



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:46 PM UTC

PDB ID : 1CU1 / pdb_00001cu1
Title : CRYSTAL STRUCTURE OF AN ENZYME COMPLEX FROM HEPATITIS C VIRUS
Authors : Yao, N.; Weber, P.C.
Deposited on : 1999-08-20
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

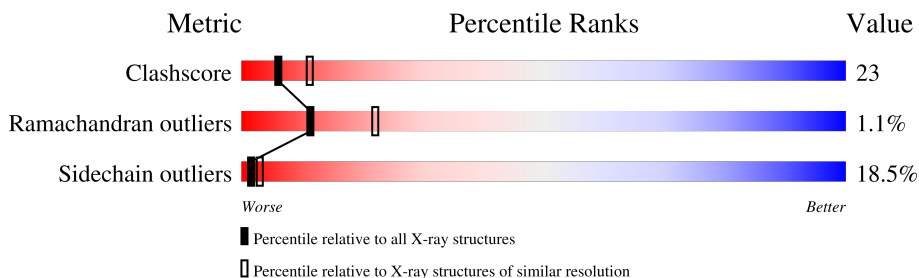
1 Overall quality at a glance

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	645	
1	B	645	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9894 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.

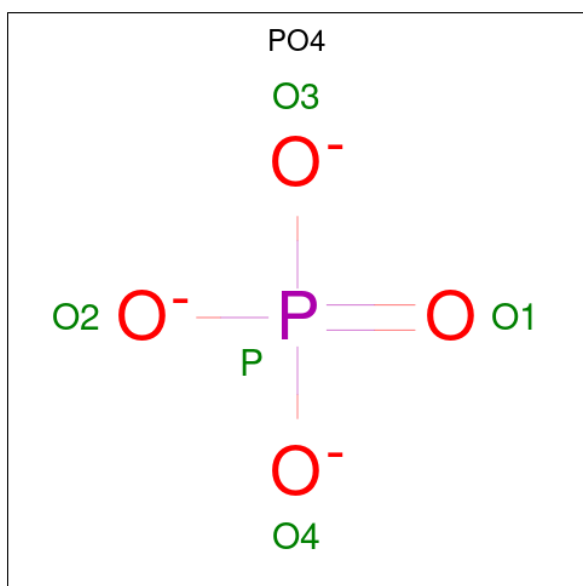
- Molecule 1 is a protein called PROTEIN (PROTEASE/HELICASE NS3).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	645	Total	C	N	O	S	0	0	0
			4807	3026	834	917	30			
1	B	645	Total	C	N	O	S	0	0	0
			4807	3026	834	917	30			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	P	0	0
			5	4	1		
3	B	1	Total	O	P	0	0
			5	4	1		

- Molecule 4 is water.

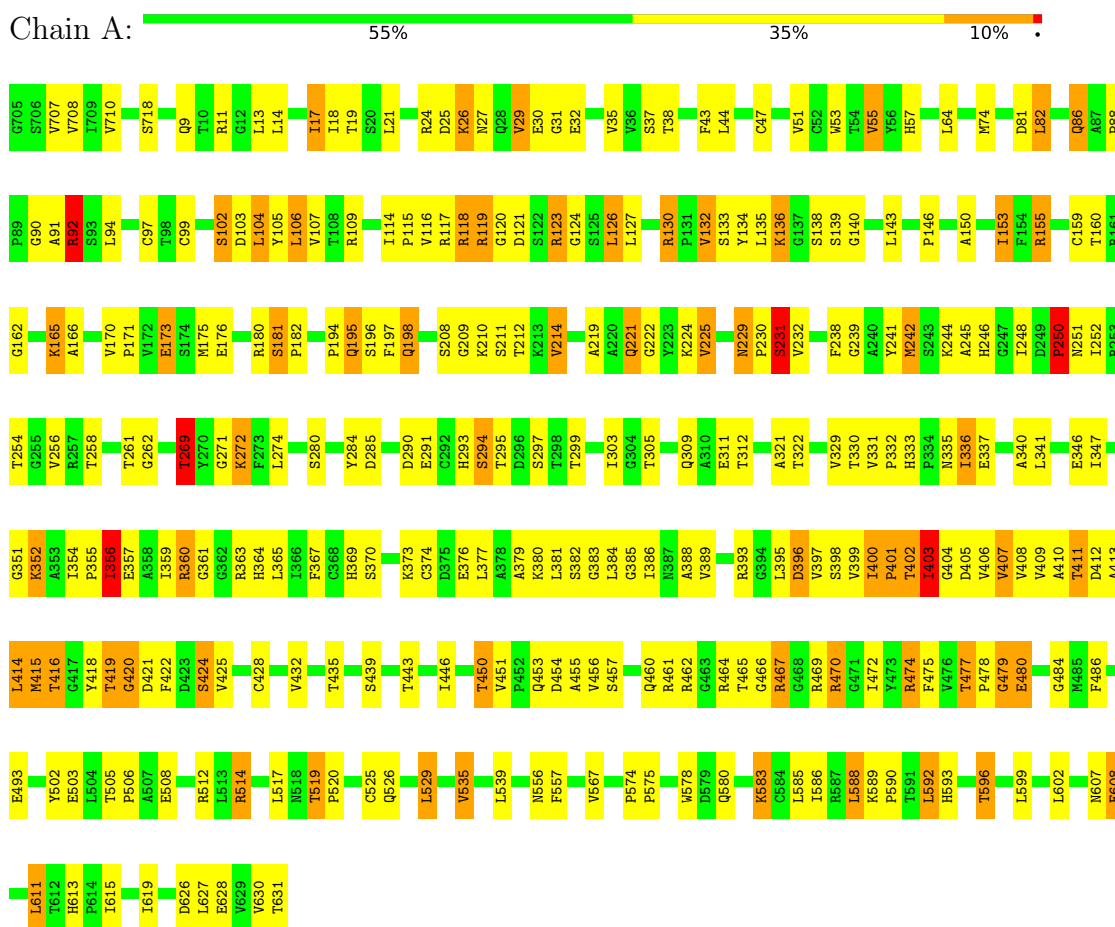
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	150	Total	O	0	0
			150	150		
4	B	118	Total	O	0	0
			118	118		

3 Residue-property plots

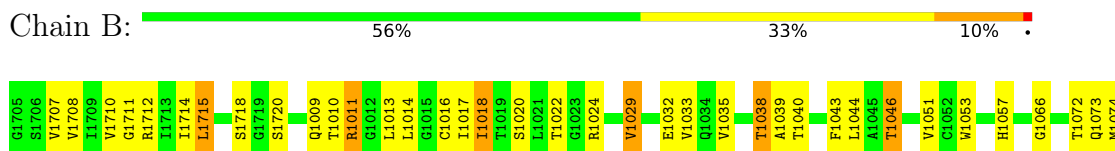
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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: PROTEIN (PROTEASE/HELICASE NS3)



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M1620	Q1549	EL447	Y1350	N1229	P1146	Y1075
L1627	D1555	T1450	G1351	P1230	S1147	T1076
V1630	M1556	V1451	K1352	S1231	A1150	M1077
T1631	F1557	P1452	I1353	S1243	I1153	G1080
	P1558		P1355		F1154	D1081
	A1562	V1456	I1356	D1249	T1155	V1082
	V1563	Q1460	E1357	P1250	G1159	G1084
	Q1564	A1358	A1358	N1251	T1160	V1085
		I1359	I1359	I1252	R1161	Q1086
	T1566	R1467	H1364	T1258	A1161	A1087
	V1567	R1470	L1365		P1088	P1089
	C1568	G1471	S1370	T1266	A1166	
	A1569	I1472	K1371	Y1267	V1170	R1092
	R1570	Y1473	K1372	S1268	P1171	S1093
	A1571	R1474	K1373	T1269	E1172	L1094
	Q1572	F1475	L1381	K1272	V1173	T1095
	A1573	V1476	I1386	F1273	E1174	P1096
	P1575	G1479	I1392	L1274	M1175	
	P1576	E1480	V1389	C1279	S1176	D1103
	S1577	R1481	A1390	S1280	E1176	L1104
	V1578	P1482	I1391	Y1284	T1177	Y1105
	D1579	S1483	Y1392		T1178	
	Q1580	D1487	L1395	I1287	S1181	T1108
	M1581	L1491	D1396	S1294	P1182	R1109
	V1582	G1492	I1397	T1295	V1183	H1110
	C1584	E1493	S1398	D1296	F1184	A1111
	T1586		I1403	T1305	T1185	D1112
	R1587	E1503	V1407	Q1309	D1186	V1113
	L1588	L1504			P1115	P1115
	K1589	T1505	I1407		S1187	V1116
	P1590	E1508	V1407		S1189	R1117
	T1591				P1190	R1118
	L1592	R1514	A1410	T1312	P1191	R1119
	H1593	V1515	T1411	A1312	A1192	G1120
	G1594	A1516	D1412	A1314	V1193	D1121
	P1595	Y1516	A1413	A1315	P1194	
	T1596	L1517	L1414	R1316	Q1195	
	P1597	N1518	M1415		S1196	
	L1598	T1519	T1416	V1329	P1197	S1125
	L1599	P1520	G1417	T1330	Q1198	L1126
	V1600	G1521	Y1418	V1331	T1199	L1127
	R1601		T1419	P1332	H1201	S1128
	L1602	Q1526	V1425		I1202	P1129
		L1529		N1335	A1203	P1131
	M1607	F1536	C1428	E1338	A1204	V1132
	E1608	V1609	N1429	I1339	K1210	S1133
	T1610	L1539	Q1434	A1340	S1211	Y1134
	L1611		T1435	L1341	T1212	K1136
	T1612	I1542	S1439	T1344	K1213	G1137
	H1613	D1543				S1138
	P1614	A1544	L1440	G1345	K1224	S1139
		H1545	D1441	I1347	V1225	G1140
					L1226	L1143
					V1227	L1144
						V1145

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 21	Depositor
Cell constants a, b, c, α , β , γ	91.36Å 110.51Å 141.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.50)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 98.1	Depositor
R, R_{free}	0.200 , 0.260	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9894	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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: ZN, PO4

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	0.85	2/4916 (0.0%)	1.26	46/6714 (0.7%)
1	B	0.84	4/4916 (0.1%)	1.20	41/6714 (0.6%)
All	All	0.85	6/9832 (0.1%)	1.23	87/13428 (0.6%)

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
1	B	0	2
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	245	ALA	C-N	15.31	1.56	1.33
1	B	1183	VAL	C-N	-8.14	1.15	1.33
1	B	1081	ASP	C-N	-7.57	1.21	1.33
1	B	1084	GLY	C-N	6.90	1.43	1.33
1	B	1094	LEU	C-N	-5.81	1.24	1.33
1	A	535	VAL	CA-CB	5.04	1.61	1.54

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	556	ASN	N-CA-C	15.31	128.05	111.36
1	B	1183	VAL	CA-C-N	14.09	143.66	120.70
1	B	1183	VAL	C-N-CA	14.09	143.66	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	PRO	O-C-N	-13.78	104.04	122.64
1	A	245	ALA	CA-C-N	-12.22	103.23	122.29
1	A	245	ALA	C-N-CA	-12.22	103.23	122.29
1	B	1556	ASN	N-CA-C	10.00	122.18	111.28
1	A	420	GLY	N-CA-C	8.84	122.05	112.33
1	A	222	GLY	N-CA-C	8.80	126.36	114.92
1	B	1184	PHE	O-C-N	8.79	130.91	121.85
1	A	519	THR	CA-C-N	8.70	128.64	120.03
1	A	519	THR	C-N-CA	8.70	128.64	120.03
1	A	94	LEU	N-CA-C	-7.84	99.22	110.59
1	A	336	ILE	N-CA-C	7.35	118.48	107.75
1	B	1225	VAL	N-CA-C	7.23	118.29	108.17
1	B	1612	THR	N-CA-C	7.19	121.88	113.18
1	A	245	ALA	O-C-N	7.11	130.91	121.67
1	B	1143	LEU	N-CA-C	-7.08	96.86	108.41
1	A	143	LEU	N-CA-C	-6.98	97.15	108.52
1	B	1439	SER	N-CA-C	6.95	121.01	112.54
1	B	1564	GLN	N-CA-C	-6.88	103.71	111.14
1	B	1250	PRO	N-CA-C	6.86	121.70	111.41
1	B	1114	ILE	CA-C-N	6.85	126.61	119.76
1	B	1114	ILE	C-N-CA	6.85	126.61	119.76
1	B	1407	VAL	N-CA-C	-6.55	98.19	107.75
1	A	707	VAL	N-CA-C	-6.54	98.97	108.71
1	A	502	TYR	N-CA-C	6.49	120.12	112.72
1	A	225	VAL	N-CA-C	6.47	117.16	108.11
1	B	1159	CYS	N-CA-C	6.42	120.09	110.14
1	B	1410	ALA	N-CA-C	6.42	118.93	109.24
1	B	1066	GLY	CA-C-N	6.33	127.76	119.84
1	B	1066	GLY	C-N-CA	6.33	127.76	119.84
1	A	297	SER	N-CA-C	6.33	118.17	111.28
1	B	1519	THR	CA-C-N	6.27	126.79	120.14
1	B	1519	THR	C-N-CA	6.27	126.79	120.14
1	B	1185	THR	O-C-N	6.19	130.82	122.59
1	A	92	ARG	N-CA-C	-6.17	100.57	110.14
1	B	1249	ASP	CA-C-N	6.14	126.11	120.03
1	B	1249	ASP	C-N-CA	6.14	126.11	120.03
1	A	150	ALA	N-CA-C	6.07	119.42	109.76
1	A	410	ALA	N-CA-C	6.04	118.89	109.52
1	A	359	ILE	N-CA-C	6.00	117.95	112.43
1	A	455	ALA	N-CA-C	5.99	117.80	111.28
1	A	401	PRO	N-CA-C	-5.92	105.95	114.18
1	A	451	VAL	N-CA-C	5.84	115.46	108.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1081	ASP	N-CA-C	-5.73	104.00	111.74
1	A	208	SER	N-CA-C	-5.73	105.02	113.61
1	A	38	THR	N-CA-C	-5.71	101.12	109.63
1	B	1150	ALA	N-CA-C	5.70	117.97	109.59
1	A	231	SER	N-CA-C	5.68	118.51	109.24
1	A	13	LEU	N-CA-C	5.67	117.94	111.02
1	B	1335	ASN	N-CA-C	5.63	118.94	112.57
1	A	439	SER	N-CA-C	5.60	119.96	113.18
1	A	99	CYS	N-CA-C	5.58	118.30	111.82
1	A	556	ASN	CA-C-N	-5.50	116.24	123.34
1	A	556	ASN	C-N-CA	-5.50	116.24	123.34
1	A	309	GLN	N-CA-C	5.50	121.40	114.31
1	A	428	CYS	N-CA-C	-5.45	105.89	112.54
1	B	1418	TYR	N-CA-C	5.44	118.31	108.69
1	B	1419	THR	N-CA-C	-5.43	100.85	109.59
1	A	557	PHE	CA-C-N	5.38	124.84	119.24
1	A	557	PHE	C-N-CA	5.38	124.84	119.24
1	A	285	ASP	N-CA-C	-5.37	106.86	113.41
1	B	1145	CYS	N-CA-C	-5.36	103.18	110.36
1	A	55	VAL	CB-CA-C	-5.30	103.82	111.34
1	B	1476	VAL	N-CA-C	-5.26	106.56	111.45
1	B	1415	MET	N-CA-C	5.25	117.01	111.28
1	B	1347	ILE	N-CA-C	5.23	113.20	107.60
1	B	1033	VAL	N-CA-C	5.22	115.87	107.73
1	B	1176	GLU	N-CA-C	-5.21	105.29	110.97
1	B	1314	GLY	N-CA-C	5.20	123.23	115.64
1	A	484	GLY	N-CA-C	5.18	122.47	115.32
1	B	1355	PRO	N-CA-C	-5.18	103.06	111.19
1	A	477	THR	CA-C-N	5.17	126.31	119.84
1	A	477	THR	C-N-CA	5.17	126.31	119.84
1	B	1284	TYR	N-CA-C	5.17	117.24	109.23
1	A	35	VAL	N-CA-C	-5.16	101.14	108.58
1	A	181	SER	N-CA-C	5.14	116.48	110.31
1	B	1035	VAL	N-CA-C	-5.13	100.49	107.99
1	B	1110	HIS	N-CA-C	-5.13	107.53	112.97
1	A	269	THR	N-CA-C	-5.12	101.92	110.17
1	A	456	VAL	N-CA-C	-5.11	105.51	110.42
1	B	1119	ARG	N-CA-C	-5.10	107.03	114.12
1	A	583	LYS	N-CA-C	5.08	118.57	112.38
1	B	1038	THR	CB-CA-C	-5.06	102.55	110.85
1	B	1193	VAL	N-CA-C	-5.06	103.99	108.95
1	A	284	TYR	N-CA-C	5.03	117.02	109.23

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	TYR	Sidechain
1	A	250	PRO	Mainchain
1	B	1084	GLY	Mainchain
1	B	1183	VAL	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	4807	0	4781	234	0
1	B	4807	0	4780	203	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	150	0	0	9	1
4	B	118	0	0	7	1
All	All	9894	0	9561	433	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 23.

All (433) 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:400:ILE:HD12	1:A:400:ILE:H	1.18	1.07
1:A:212:THR:HG22	1:A:242:MET:HE1	1.33	1.06
1:A:596:THR:HG22	1:A:607:ASN:HD22	1.19	1.06
1:A:269:THR:HG22	1:A:272:LYS:H	1.21	1.02
1:A:360:ARG:HD2	1:A:361:GLY:H	1.27	0.99
1:B:1411:THR:HG23	1:B:1413:ALA:H	1.26	0.99
1:A:474:ARG:HG3	1:A:474:ARG:HH11	1.25	0.98
1:B:1434:GLN:HE22	1:B:1556:ASN:HD22	1.13	0.97
1:B:1434:GLN:NE2	1:B:1556:ASN:HD22	1.67	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1396:ASP:OD2	1:B:1398:SER:HB2	1.71	0.91
1:A:400:ILE:HD12	1:A:400:ILE:N	1.88	0.89
1:A:401:PRO:C	1:A:403:ILE:H	1.77	0.88
1:B:1613:HIS:HD2	1:B:1615:ILE:H	1.17	0.88
1:A:136:LYS:NZ	1:A:631:THR:HA	1.89	0.87
1:A:269:THR:CG2	1:A:272:LYS:H	1.88	0.87
1:B:1183:VAL:O	1:B:1183:VAL:HG12	1.77	0.84
1:A:360:ARG:HD2	1:A:361:GLY:N	1.93	0.83
1:A:425:VAL:HG23	1:A:465:THR:HB	1.60	0.82
1:A:474:ARG:HG3	1:A:474:ARG:NH1	1.92	0.81
1:B:1452:PRO:HB2	1:B:1481:ARG:HD2	1.63	0.81
1:A:130:ARG:HG3	1:A:130:ARG:HH11	1.46	0.80
1:B:1279:CYS:H	1:B:1309:GLN:NE2	1.80	0.80
1:A:400:ILE:H	1:A:400:ILE:CD1	1.95	0.80
1:A:401:PRO:O	1:A:403:ILE:N	2.15	0.79
1:A:399:VAL:O	1:A:401:PRO:HD3	1.83	0.79
1:B:1712:ARG:HG3	1:B:1714:ILE:HD11	1.64	0.78
1:B:1279:CYS:N	1:B:1309:GLN:HE21	1.81	0.78
1:B:1279:CYS:HB2	1:B:1309:GLN:HG3	1.66	0.77
1:B:1580:GLN:HA	1:B:1580:GLN:NE2	1.98	0.77
1:B:1279:CYS:H	1:B:1309:GLN:HE21	1.34	0.76
1:A:17:ILE:HD13	1:B:1017:ILE:HD13	1.67	0.76
1:A:251:ASN:HD21	1:A:262:GLY:H	1.34	0.75
1:A:596:THR:CG2	1:A:607:ASN:HD22	1.95	0.75
1:B:1046:THR:HG22	1:B:1140:GLY:O	1.87	0.75
1:A:194:PRO:HG3	1:A:198:GLN:HB2	1.69	0.75
1:A:346:GLU:OE2	1:A:356:ILE:HG12	1.86	0.75
1:B:1155:ARG:HH22	1:B:1526:GLN:HE22	1.35	0.74
1:B:1562:ALA:O	1:B:1566:THR:HG22	1.87	0.74
1:B:1715:LEU:H	1:B:1715:LEU:HD22	1.52	0.74
1:A:115:PRO:HB2	1:A:127:LEU:HD22	1.68	0.73
1:B:1029:VAL:HG11	1:B:1088:PRO:HG2	1.69	0.73
1:A:347:ILE:HD11	1:A:356:ILE:HG23	1.69	0.73
1:A:415:MET:HA	1:A:464:ARG:HH21	1.52	0.73
1:B:1279:CYS:N	1:B:1309:GLN:NE2	2.36	0.73
1:B:1710:VAL:HA	1:B:1011:ARG:HB2	1.72	0.72
1:B:1370:SER:OG	1:B:1372:LYS:HE2	1.89	0.72
1:A:74:MET:HE1	1:A:86:GLN:HB2	1.71	0.72
1:A:140:GLY:HA2	1:A:153:ILE:HD12	1.72	0.71
1:B:1185:THR:HG23	1:B:1185:THR:O	1.91	0.71
1:B:1279:CYS:HB2	1:B:1309:GLN:HE21	1.54	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:333:HIS:CE1	1:A:335:ASN:HB2	2.26	0.70
1:B:1139:SER:HB3	1:B:1631:THR:O	1.90	0.70
1:B:1574:PRO:O	1:B:1596:THR:HB	1.91	0.70
1:A:382:SER:HA	1:A:386:ILE:O	1.91	0.70
1:A:477:THR:CG2	1:A:478:PRO:HD2	2.22	0.70
1:B:1712:ARG:HG3	1:B:1714:ILE:CD1	2.22	0.69
1:A:74:MET:CE	1:A:86:GLN:HB2	2.22	0.69
1:B:1038:THR:O	1:B:1039:ALA:HB3	1.92	0.69
1:A:340:ALA:HB1	4:A:892:HOH:O	1.91	0.69
1:A:596:THR:HG22	1:A:607:ASN:ND2	2.02	0.69
1:B:1089:PRO:HA	4:B:1911:HOH:O	1.92	0.69
1:A:118:ARG:NH1	1:A:121:ASP:HA	2.09	0.67
1:A:269:THR:HG22	1:A:272:LYS:N	2.05	0.67
1:A:57:HIS:HE1	1:A:631:THR:O	1.77	0.66
1:A:231:SER:HB2	1:A:416:THR:HA	1.76	0.66
1:B:1411:THR:HG21	4:B:1875:HOH:O	1.95	0.66
1:A:365:LEU:HD13	1:A:408:VAL:HG23	1.78	0.66
1:B:1563:TYR:HA	1:B:1566:THR:HG23	1.76	0.66
1:B:1139:SER:HB3	1:B:1631:THR:C	2.21	0.66
1:A:130:ARG:HD2	1:A:134:TYR:CD1	2.31	0.66
1:B:1229:ASN:HD22	1:B:1231:SER:H	1.43	0.66
1:A:17:ILE:HD13	1:B:1017:ILE:CD1	2.26	0.66
1:A:197:PHE:CB	1:A:311:GLU:HG3	2.26	0.66
1:A:29:VAL:HG22	1:A:90:GLY:C	2.21	0.65
1:A:400:ILE:HD13	1:A:406:VAL:HG21	1.78	0.65
1:B:1613:HIS:CD2	1:B:1615:ILE:H	2.08	0.65
1:A:477:THR:HG22	1:A:478:PRO:HD2	1.80	0.64
1:B:1229:ASN:O	1:B:1269:THR:HA	1.98	0.64
1:B:1575:PRO:HG2	1:B:1577:SER:O	1.98	0.64
1:B:1229:ASN:ND2	1:B:1231:SER:H	1.95	0.63
1:A:365:LEU:CD1	1:A:408:VAL:HG23	2.28	0.63
1:B:1118:ARG:NH1	1:B:1121:ASP:HA	2.13	0.63
1:B:1580:GLN:O	1:B:1583:LYS:HG2	1.97	0.63
1:A:118:ARG:HD3	1:A:120:GLY:O	1.97	0.63
1:B:1536:PHE:HA	1:B:1539:LEU:HD22	1.81	0.63
1:A:514:ARG:HG2	1:A:529:LEU:HD23	1.79	0.63
1:A:414:LEU:HB3	4:A:888:HOH:O	1.97	0.62
1:A:132:VAL:HG23	1:A:162:GLY:O	1.99	0.62
1:A:403:ILE:HG23	1:A:403:ILE:O	1.98	0.62
1:B:1153:ILE:HG23	1:B:1175:MET:HE1	1.81	0.62
1:B:1074:MET:HE1	1:B:1086:GLN:HE21	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1586:ILE:CG2	1:B:1587:ARG:N	2.62	0.62
1:A:251:ASN:ND2	1:A:261:THR:H	1.98	0.61
1:A:57:HIS:HD2	1:A:81:ASP:OD1	1.82	0.61
1:A:165:LYS:HE2	1:A:626:ASP:OD1	2.00	0.61
1:A:330:THR:HB	1:A:480:GLU:OE1	2.00	0.61
1:B:1555:ASP:OD1	1:B:1557:PHE:N	2.33	0.61
1:B:1397:VAL:HG11	1:B:1417:GLY:O	1.99	0.61
1:A:239:GLY:HA2	1:A:250:PRO:HG2	1.83	0.61
1:B:1545:HIS:O	1:B:1549:GLN:HG3	2.01	0.61
1:A:613:HIS:HE1	1:A:615:ILE:HG12	1.65	0.60
1:A:432:VAL:HG22	1:A:450:THR:HG22	1.82	0.60
1:B:1451:VAL:HB	1:B:1452:PRO:HD2	1.82	0.60
1:A:24:ARG:NH1	1:A:26:LYS:HE3	2.17	0.60
1:B:1074:MET:HG2	1:B:1075:TYR:CE2	2.37	0.60
1:A:505:THR:HG23	1:A:508:GLU:OE1	2.01	0.59
1:B:1505:THR:H	1:B:1508:GLU:CD	2.11	0.59
1:B:1018:ILE:O	1:B:1022:THR:HG23	2.02	0.59
1:B:1204:ALA:HB3	1:B:1210:LYS:HD3	1.83	0.59
1:B:1032:GLU:HG2	1:B:1093:SER:O	2.02	0.58
1:A:130:ARG:HD2	1:A:134:TYR:CE1	2.39	0.58
1:B:1155:ARG:NH2	1:B:1526:GLN:HE22	2.00	0.58
1:A:382:SER:O	1:A:385:GLY:N	2.36	0.58
1:A:418:TYR:O	1:A:464:ARG:NH2	2.35	0.58
1:B:1391:TYR:HA	1:B:1395:LEU:HD23	1.84	0.58
1:A:82:LEU:HD11	1:A:175:MET:HG2	1.85	0.58
1:A:411:THR:HG23	1:A:413:ALA:H	1.68	0.58
1:A:357:GLU:HG3	4:A:890:HOH:O	2.03	0.57
1:B:1451:VAL:HB	1:B:1452:PRO:CD	2.35	0.57
1:A:474:ARG:NH1	1:A:474:ARG:CG	2.65	0.57
1:B:1082:LEU:HG	1:B:1170:VAL:HG11	1.86	0.57
1:A:613:HIS:CE1	1:A:615:ILE:HG12	2.39	0.57
1:B:1542:ILE:HG12	1:B:1543:ASP:H	1.70	0.57
1:A:53:TRP:CE3	1:A:82:LEU:HD13	2.40	0.56
1:B:1589:LYS:N	1:B:1590:PRO:HD2	2.20	0.56
1:A:588:LEU:O	1:A:592:LEU:HD22	2.06	0.56
1:B:1504:LEU:HA	1:B:1508:GLU:OE2	2.05	0.56
1:A:106:LEU:HD12	1:A:107:VAL:N	2.21	0.56
1:B:1082:LEU:HD11	1:B:1175:MET:HG2	1.88	0.56
1:A:102:SER:HB3	1:A:117:ARG:CZ	2.36	0.55
1:B:1279:CYS:CB	1:B:1309:GLN:HE21	2.19	0.55
1:A:132:VAL:HG22	1:A:159:CYS:SG	2.45	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1057:HIS:NE2	1:B:1630:VAL:HG13	2.21	0.55
1:B:1077:ASN:ND2	1:B:1080:GLN:OE1	2.39	0.55
1:A:457:SER:O	1:A:461:ARG:HG3	2.07	0.55
1:A:415:MET:SD	1:A:415:MET:C	2.89	0.55
1:A:406:VAL:HG22	1:A:407:VAL:N	2.22	0.55
1:B:1073:GLN:HG3	4:B:1960:HOH:O	2.07	0.55
1:B:1562:ALA:O	1:B:1566:THR:CG2	2.54	0.55
1:A:252:ILE:O	1:A:258:THR:HA	2.06	0.55
1:B:1456:VAL:O	1:B:1460:GLN:HG3	2.07	0.55
1:A:421:ASP:C	1:A:422:PHE:CD1	2.86	0.54
1:A:474:ARG:HH11	1:A:474:ARG:CG	2.07	0.54
1:B:1434:GLN:NE2	1:B:1556:ASN:ND2	2.49	0.54
1:B:1714:ILE:HD12	1:B:1714:ILE:N	2.23	0.54
1:A:242:MET:O	1:A:246:HIS:N	2.32	0.54
1:A:123:ARG:HH11	1:A:123:ARG:CG	2.20	0.54
1:A:347:ILE:CD1	1:A:356:ILE:HG23	2.37	0.54
1:A:104:LEU:HD21	1:A:118:ARG:HG3	1.88	0.54
1:A:210:LYS:HD2	1:A:321:ALA:HB1	1.90	0.54
1:A:421:ASP:HB3	1:A:467:ARG:HG3	1.90	0.54
1:A:411:THR:CG2	1:A:413:ALA:H	2.21	0.53
1:B:1171:PRO:HB2	1:B:1173:GLU:CD	2.33	0.53
1:B:1434:GLN:HA	1:B:1447:GLU:O	2.07	0.53
1:B:1077:ASN:ND2	1:B:1080:GLN:CD	2.67	0.53
1:A:155:ARG:NH2	1:A:628:GLU:OE1	2.42	0.53
1:A:593:HIS:HB2	4:A:919:HOH:O	2.08	0.53
1:A:251:ASN:O	1:A:252:ILE:HD13	2.09	0.53
1:A:396:ASP:O	1:A:398:SER:N	2.42	0.53
1:B:1347:ILE:HB	1:B:1354:ILE:HB	1.91	0.52
1:A:19:THR:CG2	1:A:25:ASP:HB2	2.39	0.52
1:B:1130:ARG:NH2	4:B:1822:HOH:O	2.42	0.52
1:B:1588:LEU:N	1:B:1588:LEU:HD23	2.24	0.52
1:A:336:ILE:HG12	1:A:466:GLY:HA3	1.92	0.52
1:A:425:VAL:CG2	1:A:465:THR:HB	2.37	0.52
1:B:1567:VAL:HG12	1:B:1597:PRO:HG2	1.91	0.52
1:B:1613:HIS:CG	1:B:1614:PRO:HD2	2.45	0.52
1:A:251:ASN:ND2	1:A:262:GLY:H	2.04	0.52
1:A:173:GLU:CD	1:A:173:GLU:H	2.16	0.52
1:A:180:ARG:NH2	4:A:852:HOH:O	2.42	0.52
1:B:1073:GLN:OE1	1:B:1083:VAL:HG22	2.09	0.52
1:A:195:GLN:HE21	1:A:195:GLN:HA	1.75	0.52
1:A:411:THR:HG23	1:A:412:ASP:N	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1044:LEU:HD12	1:B:1138:SER:O	2.10	0.52
1:A:567:VAL:HG21	1:A:599:LEU:HD11	1.91	0.52
1:A:210:LYS:HB2	3:A:800:PO4:O4	2.10	0.51
1:A:364:HIS:HB2	1:A:407:VAL:HG13	1.92	0.51
1:B:1370:SER:HG	1:B:1372:LYS:HE2	1.72	0.51
1:B:1595:PRO:O	1:B:1610:THR:HG22	2.11	0.51
1:A:176:GLU:HB3	1:A:180:ARG:HH21	1.76	0.51
1:A:376:GLU:O	1:A:379:ALA:HB3	2.10	0.51
1:A:293:HIS:HD2	1:A:322:THR:OG1	1.92	0.51
1:B:1136:LYS:HA	1:B:1631:THR:HG22	1.93	0.51
1:B:1583:LYS:C	1:B:1585:LEU:H	2.18	0.51
1:B:1185:THR:O	1:B:1185:THR:CG2	2.58	0.51
1:B:1252:ILE:O	1:B:1258:THR:HA	2.10	0.51
1:A:14:LEU:HD11	1:A:18:ILE:HD11	1.92	0.51
1:B:1339:VAL:O	1:B:1474:ARG:HA	2.11	0.51
1:A:116:VAL:HG22	1:A:126:LEU:HD12	1.92	0.51
1:B:1350:TYR:OH	1:B:1373:LYS:HG2	2.11	0.51
1:B:1578:TRP:CE2	1:B:1589:LYS:HG3	2.46	0.51
1:A:470:ARG:HG3	1:A:470:ARG:HH11	1.75	0.51
1:B:1563:TYR:HA	1:B:1566:THR:CG2	2.39	0.51
1:B:1580:GLN:NE2	1:B:1583:LYS:HE3	2.26	0.51
1:A:241:TYR:C	1:A:241:TYR:CD2	2.88	0.50
1:A:293:HIS:CD2	1:A:322:THR:OG1	2.63	0.50
1:A:588:LEU:C	1:A:592:LEU:HD22	2.36	0.50
1:A:269:THR:HG21	4:A:862:HOH:O	2.10	0.50
1:A:340:ALA:HB2	1:A:475:PHE:CZ	2.46	0.50
1:B:1103:ASP:O	1:B:1146:PRO:HD3	2.11	0.50
1:B:1613:HIS:CD2	1:B:1614:PRO:HD2	2.46	0.50
1:A:383:GLY:C	1:A:385:GLY:H	2.20	0.50
1:A:588:LEU:C	1:A:590:PRO:HD2	2.37	0.50
1:A:611:LEU:HD22	1:B:1620:MET:HE1	1.94	0.50
1:B:1203:HIS:HE1	4:B:1826:HOH:O	1.94	0.50
1:A:135:LEU:O	1:A:138:SER:HB2	2.12	0.50
1:A:136:LYS:HZ2	1:A:631:THR:HA	1.76	0.50
1:B:1092:ARG:O	1:B:1093:SER:HB3	2.11	0.50
1:B:1555:ASP:O	1:B:1558:PRO:HD3	2.11	0.50
1:B:1173:GLU:CD	1:B:1173:GLU:H	2.20	0.50
1:B:1211:SER:O	1:B:1267:TYR:OH	2.29	0.50
1:A:269:THR:HG22	1:A:272:LYS:HB2	1.92	0.50
1:A:130:ARG:HH11	1:A:130:ARG:CG	2.19	0.49
1:A:506:PRO:HD2	4:A:902:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1279:CYS:CA	1:B:1309:GLN:HE21	2.25	0.49
1:A:24:ARG:HH12	1:A:26:LYS:HE3	1.77	0.49
1:A:299:THR:O	1:A:303:ILE:HG13	2.11	0.49
1:A:29:VAL:HG22	1:A:91:ALA:N	2.28	0.49
1:B:1096:PRO:HB3	1:B:1172:VAL:HG21	1.94	0.49
1:B:1165:LYS:HG2	1:B:1166:ALA:N	2.27	0.49
1:B:1596:THR:HG22	1:B:1607:ASN:OD1	2.13	0.49
1:A:176:GLU:HB3	1:A:180:ARG:NH2	2.26	0.49
1:B:1572:GLN:HG2	1:B:1591:THR:O	2.13	0.49
1:A:291:GLU:OE1	4:A:954:HOH:O	2.20	0.49
1:A:381:LEU:O	1:A:386:ILE:HB	2.11	0.49
1:A:578:TRP:CE2	1:A:589:LYS:HE3	2.48	0.49
1:B:1572:GLN:CG	1:B:1591:THR:O	2.61	0.49
1:A:136:LYS:NZ	1:A:630:VAL:O	2.45	0.49
1:A:478:PRO:O	1:A:479:GLY:O	2.31	0.49
1:B:1118:ARG:HD3	1:B:1120:GLY:O	2.13	0.48
1:A:331:VAL:HB	1:A:332:PRO:HD2	1.94	0.48
1:B:1571:ALA:C	1:B:1573:ALA:H	2.21	0.48
1:A:229:ASN:ND2	1:A:230:PRO:HD2	2.28	0.48
1:B:1574:PRO:HD3	1:B:1593:HIS:C	2.38	0.48
1:A:251:ASN:HD22	1:A:261:THR:H	1.60	0.48
1:A:239:GLY:HA3	1:A:252:ILE:HD11	1.95	0.48
1:A:588:LEU:HB3	1:A:592:LEU:CD2	2.44	0.48
1:A:400:ILE:HG22	1:A:402:THR:OG1	2.14	0.48
1:B:1074:MET:CE	1:B:1075:TYR:CE2	2.97	0.48
1:B:1201:HIS:CE1	1:B:1521:GLY:HA3	2.49	0.48
1:A:312:THR:HG22	1:A:312:THR:O	2.13	0.48
1:A:574:PRO:O	1:A:596:THR:HB	2.13	0.48
1:B:1127:LEU:N	1:B:1127:LEU:HD22	2.29	0.47
1:B:1578:TRP:CZ3	1:B:1586:ILE:HA	2.49	0.47
1:B:1571:ALA:O	1:B:1573:ALA:N	2.47	0.47
1:A:221:GLN:O	1:A:221:GLN:HG3	2.13	0.47
1:B:1074:MET:HE1	1:B:1086:GLN:NE2	2.29	0.47
1:A:369:HIS:CD2	1:A:370:SER:N	2.82	0.47
1:B:1074:MET:HE3	1:B:1075:TYR:CE2	2.49	0.47
1:A:26:LYS:O	1:A:27:ASN:C	2.56	0.47
1:A:136:LYS:HZ3	1:A:631:THR:HA	1.77	0.47
1:B:1130:ARG:HD2	1:B:1134:TYR:CD2	2.49	0.47
1:A:82:LEU:HG	1:A:170:VAL:HG11	1.95	0.47
1:A:290:ASP:OD1	1:A:291:GLU:N	2.48	0.47
1:B:1038:THR:O	1:B:1039:ALA:CB	2.57	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1184:PHE:CD1	1:B:1184:PHE:C	2.93	0.47
1:A:347:ILE:HD11	1:A:356:ILE:CG2	2.43	0.47
1:A:443:THR:HG21	1:A:619:ILE:HG22	1.97	0.47
1:B:1032:GLU:N	1:B:1032:GLU:OE1	2.48	0.47
1:B:1579:ASP:CG	1:B:1580:GLN:N	2.72	0.47
1:B:1613:HIS:CD2	1:B:1614:PRO:CD	2.98	0.47
1:A:238:PHE:O	1:A:241:TYR:N	2.43	0.47
1:A:588:LEU:HB3	1:A:592:LEU:HD21	1.96	0.47
1:A:44:LEU:O	1:A:140:GLY:HA3	2.14	0.46
1:A:305:THR:OG1	1:A:512:ARG:HD3	2.14	0.46
1:B:1082:LEU:HD22	1:B:1083:VAL:N	2.30	0.46
1:B:1434:GLN:CD	1:B:1556:ASN:HD22	2.22	0.46
1:A:197:PHE:CG	1:A:311:GLU:HG3	2.50	0.46
1:A:477:THR:HG23	1:A:478:PRO:HD2	1.94	0.46
1:B:1117:ARG:HG3	1:B:1125:SER:OG	2.14	0.46
1:B:1570:ARG:O	1:B:1571:ALA:HB2	2.16	0.46
1:B:1586:ILE:HG23	1:B:1587:ARG:N	2.29	0.46
1:A:181:SER:HB3	1:A:182:PRO:CD	2.46	0.46
1:B:1117:ARG:HD2	1:B:1119:ARG:NH2	2.30	0.46
1:A:123:ARG:NH1	1:A:123:ARG:HG2	2.30	0.46
1:A:219:ALA:C	1:A:221:GLN:H	2.23	0.46
1:B:1578:TRP:CZ2	1:B:1589:LYS:HG3	2.51	0.46
1:A:136:LYS:HZ3	1:A:631:THR:HG22	1.81	0.46
1:A:415:MET:HA	1:A:464:ARG:NH2	2.24	0.46
1:B:1135:LEU:HB3	1:B:1631:THR:HG21	1.98	0.46
1:A:160:THR:OG1	1:A:165:LYS:HD3	2.15	0.46
1:A:248:ILE:O	1:A:250:PRO:HD3	2.15	0.46
1:A:346:GLU:N	1:A:346:GLU:OE1	2.48	0.46
1:A:402:THR:C	1:A:404:GLY:N	2.72	0.46
1:B:1194:PRO:O	1:B:1316:ARG:HG2	2.15	0.46
1:B:1347:ILE:HD13	1:B:1381:LEU:CD2	2.46	0.46
1:B:1588:LEU:C	1:B:1590:PRO:HD2	2.40	0.46
1:A:155:ARG:HH22	1:A:526:GLN:HE22	1.64	0.46
1:B:1571:ALA:C	1:B:1573:ALA:N	2.73	0.46
1:A:365:LEU:HD21	1:A:367:PHE:CZ	2.51	0.45
1:A:74:MET:HE3	1:A:86:GLN:HB2	1.97	0.45
1:A:181:SER:HB3	1:A:182:PRO:HD2	1.98	0.45
1:A:575:PRO:HD2	1:A:578:TRP:CZ2	2.52	0.45
1:A:47:CYS:HA	1:A:51:VAL:O	2.15	0.45
1:A:365:LEU:HD13	1:A:408:VAL:CG2	2.46	0.45
1:B:1187:ASN:HD21	1:B:1203:HIS:CD2	2.33	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1226:LEU:HD12	1:B:1266:THR:HB	1.98	0.45
1:B:1567:VAL:CG1	1:B:1597:PRO:HG2	2.46	0.45
1:A:355:PRO:O	1:A:357:GLU:N	2.49	0.45
1:A:388:ALA:O	1:A:389:VAL:HG13	2.17	0.45
1:A:477:THR:HG22	1:A:478:PRO:CD	2.45	0.45
1:B:1161:ARG:NH1	4:B:925:HOH:O	2.47	0.45
1:B:1272:LYS:O	1:B:1272:LYS:HD3	2.16	0.45
1:A:363:ARG:HD2	1:A:403:ILE:HA	1.99	0.45
1:B:1176:GLU:O	1:B:1177:THR:C	2.60	0.45
1:A:103:ASP:O	1:A:146:PRO:HD3	2.16	0.45
1:A:589:LYS:N	1:A:590:PRO:HD2	2.31	0.45
1:A:133:SER:HA	1:A:136:LYS:HG3	1.98	0.45
1:A:123:ARG:HH11	1:A:123:ARG:HG2	1.81	0.45
1:A:351:GLY:O	1:A:352:LYS:HE3	2.16	0.45
1:A:419:THR:O	1:A:467:ARG:NH2	2.45	0.45
1:B:1051:VAL:CG1	1:B:1053:TRP:CE2	3.00	0.45
1:B:1519:THR:HA	1:B:1520:PRO:HD3	1.68	0.45
1:B:1580:GLN:NE2	1:B:1580:GLN:CA	2.73	0.45
1:A:357:GLU:O	1:A:360:ARG:HG3	2.17	0.44
1:B:1555:ASP:OD1	1:B:1556:ASN:N	2.50	0.44
1:A:29:VAL:HG11	1:A:88:PRO:HG2	1.99	0.44
1:A:360:ARG:HH11	1:A:361:GLY:H	1.64	0.44
1:B:1105:TYR:HB3	1:B:1113:VAL:HG12	1.99	0.44
1:A:505:THR:OG1	1:A:508:GLU:HG3	2.18	0.44
1:B:1014:LEU:HD12	1:B:1014:LEU:O	2.17	0.44
1:B:1210:LYS:HB2	1:B:1210:LYS:HE2	1.55	0.44
1:B:1184:PHE:HD1	1:B:1185:THR:N	2.16	0.44
1:B:1358:ALA:HB1	1:B:1474:ARG:NH1	2.32	0.44
1:A:519:THR:HA	1:A:520:PRO:HD3	1.68	0.44
1:B:1115:PRO:C	1:B:1127:LEU:HD23	2.42	0.44
1:A:232:VAL:HG23	1:A:254:THR:HG21	1.99	0.44
1:B:1108:THR:OG1	1:B:1112:ASP:HB2	2.17	0.44
1:B:1351:GLY:C	1:B:1352:LYS:HG2	2.42	0.44
1:B:1583:LYS:O	1:B:1585:LEU:N	2.51	0.44
1:A:393:ARG:HD2	4:A:761:HOH:O	2.18	0.44
1:A:406:VAL:HG22	1:A:407:VAL:H	1.82	0.44
1:B:1186:ASP:OD1	1:B:1186:ASP:C	2.61	0.44
1:A:611:LEU:CD2	1:B:1620:MET:HE1	2.47	0.44
1:B:1132:VAL:O	1:B:1133:SER:C	2.60	0.44
1:B:1279:CYS:HB2	1:B:1309:GLN:NE2	2.28	0.44
1:A:333:HIS:HE1	1:A:335:ASN:HB2	1.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:580:GLN:HA	1:A:580:GLN:NE2	2.31	0.44
1:B:1032:GLU:N	4:B:1912:HOH:O	2.31	0.43
1:B:1372:LYS:H	1:B:1372:LYS:HG3	1.41	0.43
1:A:74:MET:HE3	1:A:74:MET:HB2	1.75	0.43
1:A:121:ASP:OD2	1:A:171:PRO:HG3	2.19	0.43
1:A:470:ARG:HG3	1:A:470:ARG:NH1	2.33	0.43
1:B:1555:ASP:OD1	1:B:1555:ASP:C	2.60	0.43
1:B:1589:LYS:N	1:B:1590:PRO:CD	2.81	0.43
1:A:229:ASN:O	1:A:269:THR:HA	2.19	0.43
1:A:466:GLY:HA2	1:A:469:ARG:O	2.18	0.43
1:B:1226:LEU:HD12	1:B:1226:LEU:HA	1.85	0.43
1:B:1586:ILE:HG22	1:B:1587:ARG:H	1.82	0.43
1:A:462:ARG:O	1:A:465:THR:HG22	2.19	0.43
1:B:1711:GLY:HA2	1:B:1010:THR:HG23	1.99	0.43
1:B:1581:MET:HG2	1:B:1582:TRP:CE2	2.53	0.43
1:B:1359:ILE:HA	1:B:1364:HIS:CE1	2.53	0.43
1:B:1493:GLU:HG2	1:B:1557:PHE:CE1	2.54	0.43
1:A:219:ALA:C	1:A:221:GLN:N	2.77	0.43
1:A:331:VAL:HB	1:A:332:PRO:CD	2.49	0.43
1:B:1029:VAL:HG11	1:B:1088:PRO:CG	2.46	0.43
1:B:1545:HIS:CD2	1:B:1587:ARG:HH22	2.37	0.43
1:A:402:THR:C	1:A:404:GLY:H	2.27	0.43
1:A:269:THR:HG23	1:A:271:GLY:N	2.34	0.43
1:A:486:PHE:CE2	1:A:525:CYS:HB2	2.54	0.43
1:B:1435:THR:HA	1:B:1487:ASP:OD1	2.19	0.43
1:B:1596:THR:HG23	1:B:1608:GLU:O	2.18	0.43
1:A:374:CYS:HA	1:A:409:VAL:HG11	2.01	0.42
1:B:1504:LEU:HD12	1:B:1508:GLU:OE2	2.18	0.42
1:B:1516:TYR:HD1	1:B:1517:LEU:HD23	1.83	0.42
1:B:1013:LEU:O	1:B:1017:ILE:HD12	2.19	0.42
1:B:1082:LEU:HD23	1:B:1082:LEU:HA	1.84	0.42
1:B:1331:VAL:HB	1:B:1332:PRO:HD2	2.00	0.42
1:B:1371:LYS:HD3	1:B:1392:TYR:CD1	2.54	0.42
1:A:404:GLY:O	1:A:405:ASP:C	2.62	0.42
1:B:1213:LYS:HB3	1:B:1213:LYS:HE3	1.77	0.42
1:B:1294:SER:OG	1:B:1296:ASP:OD2	2.37	0.42
1:A:424:SER:HB2	1:A:472:ILE:HB	2.01	0.42
1:B:1575:PRO:O	1:B:1576:PRO:C	2.60	0.42
1:A:124:GLY:O	1:A:166:ALA:HB1	2.20	0.42
1:A:401:PRO:C	1:A:403:ILE:N	2.48	0.42
1:B:1087:ALA:HA	1:B:1088:PRO:HD3	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1190:PRO:O	1:B:1191:PRO:C	2.62	0.42
1:A:421:ASP:CB	1:A:467:ARG:HG3	2.49	0.42
1:B:1139:SER:CB	1:B:1631:THR:O	2.63	0.42
1:B:1365:LEU:O	1:B:1425:VAL:HA	2.20	0.42
1:B:1542:ILE:HG12	1:B:1543:ASP:N	2.33	0.42
1:B:1130:ARG:HE	1:B:1130:ARG:HB2	1.68	0.41
1:B:1228:LEU:HA	1:B:1268:SER:O	2.20	0.41
1:B:1305:THR:O	1:B:1309:GLN:HG2	2.19	0.41
1:B:1396:ASP:C	1:B:1398:SER:N	2.77	0.41
1:B:1583:LYS:C	1:B:1585:LEU:N	2.77	0.41
1:A:710:VAL:HA	1:A:11:ARG:HB2	2.01	0.41
1:A:583:LYS:HA	1:A:586:ILE:HG13	2.02	0.41
1:A:136:LYS:NZ	1:A:631:THR:HG22	2.34	0.41
1:B:1586:ILE:HG22	1:B:1587:ARG:N	2.35	0.41
1:A:53:TRP:CD1	1:A:175:MET:HE3	2.56	0.41
1:A:209:GLY:O	1:A:214:VAL:HG13	2.20	0.41
1:A:403:ILE:O	1:A:403:ILE:CG2	2.66	0.41
1:A:418:TYR:CE2	1:A:420:GLY:N	2.89	0.41
1:A:588:LEU:HD12	1:A:588:LEU:HA	1.83	0.41
1:B:1043:PHE:CD1	1:B:1043:PHE:N	2.89	0.41
1:B:1441:ASP:O	1:B:1601:ARG:NE	2.37	0.41
1:B:1579:ASP:O	1:B:1580:GLN:C	2.63	0.41
1:A:31:GLY:CA	1:A:92:ARG:HG3	2.51	0.41
1:A:470:ARG:HA	1:A:470:ARG:HD2	1.56	0.41
1:B:1016:CYS:O	1:B:1020:SER:HB2	2.21	0.41
1:A:197:PHE:HB3	1:A:311:GLU:HG3	2.00	0.41
1:A:608:GLU:H	1:A:608:GLU:HG2	1.55	0.41
1:B:1569:ALA:C	1:B:1571:ALA:H	2.29	0.41
1:A:212:THR:HG22	1:A:242:MET:CE	2.25	0.41
1:A:291:GLU:O	1:A:294:SER:HB3	2.21	0.41
1:A:295:THR:HG21	1:A:486:PHE:HB3	2.03	0.41
1:A:354:ILE:HA	1:A:355:PRO:HD3	1.84	0.41
1:B:1428:CYS:O	1:B:1429:ASN:HB2	2.21	0.41
1:B:1456:VAL:O	1:B:1460:GLN:CG	2.67	0.41
1:A:114:ILE:HA	1:A:115:PRO:HD3	1.90	0.41
1:A:118:ARG:C	1:A:119:ARG:HG2	2.46	0.41
1:A:130:ARG:CG	1:A:130:ARG:NH1	2.83	0.41
1:B:1575:PRO:C	1:B:1577:SER:N	2.79	0.41
1:A:19:THR:HG21	1:A:25:ASP:HB2	2.02	0.40
1:A:274:LEU:HD23	1:A:274:LEU:HA	1.92	0.40
1:A:337:GLU:HG2	1:A:470:ARG:HH22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1038:THR:C	1:B:1040:THR:H	2.29	0.40
1:B:1195:GLN:OE1	1:B:1195:GLN:N	2.54	0.40
1:B:1279:CYS:CB	1:B:1309:GLN:HG3	2.45	0.40
1:B:1135:LEU:HD12	1:B:1135:LEU:HA	1.79	0.40
1:A:25:ASP:OD2	1:A:25:ASP:C	2.64	0.40
1:A:195:GLN:HA	1:A:195:GLN:NE2	2.37	0.40
1:A:365:LEU:HD12	1:A:408:VAL:HG23	2.01	0.40
1:B:1226:LEU:CD1	1:B:1266:THR:HB	2.51	0.40
1:A:43:PHE:HA	1:A:109:ARG:HH21	1.85	0.40
1:B:1456:VAL:HG13	1:B:1483:SER:HB2	2.04	0.40
1:A:114:ILE:HD12	1:A:130:ARG:NH2	2.37	0.40
1:A:346:GLU:CD	1:A:355:PRO:HA	2.47	0.40
1:A:413:ALA:O	1:A:414:LEU:C	2.65	0.40
1:A:453:GLN:HB2	1:A:457:SER:OG	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)
4:A:783:HOH:O	4:B:1838:HOH:O[4_567]	2.11	0.09

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	643/645 (100%)	609 (95%)	28 (4%)	6 (1%)	14	27
1	B	643/645 (100%)	609 (95%)	26 (4%)	8 (1%)	10	20
All	All	1286/1290 (100%)	1218 (95%)	54 (4%)	14 (1%)	11	22

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	402	THR
1	B	1571	ALA
1	A	356	ILE
1	A	397	VAL
1	A	479	GLY
1	B	1572	GLN
1	B	1584	CYS
1	A	480	GLU
1	B	1185	THR
1	B	1479	GLY
1	B	1480	GLU
1	B	1586	ILE
1	A	403	ILE
1	B	1183	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	526/526 (100%)	435 (83%)	91 (17%)	2	4
1	B	526/526 (100%)	422 (80%)	104 (20%)	1	2
All	All	1052/1052 (100%)	857 (82%)	195 (18%)	1	3

All (195) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	708	VAL
1	A	718	SER
1	A	9	GLN
1	A	17	ILE
1	A	21	LEU
1	A	26	LYS
1	A	29	VAL
1	A	30	GLU
1	A	32	GLU
1	A	37	SER

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Mol	Chain	Res	Type
1	A	55	VAL
1	A	64	LEU
1	A	82	LEU
1	A	86	GLN
1	A	92	ARG
1	A	97	CYS
1	A	102	SER
1	A	104	LEU
1	A	106	LEU
1	A	118	ARG
1	A	119	ARG
1	A	123	ARG
1	A	126	LEU
1	A	130	ARG
1	A	132	VAL
1	A	136	LYS
1	A	139	SER
1	A	153	ILE
1	A	155	ARG
1	A	165	LYS
1	A	173	GLU
1	A	195	GLN
1	A	196	SER
1	A	198	GLN
1	A	211	SER
1	A	214	VAL
1	A	221	GLN
1	A	224	LYS
1	A	225	VAL
1	A	229	ASN
1	A	231	SER
1	A	242	MET
1	A	244	LYS
1	A	256	VAL
1	A	269	THR
1	A	272	LYS
1	A	280	SER
1	A	294	SER
1	A	329	VAL
1	A	341	LEU
1	A	352	LYS
1	A	356	ILE

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Mol	Chain	Res	Type
1	A	360	ARG
1	A	373	LYS
1	A	377	LEU
1	A	380	LYS
1	A	384	LEU
1	A	395	LEU
1	A	396	ASP
1	A	400	ILE
1	A	403	ILE
1	A	407	VAL
1	A	411	THR
1	A	414	LEU
1	A	415	MET
1	A	416	THR
1	A	419	THR
1	A	424	SER
1	A	435	THR
1	A	446	ILE
1	A	450	THR
1	A	454	ASP
1	A	460	GLN
1	A	467	ARG
1	A	470	ARG
1	A	474	ARG
1	A	493	GLU
1	A	503	GLU
1	A	514	ARG
1	A	517	LEU
1	A	529	LEU
1	A	535	VAL
1	A	539	LEU
1	A	585	LEU
1	A	588	LEU
1	A	592	LEU
1	A	596	THR
1	A	602	LEU
1	A	608	GLU
1	A	611	LEU
1	A	627	LEU
1	B	1707	VAL
1	B	1708	VAL
1	B	1715	LEU

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Mol	Chain	Res	Type
1	B	1718	SER
1	B	1720	SER
1	B	1009	GLN
1	B	1011	ARG
1	B	1018	ILE
1	B	1024	ARG
1	B	1029	VAL
1	B	1046	THR
1	B	1072	THR
1	B	1082	LEU
1	B	1083	VAL
1	B	1086	GLN
1	B	1104	LEU
1	B	1114	ILE
1	B	1118	ARG
1	B	1128	SER
1	B	1130	ARG
1	B	1132	VAL
1	B	1133	SER
1	B	1135	LEU
1	B	1147	SER
1	B	1155	ARG
1	B	1165	LYS
1	B	1173	GLU
1	B	1178	THR
1	B	1181	SER
1	B	1184	PHE
1	B	1187	ASN
1	B	1188	SER
1	B	1193	VAL
1	B	1196	SER
1	B	1198	GLN
1	B	1210	LYS
1	B	1213	LYS
1	B	1224	LYS
1	B	1227	VAL
1	B	1228	LEU
1	B	1243	SER
1	B	1249	ASP
1	B	1272	LYS
1	B	1274	LEU
1	B	1280	SER

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Mol	Chain	Res	Type
1	B	1287	ILE
1	B	1312	THR
1	B	1316	ARG
1	B	1329	VAL
1	B	1338	GLU
1	B	1341	LEU
1	B	1344	THR
1	B	1346	GLU
1	B	1352	LYS
1	B	1356	ILE
1	B	1372	LYS
1	B	1373	LYS
1	B	1386	ILE
1	B	1389	VAL
1	B	1395	LEU
1	B	1397	VAL
1	B	1398	SER
1	B	1403	ILE
1	B	1419	THR
1	B	1425	VAL
1	B	1450	THR
1	B	1456	VAL
1	B	1460	GLN
1	B	1467	ARG
1	B	1470	ARG
1	B	1472	ILE
1	B	1474	ARG
1	B	1481	ARG
1	B	1491	LEU
1	B	1503	GLU
1	B	1504	LEU
1	B	1508	GLU
1	B	1514	ARG
1	B	1529	LEU
1	B	1539	LEU
1	B	1555	ASP
1	B	1566	THR
1	B	1567	VAL
1	B	1579	ASP
1	B	1580	GLN
1	B	1581	MET
1	B	1583	LYS

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Mol	Chain	Res	Type
1	B	1584	CYS
1	B	1586	ILE
1	B	1587	ARG
1	B	1588	LEU
1	B	1591	THR
1	B	1593	HIS
1	B	1596	THR
1	B	1598	LEU
1	B	1600	TYR
1	B	1602	LEU
1	B	1606	GLN
1	B	1609	VAL
1	B	1611	LEU
1	B	1615	ILE
1	B	1627	LEU
1	B	1630	VAL
1	B	1631	THR

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	9	GLN
1	A	27	ASN
1	A	57	HIS
1	A	80	GLN
1	A	86	GLN
1	A	110	HIS
1	A	195	GLN
1	A	198	GLN
1	A	251	ASN
1	A	293	HIS
1	A	434	GLN
1	A	526	GLN
1	A	541	HIS
1	A	556	ASN
1	A	580	GLN
1	A	593	HIS
1	B	1027	ASN
1	B	1034	GLN
1	B	1086	GLN
1	B	1149	HIS
1	B	1187	ASN

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Mol	Chain	Res	Type
1	B	1198	GLN
1	B	1203	HIS
1	B	1229	ASN
1	B	1309	GLN
1	B	1333	HIS
1	B	1364	HIS
1	B	1526	GLN
1	B	1545	HIS
1	B	1556	ASN
1	B	1572	GLN
1	B	1580	GLN
1	B	1613	HIS

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](#)

Of 4 ligands modelled in this entry, 2 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	PO4	A	800	-	4,4,4	1.61	0	6,6,6	0.54	0
3	PO4	B	1800	-	4,4,4	1.68	0	6,6,6	0.80	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.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	800	PO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1183:VAL	C	1184:PHE	N	1.15

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.