



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 08:55 pm BST

PDB ID : 1CJY  
Title : HUMAN CYTOSOLIC PHOSPHOLIPASE A2  
Authors : Dessen, A.; Tang, J.; Schmidt, H.; Stahl, M.; Clark, J.D.; Seehra, J.; Somers, W.S.  
Deposited on : 1999-04-20  
Resolution : 2.50 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

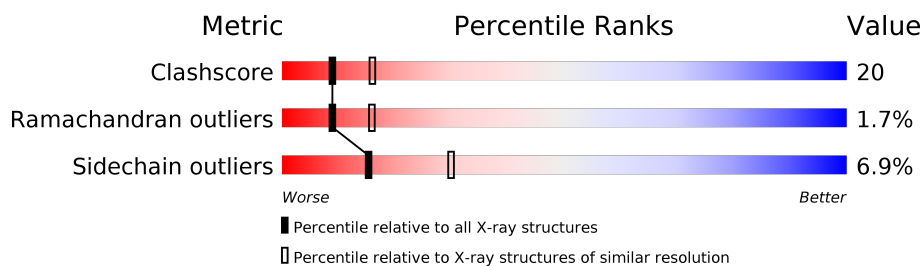
# 1 Overall quality at a glance

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	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	749	
1	B	749	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9706 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.

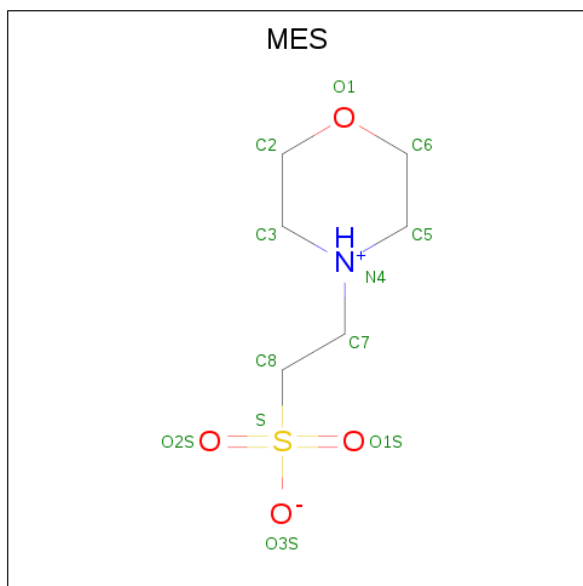
- Molecule 1 is a protein called PROTEIN (CYTOSOLIC PHOSPHOLIPASE A2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	633	Total	C	N	O	S	0	0	0
			4876	3144	804	895	33			
1	B	614	Total	C	N	O	S	0	0	0
			4744	3066	773	871	34			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Ca	0	0
			2	2		
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 4 is water.

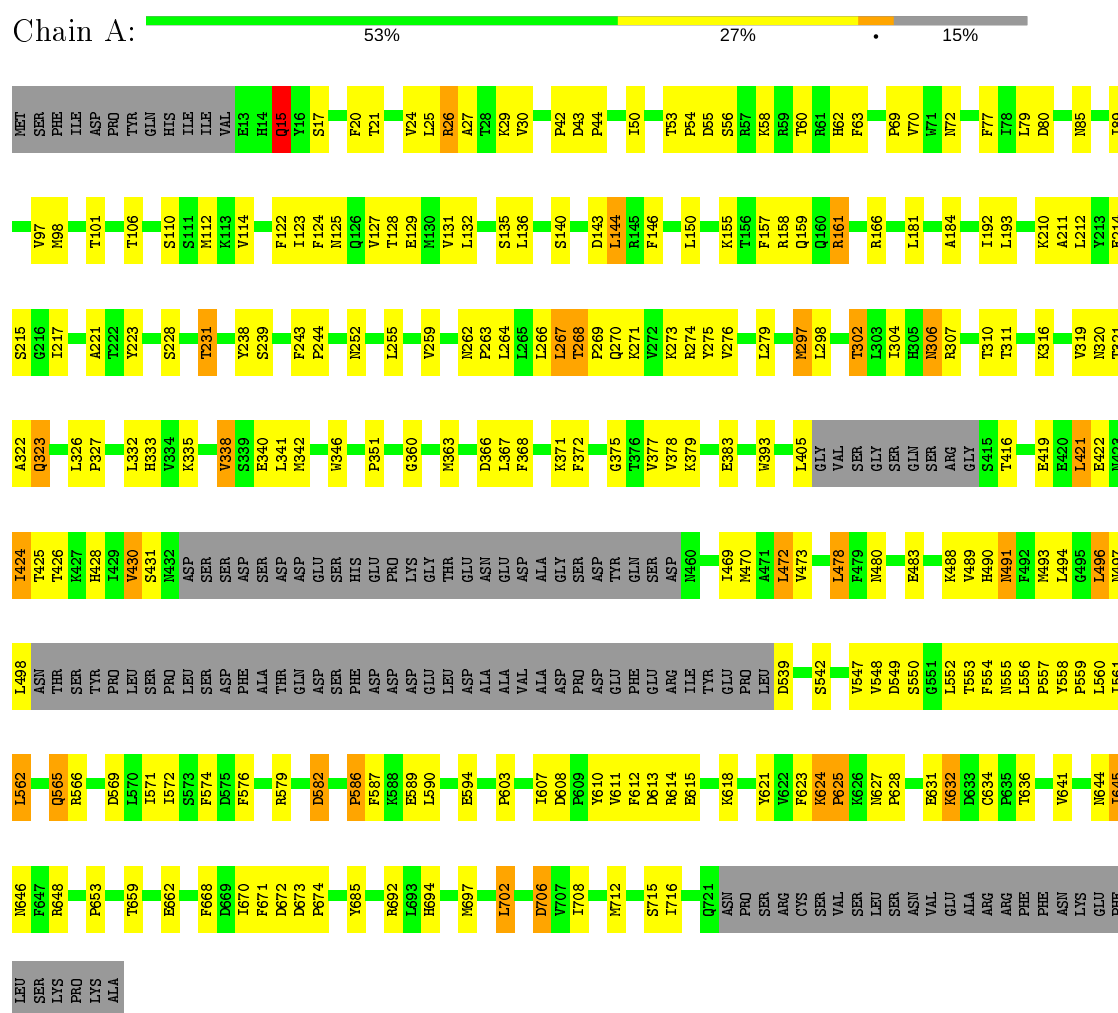
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	32	Total	O	0	0
			32	32		
4	B	26	Total	O	0	0
			26	26		

### 3 Residue-property plots

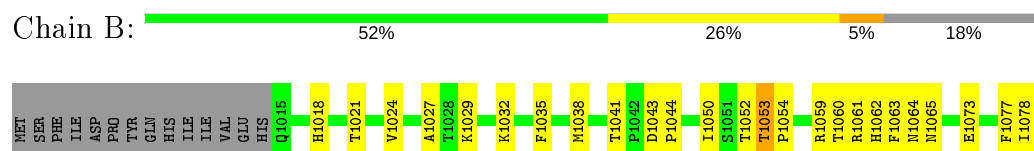
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according 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: PROTEIN (CYTOSOLIC PHOSPHOLIPASE A2)



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SER	V1641	LEU	S1476	SER	V1320	E1214	V1086
ASN	L1642	D1639	A1477	GLY	T1321	E1214	L091
VAL	A1643	I1545	L1478	GLN	Q1323	I1217	V1097
GLU	M1644	H1546	F1479	SER	P1324	D1219	M1098
ALA	I1645	V1547	M1480	ARG	P1325	C1220	V1097
ARG	M1646	V1548	T1481	GLY	F1329	L1227	T1101
ARG	Y1650	D1549	R1482	S1415	L1332	S1228	L1102
PHE	LYS	S1550	E1483	T1416	L1335	E1231	G1103
PHE	A1652	M1555	R1485	E1418	K1335	W1232	K1113
ASN		L1556	V1489	E1419	V1338	E1116	
LYS		P1557	H1490	E1420	S1339	Y1238	
GLU	E1658	Y1558	M1491	L1421	E1340	I1123	
PHE	E1659	I1561	F1492	I1424	L1341	F1124	
LEU	E1660	R1562	M1493	T1425	M1342	N1125	
SER	E1661	R1563	L1494	T1426	F1343	Q1126	
LYS	E1662	P1564		K1427	F1349	V1127	
PRO	I1670	Q1565	M1497	H1428	Y1352	T1128	
LYS		R1566	LEU	I1429	ASN	E1130	
ALA	E1675	G1567	THR	V1430	Y1352	V1259	
	S1676	V1568	SER	ASN	M1363	S1260	
	T1680		TVR	ASP	H1261	V1131	
	Y1685	D1582	PRO	SER	A1364	L1132	
	F1686	S1583	LEU	SER	P1365	N1262	
	M1687	S1584	ASP	ASP	D1366	L1264	
	F1690	P1585	PRO	SER	L1367	D1143	
	L1696	P1586	LEU	ASP	F1368	T1268	
	H1697	L1590	SER	ASP	G1369	P1269	
	H1698	K1595	ASP	GLU	S1370	Q1270	
			PHE	SER	K1371	R1157	
	L1702	M1600	ALA	ALA	F1372	R1158	
		THR	GLN	GLU	M1374	R1161	
	I1705	K1601	ASP	PRO	G1375		
	D1706	L1602	SER	LYS	T1376	I1165	
	V1707	D1608	THR	GLY	V1377	L1172	
	I1708	V1611	PHE	THR	Y1381	L1173	
	K1709	F1612	ASP	GLU	E1382	G1174	
	M1712	G1616	GLU	GLU	E1383	N1177	
	V1713	L1617	LEU	ASP	N1384	S1178	
		K1618	ASP	ALA	H1387	E1179	
	I1716	E1619	ALA	SER		G1180	
	E1717	P1625	VAL	ASP	Y1393	L1181	
	ARG	LYS	ALA	TYR	M1297	A1184	
	ARG	ASN	ASP	GLN	L1298	R1185	
	GLN	PRO	PRO	SER		D1186	
	ASN	ASP	ASP	ASP	E1301	V1187	
	PRO	ASP	GLU	ASN	T1302	P1188	
	SER	MET	PHE	GLN	H1305	V1189	
	PRO	GLU	ARG	ALA	N1402	V1190	
	ARG	LYS	GLU	S1463	R1403	A1191	
	CYS		ARG	K1465	V1404	I1192	
	SER	D1633	ILE	I1466	L1406	L1193	
	VAL	T1636	TYR	H1466	G1406	K1318	
	SER		GLU			V1319	
	LEU		PRO	M1470		K1210	

## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	153.59 Å 95.49 Å 139.13 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 2.50	Depositor
% Data completeness (in resolution range)	93.3 (12.00-2.50)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.843	Depositor
R, $R_{free}$	0.229 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9706	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.39	0/4999	0.63	0/6796
1	B	0.40	0/4862	0.64	1/6603 (0.0%)
All	All	0.39	0/9861	0.63	1/13399 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1227	LEU	CA-CB-CG	5.49	127.94	115.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	4876	0	4668	203	0
1	B	4744	0	4576	181	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	12	0	13	0	0
3	B	12	0	13	1	0
4	A	32	0	0	1	0
4	B	26	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	9706	0	9270	384	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (384) 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:323:GLN:N	1:A:323:GLN:HE21	1.54	1.04
1:A:79:LEU:HD22	1:A:85:ASN:HD22	1.23	1.03
1:A:323:GLN:NE2	1:A:323:GLN:H	1.59	0.99
1:B:1323:GLN:HE21	1:B:1323:GLN:H	1.08	0.98
1:B:1465:ILE:HD12	1:B:1465:ILE:H	1.26	0.97
1:A:565:GLN:H	1:A:565:GLN:NE2	1.64	0.95
1:B:1429:ILE:HD12	1:B:1548:VAL:HG11	1.51	0.91
1:B:1323:GLN:NE2	1:B:1323:GLN:H	1.69	0.90
1:A:425:THR:HG23	1:A:428:HIS:H	1.37	0.89
1:B:1262:ASN:HD21	1:B:1264:LEU:HD23	1.37	0.89
1:A:268:THR:HG22	1:A:271:LYS:H	1.38	0.87
1:A:193:LEU:HD11	1:A:561:ILE:HD13	1.54	0.87
1:A:608:ASP:OD1	1:A:611:VAL:HB	1.75	0.87
1:B:1323:GLN:HE21	1:B:1323:GLN:N	1.74	0.85
1:B:1491:ASN:ND2	1:B:1493:MET:H	1.76	0.83
1:A:323:GLN:HE21	1:A:323:GLN:H	0.86	0.83
1:A:97:VAL:HG23	1:A:98:MET:H	1.45	0.81
1:B:1029:LYS:O	1:B:1128:THR:HB	1.81	0.81
1:A:26:ARG:HB2	1:A:69:PRO:O	1.82	0.80
1:A:79:LEU:HD22	1:A:85:ASN:ND2	1.98	0.79
1:B:1268:THR:HG22	1:B:1271:LYS:H	1.49	0.77
1:A:363:MET:HE2	1:A:368:PHE:HA	1.66	0.76
1:A:306:ASN:HD21	1:A:307:ARG:HH11	1.32	0.76
1:A:238:TYR:CE2	1:A:327:PRO:HG3	2.21	0.75
1:B:1187:VAL:HG12	1:B:1188:PRO:HD2	1.67	0.75
1:A:321:THR:H	1:A:323:GLN:HE22	1.31	0.75
1:B:1321:THR:H	1:B:1323:GLN:HE22	1.33	0.75
1:A:29:LYS:O	1:A:128:THR:HB	1.86	0.74
1:A:298:LEU:O	1:A:302:THR:HG23	1.88	0.74
1:B:1097:VAL:HG23	1:B:1098:MET:H	1.53	0.73
1:B:1187:VAL:CG1	1:B:1188:PRO:HD2	2.18	0.73
1:A:157:PHE:CE1	1:A:319:VAL:HG23	2.23	0.73
1:A:15:GLN:NE2	1:A:17:SER:H	1.87	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1425:THR:HB	1:B:1428:HIS:H	1.53	0.71
1:B:1024:VAL:HA	1:B:1132:LEU:HD22	1.72	0.71
1:A:155:LYS:O	1:A:159:GLN:HG3	1.91	0.70
1:B:1608:ASP:O	1:B:1611:VAL:HG23	1.91	0.70
1:B:1264:LEU:H	1:B:1264:LEU:HD22	1.56	0.69
1:A:316:LYS:HE3	1:A:351:PRO:O	1.91	0.69
1:B:1268:THR:CG2	1:B:1271:LYS:H	2.05	0.69
1:A:306:ASN:ND2	1:A:307:ARG:HG2	2.07	0.69
1:B:1645:ILE:HG22	1:B:1646:ASN:N	2.08	0.69
1:A:556:LEU:HD11	1:A:589:GLU:HG2	1.75	0.68
1:A:279:LEU:HG	1:A:297:MET:HE2	1.74	0.68
1:A:565:GLN:H	1:A:565:GLN:HE21	1.41	0.68
1:A:306:ASN:HD21	1:A:307:ARG:NH1	1.90	0.68
1:A:210:LYS:O	1:A:214:GLU:HG3	1.94	0.68
1:A:366:ASP:HA	1:A:383:GLU:HG3	1.75	0.68
1:B:1430:VAL:HG13	1:B:1546:HIS:CE1	2.30	0.67
1:A:181:LEU:HA	1:A:184:ALA:HB2	1.75	0.67
1:B:1113:LYS:O	1:B:1116:GLU:HB3	1.95	0.66
1:B:1298:LEU:O	1:B:1302:THR:HG23	1.95	0.66
1:B:1645:ILE:HG22	1:B:1646:ASN:H	1.59	0.66
1:A:491:ASN:ND2	1:A:493:MET:H	1.94	0.65
1:A:15:GLN:HE22	1:A:17:SER:H	1.42	0.65
1:A:269:PRO:O	1:A:273:LYS:HG3	1.97	0.65
1:B:1342:MET:HE2	1:B:1595:LYS:HG2	1.77	0.65
1:B:1097:VAL:HG23	1:B:1098:MET:N	2.12	0.65
1:B:1405:LEU:HD12	1:B:1466:HIS:HB2	1.79	0.65
1:A:161:ARG:HB2	1:A:322:ALA:HB1	1.79	0.64
1:B:1144:LEU:HD22	1:B:1375:GLY:HA2	1.80	0.64
1:A:610:TYR:O	1:A:614:ARG:HG2	1.98	0.64
1:A:144:LEU:HD22	1:A:375:GLY:HA2	1.79	0.63
1:B:1702:LEU:HD12	1:B:1705:ILE:HD11	1.80	0.63
1:B:1218:LEU:HD22	1:B:1325:PRO:HG2	1.80	0.63
1:A:193:LEU:CD1	1:A:561:ILE:HD13	2.27	0.63
1:B:1311:THR:HB	1:B:1383:GLU:OE2	2.00	0.62
1:A:416:THR:OG1	1:A:419:GLU:HG3	2.00	0.61
1:A:158:ARG:HH21	1:A:566:ARG:HA	1.64	0.61
1:B:1123:ILE:HD12	1:B:1128:THR:O	2.01	0.61
1:A:603:PRO:HB3	1:A:634:CYS:HB2	1.82	0.61
1:B:1078:ILE:HG22	1:B:1373:PHE:HD2	1.64	0.61
1:A:89:ILE:HD13	1:A:132:LEU:HD12	1.83	0.61
1:B:1255:LEU:HD12	1:B:1690:PHE:CE1	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1465:ILE:CD1	1:B:1465:ILE:H	2.02	0.61
1:A:89:ILE:HD13	1:A:132:LEU:CD1	2.31	0.60
1:B:1187:VAL:HG12	1:B:1188:PRO:CD	2.31	0.60
1:B:1369:GLY:HA2	1:B:1489:VAL:HG22	1.83	0.60
1:A:579:ARG:HD3	1:A:586:PRO:HB3	1.83	0.60
1:B:1255:LEU:HD12	1:B:1690:PHE:HE1	1.65	0.60
1:B:1387:HIS:HD2	4:B:77:HOH:O	1.85	0.60
1:A:161:ARG:NH1	1:A:221:ALA:O	2.34	0.60
1:A:275:TYR:HA	1:A:297:MET:HE1	1.82	0.60
1:A:548:VAL:HG22	1:A:549:ASP:N	2.15	0.60
1:B:1369:GLY:HA2	1:B:1489:VAL:CG2	2.30	0.60
1:B:1565:GLN:H	1:B:1565:GLN:NE2	2.00	0.60
1:B:1018:HIS:CE1	1:B:1081:PRO:HB3	2.36	0.60
1:B:1425:THR:HB	1:B:1428:HIS:N	2.15	0.60
1:B:1228:SER:O	1:B:1231:THR:HB	2.02	0.60
1:A:228:SER:O	1:A:231:THR:HB	2.02	0.59
1:A:125:ASN:O	1:A:127:VAL:HG23	2.02	0.59
1:A:97:VAL:HG23	1:A:98:MET:N	2.16	0.58
1:A:53:THR:HG23	1:A:54:PRO:HD2	1.85	0.58
1:A:21:THR:HB	1:A:135:SER:HB2	1.84	0.58
1:A:645:ILE:O	1:A:648:ARG:HG3	2.03	0.58
1:A:25:LEU:HA	1:A:72:ASN:HD22	1.67	0.58
1:A:553:THR:HG22	1:A:554:PHE:CD2	2.38	0.58
1:A:558:TYR:HB3	1:A:562:LEU:HD22	1.84	0.58
1:A:166:ARG:HH12	1:A:184:ALA:HB3	1.69	0.57
1:B:1582:ASP:O	1:B:1617:LEU:HD22	2.03	0.57
1:A:426:THR:O	1:A:430:VAL:HG22	2.04	0.57
1:A:430:VAL:HG23	1:A:431:SER:H	1.70	0.57
1:B:1021:THR:HB	1:B:1135:SER:HB2	1.86	0.57
1:A:627:ASN:N	1:A:628:PRO:HD2	2.20	0.57
1:B:1416:THR:OG1	1:B:1419:GLU:HG3	2.05	0.57
1:A:15:GLN:HA	1:A:497:ASN:CG	2.24	0.57
1:B:1189:VAL:HB	1:B:1568:VAL:HA	1.86	0.57
1:B:1157:PHE:CE1	1:B:1319:VAL:HG22	2.40	0.56
1:A:319:VAL:O	1:A:319:VAL:HG22	2.06	0.56
1:A:470:MET:HA	1:A:470:MET:HE2	1.86	0.56
1:A:659:THR:OG1	1:A:662:GLU:HG3	2.06	0.56
1:B:1264:LEU:N	1:B:1264:LEU:HD22	2.21	0.56
1:A:430:VAL:HG23	1:A:431:SER:N	2.21	0.56
1:B:1127:VAL:HB	4:B:62:HOH:O	2.04	0.56
1:A:493:MET:O	1:A:496:LEU:HD23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:480:ASN:O	1:A:483:GLU:HG2	2.06	0.56
1:B:1259:VAL:HG12	1:B:1685:TYR:HB2	1.87	0.55
1:A:366:ASP:OD2	1:A:367:LEU:HD13	2.05	0.55
1:A:335:LYS:NZ	1:A:539:ASP:HB2	2.20	0.55
1:A:498:LEU:C	1:A:498:LEU:HD13	2.27	0.55
1:B:1583:SER:O	1:B:1584:SER:O	2.24	0.55
1:A:157:PHE:CD1	1:A:319:VAL:HG23	2.41	0.55
1:B:1174:GLY:O	1:B:1177:ASN:ND2	2.40	0.55
1:B:1259:VAL:O	1:B:1259:VAL:HG12	2.04	0.55
1:B:1184:ALA:HB1	1:B:1186:ASP:O	2.08	0.54
1:A:332:LEU:O	1:A:547:VAL:HA	2.07	0.54
1:B:1332:LEU:HG	1:B:1550:SER:HA	1.88	0.54
1:B:1650:TYR:O	1:B:1652:ALA:N	2.40	0.54
1:A:259:VAL:HG12	1:A:685:TYR:HB2	1.90	0.54
1:B:1321:THR:OG1	1:B:1323:GLN:NE2	2.41	0.54
1:A:181:LEU:HA	1:A:184:ALA:CB	2.37	0.54
1:A:158:ARG:NH2	1:A:566:ARG:O	2.40	0.54
1:B:1335:LYS:O	1:B:1338:VAL:HG22	2.08	0.54
1:B:1238:TYR:O	1:B:1318:LYS:HG3	2.07	0.53
1:A:335:LYS:O	1:A:338:VAL:HG12	2.08	0.53
1:A:363:MET:HE2	1:A:368:PHE:CA	2.35	0.53
1:B:1268:THR:HG22	1:B:1271:LYS:CB	2.38	0.53
1:B:1158:ARG:NH2	1:B:1566:ARG:O	2.39	0.53
1:B:1054:PRO:HG2	1:B:1494:LEU:HD13	1.89	0.53
1:A:79:LEU:HB3	1:A:85:ASN:ND2	2.24	0.53
1:B:1424:ILE:HD12	1:B:1424:ILE:O	2.08	0.53
1:B:1400:LEU:O	1:B:1404:VAL:HG23	2.08	0.53
1:A:419:GLU:O	1:A:422:GLU:HG2	2.09	0.53
1:B:1165:ILE:HD12	1:B:1220:CYS:O	2.08	0.53
1:A:556:LEU:CD1	1:A:589:GLU:HG2	2.39	0.52
1:B:1480:ASN:CG	1:B:1482:ARG:H	2.12	0.52
1:B:1131:VAL:O	1:B:1132:LEU:HD23	2.09	0.52
1:A:469:ILE:HG22	1:A:470:MET:HE3	1.92	0.52
1:B:1243:PHE:CD1	1:B:1244:PRO:HA	2.44	0.52
1:A:631:GLU:O	1:A:632:LYS:O	2.27	0.52
1:A:306:ASN:HD22	1:A:306:ASN:C	2.13	0.52
1:B:1027:ALA:HA	1:B:1129:GLU:O	2.09	0.52
1:A:589:GLU:OE2	1:A:589:GLU:N	2.34	0.52
1:A:469:ILE:HG22	1:A:470:MET:CE	2.41	0.51
1:A:607:ILE:HG23	1:A:623:PHE:CE2	2.45	0.51
1:A:252:ASN:HD22	1:A:694:HIS:HE1	1.56	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1659:THR:O	1:B:1662:GLU:N	2.38	0.51
1:B:1329:PHE:HB2	1:B:1349:PHE:HB2	1.93	0.51
1:A:268:THR:CG2	1:A:271:LYS:H	2.18	0.51
1:B:1465:ILE:N	1:B:1465:ILE:HD12	2.09	0.51
1:B:1371:LYS:HE2	1:B:1490:HIS:CE1	2.46	0.51
1:B:1210:LYS:O	1:B:1214:GLU:HG3	2.10	0.51
1:B:1231:THR:CG2	1:B:1393:TRP:HE3	2.23	0.51
1:B:1264:LEU:H	1:B:1264:LEU:CD2	2.23	0.51
1:B:1491:ASN:ND2	1:B:1491:ASN:C	2.64	0.51
1:B:1491:ASN:HD22	1:B:1491:ASN:C	2.12	0.51
1:B:1262:ASN:HD22	1:B:1262:ASN:C	2.14	0.51
1:B:1259:VAL:CG1	1:B:1685:TYR:HB2	2.41	0.51
1:A:332:LEU:HG	1:A:550:SER:HA	1.93	0.50
1:A:708:ILE:HG22	1:A:712:MET:HE3	1.93	0.50
1:B:1301:GLU:O	1:B:1305:HIS:HB3	2.11	0.50
1:A:259:VAL:HG12	1:A:259:VAL:O	2.10	0.50
1:B:1035:PHE:HA	1:B:1038:MET:HE3	1.93	0.50
1:A:587:PHE:HE2	1:A:612:PHE:HB2	1.77	0.50
1:B:1041:THR:HG22	1:B:1065:ASN:HA	1.93	0.50
1:A:181:LEU:HG	1:A:716:ILE:HD13	1.93	0.50
1:B:1191:ALA:CB	1:B:1561:ILE:HG12	2.42	0.50
1:B:1078:ILE:HG22	1:B:1373:PHE:CD2	2.46	0.50
1:B:1282:LYS:NZ	1:B:1384:ASN:HD21	2.09	0.50
1:B:1231:THR:HG23	1:B:1393:TRP:HE3	1.76	0.50
1:B:1279:LEU:HG	1:B:1297:MET:CE	2.42	0.50
1:A:306:ASN:HD21	1:A:307:ARG:HG2	1.77	0.49
1:B:1712:MET:O	1:B:1716:ILE:HG13	2.12	0.49
1:A:215:SER:OG	1:A:217:ILE:HG12	2.13	0.49
1:A:30:VAL:HG11	1:A:44:PRO:HG3	1.93	0.49
1:A:143:ASP:OD2	1:A:377:VAL:HG13	2.12	0.49
1:A:469:ILE:O	1:A:473:VAL:HG23	2.12	0.49
1:A:548:VAL:HG22	1:A:549:ASP:H	1.75	0.49
1:B:1645:ILE:CG2	1:B:1646:ASN:H	2.22	0.49
1:A:123:ILE:HD12	1:A:123:ILE:N	2.27	0.49
1:B:1043:ASP:HA	1:B:1063:PHE:O	2.13	0.49
1:A:238:TYR:CZ	1:A:327:PRO:HG3	2.48	0.49
1:B:1123:ILE:HD11	1:B:1126:GLN:C	2.32	0.49
1:B:1421:LEU:O	1:B:1421:LEU:HD23	2.13	0.49
1:A:122:PHE:C	1:A:123:ILE:HD12	2.34	0.49
1:A:20:PHE:HD1	1:A:135:SER:O	1.96	0.49
1:A:306:ASN:HD22	1:A:307:ARG:N	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1079:LEU:HB3	1:B:1085:ASN:OD1	2.12	0.49
1:A:211:ALA:HB1	1:A:702:LEU:HD13	1.95	0.49
1:B:1143:ASP:OD2	1:B:1377:VAL:HG13	2.13	0.49
1:A:624:LYS:HG3	1:A:625:PRO:HD2	1.94	0.48
1:B:1421:LEU:HA	1:B:1424:ILE:CG2	2.43	0.48
1:B:1659:THR:O	1:B:1660:GLU:C	2.50	0.48
1:A:212:LEU:HD22	1:A:217:ILE:HG21	1.95	0.48
1:B:1231:THR:HG23	1:B:1393:TRP:CE3	2.48	0.48
1:A:668:PHE:CD2	1:A:692:ARG:HD3	2.48	0.48
1:A:279:LEU:HG	1:A:297:MET:CE	2.44	0.48
1:A:611:VAL:O	1:A:615:GLU:HB2	2.14	0.48
1:B:1399:ILE:HA	1:B:1485:ARG:HG3	1.94	0.48
1:B:1650:TYR:HB3	1:B:1652:ALA:O	2.14	0.48
1:A:239:SER:HB2	1:A:310:THR:HG21	1.96	0.48
1:B:1178:SER:O	1:B:1180:GLY:N	2.47	0.48
1:B:1430:VAL:HG13	1:B:1546:HIS:HE1	1.79	0.48
1:B:1480:ASN:HD21	1:B:1482:ARG:CB	2.26	0.48
1:B:1561:ILE:HG13	1:B:1568:VAL:HG11	1.95	0.48
1:B:1231:THR:HG21	1:B:1393:TRP:HB2	1.96	0.47
1:A:610:TYR:HA	1:A:613:ASP:OD1	2.13	0.47
1:B:1032:LYS:HG2	1:B:1102:LEU:HD22	1.96	0.47
1:B:1321:THR:N	1:B:1323:GLN:HE22	2.08	0.47
1:A:150:LEU:CD1	1:A:158:ARG:HE	2.26	0.47
1:A:645:ILE:HG22	1:A:646:ASN:N	2.29	0.47
1:B:1193:LEU:HG	1:B:1557:PRO:HG2	1.96	0.47
1:B:1214:GLU:OE1	1:B:1698:HIS:HE1	1.97	0.47
1:A:311:THR:HB	1:A:383:GLU:OE2	2.14	0.47
1:A:333:HIS:HE1	4:A:3029:HOH:O	1.98	0.47
1:B:1421:LEU:C	1:B:1421:LEU:HD23	2.34	0.47
1:B:1387:HIS:CD2	4:B:77:HOH:O	2.63	0.47
1:B:1687:ASN:HD22	1:B:1687:ASN:N	2.12	0.47
1:A:24:VAL:HA	1:A:132:LEU:HD23	1.97	0.47
1:A:670:ILE:N	1:A:670:ILE:HD12	2.30	0.47
1:B:1491:ASN:HB2	1:B:1545:ILE:HG23	1.96	0.46
1:B:1261:HIS:O	1:B:1263:PRO:HD3	2.15	0.46
1:A:708:ILE:HG22	1:A:712:MET:CE	2.45	0.46
1:A:421:LEU:O	1:A:424:ILE:HG22	2.15	0.46
1:A:670:ILE:HG22	1:A:671:PHE:CD1	2.50	0.46
1:B:1165:ILE:HD12	1:B:1220:CYS:C	2.36	0.46
1:B:1370:SER:HA	1:B:1381:TYR:CD1	2.51	0.46
1:A:124:PHE:O	1:A:128:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:THR:HG23	1:A:270:GLN:H	1.80	0.46
1:B:1558:TYR:HB3	1:B:1562:LEU:HD22	1.98	0.46
1:B:1268:THR:HG22	1:B:1271:LYS:HB2	1.97	0.46
1:A:586:PRO:CB	1:A:641:VAL:HG21	2.45	0.46
1:A:576:PHE:HE2	1:A:697:MET:HG3	1.81	0.46
1:B:1332:LEU:O	1:B:1547:VAL:HA	2.16	0.46
1:A:24:VAL:HG11	1:A:60:THR:HG21	1.98	0.46
1:A:491:ASN:HD21	1:A:493:MET:HB2	1.80	0.46
1:B:1157:PHE:CE1	1:B:1319:VAL:CG2	2.98	0.46
1:A:15:GLN:NE2	1:A:17:SER:N	2.61	0.46
1:B:1675:GLU:O	1:B:1676:SER:O	2.34	0.46
1:A:346:TRP:CE2	1:A:559:PRO:HG2	2.52	0.45
1:A:561:ILE:HD12	1:A:571:ILE:HG12	1.98	0.45
1:B:1280:TRP:O	1:B:1284:SER:HB2	2.16	0.45
1:B:1491:ASN:HD22	1:B:1492:PHE:N	2.13	0.45
1:A:25:LEU:HD12	1:A:131:VAL:HG12	1.98	0.45
1:A:306:ASN:ND2	1:A:306:ASN:C	2.68	0.45
1:A:712:MET:O	1:A:716:ILE:HG13	2.16	0.45
1:A:231:THR:HG23	1:A:393:TRP:CE3	2.51	0.45
1:A:267:LEU:HD11	1:A:298:LEU:HD22	1.98	0.45
1:A:594:GLU:OE1	1:A:607:ILE:HG12	2.17	0.45
1:A:157:PHE:CD1	1:A:319:VAL:CG2	3.00	0.45
1:A:346:TRP:CD2	1:A:559:PRO:HG2	2.51	0.45
1:A:706:ASP:OD1	1:A:706:ASP:N	2.47	0.45
1:B:1244:PRO:O	1:B:1245:GLU:C	2.55	0.45
1:B:1274:ARG:HG2	1:B:1274:ARG:HH11	1.82	0.45
1:A:262:ASN:HD22	1:A:263:PRO:CD	2.29	0.45
1:A:335:LYS:HZ2	1:A:539:ASP:HB2	1.82	0.45
1:B:1633:ASP:N	1:B:1633:ASP:OD1	2.50	0.45
1:A:223:TYR:CZ	1:A:566:ARG:HD3	2.52	0.45
1:A:263:PRO:O	1:A:266:LEU:HB2	2.17	0.45
1:B:1053:THR:HG22	1:B:1054:PRO:HD2	1.98	0.45
1:A:340:GLU:OE1	1:A:342:MET:HB3	2.16	0.44
1:B:1659:THR:O	1:B:1661:GLU:N	2.50	0.44
1:A:553:THR:HG22	1:A:554:PHE:HD2	1.79	0.44
1:B:1491:ASN:HD21	1:B:1493:MET:HB2	1.82	0.44
1:A:231:THR:CG2	1:A:393:TRP:CE3	3.00	0.44
1:B:1050:ILE:HD12	1:B:1077:PHE:CD1	2.52	0.44
1:B:1566:ARG:O	1:B:1567:GLY:C	2.55	0.44
1:A:124:PHE:HB2	1:A:128:THR:HG23	1.99	0.44
1:A:618:LYS:HG3	1:A:621:TYR:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1612:PHE:O	1:B:1616:GLY:N	2.45	0.44
1:A:243:PHE:CD1	1:A:244:PRO:HA	2.53	0.44
1:A:378:VAL:HG23	1:A:379:LYS:N	2.32	0.44
1:A:342:MET:HG3	1:A:342:MET:O	2.17	0.44
1:A:56:SER:O	1:A:58:LYS:HG3	2.17	0.44
1:A:621:TYR:CD1	1:A:621:TYR:N	2.86	0.44
1:B:1352:TYR:O	1:B:1365:PRO:HD3	2.18	0.44
1:B:1644:ASN:HA	1:B:1696:LEU:HD11	2.00	0.44
1:A:274:ARG:HH11	1:A:274:ARG:HG2	1.82	0.44
1:A:558:TYR:N	1:A:559:PRO:CD	2.80	0.44
1:B:1273:LYS:HB2	1:B:1273:LYS:HE3	1.90	0.44
1:B:1617:LEU:HD21	1:B:1643:ALA:CB	2.47	0.44
1:A:25:LEU:HD23	1:A:72:ASN:ND2	2.32	0.43
1:A:97:VAL:CG2	1:A:98:MET:H	2.25	0.43
1:A:341:LEU:HD13	1:A:552:LEU:HB3	1.99	0.43
1:B:1035:PHE:HA	1:B:1038:MET:CE	2.47	0.43
1:B:1123:ILE:HD11	1:B:1127:VAL:N	2.33	0.43
1:B:1642:LEU:HG	1:B:1670:ILE:HD13	2.00	0.43
1:A:582:ASP:OD1	1:A:672:ASP:N	2.51	0.43
1:B:1231:THR:CG2	1:B:1393:TRP:CE3	3.01	0.43
1:B:1619:GLU:OE2	1:B:1646:ASN:HB2	2.19	0.43
1:A:114:VAL:HA	1:A:136:LEU:O	2.18	0.43
1:A:44:PRO:O	1:A:62:HIS:HA	2.18	0.43
1:B:1708:ILE:O	1:B:1712:MET:HG3	2.18	0.43
1:A:146:PHE:HA	1:A:360:GLY:O	2.19	0.43
1:A:231:THR:CG2	1:A:393:TRP:HE3	2.32	0.43
1:A:590:LEU:O	1:A:590:LEU:HD23	2.18	0.43
1:B:1060:THR:HB	1:B:1073:GLU:OE2	2.19	0.43
1:B:1161:ARG:HB2	1:B:1322:ALA:HB1	2.01	0.42
1:B:1259:VAL:O	1:B:1259:VAL:CG1	2.66	0.42
1:A:192:ILE:N	1:A:192:ILE:HD12	2.35	0.42
1:A:304:ILE:HB	1:A:307:ARG:HG3	2.02	0.42
1:A:557:PRO:HB2	1:A:560:LEU:HD12	2.01	0.42
1:A:43:ASP:HA	1:A:63:PHE:O	2.19	0.42
1:B:1600:ASN:O	1:B:1602:LEU:HD22	2.20	0.42
1:B:1645:ILE:CG2	1:B:1646:ASN:N	2.74	0.42
1:B:1698:HIS:CE1	1:B:1702:LEU:HD22	2.54	0.42
1:A:259:VAL:CG1	1:A:685:TYR:HB2	2.49	0.42
1:A:712:MET:O	1:A:715:SER:HB2	2.20	0.42
1:A:80:ASP:OD1	1:A:80:ASP:C	2.57	0.42
1:B:1274:ARG:HG2	1:B:1274:ARG:NH1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:SER:C	1:A:112:MET:H	2.21	0.42
1:B:1177:ASN:O	1:B:1178:SER:C	2.57	0.42
1:B:1641:VAL:CG1	1:B:1642:LEU:N	2.82	0.42
1:A:264:LEU:CD2	1:A:405:LEU:HD23	2.50	0.42
1:A:42:PRO:C	1:A:44:PRO:HD3	2.40	0.42
1:A:548:VAL:CG2	1:A:549:ASP:N	2.83	0.42
1:B:1231:THR:HG22	1:B:1232:TRP:N	2.33	0.42
1:A:267:LEU:HD13	1:A:469:ILE:HD11	2.00	0.42
1:A:371:LYS:NZ	1:A:490:HIS:NE2	2.67	0.42
1:A:50:ILE:HD12	1:A:77:PHE:CD2	2.55	0.42
1:B:1172:LEU:CD2	1:B:1217:ILE:HD13	2.50	0.42
1:A:144:LEU:HD12	1:A:144:LEU:HA	1.85	0.42
1:A:193:LEU:HD11	1:A:561:ILE:CD1	2.36	0.42
1:A:27:ALA:HA	1:A:129:GLU:O	2.19	0.42
1:B:1097:VAL:CG2	1:B:1098:MET:H	2.28	0.42
1:B:1397:PHE:CE2	1:B:1417:MET:HE3	2.55	0.42
1:B:1181:LEU:HG	1:B:1716:ILE:HD13	2.02	0.42
1:A:472:LEU:HD12	1:A:472:LEU:HA	1.85	0.42
1:B:1262:ASN:HD21	1:B:1264:LEU:CD2	2.20	0.42
1:A:326:LEU:HA	1:A:327:PRO:HD3	1.94	0.42
1:A:425:THR:HG23	1:A:428:HIS:N	2.18	0.42
1:A:430:VAL:CG2	1:A:431:SER:H	2.29	0.42
1:B:1421:LEU:HA	1:B:1424:ILE:HG21	2.01	0.42
1:A:166:ARG:NH1	1:A:184:ALA:HB3	2.35	0.41
1:B:1262:ASN:HD22	1:B:1263:PRO:N	2.18	0.41
1:B:1363:MET:HE3	1:B:1492:PHE:CD2	2.55	0.41
1:B:1064:ASN:OD1	3:B:4000:MES:H31	2.20	0.41
1:B:1262:ASN:ND2	1:B:1262:ASN:C	2.74	0.41
1:A:589:GLU:CD	1:A:589:GLU:H	2.19	0.41
1:B:1044:PRO:O	1:B:1062:HIS:HA	2.20	0.41
1:B:1268:THR:HG23	1:B:1270:GLN:H	1.84	0.41
1:B:1489:VAL:HG22	4:B:74:HOH:O	2.19	0.41
1:A:26:ARG:HB3	1:A:70:VAL:HA	2.01	0.41
1:A:319:VAL:O	1:A:319:VAL:CG2	2.68	0.41
1:A:26:ARG:CB	1:A:70:VAL:HA	2.50	0.41
1:A:192:ILE:N	1:A:192:ILE:CD1	2.83	0.41
1:A:320:ASN:OD1	1:A:321:THR:HG23	2.21	0.41
1:B:1617:LEU:HD21	1:B:1643:ALA:HB1	2.02	0.41
1:A:15:GLN:HA	1:A:497:ASN:OD1	2.20	0.41
1:B:1052:THR:OG1	1:B:1085:ASN:ND2	2.54	0.41
1:B:1276:VAL:HG11	1:B:1476:SER:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:MET:CE	1:A:470:MET:HA	2.49	0.41
1:B:1086:VAL:HG23	1:B:1086:VAL:O	2.20	0.41
1:B:1339:SER:HA	1:B:1426:THR:HG21	2.02	0.41
1:B:1103:GLY:HA3	1:B:1124:PHE:HD2	1.86	0.41
1:A:266:LEU:HD12	1:A:302:THR:HG22	2.02	0.41
1:A:572:ILE:HG22	1:A:574:PHE:CE1	2.55	0.41
1:A:673:ASP:OD1	1:A:674:PRO:HD2	2.21	0.41
1:B:1279:LEU:HG	1:B:1297:MET:HE2	2.02	0.41
1:B:1709:LYS:O	1:B:1713:VAL:HG23	2.21	0.41
1:A:274:ARG:NH1	1:A:274:ARG:HG2	2.35	0.40
1:B:1291:PHE:CE1	1:B:1470:MET:HE3	2.56	0.40
1:B:1480:ASN:ND2	1:B:1483:GLU:N	2.69	0.40
1:B:1563:ARG:HA	1:B:1564:PRO:HD2	1.90	0.40
1:A:262:ASN:HD22	1:A:263:PRO:HD2	1.85	0.40
1:A:276:VAL:HG13	1:A:478:LEU:HG	2.02	0.40
1:A:372:PHE:CE1	1:A:377:VAL:HG12	2.56	0.40
1:A:702:LEU:HA	1:A:702:LEU:HD12	1.94	0.40
1:B:1061:ARG:HG2	1:B:1061:ARG:HH11	1.86	0.40
1:B:1340:GLU:HB3	1:B:1343:PHE:HD2	1.87	0.40
1:A:124:PHE:HB2	1:A:128:THR:CG2	2.52	0.40
1:A:608:ASP:OD2	1:A:614:ARG:NH1	2.53	0.40
1:B:1417:MET:HG2	1:B:1680:THR:HG21	2.04	0.40
1:B:1418:GLU:H	1:B:1418:GLU:CD	2.24	0.40

There are no symmetry-related clashes.

## 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	625/749 (83%)	565 (90%)	48 (8%)	12 (2%)	8	13
1	B	602/749 (80%)	553 (92%)	40 (7%)	9 (2%)	10	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	1227/1498 (82%)	1118 (91%)	88 (7%)	21 (2%)	9	16

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	430	VAL
1	A	625	PRO
1	A	632	LYS
1	B	1178	SER
1	B	1584	SER
1	B	1660	GLU
1	B	1676	SER
1	A	15	GLN
1	A	424	ILE
1	B	1179	GLU
1	A	267	LEU
1	A	542	SER
1	B	1180	GLY
1	A	140	SER
1	A	338	VAL
1	B	1184	ALA
1	B	1645	ILE
1	A	55	ASP
1	A	586	PRO
1	B	1177	ASN
1	A	645	ILE

### 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	519/677 (77%)	487 (94%)	32 (6%)	18	35
1	B	511/677 (76%)	472 (92%)	39 (8%)	13	25
All	All	1030/1354 (76%)	959 (93%)	71 (7%)	15	30

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

Mol	Chain	Res	Type
1	A	15	GLN
1	A	26	ARG
1	A	101	THR
1	A	106	THR
1	A	144	LEU
1	A	161	ARG
1	A	231	THR
1	A	255	LEU
1	A	268	THR
1	A	297	MET
1	A	302	THR
1	A	306	ASN
1	A	323	GLN
1	A	421	LEU
1	A	472	LEU
1	A	478	LEU
1	A	488	LYS
1	A	489	VAL
1	A	491	ASN
1	A	494	LEU
1	A	496	LEU
1	A	555	ASN
1	A	562	LEU
1	A	565	GLN
1	A	569	ASP
1	A	582	ASP
1	A	624	LYS
1	A	636	THR
1	A	644	ASN
1	A	653	PRO
1	A	702	LEU
1	A	706	ASP
1	B	1053	THR
1	B	1059	ARG
1	B	1091	LEU
1	B	1101	THR
1	B	1128	THR
1	B	1144	LEU
1	B	1186	ASP
1	B	1227	LEU
1	B	1231	THR
1	B	1262	ASN

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Mol	Chain	Res	Type
1	B	1268	THR
1	B	1284	SER
1	B	1302	THR
1	B	1319	VAL
1	B	1323	GLN
1	B	1340	GLU
1	B	1367	LEU
1	B	1402	ASN
1	B	1425	THR
1	B	1429	ILE
1	B	1465	ILE
1	B	1478	LEU
1	B	1481	THR
1	B	1485	ARG
1	B	1491	ASN
1	B	1494	LEU
1	B	1548	VAL
1	B	1555	ASN
1	B	1562	LEU
1	B	1565	GLN
1	B	1568	VAL
1	B	1582	ASP
1	B	1586	PRO
1	B	1590	LEU
1	B	1595	LYS
1	B	1636	THR
1	B	1658	GLU
1	B	1702	LEU
1	B	1706	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	72	ASN
1	A	82	ASN
1	A	85	ASN
1	A	153	GLN
1	A	258	ASN
1	A	262	ASN
1	A	306	ASN
1	A	323	GLN

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Mol	Chain	Res	Type
1	A	461	GLN
1	A	491	ASN
1	A	565	GLN
1	A	627	ASN
1	A	644	ASN
1	A	684	GLN
1	A	687	ASN
1	A	694	HIS
1	A	704	ASN
1	B	1018	HIS
1	B	1072	ASN
1	B	1082	ASN
1	B	1085	ASN
1	B	1258	ASN
1	B	1262	ASN
1	B	1287	GLN
1	B	1309	ASN
1	B	1323	GLN
1	B	1384	ASN
1	B	1387	HIS
1	B	1480	ASN
1	B	1491	ASN
1	B	1565	GLN
1	B	1684	GLN
1	B	1687	ASN
1	B	1694	HIS
1	B	1698	HIS
1	B	1703	ASN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	MES	A	3000	2	12,12,12	9.06	8 (66%)	14,16,16	2.68	6 (42%)
3	MES	B	4000	2	12,12,12	8.86	8 (66%)	14,16,16	2.61	6 (42%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MES	A	3000	2	-	1/6/14/14	0/1/1/1
3	MES	B	4000	2	-	2/6/14/14	0/1/1/1

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	3000	MES	C8-S	-24.05	1.43	1.77
3	B	4000	MES	C8-S	-23.50	1.44	1.77
3	A	3000	MES	O1S-S	11.83	1.80	1.45
3	B	4000	MES	O2S-S	11.60	1.79	1.45
3	A	3000	MES	O2S-S	11.40	1.78	1.45
3	B	4000	MES	O1S-S	11.21	1.78	1.45
3	A	3000	MES	O3S-S	9.11	1.79	1.47
3	B	4000	MES	O3S-S	8.79	1.78	1.47
3	A	3000	MES	C7-C8	-4.93	1.39	1.52
3	B	4000	MES	C7-C8	-4.83	1.39	1.52
3	A	3000	MES	C3-C2	-3.16	1.38	1.50
3	B	4000	MES	C3-C2	-3.09	1.38	1.50
3	B	4000	MES	C7-N4	-2.55	1.41	1.47
3	A	3000	MES	C7-N4	-2.44	1.41	1.47
3	B	4000	MES	C5-C6	-2.37	1.41	1.50
3	A	3000	MES	C5-C6	-2.33	1.41	1.50

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3000	MES	O3S-S-C8	5.79	115.14	105.77
3	B	4000	MES	O3S-S-C8	5.43	114.55	105.77
3	A	3000	MES	O1S-S-C8	5.26	113.24	106.92
3	B	4000	MES	O1S-S-C8	5.06	113.01	106.92
3	B	4000	MES	O2S-S-C8	3.52	111.15	106.92
3	A	3000	MES	O2S-S-C8	3.24	110.82	106.92
3	A	3000	MES	O3S-S-O2S	-3.03	103.87	111.27
3	B	4000	MES	O1-C2-C3	-2.57	106.13	111.80
3	A	3000	MES	O1-C2-C3	-2.56	106.15	111.80
3	B	4000	MES	O3S-S-O2S	-2.51	105.13	111.27
3	B	4000	MES	O3S-S-O1S	-2.46	105.27	111.27
3	A	3000	MES	O3S-S-O1S	-2.29	105.67	111.27

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	3000	MES	N4-C7-C8-S
3	B	4000	MES	N4-C7-C8-S
3	B	4000	MES	C7-C8-S-O2S

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	4000	MES	1	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.