



# Full wwPDB X-ray Structure Validation Report i

Jun 23, 2024 – 06:12 PM EDT

PDB ID : 4RTD  
Title : Escherichia coli alpha-2-macroglobulin activated by porcine elastase  
Authors : Fyfe, C.D.; Grinter, R.; Roszak, A.W.; Josts, I.; Cogdell, R.J.; Walker, D.  
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](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 i symbol.

The types of validation reports are described at  
<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.37.1

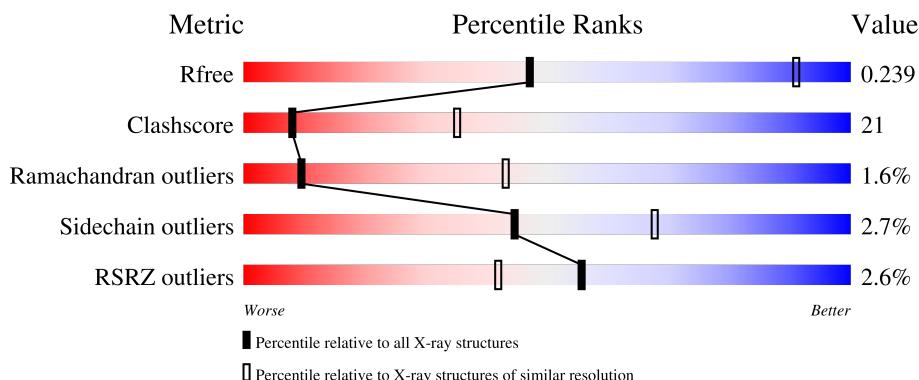
# 1 Overall quality at a glance

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))
$R_{free}$	130704	1557 (3.82-3.50)
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)
RSRZ outliers	127900	1441 (3.82-3.50)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	2%	43%	24%	.	32%

## 2 Entry composition (i)

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 8699	C 5497	N 1505	O 1677	S 1	Se 19	0	0	0

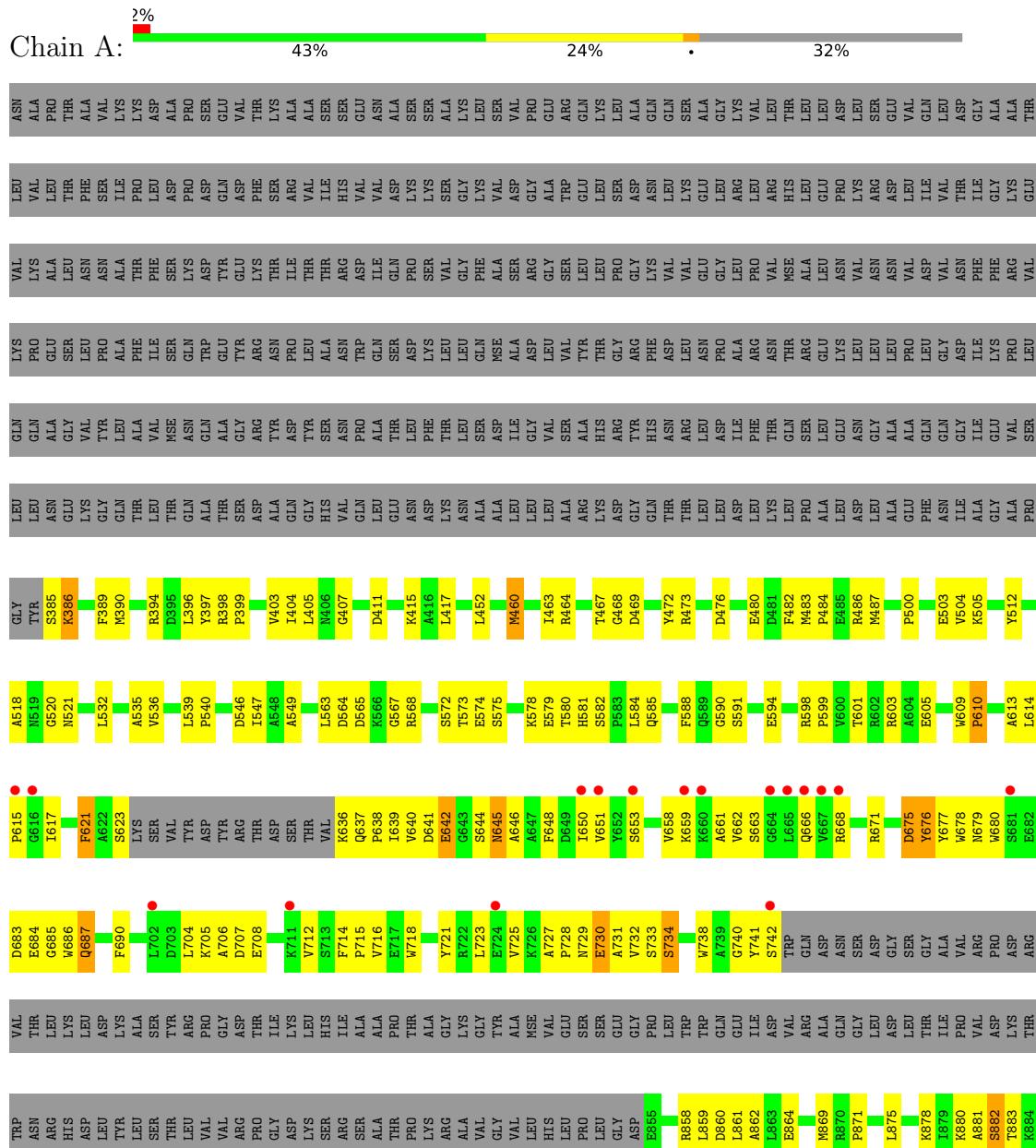
There are 11 discrepancies between the modelled and reference sequences:

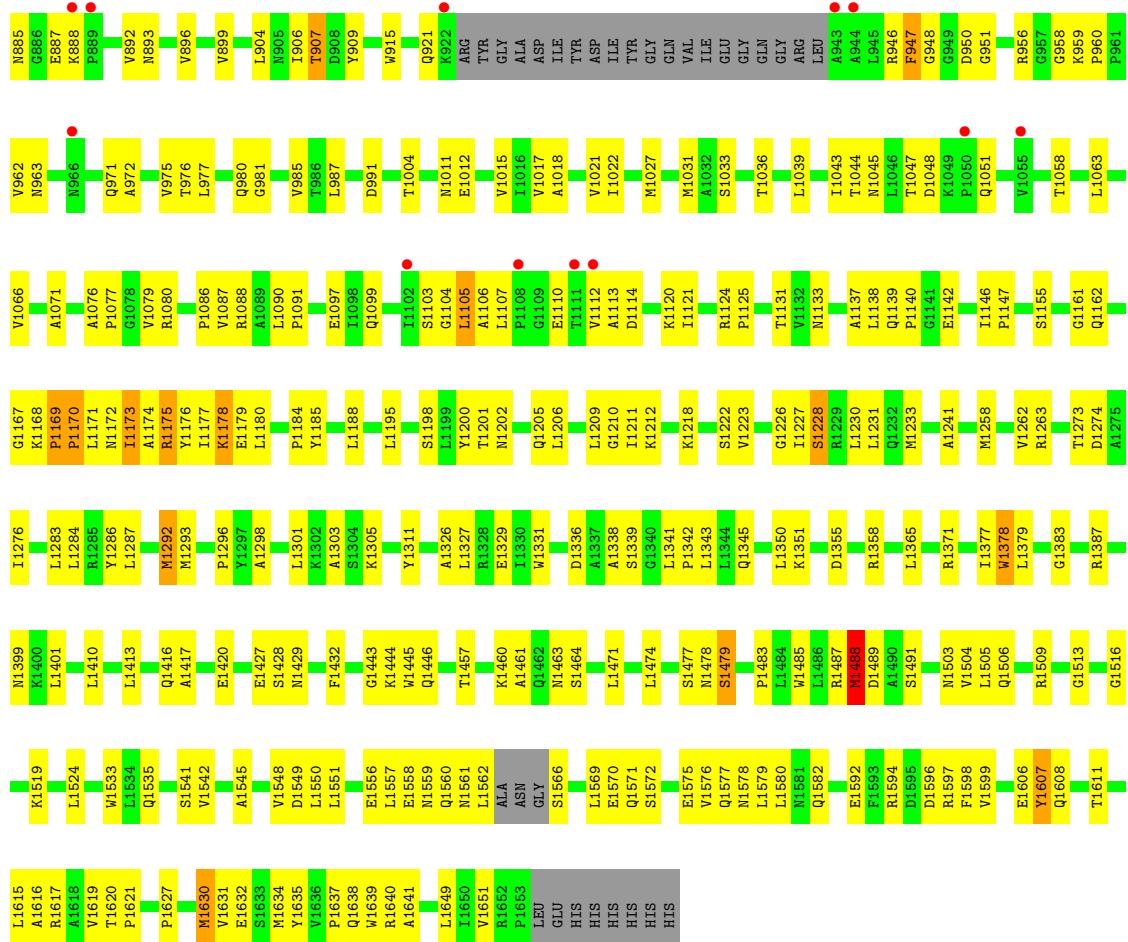
Chain	Residue	Modelled	Actual	Comment	Reference
A	219	PRO	SER	ENGINEERED MUTATION	UNP P76578
A	606	ARG	GLN	ENGINEERED MUTATION	UNP P76578
A	1587	ASN	SER	ENGINEERED MUTATION	UNP P76578
A	1654	LEU	-	EXPRESSION TAG	UNP P76578
A	1655	GLU	-	EXPRESSION TAG	UNP P76578
A	1656	HIS	-	EXPRESSION TAG	UNP P76578
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





## 4 Data and refinement statistics i

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.06 Å    176.06 Å    161.13 Å 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) 100.0 (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 3.66 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
$R$ , $R_{free}$	0.177 , 0.238 0.183 , 0.239	Depositor DCC
$R_{free}$ test set	1033 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	126.2	Xtriage
Anisotropy	0.162	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 113.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.037 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8699	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [\(i\)](#)

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

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	0.50	0/8863	0.75	3/12024 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	460	MSE	CG-SE-CE	7.75	115.94	98.90
1	A	1105	LEU	CA-CB-CG	5.31	127.52	115.30
1	A	1488	MSE	CA-CB-CG	-5.20	104.46	113.30

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	8699	0	8589	370	0
All	All	8699	0	8589	370	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 21.

All (370) 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
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: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: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: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:661:ALA:HB2	1:A:705:LYS:C	2.17	0.65
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1582:GLN:OE1	1:A:1611:THR:OG1	2.11	0.64
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: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:883:THR:HG21	1:A:887:GLU:C	2.19	0.62
1:A:1569:LEU:HD23	1:A:1570:GLU:N	2.14	0.62
1:A:661:ALA:HB2	1:A:706:ALA:N	2.14	0.62
1:A:1558:GLU:CD	1:A:1569:LEU:HD13	2.20	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:869:MSE:SE	1:A:875:LEU:HD12	2.50	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:1571:GLN:HA	1:A:1571:GLN:OE1	2.02	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:1410:LEU:HD23	1:A:1410:LEU:C	2.23	0.58
1:A:1570:GLU:HG2	1:A:1571:GLN:N	2.19	0.58
1:A:1167:GLY:C	1:A:1485:TRP:HZ3	2.07	0.58
1:A:639:ILE:HG12	1:A:738:TRP:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:398:ARG:O	1:A:399:PRO:C	2.44	0.56
1:A:532:LEU:HD12	1:A:585:GLN:HB3	1.87	0.56
1:A:1569:LEU:HD23	1:A:1569:LEU:C	2.26	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:1577:GLN:O	1:A:1578:ASN:C	2.45	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1350:LEU:O	1:A:1351:LYS:C	2.45	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
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: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:1176:TYR:C	1:A:1177:ILE:HD12	2.30	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: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:888:LYS:NZ	1:A:892:VAL:HG13	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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:1161:GLY:C	1:A:1162:GLN:OE1	2.51	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:467:THR:C	1:A:469:ASP:H	2.17	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:906:ILE:HD12	1:A:906:ILE:C	2.35	0.47
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1303:ALA:HB1	1:A:1338:ALA:HB2	1.96	0.47
1:A:1596:ASP:C	1:A:1597:ARG:HG2	2.34	0.47
1:A:1173:ILE:HD11	1:A:1420:GLU:OE2	2.15	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1169:PRO:HA	1:A:1170:PRO:HD3	1.82	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: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: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: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:460:MSE:HE2	1:A:476:ASP:CB	2.49	0.43
1:A:661:ALA:CB	1:A:705:LYS:C	2.86	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:888:LYS:HZ3	1:A:1004:THR:CG2	2.31	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:1177:ILE:C	1:A:1178:LYS:HG2	2.39	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:1428:SER:O	1:A:1429:ASN:C	2.57	0.43
1:A:1550:LEU:CD2	1:A:1597:ARG:HD2	2.49	0.43
1:A:613:ALA:HB1	1:A:653:SER:C	2.40	0.42
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: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: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:640:VAL:HG21	1:A:644:SER:C	2.39	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: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: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: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:532:LEU:HD23	1:A:532:LEU:C	2.40	0.41
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:991:ASP:C	1:A:991:ASP:OD1	2.59	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: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:888:LYS:HZ2	1:A:892:VAL:HG13	1.85	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: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:1045:ASN:CG	1:A:1047:THR:HG22	2.40	0.40
1:A:1343:LEU:HD13	1:A:1365:LEU:HD23	2.03	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
1:A:648:PHE:CD2	1:A:723:LEU:HD22	2.57	0.40
1:A:1513:GLY:CA	1:A:1519:LYS:HG3	2.52	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 [\(i\)](#)

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	1112/1639 (68%)	989 (89%)	105 (9%)	18 (2%)	9 / 43

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	642	GLU
1	A	730	GLU
1	A	1169	PRO
1	A	1178	LYS
1	A	947	PHE
1	A	948	GLY
1	A	687	GLN
1	A	1170	PRO
1	A	386	LYS
1	A	610	PRO
1	A	1071	ALA
1	A	1173	ILE
1	A	1175	ARG
1	A	567	GLY
1	A	676	TYR
1	A	1048	ASP
1	A	1296	PRO
1	A	468	GLY

#### 5.3.2 Protein sidechains [\(i\)](#)

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	927/1340 (69%)	902 (97%)	25 (3%)	44 68

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	563	LEU
1	A	605	GLU
1	A	621	PHE
1	A	645	ASN
1	A	675	ASP
1	A	686	TRP
1	A	734	SER
1	A	882	SER
1	A	907	THR
1	A	921	GLN
1	A	962	VAL
1	A	1155	SER
1	A	1198	SER
1	A	1228	SER
1	A	1274	ASP
1	A	1292	MSE
1	A	1336	ASP
1	A	1378	TRP
1	A	1477	SER
1	A	1479	SER
1	A	1488	MSE
1	A	1541	SER
1	A	1572	SER
1	A	1607	TYR
1	A	1630	MSE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1139	GLN
1	A	1172	ASN
1	A	1470	GLN
1	A	1590	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 monosaccharides 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1103/1639 (67%)	0.05	29 (2%) 56 42	85, 139, 205, 267	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1108	PRO	4.9
1	A	943	ALA	4.0
1	A	616	GLY	3.3
1	A	615	PRO	3.2
1	A	651	VAL	3.1
1	A	665	LEU	3.1
1	A	653	SER	3.0
1	A	650	ILE	2.9
1	A	1111	THR	2.7
1	A	922	LYS	2.7
1	A	667	VAL	2.6
1	A	702	LEU	2.6
1	A	889	PRO	2.4
1	A	888	LYS	2.4
1	A	664	GLY	2.4
1	A	1112	VAL	2.4
1	A	659	LYS	2.3
1	A	966	ASN	2.3
1	A	666	GLN	2.3
1	A	1102	ILE	2.3
1	A	742	SER	2.3
1	A	1050	PRO	2.2
1	A	668	ARG	2.2
1	A	711	LYS	2.2
1	A	681	SER	2.2
1	A	660	LYS	2.2
1	A	724	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	1055	VAL	2.1
1	A	944	ALA	2.0

## 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 monosaccharides 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.