:D:66:ARG:CG	2.80	0.44
1:A:1073:GLU:HG2	1:A:1075:PHE:CD1	2.52	0.44
2:H:158:SER:O	2:H:162:GLN:N	2.50	0.44
2:H:66:ARG:NH1	2:H:66:ARG:HG3	2.31	0.44
1:E:1344:ALA:HB2	1:E:1387:LEU:CD1	2.48	0.44
2:H:23:TYR:HE1	2:H:166:LYS:HD3	1.83	0.44
1:E:1052:GLU:HG3	1:E:1099:LEU:HD13	2.00	0.44
1:C:1153:PRO:O	1:C:1157:VAL:HG23	2.18	0.44
1:C:1168:PHE:O	1:C:1172:GLN:HG2	2.18	0.44
2:F:96:LYS:O	2:F:99:PRO:HD2	2.17	0.44
1:A:1277:ASN:OD1	1:A:1374:HIS:HB2	2.18	0.44
1:A:1208:ASP:O	1:A:1214:HIS:HB2	2.17	0.44
2:H:129:LEU:HD12	2:H:136:PRO:HG3	2.00	0.44
1:C:1247:GLN:HB3	1:C:1332:ARG:HH11	1.83	0.43
1:A:1149:HIS:CE1	1:A:1186:LEU:O	2.71	0.43
1:A:1201:ARG:HG2	1:A:1221:ILE:HD13	2.00	0.43
1:A:1068:LYS:N	1:A:1069:PRO:HD2	2.33	0.43
1:A:1042:ARG:HH11	1:A:1042:ARG:HB3	1.83	0.43
1:E:1365:SER:C	1:E:1367:GLY:N	2.70	0.43
1:C:1042:ARG:NE	1:C:1113:GLU:HA	2.31	0.43
1:C:1368:ARG:HD2	1:C:1369:PRO:O	2.18	0.43
2:H:161:THR:HB	2:H:163:ARG:HG2	2.00	0.43
1:C:1327:ASP:HA	1:C:1328:PRO:HD2	1.85	0.43
1:A:1287:LYS:CD	1:A:1287:LYS:N	2.76	0.43
2:F:17:THR:O	2:F:21:ILE:HG13	2.18	0.43
2:H:128:LYS:HD3	2:H:128:LYS:C	2.38	0.43
1:G:1201:ARG:HG2	1:G:1221:ILE:HD13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:1042:ARG:HB3	1:E:1042:ARG:HH11	1.82	0.43
1:E:1234:MSE:CE	1:E:1267:LEU:HD23	2.47	0.43
1:G:1368:ARG:HD2	1:G:1369:PRO:O	2.18	0.43
1:C:1239:GLU:OE2	2:D:66:ARG:HG3	2.18	0.43
2:D:162:GLN:HG3	2:D:165:LEU:HD22	1.99	0.43
2:H:155:LEU:CD1	2:H:155:LEU:N	2.82	0.43
1:C:1187:ILE:O	1:C:1191:GLN:HG3	2.19	0.43
1:E:1344:ALA:HB2	1:E:1387:LEU:HD13	2.00	0.43
1:A:1152:VAL:HB	1:A:1153:PRO:HD3	1.99	0.43
1:G:1156:LEU:HD21	1:G:1182:LEU:HD23	2.00	0.43
2:B:11:ASP:OD1	2:B:92:ASN:ND2	2.47	0.43
2:F:85:VAL:HG11	2:F:125:THR:HG21	2.00	0.43
1:C:1213:GLU:H	1:C:1213:GLU:CD	2.22	0.43
1:C:1052:GLU:O	1:C:1056:VAL:HG23	2.19	0.43
1:E:1157:VAL:CG1	1:E:1157:VAL:O	2.64	0.43
1:C:1363:SER:N	1:C:1368:ARG:O	2.49	0.43
1:G:1086:GLY:O	1:G:1087:ASN:OD1	2.37	0.43
1:G:1073:GLU:HG2	1:G:1075:PHE:CD1	2.54	0.43
2:F:161:THR:HG22	2:F:163:ARG:HB3	2.00	0.43
1:G:1365:SER:C	1:G:1367:GLY:N	2.72	0.43
1:G:1077:THR:OG1	1:G:1080:GLU:HG3	2.19	0.43
1:A:1344:ALA:HB2	1:A:1387:LEU:HD13	1.99	0.43
1:A:1197:PRO:HB2	1:A:1201:ARG:HH12	1.84	0.43
1:E:1213:GLU:CD	1:E:1213:GLU:H	2.22	0.43
2:F:68:ARG:HD2	2:F:100:GLU:OE2	2.19	0.43
1:A:1380:PRO:HG2	1:A:1381:GLU:OE2	2.19	0.43
1:C:1286:LYS:HB3	1:C:1289:PRO:HG3	2.01	0.43
2:D:137:ILE:HG23	2:D:141:GLN:HB2	2.00	0.43
1:G:1260:ALA:O	1:G:1261:ASP:CB	2.66	0.43
1:G:1368:ARG:HA	1:G:1369:PRO:HD3	1.75	0.43
1:G:1115:LEU:HA	1:G:1120:GLN:NE2	2.34	0.43
1:E:1103:GLU:O	1:E:1107:ARG:HG3	2.18	0.43
2:B:8:VAL:HG21	2:B:20:LEU:HD21	2.01	0.43
1:C:1118:VAL:HG23	1:C:1119:ASP:N	2.34	0.43
1:G:1118:VAL:HG23	1:G:1119:ASP:N	2.33	0.43
1:A:1176:GLN:NE2	2:B:1:MET:N	2.67	0.43
2:F:66:ARG:HG3	2:F:66:ARG:NH1	2.30	0.42
1:C:1365:SER:C	1:C:1367:GLY:N	2.71	0.42
1:E:1118:VAL:HG23	1:E:1119:ASP:N	2.34	0.42
2:H:66:ARG:CG	2:H:66:ARG:HH11	2.28	0.42
1:A:1365:SER:O	1:A:1367:GLY:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1282:LEU:HD21	1:C:1289:PRO:CB	2.48	0.42
2:F:129:LEU:HD12	2:F:136:PRO:HG3	2.01	0.42
1:G:1055:TYR:CD2	1:G:1192:ARG:HG2	2.54	0.42
2:B:120:ARG:HH21	2:B:139:TYR:N	2.15	0.42
1:G:1234:MSE:HE2	1:G:1237:ILE:HD12	2.00	0.42
1:G:1168:PHE:O	1:G:1172:GLN:HG2	2.19	0.42
1:A:1275:TRP:O	1:A:1278:PRO:HD3	2.19	0.42
2:H:49:LYS:HD3	2:H:177:LEU:HD13	2.01	0.42
1:G:1389:SER:O	1:G:1392:SER:HB3	2.20	0.42
2:H:85:VAL:HG11	2:H:125:THR:HG21	2.01	0.42
2:H:137:ILE:HG23	2:H:141:GLN:HB2	2.00	0.42
1:E:1042:ARG:NE	1:E:1113:GLU:HA	2.30	0.42
1:C:1365:SER:O	1:C:1367:GLY:N	2.50	0.42
1:E:1094:PHE:CE1	1:E:1135:TYR:HD2	2.36	0.42
1:G:1380:PRO:HG2	1:G:1381:GLU:OE2	2.19	0.42
1:A:1342:VAL:HG13	1:A:1342:VAL:O	2.20	0.42
1:E:1065:ARG:HH11	1:E:1065:ARG:HG2	1.84	0.42
1:C:1344:ALA:HB2	1:C:1387:LEU:CD1	2.49	0.42
1:C:1389:SER:O	1:C:1392:SER:HB3	2.19	0.42
1:A:1241:PHE:O	1:A:1242:GLY:C	2.57	0.42
2:D:120:ARG:NH2	2:D:139:TYR:H	2.16	0.42
1:E:1368:ARG:NH1	1:E:1368:ARG:CG	2.76	0.42
1:G:1036:SER:O	1:G:1039:ASP:N	2.53	0.42
2:B:17:THR:O	2:B:21:ILE:HG13	2.20	0.42
1:A:1118:VAL:HG23	1:A:1119:ASP:N	2.33	0.42
2:F:138:THR:HG23	2:F:141:GLN:HE21	1.84	0.42
1:E:1234:MSE:O	1:E:1264:MSE:HE2	2.19	0.42
1:E:1178:HIS:C	1:E:1180:SER:H	2.23	0.42
1:A:1355:VAL:HG12	1:A:1356:CYS:N	2.34	0.42
1:C:1244:VAL:HG21	1:C:1329:PHE:CD2	2.55	0.42
2:B:5:LYS:HE3	2:B:56:TRP:CE3	2.53	0.42
2:D:160:LEU:HD13	2:D:160:LEU:C	2.40	0.42
1:E:1086:GLY:O	1:E:1087:ASN:OD1	2.38	0.42
1:G:1215:TYR:O	1:G:1219:VAL:HG23	2.20	0.42
2:H:57:ASP:OD1	2:H:58:THR:N	2.53	0.42
1:E:1239:GLU:OE1	2:F:66:ARG:NH1	2.53	0.42
1:G:1115:LEU:N	1:G:1115:LEU:CD1	2.83	0.42
2:F:146:ALA:HB2	2:F:154:TYR:HB2	2.02	0.42
1:E:1107:ARG:C	1:E:1109:VAL:H	2.23	0.42
1:A:1107:ARG:C	1:A:1109:VAL:H	2.23	0.42
1:G:1244:VAL:HG21	1:G:1329:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1097:GLU:O	1:C:1101:THR:HG23	2.19	0.42
2:D:108:THR:HA	2:D:109:PRO:HD2	1.90	0.42
1:E:1287:LYS:CG	1:E:1288:GLU:H	2.32	0.42
1:G:1042:ARG:HB3	1:G:1042:ARG:HH11	1.85	0.42
1:G:1363:SER:N	1:G:1368:ARG:O	2.48	0.42
2:F:108:THR:HA	2:F:109:PRO:HD2	1.92	0.42
1:A:1178:HIS:HA	1:A:1181:THR:CG2	2.50	0.42
1:C:1282:LEU:HD22	1:G:1285:TRP:CZ3	2.55	0.42
2:D:68:ARG:N	2:D:69:PRO:HD2	2.34	0.42
2:D:5:LYS:HG3	2:D:75:THR:HA	2.00	0.42
1:G:1295:VAL:HG11	1:G:1389:SER:OG	2.20	0.42
2:B:5:LYS:HG3	2:B:75:THR:HA	2.00	0.42
1:G:1065:ARG:HH11	1:G:1065:ARG:HG2	1.84	0.42
2:H:120:ARG:HH21	2:H:139:TYR:N	2.17	0.42
2:D:87:PRO:O	2:D:90:PHE:HB3	2.20	0.42
1:C:1042:ARG:HH11	1:C:1042:ARG:HB3	1.85	0.42
1:A:1168:PHE:O	1:A:1172:GLN:HG2	2.20	0.42
2:D:161:THR:HG22	2:D:161:THR:O	2.20	0.42
1:C:1178:HIS:C	1:C:1180:SER:H	2.22	0.42
1:A:1115:LEU:N	1:A:1115:LEU:CD1	2.83	0.42
2:H:8:VAL:HG21	2:H:20:LEU:HD21	2.02	0.42
1:E:1295:VAL:HG11	1:E:1389:SER:OG	2.19	0.42
1:C:1201:ARG:HG2	1:C:1221:ILE:HD13	2.02	0.42
2:B:24:THR:HG22	2:B:40:TYR:CE2	2.55	0.42
1:C:1065:ARG:HH11	1:C:1065:ARG:HG2	1.85	0.42
1:E:1275:TRP:O	1:E:1278:PRO:HD3	2.20	0.42
2:F:57:ASP:OD1	2:F:58:THR:N	2.51	0.41
1:E:1277:ASN:OD1	1:E:1374:HIS:HB2	2.20	0.41
1:E:1115:LEU:H	1:E:1115:LEU:CD1	2.34	0.41
1:E:1115:LEU:CD1	1:E:1115:LEU:N	2.83	0.41
2:H:146:ALA:HB2	2:H:154:TYR:HB2	2.02	0.41
1:G:1107:ARG:C	1:G:1109:VAL:H	2.23	0.41
1:A:1373:PHE:HB3	1:A:1375:LEU:HD21	2.02	0.41
1:C:1197:PRO:HB2	1:C:1201:ARG:HH12	1.85	0.41
2:B:129:LEU:HD12	2:B:136:PRO:HG3	2.01	0.41
1:E:1063:MSE:HG3	1:E:1068:LYS:HE3	2.03	0.41
2:F:66:ARG:NH1	2:F:66:ARG:CG	2.82	0.41
1:A:1365:SER:C	1:A:1367:GLY:N	2.72	0.41
2:F:5:LYS:HG3	2:F:75:THR:HA	2.03	0.41
2:D:68:ARG:HB3	2:D:69:PRO:HD3	2.02	0.41
1:G:1304:TYR:CB	1:G:1331:PHE:HB3	2.43	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1240:GLU:CG	1:C:1305:LYS:NZ	2.82	0.41
2:D:17:THR:O	2:D:21:ILE:HG13	2.20	0.41
2:B:146:ALA:HB2	2:B:154:TYR:HB2	2.02	0.41
1:E:1094:PHE:HE1	1:E:1135:TYR:CD2	2.37	0.41
1:E:1399:ARG:C	1:E:1401:GLN:H	2.22	0.41
1:G:1197:PRO:HB2	1:G:1201:ARG:HH12	1.84	0.41
1:A:1287:LYS:CG	1:A:1288:GLU:H	2.33	0.41
1:E:1368:ARG:HA	1:E:1369:PRO:HD3	1.76	0.41
1:G:1052:GLU:O	1:G:1056:VAL:HG23	2.21	0.41
1:A:1359:VAL:HG22	1:A:1372:VAL:HG22	2.03	0.41
1:G:1252:GLN:HE21	1:G:1252:GLN:HB2	1.66	0.41
2:D:85:VAL:HG11	2:D:125:THR:HG21	2.03	0.41
2:D:12:GLY:O	2:D:13:ALA:HB3	2.21	0.41
1:C:1059:LEU:HA	1:C:1059:LEU:HD12	1.94	0.41
2:B:162:GLN:HE21	2:B:162:GLN:HB2	1.66	0.41
2:F:158:SER:HB3	2:F:161:THR:HB	2.03	0.41
2:B:161:THR:HG22	2:B:161:THR:O	2.20	0.41
1:G:1327:ASP:HA	1:G:1328:PRO:HD2	1.86	0.41
2:F:87:PRO:O	2:F:90:PHE:HB3	2.20	0.41
1:G:1052:GLU:HG3	1:G:1099:LEU:HD13	2.03	0.41
1:A:1234:MSE:HE2	1:A:1237:ILE:HD12	2.02	0.41
1:A:1076:LEU:HA	1:A:1080:GLU:OE1	2.21	0.41
1:A:1177:GLN:HG3	2:B:41:SER:CB	2.50	0.41
1:G:1250:ALA:C	1:G:1252:GLN:N	2.73	0.41
1:A:1174:PRO:HG2	1:A:1175:ARG:H	1.86	0.41
1:C:1068:LYS:N	1:C:1069:PRO:HD2	2.35	0.41
2:D:11:ASP:OD1	2:D:92:ASN:ND2	2.51	0.41
2:F:137:ILE:HG23	2:F:141:GLN:HB2	2.02	0.41
2:F:37:PHE:HD2	2:F:57:ASP:HB2	1.86	0.41
2:H:66:ARG:NH1	2:H:66:ARG:CG	2.84	0.41
2:H:161:THR:HG22	2:H:161:THR:O	2.21	0.41
1:A:1115:LEU:H	1:A:1115:LEU:CD1	2.34	0.41
1:G:1250:ALA:C	1:G:1252:GLN:H	2.22	0.41
2:B:66:ARG:CG	2:B:66:ARG:NH1	2.84	0.41
2:F:161:THR:HG22	2:F:161:THR:O	2.20	0.41
1:A:1178:HIS:C	1:A:1180:SER:H	2.24	0.41
1:C:1115:LEU:CD1	1:C:1115:LEU:H	2.33	0.41
1:C:1115:LEU:CD1	1:C:1115:LEU:N	2.84	0.41
2:D:146:ALA:HB2	2:D:154:TYR:HB2	2.03	0.41
1:E:1106:VAL:CG2	1:E:1112:LEU:HD11	2.51	0.41
1:G:1355:VAL:HG12	1:G:1356:CYS:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:68:ARG:HB3	2:B:69:PRO:HD3	2.03	0.41
1:C:1208:ASP:O	1:C:1214:HIS:HB2	2.21	0.41
1:E:1047:GLU:O	1:E:1051:THR:HG23	2.21	0.41
1:G:1213:GLU:H	1:G:1213:GLU:CD	2.23	0.41
1:C:1380:PRO:HG2	1:C:1381:GLU:OE2	2.20	0.41
1:A:1065:ARG:HG2	1:A:1065:ARG:HH11	1.85	0.41
1:C:1250:ALA:C	1:C:1252:GLN:H	2.23	0.41
2:F:160:LEU:HD13	2:F:160:LEU:C	2.41	0.41
1:E:1250:ALA:O	1:E:1251:GLU:HB3	2.20	0.41
1:E:1355:VAL:HG12	1:E:1356:CYS:N	2.36	0.41
1:G:1178:HIS:C	1:G:1180:SER:H	2.24	0.41
1:A:1103:GLU:O	1:A:1107:ARG:HG3	2.21	0.41
1:C:1345:LEU:H	1:C:1356:CYS:HA	1.86	0.41
1:G:1340:LEU:HD12	1:G:1394:LEU:HD21	2.03	0.41
2:H:11:ASP:OD1	2:H:92:ASN:ND2	2.47	0.41
1:C:1252:GLN:HE21	1:C:1252:GLN:HB2	1.64	0.41
1:A:1210:GLU:OE1	1:A:1210:GLU:HA	2.21	0.41
1:G:1287:LYS:N	1:G:1287:LYS:CD	2.80	0.40
2:D:37:PHE:HD2	2:D:57:ASP:HB2	1.87	0.40
1:E:1086:GLY:C	1:E:1088:LEU:N	2.74	0.40
1:G:1086:GLY:C	1:G:1088:LEU:N	2.74	0.40
1:G:1365:SER:O	1:G:1367:GLY:N	2.55	0.40
1:C:1344:ALA:HB2	1:C:1387:LEU:HD13	2.01	0.40
1:E:1098:PHE:CE2	1:E:1102:LEU:HD11	2.56	0.40
1:E:1208:ASP:O	1:E:1214:HIS:HB2	2.21	0.40
1:A:1346:PRO:HG2	1:E:1345:LEU:CD1	2.52	0.40
1:C:1303:VAL:CG1	1:C:1329:PHE:HD2	2.35	0.40
1:C:1342:VAL:O	1:C:1342:VAL:HG13	2.21	0.40
2:B:137:ILE:HG23	2:B:141:GLN:HB2	2.03	0.40
1:E:1249:ILE:CD1	1:E:1261:ASP:H	2.14	0.40
1:C:1106:VAL:CG2	1:C:1112:LEU:HD11	2.51	0.40
1:G:1344:ALA:HB2	1:G:1387:LEU:CD1	2.51	0.40
1:E:1085:PHE:O	1:E:1088:LEU:HB2	2.20	0.40
1:A:1237:ILE:HD11	1:A:1270:HIS:CD2	2.56	0.40
2:H:98:TYR:OH	2:H:102:ARG:HD2	2.21	0.40
2:F:40:TYR:HB3	2:F:55:LEU:HB2	2.04	0.40
1:C:1273:VAL:CG2	1:C:1375:LEU:HB3	2.51	0.40
1:G:1340:LEU:HD11	1:G:1390:VAL:HG13	2.03	0.40
1:C:1234:MSE:CE	1:C:1234:MSE:HA	2.44	0.40
1:A:1179:SER:HB3	2:B:41:SER:HB2	2.03	0.40
1:C:1386:PHE:O	1:C:1390:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1156:LEU:HD21	1:A:1182:LEU:HD23	2.03	0.40
1:C:1250:ALA:C	1:C:1252:GLN:N	2.75	0.40
1:G:1068:LYS:N	1:G:1069:PRO:HD2	2.35	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:139:TYR:OH	2:H:107:ASN:OD1[2_657]	2.06	0.14

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/377 (97%)	313 (86%)	43 (12%)	10 (3%)	6	21
1	C	364/377 (97%)	315 (86%)	41 (11%)	8 (2%)	8	28
1	E	365/377 (97%)	322 (88%)	30 (8%)	13 (4%)	4	14
1	G	365/377 (97%)	322 (88%)	31 (8%)	12 (3%)	5	16
2	B	175/177 (99%)	164 (94%)	9 (5%)	2 (1%)	17	50
2	D	175/177 (99%)	164 (94%)	9 (5%)	2 (1%)	17	50
2	F	175/177 (99%)	162 (93%)	12 (7%)	1 (1%)	30	65
2	H	175/177 (99%)	163 (93%)	11 (6%)	1 (1%)	30	65
All	All	2160/2216 (98%)	1925 (89%)	186 (9%)	49 (2%)	8	26

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1087	ASN
1	A	1253	THR

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Mol	Chain	Res	Type
1	A	1261	ASP
1	C	1087	ASN
1	C	1253	THR
1	C	1261	ASP
1	E	1087	ASN
1	E	1253	THR
1	E	1261	ASP
1	G	1087	ASN
1	G	1253	THR
1	G	1261	ASP
1	A	1086	GLY
1	A	1252	GLN
2	B	11	ASP
1	C	1086	GLY
1	C	1252	GLN
2	D	11	ASP
1	E	1086	GLY
1	E	1305	LYS
1	E	1306	ASP
2	F	11	ASP
1	G	1086	GLY
1	G	1252	GLN
1	G	1325	GLU
1	A	1085	PHE
1	A	1312	LYS
1	A	1322	ILE
1	C	1085	PHE
1	E	1085	PHE
1	E	1252	GLN
1	G	1085	PHE
2	H	11	ASP
1	C	1311	LYS
1	E	1325	GLU
1	A	1254	GLY
1	A	1328	PRO
1	C	1254	GLY
2	D	65	ASP
1	E	1254	GLY
1	G	1254	GLY
1	G	1324	GLU
1	G	1399	ARG
2	B	65	ASP

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Mol	Chain	Res	Type
1	E	1350	ALA
1	G	1311	LYS
1	E	1327	ASP
1	G	1157	VAL
1	E	1157	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	332/332 (100%)	322 (97%)	10 (3%)	48	82
1	C	330/332 (99%)	320 (97%)	10 (3%)	48	82
1	E	331/332 (100%)	318 (96%)	13 (4%)	39	74
1	G	331/332 (100%)	319 (96%)	12 (4%)	42	76
2	B	153/153 (100%)	146 (95%)	7 (5%)	33	67
2	D	153/153 (100%)	146 (95%)	7 (5%)	33	67
2	F	153/153 (100%)	147 (96%)	6 (4%)	39	74
2	H	153/153 (100%)	147 (96%)	6 (4%)	39	74
All	All	1936/1940 (100%)	1865 (96%)	71 (4%)	41	76

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1048	LEU
1	A	1059	LEU
1	A	1062	LEU
1	A	1194	LEU
1	A	1252	GLN
1	A	1284	LYS
1	A	1287	LYS
1	A	1343	ARG
1	A	1368	ARG
1	A	1371	ARG

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Mol	Chain	Res	Type
2	B	50	PRO
2	B	62	GLU
2	B	66	ARG
2	B	77	VAL
2	B	116	LYS
2	B	143	LEU
2	B	170	ASP
1	C	1048	LEU
1	C	1059	LEU
1	C	1062	LEU
1	C	1194	LEU
1	C	1252	GLN
1	C	1284	LYS
1	C	1287	LYS
1	C	1343	ARG
1	C	1368	ARG
1	C	1371	ARG
2	D	50	PRO
2	D	62	GLU
2	D	66	ARG
2	D	77	VAL
2	D	116	LYS
2	D	143	LEU
2	D	170	ASP
1	E	1035	LEU
1	E	1048	LEU
1	E	1059	LEU
1	E	1062	LEU
1	E	1173	ASN
1	E	1194	LEU
1	E	1252	GLN
1	E	1284	LYS
1	E	1287	LYS
1	E	1313	LYS
1	E	1343	ARG
1	E	1368	ARG
1	E	1371	ARG
2	F	50	PRO
2	F	62	GLU
2	F	66	ARG
2	F	77	VAL
2	F	116	LYS

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Mol	Chain	Res	Type
2	F	170	ASP
1	G	1048	LEU
1	G	1059	LEU
1	G	1062	LEU
1	G	1194	LEU
1	G	1252	GLN
1	G	1284	LYS
1	G	1287	LYS
1	G	1313	LYS
1	G	1343	ARG
1	G	1368	ARG
1	G	1371	ARG
1	G	1397	LYS
2	H	62	GLU
2	H	66	ARG
2	H	77	VAL
2	H	116	LYS
2	H	143	LEU
2	H	170	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1120	GLN
1	A	1149	HIS
1	A	1173	ASN
1	A	1176	GLN
1	A	1230	HIS
1	A	1235	GLN
1	A	1374	HIS
2	B	2	GLN
2	B	74	GLN
2	B	141	GLN
1	C	1120	GLN
1	C	1149	HIS
1	C	1173	ASN
1	C	1230	HIS
1	C	1235	GLN
1	C	1374	HIS
2	D	2	GLN
2	D	74	GLN
2	D	141	GLN

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Mol	Chain	Res	Type
1	E	1120	GLN
1	E	1149	HIS
1	E	1173	ASN
1	E	1176	GLN
1	E	1230	HIS
1	E	1235	GLN
1	E	1374	HIS
2	F	2	GLN
2	F	74	GLN
2	F	141	GLN
1	G	1120	GLN
1	G	1149	HIS
1	G	1173	ASN
1	G	1176	GLN
1	G	1230	HIS
1	G	1235	GLN
1	G	1374	HIS
2	H	2	GLN
2	H	74	GLN
2	H	141	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	$\# Z > 2$
3	SO4	B	4001	-	4,4,4	0.24	0	6,6,6	0.17	0
3	SO4	D	4002	-	4,4,4	0.21	0	6,6,6	0.21	0
3	SO4	F	4003	-	4,4,4	0.24	0	6,6,6	0.15	0
3	SO4	H	4004	-	4,4,4	0.31	0	6,6,6	0.26	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
3	SO4	B	4001	-	-	0/0/0/0	0/0/0/0
3	SO4	D	4002	-	-	0/0/0/0	0/0/0/0
3	SO4	F	4003	-	-	0/0/0/0	0/0/0/0
3	SO4	H	4004	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.