



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 01:22 AM UTC

PDB ID : 1LLW / pdb_00001llw
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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

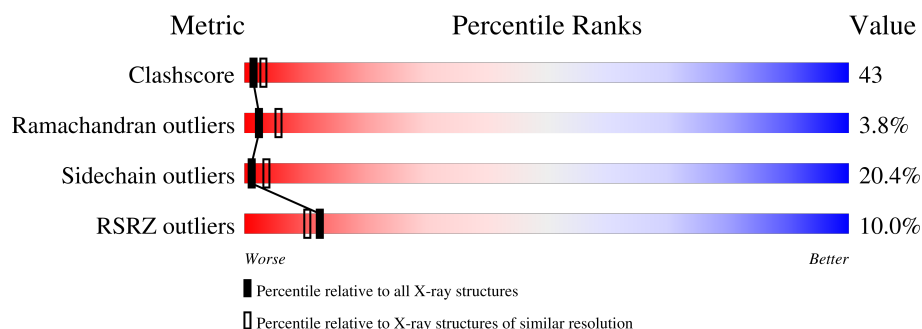
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	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	-
4	AKG	A	2073	-	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.

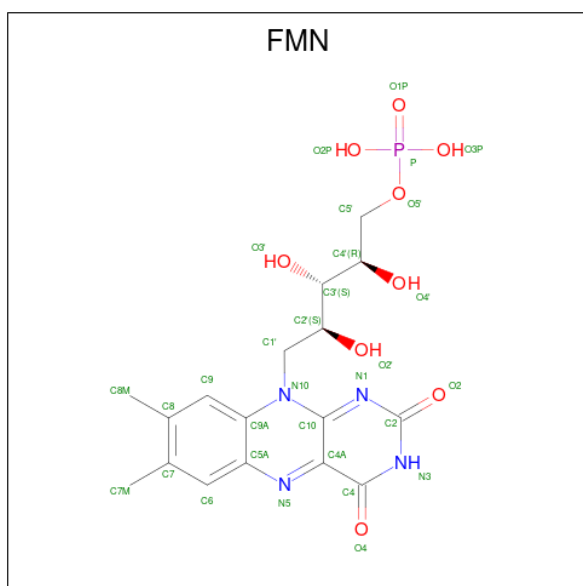
- Molecule 1 is a protein called Ferredoxin-dependent glutamate synthase.

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:

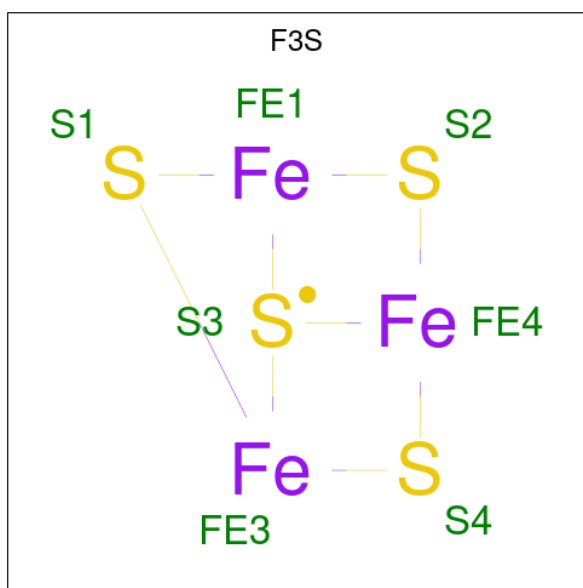
Chain	Residue	Modelled	Actual	Comment	Reference
A	578	ASP	THR	conflict	UNP P55038
A	581	THR	ASP	conflict	UNP P55038
A	1507	ASN	GLY	conflict	UNP P55038

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



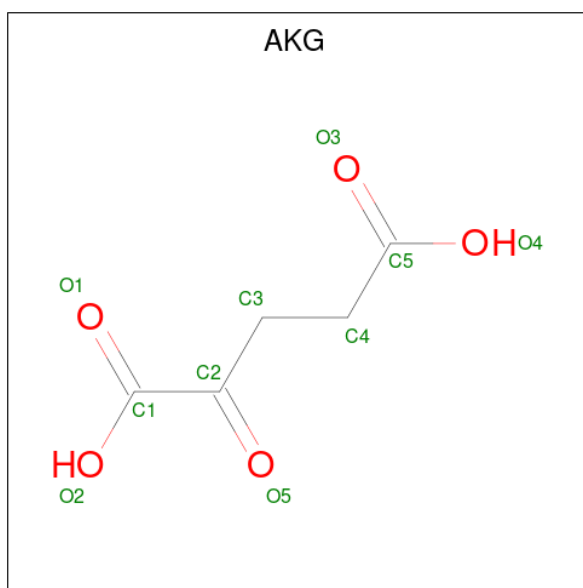
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	17	4	9	1	0	0

- Molecule 3 is FE3-S4 CLUSTER (CCD ID: 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 (CCD ID: 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		

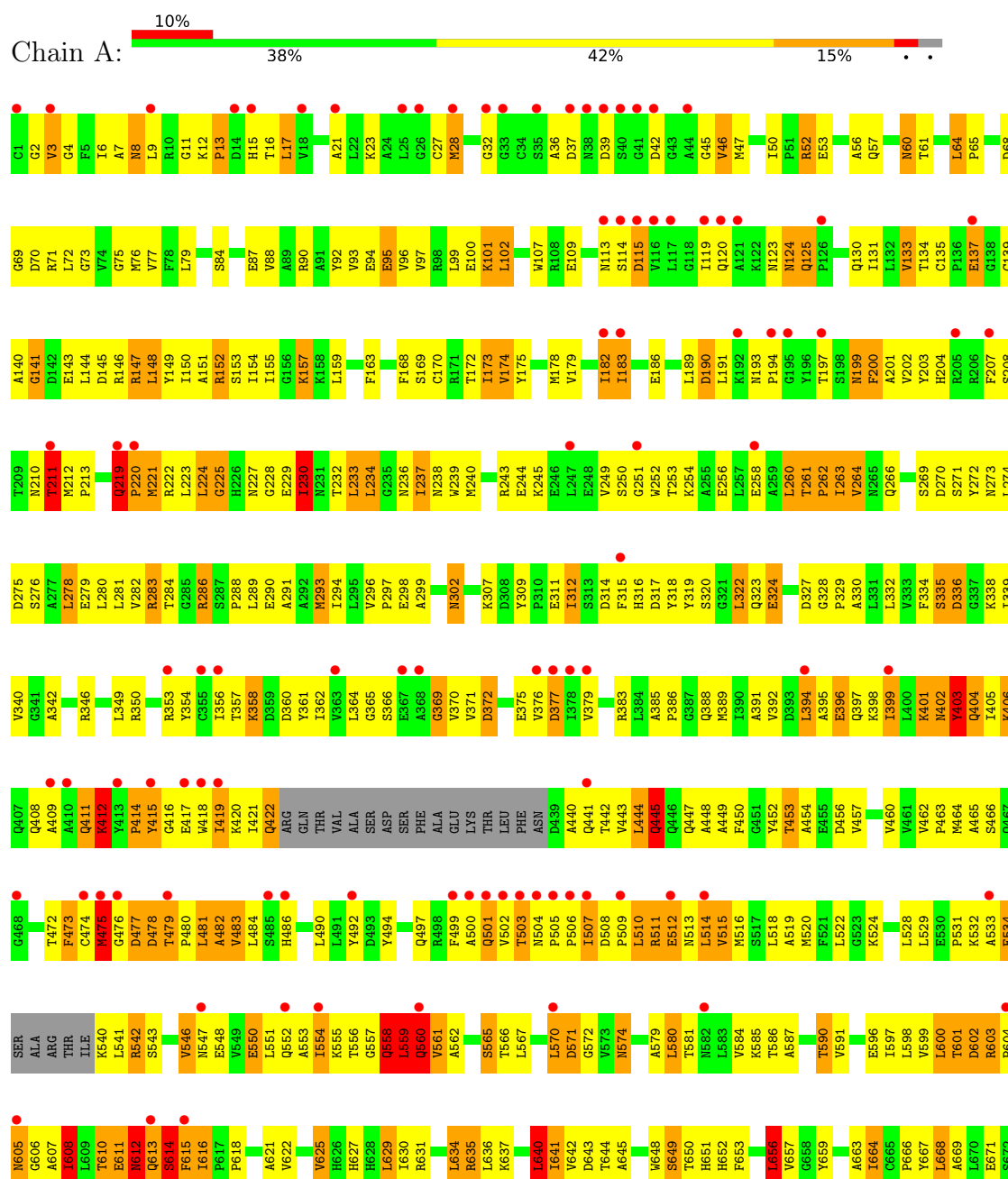
- Molecule 5 is water.

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

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Ferredoxin-dependent glutamate synthase



G1489	K1490	F1491	W1492	Q1493	A1494	P1497	S1498	E1499	K1500	P1503	E1504	N1507	ASP	VAL	SER	LEU	THR	GLY	LVS	THR	LEU	THR	SER	VAL																															
G1421	A1422	G1423	M1424	T1425	L1428	A1429	Y1430	F1431	L1432	L1433	E1434	V1435	L1438	P1439	E1440	K1441	I1442	M1443	I1446	I1447	T1448	L1449	Q1450	L1451	L1452	T1453	A1454	S1455	K1456	E1458	E1459	G1460	L1461	K1462	S1463	L1464	I1465	T1466	V1469	T1472	G1473	S1474	P1475	K1476	L1480	L1481	A1482	M1483	W1484	Y1487	L1488				
F1352	A1353	P1354	E1355	D1356	N1357	V1358	I1359	I1360	G1361	N1362	T1363	C1364	L1365	Y1366	T1369	G1370	G1371	N1372	L1373	Y1374	A1375	N1376	G1380	E1381	Q1382	F1383	A1384	V1385	R1386	N1387	S1388	V1389	I1394	D1399	H1400	C1401	C1402	E1403	Y1404	M1405	T1406	V1409	I1410	V1411	V1412	L1413	G1414	P1415	V1416	G1417	R1418	N1419	V1420		
L1273	V1274	N1275	T1279	L1280	G1281	T1282	R1283	L1284	S1285	T1286	Q1287	I1288	Y1292	G1293	N1294	N1295	G1296	F1297	L1298	G1299	N1300	I1301	F1305	Q1306	G1307	L1308	A1309	G1310	Q1311	A1315	F1316	N1317	L1318	M1321	H1324	L1325	Q1326	G1327	E1328	A1329	K1335	G1336	M1337	N1338	T1344	V1345	P1346	H1347	P1348	S1351					
R1199	T1200	L1203	D1208	V1209	Q1210	L1211	S1212	K1213	R1141	T1214	Q1215	N1216	L1225	G1226	P1227	T1228	K1229	R1232	Q1233	W1234	L1235	E1238	P1239	V1240	H1241	S1242	H1243	G1244	V1245	P1246	D1249	L1250	L1251	L1252	A1253	D1254	P1255	D1256	L1257	Q1258	E1259	A1260	L1261	N1262	H1263	Q1264	T1265	L1266	A1267	T1268	K1269	T1270	R1272		
I1130	A1131	M1132	I1133	G1136	C1137	I1138	M1139	A1140	R1141	T1142	C1143	H1144	T1145	N1146	M1147	C1148	P1149	V1150	G1151	V1152	A1153	T1154	R1158	L1159	R1160	Q1161	K1164	Q1169	V1170	N1171	N1172	F1173	F1174	Y1175	F1176	I1177	A1178	E1179	E1180	V1181	R1182	L1185	L1188	G1189	Y1190	S1192	L1193	D1194	D1195	L1196	I1197	G1198	C1199		
N1052	A1053	I1055	H1061	D1062	T1065	G1066	A1067	S1068	P1069	L1070	S1071	G1077	W1080	E1081	T1085	E1086	V1087	H1088	R1089	M1092	E1093	N1094	Q1095	A1096	Q1017	L1018	D1021	L1022	H1023	Q1024	I1025	Q1030	V1031	S1032	V1033	K1034	L1035	V1036	A1037	E1038	I1039	I1041	I1044	A1045	A1046	G1047									
A988	Q989	G970	A971	K972	P973	Q978	T988	L991	R992	R993	S994	N900	S901	G902	G903	D907	V908	V909	R910	Y911	L912	D916	R937	S919	E920	P924	T937	N939	S940	A941	I942	A946	R949	F950	G951	V952	T953	P954	E955	Y956	L957	M958	K961	Q962	L963	E964	P965	K966	N967						
A810	A811	Y812	VAL	GLY	GLY	ASN	GLY	ASN	ASN	GLY	GLU	ALA	Y824	D825	H826	Y827	E828	L829	Y830	R831	Q832	Y833	L834	K835	D836	R837	P838	V839	T840	R843	L846	D847	F848	T855	S856	L857	V860	E861	S862	V863	V867	T872	Q873	G874	N875	S876	L877	Q878	S881	R882	E883				
L737	E740	L744	Y745	F746	T749	S750	S751	R752	W753	G754	L755	L756	T757	A759	D760	V761	A762	W765	W766	Y767	F768	H769	G770	W771	A772	F773	F774	E775	A777	K778	Y779	L780	F783	G784	P790	G791	G792	E793	Y794	H795	W796	X797	S798	P799	E800	N801	S802	L805	V809						
V673	R674	Q675	W676	W677	L678	D679	E680	K681	T682	Q683	K684	L685	M686	E687	N688	G689	R690	L691	D692	R693	I694	D695	L696	P697	T698	K701	N702	W703	R704	Q705	S706	V707	L711	F712	F713	I714	L715	S716	K717	I720	S721	L722	L723	A724	S725	Y726	H727	G728	A729	Q730	L731	F732	E733	A734	G736

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 12.00 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.6 (12.00-2.70) 96.6 (12.00-2.70)	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 0.231 , (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)	0.31 , 64.0	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	0.91	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: F3S, FMN, 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	1.15	28/11533 (0.2%)	1.44	122/15639 (0.8%)

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 (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	293	MET	SD-CE	11.69	2.08	1.79
1	A	221	MET	SD-CE	9.08	2.02	1.79
1	A	240	MET	SD-CE	7.64	1.98	1.79
1	A	237	ILE	CA-CB	7.57	1.64	1.54
1	A	1120	MET	SD-CE	-6.44	1.63	1.79
1	A	796	MET	CG-SD	6.41	1.96	1.80
1	A	998	VAL	C-O	-6.17	1.15	1.24
1	A	1433	ASP	CB-CG	6.10	1.67	1.52
1	A	1139	MET	SD-CE	5.96	1.94	1.79
1	A	28	MET	SD-CE	-5.89	1.64	1.79
1	A	965	ILE	CA-CB	-5.79	1.47	1.54
1	A	707	VAL	CA-CB	5.77	1.61	1.54
1	A	1100	VAL	CA-CB	5.75	1.61	1.55
1	A	715	LEU	C-O	5.68	1.30	1.24
1	A	1181	VAL	CA-CB	5.62	1.61	1.54
1	A	1036	VAL	CA-CB	-5.44	1.47	1.54
1	A	717	LYS	C-O	-5.36	1.17	1.24
1	A	542	ARG	CA-C	5.26	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	202	VAL	CA-CB	-5.23	1.48	1.54
1	A	1361	GLY	C-O	-5.22	1.19	1.24
1	A	875	MET	SD-CE	5.22	1.92	1.79
1	A	219	GLN	CA-C	-5.21	1.46	1.52
1	A	771	MET	SD-CE	5.19	1.92	1.79
1	A	891	ALA	CA-CB	-5.12	1.45	1.53
1	A	211	THR	N-CA	-5.12	1.40	1.46
1	A	872	THR	N-CA	-5.07	1.40	1.46
1	A	1347	HIS	CA-C	5.04	1.58	1.52
1	A	1085	THR	CA-CB	-5.01	1.45	1.53

All (122) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	872	THR	N-CA-C	-10.19	100.25	111.36
1	A	219	GLN	N-CA-C	8.90	129.48	109.81
1	A	768	PHE	N-CA-C	8.69	123.61	112.92
1	A	402	ASN	N-CA-C	8.62	120.37	110.97
1	A	693	ARG	N-CA-C	-8.47	100.27	110.44
1	A	1052	ASN	N-CA-C	8.32	123.06	111.92
1	A	574	ASN	N-CA-C	7.97	120.74	111.02
1	A	1138	ILE	CA-C-N	-7.90	110.71	122.24
1	A	1138	ILE	C-N-CA	-7.90	110.71	122.24
1	A	1170	VAL	N-CA-C	-7.76	103.35	111.58
1	A	1044	ILE	N-CA-C	-7.74	102.91	110.72
1	A	501	GLN	CA-C-N	-7.67	110.66	121.55
1	A	501	GLN	C-N-CA	-7.67	110.66	121.55
1	A	607	ALA	N-CA-C	7.51	120.29	108.79
1	A	1376	ASN	CB-CA-C	-7.45	100.58	111.91
1	A	608	ILE	N-CA-C	7.36	117.54	106.42
1	A	640	LEU	N-CA-C	7.36	121.68	109.46
1	A	1240	VAL	CB-CA-C	-7.24	99.42	111.29
1	A	792	GLY	N-CA-C	7.08	121.29	112.79
1	A	336	ASP	N-CA-C	-7.07	104.81	113.50
1	A	21	ALA	N-CA-C	-7.00	103.58	111.07
1	A	123	ASN	CA-C-N	6.97	130.18	120.29
1	A	123	ASN	C-N-CA	6.97	130.18	120.29
1	A	909	VAL	CB-CA-C	-6.91	99.95	111.29
1	A	559	LEU	N-CA-C	6.90	120.40	109.50
1	A	951	GLY	CA-C-N	-6.89	114.41	122.95
1	A	951	GLY	C-N-CA	-6.89	114.41	122.95
1	A	1481	LEU	N-CA-C	6.79	118.34	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	ASN	CA-C-N	-6.70	114.92	123.16
1	A	302	ASN	C-N-CA	-6.70	114.92	123.16
1	A	512	GLU	N-CA-C	-6.68	103.28	112.03
1	A	442	THR	N-CA-C	-6.55	105.11	113.23
1	A	225	GLY	N-CA-C	-6.51	100.74	110.71
1	A	124	ASN	N-CA-C	6.47	118.41	111.36
1	A	261	THR	O-C-N	6.44	125.47	120.38
1	A	1286	GLY	N-CA-C	-6.41	104.85	113.24
1	A	1288	ILE	N-CA-C	-6.38	104.53	110.53
1	A	1228	THR	N-CA-C	6.30	121.00	112.88
1	A	606	GLY	N-CA-C	6.21	123.00	114.92
1	A	505	PRO	N-CA-C	6.21	118.27	110.70
1	A	1281	GLY	N-CA-C	-6.20	107.31	114.69
1	A	731	ILE	CB-CA-C	6.20	121.45	111.29
1	A	220	PRO	N-CD-CG	-6.12	94.02	103.20
1	A	1164	LYS	N-CA-C	-6.10	102.90	110.41
1	A	335	SER	CA-C-N	6.10	132.48	121.92
1	A	335	SER	C-N-CA	6.10	132.48	121.92
1	A	396	GLU	N-CA-C	6.09	120.29	112.86
1	A	473	PHE	N-CA-C	6.05	116.23	108.24
1	A	372	ASP	N-CA-C	6.04	118.98	107.75
1	A	558	GLN	N-CA-C	6.04	118.38	111.02
1	A	656	LEU	N-CA-C	5.99	117.50	110.97
1	A	998	VAL	N-CA-C	5.99	117.97	108.87
1	A	695	ASP	N-CA-C	-5.98	102.60	110.43
1	A	1144	HIS	N-CA-C	-5.97	105.86	113.02
1	A	1492	TRP	N-CA-C	5.88	118.11	110.53
1	A	244	GLU	N-CA-C	5.86	117.74	111.36
1	A	1062	ASP	N-CA-C	5.85	118.41	111.33
1	A	445	GLN	N-CA-C	5.84	121.97	114.56
1	A	1065	THR	N-CA-C	-5.83	99.67	108.46
1	A	1318	LEU	N-CA-C	5.72	118.89	110.59
1	A	1357	ASN	CA-C-N	5.71	128.16	120.50
1	A	1357	ASN	C-N-CA	5.71	128.16	120.50
1	A	502	VAL	N-CA-C	-5.71	104.99	113.39
1	A	477	ASP	CA-C-N	5.71	129.73	120.60
1	A	477	ASP	C-N-CA	5.71	129.73	120.60
1	A	1065	THR	CB-CA-C	-5.69	100.56	109.72
1	A	1497	PRO	N-CA-C	-5.68	100.77	112.47
1	A	230	ILE	N-CA-C	-5.64	101.45	108.89
1	A	503	THR	N-CA-C	-5.63	106.25	113.23
1	A	729	ALA	CA-C-N	-5.59	113.13	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	729	ALA	C-N-CA	-5.59	113.13	122.92
1	A	612	ASN	N-CA-C	-5.56	98.96	110.80
1	A	336	ASP	N-CA-CB	-5.56	102.36	110.53
1	A	877	LEU	CA-CB-CG	-5.55	96.87	116.30
1	A	1132	MET	N-CA-C	-5.55	104.87	111.03
1	A	174	VAL	N-CA-C	5.54	115.93	108.17
1	A	1061	HIS	CA-C-N	5.53	127.96	120.38
1	A	1061	HIS	C-N-CA	5.53	127.96	120.38
1	A	608	ILE	N-CA-CB	-5.53	107.12	112.65
1	A	968	ALA	N-CA-C	5.52	117.24	108.79
1	A	996	PRO	CA-C-N	-5.51	113.86	120.03
1	A	996	PRO	C-N-CA	-5.51	113.86	120.03
1	A	502	VAL	CA-C-O	5.50	124.48	119.20
1	A	61	THR	N-CA-C	-5.46	105.89	112.54
1	A	1077	GLY	N-CA-C	5.44	121.31	112.61
1	A	825	ASP	N-CA-C	-5.43	105.92	112.54
1	A	1362	ASN	N-CA-C	5.41	117.51	110.43
1	A	811	ALA	N-CA-C	5.40	117.03	111.03
1	A	238	ASN	N-CA-C	5.38	117.23	111.36
1	A	1347	HIS	CB-CA-C	5.38	118.54	109.67
1	A	1061	HIS	N-CA-C	-5.35	106.02	112.54
1	A	200	PHE	N-CA-C	5.34	115.08	108.19
1	A	610	THR	N-CA-C	-5.32	105.56	111.36
1	A	753	VAL	CB-CA-C	5.26	119.92	111.29
1	A	691	LEU	N-CA-C	5.23	117.00	108.63
1	A	1154	THR	CB-CA-C	-5.23	98.57	110.07
1	A	899	SER	N-CA-C	-5.22	101.43	109.52
1	A	546	VAL	CB-CA-C	5.21	118.17	110.77
1	A	950	PHE	CA-C-N	-5.20	111.22	121.41
1	A	950	PHE	C-N-CA	-5.20	111.22	121.41
1	A	72	LEU	CA-C-N	-5.20	111.23	121.41
1	A	72	LEU	C-N-CA	-5.20	111.23	121.41
1	A	1046	ALA	CA-C-N	5.17	125.68	119.94
1	A	1046	ALA	C-N-CA	5.17	125.68	119.94
1	A	445	GLN	CB-CA-C	5.16	117.18	109.13
1	A	11	GLY	N-CA-C	-5.14	101.00	113.18
1	A	391	ALA	N-CA-C	5.13	115.07	108.34
1	A	302	ASN	CB-CA-C	-5.13	104.98	111.86
1	A	1264	GLN	CA-C-N	-5.13	113.83	122.29
1	A	1264	GLN	C-N-CA	-5.13	113.83	122.29
1	A	440	ALA	N-CA-C	-5.13	102.03	109.31
1	A	1370	GLY	N-CA-C	-5.12	103.77	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1351	SER	N-CA-C	-5.11	106.90	112.72
1	A	707	VAL	CB-CA-C	-5.10	105.18	112.22
1	A	1229	LYS	N-CA-C	5.10	117.22	111.11
1	A	1499	GLU	N-CA-C	-5.08	106.21	114.09
1	A	230	ILE	CA-C-N	-5.06	114.56	122.65
1	A	230	ILE	C-N-CA	-5.06	114.56	122.65
1	A	610	THR	CB-CA-C	-5.05	102.26	110.85
1	A	997	GLY	N-CA-C	5.04	118.98	112.83
1	A	756	LEU	N-CA-C	5.04	117.34	110.24
1	A	501	GLN	N-CA-C	5.03	116.78	108.48

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	977	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	977	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 43.

All (977) 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:1337:MET:HE2	1:A:1365:LEU:HD21	1.25	1.18
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:OE1	1:A:558:GLN:HA	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:460:VAL:CG1	1:A:464:MET:HE2	1.89	1.02
1:A:1263:HIS:HE1	1:A:1297:PHE:HA	0.86	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:559:LEU:HD21	1:A:560:GLN:O	1.59	1.02
1:A:1263:HIS:HE1	1:A:1297:PHE:CA	1.71	1.02
1:A:383:ARG:NH1	1:A:1380:GLY:CA	2.13	1.02
1:A:1254:ASP:CB	1:A:1255:PRO:HD3	1.88	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:HD1	1:A:403:TYR:H	1.06	1.00
1:A:243:ARG:NH1	1:A:528:LEU:HB2	1.75	1.00
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:1254:ASP:CB	1:A:1255:PRO:CD	2.42	0.97
1:A:1491:PHE:O	1:A:1491:PHE:CD1	2.18	0.96
1:A:1254:ASP:HB3	1:A:1255:PRO:HD3	1.45	0.96
1:A:686:MET:HE1	1:A:694:ILE:HB	1.47	0.95
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:1337:MET:HE2	1:A:1365:LEU:CD2	1.97	0.94
1:A:686:MET:O	1:A:692:ASP:HB2	1.68	0.93
1:A:460:VAL:HG12	1:A:464:MET:HE2	1.47	0.93
1:A:846:LEU:HB2	1:A:1116:MET:HE1	1.48	0.93
1:A:1355:GLU:HG2	1:A:1476:LYS:CB	1.99	0.93
1:A:318:TYR:HD1	1:A:418:TRP:HE1	1.13	0.92
1:A:686:MET:HE3	1:A:692:ASP:HA	1.52	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:657:VAL:HG11	1:A:723:LEU:HD11	1.52	0.91
1:A:1130:ILE:HD13	1:A:1130:ILE:H	1.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:953:THR:HG23	1:A:1294:ASN:ND2	1.85	0.90
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:OE1	1:A:1311:GLN:HA	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:HG3	1:A:993:ARG:HH11	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:383:ARG:HH11	1:A:1380:GLY:HA2	1.35	0.87
1:A:1119:LEU:CD2	1:A:1196:ILE:HG22	2.04	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: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:O	1:A:603:ARG:HG2	1.72	0.85
1:A:289:LEU:HD22	1:A:389:MET:HE3	1.58	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:1288:ILE:HD12	1:A:1321:MET:HE2	1.57	0.84
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:878:GLY:HA2	1:A:988:ILE:HD12	1.60	0.84
1:A:1251:ILE:HD13	1:A:1271:TYR:CE1	2.13	0.84
1:A:1420:VAL:HG12	1:A:1420:VAL:O	1.77	0.84
1:A:558:GLN:OE1	1:A:558:GLN:CA	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:399:ILE:HG22	1:A:404:GLN:HG2	1.62	0.82
1:A:475:MET:HE1	1:A:1129:SER:OG	1.79	0.82
1:A:1347:HIS:CE1	1:A:1348:PRO:HD2	2.14	0.82
1:A:509:PRO:HA	1:A:516:MET:HE1	1.61	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:1081:GLU:HG3	1:A:1120:MET:HE1	1.63	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:OD1	1:A:1208:ASP:N	2.13	0.80
1:A:1491:PHE:HD1	1:A:1491:PHE:C	1.88	0.79
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:179:VAL:HB	1:A:183:ILE:HG22	1.63	0.78
1:A:1491:PHE:CD1	1:A:1491:PHE:C	2.60	0.78
1:A:1318:LEU:HB2	1:A:1321:MET:HE3	1.63	0.78
1:A:1360:ILE:HG23	1:A:1364:CYS:SG	2.23	0.78
1:A:445:GLN:OE1	1:A:777:ALA:HB2	1.84	0.78
1:A:1409:VAL:O	1:A:1410:ILE:HD13	1.83	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:460:VAL:HG13	1:A:464:MET:HE2	1.66	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:464:MET:HB3	1:A:706:SER:OG	1.85	0.77
1:A:1119:LEU:O	1:A:1198:GLY:HA2	1.84	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:499:PHE:CD1	1:A:973:PRO:HB3	2.20	0.77
1:A:610:THR:HG23	1:A:773:PHE:HB3	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:294:ILE:HG21	1:A:528:LEU:HD11	1.67	0.76
1:A:1191:ARG:HG2	5:A:2084:HOH:O	1.85	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:HG12	1:A:182:ILE:O	1.85	0.76
1:A:885:HIS:HD2	1:A:910:ARG:HH22	0.79	0.76
1:A:811:ALA:O	1:A:812:TYR:HB2	1.84	0.76
1:A:1355:GLU:CD	1:A:1355:GLU:H	1.93	0.76
1:A:1119:LEU:HD23	1:A:1196:ILE:CG2	2.15	0.75
1:A:1254:ASP:C	1:A:1256:ASP:H	1.94	0.75
1:A:1461:LEU:HD21	1:A:1491:PHE:HZ	1.52	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:354:TYR:HB3	1:A:364:LEU:CD1	2.16	0.74
1:A:1376:ASN:OD1	1:A:1472:THR:HG21	1.87	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:1461:LEU:HD21	1:A:1491:PHE:CZ	2.22	0.74
1:A:475:MET:CA	1:A:475:MET:HE3	2.18	0.74
1:A:1142:VAL:O	1:A:1142:VAL:CG1	2.35	0.74
1:A:1130:ILE:H	1:A:1130:ILE:CD1	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:443:VAL:CG2	1:A:675:GLN:HE21	1.99	0.73
1:A:581:THR:CG2	1:A:585:LYS:HE3	2.18	0.73
1:A:9:LEU:HD21	1:A:392:VAL:CG1	2.19	0.73
1:A:472:THR:HG22	1:A:473:PHE:N	2.01	0.73
1:A:1119:LEU:HD21	1:A:1196:ILE:CG2	2.18	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:258:GLU:O	1:A:261:THR:OG1	2.04	0.72
1:A:404:GLN:OE1	1:A:404:GLN:CA	2.35	0.72
1:A:1148:CYS:SG	3:A:2072:F3S:S3	2.86	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TYR:HD1	1:A:418:TRP:NE1	1.86	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:883:GLU:OE1	1:A:1160:ARG:CD	2.35	0.72
1:A:1147:ASN:O	1:A:1148:CYS:C	2.31	0.71
1:A:1347:HIS:CD2	1:A:1348:PRO:HD2	2.25	0.71
1:A:497:GLN:HE21	1:A:651:HIS:CD2	2.06	0.71
1:A:506:PRO:HD2	1:A:1005:PRO:HB3	1.72	0.71
1:A:45:GLY:HA3	1:A:220:PRO:CD	2.20	0.71
1:A:560:GLN:OE1	1:A:560:GLN:CA	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:475:MET:HE3	1:A:475:MET:HA	1.71	0.71
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:418:TRP:C	1:A:418:TRP:CD2	2.70	0.70
1:A:460:VAL:O	1:A:464:MET:HG3	1.92	0.70
1:A:403:TYR:HD1	1:A:403:TYR:N	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:402:ASN:O	1:A:403:TYR:O	2.09	0.70
1:A:1372:ASN:N	1:A:1372:ASN:ND2	2.34	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:901:SER:O	1:A:902:GLY:C	2.35	0.69
1:A:567:LEU:HD12	1:A:604:PRO:HD2	1.73	0.69
1:A:1101:LEU:HA	1:A:1123:GLU:OE2	1.92	0.69
1:A:296:VAL:HG12	1:A:296:VAL:O	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:1325:LEU:HD21	1:A:1328:GLU:O	1.93	0.69
1:A:460:VAL:CG1	1:A:464:MET:CE	2.60	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:611:GLU:C	1:A:613:GLN:N	2.48	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1347:HIS:ND1	1:A:1348:PRO:CD	2.53	0.68
1:A:445:GLN:HG3	1:A:777:ALA:CB	2.22	0.67
1:A:1294:ASN:HB3	1:A:1338:ASN:HD21	1.59	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:1409:VAL:C	1:A:1410:ILE:HD13	2.20	0.67
1:A:501:GLN:HE22	1:A:1035:LEU:CB	2.07	0.67
1:A:1338:ASN:O	1:A:1370:GLY:HA3	1.94	0.67
1:A:1263:HIS:CE1	1:A:1298:GLU:H	2.13	0.66
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:1246:VAL:O	1:A:1249:ASP:HB2	1.95	0.66
1:A:1360:ILE:CG2	1:A:1364:CYS:SG	2.83	0.66
1:A:9:LEU:HD21	1:A:392:VAL:HG13	1.78	0.66
1:A:645:ALA:HB1	1:A:668:LEU:HB2	1.76	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: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: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:315:PHE:HD2	1:A:319:TYR:CE1	2.14	0.66
1:A:688:ASN:CG	1:A:688:ASN:O	2.39	0.66
1:A:907:ASP:CG	1:A:909:VAL:HG23	2.20	0.65
1:A:509:PRO:CA	1:A:516:MET:HE1	2.25	0.65
1:A:1311:GLN:OE1	1:A:1311:GLN:CA	2.45	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:1402:CYS:O	1:A:1403:GLU:O	2.14	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:1251:ILE:CD1	1:A:1271:TYR:CE1	2.80	0.65
1:A:406:LYS:O	1:A:409:ALA:HB3	1.96	0.65
1:A:311:GLU:CB	1:A:409:ALA:HB1	2.26	0.65
1:A:1282:THR:OG1	1:A:1315:ALA:HB3	1.97	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:529:LEU:O	1:A:531:PRO:HD3	1.96	0.64
1:A:1032:SER:HA	1:A:1055:ILE:O	1.97	0.64
1:A:602:ASP:O	1:A:608:ILE:HD13	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:MET:HE1	1:A:888:LEU:HD11	1.79	0.64
1:A:146:ARG:NH2	1:A:256:GLU:OE1	2.29	0.64
1:A:234:LEU:CD1	1:A:234:LEU:C	2.70	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:1137:CYS:SG	1:A:1138:ILE:O	2.54	0.64
1:A:891:ALA:CB	1:A:1170:VAL:CG2	2.75	0.64
1:A:715:LEU:HD22	1:A:726:TYR:CG	2.32	0.64
1:A:1432:LEU:HG	1:A:1432:LEU:O	1.96	0.64
1:A:234:LEU:C	1:A:234:LEU:HD12	2.23	0.64
1:A:501:GLN:NE2	1:A:1035:LEU:HA	2.13	0.64
1:A:612:ASN:O	1:A:614:SER:N	2.31	0.64
1:A:1462:LYS:HB2	1:A:1484:TRP:CZ2	2.33	0.64
1:A:611:GLU:O	1:A:613:GLN:N	2.29	0.64
1:A:1430:TYR:CE2	1:A:1493:GLN:OE1	2.50	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:686:MET:CE	1:A:694:ILE:HB	2.26	0.63
1:A:1216:ASN:C	1:A:1216:ASN:HD22	2.05	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: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: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:875:MET:SD	1:A:1132:MET:HE1	2.39	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:32:GLY:HA2	1:A:207:PHE:HB2	1.81	0.62
1:A:1142:VAL:HG11	1:A:1147:ASN:HB2	1.81	0.62
1:A:414:PRO:HB2	1:A:418:TRP:HB3	1.81	0.62
1:A:1388:SER:HA	1:A:1406:THR:HG22	1.82	0.62
1:A:358:LYS:HD2	1:A:377:ASP:HB2	1.81	0.62
1:A:1142:VAL:O	1:A:1142:VAL:HG12	1.98	0.62
1:A:6:ILE:HD11	1:A:371:VAL:HG21	1.80	0.62
1:A:1101:LEU:HD11	1:A:1124:GLU:HG3	1.81	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:1363:THR:CG2	1:A:1385:VAL:HG21	2.31	0.61
1:A:2:GLY:HA3	1:A:28:MET:HE3	1.82	0.61
1:A:875:MET:SD	1:A:1132:MET:CE	2.89	0.61
1:A:311:GLU:HB3	1:A:409:ALA:HB1	1.81	0.61
1:A:509:PRO:HA	1:A:516:MET:CE	2.29	0.61
1:A:28:MET:HE1	1:A:366:SER:HB2	1.80	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:499:PHE:CE1	1:A:973:PRO:HB3	2.36	0.61
1:A:570:LEU:HG	1:A:613:GLN:HG2	1.83	0.61
1:A:971:ALA:HB3	1:A:1065:THR:HG23	1.82	0.61
1:A:388:GLN:HG2	1:A:401:LYS:HD3	1.81	0.61
1:A:560:GLN:C	1:A:561:VAL:HG23	2.26	0.61
1:A:645:ALA:HB1	1:A:668:LEU:CB	2.31	0.61
1:A:1092:MET:HE2	1:A:1226:PRO:HB2	1.83	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:221:MET:CE	1:A:221:MET:CG	2.79	0.60
1:A:289:LEU:CD2	1:A:389:MET:HE3	2.31	0.60
1:A:1250:ASP:O	1:A:1253:ALA:N	2.32	0.60
1:A:13:PRO:O	1:A:197:THR:HB	2.00	0.60
1:A:441:GLN:OE1	1:A:441:GLN:N	2.35	0.60
1:A:603:ARG:HD2	1:A:667:TYR:CE2	2.37	0.60
1:A:616:ILE:HG21	1:A:621:ALA:HB2	1.83	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:9:LEU:O	1:A:396:GLU:HG2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1228:THR:O	1:A:1228:THR:CG2	2.49	0.60
1:A:1371:GLY:C	1:A:1372:ASN:ND2	2.60	0.60
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:679:ASP:OD1	1:A:679:ASP:C	2.45	0.59
1:A:1200:THR:HG21	1:A:1225:LEU:HB2	1.83	0.59
1:A:663:ALA:C	1:A:664:ILE:HG12	2.27	0.59
1:A:1325:LEU:HB3	1:A:1344:ILE:HG12	1.83	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
1:A:9:LEU:HD12	1:A:360:ASP:HB3	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:1023:HIS:HE1	1:A:1054:ASP:OD2	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: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: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:316:HIS:O	1:A:320:SER:CB	2.52	0.58
1:A:518:LEU:HD13	1:A:712:PHE:CE2	2.38	0.58
1:A:642:VAL:HG13	1:A:664:ILE:HG23	1.86	0.58
1:A:941:ALA:HB1	1:A:961:LYS:HD2	1.85	0.58
1:A:1137:CYS:SG	3:A:2072:F3S:S1	3.01	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:445:GLN:CG	1:A:777:ALA:HB1	2.29	0.58
1:A:591:VAL:HG22	1:A:598:LEU:HD11	1.86	0.58
1:A:769:HIS:C	1:A:769:HIS:CD2	2.81	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:450:PHE:CZ	1:A:615:PHE:CZ	2.92	0.57
1:A:511:ARG:HD3	1:A:1423:GLY:HA3	1.86	0.57
1:A:358:LYS:CD	1:A:377:ASP:HB2	2.34	0.57
1:A:993:ARG:CG	1:A:993:ARG:NH1	2.60	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1315:ALA:O	1:A:1317:ASN:N	2.37	0.57
1:A:602:ASP:O	1:A:608:ILE:CD1	2.53	0.57
1:A:1154:THR:HG21	1:A:1159:LEU:HD12	1.87	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: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: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:668:LEU:O	1:A:669:ALA:C	2.46	0.57
1:A:953:THR:O	1:A:956:TYR:HB3	2.04	0.57
1:A:1105:ASP:OD1	1:A:1105:ASP:C	2.47	0.57
1:A:492:TYR:HE2	1:A:656:LEU:CD1	2.15	0.57
1:A:1371:GLY:C	1:A:1372:ASN:HD22	2.12	0.57
1:A:1376:ASN:HD21	1:A:1472:THR:CG2	2.15	0.57
1:A:774:PRO:HD2	5:A:2116:HOH:O	2.04	0.56
1:A:883:GLU:CD	1:A:1160:ARG:HD2	2.29	0.56
1:A:1087:VAL:O	1:A:1088:HIS:C	2.47	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:71:ARG:HG3	1:A:139:CYS:O	2.06	0.56
1:A:289:LEU:HD22	1:A:404:GLN:HE22	1.70	0.56
1:A:383:ARG:HH12	1:A:1380:GLY:C	2.10	0.56
1:A:875:MET:CE	1:A:888:LEU:CD1	2.84	0.56
1:A:73:GLY:CA	1:A:170:CYS:HA	2.33	0.56
1:A:75:GLY:O	1:A:130:GLN:HA	2.05	0.56
1:A:232:THR:O	1:A:233:LEU:C	2.48	0.56
1:A:519:ALA:O	1:A:520:MET:CG	2.54	0.56
1:A:1279:THR:HG22	1:A:1282:THR:HB	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:1442:ILE:HD12	1:A:1449:LEU:HD22	1.87	0.56
1:A:157:LYS:HZ1	1:A:261:THR:CB	2.19	0.56
1:A:445:GLN:OE1	1:A:776:MET:O	2.24	0.56
1:A:548:GLU:CD	1:A:603:ARG:HH22	2.14	0.56
1:A:1420:VAL:O	1:A:1420:VAL:CG1	2.48	0.56
1:A:56:ALA:O	1:A:60:ASN:HB2	2.05	0.56
1:A:501:GLN:NE2	1:A:1035:LEU:CA	2.68	0.56
1:A:627:HIS:O	1:A:631:ARG:HG3	2.06	0.56
1:A:1402:CYS:O	1:A:1403:GLU:C	2.48	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1228:THR:HG21	1:A:1232:ARG:HH21	1.71	0.56
1:A:275:ASP:O	1:A:276:SER:C	2.49	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: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:449:ALA:HA	1:A:768:PHE:O	2.07	0.55
1:A:1251:ILE:HD13	1:A:1271:TYR:CZ	2.41	0.55
1:A:501:GLN:NE2	1:A:1035:LEU:HB3	2.17	0.55
1:A:316:HIS:O	1:A:320:SER:HB3	2.07	0.55
1:A:827:TYR:CE1	1:A:1176:PHE:CD1	2.95	0.55
1:A:875:MET:CE	1:A:888:LEU:HD11	2.37	0.55
1:A:1085:THR:HG22	1:A:1086:GLU:N	2.20	0.55
1:A:1250:ASP:O	1:A:1251:ILE:C	2.49	0.55
1:A:1294:ASN:HB3	1:A:1338:ASN:ND2	2.22	0.55
1:A:514:LEU:HD13	1:A:514:LEU:C	2.31	0.55
1:A:84:SER:O	1:A:88:VAL:HG23	2.07	0.55
1:A:744:TYR:C	1:A:744:TYR:CD2	2.84	0.55
1:A:768:PHE:CE1	1:A:783:PHE:HZ	2.24	0.55
1:A:399:ILE:CG2	1:A:404:GLN:HG2	2.35	0.55
1:A:750:THR:CG2	1:A:1039:ILE:HG21	2.33	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:460:VAL:HG12	1:A:464:MET:HE3	1.85	0.54
1:A:600:LEU:HD21	1:A:625:VAL:HG11	1.87	0.54
1:A:1139:MET:O	1:A:1140:ALA:C	2.48	0.54
1:A:271:SER:O	1:A:272:TYR:C	2.50	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:207:PHE:C	1:A:207:PHE:CD2	2.84	0.54
1:A:499:PHE:CG	1:A:973:PRO:HB3	2.42	0.54
1:A:402:ASN:O	1:A:403:TYR:C	2.50	0.54
1:A:972:LYS:HD3	1:A:1068:SER:OG	2.07	0.54
1:A:1138:ILE:CG2	1:A:1139:MET:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1363:THR:HG22	1:A:1385:VAL:HG21	1.89	0.54
1:A:311:GLU:HB2	1:A:409:ALA:HB1	1.90	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:1325:LEU:HD21	1:A:1328:GLU:C	2.33	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:445:GLN:CD	1:A:777:ALA:CB	2.80	0.53
1:A:559:LEU:CG	1:A:560:GLN:O	2.56	0.53
1:A:560:GLN:C	1:A:561:VAL:CG2	2.81	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:1254:ASP:C	1:A:1256:ASP:N	2.65	0.53
1:A:312:ILE:C	1:A:312:ILE:HD13	2.33	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: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:1442:ILE:HD12	1:A:1449:LEU:HD13	1.90	0.53
1:A:481:LEU:O	1:A:483:VAL:N	2.41	0.53
1:A:263:ILE:CD1	1:A:280:LEU:HD22	2.35	0.53
1:A:1089:ARG:NH2	1:A:1225:LEU:CD2	2.72	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
1:A:224:LEU:HD12	1:A:225:GLY:O	2.08	0.53
1:A:408:GLN:CD	1:A:408:GLN:O	2.52	0.53
1:A:478:ASP:OD2	1:A:1141:ARG:NH2	2.39	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:157:LYS:HZ1	1:A:261:THR:HB	1.74	0.53
1:A:394:LEU:C	1:A:396:GLU:H	2.16	0.53
1:A:481:LEU:O	1:A:482:ALA:C	2.51	0.53
1:A:704:ARG:O	1:A:707:VAL:HB	2.09	0.53
1:A:173:ILE:HD13	1:A:175:TYR:HE1	1.74	0.53
1:A:290:GLU:CD	1:A:408:GLN:HG3	2.33	0.53
1:A:524:LYS:HB3	1:A:637:LYS:O	2.09	0.53
1:A:1137:CYS:SG	3:A:2072:F3S:S3	3.07	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:13:PRO:HB2	1:A:197:THR:OG1	2.08	0.52
1:A:559:LEU:HD23	1:A:560:GLN:O	2.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1419:ASN:HD21	1:A:1443:ASN:ND2	2.07	0.52
1:A:635:ARG:HH11	1:A:635:ARG:CG	2.22	0.52
1:A:720:ILE:HD11	1:A:731:ILE:HD12	1.91	0.52
1:A:1021:ASP:O	1:A:1024:GLN:HB3	2.10	0.52
1:A:1338:ASN:OD1	1:A:1369:THR:HG23	2.10	0.52
1:A:289:LEU:HB3	1:A:389:MET:HE1	1.91	0.52
1:A:375:GLU:N	1:A:375:GLU:OE1	2.43	0.52
1:A:418:TRP:O	1:A:418:TRP:CD2	2.62	0.52
1:A:768:PHE:HE1	1:A:783:PHE:HZ	1.57	0.52
1:A:798:SER:H	1:A:801:MET:HE2	1.74	0.52
1:A:887:THR:O	1:A:888:LEU:C	2.50	0.52
1:A:677:TRP:NE1	1:A:694:ILE:O	2.27	0.52
1:A:872:THR:O	1:A:1127:PHE:O	2.27	0.52
1:A:877:LEU:HG	1:A:877:LEU:O	2.09	0.52
1:A:1081:GLU:HG3	1:A:1120:MET:CE	2.38	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:602:ASP:C	1:A:604:PRO:HD3	2.35	0.52
1:A:876:SER:HA	1:A:902:GLY:HA3	1.90	0.52
1:A:1008:ASP:HB2	1:A:1366:TYR:HE1	1.75	0.52
1:A:52:ARG:HD2	5:A:2076:HOH:O	2.09	0.52
1:A:353:ARG:NH2	1:A:1329:ALA:O	2.43	0.52
1:A:447:GLN:HB3	1:A:780:LEU:HD21	1.92	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:686:MET:C	1:A:692:ASP:HB2	2.34	0.52
1:A:92:TYR:O	1:A:93:VAL:C	2.52	0.51
1:A:910:ARG:C	1:A:912:LEU:H	2.18	0.51
1:A:221:MET:HE1	1:A:271:SER:C	2.36	0.51
1:A:329:PRO:HB3	1:A:349:LEU:CB	2.40	0.51
1:A:978:GLN:O	4:A:2073:AKG:H41	2.10	0.51
1:A:1081:GLU:HA	1:A:1120:MET:HE3	1.92	0.51
1:A:204:HIS:CG	1:A:219:GLN:O	2.63	0.51
1:A:484:LEU:HD23	1:A:1211:LEU:HD13	1.91	0.51
1:A:1198:GLY:C	1:A:1200:THR:H	2.19	0.51
1:A:445:GLN:CD	1:A:777:ALA:HB2	2.36	0.51
1:A:686:MET:O	1:A:692:ASP:CB	2.52	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1130:ILE:CD1	1:A:1130:ILE:N	2.69	0.51
1:A:872:THR:HB	1:A:892:MET:HG3	1.92	0.51
1:A:1317:ASN:OD1	1:A:1321:MET:HB3	2.10	0.51
1:A:2:GLY:CA	1:A:28:MET:CE	2.89	0.51
1:A:179:VAL:HB	1:A:183:ILE:CG2	2.39	0.51
1:A:744:TYR:CD2	1:A:744:TYR:O	2.63	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:514:LEU:C	1:A:514:LEU:CD1	2.83	0.51
1:A:768:PHE:CE2	1:A:771:MET:CB	2.94	0.51
1:A:1461:LEU:HD11	1:A:1465:ILE:HD11	1.93	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:124:ASN:ND2	1:A:213:PRO:O	2.44	0.51
1:A:140:ALA:O	1:A:141:GLY:C	2.53	0.51
1:A:204:HIS:CE1	1:A:219:GLN:HB3	2.45	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:1173:PHE:O	1:A:1177:ILE:HG12	2.11	0.51
1:A:377:ASP:C	1:A:377:ASP:OD1	2.53	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:1228:THR:CG2	1:A:1232:ARG:HH21	2.24	0.51
1:A:403:TYR:O	1:A:406:LYS:N	2.43	0.50
1:A:540:LYS:N	5:A:2080:HOH:O	2.44	0.50
1:A:1354:PRO:HB3	5:A:2110:HOH:O	2.10	0.50
1:A:77:VAL:HG12	1:A:79:LEU:HG	1.93	0.50
1:A:843:ARG:HG3	1:A:1112:TRP:CH2	2.46	0.50
1:A:874:GLY:CA	1:A:900:ASN:HB3	2.41	0.50
1:A:877:LEU:HD23	1:A:988:ILE:HD13	1.93	0.50
1:A:480:PRO:HB3	1:A:840:THR:HA	1.93	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
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:1119:LEU:HD13	1:A:1203:LEU:HD21	1.94	0.50
1:A:801:MET:HE3	1:A:802:SER:HB3	1.92	0.50
1:A:1080:TRP:CZ3	1:A:1120:MET:CE	2.94	0.50
1:A:452:TYR:CE1	1:A:668:LEU:HD13	2.47	0.50
1:A:1065:THR:HB	1:A:1067:ALA:H	1.77	0.50
1:A:1185:LEU:O	1:A:1189:GLY:N	2.39	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:971:ALA:HB3	1:A:1065:THR:CG2	2.42	0.49
1:A:269:SER:O	1:A:270:ASP:C	2.55	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:4:GLY:HA3	1:A:203:TYR:CZ	2.48	0.49
1:A:338:LYS:O	1:A:394:LEU:CD2	2.58	0.49
1:A:559:LEU:HD22	1:A:596:GLU:N	2.27	0.49
1:A:1418:ARG:HA	1:A:1441:LYS:HB3	1.94	0.49
1:A:207:PHE:C	1:A:207:PHE:HD2	2.21	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:574:ASN:C	1:A:574:ASN:OD1	2.55	0.49
1:A:608:ILE:HG21	1:A:615:PHE:CZ	2.47	0.49
1:A:955:GLU:O	1:A:956:TYR:C	2.56	0.49
1:A:1024:GLN:HA	1:A:1283:ARG:HH21	1.78	0.49
1:A:1404:TYR:CD1	1:A:1404:TYR:N	2.80	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:532:LYS:C	1:A:534:GLU:H	2.21	0.49
1:A:696:LEU:N	1:A:697:PRO:HD2	2.28	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: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: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:473:PHE:CG	1:A:474:CYS:N	2.77	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:1315:ALA:O	1:A:1316:PHE:C	2.56	0.49
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:711:LEU:O	1:A:712:PHE:C	2.55	0.48
1:A:490:LEU:N	1:A:490:LEU:HD23	2.28	0.48
1:A:663:ALA:C	1:A:664:ILE:CG1	2.86	0.48
1:A:911:TYR:O	1:A:912:LEU:HD23	2.14	0.48
1:A:1285:SER:HA	1:A:1321:MET:HE1	1.94	0.48
1:A:671:GLU:OE1	1:A:674:ARG:NH1	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1008:ASP:HB2	1:A:1366:TYR:CE1	2.48	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:693:ARG:C	1:A:694:ILE:HG12	2.38	0.48
1:A:1148:CYS:C	1:A:1150:VAL:H	2.21	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:797:ASN:HA	1:A:801:MET:HE2	1.95	0.48
1:A:1054:ASP:C	1:A:1055:ILE:HG13	2.38	0.48
1:A:148:LEU:O	1:A:151:ALA:N	2.46	0.48
1:A:189:LEU:O	1:A:190:ASP:C	2.57	0.48
1:A:759:ALA:O	1:A:762:ALA:HB3	2.13	0.48
1:A:1420:VAL:HB	1:A:1442:ILE:HA	1.96	0.48
1:A:284:THR:OG1	1:A:529:LEU:HD22	2.13	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:145:ASP:OD2	1:A:169:SER:HB2	2.13	0.48
1:A:314:ASP:CG	1:A:415:TYR:HD1	2.21	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:875:MET:SD	1:A:1132:MET:HE2	2.54	0.48
1:A:1065:THR:HG21	1:A:1068:SER:HG	1.76	0.48
1:A:145:ASP:O	1:A:146:ARG:C	2.57	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:1316:PHE:CD2	1:A:1336:GLY:HA3	2.49	0.48
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:954:PRO:HG3	1:A:1316:PHE:HB3	1.95	0.47
1:A:1021:ASP:OD2	1:A:1335:LYS:NZ	2.43	0.47
1:A:484:LEU:HD23	1:A:1211:LEU:CD1	2.44	0.47
1:A:149:TYR:CG	1:A:283:ARG:HG3	2.49	0.47
1:A:1000:LEU:HA	1:A:1000:LEU:HD23	1.59	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1017:GLN:HG3	1:A:1311:GLN:HG3	1.97	0.47
1:A:219:GLN:O	1:A:219:GLN:CG	2.52	0.47
1:A:794:TYR:CE1	1:A:837:ARG:HB3	2.50	0.47
1:A:1146:ASN:C	1:A:1154:THR:HG23	2.39	0.47
1:A:1363:THR:HG23	1:A:1385:VAL:HG21	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: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:1030:GLN:HG2	1:A:1240:VAL:HG13	1.97	0.47
1:A:1275:ASN:OD1	1:A:1275:ASN:C	2.57	0.47
1:A:135:CYS:HB3	1:A:139:CYS:HB2	1.97	0.47
1:A:519:ALA:C	1:A:520:MET:HG2	2.40	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:223:LEU:HD12	1:A:335:SER:O	2.15	0.47
1:A:239:TRP:NE1	1:A:728:GLY:HA3	2.29	0.47
1:A:403:TYR:N	1:A:403:TYR:CD1	2.60	0.47
1:A:486:HIS:CE1	1:A:838:PRO:HB3	2.50	0.47
1:A:1264:GLN:NE2	1:A:1298:GLU:OE1	2.47	0.47
1:A:2:GLY:CA	1:A:28:MET:HE2	2.44	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:1145:THR:HG22	1:A:1147:ASN:CG	2.40	0.46
1:A:1451:ARG:O	1:A:1452:ILE:C	2.58	0.46
1:A:364:LEU:HG	1:A:365:GLY:N	2.31	0.46
1:A:1119:LEU:O	1:A:1198:GLY:CA	2.60	0.46
1:A:453:THR:O	1:A:454:ALA:C	2.59	0.46
1:A:477:ASP:OD1	1:A:479:THR:HG23	2.15	0.46
1:A:548:GLU:OE2	1:A:603:ARG:NH2	2.49	0.46
1:A:770:GLY:C	1:A:771:MET:SD	2.98	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:212:MET:CE	1:A:1094:ASN:HA	2.46	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:722:LEU:C	1:A:724:ALA:N	2.72	0.46
1:A:831:ARG:O	1:A:834:LEU:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1118:ALA:O	1:A:1197:ILE:HA	2.16	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:1070:LEU:O	1:A:1071:SER:C	2.58	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:1139:MET:HB3	1:A:1139:MET:HE3	1.52	0.46
1:A:1228:THR:HG23	1:A:1232:ARG:HE	1.80	0.46
1:A:342:ALA:O	1:A:389:MET:HA	2.15	0.46
1:A:349:LEU:O	1:A:350:ARG:NH1	2.44	0.46
1:A:513:ASN:HA	1:A:516:MET:CE	2.46	0.46
1:A:682:THR:O	1:A:683:GLN:C	2.59	0.46
1:A:513:ASN:HA	1:A:516:MET:HE2	1.97	0.46
1:A:418:TRP:O	1:A:418:TRP:HE3	1.92	0.46
1:A:727:HIS:O	1:A:728:GLY:C	2.56	0.46
1:A:1383:PHE:O	1:A:1384:ALA:HB3	2.15	0.46
1:A:100:GLU:C	1:A:102:LEU:H	2.17	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:501:GLN:NE2	1:A:1035:LEU:CB	2.77	0.46
1:A:867:VAL:CG1	1:A:895:LEU:CB	2.89	0.46
1:A:1004:PRO:HB2	1:A:1005:PRO:HD3	1.96	0.46
1:A:1096:LEU:O	1:A:1099:ARG:HB2	2.16	0.46
1:A:289:LEU:HB3	1:A:389:MET:CE	2.46	0.45
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: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:221:MET:HE1	1:A:272:TYR:N	2.31	0.45
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: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
1:A:113:ASN:OD1	1:A:115:ASP:HB2	2.15	0.45
1:A:212:MET:HE2	1:A:1094:ASN:HA	1.99	0.45
1:A:698:THR:O	1:A:702:ASN:HB2	2.17	0.45
1:A:832:GLN:HG2	5:A:2092:HOH:O	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:324:GLU:H	1:A:324:GLU:HG3	1.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:418:TRP:HZ3	1:A:422:GLN:HB3	1.79	0.45
1:A:722:LEU:O	1:A:723:LEU:C	2.60	0.45
1:A:12:LYS:HD3	1:A:12:LYS:HA	1.67	0.45
1:A:94:GLU:O	1:A:95:GLU:C	2.59	0.45
1:A:186:GLU:OE1	1:A:186:GLU:HA	2.17	0.45
1:A:250:SER:C	1:A:252:TRP:H	2.25	0.45
1:A:561:VAL:HG11	1:A:599:VAL:HG23	1.97	0.45
1:A:567:LEU:HD23	1:A:567:LEU:HA	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:996:PRO:O	1:A:997:GLY:C	2.58	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:843:ARG:HB2	1:A:1116:MET:HE3	1.98	0.45
1:A:1216:ASN:C	1:A:1216:ASN:ND2	2.74	0.45
1:A:239:TRP:HE1	1:A:728:GLY:CA	2.28	0.45
1:A:418:TRP:HB2	1:A:533:ALA:HB1	1.99	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:1273:LEU:HD21	1:A:1305:PHE:CD2	2.52	0.45
1:A:87:GLU:O	1:A:88:VAL:C	2.59	0.44
1:A:152:ARG:HD3	1:A:222:ARG:NH1	2.32	0.44
1:A:474:CYS:CB	1:A:1143:CYS:HB2	2.47	0.44
1:A:570:LEU:HG	1:A:613:GLN:CG	2.46	0.44
1:A:1354:PRO:CB	5:A:2110:HOH:O	2.64	0.44
1:A:443:VAL:CG2	1:A:675:GLN:NE2	2.68	0.44
1:A:514:LEU:CD1	1:A:515:VAL:N	2.80	0.44
1:A:1499:GLU:O	1:A:1500:LYS:C	2.58	0.44
1:A:17:LEU:CD1	1:A:201:ALA:HB2	2.47	0.44
1:A:53:GLU:O	1:A:56:ALA:HB3	2.17	0.44
1:A:296:VAL:N	1:A:297:PRO:CD	2.79	0.44
1:A:508:ASP:OD1	1:A:508:ASP:C	2.60	0.44
1:A:910:ARG:O	1:A:939:ASN:HB2	2.17	0.44
1:A:1080:TRP:HZ3	1:A:1120:MET:HE2	1.81	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: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:546:VAL:HB	1:A:550:GLU:HB2	2.00	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:547:ASN:N	1:A:550:GLU:HG3	2.32	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:1395:GLU:O	1:A:1414:GLY:HA3	2.17	0.44
1:A:309:TYR:HB3	1:A:312:ILE:CG2	2.48	0.44
1:A:322:LEU:HA	1:A:322:LEU:HD12	1.70	0.44
1:A:501:GLN:HE21	1:A:1035:LEU:HA	1.81	0.44
1:A:443:VAL:O	1:A:447:GLN:HB2	2.18	0.44
1:A:860:VAL:HG21	1:A:1182:ARG:O	2.18	0.44
1:A:1148:CYS:C	1:A:1150:VAL:N	2.73	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:1021:ASP:HA	1:A:1279:THR:HG21	2.00	0.44
1:A:552:GLN:O	1:A:553:ALA:C	2.61	0.44
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:1259:GLU:CD	1:A:1267:ALA:HB2	2.43	0.43
1:A:2:GLY:O	1:A:204:HIS:HA	2.18	0.43
1:A:146:ARG:O	1:A:149:TYR:HB3	2.18	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:554:ILE:HG21	1:A:641:ILE:HD11	1.99	0.43
1:A:629:LEU:HD23	1:A:635:ARG:HD2	2.01	0.43
1:A:1175:TYR:HD2	1:A:1175:TYR:HA	1.63	0.43
1:A:1309:ALA:HB3	1:A:1329:ALA:CB	2.48	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:155:ILE:HG23	1:A:163:PHE:CZ	2.53	0.43
1:A:406:LYS:HA	1:A:409:ALA:HB3	2.00	0.43
1:A:601:THR:HG23	1:A:643:ASP:OD2	2.19	0.43
1:A:1325:LEU:CD2	1:A:1329:ALA:HB2	2.49	0.43
1:A:17:LEU:HD11	1:A:200:PHE:C	2.43	0.43
1:A:289:LEU:CA	1:A:389:MET:HE1	2.49	0.43
1:A:385:ALA:HB3	1:A:388:GLN:CD	2.42	0.43
1:A:832:GLN:HA	1:A:835:LYS:HG3	2.01	0.43
1:A:1136:GLY:O	1:A:1150:VAL:HG11	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1419:ASN:HD22	1:A:1443:ASN:HB2	1.84	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:148:LEU:O	1:A:149:TYR:C	2.61	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: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:580:LEU:O	1:A:581:THR:C	2.61	0.43
1:A:768:PHE:CD2	1:A:771:MET:CG	2.92	0.43
1:A:1244:GLY:O	1:A:1245:PRO:C	2.61	0.43
1:A:848:PHE:HB3	1:A:1188:LEU:HD21	2.00	0.43
1:A:315:PHE:O	1:A:319:TYR:CD1	2.72	0.42
1:A:474:CYS:HB2	1:A:1143:CYS:HB2	2.01	0.42
1:A:634:LEU:O	1:A:635:ARG:C	2.62	0.42
1:A:636:LEU:HA	1:A:636:LEU:HD12	1.70	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:1065:THR:HG22	4:A:2073:AKG:O1	2.18	0.42
1:A:323:GLN:HE21	1:A:528:LEU:HD22	1.85	0.42
1:A:1005:PRO:HG2	1:A:1007:HIS:CE1	2.54	0.42
1:A:1430:TYR:HE2	1:A:1493:GLN:OE1	2.00	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:500:ALA:HB1	1:A:504:ASN:O	2.19	0.42
1:A:910:ARG:HD2	1:A:938:ALA:O	2.19	0.42
1:A:1082:LEU:HD23	1:A:1082:LEU:HA	1.75	0.42
1:A:288:PRO:HB2	1:A:334:PHE:CD1	2.54	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:694:ILE:HD12	1:A:694:ILE:HG23	1.36	0.42
1:A:728:GLY:O	1:A:729:ALA:O	2.37	0.42
1:A:809:VAL:HG12	1:A:1172:ASN:HB2	2.02	0.42
1:A:551:LEU:HD12	1:A:551:LEU:HA	1.79	0.42
1:A:561:VAL:HG13	1:A:597:ILE:HG22	2.01	0.42
1:A:1451:ARG:NH1	1:A:1491:PHE:H	2.16	0.42
1:A:421:ILE:C	1:A:422:GLN:O	2.63	0.42
1:A:97:VAL:HG11	1:A:133:VAL:CG2	2.50	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:HD12	1:A:1446:ILE:HG21	1.84	0.42
1:A:193:ASN:HA	1:A:194:PRO:HD3	1.90	0.41
1:A:499:PHE:CG	1:A:973:PRO:CB	3.02	0.41
1:A:522:LEU:HD23	1:A:522:LEU:HA	1.83	0.41
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:50:ILE:CD1	1:A:170:CYS:C	2.93	0.41
1:A:53:GLU:O	1:A:56:ALA:CB	2.67	0.41
1:A:350:ARG:HD2	1:A:350:ARG:HH11	1.59	0.41
1:A:421:ILE:O	1:A:421:ILE:CG2	2.68	0.41
1:A:509:PRO:HB3	1:A:716:SER:HB3	2.01	0.41
1:A:299:ALA:HB2	1:A:346:ARG:NH2	2.35	0.41
1:A:399:ILE:HG22	1:A:399:ILE:O	2.21	0.41
1:A:399:ILE:HG22	1:A:404:GLN:CG	2.42	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:148:LEU:HD23	1:A:169:SER:CA	2.49	0.41
1:A:357:THR:OG1	1:A:361:TYR:CB	2.68	0.41
1:A:358:LYS:H	1:A:358:LYS:HG3	1.55	0.41
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:7:ALA:HB3	1:A:362:ILE:HG23	2.01	0.41
1:A:131:ILE:HG12	1:A:133:VAL:HG23	2.03	0.41
1:A:237:ILE:HD13	1:A:237:ILE:HG21	1.81	0.41
1:A:1132:MET:HB2	1:A:1132:MET:HE3	1.27	0.41
1:A:1385:VAL:O	1:A:1404:TYR:N	2.53	0.41
1:A:47:MET:O	1:A:201:ALA:HA	2.21	0.41
1:A:64:LEU:HA	1:A:65:PRO:HD3	1.92	0.41
1:A:233:LEU:HD12	1:A:233:LEU:HA	1.81	0.41
1:A:566:THR:HB	1:A:601:THR:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:882:ARG:HB2	1:A:886:GLU:OE2	2.19	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:309:TYR:O	1:A:312:ILE:CG2	2.68	0.41
1:A:475:MET:HB3	1:A:475:MET:HE2	1.39	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:1053:ALA:O	1:A:1241:HIS:HD2	2.04	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:1292:TYR:O	1:A:1293:GLY:C	2.63	0.41
1:A:8:ASN:N	1:A:199:ASN:O	2.52	0.41
1:A:212:MET:HE3	1:A:1094:ASN:OD1	2.21	0.41
1:A:219:GLN:O	1:A:219:GLN:HG2	2.20	0.41
1:A:229:GLU:O	1:A:328:GLY:HA3	2.21	0.41
1:A:275:ASP:HB3	1:A:276:SER:H	1.76	0.41
1:A:603:ARG:N	1:A:604:PRO:HD3	2.36	0.41
1:A:1145:THR:CG2	1:A:1147:ASN:ND2	2.84	0.41
1:A:1416:VAL:O	1:A:1441:LYS:NZ	2.40	0.41
1:A:475:MET:HE3	1:A:476:GLY:H	1.86	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:1081:GLU:CG	1:A:1120:MET:HE1	2.42	0.41
1:A:1258:GLN:O	1:A:1262:ASN:HB2	2.21	0.41
1:A:46:VAL:N	1:A:220:PRO:HG2	2.36	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:101:LYS:HE3	1:A:137:GLU:CD	2.46	0.40
1:A:145:ASP:O	1:A:149:TYR:N	2.41	0.40
1:A:234:LEU:C	1:A:234:LEU:HD13	2.47	0.40
1:A:411:GLN:CG	1:A:412:LYS:H	2.35	0.40
1:A:1012:ILE:HD11	1:A:1047:GLY:C	2.46	0.40
1:A:1382:ARG:O	1:A:1385:VAL:HG22	2.21	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:903:GLU:HG2	1:A:946:ALA:CB	2.51	0.40
1:A:1080:TRP:CZ3	1:A:1120:MET:HE2	2.56	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:386:PRO:HD3	1:A:1381:GLU:OE1	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:ILE:O	1:A:421:ILE:HG22	2.21	0.40
1:A:570:LEU:HD13	1:A:571:ASP:CG	2.47	0.40
1:A:916:ASP:OD1	1:A:916:ASP:N	2.53	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

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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1467/1520 (96%)	1215 (83%)	196 (13%)	56 (4%)	2 5

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	955 (80%)	245 (20%)	1 3

All (245) 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	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
1	A	95	GLU
1	A	96	VAL
1	A	99	LEU
1	A	102	LEU
1	A	109	GLU
1	A	115	ASP
1	A	125	GLN
1	A	133	VAL
1	A	137	GLU
1	A	147	ARG
1	A	148	LEU

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Mol	Chain	Res	Type
1	A	152	ARG
1	A	154	ILE
1	A	157	LYS
1	A	159	LEU
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	211	THR
1	A	219	GLN
1	A	224	LEU
1	A	230	ILE
1	A	234	LEU
1	A	245	LYS
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	340	VAL
1	A	356	ILE
1	A	358	LYS
1	A	370	VAL
1	A	372	ASP
1	A	376	VAL
1	A	377	ASP
1	A	379	VAL
1	A	394	LEU
1	A	397	GLN
1	A	398	LYS
1	A	401	LYS

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Mol	Chain	Res	Type
1	A	403	TYR
1	A	406	LYS
1	A	411	GLN
1	A	419	ILE
1	A	422	GLN
1	A	444	LEU
1	A	453	THR
1	A	457	VAL
1	A	466	SER
1	A	475	MET
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	554	ILE
1	A	558	GLN
1	A	559	LEU
1	A	560	GLN
1	A	570	LEU
1	A	580	LEU
1	A	584	VAL
1	A	590	THR
1	A	600	LEU
1	A	601	THR
1	A	602	ASP
1	A	603	ARG
1	A	605	ASN
1	A	608	ILE
1	A	611	GLU
1	A	614	SER
1	A	616	ILE
1	A	625	VAL

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Mol	Chain	Res	Type
1	A	629	LEU
1	A	630	ILE
1	A	634	LEU
1	A	635	ARG
1	A	640	LEU
1	A	641	ILE
1	A	649	SER
1	A	650	THR
1	A	656	LEU
1	A	664	ILE
1	A	668	LEU
1	A	678	LEU
1	A	679	ASP
1	A	684	LYS
1	A	686	MET
1	A	693	ARG
1	A	704	ARG
1	A	705	GLN
1	A	706	SER
1	A	715	LEU
1	A	731	ILE
1	A	735	ILE
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	797	ASN
1	A	801	MET
1	A	809	VAL
1	A	824	TYR
1	A	829	LEU
1	A	834	LEU
1	A	843	ARG
1	A	855	ILE
1	A	857	LEU
1	A	863	VAL

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Mol	Chain	Res	Type
1	A	867	VAL
1	A	872	THR
1	A	877	LEU
1	A	895	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	1017	GLN
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	1110	THR
1	A	1120	MET
1	A	1130	ILE
1	A	1132	MET
1	A	1133	ILE
1	A	1139	MET
1	A	1142	VAL
1	A	1145	THR
1	A	1148	CYS
1	A	1150	VAL
1	A	1154	THR
1	A	1161	GLN
1	A	1175	TYR
1	A	1179	GLU
1	A	1191	ARG
1	A	1192	SER
1	A	1193	LEU
1	A	1194	ASP

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Mol	Chain	Res	Type
1	A	1200	THR
1	A	1208	ASP
1	A	1211	LEU
1	A	1214	THR
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	1282	THR
1	A	1311	GLN
1	A	1355	GLU
1	A	1359	ILE
1	A	1360	ILE
1	A	1363	THR
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	1416	VAL
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

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Mol	Chain	Res	Type
1	A	1449	LEU
1	A	1451	ARG
1	A	1452	ILE
1	A	1453	THR
1	A	1463	SER
1	A	1464	LEU
1	A	1466	THR
1	A	1469	VAL
1	A	1488	LEU
1	A	1490	LYS
1	A	1491	PHE
1	A	1504	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	120	GLN
1	A	127	HIS
1	A	204	HIS
1	A	226	HIS
1	A	236	ASN
1	A	323	GLN
1	A	486	HIS
1	A	501	GLN
1	A	513	ASN
1	A	527	ASN
1	A	552	GLN
1	A	646	GLN
1	A	651	HIS
1	A	652	HIS
1	A	675	GLN
1	A	730	GLN
1	A	769	HIS
1	A	797	ASN
1	A	885	HIS
1	A	934	ASN
1	A	978	GLN
1	A	1023	HIS
1	A	1052	ASN
1	A	1147	ASN
1	A	1216	ASN

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Mol	Chain	Res	Type
1	A	1263	HIS
1	A	1294	ASN
1	A	1304	ASN
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

3 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	AKG	A	2073	-	9,9,9	2.26	3 (33%)	11,11,11	1.60	4 (36%)
3	F3S	A	2072	1	0,9,9	-	-	-		
2	FMN	A	2070	-	33,33,33	1.21	4 (12%)	48,50,50	1.19	6 (12%)

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
4	AKG	A	2073	-	-	6/9/9/9	-
3	F3S	A	2072	1	-	-	0/3/3/3
2	FMN	A	2070	-	-	5/18/18/18	0/3/3/3

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2073	AKG	O5-C2	4.70	1.32	1.23
4	A	2073	AKG	O1-C1	3.86	1.32	1.22
2	A	2070	FMN	C4A-N5	3.23	1.37	1.30
4	A	2073	AKG	O3-C5	2.72	1.31	1.22
2	A	2070	FMN	C4A-C10	-2.21	1.37	1.44
2	A	2070	FMN	O2'-C2'	-2.04	1.39	1.43
2	A	2070	FMN	C9A-N10	-2.03	1.37	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2070	FMN	C4A-C10-N10	3.13	120.96	116.48
2	A	2070	FMN	C4-C4A-N5	2.72	121.97	118.21
4	A	2073	AKG	O4-C5-O3	-2.71	116.36	123.33
2	A	2070	FMN	C4-N3-C2	-2.68	120.89	125.64
2	A	2070	FMN	C10-C4A-N5	-2.57	119.57	124.81
2	A	2070	FMN	O4-C4-C4A	-2.34	120.36	126.53
4	A	2073	AKG	O4-C5-C4	2.30	121.28	114.00
2	A	2070	FMN	C4A-C4-N3	2.30	119.11	113.25
4	A	2073	AKG	O5-C2-C1	-2.17	116.57	119.67
4	A	2073	AKG	C3-C2-C1	2.02	119.29	115.86

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2073	AKG	O2-C1-C2-C3
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	O1-C1-C2-C3

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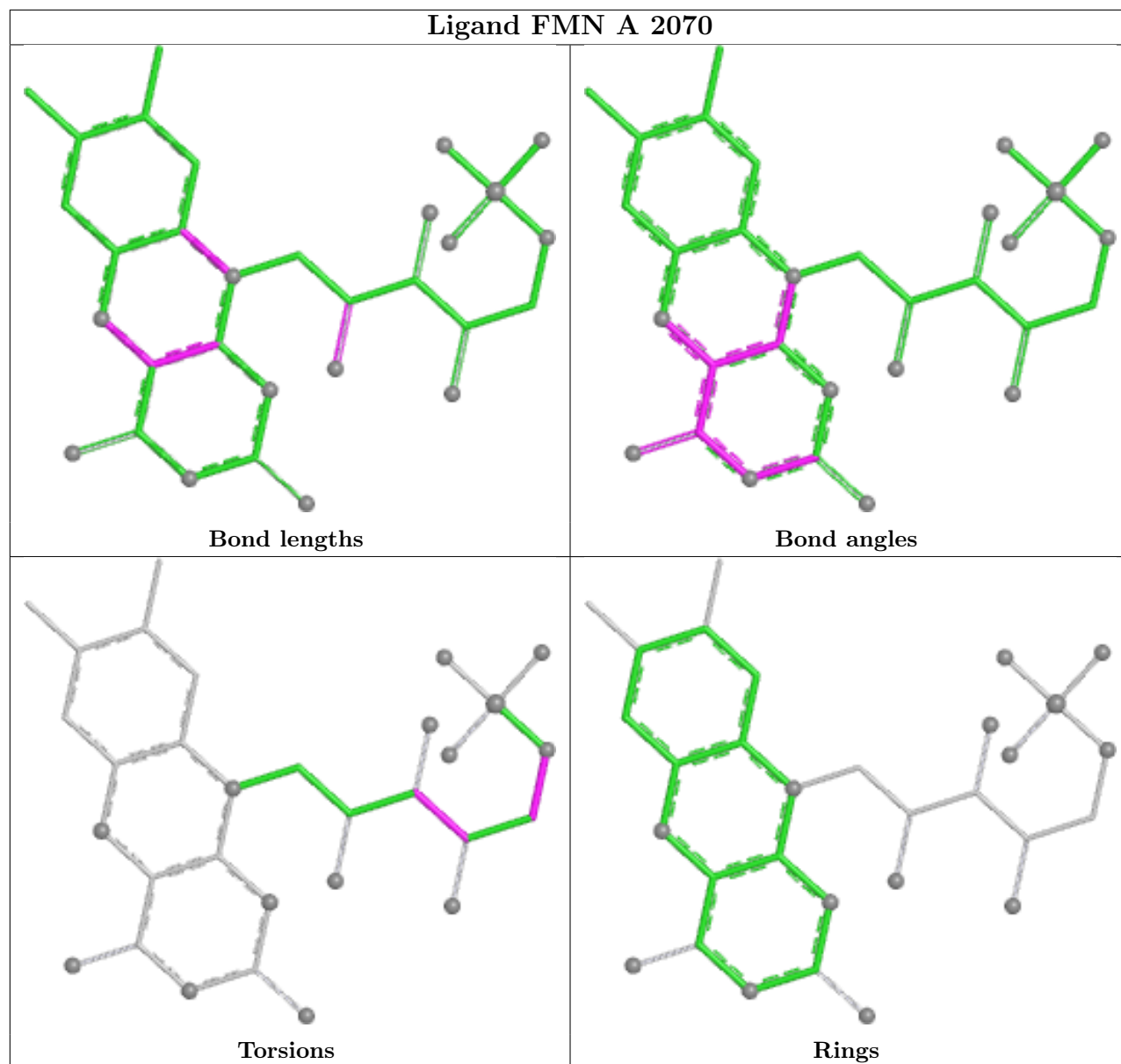
Mol	Chain	Res	Type	Atoms
4	A	2073	AKG	O2-C1-C2-O5
2	A	2070	FMN	C4'-C5'-O5'-P
4	A	2073	AKG	O1-C1-C2-O5
4	A	2073	AKG	C3-C4-C5-O3
4	A	2073	AKG	C3-C4-C5-O4

There are no ring outliers.

2 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2073	AKG	2	0
3	A	2072	F3S	4	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%)	0.61	147 (9%)	12 10	8, 42, 64, 100	0

All (147) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	418	TRP	6.7
1	A	376	VAL	6.3
1	A	500	ALA	5.2
1	A	41	GLY	5.2
1	A	1263	HIS	4.8
1	A	1265	THR	4.7
1	A	501	GLN	4.6
1	A	776	MET	4.6
1	A	502	VAL	4.5
1	A	377	ASP	4.5
1	A	474	CYS	4.4
1	A	35	SER	4.3
1	A	413	TYR	4.2
1	A	504	ASN	4.2
1	A	353	ARG	4.0
1	A	194	PRO	4.0
1	A	560	GLN	4.0
1	A	468	GLY	3.9
1	A	755	GLY	3.8
1	A	40	SER	3.8
1	A	415	TYR	3.8
1	A	251	GLY	3.8
1	A	1264	GLN	3.7
1	A	475	MET	3.7
1	A	692	ASP	3.6
1	A	1433	ASP	3.6
1	A	678	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	745	ALA	3.5
1	A	773	PHE	3.5
1	A	409	ALA	3.5
1	A	605	ASN	3.5
1	A	492	TYR	3.4
1	A	192	LYS	3.3
1	A	680	GLU	3.3
1	A	219	GLN	3.3
1	A	552	GLN	3.3
1	A	750	THR	3.3
1	A	9	LEU	3.3
1	A	207	PHE	3.3
1	A	220	PRO	3.2
1	A	28	MET	3.2
1	A	1490	LYS	3.2
1	A	547	ASN	3.2
1	A	615	PHE	3.2
1	A	205	ARG	3.2
1	A	378	ILE	3.2
1	A	1475	PRO	3.1
1	A	1260	ALA	3.1
1	A	777	ALA	3.1
1	A	419	ILE	3.0
1	A	476	GLY	3.0
1	A	507	ILE	3.0
1	A	554	ILE	3.0
1	A	315	PHE	3.0
1	A	505	PRO	2.9
1	A	1	CYS	2.9
1	A	1487	TYR	2.9
1	A	1353	ALA	2.9
1	A	582	ASN	2.9
1	A	195	GLY	2.9
1	A	902	GLY	2.9
1	A	826	HIS	2.9
1	A	509	PRO	2.8
1	A	752	ARG	2.8
1	A	42	ASP	2.8
1	A	114	SER	2.8
1	A	211	THR	2.8
1	A	137	GLU	2.8
1	A	613	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	182	ILE	2.7
1	A	715	LEU	2.7
1	A	1483	ASN	2.7
1	A	33	GLY	2.7
1	A	356	ILE	2.6
1	A	258	GLU	2.6
1	A	733	GLU	2.6
1	A	1259	GLU	2.6
1	A	126	PRO	2.6
1	A	39	ASP	2.6
1	A	44	ALA	2.6
1	A	499	PHE	2.5
1	A	772	ALA	2.5
1	A	121	ALA	2.5
1	A	25	LEU	2.5
1	A	1500	LYS	2.5
1	A	1507	ASN	2.5
1	A	37	ASP	2.5
1	A	26	GLY	2.5
1	A	1351	SER	2.4
1	A	14	ASP	2.4
1	A	506	PRO	2.4
1	A	399	ILE	2.4
1	A	417	GLU	2.4
1	A	512	GLU	2.4
1	A	479	THR	2.4
1	A	363	VAL	2.4
1	A	824	TYR	2.4
1	A	1491	PHE	2.4
1	A	829	LEU	2.4
1	A	728	GLY	2.4
1	A	514	LEU	2.3
1	A	901	SER	2.3
1	A	247	LEU	2.3
1	A	15	HIS	2.3
1	A	920	GLU	2.3
1	A	1446	ILE	2.3
1	A	410	ALA	2.2
1	A	367	GLU	2.2
1	A	832	GLN	2.2
1	A	119	ILE	2.2
1	A	355	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	38	ASN	2.2
1	A	115	ASP	2.2
1	A	1301	ILE	2.2
1	A	503	THR	2.2
1	A	485	SER	2.2
1	A	780	LEU	2.2
1	A	825	ASP	2.2
1	A	18	VAL	2.2
1	A	1240	VAL	2.2
1	A	533	ALA	2.2
1	A	197	THR	2.2
1	A	32	GLY	2.2
1	A	117	LEU	2.2
1	A	756	LEU	2.2
1	A	810	ALA	2.1
1	A	1435	VAL	2.1
1	A	368	ALA	2.1
1	A	749	THR	2.1
1	A	113	ASN	2.1
1	A	120	GLN	2.1
1	A	441	GLN	2.1
1	A	768	PHE	2.1
1	A	693	ARG	2.1
1	A	604	PRO	2.1
1	A	394	LEU	2.1
1	A	827	TYR	2.1
1	A	116	VAL	2.1
1	A	379	VAL	2.1
1	A	570	LEU	2.1
1	A	486	HIS	2.1
1	A	784	GLY	2.1
1	A	183	ILE	2.1
1	A	21	ALA	2.0
1	A	1254	ASP	2.0
1	A	697	PRO	2.0
1	A	3	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

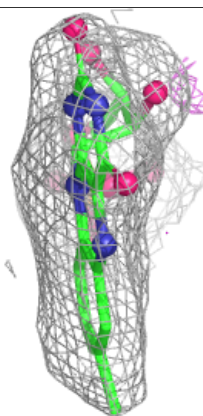
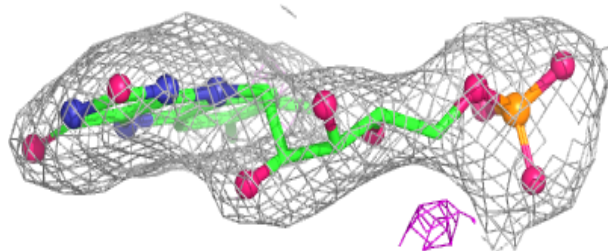
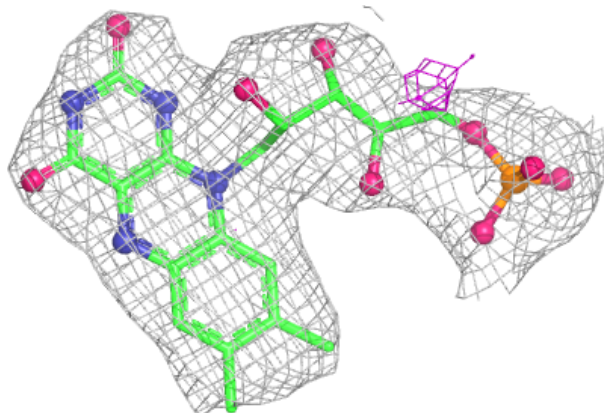
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	AKG	A	2073	10/10	0.93	0.11	81,85,87,89	0
2	FMN	A	2070	31/31	0.96	0.10	80,85,88,88	0
3	F3S	A	2072	7/7	0.97	0.09	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.

Electron density around FMN A 2070:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.