



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:50 AM UTC

PDB ID : 1EG7 / pdb_00001eg7
Title : THE CRYSTAL STRUCTURE OF FORMYLTETRAHYDROFOLATE
SYNTHETASE FROM MOORELLA THERMOACETICA
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Deposited on : 2000-02-14
Resolution : 2.50 Å(reported)

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

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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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

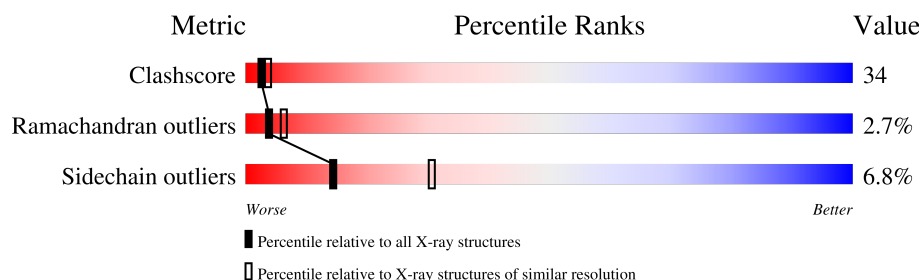
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	557	
1	B	557	

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
2	SO4	A	3	-	-	X	-
2	SO4	A	5	-	-	X	-
2	SO4	A	7	-	-	X	-
2	SO4	A	8	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8586 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.

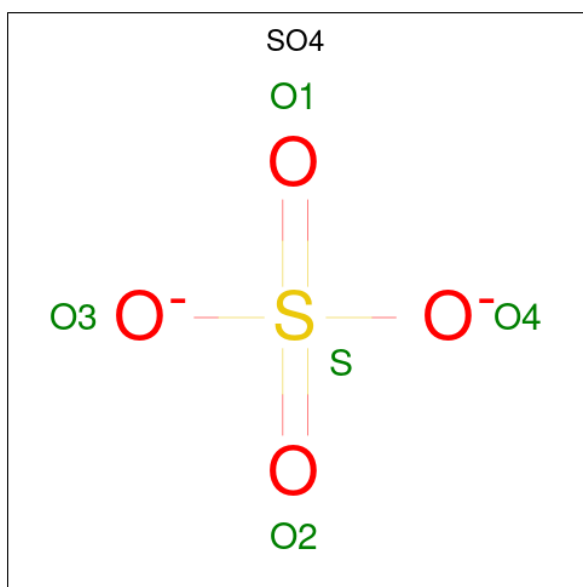
- Molecule 1 is a protein called FORMYLTETRAHYDROFOLATE SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4135	2618	716	780	21			
1	B	548	Total	C	N	O	S	0	0	0
			4127	2614	715	777	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1174	GLU	ASP	conflict	UNP P21164
A	1225	LYS	ILE	conflict	UNP P21164
A	?	-	GLU	deletion	UNP P21164
A	?	-	VAL	deletion	UNP P21164
B	1174	GLU	ASP	conflict	UNP P21164
B	1225	LYS	ILE	conflict	UNP P21164
B	?	-	GLU	deletion	UNP P21164
B	?	-	VAL	deletion	UNP P21164

- Molecule 2 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	198	Total	O	0	0
			198	198		

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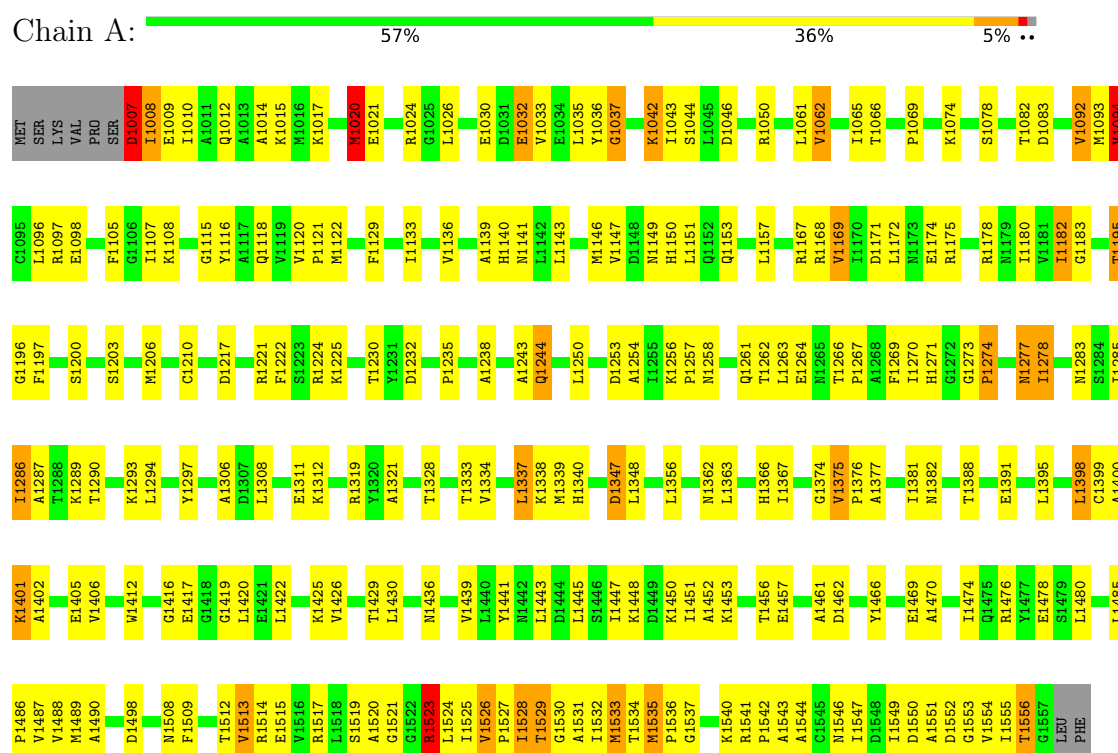
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	71	Total	O	0	0
			71	71		

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. 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. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

• Molecule 1: FORMYLTETRAHYDROFOLATE SYNTHETASE



• Molecule 1: FORMYLTETRAHYDROFOLATE SYNTHETASE



T1529	L1445	G1371	A1295	D1217
G1530	S1446	K1372	D1296	A1218
A1531	I1447	F1373	D1297	K1219
T1532	K1448	G1374	V1298	E1220
M1533	D1449	V1375	T1299	V1221
T1534	K1450	P1376	T1300	F1222
M1535	I1451	A1377	E1301	S1223
P1536		V1378	A1302	R1224
G1537	I1454	V1379	G1303	K1225
	A1455	A1380	F1304	V1226
		I1381		V1227
K1540		N1382	E1311	
R1541	I1458	A1383	K1312	V1236
P1542	Y1459	F1384	F1313	
A1543	G1460	P1385	Y1314	Q1244
A1544	A1461	T1386	D1315	
G1545	D1462	D1387	V1316	L1250
N1546		T1388		
I1547	Y1466	E1389		
D1548			R1319	D1253
T1549	K1472	N1393	Y1320	A1254
D1550		L1394	A1321	I1255
A1551	R1476		P1325	K1256
D1552	Y1477		D1326	P1257
G1553	E1478	L1398		N1258
V1554	S1479	C1399		L1259
T1555	L1480	A1400	V1329	V1260
T1556	G1481	K1401	I1330	Q1261
G1557	Y1482		V1331	T1262
LEU	G1483	E1405	A1332	L1263
PHE	N1484		T1333	E1264
	L1485		V1334	N1265
	P1486	L1408	R1335	T1266
	V1487	S1409	A1336	P1267
	M1488	W1412		A1268
	M1489	A1413	L1337	F1269
	A1490	K1414	K1338	
		G1415	M1339	I1270
		G1416		H1271
	D1498	E1417	V1343	G1272
		G1418	P1344	G1273
	P1506	G1419	K1345	P1274
		L1420		F1275
	F1509	E1421	T1350	A1276
	T1510	L1422	E1351	N1277
	I1511		M1352	I1278
	T1512	K1425	L1353	A1279
	V1513	V1426		H1280
	R1514		L1356	G1281
	E1515	L1430	R1357	C1282
	V1516	E1431		N1283
	R1517	S1432	F1360	S1284
	L1518	R1433	A1361	I1285
	S1519	P1434	M1362	I1286
	A1520	S1435	L1363	A1287
		N1436	E1364	T1288
	R1523	F1437	K1365	T1289
	L1524		H1366	T1290
	I1525	L1440	I1367	A1291
	V1526		E1368	L1292
	P1527	L1443	M1369	K1293
	I1528	D1444	I1370	L1294

4 Data and refinement statistics

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

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	160.88Å 160.88Å 256.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.99 – 2.50	Depositor
% Data completeness (in resolution range)	90.6 (19.99-2.50)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.253 , 0.301	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	8586	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.57	5/4203 (0.1%)	1.05	27/5691 (0.5%)
1	B	0.50	1/4195 (0.0%)	0.99	14/5680 (0.2%)
All	All	0.53	6/8398 (0.1%)	1.02	41/11371 (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	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1008	ILE	CA-C	13.05	1.67	1.52
1	A	1008	ILE	N-CA	11.76	1.64	1.45
1	A	1007	ASP	CA-C	6.23	1.66	1.52
1	A	1007	ASP	C-N	5.58	1.42	1.33
1	A	1007	ASP	CA-CB	5.21	1.63	1.53
1	B	1435	SER	N-CA	5.15	1.52	1.45

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1008	ILE	N-CA-C	-9.46	94.59	109.17
1	B	1015	LYS	N-CA-C	9.44	130.92	110.80
1	A	1008	ILE	CB-CA-C	-9.33	98.32	111.38
1	A	1007	ASP	CA-C-O	-8.81	105.83	120.80
1	A	1523	ARG	N-CA-C	8.45	118.20	108.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1007	ASP	N-CA-C	7.12	130.92	111.00
1	A	1007	ASP	CB-CA-C	7.02	123.44	110.10
1	B	1037	GLY	N-CA-C	-6.99	101.76	111.76
1	B	1553	GLY	N-CA-C	6.92	121.24	111.14
1	A	1007	ASP	CA-C-N	-6.76	112.94	122.34
1	A	1007	ASP	C-N-CA	-6.76	112.94	122.34
1	A	1008	ILE	N-CA-CB	6.55	124.96	112.24
1	A	1007	ASP	N-CA-CB	-6.35	99.70	110.50
1	B	1204	GLU	N-CA-C	-6.33	104.81	112.54
1	B	1169	VAL	N-CA-C	5.91	116.86	108.42
1	A	1238	ALA	N-CA-C	-5.88	104.95	111.36
1	A	1014	ALA	N-CA-C	5.88	117.34	108.46
1	B	1378	VAL	N-CA-C	5.81	116.23	108.27
1	A	1020	MET	N-CA-C	-5.64	105.03	111.07
1	A	1290	THR	N-CA-C	-5.59	105.26	111.36
1	A	1042	LYS	N-CA-C	-5.58	100.60	109.59
1	B	1051	LEU	N-CA-C	-5.57	107.07	112.97
1	A	1094	VAL	CB-CA-C	-5.55	102.35	110.62
1	B	1261	GLN	N-CA-C	5.49	116.62	108.60
1	B	1283	ASN	N-CA-C	-5.47	103.68	110.41
1	A	1074	LYS	N-CA-C	5.45	117.02	111.14
1	A	1037	GLY	N-CA-C	-5.40	103.65	112.83
1	A	1092	VAL	N-CA-C	5.37	116.10	108.42
1	A	1375	VAL	N-CA-C	5.36	113.73	107.89
1	A	1531	ALA	N-CA-C	-5.34	106.80	113.15
1	B	1435	SER	N-CA-C	5.33	117.20	110.33
1	B	1436	ASN	N-CA-CB	5.32	119.10	111.65
1	A	1139	ALA	N-CA-C	-5.27	105.43	111.07
1	A	1182	ILE	N-CA-CB	-5.22	106.12	112.07
1	A	1151	LEU	N-CA-C	-5.20	105.06	111.40
1	B	1303	GLY	N-CA-C	5.08	117.78	111.93
1	B	1182	ILE	N-CA-CB	-5.07	106.56	112.34
1	A	1283	ASN	N-CA-C	-5.04	104.03	110.53
1	B	1263	LEU	N-CA-C	-5.02	106.66	112.89
1	A	1032	GLU	N-CA-C	-5.00	105.88	112.94
1	A	1457	GLU	N-CA-C	5.00	117.62	111.82

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1007	ASP	Mainchain,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	4135	0	4223	233	1
1	B	4127	0	4219	337	0
2	A	35	0	0	12	0
2	B	20	0	0	2	0
3	A	198	0	0	14	0
3	B	71	0	0	4	0
All	All	8586	0	8442	570	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 34.

All (570) 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:B:1009:GLU:OE2	1:B:1111:ALA:HB2	1.33	1.27
1:A:1175:ARG:HD3	2:A:5:SO4:O3	1.55	1.07
1:A:1244:GLN:H	1:A:1244:GLN:NE2	1.55	1.03
1:B:1277:ASN:ND2	1:B:1278:ILE:H	1.59	1.01
1:B:1244:GLN:H	1:B:1244:GLN:NE2	1.59	0.99
1:B:1009:GLU:OE2	1:B:1111:ALA:CB	2.10	0.97
1:B:1517:ARG:HH22	1:B:1532:ILE:HG13	1.28	0.97
1:A:1244:GLN:HE21	1:A:1244:GLN:N	1.62	0.97
1:A:1517:ARG:HH22	1:A:1532:ILE:HG13	1.27	0.96
1:A:1257:PRO:HD3	1:A:1286:ILE:HD13	1.48	0.94
1:B:1277:ASN:HD22	1:B:1278:ILE:H	1.06	0.93
1:A:1277:ASN:HD22	1:A:1278:ILE:H	1.13	0.91
1:B:1212:ALA:O	1:B:1286:ILE:HG23	1.72	0.89
1:A:1533:MET:HB2	2:A:3:SO4:O2	1.73	0.89
1:B:1353:LEU:HD12	1:B:1353:LEU:H	1.37	0.88
1:B:1498:ASP:CB	1:B:1528:ILE:HG21	2.03	0.88
1:A:1498:ASP:CB	1:A:1528:ILE:HG21	2.04	0.88
1:B:1012:GLN:NE2	1:B:1116:TYR:CE2	2.42	0.88
1:A:1523:ARG:HH11	1:A:1525:ILE:HD11	1.39	0.87
1:B:1394:LEU:O	1:B:1398:LEU:HD23	1.73	0.87
1:B:1149:ASN:O	1:B:1153:GLN:HG2	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1244:GLN:H	1:B:1244:GLN:HE21	1.17	0.86
1:B:1557:GLY:HA3	3:B:164:HOH:O	1.77	0.84
1:B:1277:ASN:HD22	1:B:1278:ILE:N	1.74	0.84
1:B:1523:ARG:HH11	1:B:1525:ILE:HD11	1.41	0.84
1:A:1515:GLU:O	1:A:1527:PRO:HD2	1.78	0.83
1:A:1017:LYS:H	1:A:1261:GLN:HE22	1.27	0.83
1:A:1286:ILE:HD12	1:A:1286:ILE:C	2.05	0.82
1:B:1022:LEU:HD11	1:B:1261:GLN:NE2	1.96	0.80
1:A:1546:ASN:HB3	1:A:1556:THR:HG21	1.63	0.79
1:B:1049:ARG:HD3	1:B:1049:ARG:C	2.08	0.79
1:A:1451:ILE:HG12	1:A:1489:MET:HE1	1.65	0.79
1:B:1498:ASP:HB2	1:B:1528:ILE:HG21	1.65	0.78
1:B:1319:ARG:HE	1:B:1443:LEU:HD13	1.48	0.77
1:A:1244:GLN:H	1:A:1244:GLN:HE21	0.83	0.76
1:A:1512:THR:O	1:A:1528:ILE:HG23	1.86	0.76
1:B:1212:ALA:O	1:B:1286:ILE:CG2	2.33	0.76
1:B:1498:ASP:HB3	1:B:1528:ILE:HG21	1.66	0.76
1:B:1368:GLU:HG2	1:B:1401:LYS:HE2	1.69	0.75
1:B:1443:LEU:HG	1:B:1484:ASN:O	1.87	0.75
1:A:1498:ASP:HB2	1:A:1528:ILE:HG21	1.68	0.75
1:B:1262:THR:HG22	1:B:1263:LEU:H	1.49	0.75
1:A:1082:THR:HG21	1:A:1094:VAL:HG22	1.69	0.75
1:B:1356:LEU:HD12	1:B:1394:LEU:HD23	1.68	0.75
1:B:1550:ASP:C	1:B:1552:ASP:H	1.92	0.74
1:A:1277:ASN:HD22	1:A:1278:ILE:N	1.85	0.74
1:A:1277:ASN:ND2	1:A:1278:ILE:H	1.85	0.74
1:B:1523:ARG:NH1	1:B:1525:ILE:HD11	2.03	0.73
1:B:1244:GLN:HE21	1:B:1244:GLN:N	1.87	0.73
1:A:1195:THR:HG21	3:A:134:HOH:O	1.89	0.72
1:B:1161:PRO:HA	1:B:1164:ILE:HD12	1.70	0.72
1:B:1472:LYS:O	1:B:1476:ARG:HG3	1.90	0.72
1:B:1012:GLN:NE2	1:B:1116:TYR:CD2	2.58	0.72
1:B:1093:MET:HG2	1:B:1267:PRO:HB2	1.72	0.72
1:B:1061:LEU:HD22	1:B:1313:PHE:CD2	2.25	0.71
1:B:1319:ARG:NE	1:B:1443:LEU:HD13	2.03	0.71
1:B:1074:LYS:HZ2	1:B:1074:LYS:HB2	1.56	0.71
1:A:1271:HIS:ND1	1:A:1286:ILE:HD11	2.05	0.71
1:B:1455:ALA:HA	1:B:1459:TYR:HD2	1.54	0.71
1:B:1074:LYS:HB2	1:B:1074:LYS:NZ	2.06	0.70
1:A:1523:ARG:NH1	1:A:1525:ILE:HD11	2.06	0.70
1:B:1373:PHE:O	1:B:1375:VAL:HG13	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1149:ASN:ND2	1:B:1153:GLN:HE21	1.90	0.69
1:A:1020:MET:HE1	1:A:1030:GLU:HA	1.73	0.69
1:B:1360:PHE:CE2	1:B:1364:GLU:HB2	2.27	0.69
1:A:1174:GLU:HG3	3:A:237:HOH:O	1.93	0.69
1:A:1150:HIS:HE1	1:A:1157:LEU:H	1.39	0.69
1:B:1090:LYS:HD2	1:B:1297:TYR:HE2	1.57	0.69
1:B:1334:VAL:HB	1:B:1387:ASP:OD1	1.93	0.69
1:A:1277:ASN:HD22	1:A:1277:ASN:H	1.41	0.69
1:B:1175:ARG:HD3	2:B:9:SO4:O3	1.93	0.68
1:B:1079:VAL:HB	1:B:1117:ALA:O	1.94	0.68
1:A:1042:LYS:HE3	1:A:1258:ASN:OD1	1.94	0.68
1:A:1476:ARG:O	1:A:1480:LEU:HB2	1.93	0.68
1:A:1143:LEU:O	1:A:1147:VAL:HG23	1.94	0.68
1:B:1082:THR:HG21	1:B:1094:VAL:HG22	1.76	0.68
1:A:1533:MET:CB	2:A:3:SO4:O2	2.42	0.68
1:A:1486:PRO:HD2	1:A:1523:ARG:HB3	1.75	0.67
1:B:1275:PHE:O	1:B:1279:ALA:HB3	1.94	0.67
1:B:1019:VAL:HG13	1:B:1259:LEU:HG	1.75	0.67
1:B:1353:LEU:HD12	1:B:1353:LEU:N	2.08	0.67
1:B:1075:THR:HG22	1:B:1113:GLY:HA2	1.76	0.67
1:A:1286:ILE:HD12	1:A:1287:ALA:N	2.10	0.66
1:B:1020:MET:HE1	1:B:1030:GLU:HA	1.76	0.66
1:B:1373:PHE:CE2	1:B:1440:LEU:HB2	2.30	0.66
1:B:1517:ARG:NH2	1:B:1532:ILE:HG13	2.07	0.66
1:A:1533:MET:HA	2:A:3:SO4:O4	1.96	0.66
1:B:1477:TYR:HE2	1:B:1516:VAL:HG12	1.60	0.66
1:B:1448:LYS:HE2	1:B:1466:TYR:CD2	2.31	0.66
1:A:1167:ARG:NH2	1:A:1178:ARG:O	2.29	0.66
1:A:1382:ASN:OD1	2:A:7:SO4:O1	2.13	0.66
1:B:1120:VAL:HB	1:B:1121:PRO:HA	1.77	0.66
1:A:1277:ASN:ND2	1:A:1277:ASN:H	1.94	0.65
1:A:1540:LYS:O	1:A:1542:PRO:HD3	1.97	0.65
1:B:1447:ILE:O	1:B:1451:ILE:HG13	1.96	0.65
1:B:1262:THR:HG22	1:B:1263:LEU:N	2.10	0.65
1:B:1546:ASN:HB3	1:B:1556:THR:HG21	1.78	0.65
1:A:1082:THR:HG21	1:A:1094:VAL:CG2	2.27	0.65
1:A:1032:GLU:OE2	1:A:1050:ARG:NH1	2.30	0.65
1:A:1469:GLU:HG3	3:A:274:HOH:O	1.96	0.65
1:A:1257:PRO:HD3	1:A:1286:ILE:CD1	2.23	0.64
1:A:1009:GLU:HG2	1:A:1115:GLY:H	1.61	0.64
1:A:1169:VAL:HG22	1:A:1200:SER:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1312:LYS:HD3	1:B:1488:VAL:HG13	1.79	0.64
1:A:1417:GLU:HA	1:A:1420:LEU:CD2	2.27	0.64
1:A:1020:MET:CE	1:A:1030:GLU:HG3	2.28	0.64
1:B:1482:TYR:HB3	1:B:1485:LEU:HD12	1.80	0.64
1:B:1161:PRO:HA	1:B:1164:ILE:CD1	2.27	0.64
1:B:1445:LEU:O	1:B:1450:LYS:HE3	1.96	0.64
1:B:1315:ASP:O	1:B:1319:ARG:HD2	1.98	0.63
1:B:1384:PHE:CD1	1:B:1385:PRO:HD2	2.33	0.63
1:A:1398:LEU:C	1:A:1400:ALA:H	2.06	0.63
1:B:1446:SER:HB3	1:B:1449:ASP:OD2	1.97	0.63
1:A:1169:VAL:CG2	1:A:1200:SER:HA	2.29	0.63
1:A:1412:TRP:CG	2:A:7:SO4:O4	2.51	0.63
1:B:1417:GLU:HA	1:B:1420:LEU:HD23	1.81	0.63
1:A:1035:LEU:HD22	1:A:1037:GLY:O	1.98	0.63
1:B:1051:LEU:HD22	1:B:1054:LYS:HG3	1.80	0.63
1:B:1082:THR:HG21	1:B:1094:VAL:CG2	2.29	0.63
1:B:1546:ASN:C	1:B:1556:THR:HG21	2.23	0.63
1:A:1381:ILE:HD12	1:A:1395:LEU:HD21	1.80	0.62
1:B:1277:ASN:ND2	1:B:1278:ILE:N	2.37	0.62
1:A:1262:THR:HG22	1:A:1263:LEU:N	2.13	0.62
1:A:1417:GLU:HA	1:A:1420:LEU:HD23	1.81	0.62
1:B:1062:VAL:HG13	1:B:1301:GLU:HB3	1.80	0.62
1:A:1093:MET:HG2	1:A:1267:PRO:HB2	1.82	0.62
1:B:1042:LYS:NZ	1:B:1254:ALA:HA	2.14	0.62
1:B:1303:GLY:HA2	2:B:2:SO4:O1	2.00	0.62
1:B:1490:ALA:O	1:B:1527:PRO:HA	1.99	0.62
1:B:1105:PHE:HB3	1:B:1544:ALA:HB2	1.82	0.62
1:A:1066:THR:H	1:A:1362:ASN:HD21	1.48	0.62
1:A:1554:VAL:HG12	1:A:1555:ILE:N	2.14	0.62
1:B:1326:ASP:O	1:B:1376:PRO:HG2	2.00	0.61
1:B:1066:THR:H	1:B:1362:ASN:HD21	1.47	0.61
1:B:1142:LEU:O	1:B:1146:MET:HG3	2.00	0.61
1:A:1020:MET:HE3	1:A:1030:GLU:HG3	1.82	0.61
1:B:1074:LYS:NZ	1:B:1074:LYS:CB	2.62	0.61
1:B:1353:LEU:H	1:B:1353:LEU:CD1	2.10	0.61
1:B:1417:GLU:HA	1:B:1420:LEU:CD2	2.30	0.61
1:A:1533:MET:CA	2:A:3:SO4:O2	2.49	0.61
1:B:1363:LEU:O	1:B:1367:ILE:HG12	2.00	0.61
1:A:1043:ILE:HD12	1:A:1269:PHE:HE1	1.65	0.60
1:A:1010:ILE:C	1:A:1012:GLN:H	2.07	0.60
1:B:1042:LYS:HD3	1:B:1256:LYS:HB2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1337:LEU:HD23	1:B:1360:PHE:HA	1.83	0.60
1:B:1086:ALA:HB2	1:B:1092:VAL:HG12	1.83	0.60
1:B:1140:HIS:HD2	1:B:1203:SER:OG	1.85	0.60
1:B:1550:ASP:C	1:B:1552:ASP:N	2.54	0.60
1:A:1487:VAL:HG12	1:A:1489:MET:HE2	1.83	0.60
1:B:1488:VAL:CG2	1:B:1523:ARG:HD3	2.31	0.60
1:B:1528:ILE:HG22	1:B:1529:THR:N	2.17	0.60
1:A:1517:ARG:NH2	1:A:1532:ILE:HG13	2.08	0.60
1:B:1331:VAL:HG12	1:B:1332:ALA:N	2.17	0.60
1:A:1083:ASP:CG	1:A:1262:THR:HG21	2.27	0.59
1:A:1133:ILE:HG21	1:A:1171:ASP:OD1	2.01	0.59
1:A:1140:HIS:HD2	1:A:1203:SER:OG	1.85	0.59
1:B:1083:ASP:OD2	1:B:1262:THR:HG21	2.02	0.59
1:A:1513:VAL:HB	1:A:1526:VAL:HG23	1.84	0.59
1:B:1082:THR:HG22	1:B:1266:THR:HG21	1.84	0.59
1:A:1319:ARG:NH2	1:A:1439:VAL:HG21	2.18	0.59
1:A:1486:PRO:O	1:A:1523:ARG:HB2	2.02	0.59
1:B:1062:VAL:HG11	1:B:1078:SER:OG	2.02	0.59
1:A:1082:THR:HG22	1:A:1266:THR:HG21	1.84	0.59
1:B:1009:GLU:OE1	1:B:1114:GLY:HA2	2.03	0.59
1:A:1107:ILE:O	1:A:1108:LYS:HB2	2.02	0.59
1:A:1319:ARG:NH2	1:A:1441:TYR:O	2.33	0.58
1:B:1107:ILE:O	1:B:1108:LYS:HB2	2.02	0.58
1:A:1363:LEU:O	1:A:1367:ILE:HG12	2.03	0.58
1:A:1533:MET:HA	2:A:3:SO4:S	2.43	0.58
1:B:1133:ILE:HG21	1:B:1171:ASP:OD1	2.03	0.58
1:B:1286:ILE:C	1:B:1286:ILE:HD12	2.28	0.58
1:B:1365:LYS:HE3	1:B:1369:ASN:HD21	1.67	0.58
1:B:1555:ILE:HG23	1:B:1555:ILE:O	2.04	0.58
1:B:1020:MET:O	1:B:1024:ARG:HG3	2.02	0.58
1:A:1222:PHE:HA	1:A:1225:LYS:HD2	1.85	0.58
1:B:1110:GLY:HA2	3:B:191:HOH:O	2.03	0.58
1:B:1172:LEU:O	1:B:1535:MET:HE1	2.03	0.58
1:A:1462:ASP:OD2	1:A:1508:ASN:HA	2.03	0.58
1:B:1515:GLU:O	1:B:1527:PRO:HD2	2.03	0.58
1:A:1036:TYR:CE1	1:A:1042:LYS:HG3	2.39	0.58
1:B:1026:LEU:HD23	1:B:1028:ILE:HD11	1.84	0.58
1:B:1092:VAL:HG23	1:B:1297:TYR:O	2.03	0.58
1:A:1222:PHE:HA	1:A:1225:LYS:CD	2.34	0.58
1:B:1042:LYS:HE2	1:B:1258:ASN:OD1	2.03	0.58
1:B:1175:ARG:HG2	1:B:1178:ARG:CZ	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1283:ASN:ND2	1:B:1300:THR:OG1	2.36	0.57
1:B:1353:LEU:HB3	1:B:1394:LEU:HD22	1.86	0.57
1:A:1120:VAL:HB	1:A:1121:PRO:HA	1.86	0.57
1:A:1083:ASP:OD2	1:A:1262:THR:HG21	2.05	0.57
1:B:1214:ASP:O	1:B:1215:LEU:C	2.48	0.57
1:B:1277:ASN:ND2	1:B:1277:ASN:H	2.03	0.57
1:B:1376:PRO:HD3	1:B:1435:SER:HB3	1.86	0.57
1:B:1169:VAL:HG13	1:B:1200:SER:HA	1.86	0.56
1:A:1554:VAL:HG12	1:A:1555:ILE:H	1.69	0.56
1:B:1540:LYS:C	1:B:1542:PRO:HD3	2.30	0.56
1:A:1405:GLU:HG3	1:A:1425:LYS:HB2	1.88	0.56
1:A:1523:ARG:HD2	1:A:1523:ARG:N	2.19	0.56
1:A:1532:ILE:HG12	1:A:1532:ILE:O	2.04	0.56
1:B:1331:VAL:HG12	1:B:1332:ALA:H	1.70	0.56
1:A:1514:ARG:HD3	3:A:295:HOH:O	2.05	0.56
1:A:1083:ASP:OD1	1:A:1262:THR:HG21	2.06	0.56
1:B:1204:GLU:CD	1:B:1225:LYS:HZ1	2.13	0.56
1:A:1150:HIS:CE1	1:A:1157:LEU:H	2.23	0.56
1:A:1530:GLY:C	1:A:1532:ILE:H	2.13	0.56
1:B:1515:GLU:HB3	1:B:1527:PRO:CG	2.36	0.56
1:B:1515:GLU:HB3	1:B:1527:PRO:HG2	1.87	0.56
1:B:1370:ILE:HG21	1:B:1377:ALA:HB2	1.88	0.56
1:A:1020:MET:HE2	1:A:1033:VAL:HB	1.88	0.55
1:A:1092:VAL:HG23	1:A:1297:TYR:O	2.06	0.55
1:A:1116:TYR:CZ	2:A:8:SO4:O1	2.59	0.55
1:B:1043:ILE:HD11	1:B:1259:LEU:HD22	1.88	0.55
1:B:1408:LEU:HD13	1:B:1414:LYS:NZ	2.21	0.55
1:A:1540:LYS:C	1:A:1542:PRO:HD3	2.31	0.55
1:B:1416:GLY:O	1:B:1420:LEU:HD22	2.06	0.55
1:B:1043:ILE:HD12	1:B:1269:PHE:CZ	2.41	0.55
1:B:1010:ILE:C	1:B:1012:GLN:N	2.63	0.55
1:B:1417:GLU:C	1:B:1419:GLY:H	2.15	0.55
1:B:1476:ARG:O	1:B:1480:LEU:HD13	2.05	0.55
1:B:1275:PHE:HD2	1:B:1277:ASN:HD21	1.55	0.55
1:B:1285:ILE:HD13	1:B:1321:ALA:HB2	1.89	0.55
1:A:1333:THR:HG22	1:A:1382:ASN:HB3	1.89	0.55
1:A:1445:LEU:O	1:A:1450:LYS:HE3	2.07	0.55
1:B:1284:SER:HB2	3:B:283:HOH:O	2.06	0.55
1:B:1288:THR:O	1:B:1292:LEU:HG	2.06	0.55
1:B:1422:LEU:O	1:B:1426:VAL:HG23	2.07	0.55
1:A:1140:HIS:HE1	1:A:1167:ARG:O	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1533:MET:HA	2:A:3:SO4:O2	2.07	0.54
1:B:1011:ALA:C	1:B:1013:ALA:H	2.14	0.54
1:B:1498:ASP:HB2	1:B:1528:ILE:CG2	2.36	0.54
1:B:1436:ASN:O	1:B:1436:ASN:CG	2.50	0.54
1:B:1095:CYS:O	1:B:1283:ASN:ND2	2.41	0.54
1:B:1547:ILE:HA	1:B:1556:THR:HB	1.90	0.54
1:A:1007:ASP:OD2	3:A:131:HOH:O	2.19	0.54
1:B:1204:GLU:HB3	1:B:1225:LYS:HZ3	1.73	0.54
1:A:1217:ASP:O	1:A:1221:ARG:HG3	2.07	0.53
1:B:1058:LYS:HB2	1:B:1297:TYR:HD1	1.73	0.53
1:B:1214:ASP:O	1:B:1217:ASP:N	2.33	0.53
1:A:1550:ASP:C	1:A:1552:ASP:H	2.15	0.53
1:A:1550:ASP:OD1	1:A:1551:ALA:N	2.41	0.53
1:B:1049:ARG:HD3	1:B:1049:ARG:O	2.08	0.53
1:B:1280:HIS:CD2	1:B:1282:CYS:HB2	2.43	0.53
1:B:1530:GLY:C	1:B:1532:ILE:H	2.15	0.53
1:A:1417:GLU:O	1:A:1420:LEU:HD23	2.08	0.53
1:B:1555:ILE:O	1:B:1556:THR:CB	2.55	0.53
1:A:1082:THR:CG2	1:A:1094:VAL:HG22	2.38	0.53
1:A:1140:HIS:CD2	1:A:1203:SER:OG	2.62	0.53
1:B:1088:LEU:HD21	1:B:1420:LEU:HD12	1.91	0.53
1:B:1398:LEU:C	1:B:1400:ALA:H	2.17	0.53
1:B:1019:VAL:CG1	1:B:1259:LEU:HG	2.37	0.53
1:A:1174:GLU:HA	3:A:214:HOH:O	2.09	0.53
1:A:1556:THR:O	1:A:1556:THR:HG22	2.09	0.53
1:A:1141:ASN:OD1	1:A:1168:ARG:HG3	2.09	0.53
1:B:1174:GLU:HG3	3:B:298:HOH:O	2.09	0.53
1:B:1286:ILE:HD12	1:B:1287:ALA:N	2.23	0.53
1:B:1286:ILE:HA	1:B:1289:LYS:HE2	1.91	0.53
1:B:1448:LYS:HE2	1:B:1466:TYR:CG	2.44	0.53
1:B:1271:HIS:CE1	1:B:1286:ILE:HD11	2.44	0.53
1:B:1211:LEU:HD21	1:B:1280:HIS:NE2	2.24	0.52
1:B:1510:THR:HG22	1:B:1511:ILE:N	2.23	0.52
1:B:1080:GLY:HA3	1:B:1409:SER:HB3	1.92	0.52
1:B:1222:PHE:HA	1:B:1225:LYS:HD2	1.91	0.52
1:B:1414:LYS:O	1:B:1417:GLU:HB3	2.09	0.52
1:B:1149:ASN:ND2	1:B:1153:GLN:NE2	2.56	0.52
1:B:1150:HIS:HE1	1:B:1157:LEU:H	1.57	0.52
1:A:1175:ARG:HG2	1:A:1178:ARG:CZ	2.39	0.52
1:B:1350:THR:HG22	1:B:1351:GLU:N	2.25	0.52
1:B:1515:GLU:C	1:B:1527:PRO:HD2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1083:ASP:O	1:B:1087:ARG:HB2	2.09	0.52
1:A:1017:LYS:H	1:A:1261:GLN:NE2	2.01	0.52
1:B:1405:GLU:HG3	1:B:1425:LYS:HB2	1.92	0.52
1:A:1182:ILE:CG2	1:A:1183:GLY:N	2.72	0.51
1:B:1374:GLY:O	1:B:1435:SER:HB2	2.09	0.51
1:A:1017:LYS:HD3	1:A:1021:GLU:OE2	2.10	0.51
1:A:1540:LYS:HG3	1:A:1541:ARG:N	2.25	0.51
1:B:1488:VAL:HG21	1:B:1523:ARG:HD3	1.92	0.51
1:B:1526:VAL:O	1:B:1526:VAL:HG22	2.09	0.51
1:A:1485:LEU:HD13	1:A:1523:ARG:HA	1.91	0.51
1:B:1008:ILE:HG13	1:B:1011:ALA:HB2	1.92	0.51
1:A:1010:ILE:C	1:A:1012:GLN:N	2.67	0.51
1:A:1461:ALA:HB2	1:A:1509:PHE:CE1	2.45	0.51
1:B:1204:GLU:HB3	1:B:1225:LYS:NZ	2.25	0.51
1:A:1347:ASP:OD2	1:A:1347:ASP:N	2.43	0.51
1:B:1062:VAL:HG12	1:B:1300:THR:O	2.11	0.51
1:B:1092:VAL:HA	1:B:1297:TYR:O	2.11	0.51
1:B:1143:LEU:HD23	1:B:1166:TRP:CE2	2.45	0.51
1:B:1405:GLU:OE1	1:B:1421:GLU:HG2	2.10	0.51
1:A:1277:ASN:HD22	1:A:1277:ASN:N	2.04	0.51
1:A:1334:VAL:O	1:A:1338:LYS:HG3	2.11	0.51
1:A:1425:LYS:O	1:A:1429:THR:HG23	2.10	0.51
1:B:1518:LEU:HD12	1:B:1519:SER:N	2.26	0.51
1:B:1523:ARG:H	1:B:1523:ARG:HD2	1.76	0.50
1:A:1062:VAL:HG11	1:A:1078:SER:OG	2.11	0.50
1:A:1405:GLU:OE2	1:A:1425:LYS:HD3	2.11	0.50
1:B:1061:LEU:HD13	1:B:1313:PHE:CE1	2.46	0.50
1:A:1523:ARG:HD2	1:A:1523:ARG:H	1.76	0.50
1:B:1040:LYS:HE2	1:B:1124:ASP:OD2	2.11	0.50
1:B:1394:LEU:C	1:B:1398:LEU:HD23	2.35	0.50
1:B:1517:ARG:HH22	1:B:1532:ILE:CG1	2.10	0.50
1:A:1262:THR:CG2	1:A:1263:LEU:N	2.75	0.50
1:B:1149:ASN:HD21	1:B:1153:GLN:NE2	2.09	0.50
1:A:1451:ILE:HG12	1:A:1489:MET:CE	2.40	0.50
1:A:1550:ASP:C	1:A:1552:ASP:N	2.70	0.50
1:A:1377:ALA:O	1:A:1402:ALA:HB1	2.12	0.50
1:A:1447:ILE:O	1:A:1451:ILE:HG13	2.12	0.50
1:B:1050:ARG:HG3	1:B:1051:LEU:N	2.26	0.50
1:A:1517:ARG:HH22	1:A:1532:ILE:CG1	2.13	0.50
1:B:1169:VAL:CG1	1:B:1200:SER:HA	2.41	0.50
1:B:1047:VAL:CG1	1:B:1294:LEU:HD21	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1225:LYS:HA	1:B:1520:ALA:HB3	1.94	0.49
1:B:1523:ARG:HD2	1:B:1523:ARG:N	2.27	0.49
1:A:1149:ASN:O	1:A:1153:GLN:HG2	2.12	0.49
1:B:1149:ASN:HD21	1:B:1153:GLN:HE21	1.58	0.49
1:B:1177:LEU:HB3	1:B:1197:PHE:HB2	1.93	0.49
1:B:1210:CYS:O	1:B:1211:LEU:HD23	2.12	0.49
1:B:1219:LYS:O	1:B:1222:PHE:HB2	2.11	0.49
1:B:1356:LEU:HD13	1:B:1356:LEU:C	2.38	0.49
1:A:1210:CYS:SG	1:A:1274:PRO:HD3	2.51	0.49
1:A:1398:LEU:O	1:A:1400:ALA:N	2.43	0.49
1:B:1115:GLY:O	1:B:1118:GLN:HG2	2.13	0.49
1:B:1515:GLU:HG2	1:B:1516:VAL:H	1.76	0.49
1:A:1043:ILE:HD12	1:A:1269:PHE:CE1	2.47	0.49
1:A:1381:ILE:HD12	1:A:1395:LEU:CD2	2.43	0.49
1:B:1114:GLY:O	1:B:1115:GLY:C	2.55	0.49
1:A:1168:ARG:HG2	1:A:1197:PHE:CE2	2.48	0.49
1:A:1519:SER:C	1:A:1521:GLY:H	2.20	0.49
1:A:1065:ILE:CD1	1:A:1337:LEU:HD13	2.42	0.49
1:B:1136:VAL:HG13	1:B:1205:VAL:CG1	2.43	0.49
1:B:1244:GLN:NE2	1:B:1244:GLN:N	2.42	0.49
1:B:1550:ASP:O	1:B:1552:ASP:N	2.46	0.49
1:A:1490:ALA:O	1:A:1527:PRO:HA	2.13	0.49
1:B:1455:ALA:HA	1:B:1459:TYR:CD2	2.41	0.49
1:A:1474:ILE:O	1:A:1478:GLU:HG3	2.13	0.49
1:B:1335:ARG:HH21	1:B:1386:THR:HG21	1.78	0.49
1:B:1459:TYR:HE2	1:B:1489:MET:HG3	1.78	0.49
1:A:1339:MET:HG2	1:A:1348:LEU:HD21	1.95	0.48
1:A:1116:TYR:CE1	2:A:8:SO4:O1	2.66	0.48
1:B:1148:ASP:OD2	1:B:1168:ARG:NH2	2.46	0.48
1:B:1488:VAL:HG23	1:B:1523:ARG:HD3	1.94	0.48
1:B:1182:ILE:O	1:B:1192:PRO:HA	2.13	0.48
1:B:1024:ARG:C	1:B:1026:LEU:H	2.21	0.48
1:A:1286:ILE:C	1:A:1286:ILE:CD1	2.77	0.48
1:A:1042:LYS:NZ	1:A:1254:ALA:HA	2.28	0.48
1:B:1370:ILE:CG2	1:B:1377:ALA:HB2	2.43	0.48
1:B:1486:PRO:HD2	1:B:1523:ARG:HB3	1.95	0.48
1:B:1068:THR:C	1:B:1070:ALA:H	2.21	0.47
1:B:1440:LEU:HD22	1:B:1458:ILE:HD11	1.96	0.47
1:A:1129:PHE:CZ	1:A:1270:ILE:HG21	2.49	0.47
1:A:1182:ILE:HG22	1:A:1183:GLY:N	2.29	0.47
1:B:1069:PRO:HG2	1:B:1339:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1092:VAL:HG23	1:B:1297:TYR:C	2.39	0.47
1:B:1292:LEU:HD23	1:B:1298:VAL:HG21	1.96	0.47
1:B:1380:ALA:O	1:B:1381:ILE:HD13	2.13	0.47
1:B:1220:GLU:O	1:B:1224:ARG:HG3	2.15	0.47
1:A:1277:ASN:ND2	1:A:1278:ILE:N	2.53	0.47
1:A:1417:GLU:CA	1:A:1420:LEU:HD23	2.45	0.47
1:B:1058:LYS:N	1:B:1296:ASP:O	2.41	0.47
1:B:1339:MET:HE3	1:B:1345:LYS:HA	1.97	0.47
1:A:1105:PHE:HB3	1:A:1544:ALA:HB2	1.96	0.47
1:B:1010:ILE:HA	1:B:1122:MET:HE1	1.97	0.47
1:B:1031:ASP:OD2	1:B:1032:GLU:HG3	2.15	0.47
1:B:1222:PHE:HA	1:B:1225:LYS:CD	2.44	0.47
1:B:1375:VAL:CG1	1:B:1437:PHE:HD2	2.28	0.47
1:B:1417:GLU:C	1:B:1419:GLY:N	2.71	0.47
1:A:1417:GLU:C	1:A:1420:LEU:HD23	2.39	0.47
1:B:1210:CYS:SG	1:B:1274:PRO:HD3	2.55	0.47
1:A:1398:LEU:C	1:A:1400:ALA:N	2.73	0.47
1:B:1098:GLU:N	1:B:1272:GLY:O	2.37	0.47
1:A:1096:LEU:O	1:A:1270:ILE:HA	2.15	0.46
1:A:1532:ILE:O	1:A:1534:THR:N	2.47	0.46
1:B:1091:ARG:HB3	1:B:1296:ASP:H	1.80	0.46
1:B:1278:ILE:HD12	1:B:1490:ALA:HB1	1.97	0.46
1:B:1338:LYS:HB3	1:B:1343:VAL:HG21	1.97	0.46
1:A:1270:ILE:HG23	1:A:1270:ILE:O	2.15	0.46
1:A:1285:ILE:HD13	1:A:1321:ALA:HB2	1.96	0.46
1:A:1476:ARG:HD3	3:A:148:HOH:O	2.16	0.46
1:A:1523:ARG:N	1:A:1523:ARG:CD	2.77	0.46
1:B:1203:SER:OG	1:B:1205:VAL:HB	2.15	0.46
1:B:1376:PRO:HB3	1:B:1433:ARG:HG2	1.97	0.46
1:B:1010:ILE:C	1:B:1012:GLN:H	2.22	0.46
1:B:1482:TYR:HB3	1:B:1485:LEU:CD1	2.46	0.46
1:B:1550:ASP:OD1	1:B:1551:ALA:N	2.49	0.46
1:A:1020:MET:HE1	1:A:1030:GLU:HG3	1.96	0.46
1:A:1172:LEU:O	1:A:1535:MET:HE1	2.16	0.46
1:B:1032:GLU:CD	1:B:1050:ARG:HH12	2.24	0.46
1:B:1257:PRO:HD3	1:B:1286:ILE:HD13	1.97	0.46
1:A:1417:GLU:HA	1:A:1420:LEU:HD21	1.97	0.46
1:A:1487:VAL:CG1	1:A:1489:MET:HE2	2.45	0.46
1:B:1271:HIS:ND1	1:B:1286:ILE:HD11	2.31	0.46
1:B:1523:ARG:HB2	1:B:1524:LEU:H	1.52	0.46
1:B:1506:PRO:HB2	1:B:1509:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1549:ILE:HG23	1:B:1549:ILE:O	2.16	0.46
1:A:1007:ASP:CG	3:A:131:HOH:O	2.59	0.46
1:B:1375:VAL:HG23	1:B:1375:VAL:O	2.15	0.46
1:A:1419:GLY:HA2	3:A:310:HOH:O	2.15	0.45
1:B:1140:HIS:HE1	1:B:1167:ARG:O	1.98	0.45
1:B:1451:ILE:HG23	1:B:1489:MET:HE1	1.98	0.45
1:B:1448:LYS:HG2	1:B:1466:TYR:CE2	2.51	0.45
1:A:1555:ILE:O	1:A:1556:THR:CB	2.64	0.45
1:B:1065:ILE:HG23	1:B:1332:ALA:HB2	1.99	0.45
1:B:1415:GLY:C	1:B:1417:GLU:N	2.74	0.45
1:B:1368:GLU:O	1:B:1372:LYS:HG3	2.15	0.45
1:B:1079:VAL:CB	1:B:1117:ALA:O	2.64	0.45
1:B:1093:MET:HE3	1:B:1267:PRO:HB3	1.98	0.45
1:B:1515:GLU:O	1:B:1516:VAL:HG23	2.16	0.45
1:B:1548:ASP:OD1	1:B:1549:ILE:N	2.49	0.45
1:A:1009:GLU:HG2	1:A:1115:GLY:N	2.31	0.45
1:A:1543:ALA:O	1:A:1547:ILE:HG12	2.17	0.45
1:B:1061:LEU:HD22	1:B:1313:PHE:CE2	2.52	0.45
1:B:1262:THR:CG2	1:B:1263:LEU:H	2.26	0.45
1:A:1098:GLU:HA	1:A:1270:ILE:HD11	1.97	0.45
1:B:1432:SER:O	1:B:1434:PRO:HD3	2.17	0.45
1:B:1447:ILE:HG13	1:B:1478:GLU:OE1	2.17	0.45
1:A:1498:ASP:OD2	1:A:1528:ILE:HG21	2.17	0.45
1:B:1459:TYR:CE2	1:B:1489:MET:HG3	2.52	0.45
1:A:1042:LYS:HZ3	1:A:1253:ASP:C	2.24	0.45
1:A:1519:SER:C	1:A:1521:GLY:N	2.75	0.45
1:B:1466:TYR:CE2	1:B:1513:VAL:HG11	2.52	0.45
1:A:1308:LEU:O	1:A:1312:LYS:HG3	2.16	0.44
1:B:1143:LEU:O	1:B:1147:VAL:HG23	2.17	0.44
1:B:1379:VAL:HG21	1:B:1399:CYS:SG	2.56	0.44
1:B:1379:VAL:HG12	1:B:1380:ALA:N	2.31	0.44
1:A:1065:ILE:HB	1:A:1362:ASN:ND2	2.33	0.44
1:A:1178:ARG:NH2	2:A:5:SO4:O2	2.49	0.44
1:A:1230:THR:C	1:A:1232:ASP:H	2.26	0.44
1:A:1235:PRO:HG3	1:A:1480:LEU:HD21	1.99	0.44
1:B:1058:LYS:HB3	1:B:1430:LEU:HD21	1.99	0.44
1:B:1125:ILE:HA	1:B:1129:PHE:CD1	2.51	0.44
1:B:1382:ASN:HD22	1:B:1382:ASN:HA	1.56	0.44
1:B:1032:GLU:OE1	1:B:1050:ARG:NH1	2.47	0.44
1:B:1489:MET:HE2	1:B:1526:VAL:HG13	1.99	0.44
1:B:1509:PHE:CD1	1:B:1509:PHE:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1523:ARG:N	1:B:1523:ARG:CD	2.76	0.44
1:A:1517:ARG:HH12	1:A:1532:ILE:HD12	1.83	0.44
1:A:1032:GLU:CD	1:A:1050:ARG:HH12	2.25	0.44
1:A:1498:ASP:CG	1:A:1528:ILE:HG21	2.42	0.44
1:B:1222:PHE:HD2	1:B:1225:LYS:HD2	1.83	0.44
1:A:1020:MET:CE	1:A:1033:VAL:HB	2.48	0.44
1:A:1044:SER:C	1:A:1046:ASP:H	2.25	0.44
1:B:1227:VAL:HG22	1:B:1236:VAL:O	2.18	0.44
1:A:1319:ARG:HA	3:A:352:HOH:O	2.17	0.44
1:B:1408:LEU:HD13	1:B:1414:LYS:CE	2.47	0.44
1:A:1092:VAL:HG22	1:A:1093:MET:N	2.33	0.43
1:A:1398:LEU:HD13	1:A:1398:LEU:HA	1.86	0.43
1:A:1416:GLY:O	1:A:1420:LEU:CD2	2.66	0.43
1:A:1498:ASP:HB3	1:A:1528:ILE:HG21	1.93	0.43
1:B:1276:ALA:HB3	1:B:1304:PHE:CE2	2.53	0.43
1:A:1175:ARG:HG2	1:A:1178:ARG:NH2	2.33	0.43
1:A:1277:ASN:ND2	1:A:1277:ASN:N	2.56	0.43
1:A:1374:GLY:HA3	1:A:1436:ASN:O	2.18	0.43
1:B:1035:LEU:HB3	1:B:1037:GLY:O	2.18	0.43
1:B:1389:GLU:O	1:B:1393:ASN:ND2	2.51	0.43
1:B:1488:VAL:HB	1:B:1525:ILE:HD13	1.99	0.43
1:A:1175:ARG:HG3	1:A:1537:GLY:HA3	2.00	0.43
1:B:1008:ILE:CG1	1:B:1011:ALA:HB2	2.49	0.43
1:B:1042:LYS:HZ3	1:B:1254:ALA:HA	1.84	0.43
1:B:1095:CYS:SG	1:B:1288:THR:HA	2.57	0.43
1:B:1334:VAL:HB	1:B:1387:ASP:CG	2.43	0.43
1:A:1544:ALA:HA	1:A:1547:ILE:HG12	2.01	0.43
1:B:1376:PRO:CD	1:B:1435:SER:HB3	2.49	0.43
1:A:1024:ARG:C	1:A:1026:LEU:H	2.26	0.43
1:A:1061:LEU:O	1:A:1328:THR:HA	2.19	0.43
1:A:1422:LEU:O	1:A:1426:VAL:HG23	2.19	0.43
1:A:1488:VAL:CG2	1:A:1523:ARG:HD3	2.48	0.43
1:B:1451:ILE:HG23	1:B:1489:MET:CE	2.49	0.43
1:A:1066:THR:HB	1:A:1340:HIS:CE1	2.53	0.43
1:B:1357:ARG:O	1:B:1360:PHE:HB3	2.19	0.43
1:A:1042:LYS:HZ3	1:A:1254:ALA:HA	1.84	0.43
1:A:1498:ASP:HB2	1:A:1528:ILE:CG2	2.44	0.43
1:B:1262:THR:CG2	1:B:1263:LEU:N	2.81	0.43
1:B:1454:ILE:O	1:B:1458:ILE:HB	2.17	0.43
1:A:1093:MET:HE1	1:A:1269:PHE:CE2	2.53	0.43
1:B:1044:SER:C	1:B:1046:ASP:H	2.26	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1075:THR:HA	1:B:1301:GLU:OE2	2.18	0.43
1:B:1386:THR:O	1:B:1387:ASP:C	2.61	0.43
1:A:1333:THR:O	1:A:1337:LEU:HB2	2.18	0.43
1:B:1335:ARG:NH2	1:B:1386:THR:HG21	2.33	0.43
1:B:1408:LEU:C	1:B:1412:TRP:H	2.26	0.43
1:A:1271:HIS:CE1	1:A:1286:ILE:HD11	2.53	0.42
1:B:1062:VAL:CG1	1:B:1301:GLU:HB3	2.46	0.42
1:B:1175:ARG:HG3	1:B:1537:GLY:HA3	2.00	0.42
1:A:1530:GLY:C	1:A:1532:ILE:N	2.77	0.42
1:A:1549:ILE:HG23	1:A:1549:ILE:O	2.19	0.42
1:B:1042:LYS:NZ	1:B:1253:ASP:O	2.42	0.42
1:B:1337:LEU:HD21	1:B:1363:LEU:HB2	2.01	0.42
1:B:1555:ILE:O	1:B:1556:THR:HB	2.18	0.42
1:A:1010:ILE:HB	1:A:1122:MET:HE1	2.00	0.42
1:A:1069:PRO:HG2	1:A:1339:MET:HE1	2.00	0.42
1:A:1257:PRO:HB3	1:A:1286:ILE:CD1	2.50	0.42
1:A:1376:PRO:HA	3:A:202:HOH:O	2.18	0.42
1:A:1448:LYS:HG3	3:A:173:HOH:O	2.18	0.42
1:B:1101:LEU:HD13	1:B:1127:LEU:HA	2.01	0.42
1:B:1312:LYS:O	1:B:1316:VAL:HB	2.19	0.42
1:B:1461:ALA:HB2	1:B:1511:ILE:HG12	2.01	0.42
1:A:1312:LYS:HD3	1:A:1488:VAL:HG13	2.01	0.42
1:A:1533:MET:SD	1:A:1536:PRO:HA	2.59	0.42
1:B:1376:PRO:HB3	1:B:1433:ARG:CG	2.50	0.42
1:B:1513:VAL:CG2	1:B:1526:VAL:HG23	2.49	0.42
1:A:1546:ASN:CB	1:A:1556:THR:HG21	2.43	0.42
1:A:1118:GLN:HG2	1:A:1263:LEU:HD11	2.02	0.42
1:A:1400:ALA:O	1:A:1401:LYS:HB2	2.20	0.42
1:B:1026:LEU:HG	1:B:1294:LEU:HB3	2.02	0.42
1:B:1408:LEU:C	1:B:1412:TRP:N	2.77	0.42
1:A:1167:ARG:NH2	1:A:1196:GLY:HA3	2.35	0.42
1:B:1062:VAL:HG13	1:B:1301:GLU:CB	2.46	0.42
1:A:1286:ILE:HG23	3:A:169:HOH:O	2.18	0.42
1:A:1416:GLY:O	1:A:1420:LEU:HD22	2.20	0.42
1:A:1466:TYR:CD2	1:A:1513:VAL:HG22	2.55	0.41
1:B:1040:LYS:HB2	1:B:1040:LYS:NZ	2.35	0.41
1:B:1257:PRO:HA	1:B:1271:HIS:CG	2.55	0.41
1:A:1097:ARG:HG3	3:A:102:HOH:O	2.21	0.41
1:A:1289:LYS:O	1:A:1293:LYS:HD3	2.21	0.41
1:A:1528:ILE:HB	1:A:1529:THR:H	1.66	0.41
1:A:1529:THR:HB	1:A:1530:GLY:H	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1550:ASP:N	1:A:1553:GLY:O	2.53	0.41
1:B:1047:VAL:HG11	1:B:1294:LEU:HD21	2.02	0.41
1:B:1436:ASN:O	1:B:1437:PHE:C	2.63	0.41
1:A:1306:ALA:HB3	1:A:1366:HIS:ND1	2.36	0.41
1:A:1441:TYR:HB3	1:A:1453:LYS:HD3	2.02	0.41
1:A:1470:ALA:O	1:A:1474:ILE:HG13	2.20	0.41
1:A:1523:ARG:HB2	1:A:1524:LEU:H	1.62	0.41
1:B:1011:ALA:O	1:B:1013:ALA:N	2.47	0.41
1:B:1506:PRO:HG2	1:B:1509:PHE:CE2	2.55	0.41
1:A:1180:ILE:HG12	1:A:1196:GLY:HA2	2.01	0.41
1:B:1488:VAL:HB	1:B:1525:ILE:CD1	2.49	0.41
1:B:1400:ALA:O	1:B:1401:LYS:HB2	2.20	0.41
1:B:1415:GLY:C	1:B:1417:GLU:H	2.28	0.41
1:B:1541:ARG:N	1:B:1542:PRO:HD3	2.35	0.41
1:A:1042:LYS:HE2	1:A:1256:LYS:O	2.20	0.41
1:A:1388:THR:OG1	1:A:1391:GLU:HG3	2.21	0.41
1:A:1136:VAL:HG21	1:A:1206:MET:HE2	2.02	0.41
1:B:1369:ASN:O	1:B:1372:LYS:HB2	2.21	0.41
1:A:1452:ALA:O	1:A:1456:THR:HB	2.21	0.41
1:A:1488:VAL:HG23	1:A:1523:ARG:HD3	2.02	0.41
1:B:1017:LYS:HA	1:B:1018:PRO:HD3	1.97	0.41
1:B:1030:GLU:C	1:B:1032:GLU:H	2.29	0.41
1:B:1043:ILE:HD12	1:B:1269:PHE:HZ	1.83	0.41
1:B:1061:LEU:HD13	1:B:1313:PHE:CZ	2.56	0.41
1:B:1063:THR:N	1:B:1329:VAL:O	2.48	0.41
1:B:1085:LEU:CD2	1:B:1090:LYS:HG3	2.50	0.41
1:B:1169:VAL:CG1	1:B:1200:SER:OG	2.68	0.41
1:B:1215:LEU:HD23	1:B:1215:LEU:HA	1.85	0.41
1:B:1277:ASN:ND2	1:B:1277:ASN:N	2.62	0.41
1:B:1287:ALA:O	1:B:1290:THR:HB	2.20	0.41
1:B:1350:THR:CG2	1:B:1351:GLU:N	2.84	0.41
1:B:1376:PRO:HB3	1:B:1433:ARG:HD3	2.03	0.41
1:B:1420:LEU:O	1:B:1421:GLU:C	2.63	0.41
1:B:1432:SER:C	1:B:1434:PRO:HD3	2.46	0.41
1:B:1482:TYR:CD1	1:B:1482:TYR:N	2.89	0.41
1:A:1146:MET:SD	1:A:1243:ALA:HB2	2.61	0.41
1:B:1119:VAL:HG13	1:B:1261:GLN:O	2.21	0.41
1:B:1373:PHE:CZ	1:B:1440:LEU:HB2	2.56	0.41
1:B:1394:LEU:CD1	1:B:1398:LEU:HD21	2.51	0.41
1:A:1262:THR:HG22	1:A:1263:LEU:H	1.86	0.40
1:A:1554:VAL:CG1	1:A:1555:ILE:N	2.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1277:ASN:HD22	1:B:1277:ASN:N	2.17	0.40
1:A:1026:LEU:HG	1:A:1294:LEU:HB3	2.04	0.40
1:B:1082:THR:CG2	1:B:1094:VAL:HG22	2.48	0.40
1:B:1085:LEU:HD22	1:B:1090:LYS:HB2	2.04	0.40
1:B:1270:ILE:HG23	1:B:1270:ILE:O	2.20	0.40
1:B:1010:ILE:O	1:B:1012:GLN:N	2.54	0.40
1:B:1060:ILE:O	1:B:1060:ILE:HG22	2.21	0.40
1:B:1167:ARG:NH2	1:B:1178:ARG:O	2.53	0.40
1:B:1312:LYS:CD	1:B:1488:VAL:HG13	2.49	0.40
1:B:1405:GLU:HG3	1:B:1425:LYS:CB	2.52	0.40
1:B:1466:TYR:CD2	1:B:1513:VAL:HG11	2.56	0.40
1:A:1262:THR:HG22	1:A:1264:GLU:H	1.86	0.40
1:A:1490:ALA:HB3	1:A:1527:PRO:HB3	2.04	0.40
1:B:1043:ILE:HD12	1:B:1269:PHE:CE1	2.56	0.40
1:B:1415:GLY:O	1:B:1417:GLU:N	2.54	0.40
1:B:1455:ALA:O	1:B:1459:TYR:HB2	2.21	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:1462:ASP:O	1:A:1462:ASP:O[12_555]	2.02	0.18

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	547/557 (98%)	485 (89%)	54 (10%)	8 (2%)	8	16
1	B	546/557 (98%)	444 (81%)	81 (15%)	21 (4%)	2	3
All	All	1093/1114 (98%)	929 (85%)	135 (12%)	29 (3%)	4	6

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1015	LYS
1	A	1401	LYS
1	B	1015	LYS
1	A	1399	CYS
1	B	1065	ILE
1	B	1352	ASN
1	B	1401	LYS
1	B	1529	THR
1	B	1556	THR
1	B	1018	PRO
1	B	1273	GLY
1	B	1400	ALA
1	B	1437	PHE
1	A	1520	ALA
1	A	1529	THR
1	B	1072	GLU
1	B	1325	PRO
1	B	1551	ALA
1	A	1556	THR
1	B	1265	ASN
1	B	1399	CYS
1	B	1421	GLU
1	B	1528	ILE
1	B	1026	LEU
1	B	1077	THR
1	A	1528	ILE
1	B	1154	GLY
1	A	1273	GLY
1	B	1260	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	432/440 (98%)	405 (94%)	27 (6%)	16	34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	431/440 (98%)	399 (93%)	32 (7%)	13	27
All	All	863/880 (98%)	804 (93%)	59 (7%)	14	31

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1008	ILE
1	A	1020	MET
1	A	1062	VAL
1	A	1094	VAL
1	A	1169	VAL
1	A	1195	THR
1	A	1224	ARG
1	A	1244	GLN
1	A	1250	LEU
1	A	1274	PRO
1	A	1277	ASN
1	A	1278	ILE
1	A	1286	ILE
1	A	1311	GLU
1	A	1337	LEU
1	A	1347	ASP
1	A	1356	LEU
1	A	1375	VAL
1	A	1398	LEU
1	A	1406	VAL
1	A	1430	LEU
1	A	1443	LEU
1	A	1513	VAL
1	A	1523	ARG
1	A	1526	VAL
1	A	1533	MET
1	A	1535	MET
1	B	1012	GLN
1	B	1020	MET
1	B	1040	LYS
1	B	1062	VAL
1	B	1072	GLU
1	B	1074	LYS
1	B	1085	LEU
1	B	1094	VAL
1	B	1165	THR

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Mol	Chain	Res	Type
1	B	1169	VAL
1	B	1182	ILE
1	B	1195	THR
1	B	1244	GLN
1	B	1250	LEU
1	B	1269	PHE
1	B	1275	PHE
1	B	1277	ASN
1	B	1278	ILE
1	B	1290	THR
1	B	1311	GLU
1	B	1330	ILE
1	B	1353	LEU
1	B	1382	ASN
1	B	1444	ASP
1	B	1462	ASP
1	B	1480	LEU
1	B	1513	VAL
1	B	1523	ARG
1	B	1526	VAL
1	B	1533	MET
1	B	1535	MET
1	B	1546	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1012	GLN
1	A	1029	GLN
1	A	1140	HIS
1	A	1149	ASN
1	A	1150	HIS
1	A	1158	ASN
1	A	1244	GLN
1	A	1261	GLN
1	A	1265	ASN
1	A	1277	ASN
1	A	1283	ASN
1	A	1362	ASN
1	A	1382	ASN
1	B	1029	GLN
1	B	1140	HIS

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Mol	Chain	Res	Type
1	B	1149	ASN
1	B	1150	HIS
1	B	1158	ASN
1	B	1244	GLN
1	B	1277	ASN
1	B	1283	ASN
1	B	1362	ASN
1	B	1369	ASN
1	B	1382	ASN
1	B	1393	ASN
1	B	1436	ASN
1	B	1465	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	4	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	8	-	4,4,4	0.69	0	6,6,6	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	B	9	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	1	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	A	5	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	7	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	B	10	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	11	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	6	-	4,4,4	0.68	0	6,6,6	0.49	0
2	SO4	B	2	-	4,4,4	0.69	0	6,6,6	0.49	0
2	SO4	A	3	-	4,4,4	0.68	0	6,6,6	0.49	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	8	SO4	2	0
2	B	9	SO4	1	0
2	A	5	SO4	2	0
2	A	7	SO4	2	0
2	B	2	SO4	1	0
2	A	3	SO4	6	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.