



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:34 AM UTC

PDB ID : 4RTD / pdb_00004rtd
Title : Escherichia coli alpha-2-macroglobulin activated by porcine elastase
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Deposited on : 2014-11-14
Resolution : 3.65 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

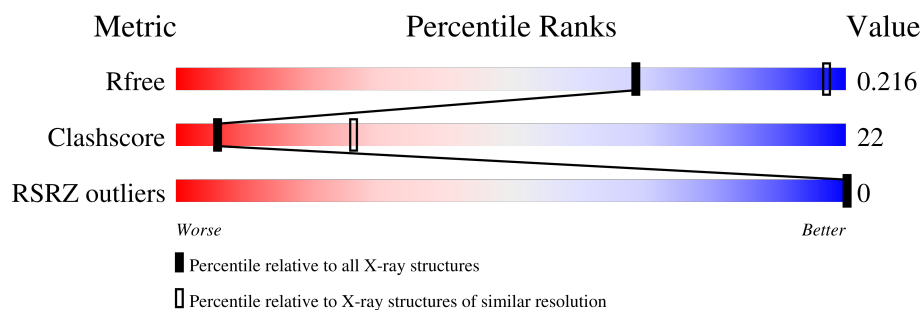
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.65 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))
R_{free}	180053	1062 (3.78-3.54)
Clashscore	190562	1009 (3.76-3.56)
RSRZ outliers	180081	1061 (3.78-3.54)

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

Mol	Chain	Length	Quality of chain
1	A	1639	42% 25% . 32%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 8699 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 Uncharacterized lipoprotein YfhM.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1122	Total	C	N	O	S	Se	0	0	0
			8699	5497	1505	1677	1	19			

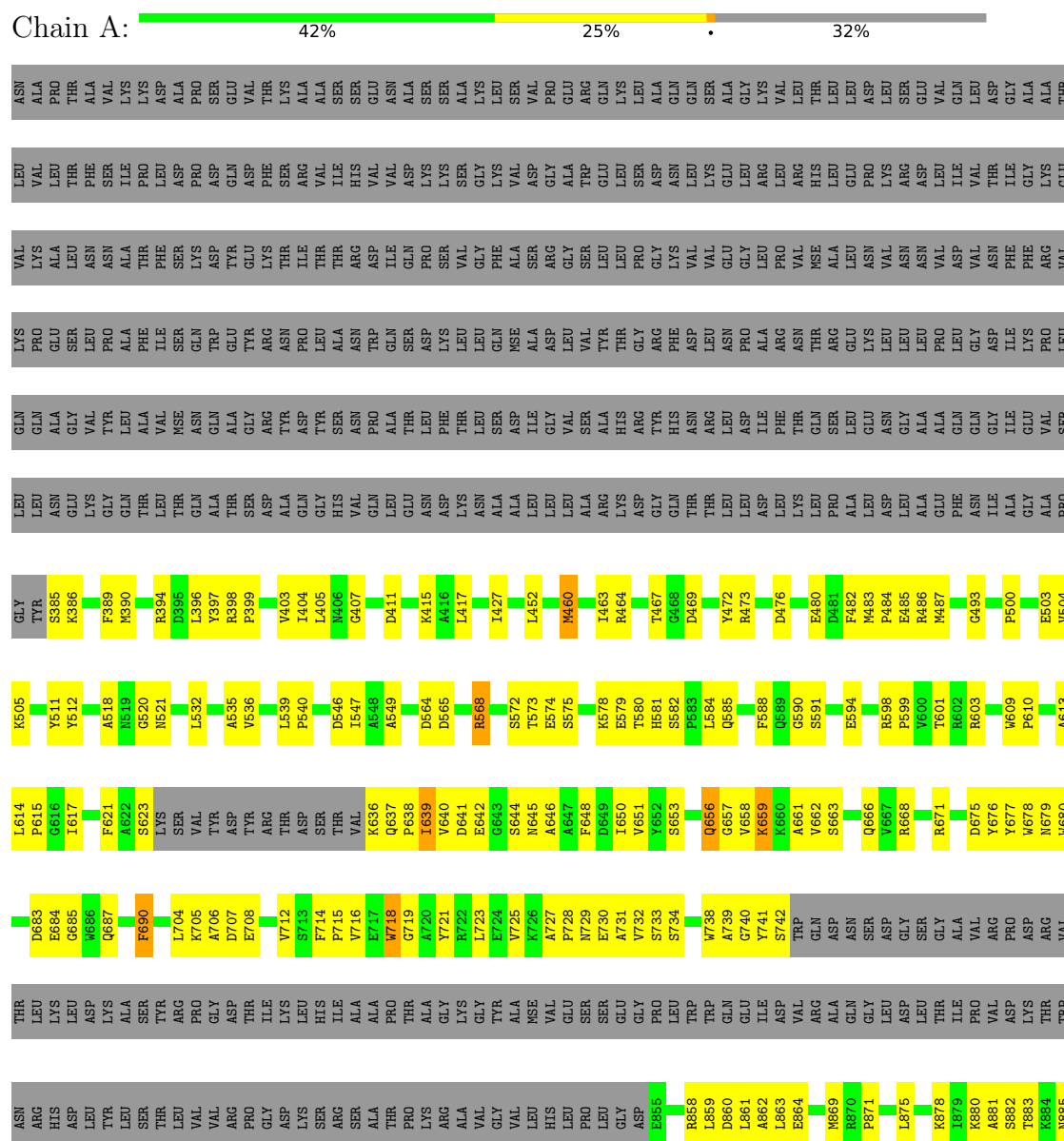
There are 11 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	PRO	SER	engineered mutation	UNP P76578
A	606	ARG	GLN	engineered mutation	UNP P76578
A	1587	ASN	SER	engineered mutation	UNP P76578
A	1654	LEU	-	expression tag	UNP P76578
A	1655	GLU	-	expression tag	UNP P76578
A	1656	HIS	-	expression tag	UNP P76578
A	1657	HIS	-	expression tag	UNP P76578
A	1658	HIS	-	expression tag	UNP P76578
A	1659	HIS	-	expression tag	UNP P76578
A	1660	HIS	-	expression tag	UNP P76578
A	1661	HIS	-	expression tag	UNP P76578

3 Residue-property plots

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

• Molecule 1: Uncharacterized lipoprotein YfhM



S1633	M1634	E1420	L1301	I1177	P1086	W975	G886
	Y1635	E1427	K1302	K1178	V1087	T976	E887
	V1636	A1428	A1303	E1179	R1088	L977	K888
	P1637	N1429	S1304	L1180	A1089		
	Q1638		K1305	P1184	P1091	Q980	V892
	W1639	F1432		Y1185	G1092		N893
	R1640		Y1311	L1188	E1097	V985	V896
	A1641	G1443	A1326	L1195	I1098	L987	V899
	L1649	W1445	L1327		Q1099		
	I1650	Q1446	R1328	Y1200		D991	L904
V1651	T1457	E1329	N1202	S1103	F992	N905	
R1652		I1330		G1104	N993	V906	
P1653	ALA	W1331		N1202	G994	T907	
LEU	ASN	K1460	A1338	Q1205	L1106	M1011	D108
GLY	A1461	A1461	S1339	L1206	L1107	E1012	Y909
HIS	S1566	Q1462	G1340				W915
HIS	N1463	L1341	L1209	E1110	V1015		W915
HIS	S1464	P1342	G1210	V1111	I1016		K922
HIS	E1570	L1343	I1211	V1112	V1017		T978
HIS	Q1571	L1471	K1212	A1113	A1018		GLY
HIS			L1344	K1212	D1114		ALA
	E1575	L1474	Q1345	K1218		V1021	ALA
	V1576		L1350	S1222	K1120	I1022	ASP
	Q1577	S1479	K1351	V1223	I1121		ILE
	N1578		D1355			M1027	T979
	L1580	Q1482			R1124		ASP
	N1581	P1483	R1358	G1226	P1125	M1031	ILE
	Q1582	L1484	W1485	I1227	S1228	A1032	T979
	E1592	W1485	L1365	V1132	T1131	S1033	GLY
	F1593	R1487	L1486	R1229	V1132	T1036	VAL
R1594	M1488	A1366	L1230	N1133		ILE	
D1595	D1489	R1371	L1231		L1039	GLU	
D1596	A1490		Q1232	A1137	L1138	GLY	
F1597	S1491	I1377	M1233	L1138	T1043	GLN	
F1598		W1378	A1241	Q1139	T1044	GLY	
V1599		L1379	A1241	P1140	N1045	ARG	
	N1503		E1141	G1141	L1046	LEU	
E1606	V1504	G1383	M1268	E1142	T1047	K943	
Y1607	L1505				D1048		
Q1608	Q1506	L1386	V1262	I1146	R946		
	R1509	R1387	P1147	P1147	Q1051	F947	
T1611			S1155				
	G1513	M1399	T1273	S1155	T1058	D950	
L1615		K1400	D1274	G1161	L1063	G951	
A1616	G1516	L1401	A1275	Q1162	E1064		
R1617			I1276		L1064	R956	
A1618	K1519	E1405	L1283	G1167	L1065	G957	
V1619	L1284	Q1406	L1284	K1168	G958		
T1620	L1524		R1285	P1169	V1066	K959	
P1621		L1410	Y1286	P1170	A1076	P960	
	W1533		L1287		P1077		
P1627	L1413	L1413	L1287	N1171	G1078	N963	
	Q1535	M1293	M1292	I1173	V1079		
M1630	Q1416	I1173	A1174	R1080	R1081	Q971	
V1631	A1417	M1293	A1417	R1175	T1081	A972	
F1632	V1542			X1176			
			A1298				

4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	176.06Å 176.06Å 161.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	46.87 – 3.65 46.87 – 3.65	Depositor EDS
% Data completeness (in resolution range)	99.9 (46.87-3.65) 82.5 (46.87-3.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 3.66Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.177 , 0.238 (Not available) , 0.216	Depositor DCC
R_{free} test set	1033 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	126.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 120.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8699	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	0.71	1/8863 (0.0%)	1.01	29/12024 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	719	GLY	N-CA	6.09	1.50	1.44

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1169	PRO	CA-C-N	11.63	134.38	119.84
1	A	1169	PRO	C-N-CA	11.63	134.38	119.84
1	A	460	MSE	CG-SE-CE	7.73	115.94	98.92
1	A	639	ILE	N-CA-C	7.23	117.86	107.88
1	A	1168	LYS	CA-C-N	-6.97	113.20	120.38
1	A	1168	LYS	C-N-CA	-6.97	113.20	120.38
1	A	690	PHE	N-CA-C	6.62	119.83	110.50
1	A	639	ILE	CB-CA-C	-6.61	102.61	111.80
1	A	485	GLU	N-CA-C	5.94	119.00	111.69
1	A	739	ALA	N-CA-C	5.92	119.76	112.54
1	A	1524	LEU	N-CA-C	5.79	118.11	108.20
1	A	718	TRP	N-CA-C	5.69	121.47	113.56
1	A	1571	GLN	N-CA-C	5.54	119.66	113.02
1	A	427	ILE	N-CA-C	5.51	115.93	107.77
1	A	1081	THR	N-CA-C	-5.50	100.70	109.23
1	A	493	GLY	N-CA-C	-5.50	102.49	110.90
1	A	1570	GLU	N-CA-C	5.47	117.30	109.14
1	A	568	ARG	N-CA-C	5.46	115.32	108.45
1	A	1386	LEU	N-CA-C	5.40	117.17	111.28
1	A	656	GLN	N-CA-C	-5.38	107.36	114.04
1	A	1155	SER	CA-C-N	5.26	124.88	119.56
1	A	1155	SER	C-N-CA	5.26	124.88	119.56
1	A	888	LYS	CA-C-N	5.19	126.33	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	888	LYS	C-N-CA	5.19	126.33	119.84
1	A	863	LEU	N-CA-C	5.17	116.84	108.41
1	A	511	TYR	N-CA-C	5.17	117.02	108.13
1	A	659	LYS	N-CA-C	5.14	121.74	110.80
1	A	1107	LEU	CA-C-N	5.00	125.44	120.04
1	A	1107	LEU	C-N-CA	5.00	125.44	120.04

There are no chirality outliers.

There are no planarity outliers.

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	8699	0	8589	388	0
All	All	8699	0	8589	388	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 22.

All (388) 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:639:ILE:HG21	1:A:738:TRP:O	1.73	0.89
1:A:396:LEU:HD22	1:A:906:ILE:HD11	1.56	0.87
1:A:1045:ASN:OD1	1:A:1047:THR:HG22	1.77	0.84
1:A:1504:VAL:HG21	1:A:1639:TRP:CD1	2.15	0.81
1:A:1106:ALA:HA	1:A:1113:ALA:HA	1.62	0.81
1:A:1578:ASN:HB2	1:A:1579:LEU:HD12	1.64	0.79
1:A:1417:ALA:HA	1:A:1420:GLU:HG3	1.65	0.78
1:A:661:ALA:HB1	1:A:704:LEU:O	1.83	0.78
1:A:1033:SER:HB2	1:A:1091:PRO:HA	1.65	0.78
1:A:411:ASP:HB3	1:A:417:LEU:HD11	1.66	0.78
1:A:1273:THR:O	1:A:1276:ILE:HG22	1.83	0.78
1:A:1488:MSE:HG3	1:A:1489:ASP:N	2.00	0.77
1:A:1509:ARG:NH1	1:A:1549:ASP:OD1	2.19	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1170:PRO:HG2	1:A:1410:LEU:HD21	1.69	0.75
1:A:658:VAL:HG22	1:A:659:LYS:HG2	1.68	0.75
1:A:1562:LEU:HB2	1:A:1566:SER:OG	1.86	0.74
1:A:946:ARG:NH2	1:A:1545:ALA:O	2.21	0.74
1:A:893:ASN:OD1	1:A:976:THR:HG22	1.86	0.73
1:A:396:LEU:HD22	1:A:906:ILE:CD1	2.18	0.73
1:A:1383:GLY:HA2	1:A:1387:ARG:HD3	1.70	0.73
1:A:1460:LYS:HG3	1:A:1461:ALA:H	1.55	0.72
1:A:864:GLU:HB2	1:A:878:LYS:HB2	1.72	0.72
1:A:882:SER:O	1:A:883:THR:HG22	1.89	0.71
1:A:906:ILE:HD12	1:A:907:THR:N	2.06	0.71
1:A:1021:VAL:HG12	1:A:1045:ASN:HA	1.74	0.70
1:A:500:PRO:HD3	1:A:609:TRP:O	1.92	0.70
1:A:661:ALA:HB2	1:A:705:LYS:C	2.17	0.69
1:A:683:ASP:HB3	1:A:685:GLY:O	1.93	0.69
1:A:397:TYR:CE2	1:A:403:VAL:HA	2.28	0.69
1:A:487:MSE:HE2	1:A:512:TYR:CZ	2.29	0.68
1:A:565:ASP:HB3	1:A:568:ARG:O	1.93	0.68
1:A:883:THR:HG21	1:A:887:GLU:C	2.19	0.67
1:A:1173:ILE:HB	1:A:1176:TYR:CD1	2.30	0.67
1:A:875:LEU:HD11	1:A:1015:VAL:HG11	1.76	0.67
1:A:859:LEU:HD13	1:A:888:LYS:HE2	1.77	0.66
1:A:1107:LEU:HD12	1:A:1110:GLU:HB2	1.76	0.66
1:A:1168:LYS:HB2	1:A:1443:GLY:HA2	1.77	0.66
1:A:1558:GLU:CD	1:A:1569:LEU:HD13	2.20	0.66
1:A:1175:ARG:NH1	1:A:1210:GLY:O	2.28	0.66
1:A:480:GLU:OE2	1:A:1561:ASN:ND2	2.27	0.66
1:A:621:PHE:CD2	1:A:638:PRO:HB2	2.32	0.65
1:A:1178:LYS:HB3	1:A:1179:GLU:HA	1.79	0.64
1:A:1011:ASN:OD1	1:A:1012:GLU:N	2.30	0.64
1:A:1133:ASN:HB2	1:A:1637:PRO:HG3	1.78	0.64
1:A:1582:GLN:OE1	1:A:1611:THR:OG1	2.11	0.64
1:A:888:LYS:HZ2	1:A:892:VAL:HG13	1.62	0.63
1:A:1162:GLN:OE1	1:A:1162:GLN:N	2.32	0.63
1:A:1378:TRP:HA	1:A:1378:TRP:CE3	2.34	0.63
1:A:536:VAL:HG11	1:A:539:LEU:HD12	1.80	0.63
1:A:1167:GLY:C	1:A:1485:TRP:HZ3	2.07	0.63
1:A:1378:TRP:HA	1:A:1378:TRP:HE3	1.64	0.63
1:A:741:TYR:HD1	1:A:742:SER:HB2	1.63	0.62
1:A:1410:LEU:HD23	1:A:1410:LEU:C	2.23	0.62
1:A:1569:LEU:HD23	1:A:1570:GLU:N	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:ALA:HB2	1:A:706:ALA:N	2.14	0.62
1:A:958:GLY:O	1:A:1597:ARG:NH1	2.31	0.62
1:A:1556:GLU:OE2	1:A:1619:VAL:HG21	2.00	0.62
1:A:1124:ARG:HG3	1:A:1125:PRO:O	1.99	0.62
1:A:679:ASN:HB3	1:A:687:GLN:HA	1.80	0.62
1:A:1509:ARG:NH2	1:A:1627:PRO:O	2.32	0.62
1:A:1170:PRO:HG2	1:A:1410:LEU:CD2	2.30	0.61
1:A:639:ILE:HG22	1:A:640:VAL:O	2.00	0.61
1:A:678:TRP:HE3	1:A:687:GLN:HB2	1.65	0.61
1:A:398:ARG:O	1:A:399:PRO:C	2.44	0.61
1:A:869:MSE:SE	1:A:875:LEU:HD12	2.50	0.60
1:A:1569:LEU:HD23	1:A:1569:LEU:C	2.26	0.60
1:A:1133:ASN:HB2	1:A:1637:PRO:CG	2.30	0.60
1:A:1200:TYR:OH	1:A:1263:ARG:HD3	2.01	0.60
1:A:1178:LYS:CD	1:A:1180:LEU:HB2	2.32	0.60
1:A:1178:LYS:HG3	1:A:1211:ILE:HD12	1.84	0.60
1:A:396:LEU:CD2	1:A:906:ILE:HD11	2.28	0.60
1:A:1478:ASN:OD1	1:A:1479:SER:N	2.35	0.60
1:A:1577:GLN:O	1:A:1578:ASN:C	2.45	0.60
1:A:615:PRO:HG3	1:A:727:ALA:HB2	1.83	0.60
1:A:1535:GLN:OE1	1:A:1535:GLN:HA	2.00	0.60
1:A:639:ILE:HG22	1:A:640:VAL:N	2.16	0.60
1:A:1168:LYS:HB3	1:A:1169:PRO:HD3	1.82	0.59
1:A:1104:GLY:O	1:A:1105:LEU:HG	2.02	0.59
1:A:1445:TRP:NE1	1:A:1460:LYS:O	2.30	0.59
1:A:1558:GLU:OE2	1:A:1617:ARG:NE	2.30	0.59
1:A:1177:ILE:O	1:A:1178:LYS:CB	2.50	0.59
1:A:486:ARG:NH2	1:A:594:GLU:OE1	2.36	0.59
1:A:892:VAL:HG11	1:A:977:LEU:HD12	1.83	0.58
1:A:1619:VAL:HG23	1:A:1620:THR:N	2.18	0.58
1:A:1571:GLN:HA	1:A:1571:GLN:OE1	2.02	0.58
1:A:1570:GLU:HG2	1:A:1571:GLN:N	2.19	0.58
1:A:639:ILE:HG12	1:A:738:TRP:O	2.03	0.57
1:A:871:PRO:HD3	1:A:1018:ALA:O	2.03	0.57
1:A:1031:MSE:HE1	1:A:1063:LEU:HD11	1.85	0.57
1:A:1350:LEU:O	1:A:1351:LYS:C	2.45	0.57
1:A:1632:GLU:HG2	1:A:1640:ARG:HB3	1.85	0.57
1:A:483:MSE:HE2	1:A:963:ASN:HD21	1.70	0.57
1:A:1487:ARG:NH2	1:A:1635:TYR:O	2.33	0.57
1:A:1167:GLY:HA3	1:A:1445:TRP:HB3	1.85	0.57
1:A:638:PRO:O	1:A:639:ILE:HG13	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1176:TYR:C	1:A:1177:ILE:HD12	2.30	0.56
1:A:1578:ASN:HB2	1:A:1579:LEU:CD1	2.35	0.56
1:A:1039:LEU:HD13	1:A:1087:VAL:HG21	1.86	0.56
1:A:532:LEU:HD12	1:A:585:GLN:HB3	1.87	0.56
1:A:718:TRP:CG	1:A:718:TRP:O	2.59	0.56
1:A:640:VAL:HG11	1:A:716:VAL:CG2	2.35	0.55
1:A:1131:THR:HG23	1:A:1491:SER:OG	2.06	0.55
1:A:1562:LEU:HB2	1:A:1566:SER:CB	2.36	0.55
1:A:460:MSE:CE	1:A:476:ASP:HB3	2.37	0.55
1:A:645:ASN:OD1	1:A:645:ASN:N	2.39	0.55
1:A:1076:ALA:HB3	1:A:1079:VAL:HG21	1.89	0.55
1:A:1503:ASN:ND2	1:A:1638:GLN:O	2.39	0.55
1:A:1146:ILE:HG13	1:A:1147:PRO:HD2	1.88	0.55
1:A:1177:ILE:O	1:A:1178:LYS:HB2	2.06	0.55
1:A:684:GLU:N	1:A:685:GLY:O	2.39	0.55
1:A:1506:GLN:HA	1:A:1641:ALA:CB	2.37	0.55
1:A:658:VAL:CG2	1:A:659:LYS:HG2	2.36	0.54
1:A:1076:ALA:HB1	1:A:1077:PRO:HD2	1.90	0.54
1:A:1195:LEU:HD22	1:A:1223:VAL:HA	1.88	0.54
1:A:394:ARG:HA	1:A:909:TYR:CE2	2.42	0.54
1:A:1161:GLY:C	1:A:1162:GLN:OE1	2.51	0.54
1:A:858:ARG:HB3	1:A:915:TRP:CD1	2.43	0.54
1:A:859:LEU:HD13	1:A:888:LYS:CE	2.36	0.54
1:A:1171:LEU:HG	1:A:1173:ILE:HG23	1.89	0.54
1:A:1615:LEU:HD12	1:A:1616:ALA:N	2.22	0.54
1:A:959:LYS:HD2	1:A:960:PRO:HD2	1.89	0.54
1:A:1619:VAL:HG23	1:A:1620:THR:H	1.72	0.54
1:A:590:GLY:O	1:A:601:THR:HG23	2.09	0.53
1:A:1139:GLN:HG2	1:A:1140:PRO:HD2	1.90	0.53
1:A:1036:THR:HG22	1:A:1088:ARG:HA	1.90	0.53
1:A:705:LYS:O	1:A:708:GLU:HB3	2.08	0.53
1:A:729:ASN:O	1:A:730:GLU:HB2	2.09	0.53
1:A:1172:ASN:O	1:A:1174:ALA:N	2.42	0.53
1:A:1575:GLU:OE1	1:A:1576:VAL:HG13	2.08	0.53
1:A:718:TRP:O	1:A:718:TRP:CD1	2.61	0.53
1:A:1177:ILE:O	1:A:1178:LYS:CG	2.56	0.53
1:A:581:HIS:HB3	1:A:730:GLU:O	2.08	0.53
1:A:467:THR:C	1:A:469:ASP:H	2.17	0.53
1:A:505:LYS:HB3	1:A:572:SER:CB	2.39	0.53
1:A:1205:GLN:O	1:A:1209:LEU:HB2	2.09	0.53
1:A:1524:LEU:HD12	1:A:1649:LEU:HD11	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:ASN:HA	1:A:715:PRO:HA	1.91	0.52
1:A:464:ARG:HD2	1:A:472:TYR:HD2	1.73	0.52
1:A:906:ILE:HD12	1:A:906:ILE:C	2.35	0.52
1:A:1562:LEU:CB	1:A:1566:SER:OG	2.56	0.52
1:A:639:ILE:CG2	1:A:640:VAL:N	2.73	0.52
1:A:1542:VAL:HG22	1:A:1639:TRP:CZ3	2.45	0.52
1:A:650:ILE:CD1	1:A:712:VAL:HG22	2.40	0.52
1:A:1607:TYR:CE1	1:A:1608:GLN:HG3	2.45	0.52
1:A:651:VAL:CG1	1:A:659:LYS:HE3	2.39	0.52
1:A:1090:LEU:HB3	1:A:1091:PRO:HD2	1.90	0.52
1:A:1339:SER:HB2	1:A:1371:ARG:HE	1.74	0.52
1:A:1569:LEU:HD21	1:A:1615:LEU:HD23	1.89	0.52
1:A:1413:LEU:HA	1:A:1416:GLN:HG2	1.92	0.51
1:A:1551:LEU:HD11	1:A:1557:LEU:HD13	1.92	0.51
1:A:1417:ALA:HA	1:A:1420:GLU:CG	2.39	0.51
1:A:1463:ASN:OD1	1:A:1464:SER:N	2.44	0.51
1:A:1596:ASP:C	1:A:1597:ARG:HG2	2.34	0.51
1:A:662:VAL:HG12	1:A:663:SER:O	2.10	0.51
1:A:883:THR:HG23	1:A:885:ASN:HB2	1.92	0.51
1:A:662:VAL:HG11	1:A:728:PRO:HG2	1.93	0.51
1:A:1103:SER:HA	1:A:1114:ASP:OD1	2.11	0.51
1:A:1446:GLN:HG2	1:A:1457:THR:HG23	1.91	0.51
1:A:1058:THR:HB	1:A:1099:GLN:HB2	1.93	0.51
1:A:1178:LYS:CD	1:A:1211:ILE:HD12	2.40	0.51
1:A:1228:SER:HA	1:A:1231:LEU:HD12	1.93	0.51
1:A:1341:LEU:O	1:A:1345:GLN:HG3	2.12	0.51
1:A:893:ASN:HA	1:A:975:VAL:O	2.10	0.50
1:A:1188:LEU:HD13	1:A:1233:MSE:SE	2.61	0.50
1:A:1341:LEU:HB3	1:A:1342:PRO:HD3	1.92	0.50
1:A:676:TYR:O	1:A:690:PHE:HA	2.11	0.50
1:A:678:TRP:CE3	1:A:687:GLN:HB2	2.44	0.50
1:A:671:ARG:NH1	1:A:721:TYR:OH	2.44	0.50
1:A:675:ASP:HA	1:A:690:PHE:HE1	1.75	0.50
1:A:580:THR:HG21	1:A:584:LEU:HD21	1.94	0.50
1:A:972:ALA:HB2	1:A:987:LEU:HD21	1.94	0.50
1:A:639:ILE:HG12	1:A:738:TRP:N	2.27	0.50
1:A:678:TRP:HZ3	1:A:687:GLN:HG3	1.77	0.50
1:A:1139:GLN:N	1:A:1142:GLU:OE2	2.45	0.50
1:A:1177:ILE:O	1:A:1178:LYS:HG2	2.12	0.50
1:A:500:PRO:O	1:A:575:SER:OG	2.15	0.50
1:A:661:ALA:HB1	1:A:705:LYS:HA	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:ASP:OD1	1:A:675:ASP:N	2.45	0.49
1:A:1579:LEU:HD12	1:A:1579:LEU:N	2.27	0.49
1:A:888:LYS:NZ	1:A:892:VAL:HG13	2.25	0.49
1:A:1331:TRP:CD1	1:A:1358:ARG:HD2	2.48	0.49
1:A:503:GLU:HG2	1:A:574:GLU:HA	1.94	0.49
1:A:588:PHE:O	1:A:603:ARG:HA	2.13	0.49
1:A:386:LYS:O	1:A:473:ARG:NH2	2.46	0.49
1:A:1188:LEU:HD22	1:A:1241:ALA:O	2.13	0.49
1:A:396:LEU:HD21	1:A:482:PHE:CG	2.47	0.49
1:A:980:GLN:N	1:A:980:GLN:OE1	2.46	0.49
1:A:1178:LYS:HD3	1:A:1180:LEU:HB2	1.95	0.49
1:A:1576:VAL:O	1:A:1576:VAL:HG23	2.13	0.49
1:A:411:ASP:OD1	1:A:415:LYS:N	2.45	0.48
1:A:651:VAL:HG11	1:A:659:LYS:HE3	1.94	0.48
1:A:1031:MSE:HE2	1:A:1121:ILE:HD13	1.93	0.48
1:A:1533:TRP:CD1	1:A:1579:LEU:HD23	2.47	0.48
1:A:472:TYR:CD1	1:A:472:TYR:N	2.81	0.48
1:A:1137:ALA:O	1:A:1138:LEU:HD23	2.12	0.48
1:A:1178:LYS:CG	1:A:1211:ILE:HD12	2.42	0.48
1:A:639:ILE:HG12	1:A:738:TRP:H	1.79	0.48
1:A:1137:ALA:HB2	1:A:1485:TRP:CD1	2.48	0.48
1:A:1177:ILE:C	1:A:1178:LYS:HG2	2.39	0.48
1:A:1201:THR:HG21	1:A:1432:PHE:HZ	1.78	0.47
1:A:1569:LEU:HD21	1:A:1615:LEU:CD2	2.43	0.47
1:A:1106:ALA:CA	1:A:1113:ALA:HA	2.40	0.47
1:A:1428:SER:O	1:A:1429:ASN:C	2.57	0.47
1:A:487:MSE:HE2	1:A:512:TYR:CE1	2.49	0.47
1:A:741:TYR:HD1	1:A:742:SER:CB	2.25	0.47
1:A:1471:LEU:HA	1:A:1474:LEU:HB2	1.96	0.47
1:A:1559:ASN:OD1	1:A:1561:ASN:N	2.46	0.47
1:A:472:TYR:N	1:A:472:TYR:HD1	2.13	0.47
1:A:532:LEU:HD21	1:A:535:ALA:HA	1.95	0.47
1:A:590:GLY:O	1:A:601:THR:HA	2.14	0.47
1:A:1047:THR:HG21	1:A:1051:GLN:HE21	1.78	0.47
1:A:1292:MSE:CG	1:A:1293:MSE:N	2.77	0.47
1:A:460:MSE:HE2	1:A:476:ASP:HB3	1.95	0.47
1:A:1371:ARG:HH12	1:A:1383:GLY:HA3	1.80	0.47
1:A:1387:ARG:HB3	1:A:1427:GLU:HG2	1.97	0.47
1:A:1558:GLU:HB3	1:A:1569:LEU:HD22	1.97	0.47
1:A:1562:LEU:O	1:A:1566:SER:HA	2.15	0.47
1:A:599:PRO:HG2	1:A:1617:ARG:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:ALA:HB1	1:A:653:SER:C	2.40	0.47
1:A:640:VAL:HG21	1:A:644:SER:C	2.39	0.47
1:A:1303:ALA:HB1	1:A:1338:ALA:HB2	1.96	0.47
1:A:1173:ILE:HD11	1:A:1420:GLU:OE2	2.15	0.47
1:A:661:ALA:CB	1:A:705:LYS:C	2.86	0.47
1:A:599:PRO:HG2	1:A:1617:ARG:CD	2.45	0.47
1:A:1326:ALA:O	1:A:1329:GLU:HG2	2.14	0.47
1:A:598:ARG:NH2	1:A:1027:MSE:O	2.45	0.46
1:A:1139:GLN:HA	1:A:1483:PRO:HB3	1.97	0.46
1:A:1039:LEU:HD13	1:A:1087:VAL:CG2	2.45	0.46
1:A:532:LEU:HD23	1:A:532:LEU:C	2.40	0.46
1:A:578:LYS:HG3	1:A:579:GLU:N	2.30	0.46
1:A:880:LYS:HA	1:A:981:GLY:O	2.14	0.46
1:A:535:ALA:HB1	1:A:609:TRP:CZ2	2.50	0.46
1:A:723:LEU:O	1:A:734:SER:HA	2.16	0.46
1:A:1505:LEU:O	1:A:1641:ALA:HB2	2.16	0.46
1:A:1630:MSE:HG3	1:A:1640:ARG:HH21	1.81	0.46
1:A:861:LEU:HD23	1:A:862:ALA:N	2.31	0.46
1:A:1168:LYS:CB	1:A:1169:PRO:HD3	2.46	0.46
1:A:1106:ALA:HA	1:A:1112:VAL:O	2.15	0.46
1:A:896:VAL:HG11	1:A:985:VAL:HG21	1.98	0.46
1:A:1047:THR:HG21	1:A:1051:GLN:HG3	1.98	0.46
1:A:1283:LEU:O	1:A:1286:TYR:HB2	2.16	0.46
1:A:1570:GLU:HG2	1:A:1571:GLN:H	1.81	0.46
1:A:1105:LEU:O	1:A:1105:LEU:HD12	2.16	0.46
1:A:888:LYS:CE	1:A:892:VAL:HG13	2.46	0.45
1:A:1577:GLN:HA	1:A:1580:LEU:HD12	1.98	0.45
1:A:1548:VAL:HG22	1:A:1599:VAL:HG22	1.98	0.45
1:A:637:GLN:O	1:A:639:ILE:HD12	2.16	0.45
1:A:892:VAL:HB	1:A:977:LEU:HB2	1.97	0.45
1:A:1226:GLY:O	1:A:1230:LEU:HG	2.16	0.45
1:A:390:MSE:HE1	1:A:473:ARG:O	2.17	0.45
1:A:1503:ASN:OD1	1:A:1504:VAL:HG23	2.16	0.45
1:A:617:ILE:HD11	1:A:725:VAL:HG23	1.99	0.45
1:A:991:ASP:OD1	1:A:991:ASP:C	2.59	0.45
1:A:1045:ASN:CG	1:A:1047:THR:HG22	2.40	0.45
1:A:1202:ASN:OD1	1:A:1202:ASN:N	2.49	0.45
1:A:659:LYS:CB	1:A:707:ASP:HA	2.46	0.45
1:A:1410:LEU:HD23	1:A:1410:LEU:O	2.15	0.45
1:A:1558:GLU:O	1:A:1560:GLN:NE2	2.50	0.45
1:A:521:ASN:OD1	1:A:1080:ARG:NH2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:PRO:HA	1:A:1170:PRO:HD3	1.82	0.44
1:A:992:PHE:HE1	1:A:994:GLY:C	2.26	0.44
1:A:1227:ILE:HG22	1:A:1228:SER:N	2.32	0.44
1:A:1578:ASN:CB	1:A:1579:LEU:HD12	2.41	0.44
1:A:621:PHE:HD2	1:A:638:PRO:HB2	1.79	0.44
1:A:1218:LYS:O	1:A:1222:SER:HB2	2.17	0.44
1:A:661:ALA:CB	1:A:706:ALA:N	2.80	0.44
1:A:860:ASP:O	1:A:881:ALA:HA	2.17	0.44
1:A:1097:GLU:HB3	1:A:1120:LYS:HG2	2.00	0.44
1:A:1031:MSE:HE1	1:A:1063:LEU:CD1	2.46	0.44
1:A:1444:LYS:HD3	1:A:1444:LYS:N	2.33	0.44
1:A:1505:LEU:C	1:A:1505:LEU:HD12	2.41	0.44
1:A:613:ALA:HB1	1:A:653:SER:O	2.17	0.44
1:A:956:ARG:NH2	1:A:1634:MSE:O	2.51	0.44
1:A:1047:THR:O	1:A:1048:ASP:CG	2.61	0.44
1:A:1169:PRO:HB2	1:A:1172:ASN:HB3	1.99	0.44
1:A:882:SER:O	1:A:883:THR:CG2	2.62	0.44
1:A:1327:LEU:HB3	1:A:1350:LEU:CD2	2.47	0.44
1:A:546:ASP:HB3	1:A:549:ALA:HB2	1.99	0.44
1:A:1178:LYS:HG3	1:A:1211:ILE:CD1	2.46	0.44
1:A:1559:ASN:OD1	1:A:1559:ASN:C	2.60	0.43
1:A:385:SER:O	1:A:386:LYS:HB2	2.18	0.43
1:A:505:LYS:HB3	1:A:572:SER:HB2	2.00	0.43
1:A:1482:GLN:CD	1:A:1482:GLN:N	2.76	0.43
1:A:1562:LEU:HB2	1:A:1566:SER:HG	1.79	0.43
1:A:460:MSE:HE2	1:A:476:ASP:CB	2.49	0.43
1:A:1377:ILE:HD13	1:A:1377:ILE:N	2.32	0.43
1:A:1607:TYR:CD1	1:A:1608:GLN:HG3	2.53	0.43
1:A:397:TYR:CD2	1:A:403:VAL:HG22	2.53	0.43
1:A:464:ARG:CD	1:A:472:TYR:HD2	2.32	0.43
1:A:504:VAL:O	1:A:572:SER:HA	2.18	0.43
1:A:639:ILE:CG2	1:A:738:TRP:O	2.56	0.43
1:A:1179:GLU:OE1	1:A:1212:LYS:N	2.52	0.43
1:A:1201:THR:HG22	1:A:1205:GLN:OE1	2.19	0.43
1:A:614:LEU:HD22	1:A:731:ALA:HB1	2.01	0.43
1:A:1178:LYS:HE2	1:A:1211:ILE:HD12	2.01	0.43
1:A:1592:GLU:OE1	1:A:1594:ARG:NH1	2.45	0.43
1:A:623:SER:HA	1:A:636:LYS:HE2	2.01	0.43
1:A:641:ASP:O	1:A:642:GLU:HB2	2.19	0.43
1:A:460:MSE:CE	1:A:476:ASP:CB	2.97	0.43
1:A:661:ALA:CB	1:A:705:LYS:HA	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:729:ASN:O	1:A:730:GLU:CB	2.67	0.43
1:A:1550:LEU:CD2	1:A:1597:ARG:HD2	2.49	0.43
1:A:732:VAL:HG12	1:A:733:SER:N	2.33	0.42
1:A:899:VAL:HG11	1:A:904:LEU:HD21	2.01	0.42
1:A:1549:ASP:HB3	1:A:1598:PHE:HB3	2.00	0.42
1:A:1571:GLN:OE1	1:A:1571:GLN:CA	2.67	0.42
1:A:656:GLN:O	1:A:657:GLY:C	2.61	0.42
1:A:1064:GLU:CD	1:A:1090:LEU:HD21	2.44	0.42
1:A:1184:PRO:HG2	1:A:1185:TYR:CE2	2.54	0.42
1:A:859:LEU:HD22	1:A:888:LYS:HE2	2.01	0.42
1:A:950:ASP:HA	1:A:951:GLY:HA2	1.78	0.42
1:A:1206:LEU:C	1:A:1211:ILE:O	2.62	0.42
1:A:405:LEU:HD22	1:A:463:ILE:HG21	2.01	0.42
1:A:520:GLY:HA2	1:A:564:ASP:HA	2.01	0.42
1:A:487:MSE:CE	1:A:512:TYR:CZ	3.02	0.42
1:A:487:MSE:HE1	1:A:594:GLU:HA	2.01	0.42
1:A:504:VAL:HB	1:A:573:THR:HG22	2.00	0.42
1:A:718:TRP:CD1	1:A:740:GLY:HA3	2.54	0.42
1:A:1405:GLU:O	1:A:1406:GLN:C	2.63	0.42
1:A:399:PRO:HA	1:A:452:LEU:CD2	2.49	0.42
1:A:680:TRP:NE1	1:A:683:ASP:HA	2.34	0.42
1:A:1175:ARG:HG3	1:A:1176:TYR:H	1.84	0.42
1:A:1274:ASP:O	1:A:1275:ALA:C	2.61	0.42
1:A:389:PHE:O	1:A:407:GLY:HA2	2.20	0.42
1:A:483:MSE:HA	1:A:484:PRO:HD2	1.93	0.42
1:A:875:LEU:CD1	1:A:1015:VAL:HG11	2.47	0.42
1:A:1066:VAL:CG1	1:A:1086:PRO:HB2	2.50	0.42
1:A:518:ALA:HB1	1:A:521:ASN:HB2	2.02	0.42
1:A:1063:LEU:HD12	1:A:1063:LEU:HA	1.83	0.42
1:A:1171:LEU:CD2	1:A:1417:ALA:CB	2.98	0.42
1:A:646:ALA:N	1:A:714:PHE:O	2.40	0.42
1:A:1066:VAL:HG12	1:A:1086:PRO:C	2.44	0.42
1:A:1138:LEU:HB3	1:A:1142:GLU:HB2	2.00	0.42
1:A:1378:TRP:CE3	1:A:1378:TRP:CA	3.03	0.42
1:A:1621:PRO:HA	1:A:1651:VAL:HB	2.01	0.42
1:A:677:TYR:CD1	1:A:690:PHE:CZ	3.08	0.42
1:A:1124:ARG:NH1	1:A:1125:PRO:O	2.46	0.42
1:A:1170:PRO:O	1:A:1172:ASN:ND2	2.48	0.42
1:A:591:SER:HB3	1:A:599:PRO:HB3	2.01	0.41
1:A:684:GLU:OE1	1:A:684:GLU:HA	2.20	0.41
1:A:1258:MSE:HE2	1:A:1258:MSE:HB2	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1606:GLU:C	1:A:1608:GLN:H	2.27	0.41
1:A:582:SER:O	1:A:584:LEU:HD13	2.20	0.41
1:A:869:MSE:HG3	1:A:1017:VAL:HG22	2.02	0.41
1:A:1137:ALA:HB2	1:A:1485:TRP:HD1	1.84	0.41
1:A:1505:LEU:CD1	1:A:1631:VAL:HG13	2.50	0.41
1:A:1516:GLY:HA3	1:A:1576:VAL:HG11	2.02	0.41
1:A:1206:LEU:HB3	1:A:1211:ILE:O	2.21	0.41
1:A:396:LEU:HD21	1:A:482:PHE:CD2	2.55	0.41
1:A:539:LEU:N	1:A:540:PRO:HD3	2.36	0.41
1:A:1298:ALA:HB1	1:A:1379:LEU:HA	2.02	0.41
1:A:1301:LEU:O	1:A:1305:LYS:HG2	2.21	0.41
1:A:1399:ASN:HB3	1:A:1401:LEU:HG	2.02	0.41
1:A:883:THR:HG21	1:A:887:GLU:O	2.21	0.41
1:A:1044:THR:HA	1:A:1080:ARG:HB3	2.03	0.41
1:A:623:SER:H	1:A:636:LYS:HD3	1.84	0.41
1:A:680:TRP:HE1	1:A:683:ASP:HA	1.85	0.41
1:A:1262:VAL:HG22	1:A:1276:ILE:HD11	2.03	0.41
1:A:1311:TYR:HA	1:A:1345:GLN:OE1	2.20	0.41
1:A:1606:GLU:O	1:A:1607:TYR:CG	2.73	0.41
1:A:564:ASP:O	1:A:565:ASP:C	2.63	0.41
1:A:610:PRO:HD2	1:A:614:LEU:HD21	2.03	0.41
1:A:547:ILE:HG22	1:A:734:SER:HB2	2.02	0.41
1:A:946:ARG:O	1:A:947:PHE:HB3	2.19	0.41
1:A:1107:LEU:N	1:A:1112:VAL:O	2.40	0.41
1:A:623:SER:N	1:A:636:LYS:HD3	2.36	0.41
1:A:963:ASN:OD1	1:A:963:ASN:C	2.63	0.41
1:A:1022:ILE:O	1:A:1043:ILE:HA	2.21	0.41
1:A:1562:LEU:HB2	1:A:1566:SER:HB2	2.01	0.41
1:A:1178:LYS:HE3	1:A:1180:LEU:HD22	2.03	0.41
1:A:1284:LEU:O	1:A:1287:LEU:N	2.51	0.41
1:A:398:ARG:HB2	1:A:482:PHE:CE1	2.56	0.40
1:A:666:GLN:OE1	1:A:668:ARG:NH2	2.53	0.40
1:A:675:ASP:HA	1:A:690:PHE:CE1	2.55	0.40
1:A:1273:THR:O	1:A:1274:ASP:C	2.64	0.40
1:A:1355:ASP:OD2	1:A:1358:ARG:HG3	2.21	0.40
1:A:1619:VAL:CG2	1:A:1620:THR:N	2.84	0.40
1:A:404:ILE:HG21	1:A:971:GLN:OE1	2.20	0.40
1:A:1343:LEU:HD13	1:A:1365:LEU:HD23	2.03	0.40
1:A:1365:LEU:O	1:A:1366:ALA:C	2.63	0.40
1:A:1548:VAL:O	1:A:1548:VAL:HG12	2.21	0.40
1:A:639:ILE:CG1	1:A:738:TRP:H	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:PHE:CD2	1:A:723:LEU:HD22	2.57	0.40
1:A:1093:TYR:CD1	1:A:1093:TYR:C	2.98	0.40
1:A:1513:GLY:CA	1:A:1519:LYS:HG3	2.52	0.40
1:A:1635:TYR:C	1:A:1635:TYR:CD1	2.99	0.40
1:A:1137:ALA:CB	1:A:1485:TRP:CD1	3.04	0.40
1:A:1413:LEU:HD12	1:A:1416:GLN:HG3	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

There are no ligands in this entry.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1103/1639 (67%)	-0.81	0 100 100	85, 139, 205, 267	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.