



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 05:35 PM BST

PDB ID : 1LLW
Title : Structural studies on the synchronization of catalytic centers in glutamate synthase: complex with 2-oxoglutarate
Authors : van den Heuvel, R.H.; Ferrari, D.; Bossi, R.T.; Ravasio, S.; Curti, B.; Vanoni, M.A.; Florencio, F.J.; Mattevi, A.
Deposited on : 2002-04-30
Resolution : 2.70 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

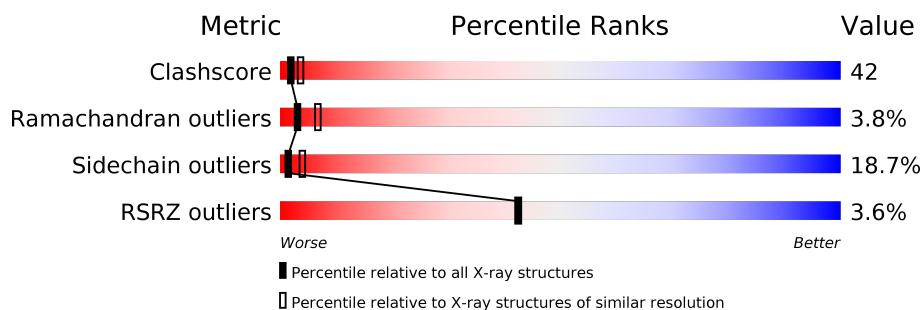
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

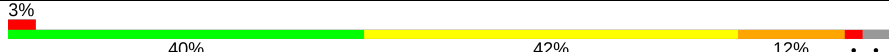
The reported resolution of this entry is 2.70 Å.

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	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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

Mol	Chain	Length	Quality of chain
1	A	1520	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	F3S	A	2072	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11408 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.

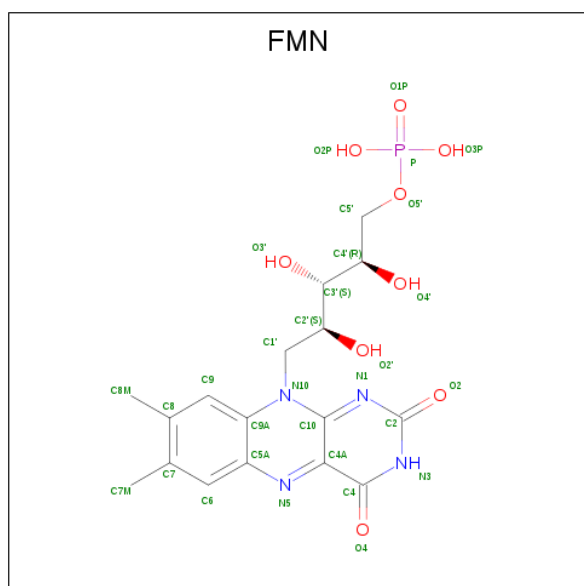
- Molecule 1 is a protein called Ferredoxin-dependent glutamate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1475	11311	7137	1970	2148	56	0	0	0

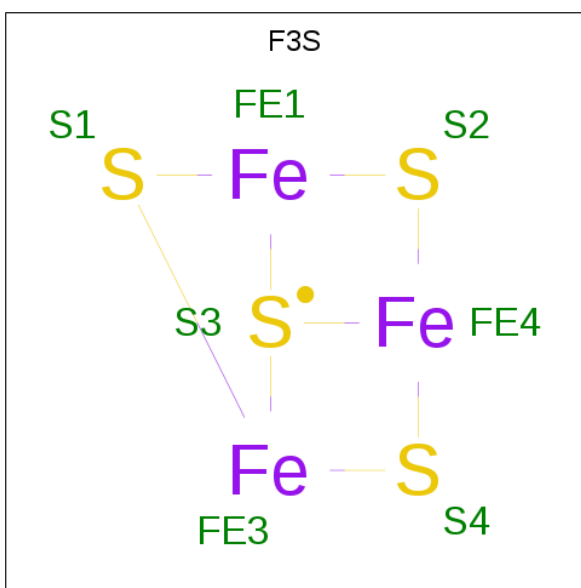
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	CONFLICT	UNP P55038
A	581	THR	ASP	CONFLICT	UNP P55038
A	1507	ASN	GLY	CONFLICT	UNP P55038

- Molecule 2 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: $C_{17}H_{21}N_4O_9P$).

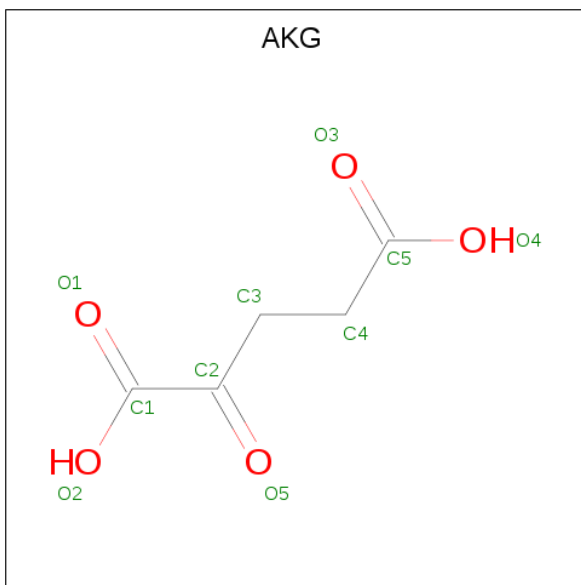


- Molecule 3 is FE3-S4 CLUSTER (three-letter code: F3S) (formula: Fe_3S_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	Fe	S	0	0
			7	3	4		

- Molecule 4 is 2-OXOGLUTARIC ACID (three-letter code: AKG) (formula: $\text{C}_5\text{H}_6\text{O}_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	5	5		

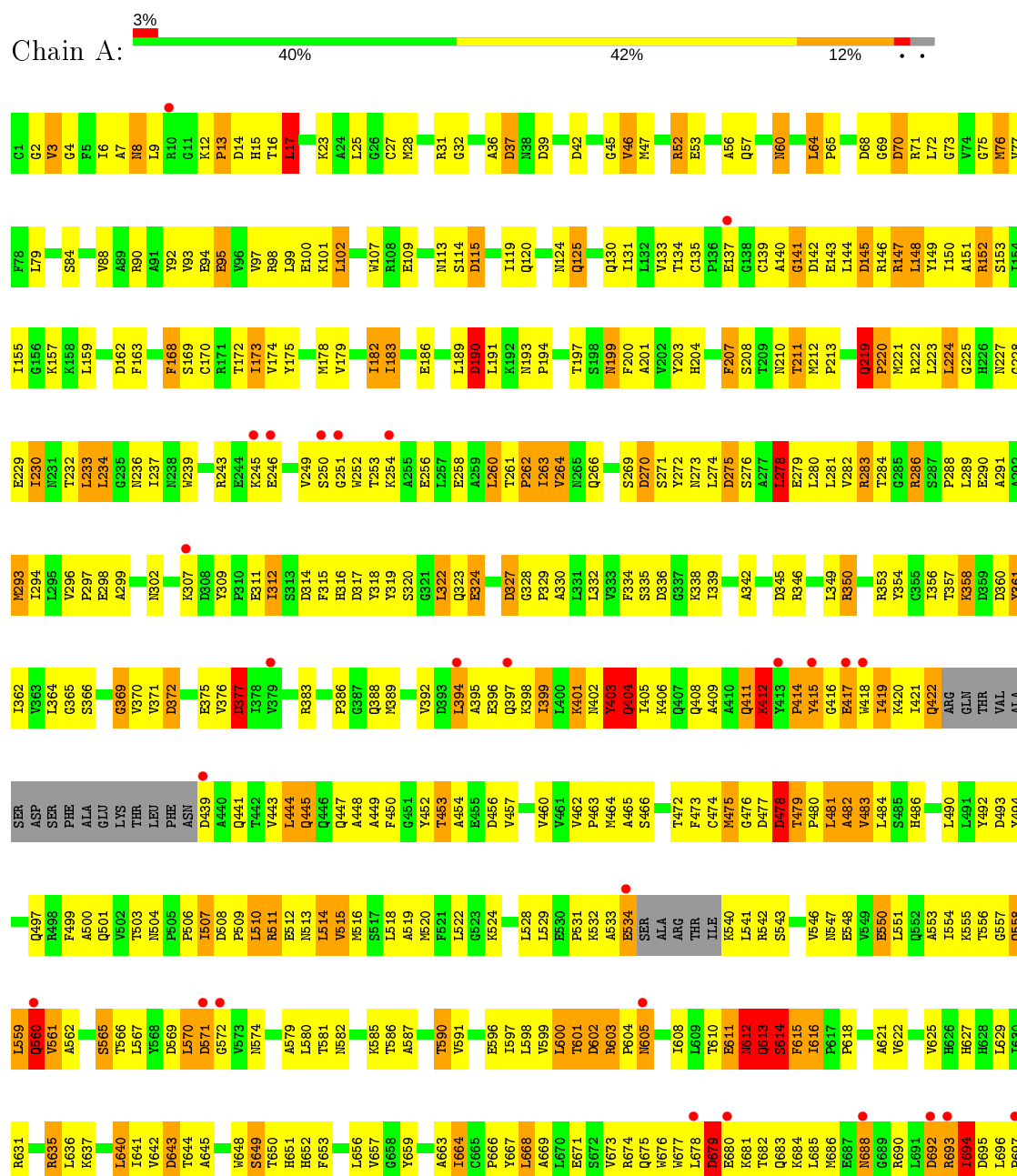
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	49	Total	O	0	0
			49	49		

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: Ferredoxin-dependent glutamate synthase



I1480	V1411	K1335	I1257	T1110	A1016	E920	R843	A772	T698
L1481	V1412	G1336	Q1258	G1111	Q1017	E921	D844	F773	
	L1413	M1337	E1259	D1113	L1018	P924	L845	P774	K701
M1484	G1414	M1338	A1260	D1113			L846	E775	N702
S1485	P1415	I1344	I1261	M1116	D1021	T937	A938	A776	N703
D1486	V1416	V1345	N1262	A1117	H1023	A938	D847	A777	R704
V1487	G1417	V1346	H1263	A1118	H1024	N939	F848		Q705
L1488	R1418	H1347	Q1264	A1119	Q1024	S940		K778	S706
G1489	N1419	H1347	L1193	M1120	I1025	I942	D851	K779	V707
K1490	V1420	P1348	D1194					L780	
G1491	G1421	K1269	I1195		Q1030		S855	F783	L711
F1492	A1422	Y1271	I1196	E1123	V1031	A946	S856		F712
G1493	R1272	R1272	I1197	E1124	S1032		L857	P790	K713
H1494	A1353	L1273	G1198		V1033	R949	V860	G791	I714
	P1354	V1274	R1199	F1127	K1034	P950	E861	Y794	L715
	T1425	N1275	T1200		L1035	G951	S862	H795	S716
		T1276	D1201		E1038	V952	V863	M796	K717
L1428	V1428	D1277	L1202	I1130	I1039	T953		N797	I720
A1429	I1359	R1278	L1203	A1131	G1040	P954	V867	S798	S721
Y1430	I1360	T1279		R1133		E955		P799	L722
F1431		V1280	R1206		M1052	Y956	T872	E800	L723
L1432	T1369	G1281	D1207	G1136	S1207	L957	G873	M801	A724
D1433	G1370	T1282	G1208	I1137	A1053	M958	G874	S802	S725
E1434	G1371	G1283	T1214	I1138	D1054	K961	M875		Y726
V1435	N1372	N1294	Q1215	M1139	I1055	Q962	S876	L805	H727
	L1373	N1295	N1216			E963			G728
N1443	G1374	G1296	L1221			E964	V809	A810	Q730
	A1375	F1297	S1212	I1141	D1062	I965	S881	A811	I731
I1446	N1376	E1298	T1214	V1142	T1065	K966	R882	Y812	
I1447		G1299	Q1215	C1143	G1066	M967	E883	LYS	G736
L1448	G1380		L1228	H1144	A1067	G970	E885	VAL	L737
L1449	E1381	F1305		T1145	S1068	A971	E886	GLY	
Q1450	R1382	Q1306	R1232	N1146	P1069	K972	T887	GLY	E740
R1451	F1383	G1307	Q1233	T1147	D1069	P973	L888	ASN	Y744
I1452	A1384	A1308	W1234	V1150	S1071			GLY	A745
A1454	V1385	A1309	L1235	G1153	W1080	Q978	A891	ASN	F746
S1455	R1386	G1310		V1152	E1081	I988	M892	GLY	
K1456	G1387	Q1311	E1238	T1154	T1085	L991	R894	ALA	T750
G1457	S1388	V1389	F1239		E1086	R992	L895		V753
E1458	V1389		W1240	R1158	V1087	R993	K898	D825	Q754
E1459		A1315	H1241	L1159	H1088	S994	S899	E826	G755
Q1460	I1394	F1316	S1242	R1160	R1089	K995	N900	Y827	L756
L1461	E1395	L1318		Q1161	M1094	P996	S901	E828	T757
K1462			P1245	Q1169	Q1095	G997	E903	L829	A758
S1463	D1399	H1321	V1246	V1170	L1096		R831	Y830	I759
L1464	H1400	H1324	L1247	V1171		L1000	Q832	D760	D760
I1465	C1401	L1325	D1248	N1172	R1099	P1004	Y833		A762
T1466	C1402	Q1326	D1249	F1173	V1100	P1005	L834		
	E1403	Q1326	D1250	Y1175	L1101	H1006	K835	V765	
Y1404	Y1404	G1327	I1251	F1176	L1102	H1007	R910	M766	
M1405	M1405	E1328	L1252	I1177	R1103	D1008	Y911	D836	
T1472	G1473	A1329	A1253		L1104		L912	R837	V767
S1474	P1475		D1254	E1180	D1105	E1013	D916	P888	F768
K1476	I1410	Y1332	P1255	V1181	K1109	D1014	T840	H769	
			D1256	R1182		L1015		G770	M771

4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	166.52Å 166.52Å 219.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.70 11.99 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (12.00-2.70) 97.9 (11.99-2.70)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.70Å)	Xtriage
Refinement program	REFMAC 5.1.06	Depositor
R, R_{free}	0.234 , 0.293 0.232 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	67.9	Xtriage
Anisotropy	0.515	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 66.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	11408	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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: FMN, F3S, AKG

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	0.89	5/11533 (0.0%)	1.15	62/15639 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	16

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1433	ASP	CB-CG	7.41	1.67	1.51
1	A	952	VAL	CB-CG2	-6.62	1.39	1.52
1	A	796	MET	CG-SD	6.00	1.96	1.81
1	A	293	MET	SD-CE	5.52	2.08	1.77
1	A	692	ASP	CB-CG	5.27	1.62	1.51

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	145	ASP	CB-CG-OD2	9.22	126.60	118.30
1	A	31	ARG	NE-CZ-NH2	-8.15	116.22	120.30
1	A	478	ASP	CB-CG-OD2	8.13	125.61	118.30
1	A	877	LEU	CA-CB-CG	-8.01	96.87	115.30
1	A	1195	ASP	CB-CG-OD2	7.79	125.31	118.30
1	A	270	ASP	CB-CG-OD2	7.69	125.22	118.30
1	A	907	ASP	CB-CG-OD2	7.55	125.09	118.30
1	A	37	ASP	CB-CG-OD2	7.52	125.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1277	ASP	CB-CG-OD2	7.50	125.05	118.30
1	A	695	ASP	CB-CG-OD2	7.46	125.02	118.30
1	A	162	ASP	CB-CG-OD2	7.32	124.89	118.30
1	A	493	ASP	CB-CG-OD2	7.25	124.83	118.30
1	A	851	ASP	CB-CG-OD2	7.21	124.78	118.30
1	A	1248	ASP	CB-CG-OD2	7.21	124.78	118.30
1	A	14	ASP	CB-CG-OD2	7.11	124.70	118.30
1	A	327	ASP	CB-CG-OD2	7.09	124.68	118.30
1	A	219	GLN	N-CA-C	6.84	129.48	111.00
1	A	278	LEU	CA-CB-CG	6.80	130.93	115.30
1	A	345	ASP	CB-CG-OD2	6.75	124.38	118.30
1	A	275	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	1101	LEU	CA-CB-CG	6.62	130.53	115.30
1	A	1201	ASP	CB-CG-OD2	6.58	124.22	118.30
1	A	692	ASP	CB-CG-OD2	6.54	124.18	118.30
1	A	350	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	A	569	ASP	CB-CG-OD2	6.47	124.13	118.30
1	A	694	ILE	CG1-CB-CG2	-6.45	97.20	111.40
1	A	17	LEU	CA-CB-CG	6.31	129.81	115.30
1	A	1240	VAL	CB-CA-C	-6.31	99.42	111.40
1	A	37	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	A	1250	ASP	CB-CG-OD2	6.28	123.95	118.30
1	A	1433	ASP	CB-CG-OD2	6.22	123.89	118.30
1	A	220	PRO	N-CD-CG	-6.12	94.02	103.20
1	A	836	ASP	CB-CG-OD2	6.10	123.79	118.30
1	A	1062	ASP	CB-CG-OD2	6.05	123.75	118.30
1	A	909	VAL	CB-CA-C	-6.02	99.95	111.40
1	A	142	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	1008	ASP	CB-CG-OD2	5.83	123.55	118.30
1	A	1113	ASP	CB-CG-OD2	5.76	123.48	118.30
1	A	377	ASP	CB-CG-OD2	5.72	123.45	118.30
1	A	571	ASP	CB-CG-OD2	5.67	123.40	118.30
1	A	1235	LEU	CB-CG-CD1	5.65	120.61	111.00
1	A	844	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	1132	MET	CG-SD-CE	-5.49	91.42	100.20
1	A	1208	ASP	CB-CG-OD2	5.49	123.24	118.30
1	A	98	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	1021	ASP	CB-CG-OD2	5.38	123.14	118.30
1	A	847	ASP	CB-CG-OD2	5.37	123.14	118.30
1	A	1227	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	1103	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	A	1399	ASP	CB-CG-OD2	5.32	123.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	950	PHE	C-N-CA	-5.28	111.22	122.30
1	A	72	LEU	C-N-CA	-5.27	111.23	122.30
1	A	70	ASP	CB-CG-OD2	5.27	123.04	118.30
1	A	679	ASP	CB-CG-OD2	5.25	123.02	118.30
1	A	1235	LEU	CA-CB-CG	5.23	127.33	115.30
1	A	643	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	1089	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	A	1141	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	722	LEU	CA-CB-CG	5.11	127.05	115.30
1	A	882	ARG	NE-CZ-NH2	-5.05	117.77	120.30
1	A	190	ASP	CB-CG-OD2	5.04	122.84	118.30
1	A	372	ASP	CB-CG-OD2	5.01	122.81	118.30

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	HIS	Peptide
1	A	1137	CYS	Peptide
1	A	219	GLN	Peptide
1	A	260	LEU	Peptide
1	A	369	GLY	Peptide
1	A	403	TYR	Peptide
1	A	412	LYS	Peptide
1	A	445	GLN	Peptide
1	A	572	GLY	Peptide
1	A	612	ASN	Peptide
1	A	615	PHE	Peptide
1	A	838	PRO	Peptide
1	A	873	GLY	Peptide
1	A	902	GLY	Peptide
1	A	952	VAL	Peptide
1	A	997	GLY	Peptide

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	11311	0	11255	947	1
2	A	31	0	19	0	0
3	A	7	0	0	4	0
4	A	10	0	4	2	0
5	A	49	0	0	14	0
All	All	11408	0	11278	947	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 42.

All (947) 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:383:ARG:NH1	1:A:1380:GLY:HA2	1.20	1.46
1:A:221:MET:SD	1:A:221:MET:CE	2.02	1.46
1:A:293:MET:SD	1:A:293:MET:CE	2.08	1.41
1:A:885:HIS:CD2	1:A:910:ARG:HH22	1.44	1.36
1:A:768:PHE:CE2	1:A:771:MET:HG2	1.68	1.28
1:A:383:ARG:HH12	1:A:1380:GLY:CA	1.45	1.27
1:A:1263:HIS:CE1	1:A:1297:PHE:HA	1.71	1.24
1:A:1355:GLU:HG2	1:A:1476:LYS:HB2	1.22	1.15
1:A:1491:PHE:HD1	1:A:1491:PHE:O	1.28	1.13
1:A:558:GLN:HA	1:A:558:GLN:OE1	1.34	1.12
1:A:768:PHE:HE2	1:A:771:MET:HG2	0.96	1.11
1:A:484:LEU:HB3	1:A:839:VAL:CG1	1.81	1.10
1:A:443:VAL:HG21	1:A:675:GLN:HE21	1.13	1.09
1:A:1347:HIS:CG	1:A:1348:PRO:HD2	1.88	1.09
1:A:802:SER:HB2	1:A:1133:ILE:HG23	1.31	1.08
1:A:1119:LEU:HD23	1:A:1196:ILE:HG22	1.35	1.07
1:A:510:LEU:HB2	1:A:511:ARG:HH21	1.11	1.07
1:A:953:THR:HG23	1:A:1294:ASN:HD21	1.06	1.07
1:A:809:VAL:HG11	1:A:1169:GLN:O	1.55	1.07
1:A:414:PRO:HB3	1:A:418:TRP:HB3	1.37	1.06
1:A:1447:ILE:HD11	1:A:1494:ALA:HB1	1.38	1.06
1:A:953:THR:CG2	1:A:1294:ASN:HD21	1.67	1.05
1:A:867:VAL:HG11	1:A:895:LEU:HB3	1.38	1.05
1:A:559:LEU:CD2	1:A:560:GLN:O	2.05	1.04
1:A:1254:ASP:HB2	1:A:1255:PRO:CD	1.87	1.03
1:A:453:THR:HB	1:A:456:ASP:OD2	1.59	1.03
1:A:1263:HIS:HE1	1:A:1297:PHE:HA	0.86	1.02
1:A:1263:HIS:HE1	1:A:1297:PHE:CA	1.71	1.02
1:A:559:LEU:HD21	1:A:560:GLN:O	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1254:ASP:CB	1:A:1255:PRO:HD3	1.88	1.02
1:A:383:ARG:NH1	1:A:1380:GLY:CA	2.13	1.02
1:A:460:VAL:HG12	1:A:464:MET:CE	1.91	1.01
1:A:885:HIS:HD2	1:A:910:ARG:NH2	1.58	1.01
1:A:883:GLU:OE1	1:A:1160:ARG:HD2	1.59	1.01
1:A:261:THR:HB	1:A:262:PRO:HD3	1.43	1.01
1:A:559:LEU:HG	1:A:560:GLN:N	1.72	1.01
1:A:403:TYR:H	1:A:403:TYR:HD1	1.06	1.00
1:A:243:ARG:NH1	1:A:528:LEU:HB2	1.75	1.00
1:A:460:VAL:HG12	1:A:464:MET:HE2	1.40	1.00
1:A:1337:MET:HE1	1:A:1365:LEU:HD21	1.42	0.99
1:A:444:LEU:O	1:A:445:GLN:HG2	1.63	0.99
1:A:885:HIS:CD2	1:A:910:ARG:NH2	2.30	0.98
1:A:1347:HIS:ND1	1:A:1348:PRO:HD2	1.77	0.98
1:A:414:PRO:CB	1:A:418:TRP:HB3	1.94	0.97
1:A:510:LEU:HB2	1:A:511:ARG:NH2	1.77	0.97
1:A:100:GLU:HB2	1:A:102:LEU:HD12	1.43	0.97
1:A:846:LEU:HB2	1:A:1116:MET:HE1	1.46	0.97
1:A:1081:GLU:HG3	1:A:1120:MET:HE1	1.44	0.97
1:A:1254:ASP:CB	1:A:1255:PRO:CD	2.42	0.97
1:A:1491:PHE:CD1	1:A:1491:PHE:O	2.18	0.96
1:A:1254:ASP:HB3	1:A:1255:PRO:HD3	1.45	0.96
1:A:354:TYR:HB3	1:A:364:LEU:HD12	1.48	0.95
1:A:445:GLN:HG3	1:A:777:ALA:HB1	1.47	0.95
1:A:71:ARG:HG2	5:A:2117:HOH:O	1.67	0.95
1:A:484:LEU:HB3	1:A:839:VAL:HG11	1.50	0.94
1:A:1101:LEU:HD13	1:A:1123:GLU:HB2	1.49	0.94
1:A:686:MET:O	1:A:692:ASP:HB2	1.68	0.93
1:A:1355:GLU:HG2	1:A:1476:LYS:CB	1.99	0.93
1:A:875:MET:SD	1:A:1132:MET:HE1	2.08	0.93
1:A:318:TYR:HD1	1:A:418:TRP:HE1	1.13	0.92
1:A:1318:LEU:HB2	1:A:1321:MET:HE3	1.50	0.92
1:A:415:TYR:CD1	1:A:416:GLY:N	2.37	0.92
1:A:768:PHE:HE2	1:A:771:MET:CG	1.83	0.91
1:A:1130:ILE:H	1:A:1130:ILE:HD13	1.36	0.91
1:A:657:VAL:HG11	1:A:723:LEU:HD11	1.52	0.91
1:A:1038:GLU:O	1:A:1041:ILE:HG22	1.70	0.90
1:A:1253:ALA:HA	5:A:2081:HOH:O	1.70	0.90
1:A:809:VAL:CG1	1:A:1169:GLN:O	2.20	0.90
1:A:907:ASP:OD2	1:A:909:VAL:HG23	1.71	0.90
1:A:953:THR:HG23	1:A:1294:ASN:ND2	1.85	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1372:ASN:N	1:A:1372:ASN:HD22	1.70	0.90
1:A:418:TRP:CE3	1:A:418:TRP:O	2.25	0.89
1:A:1138:ILE:HG22	1:A:1139:MET:N	1.87	0.89
1:A:1142:VAL:O	1:A:1145:THR:HB	1.72	0.88
1:A:757:THR:HB	5:A:2091:HOH:O	1.72	0.88
1:A:1311:GLN:HA	1:A:1311:GLN:OE1	1.74	0.88
1:A:760:ASP:OD2	1:A:1214:THR:HG23	1.73	0.88
1:A:307:LYS:HE3	1:A:1440:GLU:OE1	1.72	0.88
1:A:993:ARG:HH11	1:A:993:ARG:HG3	1.38	0.88
1:A:802:SER:HB2	1:A:1133:ILE:CG2	2.04	0.87
1:A:1337:MET:CE	1:A:1365:LEU:HD21	2.03	0.87
1:A:1119:LEU:CD2	1:A:1196:ILE:HG22	2.04	0.87
1:A:383:ARG:HH11	1:A:1380:GLY:HA2	1.35	0.87
1:A:1447:ILE:HD11	1:A:1494:ALA:CB	2.04	0.87
1:A:263:ILE:HD12	1:A:280:LEU:HD22	1.57	0.87
1:A:443:VAL:HG21	1:A:675:GLN:NE2	1.90	0.86
1:A:768:PHE:CE2	1:A:771:MET:CG	2.55	0.86
1:A:460:VAL:CG1	1:A:464:MET:HE2	2.05	0.86
1:A:560:GLN:OE1	1:A:560:GLN:HA	1.71	0.86
1:A:855:ILE:HG23	1:A:856:SER:H	1.40	0.86
1:A:286:ARG:NH2	1:A:528:LEU:O	2.07	0.86
1:A:715:LEU:HD22	1:A:726:TYR:CD1	2.11	0.85
1:A:243:ARG:HH11	1:A:528:LEU:HB2	1.41	0.85
1:A:603:ARG:HG2	1:A:603:ARG:O	1.72	0.85
1:A:404:GLN:HA	1:A:404:GLN:OE1	1.77	0.85
1:A:701:LYS:O	1:A:705:GLN:HB2	1.76	0.85
1:A:501:GLN:HE22	1:A:1035:LEU:HB3	1.42	0.84
1:A:369:GLY:HA3	1:A:1308:ALA:CB	2.08	0.84
1:A:649:SER:HB2	1:A:652:HIS:CD2	2.12	0.84
1:A:993:ARG:HH11	1:A:993:ARG:CG	1.90	0.84
1:A:1251:ILE:HD13	1:A:1271:TYR:CE1	2.13	0.84
1:A:1420:VAL:O	1:A:1420:VAL:HG12	1.77	0.84
1:A:878:GLY:HA2	1:A:988:ILE:HD12	1.60	0.84
1:A:558:GLN:CA	1:A:558:GLN:OE1	2.22	0.83
1:A:100:GLU:HB2	1:A:102:LEU:CD1	2.08	0.83
1:A:1065:THR:HG21	1:A:1068:SER:OG	1.78	0.83
1:A:414:PRO:O	1:A:418:TRP:N	2.11	0.83
1:A:492:TYR:HE2	1:A:656:LEU:HD13	1.44	0.83
1:A:867:VAL:CG1	1:A:895:LEU:HB3	2.08	0.83
1:A:881:SER:HB2	1:A:1160:ARG:HD3	1.61	0.83
1:A:750:THR:HG21	1:A:1039:ILE:HG21	1.62	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:ILE:HG22	1:A:404:GLN:HG2	1.62	0.82
1:A:1347:HIS:CE1	1:A:1348:PRO:HD2	2.14	0.82
1:A:1376:ASN:HD21	1:A:1472:THR:HG23	1.43	0.82
1:A:1119:LEU:CD2	1:A:1196:ILE:CG2	2.58	0.82
1:A:657:VAL:HG11	1:A:723:LEU:CD1	2.09	0.82
1:A:1254:ASP:HB2	1:A:1255:PRO:HD2	1.61	0.81
1:A:73:GLY:HA2	1:A:170:CYS:HA	1.63	0.81
1:A:770:GLY:O	5:A:2116:HOH:O	1.95	0.81
1:A:443:VAL:HG11	1:A:675:GLN:HG3	1.59	0.81
1:A:484:LEU:HD13	1:A:839:VAL:HG13	1.61	0.80
1:A:737:LEU:O	1:A:754:GLY:HA2	1.81	0.80
1:A:484:LEU:HB3	1:A:839:VAL:HG12	1.63	0.80
1:A:497:GLN:HE21	1:A:651:HIS:HD2	1.27	0.80
1:A:1208:ASP:N	1:A:1208:ASP:OD1	2.13	0.80
1:A:1263:HIS:CE1	1:A:1296:GLY:O	2.36	0.79
1:A:676:TRP:HE1	1:A:690:ARG:HH12	1.28	0.79
1:A:522:LEU:HB2	5:A:2080:HOH:O	1.82	0.79
1:A:460:VAL:CG1	1:A:464:MET:CE	2.60	0.79
1:A:179:VAL:HB	1:A:183:ILE:HG22	1.63	0.78
1:A:1360:ILE:HG23	1:A:1364:CYS:SG	2.23	0.78
1:A:1409:VAL:O	1:A:1410:ILE:HD13	1.83	0.78
1:A:445:GLN:OE1	1:A:777:ALA:HB2	1.84	0.78
1:A:1111:GLY:HA3	1:A:1180:GLU:HG2	1.66	0.78
1:A:827:TYR:O	1:A:831:ARG:HB2	1.83	0.78
1:A:1476:LYS:O	1:A:1480:ILE:HG13	1.84	0.78
1:A:1338:ASN:HA	1:A:1369:THR:HG22	1.64	0.77
1:A:768:PHE:CD2	1:A:771:MET:HB2	2.20	0.77
1:A:1119:LEU:O	1:A:1198:GLY:HA2	1.84	0.77
1:A:464:MET:HB3	1:A:706:SER:OG	1.85	0.77
1:A:828:GLU:O	1:A:832:GLN:HB2	1.84	0.77
1:A:12:LYS:HB3	1:A:13:PRO:HD2	1.65	0.77
1:A:610:THR:HG23	1:A:773:PHE:HB3	1.67	0.77
1:A:499:PHE:CD1	1:A:973:PRO:HB3	2.20	0.77
1:A:649:SER:HB2	1:A:652:HIS:CG	2.20	0.76
1:A:134:THR:HB	5:A:2117:HOH:O	1.86	0.76
1:A:1191:ARG:HG2	5:A:2084:HOH:O	1.85	0.76
1:A:294:ILE:HG21	1:A:528:LEU:HD11	1.67	0.76
1:A:100:GLU:O	1:A:102:LEU:N	2.18	0.76
1:A:1101:LEU:CD1	1:A:1123:GLU:HB2	2.15	0.76
1:A:182:ILE:O	1:A:182:ILE:HG12	1.85	0.76
1:A:885:HIS:HD2	1:A:910:ARG:HH22	0.79	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:811:ALA:O	1:A:812:TYR:HB2	1.84	0.76
1:A:1119:LEU:HD23	1:A:1196:ILE:CG2	2.15	0.75
1:A:1461:LEU:HD21	1:A:1491:PHE:HZ	1.52	0.75
1:A:1491:PHE:HD1	1:A:1491:PHE:C	1.88	0.75
1:A:338:LYS:O	1:A:394:LEU:HD23	1.88	0.74
1:A:649:SER:HB3	1:A:652:HIS:H	1.50	0.74
1:A:768:PHE:CD2	1:A:771:MET:HG2	2.21	0.74
1:A:949:ARG:NH2	1:A:1008:ASP:OD2	2.19	0.74
1:A:1456:LYS:HB3	1:A:1503:PRO:O	1.87	0.74
1:A:1376:ASN:OD1	1:A:1472:THR:HG21	1.87	0.74
1:A:354:TYR:HB3	1:A:364:LEU:CD1	2.16	0.74
1:A:1461:LEU:HD21	1:A:1491:PHE:CZ	2.22	0.74
1:A:567:LEU:HD12	1:A:604:PRO:CD	2.18	0.74
1:A:773:PHE:HB2	1:A:774:PRO:CD	2.16	0.74
1:A:1142:VAL:O	1:A:1142:VAL:CG1	2.35	0.74
1:A:1130:ILE:CD1	1:A:1130:ILE:H	2.00	0.74
1:A:714:ILE:HA	1:A:717:LYS:HD2	1.69	0.74
1:A:907:ASP:OD2	1:A:909:VAL:CG2	2.36	0.74
1:A:685:LEU:HD12	1:A:690:ARG:HD2	1.69	0.74
1:A:1081:GLU:CG	1:A:1120:MET:HE1	2.17	0.73
1:A:1491:PHE:CD1	1:A:1491:PHE:C	2.60	0.73
1:A:581:THR:CG2	1:A:585:LYS:HE3	2.18	0.73
1:A:443:VAL:CG2	1:A:675:GLN:HE21	1.99	0.73
1:A:9:LEU:HD21	1:A:392:VAL:CG1	2.19	0.73
1:A:1119:LEU:HD21	1:A:1196:ILE:CG2	2.18	0.73
1:A:472:THR:HG22	1:A:473:PHE:N	2.01	0.73
1:A:855:ILE:CG2	1:A:856:SER:H	2.01	0.73
1:A:616:ILE:CG2	1:A:621:ALA:HB2	2.18	0.73
1:A:1148:CYS:SG	3:A:2072:F3S:S3	2.86	0.72
1:A:404:GLN:OE1	1:A:404:GLN:CA	2.35	0.72
1:A:1455:SER:O	1:A:1459:GLU:HG2	1.88	0.72
1:A:645:ALA:CB	1:A:668:LEU:HB2	2.20	0.72
1:A:1103:ARG:HG2	1:A:1124:GLU:HB2	1.71	0.72
1:A:1138:ILE:CG2	1:A:1139:MET:N	2.51	0.72
1:A:318:TYR:HD1	1:A:418:TRP:NE1	1.86	0.72
1:A:883:GLU:OE1	1:A:1160:ARG:CD	2.35	0.72
1:A:1355:GLU:H	1:A:1355:GLU:CD	1.93	0.72
1:A:1347:HIS:CD2	1:A:1348:PRO:HD2	2.25	0.71
1:A:506:PRO:HD2	1:A:1005:PRO:HB3	1.72	0.71
1:A:497:GLN:HE21	1:A:651:HIS:CD2	2.06	0.71
1:A:45:GLY:HA3	1:A:220:PRO:CD	2.20	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:560:GLN:CA	1:A:560:GLN:OE1	2.38	0.71
1:A:37:ASP:H	1:A:120:GLN:HE21	1.38	0.71
1:A:445:GLN:HB3	1:A:772:ALA:HB1	1.73	0.71
1:A:307:LYS:CE	1:A:1440:GLU:OE1	2.37	0.71
1:A:1254:ASP:C	1:A:1256:ASP:H	1.94	0.70
1:A:211:THR:HG21	1:A:1094:ASN:O	1.91	0.70
1:A:773:PHE:CB	1:A:774:PRO:CD	2.69	0.70
1:A:1318:LEU:HB2	1:A:1321:MET:CE	2.20	0.70
1:A:460:VAL:O	1:A:464:MET:HG3	1.92	0.70
1:A:403:TYR:N	1:A:403:TYR:HD1	1.85	0.70
1:A:237:ILE:HG23	1:A:264:VAL:HG13	1.74	0.70
1:A:152:ARG:HH12	1:A:168:PHE:N	1.90	0.70
1:A:1372:ASN:N	1:A:1372:ASN:ND2	2.34	0.70
1:A:402:ASN:O	1:A:403:TYR:O	2.09	0.70
1:A:519:ALA:O	1:A:520:MET:HG2	1.92	0.69
1:A:511:ARG:HG3	1:A:1422:ALA:HB1	1.74	0.69
1:A:561:VAL:CG1	1:A:599:VAL:HG23	2.22	0.69
1:A:258:GLU:O	1:A:261:THR:OG1	2.04	0.69
1:A:1101:LEU:HA	1:A:1123:GLU:OE2	1.92	0.69
1:A:567:LEU:HD12	1:A:604:PRO:HD2	1.73	0.69
1:A:1325:LEU:HD21	1:A:1328:GLU:O	1.93	0.69
1:A:296:VAL:O	1:A:296:VAL:HG12	1.90	0.69
1:A:602:ASP:OD1	1:A:644:THR:OG1	2.07	0.69
1:A:908:VAL:HG22	1:A:911:TYR:CE1	2.26	0.69
1:A:773:PHE:HB2	1:A:774:PRO:HD3	1.72	0.69
1:A:827:TYR:O	1:A:831:ARG:N	2.26	0.69
1:A:232:THR:HG21	1:A:725:SER:HB3	1.74	0.68
1:A:559:LEU:HD22	1:A:596:GLU:H	1.58	0.68
1:A:1032:SER:CB	1:A:1055:ILE:HB	2.22	0.68
1:A:1347:HIS:ND1	1:A:1348:PRO:CD	2.53	0.68
1:A:1294:ASN:HB3	1:A:1338:ASN:HD21	1.59	0.67
1:A:445:GLN:HG3	1:A:777:ALA:CB	2.22	0.67
1:A:1130:ILE:HD13	1:A:1130:ILE:N	2.07	0.67
1:A:490:LEU:HD11	1:A:648:TRP:CH2	2.29	0.67
1:A:501:GLN:HE22	1:A:1035:LEU:CB	2.07	0.67
1:A:1147:ASN:O	1:A:1148:CYS:C	2.31	0.67
1:A:1338:ASN:O	1:A:1370:GLY:HA3	1.94	0.67
1:A:686:MET:HE3	1:A:692:ASP:HA	1.76	0.67
1:A:1263:HIS:CE1	1:A:1298:GLU:H	2.13	0.66
1:A:509:PRO:HA	1:A:516:MET:HE2	1.76	0.66
1:A:1246:VAL:O	1:A:1249:ASP:HB2	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD23	1:A:170:CYS:HB3	1.76	0.66
1:A:416:GLY:O	1:A:420:LYS:HG3	1.95	0.66
1:A:1360:ILE:CG2	1:A:1364:CYS:SG	2.83	0.66
1:A:645:ALA:HB1	1:A:668:LEU:HB2	1.76	0.66
1:A:9:LEU:HD21	1:A:392:VAL:HG13	1.78	0.66
1:A:559:LEU:CD2	1:A:596:GLU:H	2.08	0.66
1:A:676:TRP:HE1	1:A:690:ARG:NH1	1.93	0.66
1:A:450:PHE:CZ	1:A:608:ILE:HD12	2.31	0.66
1:A:1352:PHE:O	1:A:1354:PRO:HD3	1.96	0.66
1:A:1442:ILE:CD1	1:A:1449:LEU:HD13	2.25	0.66
1:A:73:GLY:HA2	1:A:169:SER:O	1.96	0.66
1:A:893:ASN:ND2	1:A:937:THR:HG23	2.11	0.66
1:A:315:PHE:HD2	1:A:319:TYR:CE1	2.14	0.66
1:A:418:TRP:CD2	1:A:418:TRP:C	2.70	0.66
1:A:1311:GLN:CA	1:A:1311:GLN:OE1	2.45	0.65
1:A:1402:CYS:O	1:A:1403:GLU:O	2.14	0.65
1:A:45:GLY:HA3	1:A:220:PRO:HD3	1.77	0.65
1:A:773:PHE:CB	1:A:774:PRO:HD3	2.26	0.65
1:A:1251:ILE:CD1	1:A:1271:TYR:CE1	2.80	0.65
1:A:37:ASP:H	1:A:120:GLN:NE2	1.92	0.65
1:A:581:THR:HG23	1:A:585:LYS:HE3	1.79	0.65
1:A:901:SER:O	1:A:902:GLY:C	2.35	0.65
1:A:406:LYS:O	1:A:409:ALA:HB3	1.96	0.65
1:A:686:MET:CE	1:A:694:ILE:HB	2.26	0.65
1:A:1282:THR:OG1	1:A:1315:ALA:HB3	1.97	0.65
1:A:311:GLU:CB	1:A:409:ALA:HB1	2.26	0.65
1:A:261:THR:CB	1:A:262:PRO:HD3	2.24	0.65
1:A:329:PRO:HB3	1:A:349:LEU:HB2	1.77	0.65
1:A:1032:SER:HA	1:A:1055:ILE:O	1.97	0.64
1:A:529:LEU:O	1:A:531:PRO:HD3	1.96	0.64
1:A:602:ASP:O	1:A:608:ILE:HD13	1.97	0.64
1:A:1137:CYS:SG	1:A:1138:ILE:O	2.54	0.64
1:A:146:ARG:NH2	1:A:256:GLU:OE1	2.29	0.64
1:A:270:ASP:OD1	1:A:271:SER:N	2.30	0.64
1:A:511:ARG:CG	1:A:1422:ALA:HB1	2.26	0.64
1:A:891:ALA:CB	1:A:1170:VAL:CG2	2.75	0.64
1:A:1432:LEU:O	1:A:1432:LEU:HG	1.96	0.64
1:A:715:LEU:HD22	1:A:726:TYR:CG	2.32	0.64
1:A:501:GLN:NE2	1:A:1035:LEU:HA	2.13	0.64
1:A:1462:LYS:HB2	1:A:1484:TRP:CZ2	2.33	0.64
1:A:612:ASN:O	1:A:614:SER:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1430:TYR:CE2	1:A:1493:GLN:OE1	2.50	0.64
1:A:611:GLU:O	1:A:613:GLN:N	2.29	0.64
1:A:611:GLU:C	1:A:613:GLN:N	2.48	0.64
1:A:315:PHE:HD2	1:A:319:TYR:HE1	1.44	0.64
1:A:148:LEU:HD23	1:A:169:SER:HA	1.79	0.64
1:A:1228:THR:HG23	1:A:1228:THR:O	1.97	0.63
1:A:1338:ASN:OD1	1:A:1369:THR:CG2	2.47	0.63
1:A:1447:ILE:CD1	1:A:1494:ALA:HB1	2.20	0.63
1:A:302:ASN:O	1:A:1418:ARG:NH1	2.31	0.63
1:A:551:LEU:HG	1:A:555:LYS:HE2	1.79	0.63
1:A:957:LEU:HD22	1:A:963:LEU:HD13	1.81	0.63
1:A:757:THR:H	1:A:760:ASP:HB2	1.62	0.63
1:A:383:ARG:HG2	1:A:1358:VAL:HG21	1.80	0.63
1:A:415:TYR:CG	1:A:416:GLY:N	2.56	0.63
1:A:453:THR:CB	1:A:456:ASP:OD2	2.40	0.63
1:A:908:VAL:HG22	1:A:911:TYR:HE1	1.64	0.63
1:A:1142:VAL:HG11	1:A:1147:ASN:HB2	1.81	0.62
1:A:32:GLY:HA2	1:A:207:PHE:HB2	1.81	0.62
1:A:1388:SER:HA	1:A:1406:THR:HG22	1.82	0.62
1:A:1409:VAL:C	1:A:1410:ILE:HD13	2.20	0.62
1:A:289:LEU:CD2	1:A:389:MET:HE3	2.29	0.62
1:A:414:PRO:HB2	1:A:418:TRP:HB3	1.81	0.62
1:A:1142:VAL:O	1:A:1142:VAL:HG12	1.98	0.62
1:A:358:LYS:HD2	1:A:377:ASP:HB2	1.81	0.62
1:A:1101:LEU:HD11	1:A:1124:GLU:HG3	1.81	0.62
1:A:6:ILE:HD11	1:A:371:VAL:HG21	1.80	0.62
1:A:318:TYR:CD1	1:A:418:TRP:NE1	2.65	0.62
1:A:679:ASP:OD1	1:A:681:LYS:N	2.33	0.62
1:A:289:LEU:HD22	1:A:389:MET:HE3	1.81	0.62
1:A:290:GLU:OE1	1:A:408:GLN:HG3	2.00	0.62
1:A:421:ILE:O	1:A:422:GLN:O	2.17	0.62
1:A:953:THR:CG2	1:A:1294:ASN:ND2	2.52	0.62
1:A:1288:ILE:HD12	1:A:1321:MET:HE1	1.81	0.62
1:A:509:PRO:HA	1:A:516:MET:CE	2.29	0.62
1:A:2:GLY:HA3	1:A:28:MET:CE	2.30	0.61
1:A:855:ILE:CG2	1:A:856:SER:N	2.60	0.61
1:A:239:TRP:HE1	1:A:728:GLY:HA3	1.65	0.61
1:A:1363:THR:CG2	1:A:1385:VAL:HG21	2.31	0.61
1:A:17:LEU:HD21	1:A:200:PHE:HA	1.80	0.61
1:A:450:PHE:HZ	1:A:608:ILE:HD12	1.63	0.61
1:A:2:GLY:HA3	1:A:28:MET:HE3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:311:GLU:HB3	1:A:409:ALA:HB1	1.81	0.61
1:A:1257:ILE:O	1:A:1261:ILE:HG12	2.01	0.61
1:A:1461:LEU:CD2	1:A:1491:PHE:HZ	2.13	0.61
1:A:28:MET:HE1	1:A:366:SER:HB2	1.80	0.61
1:A:688:ASN:O	1:A:688:ASN:CG	2.39	0.61
1:A:570:LEU:HG	1:A:613:GLN:HG2	1.83	0.61
1:A:907:ASP:CG	1:A:909:VAL:HG23	2.20	0.61
1:A:971:ALA:HB3	1:A:1065:THR:HG23	1.82	0.61
1:A:499:PHE:CE1	1:A:973:PRO:HB3	2.36	0.61
1:A:388:GLN:HG2	1:A:401:LYS:HD3	1.81	0.61
1:A:645:ALA:HB1	1:A:668:LEU:CB	2.31	0.61
1:A:1347:HIS:CE1	1:A:1348:PRO:CD	2.84	0.60
1:A:314:ASP:OD2	1:A:415:TYR:HD1	1.84	0.60
1:A:827:TYR:HE1	1:A:1176:PHE:HD1	1.50	0.60
1:A:550:GLU:O	1:A:554:ILE:HD13	2.01	0.60
1:A:586:THR:O	1:A:590:THR:OG1	2.18	0.60
1:A:147:ARG:HA	1:A:150:ILE:HD12	1.83	0.60
1:A:315:PHE:HE1	1:A:415:TYR:HB3	1.66	0.60
1:A:603:ARG:O	1:A:603:ARG:CG	2.45	0.60
1:A:1250:ASP:O	1:A:1253:ALA:N	2.32	0.60
1:A:221:MET:CE	1:A:221:MET:CG	2.79	0.60
1:A:13:PRO:O	1:A:197:THR:HB	2.00	0.60
1:A:441:GLN:N	1:A:441:GLN:OE1	2.35	0.60
1:A:603:ARG:HD2	1:A:667:TYR:CE2	2.37	0.60
1:A:1032:SER:HB3	1:A:1055:ILE:HB	1.84	0.60
1:A:1354:PRO:HB2	1:A:1355:GLU:OE2	2.02	0.60
1:A:616:ILE:HG21	1:A:621:ALA:HB2	1.83	0.60
1:A:1228:THR:CG2	1:A:1228:THR:O	2.49	0.60
1:A:9:LEU:O	1:A:396:GLU:HG2	2.01	0.60
1:A:1216:ASN:HD22	1:A:1216:ASN:C	2.05	0.59
1:A:234:LEU:CD1	1:A:234:LEU:C	2.70	0.59
1:A:239:TRP:HH2	1:A:635:ARG:HH12	1.50	0.59
1:A:567:LEU:HD21	1:A:615:PHE:CE2	2.36	0.59
1:A:450:PHE:CD2	1:A:645:ALA:HB3	2.37	0.59
1:A:1200:THR:HG21	1:A:1225:LEU:HB2	1.83	0.59
1:A:1325:LEU:HB3	1:A:1344:ILE:HG12	1.83	0.59
1:A:234:LEU:HD12	1:A:234:LEU:C	2.23	0.59
1:A:484:LEU:CB	1:A:839:VAL:CG1	2.72	0.59
1:A:6:ILE:CD1	1:A:371:VAL:HG21	2.33	0.59
1:A:9:LEU:HD21	1:A:392:VAL:HG11	1.84	0.59
1:A:1382:ARG:HG3	1:A:1385:VAL:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:HIS:HE1	1:A:1054:ASP:OD2	1.85	0.59
1:A:152:ARG:HH12	1:A:168:PHE:H	1.50	0.59
1:A:501:GLN:HE22	1:A:1035:LEU:CA	2.16	0.59
1:A:9:LEU:HD12	1:A:360:ASP:HB3	1.85	0.59
1:A:1263:HIS:CE1	1:A:1298:GLU:N	2.71	0.58
1:A:1412:VAL:HG11	1:A:1416:VAL:CG2	2.32	0.58
1:A:1438:LEU:HB3	1:A:1439:PRO:HD3	1.85	0.58
1:A:1138:ILE:HG22	1:A:1139:MET:H	1.68	0.58
1:A:1442:ILE:HD11	1:A:1449:LEU:HD13	1.85	0.58
1:A:261:THR:HB	1:A:262:PRO:CD	2.28	0.58
1:A:603:ARG:HD2	1:A:667:TYR:CD2	2.38	0.58
1:A:1137:CYS:SG	3:A:2072:F3S:S1	3.01	0.58
1:A:316:HIS:O	1:A:320:SER:CB	2.52	0.58
1:A:642:VAL:HG13	1:A:664:ILE:HG23	1.86	0.58
1:A:518:LEU:HD13	1:A:712:PHE:CE2	2.38	0.58
1:A:941:ALA:HB1	1:A:961:LYS:HD2	1.85	0.58
1:A:383:ARG:HH12	1:A:1380:GLY:HA2	0.77	0.58
1:A:445:GLN:OE1	1:A:772:ALA:HA	2.04	0.58
1:A:591:VAL:HG22	1:A:598:LEU:HD11	1.86	0.58
1:A:445:GLN:CG	1:A:777:ALA:HB1	2.29	0.58
1:A:37:ASP:OD1	1:A:119:ILE:HG22	2.04	0.58
1:A:484:LEU:HD13	1:A:839:VAL:CG1	2.33	0.58
1:A:516:MET:HG2	1:A:721:SER:HA	1.85	0.58
1:A:511:ARG:HD3	1:A:1423:GLY:HA3	1.86	0.57
1:A:450:PHE:CZ	1:A:615:PHE:CZ	2.92	0.57
1:A:1315:ALA:O	1:A:1317:ASN:N	2.37	0.57
1:A:358:LYS:CD	1:A:377:ASP:HB2	2.34	0.57
1:A:993:ARG:NH1	1:A:993:ARG:CG	2.60	0.57
1:A:1154:THR:HG21	1:A:1159:LEU:HD12	1.87	0.57
1:A:602:ASP:O	1:A:608:ILE:CD1	2.53	0.57
1:A:1451:ARG:HH12	1:A:1491:PHE:H	1.53	0.57
1:A:1461:LEU:CD2	1:A:1491:PHE:CZ	2.87	0.57
1:A:243:ARG:HG2	1:A:636:LEU:HD21	1.87	0.57
1:A:450:PHE:CE2	1:A:645:ALA:HB3	2.40	0.57
1:A:211:THR:HG22	1:A:212:MET:HE2	1.86	0.57
1:A:3:VAL:HG21	1:A:227:ASN:HB3	1.87	0.57
1:A:230:ILE:HA	1:A:327:ASP:O	2.05	0.57
1:A:953:THR:O	1:A:956:TYR:HB3	2.04	0.57
1:A:492:TYR:HE2	1:A:656:LEU:CD1	2.15	0.57
1:A:1376:ASN:HD21	1:A:1472:THR:CG2	2.15	0.57
1:A:875:MET:SD	1:A:1132:MET:CE	2.89	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:PRO:HD2	5:A:2116:HOH:O	2.04	0.56
1:A:314:ASP:OD2	1:A:415:TYR:CD1	2.57	0.56
1:A:483:VAL:HG23	1:A:494:TYR:HE2	1.69	0.56
1:A:995:LYS:HD2	1:A:1498:SER:OG	2.04	0.56
1:A:289:LEU:HD22	1:A:404:GLN:HE22	1.70	0.56
1:A:686:MET:HE3	1:A:694:ILE:HB	1.85	0.56
1:A:71:ARG:HG3	1:A:139:CYS:O	2.06	0.56
1:A:875:MET:CE	1:A:888:LEU:CD1	2.84	0.56
1:A:1279:THR:HG22	1:A:1282:THR:HB	1.87	0.56
1:A:75:GLY:O	1:A:130:GLN:HA	2.05	0.56
1:A:73:GLY:CA	1:A:170:CYS:HA	2.33	0.56
1:A:519:ALA:O	1:A:520:MET:CG	2.54	0.56
1:A:1442:ILE:HD12	1:A:1449:LEU:HD22	1.87	0.56
1:A:264:VAL:HG22	1:A:273:ASN:OD1	2.05	0.56
1:A:559:LEU:O	1:A:561:VAL:HG23	2.05	0.56
1:A:560:GLN:C	1:A:561:VAL:HG23	2.26	0.56
1:A:1420:VAL:O	1:A:1420:VAL:CG1	2.48	0.56
1:A:445:GLN:OE1	1:A:776:MET:O	2.24	0.56
1:A:501:GLN:NE2	1:A:1035:LEU:CA	2.68	0.56
1:A:56:ALA:O	1:A:60:ASN:HB2	2.05	0.56
1:A:627:HIS:O	1:A:631:ARG:HG3	2.06	0.56
1:A:1228:THR:HG21	1:A:1232:ARG:HH21	1.71	0.56
1:A:281:LEU:HD12	1:A:291:ALA:HB1	1.88	0.56
1:A:309:TYR:O	1:A:312:ILE:HG22	2.06	0.56
1:A:448:ALA:HB3	1:A:772:ALA:HB2	1.88	0.56
1:A:559:LEU:O	1:A:561:VAL:CG2	2.54	0.56
1:A:971:ALA:CB	1:A:1065:THR:HG23	2.35	0.56
1:A:1279:THR:HG22	1:A:1282:THR:CB	2.36	0.56
1:A:472:THR:CG2	1:A:473:PHE:N	2.69	0.56
1:A:805:LEU:HB2	1:A:830:TYR:CD1	2.41	0.56
1:A:1129:SER:HA	1:A:1132:MET:HE3	1.87	0.55
1:A:1251:ILE:HD13	1:A:1271:TYR:CZ	2.41	0.55
1:A:449:ALA:HA	1:A:768:PHE:O	2.07	0.55
1:A:501:GLN:NE2	1:A:1035:LEU:HB3	2.17	0.55
1:A:582:ASN:O	1:A:586:THR:OG1	2.14	0.55
1:A:219:GLN:CG	1:A:219:GLN:O	2.52	0.55
1:A:316:HIS:O	1:A:320:SER:HB3	2.07	0.55
1:A:1085:THR:HG22	1:A:1086:GLU:N	2.20	0.55
1:A:827:TYR:CE1	1:A:1176:PHE:CD1	2.95	0.55
1:A:1371:GLY:C	1:A:1372:ASN:ND2	2.60	0.55
1:A:875:MET:CE	1:A:888:LEU:HD11	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1294:ASN:HB3	1:A:1338:ASN:ND2	2.22	0.55
1:A:768:PHE:CE1	1:A:783:PHE:HZ	2.24	0.55
1:A:84:SER:O	1:A:88:VAL:HG23	2.07	0.55
1:A:750:THR:CG2	1:A:1039:ILE:HG21	2.33	0.55
1:A:399:ILE:CG2	1:A:404:GLN:HG2	2.35	0.55
1:A:679:ASP:OD1	1:A:679:ASP:C	2.45	0.55
1:A:827:TYR:HE1	1:A:1176:PHE:CD1	2.25	0.55
1:A:570:LEU:HB2	1:A:613:GLN:HB2	1.88	0.55
1:A:228:GLY:O	1:A:229:GLU:HG2	2.06	0.54
1:A:600:LEU:HD21	1:A:625:VAL:HG11	1.87	0.54
1:A:663:ALA:C	1:A:664:ILE:HG12	2.27	0.54
1:A:827:TYR:CE1	1:A:1176:PHE:HD1	2.25	0.54
1:A:450:PHE:HZ	1:A:608:ILE:CD1	2.20	0.54
1:A:499:PHE:CG	1:A:973:PRO:HB3	2.42	0.54
1:A:1138:ILE:CG2	1:A:1139:MET:H	2.21	0.54
1:A:972:LYS:HD3	1:A:1068:SER:OG	2.07	0.54
1:A:1363:THR:HG22	1:A:1385:VAL:HG21	1.89	0.54
1:A:314:ASP:HB2	1:A:415:TYR:HB2	1.87	0.54
1:A:484:LEU:CB	1:A:839:VAL:HG12	2.35	0.54
1:A:1234:TRP:CZ3	1:A:1235:LEU:HD13	2.43	0.54
1:A:1292:TYR:CE1	1:A:1297:PHE:HD1	2.26	0.54
1:A:311:GLU:HB2	1:A:409:ALA:HB1	1.90	0.54
1:A:559:LEU:HG	1:A:560:GLN:CA	2.37	0.54
1:A:861:GLU:OE1	1:A:1193:LEU:N	2.40	0.54
1:A:559:LEU:CG	1:A:560:GLN:O	2.56	0.53
1:A:565:SER:OG	1:A:567:LEU:HB2	2.09	0.53
1:A:794:TYR:CG	1:A:795:HIS:N	2.75	0.53
1:A:645:ALA:HB2	1:A:667:TYR:CZ	2.42	0.53
1:A:916:ASP:OD2	1:A:924:PRO:HD2	2.09	0.53
1:A:475:MET:HE1	1:A:1129:SER:OG	2.09	0.53
1:A:1442:ILE:HD12	1:A:1449:LEU:HD13	1.90	0.53
1:A:243:ARG:NH1	1:A:528:LEU:HD22	2.24	0.53
1:A:278:LEU:O	1:A:282:VAL:HG23	2.08	0.53
1:A:769:HIS:CD2	1:A:769:HIS:C	2.81	0.53
1:A:481:LEU:O	1:A:483:VAL:N	2.41	0.53
1:A:1089:ARG:NH2	1:A:1225:LEU:CD2	2.72	0.53
1:A:263:ILE:CD1	1:A:280:LEU:HD22	2.35	0.53
1:A:1081:GLU:O	1:A:1085:THR:HB	2.08	0.53
1:A:1399:ASP:OD1	1:A:1417:GLY:HA3	2.07	0.53
1:A:152:ARG:HG3	1:A:153:SER:N	2.23	0.53
1:A:157:LYS:NZ	1:A:261:THR:HB	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:HD12	1:A:225:GLY:O	2.08	0.53
1:A:478:ASP:OD2	1:A:1141:ARG:NH2	2.39	0.53
1:A:704:ARG:O	1:A:707:VAL:HB	2.09	0.53
1:A:1137:CYS:SG	3:A:2072:F3S:S3	3.07	0.53
1:A:173:ILE:HD13	1:A:175:TYR:HE1	1.74	0.53
1:A:524:LYS:HB3	1:A:637:LYS:O	2.09	0.53
1:A:1142:VAL:CG1	1:A:1147:ASN:HB2	2.39	0.52
1:A:1316:PHE:CE2	1:A:1336:GLY:HA3	2.44	0.52
1:A:1263:HIS:CE1	1:A:1297:PHE:CA	2.61	0.52
1:A:1354:PRO:HG2	1:A:1475:PRO:HG2	1.91	0.52
1:A:13:PRO:HB2	1:A:197:THR:OG1	2.08	0.52
1:A:1419:ASN:HD21	1:A:1443:ASN:ND2	2.07	0.52
1:A:559:LEU:HD23	1:A:560:GLN:O	2.03	0.52
1:A:1021:ASP:O	1:A:1024:GLN:HB3	2.10	0.52
1:A:1105:ASP:OD1	1:A:1105:ASP:C	2.47	0.52
1:A:1338:ASN:OD1	1:A:1369:THR:HG23	2.10	0.52
1:A:635:ARG:CG	1:A:635:ARG:HH11	2.22	0.52
1:A:668:LEU:O	1:A:669:ALA:C	2.46	0.52
1:A:720:ILE:HD11	1:A:731:ILE:HD12	1.91	0.52
1:A:1371:GLY:C	1:A:1372:ASN:HD22	2.12	0.52
1:A:375:GLU:N	1:A:375:GLU:OE1	2.43	0.52
1:A:418:TRP:CD2	1:A:418:TRP:O	2.62	0.52
1:A:768:PHE:HE1	1:A:783:PHE:HZ	1.57	0.52
1:A:872:THR:O	1:A:1127:PHE:O	2.27	0.52
1:A:677:TRP:NE1	1:A:694:ILE:O	2.27	0.52
1:A:883:GLU:CD	1:A:1160:ARG:HD2	2.29	0.52
1:A:877:LEU:HG	1:A:877:LEU:O	2.09	0.52
1:A:1008:ASP:HB2	1:A:1366:TYR:HE1	1.75	0.52
1:A:1087:VAL:O	1:A:1088:HIS:C	2.47	0.52
1:A:42:ASP:OD2	1:A:208:SER:N	2.42	0.52
1:A:541:LEU:HD23	1:A:663:ALA:HB2	1.91	0.52
1:A:876:SER:HA	1:A:902:GLY:HA3	1.90	0.52
1:A:353:ARG:NH2	1:A:1329:ALA:O	2.43	0.52
1:A:383:ARG:HH12	1:A:1380:GLY:C	2.10	0.52
1:A:447:GLN:HB3	1:A:780:LEU:HD21	1.92	0.52
1:A:52:ARG:HD2	5:A:2076:HOH:O	2.09	0.52
1:A:648:TRP:H	1:A:652:HIS:HD2	1.56	0.52
1:A:696:LEU:N	1:A:697:PRO:CD	2.73	0.52
1:A:768:PHE:CD2	1:A:771:MET:CB	2.92	0.52
1:A:418:TRP:CZ3	1:A:422:GLN:HB3	2.45	0.52
1:A:232:THR:O	1:A:233:LEU:C	2.48	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:978:GLN:O	4:A:2073:AKG:H41	2.10	0.51
1:A:329:PRO:HB3	1:A:349:LEU:CB	2.40	0.51
1:A:484:LEU:HD23	1:A:1211:LEU:HD13	1.91	0.51
1:A:204:HIS:CG	1:A:219:GLN:O	2.63	0.51
1:A:473:PHE:CG	1:A:474:CYS:N	2.77	0.51
1:A:1130:ILE:CD1	1:A:1130:ILE:N	2.69	0.51
1:A:548:GLU:CD	1:A:603:ARG:HH22	2.14	0.51
1:A:686:MET:O	1:A:692:ASP:CB	2.52	0.51
1:A:1317:ASN:OD1	1:A:1321:MET:HB3	2.10	0.51
1:A:1402:CYS:O	1:A:1403:GLU:C	2.48	0.51
1:A:872:THR:HB	1:A:892:MET:HG3	1.92	0.51
1:A:1142:VAL:HG13	1:A:1145:THR:HB	1.90	0.51
1:A:1497:PRO:O	1:A:1498:SER:HB2	2.11	0.51
1:A:179:VAL:HB	1:A:183:ILE:CG2	2.39	0.51
1:A:2:GLY:CA	1:A:28:MET:CE	2.89	0.51
1:A:744:TYR:CD2	1:A:744:TYR:O	2.63	0.51
1:A:1461:LEU:HD11	1:A:1465:ILE:HD11	1.93	0.51
1:A:275:ASP:O	1:A:276:SER:C	2.49	0.51
1:A:768:PHE:CE2	1:A:771:MET:CB	2.94	0.51
1:A:114:SER:OG	1:A:125:GLN:OE1	2.28	0.51
1:A:794:TYR:CD2	1:A:795:HIS:N	2.79	0.51
1:A:1173:PHE:O	1:A:1177:ILE:HG12	2.11	0.51
1:A:204:HIS:CE1	1:A:219:GLN:HB3	2.45	0.51
1:A:124:ASN:ND2	1:A:213:PRO:O	2.44	0.51
1:A:608:ILE:HG21	1:A:615:PHE:HZ	1.76	0.51
1:A:799:PRO:HB3	1:A:1138:ILE:HG23	1.92	0.51
1:A:798:SER:H	1:A:801:MET:HE2	1.76	0.51
1:A:1228:THR:CG2	1:A:1232:ARG:HH21	2.24	0.51
1:A:401:LYS:HE3	1:A:402:ASN:OD1	2.10	0.51
1:A:703:TYR:O	1:A:707:VAL:HG23	2.11	0.51
1:A:1354:PRO:HB3	5:A:2110:HOH:O	2.10	0.50
1:A:403:TYR:O	1:A:406:LYS:N	2.43	0.50
1:A:514:LEU:HD13	1:A:514:LEU:C	2.31	0.50
1:A:540:LYS:N	5:A:2080:HOH:O	2.44	0.50
1:A:843:ARG:HG3	1:A:1112:TRP:CH2	2.46	0.50
1:A:1250:ASP:O	1:A:1251:ILE:C	2.49	0.50
1:A:77:VAL:HG12	1:A:79:LEU:HG	1.93	0.50
1:A:877:LEU:HD23	1:A:988:ILE:HD13	1.93	0.50
1:A:874:GLY:CA	1:A:900:ASN:HB3	2.41	0.50
1:A:1119:LEU:HD21	1:A:1196:ILE:HG21	1.91	0.50
1:A:1138:ILE:O	3:A:2072:F3S:S1	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:HD22	1:A:389:MET:CE	2.41	0.50
1:A:480:PRO:HB3	1:A:840:THR:HA	1.93	0.50
1:A:1119:LEU:HD13	1:A:1203:LEU:HD21	1.94	0.50
1:A:17:LEU:HD11	1:A:201:ALA:HB2	1.91	0.50
1:A:567:LEU:HD21	1:A:615:PHE:HE2	1.77	0.50
1:A:744:TYR:CD2	1:A:744:TYR:C	2.84	0.50
1:A:1080:TRP:CZ3	1:A:1120:MET:CE	2.94	0.50
1:A:1065:THR:HB	1:A:1067:ALA:H	1.77	0.50
1:A:1139:MET:O	1:A:1140:ALA:C	2.48	0.50
1:A:1185:LEU:O	1:A:1189:GLY:N	2.39	0.50
1:A:452:TYR:CE1	1:A:668:LEU:HD13	2.47	0.50
1:A:875:MET:HE3	1:A:888:LEU:CD1	2.42	0.50
1:A:898:LYS:HE2	1:A:942:ILE:HD11	1.93	0.50
1:A:1214:THR:HG22	1:A:1215:GLN:H	1.77	0.49
1:A:271:SER:O	1:A:272:TYR:C	2.50	0.49
1:A:1337:MET:CE	1:A:1365:LEU:CD2	2.85	0.49
1:A:207:PHE:CD2	1:A:207:PHE:C	2.84	0.49
1:A:971:ALA:HB3	1:A:1065:THR:CG2	2.42	0.49
1:A:740:GLU:OE1	1:A:740:GLU:N	2.44	0.49
1:A:773:PHE:HB2	1:A:774:PRO:HD2	1.95	0.49
1:A:797:ASN:HA	1:A:801:MET:HE2	1.93	0.49
1:A:1418:ARG:HA	1:A:1441:LYS:HB3	1.94	0.49
1:A:4:GLY:HA3	1:A:203:TYR:CZ	2.48	0.49
1:A:212:MET:HE2	1:A:1094:ASN:HA	1.93	0.49
1:A:338:LYS:O	1:A:394:LEU:CD2	2.58	0.49
1:A:402:ASN:O	1:A:403:TYR:C	2.50	0.49
1:A:559:LEU:HD22	1:A:596:GLU:N	2.27	0.49
1:A:1024:GLN:HA	1:A:1283:ARG:HH21	1.78	0.49
1:A:1404:TYR:N	1:A:1404:TYR:CD1	2.80	0.49
1:A:290:GLU:O	1:A:294:ILE:HD12	2.13	0.49
1:A:447:GLN:O	1:A:452:TYR:HB2	2.13	0.49
1:A:608:ILE:HG21	1:A:615:PHE:CZ	2.47	0.49
1:A:1325:LEU:HD21	1:A:1328:GLU:C	2.33	0.49
1:A:1401:CYS:O	1:A:1402:CYS:HB2	2.12	0.49
1:A:1419:ASN:ND2	1:A:1443:ASN:ND2	2.60	0.49
1:A:178:MET:HG3	1:A:213:PRO:HB2	1.94	0.49
1:A:342:ALA:CB	1:A:364:LEU:CD2	2.91	0.49
1:A:696:LEU:N	1:A:697:PRO:HD2	2.28	0.49
1:A:616:ILE:HG22	1:A:621:ALA:HB2	1.94	0.49
1:A:657:VAL:CG1	1:A:723:LEU:HD11	2.35	0.49
1:A:445:GLN:CD	1:A:777:ALA:CB	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:LEU:HD22	1:A:833:TYR:HE1	1.77	0.49
1:A:315:PHE:CD2	1:A:319:TYR:CE1	2.99	0.49
1:A:560:GLN:C	1:A:561:VAL:CG2	2.81	0.49
1:A:768:PHE:HE1	1:A:783:PHE:CZ	2.31	0.49
1:A:954:PRO:O	1:A:958:MET:HG2	2.13	0.49
1:A:312:ILE:C	1:A:312:ILE:HD13	2.33	0.48
1:A:239:TRP:CD1	1:A:324:GLU:OE2	2.66	0.48
1:A:414:PRO:O	1:A:417:GLU:N	2.46	0.48
1:A:587:ALA:O	1:A:591:VAL:HG23	2.13	0.48
1:A:490:LEU:N	1:A:490:LEU:HD23	2.28	0.48
1:A:911:TYR:O	1:A:912:LEU:HD23	2.14	0.48
1:A:671:GLU:OE1	1:A:674:ARG:NH1	2.42	0.48
1:A:1008:ASP:HB2	1:A:1366:TYR:CE1	2.48	0.48
1:A:200:PHE:CD1	1:A:201:ALA:N	2.81	0.48
1:A:541:LEU:HD21	1:A:546:VAL:HG11	1.95	0.48
1:A:874:GLY:HA2	1:A:900:ASN:HB3	1.94	0.48
1:A:1375:ALA:O	1:A:1394:ILE:HA	2.12	0.48
1:A:1438:LEU:HA	1:A:1441:LYS:HD2	1.93	0.48
1:A:243:ARG:HH11	1:A:528:LEU:CB	2.19	0.48
1:A:445:GLN:OE1	1:A:777:ALA:CB	2.60	0.48
1:A:408:GLN:O	1:A:408:GLN:CD	2.52	0.48
1:A:1420:VAL:HB	1:A:1442:ILE:HA	1.96	0.48
1:A:148:LEU:O	1:A:151:ALA:N	2.46	0.48
1:A:157:LYS:HZ3	1:A:261:THR:HB	1.78	0.48
1:A:394:LEU:C	1:A:396:GLU:H	2.16	0.48
1:A:481:LEU:O	1:A:482:ALA:C	2.51	0.48
1:A:759:ALA:O	1:A:762:ALA:HB3	2.13	0.48
1:A:284:THR:OG1	1:A:529:LEU:HD22	2.13	0.48
1:A:290:GLU:CD	1:A:408:GLN:HG3	2.33	0.48
1:A:507:ILE:O	1:A:716:SER:HB2	2.13	0.48
1:A:893:ASN:HD22	1:A:937:THR:HG23	1.76	0.48
1:A:1065:THR:HG21	1:A:1068:SER:HG	1.76	0.48
1:A:145:ASP:OD2	1:A:169:SER:HB2	2.13	0.48
1:A:685:LEU:HD12	1:A:690:ARG:CD	2.42	0.48
1:A:756:LEU:HD12	1:A:1214:THR:OG1	2.13	0.48
1:A:1316:PHE:CD2	1:A:1336:GLY:HA3	2.49	0.48
1:A:342:ALA:HB3	1:A:364:LEU:CD2	2.44	0.48
1:A:369:GLY:HA3	1:A:1308:ALA:HB3	1.92	0.48
1:A:406:LYS:HA	1:A:409:ALA:CB	2.44	0.48
1:A:492:TYR:CE2	1:A:656:LEU:CD1	2.97	0.48
1:A:954:PRO:HG3	1:A:1316:PHE:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:PHE:CE1	1:A:415:TYR:HB3	2.47	0.47
1:A:570:LEU:HB2	1:A:613:GLN:CB	2.43	0.47
1:A:649:SER:O	1:A:653:PHE:HD2	1.97	0.47
1:A:875:MET:HE3	1:A:888:LEU:HD11	1.95	0.47
1:A:484:LEU:HD23	1:A:1211:LEU:CD1	2.44	0.47
1:A:887:THR:O	1:A:888:LEU:C	2.50	0.47
1:A:1000:LEU:HA	1:A:1000:LEU:HD23	1.59	0.47
1:A:149:TYR:CG	1:A:283:ARG:HG3	2.49	0.47
1:A:801:MET:HE3	1:A:802:SER:HB3	1.95	0.47
1:A:1017:GLN:HG3	1:A:1311:GLN:HG3	1.97	0.47
1:A:3:VAL:CG2	1:A:227:ASN:HB3	2.45	0.47
1:A:891:ALA:HB1	1:A:1171:VAL:HG23	1.96	0.47
1:A:1363:THR:HG23	1:A:1385:VAL:HG21	1.97	0.47
1:A:794:TYR:CE1	1:A:837:ARG:HB3	2.50	0.47
1:A:1030:GLN:HG2	1:A:1240:VAL:HG13	1.97	0.47
1:A:97:VAL:HG11	1:A:133:VAL:HG21	1.95	0.47
1:A:444:LEU:O	1:A:445:GLN:CG	2.47	0.47
1:A:602:ASP:C	1:A:604:PRO:HD3	2.35	0.47
1:A:625:VAL:O	1:A:629:LEU:HB2	2.14	0.47
1:A:801:MET:CE	1:A:802:SER:HB3	2.44	0.47
1:A:1288:ILE:HD12	1:A:1321:MET:CE	2.44	0.47
1:A:686:MET:C	1:A:692:ASP:HB2	2.34	0.47
1:A:135:CYS:HB3	1:A:139:CYS:HB2	1.97	0.47
1:A:561:VAL:HG12	1:A:561:VAL:O	2.15	0.47
1:A:640:LEU:N	1:A:640:LEU:HD13	2.30	0.47
1:A:92:TYR:O	1:A:93:VAL:C	2.52	0.47
1:A:1264:GLN:NE2	1:A:1298:GLU:OE1	2.47	0.47
1:A:239:TRP:NE1	1:A:728:GLY:HA3	2.29	0.47
1:A:223:LEU:HD12	1:A:335:SER:O	2.15	0.47
1:A:403:TYR:CD1	1:A:403:TYR:N	2.60	0.47
1:A:486:HIS:CE1	1:A:838:PRO:HB3	2.50	0.47
1:A:1198:GLY:C	1:A:1200:THR:H	2.19	0.47
1:A:2:GLY:CA	1:A:28:MET:HE2	2.44	0.47
1:A:460:VAL:CG1	1:A:464:MET:HE1	2.43	0.47
1:A:627:HIS:CE1	1:A:730:GLN:HE22	2.33	0.47
1:A:173:ILE:HD13	1:A:175:TYR:CE1	2.50	0.46
1:A:312:ILE:HG21	1:A:405:ILE:HD13	1.96	0.46
1:A:445:GLN:CG	1:A:777:ALA:CB	2.89	0.46
1:A:445:GLN:CD	1:A:777:ALA:HB2	2.36	0.46
1:A:910:ARG:C	1:A:912:LEU:H	2.18	0.46
1:A:1119:LEU:O	1:A:1198:GLY:CA	2.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:LEU:HG	1:A:365:GLY:N	2.31	0.46
1:A:1272:ARG:NH1	1:A:1306:GLN:HG2	2.30	0.46
1:A:1306:GLN:HA	1:A:1326:GLN:O	2.16	0.46
1:A:477:ASP:OD1	1:A:479:THR:HG23	2.15	0.46
1:A:514:LEU:CD1	1:A:514:LEU:C	2.83	0.46
1:A:548:GLU:OE2	1:A:603:ARG:NH2	2.49	0.46
1:A:1118:ALA:O	1:A:1197:ILE:HA	2.16	0.46
1:A:212:MET:CE	1:A:1094:ASN:HA	2.46	0.46
1:A:221:MET:HE1	1:A:271:SER:HB3	1.97	0.46
1:A:364:LEU:HG	1:A:365:GLY:H	1.80	0.46
1:A:562:ALA:CB	1:A:590:THR:HG21	2.46	0.46
1:A:645:ALA:HB1	1:A:668:LEU:HD12	1.97	0.46
1:A:831:ARG:O	1:A:834:LEU:HB2	2.15	0.46
1:A:210:ASN:HB2	1:A:1094:ASN:OD1	2.15	0.46
1:A:349:LEU:O	1:A:350:ARG:HD2	2.15	0.46
1:A:1228:THR:HG23	1:A:1232:ARG:HE	1.80	0.46
1:A:140:ALA:O	1:A:141:GLY:C	2.53	0.46
1:A:414:PRO:HB2	1:A:418:TRP:CD1	2.50	0.46
1:A:514:LEU:HD13	1:A:515:VAL:N	2.30	0.46
1:A:349:LEU:O	1:A:350:ARG:NH1	2.44	0.46
1:A:377:ASP:C	1:A:377:ASP:OD1	2.53	0.46
1:A:342:ALA:O	1:A:389:MET:HA	2.15	0.46
1:A:513:ASN:HA	1:A:516:MET:CE	2.46	0.46
1:A:516:MET:HE3	1:A:516:MET:HB2	1.91	0.46
1:A:1021:ASP:OD2	1:A:1335:LYS:NZ	2.43	0.46
1:A:1383:PHE:O	1:A:1384:ALA:HB3	2.15	0.46
1:A:418:TRP:HE3	1:A:418:TRP:O	1.92	0.46
1:A:1004:PRO:HB2	1:A:1005:PRO:HD3	1.96	0.46
1:A:501:GLN:NE2	1:A:1035:LEU:CB	2.77	0.46
1:A:1096:LEU:O	1:A:1099:ARG:HB2	2.16	0.46
1:A:232:THR:CB	1:A:236:ASN:HD21	2.29	0.46
1:A:342:ALA:HB3	1:A:364:LEU:HD22	1.97	0.46
1:A:867:VAL:CG1	1:A:895:LEU:CB	2.89	0.46
1:A:809:VAL:HG12	1:A:1169:GLN:O	2.12	0.45
1:A:1403:GLU:HG3	1:A:1422:ALA:HB3	1.98	0.45
1:A:289:LEU:HB3	1:A:389:MET:CE	2.46	0.45
1:A:1256:ASP:O	1:A:1259:GLU:HG2	2.15	0.45
1:A:1355:GLU:HG3	1:A:1395:GLU:OE1	2.16	0.45
1:A:1130:ILE:HA	1:A:1133:ILE:HG13	1.98	0.45
1:A:1474:SER:HA	1:A:1475:PRO:HD3	1.69	0.45
1:A:1488:LEU:HD23	1:A:1488:LEU:HA	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ILE:O	1:A:422:GLN:HG2	2.16	0.45
1:A:843:ARG:HG3	1:A:1112:TRP:CZ3	2.52	0.45
1:A:113:ASN:OD1	1:A:115:ASP:HB2	2.15	0.45
1:A:698:THR:O	1:A:702:ASN:HB2	2.17	0.45
1:A:1132:MET:HG2	1:A:1152:VAL:HG11	1.97	0.45
1:A:1432:LEU:HB2	1:A:1491:PHE:CD2	2.52	0.45
1:A:832:GLN:HG2	5:A:2092:HOH:O	2.17	0.45
1:A:324:GLU:HG3	1:A:324:GLU:H	1.25	0.45
1:A:418:TRP:HZ3	1:A:422:GLN:HB3	1.79	0.45
1:A:12:LYS:HA	1:A:12:LYS:HD3	1.67	0.45
1:A:186:GLU:HA	1:A:186:GLU:OE1	2.17	0.45
1:A:561:VAL:HG11	1:A:599:VAL:HG23	1.97	0.45
1:A:567:LEU:HA	1:A:567:LEU:HD23	1.61	0.45
1:A:825:ASP:O	1:A:828:GLU:HB3	2.17	0.45
1:A:967:MET:HB2	1:A:1034:LYS:O	2.17	0.45
1:A:711:LEU:O	1:A:712:PHE:C	2.55	0.45
1:A:135:CYS:CB	1:A:139:CYS:HB2	2.46	0.45
1:A:281:LEU:O	1:A:286:ARG:HG3	2.17	0.45
1:A:524:LYS:CB	1:A:637:LYS:O	2.64	0.45
1:A:1273:LEU:HD21	1:A:1305:PHE:CD2	2.52	0.45
1:A:239:TRP:HE1	1:A:728:GLY:CA	2.28	0.45
1:A:462:VAL:HB	1:A:463:PRO:HD3	1.99	0.45
1:A:465:ALA:HB1	1:A:673:VAL:HG13	1.99	0.45
1:A:418:TRP:HB2	1:A:533:ALA:HB1	1.99	0.45
1:A:474:CYS:CB	1:A:1143:CYS:HB2	2.47	0.44
1:A:1354:PRO:CB	5:A:2110:HOH:O	2.64	0.44
1:A:152:ARG:HD3	1:A:222:ARG:NH1	2.32	0.44
1:A:269:SER:O	1:A:270:ASP:C	2.55	0.44
1:A:513:ASN:HA	1:A:516:MET:HE3	1.99	0.44
1:A:570:LEU:HG	1:A:613:GLN:CG	2.46	0.44
1:A:514:LEU:CD1	1:A:515:VAL:N	2.80	0.44
1:A:574:ASN:C	1:A:574:ASN:OD1	2.55	0.44
1:A:443:VAL:CG2	1:A:675:GLN:NE2	2.68	0.44
1:A:955:GLU:O	1:A:956:TYR:C	2.56	0.44
1:A:1110:THR:O	1:A:1113:ASP:N	2.50	0.44
1:A:1257:ILE:HD11	5:A:2081:HOH:O	2.16	0.44
1:A:1347:HIS:CG	1:A:1348:PRO:CD	2.80	0.44
1:A:17:LEU:CD1	1:A:201:ALA:HB2	2.47	0.44
1:A:296:VAL:N	1:A:297:PRO:CD	2.79	0.44
1:A:53:GLU:O	1:A:56:ALA:HB3	2.17	0.44
1:A:910:ARG:O	1:A:939:ASN:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:LEU:HB3	1:A:1226:PRO:HD2	1.99	0.44
1:A:546:VAL:HB	1:A:550:GLU:HB2	2.00	0.44
1:A:686:MET:HE1	1:A:694:ILE:O	2.17	0.44
1:A:90:ARG:HG3	1:A:107:TRP:CZ2	2.53	0.44
1:A:90:ARG:O	1:A:90:ARG:HG2	2.17	0.44
1:A:1395:GLU:O	1:A:1414:GLY:HA3	2.17	0.44
1:A:547:ASN:N	1:A:550:GLU:HG3	2.32	0.44
1:A:663:ALA:C	1:A:664:ILE:CG1	2.86	0.44
1:A:757:THR:N	1:A:760:ASP:HB2	2.32	0.44
1:A:878:GLY:HA3	1:A:992:ARG:NH2	2.32	0.44
1:A:1315:ALA:O	1:A:1316:PHE:C	2.56	0.44
1:A:309:TYR:HB3	1:A:312:ILE:CG2	2.48	0.44
1:A:322:LEU:HD12	1:A:322:LEU:HA	1.70	0.44
1:A:501:GLN:HE21	1:A:1035:LEU:HA	1.81	0.44
1:A:1254:ASP:C	1:A:1256:ASP:N	2.65	0.44
1:A:207:PHE:HD2	1:A:207:PHE:C	2.21	0.44
1:A:443:VAL:O	1:A:447:GLN:HB2	2.18	0.44
1:A:532:LYS:C	1:A:534:GLU:H	2.21	0.44
1:A:860:VAL:HG21	1:A:1182:ARG:O	2.18	0.44
1:A:1021:ASP:HA	1:A:1279:THR:HG21	2.00	0.44
1:A:6:ILE:HD11	1:A:371:VAL:CG2	2.47	0.44
1:A:76:MET:HG2	1:A:174:VAL:O	2.18	0.44
1:A:1148:CYS:C	1:A:1150:VAL:H	2.21	0.43
1:A:9:LEU:CD2	1:A:392:VAL:HG13	2.47	0.43
1:A:486:HIS:HE1	1:A:838:PRO:HB3	1.83	0.43
1:A:796:MET:O	1:A:1109:LYS:NZ	2.48	0.43
1:A:1175:TYR:HA	1:A:1175:TYR:HD2	1.63	0.43
1:A:1309:ALA:HB3	1:A:1329:ALA:CB	2.48	0.43
1:A:146:ARG:O	1:A:149:TYR:HB3	2.18	0.43
1:A:2:GLY:O	1:A:204:HIS:HA	2.18	0.43
1:A:475:MET:CE	1:A:475:MET:CA	2.90	0.43
1:A:478:ASP:HB3	1:A:795:HIS:ND1	2.33	0.43
1:A:486:HIS:HD2	1:A:1212:SER:OG	2.01	0.43
1:A:629:LEU:HD23	1:A:635:ARG:HD2	2.01	0.43
1:A:554:ILE:HG21	1:A:641:ILE:HD11	1.99	0.43
1:A:693:ARG:C	1:A:694:ILE:HG12	2.38	0.43
1:A:1054:ASP:C	1:A:1055:ILE:HG13	2.38	0.43
1:A:15:HIS:O	1:A:15:HIS:CG	2.71	0.43
1:A:679:ASP:OD1	1:A:680:GLU:N	2.52	0.43
1:A:1325:LEU:CD2	1:A:1329:ALA:HB2	2.49	0.43
1:A:155:ILE:HG23	1:A:163:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:LEU:O	1:A:190:ASP:C	2.57	0.43
1:A:406:LYS:HA	1:A:409:ALA:HB3	2.00	0.43
1:A:475:MET:HE2	1:A:476:GLY:H	1.83	0.43
1:A:601:THR:HG23	1:A:643:ASP:OD2	2.19	0.43
1:A:1136:GLY:O	1:A:1150:VAL:HG11	2.18	0.43
1:A:832:GLN:HA	1:A:835:LYS:HG3	2.01	0.43
1:A:1419:ASN:HD22	1:A:1443:ASN:HB2	1.84	0.43
1:A:7:ALA:HB3	1:A:362:ILE:CG2	2.49	0.43
1:A:600:LEU:CD2	1:A:625:VAL:HG11	2.48	0.43
1:A:891:ALA:CB	1:A:1170:VAL:HG22	2.49	0.43
1:A:145:ASP:O	1:A:146:ARG:C	2.57	0.43
1:A:566:THR:HB	1:A:602:ASP:HA	2.01	0.43
1:A:659:TYR:CE2	1:A:746:PHE:HB3	2.54	0.43
1:A:965:ILE:HD13	1:A:1018:LEU:HD23	1.99	0.43
1:A:1409:VAL:HA	1:A:1428:LEU:O	2.18	0.43
1:A:332:LEU:O	1:A:342:ALA:HA	2.18	0.43
1:A:541:LEU:HD23	1:A:663:ALA:CB	2.48	0.43
1:A:727:HIS:O	1:A:728:GLY:C	2.56	0.43
1:A:768:PHE:CD2	1:A:771:MET:CG	2.92	0.43
1:A:848:PHE:HB3	1:A:1188:LEU:HD21	2.00	0.43
1:A:474:CYS:HB2	1:A:1143:CYS:HB2	2.01	0.42
1:A:315:PHE:O	1:A:319:TYR:CD1	2.72	0.42
1:A:636:LEU:HA	1:A:636:LEU:HD12	1.70	0.42
1:A:1065:THR:HG22	4:A:2073:AKG:O1	2.18	0.42
1:A:336:ASP:HB3	1:A:339:ILE:H	1.83	0.42
1:A:510:LEU:HD13	1:A:511:ARG:NH2	2.34	0.42
1:A:579:ALA:HB3	1:A:616:ILE:HD11	2.00	0.42
1:A:768:PHE:HD2	1:A:768:PHE:HA	1.79	0.42
1:A:912:LEU:HD23	1:A:912:LEU:HA	1.81	0.42
1:A:1005:PRO:HG2	1:A:1007:HIS:CE1	2.54	0.42
1:A:1146:ASN:C	1:A:1154:THR:HG23	2.39	0.42
1:A:1430:TYR:HE2	1:A:1493:GLN:OE1	2.00	0.42
1:A:323:GLN:HE21	1:A:528:LEU:HD22	1.85	0.42
1:A:1082:LEU:HD23	1:A:1082:LEU:HA	1.75	0.42
1:A:1080:TRP:CZ3	1:A:1120:MET:HE2	2.53	0.42
1:A:1275:ASN:C	1:A:1275:ASN:OD1	2.57	0.42
1:A:230:ILE:HG22	1:A:233:LEU:N	2.34	0.42
1:A:276:SER:O	1:A:279:GLU:HB2	2.19	0.42
1:A:315:PHE:HZ	1:A:412:LYS:O	2.02	0.42
1:A:314:ASP:CG	1:A:415:TYR:HD1	2.21	0.42
1:A:500:ALA:HB1	1:A:504:ASN:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:ARG:HD2	1:A:938:ALA:O	2.19	0.42
1:A:1110:THR:HG22	1:A:1113:ASP:H	1.85	0.42
1:A:1325:LEU:CB	1:A:1344:ILE:HG12	2.50	0.42
1:A:288:PRO:HB2	1:A:334:PHE:CD1	2.54	0.42
1:A:36:ALA:N	1:A:120:GLN:HE22	2.18	0.42
1:A:317:ASP:HB3	1:A:419:ILE:CD1	2.50	0.42
1:A:519:ALA:C	1:A:520:MET:HG2	2.40	0.42
1:A:809:VAL:HG12	1:A:1172:ASN:HB2	2.02	0.42
1:A:139:CYS:SG	1:A:143:GLU:HG3	2.59	0.42
1:A:401:LYS:O	1:A:404:GLN:HB3	2.19	0.42
1:A:445:GLN:HB3	1:A:772:ALA:CB	2.45	0.42
1:A:605:ASN:OD1	1:A:605:ASN:N	2.53	0.42
1:A:666:PRO:HB2	1:A:669:ALA:HB3	2.01	0.42
1:A:694:ILE:HG23	1:A:694:ILE:HD12	1.36	0.42
1:A:728:GLY:O	1:A:729:ALA:O	2.37	0.42
1:A:1451:ARG:NH1	1:A:1491:PHE:H	2.16	0.42
1:A:551:LEU:HA	1:A:551:LEU:HD12	1.79	0.42
1:A:561:VAL:HG13	1:A:597:ILE:HG22	2.01	0.42
1:A:1145:THR:HG22	1:A:1147:ASN:CG	2.40	0.42
1:A:1451:ARG:O	1:A:1452:ILE:C	2.58	0.42
1:A:474:CYS:SG	1:A:1143:CYS:HB2	2.60	0.42
1:A:1150:VAL:HG13	1:A:1152:VAL:HG23	2.01	0.42
1:A:1446:ILE:HG21	1:A:1446:ILE:HD12	1.84	0.42
1:A:770:GLY:C	1:A:771:MET:SD	2.98	0.42
1:A:97:VAL:HG11	1:A:133:VAL:CG2	2.50	0.42
1:A:1297:PHE:CZ	1:A:1299:GLY:HA3	2.55	0.41
1:A:1458:GLU:OE2	1:A:1488:LEU:HD11	2.20	0.41
1:A:193:ASN:HA	1:A:194:PRO:HD3	1.90	0.41
1:A:522:LEU:HA	1:A:522:LEU:HD23	1.83	0.41
1:A:499:PHE:CG	1:A:973:PRO:CB	3.02	0.41
1:A:350:ARG:HH11	1:A:350:ARG:HD2	1.59	0.41
1:A:421:ILE:CG2	1:A:421:ILE:O	2.68	0.41
1:A:453:THR:O	1:A:454:ALA:C	2.59	0.41
1:A:509:PRO:HB3	1:A:716:SER:HB3	2.01	0.41
1:A:53:GLU:O	1:A:56:ALA:CB	2.67	0.41
1:A:1070:LEU:O	1:A:1071:SER:C	2.58	0.41
1:A:1142:VAL:O	1:A:1142:VAL:HG13	2.16	0.41
1:A:1197:ILE:O	1:A:1232:ARG:NH2	2.52	0.41
1:A:299:ALA:HB2	1:A:346:ARG:NH2	2.35	0.41
1:A:399:ILE:HG22	1:A:404:GLN:CG	2.42	0.41
1:A:399:ILE:HG22	1:A:399:ILE:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1129:SER:O	1:A:1133:ILE:HG12	2.20	0.41
1:A:1173:PHE:CZ	1:A:1177:ILE:HG13	2.55	0.41
1:A:1481:LEU:O	1:A:1484:TRP:HB2	2.21	0.41
1:A:148:LEU:HD23	1:A:169:SER:CA	2.49	0.41
1:A:358:LYS:H	1:A:358:LYS:HG3	1.55	0.41
1:A:357:THR:OG1	1:A:361:TYR:CB	2.68	0.41
1:A:131:ILE:HG12	1:A:133:VAL:HG23	2.03	0.41
1:A:1385:VAL:O	1:A:1404:TYR:N	2.53	0.41
1:A:237:ILE:HG21	1:A:237:ILE:HD13	1.81	0.41
1:A:682:THR:O	1:A:683:GLN:C	2.59	0.41
1:A:7:ALA:HB3	1:A:362:ILE:HG23	2.01	0.41
1:A:957:LEU:HD13	1:A:1025:ILE:HG21	2.02	0.41
1:A:1484:TRP:O	1:A:1488:LEU:HB2	2.21	0.41
1:A:47:MET:O	1:A:201:ALA:HA	2.21	0.41
1:A:233:LEU:HA	1:A:233:LEU:HD12	1.81	0.41
1:A:566:THR:HB	1:A:601:THR:O	2.21	0.41
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.92	0.41
1:A:882:ARG:HB2	1:A:886:GLU:OE2	2.19	0.41
1:A:1053:ALA:O	1:A:1241:HIS:HD2	2.04	0.41
1:A:309:TYR:O	1:A:312:ILE:CG2	2.68	0.41
1:A:508:ASP:O	1:A:512:GLU:HB2	2.20	0.41
1:A:720:ILE:CD1	1:A:731:ILE:HD12	2.50	0.41
1:A:100:GLU:C	1:A:102:LEU:H	2.17	0.41
1:A:644:THR:O	1:A:666:PRO:HA	2.21	0.41
1:A:878:GLY:H	1:A:992:ARG:HH21	1.68	0.41
1:A:275:ASP:HB3	1:A:276:SER:H	1.76	0.41
1:A:1145:THR:CG2	1:A:1147:ASN:ND2	2.84	0.41
1:A:8:ASN:N	1:A:199:ASN:O	2.52	0.41
1:A:219:GLN:HG2	1:A:219:GLN:O	2.20	0.41
1:A:229:GLU:O	1:A:328:GLY:HA3	2.21	0.41
1:A:603:ARG:N	1:A:604:PRO:HD3	2.36	0.41
1:A:1258:GLN:O	1:A:1262:ASN:HB2	2.21	0.41
1:A:553:ALA:O	1:A:556:THR:HB	2.21	0.41
1:A:674:ARG:HH11	1:A:674:ARG:HD2	1.74	0.41
1:A:736:GLY:H	1:A:753:VAL:HG12	1.86	0.41
1:A:46:VAL:N	1:A:220:PRO:HG2	2.36	0.40
1:A:508:ASP:C	1:A:508:ASP:OD1	2.60	0.40
1:A:510:LEU:CB	1:A:511:ARG:HH21	2.04	0.40
1:A:559:LEU:HG	1:A:560:GLN:O	2.21	0.40
1:A:1382:ARG:O	1:A:1385:VAL:HG22	2.21	0.40
1:A:145:ASP:O	1:A:149:TYR:N	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:411:GLN:CG	1:A:412:LYS:H	2.35	0.40
1:A:1262:ASN:O	1:A:1264:GLN:N	2.54	0.40
1:A:1345:VAL:HA	1:A:1376:ASN:HD22	1.87	0.40
1:A:581:THR:HG22	1:A:585:LYS:HE3	1.97	0.40
1:A:618:PRO:O	1:A:622:VAL:HG23	2.21	0.40
1:A:722:LEU:O	1:A:723:LEU:C	2.60	0.40
1:A:903:GLU:HG2	1:A:946:ALA:CB	2.51	0.40
1:A:250:SER:C	1:A:252:TRP:H	2.25	0.40
1:A:386:PRO:HD3	1:A:1381:GLU:OE1	2.22	0.40
1:A:421:ILE:HG22	1:A:421:ILE:O	2.21	0.40
1:A:1216:ASN:C	1:A:1216:ASN:ND2	2.74	0.40
1:A:1269:LYS:HD3	1:A:1269:LYS:HA	1.85	0.40
1:A:1462:LYS:O	1:A:1466:THR:HB	2.22	0.40
1:A:916:ASP:N	1:A:916:ASP:OD1	2.53	0.40
1:A:94:GLU:O	1:A:95:GLU:C	2.59	0.40
1:A:996:PRO:O	1:A:997:GLY:C	2.58	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)
1:A:1158:ARG:CD	1:A:1324:HIS:CE1[4_475]	2.19	0.01

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	1467/1520 (96%)	1215 (83%)	196 (13%)	56 (4%)	3 7

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	ASP
1	A	101	LYS
1	A	403	TYR
1	A	414	PRO
1	A	415	TYR
1	A	482	ALA
1	A	560	GLN
1	A	614	SER
1	A	839	VAL
1	A	903	GLU
1	A	1254	ASP
1	A	1399	ASP
1	A	1403	GLU
1	A	1491	PHE
1	A	1498	SER
1	A	141	GLY
1	A	251	GLY
1	A	283	ARG
1	A	412	LYS
1	A	557	GLY
1	A	571	ASP
1	A	688	ASN
1	A	754	GLY
1	A	970	GLY
1	A	1200	THR
1	A	1209	VAL
1	A	1316	PHE
1	A	1442	ILE
1	A	1490	LYS
1	A	13	PRO
1	A	233	LEU
1	A	395	ALA
1	A	404	GLN
1	A	475	MET
1	A	561	VAL
1	A	773	PHE
1	A	1366	TYR
1	A	69	GLY
1	A	565	SER
1	A	613	GLN
1	A	1194	ASP
1	A	1489	GLY
1	A	39	ASP

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Mol	Chain	Res	Type
1	A	190	ASP
1	A	330	ALA
1	A	612	ASN
1	A	729	ALA
1	A	1311	GLN
1	A	694	ILE
1	A	790	PRO
1	A	1389	VAL
1	A	262	PRO
1	A	1420	VAL
1	A	973	PRO
1	A	399	ILE
1	A	1245	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	1200/1236 (97%)	976 (81%)	224 (19%)	1 4

All (224) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	VAL
1	A	8	ASN
1	A	16	THR
1	A	17	LEU
1	A	23	LYS
1	A	25	LEU
1	A	27	CYS
1	A	46	VAL
1	A	52	ARG
1	A	57	GLN
1	A	60	ASN
1	A	64	LEU
1	A	70	ASP

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Mol	Chain	Res	Type
1	A	76	MET
1	A	95	GLU
1	A	99	LEU
1	A	102	LEU
1	A	109	GLU
1	A	115	ASP
1	A	125	GLN
1	A	137	GLU
1	A	147	ARG
1	A	148	LEU
1	A	152	ARG
1	A	159	LEU
1	A	168	PHE
1	A	172	THR
1	A	173	ILE
1	A	182	ILE
1	A	183	ILE
1	A	191	LEU
1	A	199	ASN
1	A	207	PHE
1	A	211	THR
1	A	224	LEU
1	A	230	ILE
1	A	234	LEU
1	A	245	LYS
1	A	246	GLU
1	A	249	VAL
1	A	253	THR
1	A	254	LYS
1	A	260	LEU
1	A	263	ILE
1	A	264	VAL
1	A	266	GLN
1	A	274	LEU
1	A	278	LEU
1	A	286	ARG
1	A	298	GLU
1	A	312	ILE
1	A	322	LEU
1	A	324	GLU
1	A	356	ILE
1	A	358	LYS

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Mol	Chain	Res	Type
1	A	361	TYR
1	A	370	VAL
1	A	372	ASP
1	A	376	VAL
1	A	377	ASP
1	A	394	LEU
1	A	397	GLN
1	A	398	LYS
1	A	401	LYS
1	A	403	TYR
1	A	404	GLN
1	A	411	GLN
1	A	417	GLU
1	A	419	ILE
1	A	422	GLN
1	A	439	ASP
1	A	444	LEU
1	A	453	THR
1	A	457	VAL
1	A	466	SER
1	A	478	ASP
1	A	479	THR
1	A	481	LEU
1	A	483	VAL
1	A	503	THR
1	A	507	ILE
1	A	510	LEU
1	A	511	ARG
1	A	514	LEU
1	A	515	VAL
1	A	534	GLU
1	A	542	ARG
1	A	543	SER
1	A	550	GLU
1	A	558	GLN
1	A	559	LEU
1	A	560	GLN
1	A	570	LEU
1	A	580	LEU
1	A	590	THR
1	A	600	LEU
1	A	601	THR

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Mol	Chain	Res	Type
1	A	602	ASP
1	A	603	ARG
1	A	605	ASN
1	A	611	GLU
1	A	613	GLN
1	A	614	SER
1	A	616	ILE
1	A	635	ARG
1	A	640	LEU
1	A	649	SER
1	A	650	THR
1	A	664	ILE
1	A	668	LEU
1	A	678	LEU
1	A	679	ASP
1	A	684	LYS
1	A	693	ARG
1	A	701	LYS
1	A	704	ARG
1	A	705	GLN
1	A	706	SER
1	A	750	THR
1	A	753	VAL
1	A	757	THR
1	A	761	VAL
1	A	765	VAL
1	A	766	MET
1	A	769	HIS
1	A	771	MET
1	A	778	LYS
1	A	780	LEU
1	A	783	PHE
1	A	797	ASN
1	A	801	MET
1	A	809	VAL
1	A	824	TYR
1	A	827	TYR
1	A	829	LEU
1	A	834	LEU
1	A	836	ASP
1	A	843	ARG
1	A	855	ILE

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Mol	Chain	Res	Type
1	A	857	LEU
1	A	863	VAL
1	A	867	VAL
1	A	872	THR
1	A	877	LEU
1	A	899	SER
1	A	903	GLU
1	A	909	VAL
1	A	912	LEU
1	A	919	SER
1	A	953	THR
1	A	991	LEU
1	A	993	ARG
1	A	996	PRO
1	A	1013	GLU
1	A	1015	LEU
1	A	1039	ILE
1	A	1052	ASN
1	A	1062	ASP
1	A	1065	THR
1	A	1085	THR
1	A	1095	GLN
1	A	1100	VAL
1	A	1101	LEU
1	A	1105	ASP
1	A	1110	THR
1	A	1120	MET
1	A	1130	ILE
1	A	1132	MET
1	A	1142	VAL
1	A	1148	CYS
1	A	1150	VAL
1	A	1154	THR
1	A	1161	GLN
1	A	1175	TYR
1	A	1192	SER
1	A	1194	ASP
1	A	1200	THR
1	A	1208	ASP
1	A	1211	LEU
1	A	1214	THR
1	A	1215	GLN

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Mol	Chain	Res	Type
1	A	1216	ASN
1	A	1225	LEU
1	A	1228	THR
1	A	1235	LEU
1	A	1238	GLU
1	A	1240	VAL
1	A	1242	SER
1	A	1246	VAL
1	A	1254	ASP
1	A	1256	ASP
1	A	1257	ILE
1	A	1259	GLU
1	A	1274	VAL
1	A	1279	THR
1	A	1280	VAL
1	A	1311	GLN
1	A	1332	TYR
1	A	1363	THR
1	A	1366	TYR
1	A	1369	THR
1	A	1372	ASN
1	A	1373	LEU
1	A	1381	GLU
1	A	1385	VAL
1	A	1386	ARG
1	A	1389	VAL
1	A	1406	THR
1	A	1419	ASN
1	A	1425	THR
1	A	1432	LEU
1	A	1433	ASP
1	A	1442	ILE
1	A	1446	ILE
1	A	1447	ILE
1	A	1448	THR
1	A	1451	ARG
1	A	1453	THR
1	A	1456	LYS
1	A	1463	SER
1	A	1464	LEU
1	A	1488	LEU
1	A	1491	PHE

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Mol	Chain	Res	Type
1	A	1504	GLU

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

Mol	Chain	Res	Type
1	A	15	HIS
1	A	120	GLN
1	A	127	HIS
1	A	236	ASN
1	A	303	GLN
1	A	323	GLN
1	A	486	HIS
1	A	501	GLN
1	A	552	GLN
1	A	613	GLN
1	A	651	HIS
1	A	652	HIS
1	A	675	GLN
1	A	730	GLN
1	A	769	HIS
1	A	885	HIS
1	A	978	GLN
1	A	1023	HIS
1	A	1052	ASN
1	A	1216	ASN
1	A	1262	ASN
1	A	1263	HIS
1	A	1372	ASN
1	A	1376	ASN
1	A	1419	ASN
1	A	1493	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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
3	F3S	A	2072	1	0,9,9	0.00	-	-		
2	FMN	A	2070	-	31,33,33	1.39	4 (12%)	40,50,50	1.81	8 (20%)
4	AKG	A	2073	-	3,9,9	3.74	1 (33%)	4,11,11	1.43	1 (25%)

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	F3S	A	2072	1	-	-	0/3/3/3
2	FMN	A	2070	-	-	5/18/18/18	0/3/3/3
4	AKG	A	2073	-	-	2/3/9/9	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2073	AKG	O5-C2	6.45	1.32	1.22
2	A	2070	FMN	C4-N3	3.70	1.39	1.33
2	A	2070	FMN	C4A-N5	3.08	1.37	1.33
2	A	2070	FMN	C10-N1	2.67	1.36	1.33
2	A	2070	FMN	O2'-C2'	-2.03	1.39	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2070	FMN	C4-N3-C2	6.80	120.89	115.14
2	A	2070	FMN	C1'-N10-C9A	5.07	122.29	118.29
2	A	2070	FMN	C1'-N10-C10	-3.31	115.44	118.41
2	A	2070	FMN	C4A-C4-N3	-3.16	119.11	123.43
2	A	2070	FMN	C4-C4A-N5	2.95	121.97	118.60
2	A	2070	FMN	C4A-N5-C5A	2.48	119.25	116.77
2	A	2070	FMN	C10-C4A-N5	-2.44	119.57	121.26
2	A	2070	FMN	C4-C4A-C10	-2.27	118.45	119.95
4	A	2073	AKG	O5-C2-C3	2.17	124.09	120.38

There are no chirality outliers.

All (7) torsion outliers are listed below:

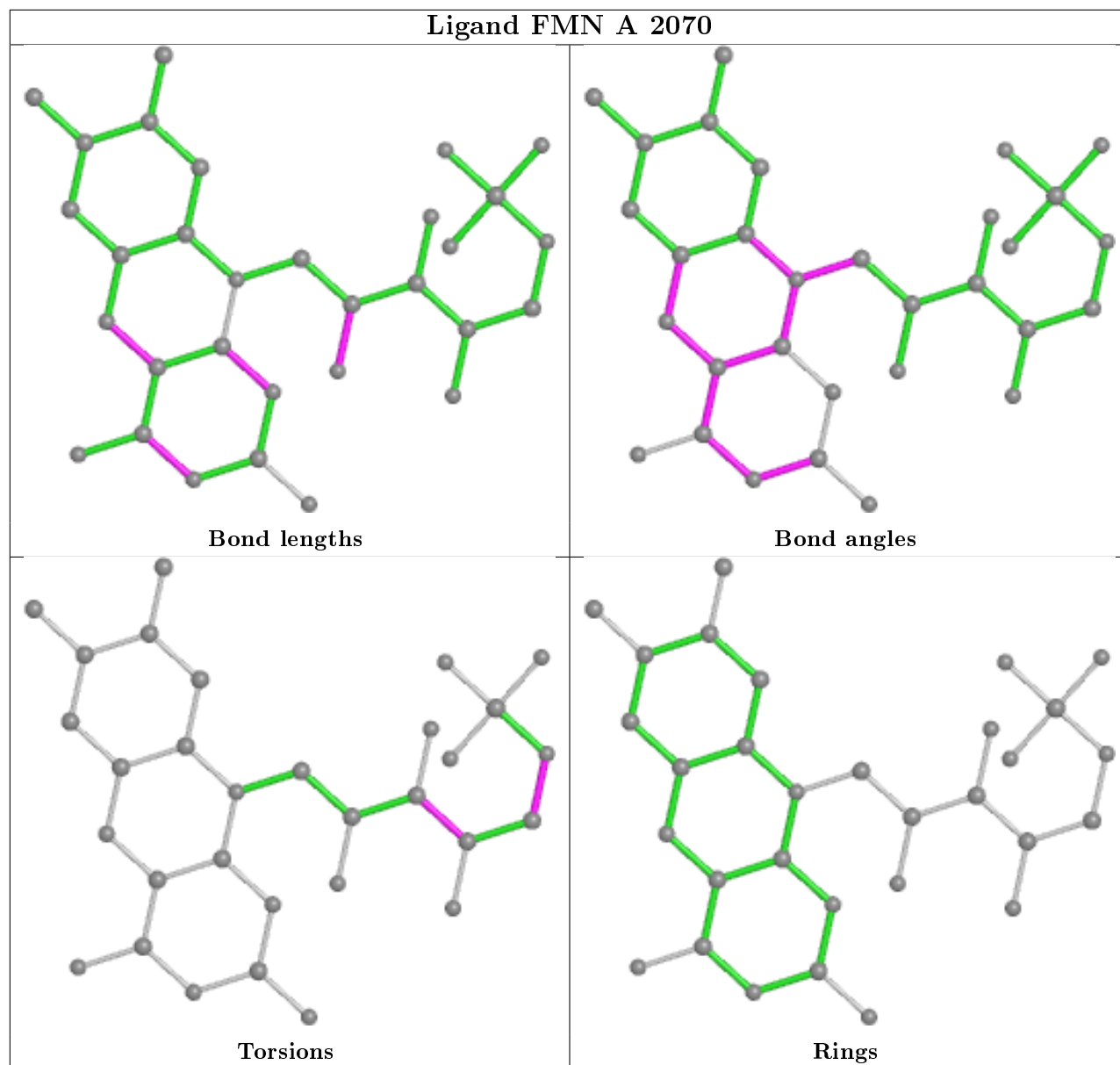
Mol	Chain	Res	Type	Atoms
2	A	2070	FMN	O3'-C3'-C4'-O4'
2	A	2070	FMN	O3'-C3'-C4'-C5'
2	A	2070	FMN	C2'-C3'-C4'-C5'
2	A	2070	FMN	C2'-C3'-C4'-O4'
4	A	2073	AKG	C1-C2-C3-C4
4	A	2073	AKG	O5-C2-C3-C4
2	A	2070	FMN	C4'-C5'-O5'-P

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2072	F3S	4	0
4	A	2073	AKG	2	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

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1475/1520 (97%)	-0.26	53 (3%) 42 42	8, 42, 64, 100	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	776	MET	7.3
1	A	10	ARG	5.0
1	A	605	ASN	4.9
1	A	1507	ASN	4.7
1	A	1264	GLN	4.4
1	A	251	GLY	4.3
1	A	560	GLN	4.3
1	A	413	TYR	4.2
1	A	418	TRP	4.2
1	A	439	ASP	3.8
1	A	774	PRO	3.8
1	A	137	GLU	3.8
1	A	693	ARG	3.7
1	A	1212	SER	3.6
1	A	1490	LYS	3.5
1	A	571	ASP	3.5
1	A	415	TYR	3.4
1	A	836	ASP	3.4
1	A	572	GLY	3.4
1	A	678	LEU	3.2
1	A	379	VAL	3.0
1	A	680	GLU	2.9
1	A	245	LYS	2.8
1	A	824	TYR	2.8
1	A	246	GLU	2.8
1	A	1263	HIS	2.8
1	A	417	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	394	LEU	2.7
1	A	920	GLU	2.6
1	A	1435	VAL	2.6
1	A	254	LYS	2.5
1	A	833	TYR	2.5
1	A	307	LYS	2.5
1	A	250	SER	2.5
1	A	829	LEU	2.4
1	A	1260	ALA	2.4
1	A	825	ASP	2.4
1	A	1456	LYS	2.4
1	A	828	GLU	2.4
1	A	791	GLY	2.3
1	A	692	ASP	2.3
1	A	397	GLN	2.3
1	A	775	GLU	2.2
1	A	1351	SER	2.2
1	A	1206	ARG	2.2
1	A	1258	GLN	2.2
1	A	1433	ASP	2.1
1	A	534	GLU	2.1
1	A	688	ASN	2.1
1	A	1486	ASP	2.1
1	A	697	PRO	2.1
1	A	772	ALA	2.0
1	A	1353	ALA	2.0

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

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

6.3 Carbohydrates [i](#)

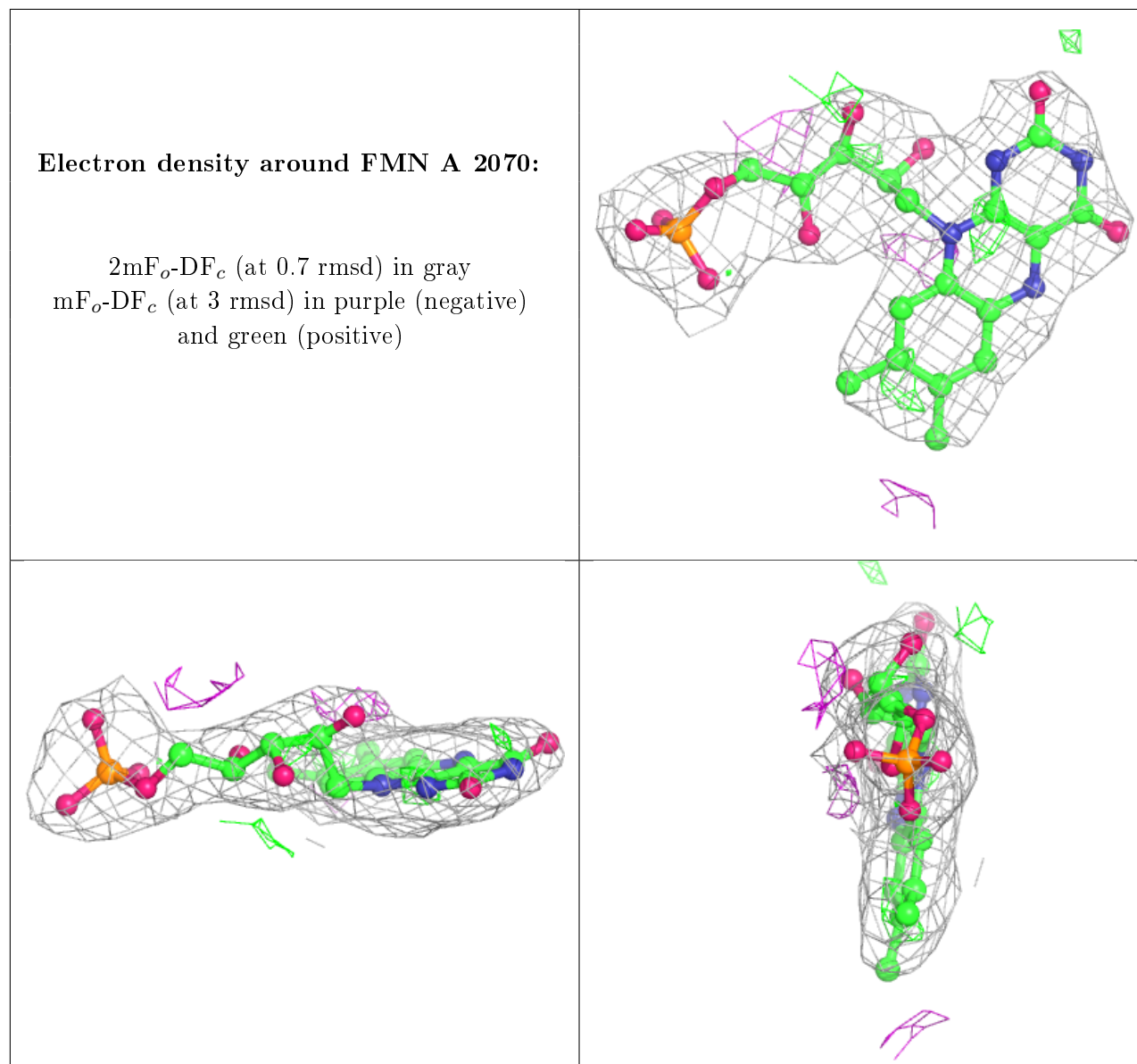
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	AKG	A	2073	10/10	0.96	0.24	81,85,87,89	0
2	FMN	A	2070	31/31	0.97	0.17	80,85,88,88	0
3	F3S	A	2072	7/7	0.98	0.12	85,91,94,96	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.



6.5 Other polymers ⓘ

There are no such residues in this entry.