



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:48 PM GMT

PDB ID : 1M74  
Title : Crystal structure of Mg-ADP-bound SecA from *Bacillus subtilis*  
Authors : Hunt, J.F.; Weinkauff, S.; Henry, L.; Fak, J.J.; McNicholas, P.; Oliver, D.B.; Deisenhofer, J.  
Deposited on : 2002-07-16  
Resolution : 3.00 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  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

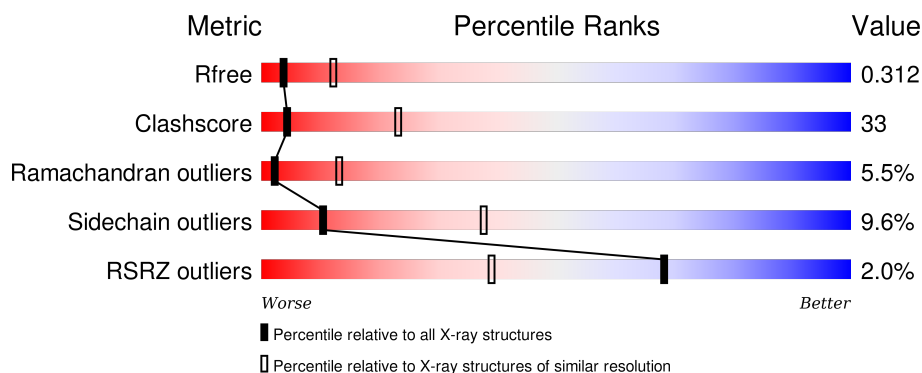
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

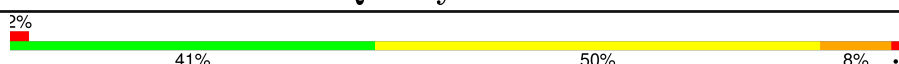
The reported resolution of this entry is 3.00 Å.

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))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	802	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SO4	A	1003	-	-	X	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6501 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 Preprotein translocase secA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	802	Total	C	N	O	S	0	0	0
			6402	4000	1117	1250	35			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



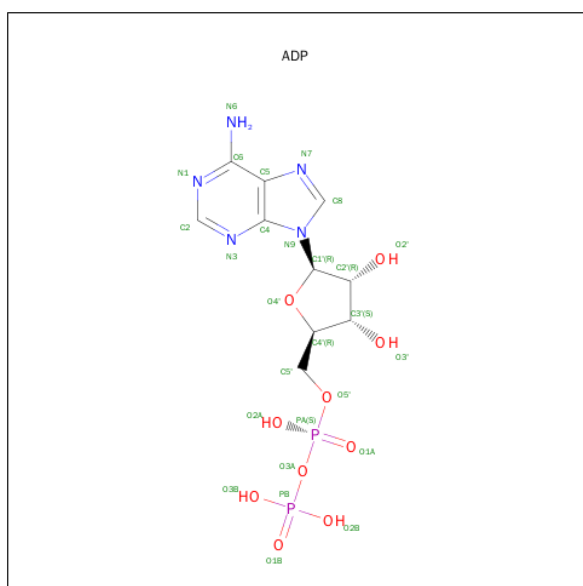
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

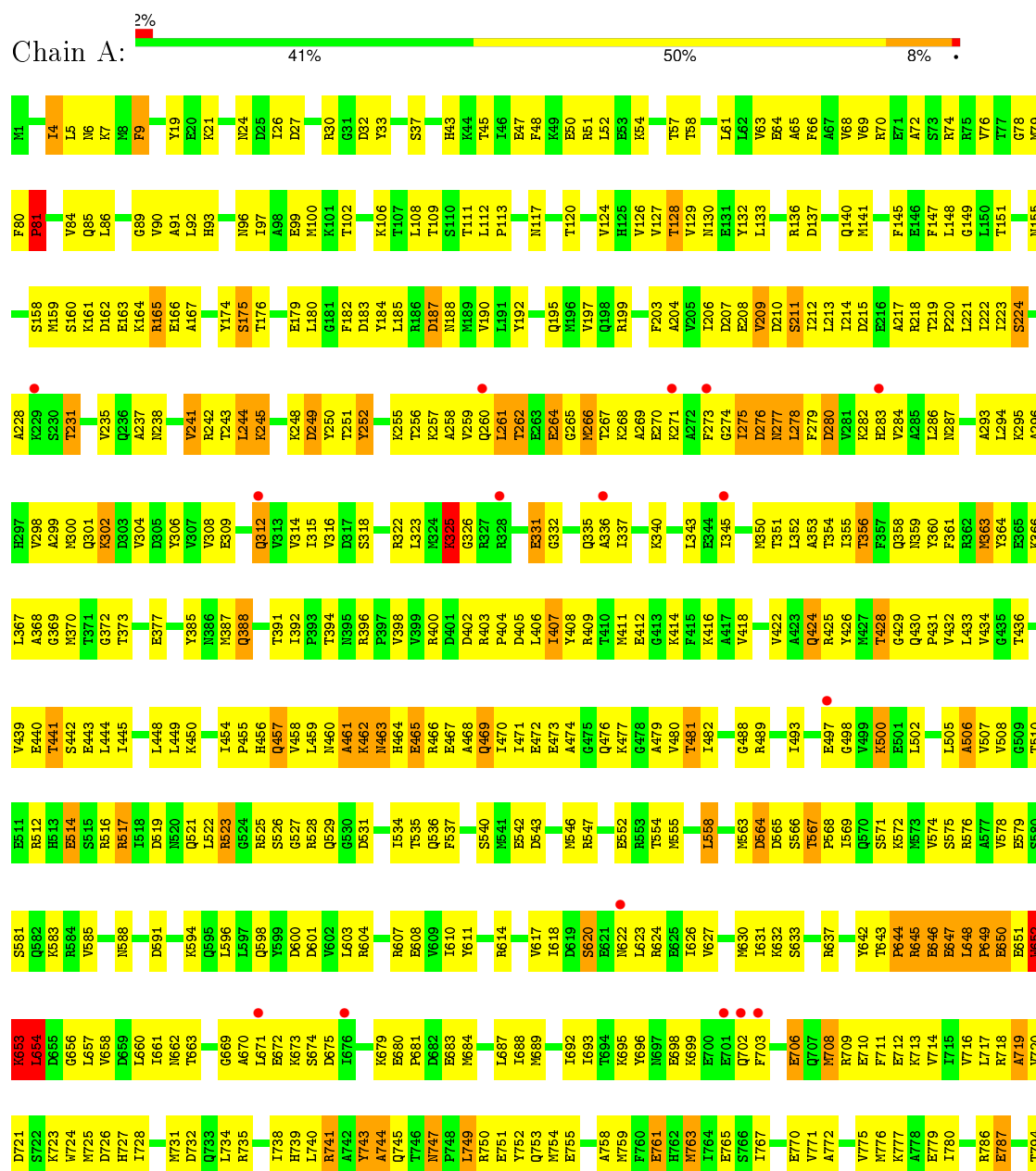
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	46	Total O 46 46	0	0

### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Preprotein translocase secA





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 31 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	131.25Å 131.25Å 150.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.45 – 3.00 49.45 – 2.70	Depositor EDS
% Data completeness (in resolution range)	76.1 (49.45-3.00) 84.0 (49.45-2.70)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.69 (at 2.69Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, $R_{free}$	0.217 , 0.291 0.233 , 0.312	Depositor DCC
$R_{free}$ test set	1491 reflections (6.00%)	DCC
Wilson B-factor (Å <sup>2</sup> )	78.9	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 104.3	EDS
Estimated twinning fraction	0.024 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Outliers	0 of 40793 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6501	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

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	0.62	0/6492	0.88	6/8731 (0.1%)

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	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	199	ARG	N-CA-C	-5.36	96.53	111.00
1	A	249	ASP	N-CA-C	-5.24	96.86	111.00
1	A	656	GLY	N-CA-C	-5.21	100.06	113.10
1	A	461	ALA	N-CA-C	5.19	125.02	111.00
1	A	7	LYS	CD-CE-NZ	-5.16	99.83	111.70
1	A	126	VAL	N-CA-C	-5.09	97.26	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	611	TYR	Sidechain



## 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	6402	0	6382	421	0
2	A	1	0	0	1	0
3	A	25	0	0	3	0
4	A	27	0	12	1	0
5	A	46	0	0	4	0
All	All	6501	0	6394	422	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 33.

All (422) 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:749:LEU:HD13	1:A:753:GLN:HE21	1.23	1.02
1:A:567:THR:HG23	1:A:568:PRO:HD3	1.41	1.01
1:A:409:ARG:HG3	1:A:564:ASP:HB3	1.48	0.95
1:A:661:ILE:HG21	1:A:688:ILE:HD11	1.50	0.93
1:A:368:ALA:HA	1:A:387:MET:HE3	1.49	0.93
1:A:111:THR:HA	1:A:145:PHE:HZ	1.36	0.90
1:A:718:ARG:HH21	1:A:787:GLU:HB2	1.32	0.90
1:A:637:ARG:HH12	1:A:765:GLU:HA	1.35	0.90
1:A:214:ILE:HG21	1:A:517:ARG:HH12	1.37	0.89
1:A:108:LEU:HA	1:A:141:MET:HE1	1.57	0.87
1:A:258:ALA:HB1	1:A:294:LEU:HD23	1.56	0.87
1:A:222:ILE:HG23	1:A:351:THR:HG23	1.56	0.86
1:A:65:ALA:O	1:A:69:VAL:HG23	1.76	0.85
1:A:425:ARG:HB3	1:A:430:GLN:HB3	1.60	0.83
1:A:654:LEU:HD12	1:A:654:LEU:H	1.44	0.83
1:A:648:LEU:HB3	1:A:651:GLU:HB2	1.60	0.83
1:A:128:THR:HG23	1:A:207:ASP:HB3	1.60	0.82
1:A:111:THR:HA	1:A:145:PHE:CZ	2.14	0.81
1:A:373:THR:HB	1:A:517:ARG:HG2	1.63	0.81
1:A:571:SER:HB3	1:A:574:VAL:HG12	1.63	0.81
1:A:710:GLU:O	1:A:714:VAL:HG23	1.81	0.81
1:A:698:GLU:HB3	1:A:702:GLN:HE22	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:LYS:HE2	1:A:510:THR:O	1.83	0.78
1:A:425:ARG:O	1:A:428:THR:HG22	1.84	0.78
1:A:217:ALA:HB1	1:A:358:GLN:HE21	1.49	0.77
1:A:431:PRO:HB3	1:A:479:ALA:HB3	1.67	0.77
1:A:679:LYS:HD3	1:A:687:LEU:HD11	1.67	0.77
1:A:279:PHE:O	1:A:283:HIS:HB3	1.85	0.77
1:A:301:GLN:HB2	1:A:304:VAL:CG1	2.16	0.76
1:A:457:GLN:HG3	1:A:481:THR:HG23	1.66	0.76
1:A:250:TYR:HB3	1:A:259:VAL:HB	1.67	0.76
1:A:252:TYR:HD2	1:A:255:LYS:H	1.35	0.75
1:A:465:GLU:O	1:A:469:GLN:HG2	1.87	0.75
1:A:251:THR:HA	1:A:257:LYS:O	1.87	0.75
1:A:445:ILE:O	1:A:449:LEU:HG	1.87	0.74
1:A:642:TYR:HB2	1:A:657:LEU:HD13	1.68	0.74
1:A:514:GLU:HB3	1:A:585:VAL:HG11	1.70	0.74
1:A:100:MET:HG2	1:A:392:ILE:HB	1.69	0.73
1:A:699:LYS:HG3	1:A:703:PHE:HD1	1.52	0.73
1:A:749:LEU:HD13	1:A:753:GLN:NE2	2.00	0.73
1:A:425:ARG:HD2	1:A:430:GLN:HG2	1.72	0.72
1:A:252:TYR:HB2	1:A:257:LYS:H	1.55	0.72
1:A:368:ALA:CA	1:A:387:MET:HE3	2.19	0.72
1:A:523:ARG:HE	1:A:537:PHE:HE1	1.35	0.72
1:A:661:ILE:HG21	1:A:688:ILE:CD1	2.20	0.71
1:A:661:ILE:CG2	1:A:688:ILE:HD11	2.21	0.71
1:A:161:LYS:HE2	1:A:165:ARG:NH2	2.06	0.71
1:A:422:VAL:HG13	1:A:432:VAL:HG21	1.73	0.70
1:A:93:HIS:HD2	1:A:117:ASN:HD21	1.40	0.70
1:A:723:LYS:HG3	1:A:767:ILE:HG12	1.73	0.69
1:A:683:GLU:O	1:A:687:LEU:HG	1.93	0.69
1:A:283:HIS:HA	1:A:287:ASN:CB	2.22	0.69
1:A:738:ILE:HD11	1:A:751:GLU:HB2	1.73	0.69
1:A:161:LYS:HE2	1:A:165:ARG:HH22	1.59	0.68
1:A:684:MET:O	1:A:688:ILE:HG22	1.94	0.68
1:A:436:THR:HB	1:A:441:THR:HB	1.75	0.68
1:A:699:LYS:HG3	1:A:703:PHE:CD1	2.29	0.67
1:A:552:GLU:HA	1:A:555:MET:HE3	1.76	0.67
1:A:637:ARG:NH1	1:A:765:GLU:HA	2.09	0.67
1:A:217:ALA:HB1	1:A:358:GLN:NE2	2.09	0.67
1:A:632:LYS:HB2	1:A:689:MET:SD	2.34	0.66
1:A:623:LEU:HD12	1:A:626:ILE:HD12	1.77	0.66
1:A:610:ILE:HG13	1:A:724:TRP:CE3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:361:PHE:HB3	1:A:367:LEU:HD21	1.77	0.66
1:A:571:SER:CB	1:A:574:VAL:HG12	2.25	0.66
1:A:412:GLU:O	1:A:416:LYS:HB2	1.96	0.66
1:A:356:THR:HG23	1:A:359:ASN:HB2	1.78	0.65
1:A:444:LEU:O	1:A:448:LEU:HG	1.96	0.65
1:A:163:GLU:O	1:A:166:GLU:HG2	1.97	0.65
1:A:630:MET:HE3	1:A:771:VAL:HG11	1.78	0.65
1:A:252:TYR:HE2	1:A:642:TYR:CE1	2.14	0.65
2:A:902:MG:MG	5:A:1146:HOH:O	1.40	0.65
1:A:741:ARG:O	1:A:741:ARG:HD3	1.97	0.64
1:A:643:THR:HA	1:A:652:TRP:CD1	2.31	0.64
1:A:440:GLU:HA	1:A:443:GLU:OE2	1.98	0.64
1:A:411:MET:HG3	1:A:542:GLU:HG3	1.80	0.64
1:A:622:ASN:HA	1:A:709:ARG:HH21	1.63	0.63
1:A:283:HIS:HA	1:A:287:ASN:HB3	1.81	0.63
1:A:610:ILE:HG13	1:A:724:TRP:CZ3	2.33	0.63
1:A:190:VAL:HG13	1:A:195:GLN:HB2	1.79	0.63
1:A:695:LYS:HD3	1:A:776:MET:HE3	1.81	0.63
1:A:721:ASP:O	1:A:725:MET:HG2	1.98	0.63
1:A:450:LYS:HG3	1:A:456:HIS:HE1	1.60	0.63
1:A:70:ARG:HG2	1:A:80:PHE:CE1	2.34	0.63
1:A:643:THR:N	1:A:644:PRO:HD3	2.13	0.63
1:A:241:VAL:HG13	1:A:294:LEU:HD12	1.81	0.62
1:A:301:GLN:HB2	1:A:304:VAL:HG12	1.80	0.62
1:A:252:TYR:HE2	1:A:642:TYR:HE1	1.46	0.62
1:A:642:TYR:CD2	1:A:657:LEU:HB2	2.34	0.62
1:A:368:ALA:HA	1:A:387:MET:CE	2.25	0.62
1:A:698:GLU:HB3	1:A:702:GLN:NE2	2.14	0.62
1:A:335:GLN:HG3	1:A:345:ILE:HG23	1.82	0.62
1:A:620:SER:HB2	1:A:713:LYS:HE2	1.80	0.62
1:A:244:LEU:HD22	1:A:268:LYS:HD2	1.81	0.62
1:A:244:LEU:HD13	1:A:265:GLY:HA2	1.81	0.62
1:A:248:LYS:HA	1:A:262:THR:HG21	1.81	0.62
1:A:527:GLY:HA2	1:A:531:ASP:O	2.00	0.62
1:A:468:ALA:HA	1:A:471:ILE:HG22	1.81	0.62
1:A:280:ASP:HB2	1:A:779:GLU:O	2.01	0.61
1:A:108:LEU:HA	1:A:141:MET:CE	2.30	0.61
1:A:711:PHE:HE2	1:A:775:VAL:HA	1.64	0.61
1:A:160:SER:OG	1:A:163:GLU:HG3	2.00	0.61
1:A:192:TYR:CE2	1:A:786:ARG:HD2	2.35	0.61
1:A:603:LEU:O	1:A:607:ARG:HG3	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HG23	1:A:212:ILE:HD12	1.83	0.61
1:A:402:ASP:HA	1:A:535:THR:OG1	2.00	0.61
1:A:112:LEU:HB2	1:A:113:PRO:CD	2.31	0.60
1:A:689:MET:O	1:A:693:ILE:HG12	2.01	0.60
1:A:601:ASP:HA	1:A:604:ARG:HG2	1.82	0.60
1:A:86:LEU:O	1:A:90:VAL:HG23	2.02	0.60
1:A:431:PRO:HB2	1:A:505:LEU:HD12	1.83	0.60
1:A:21:LYS:O	1:A:24:ASN:HB2	2.01	0.59
1:A:658:VAL:O	1:A:662:ASN:HB2	2.02	0.59
1:A:208:GLU:HG2	1:A:489:ARG:HH21	1.66	0.59
1:A:761:GLU:O	1:A:765:GLU:HG3	2.02	0.59
1:A:517:ARG:O	1:A:521:GLN:HG3	2.03	0.59
1:A:653:LYS:O	1:A:653:LYS:HD2	2.03	0.59
1:A:204:ALA:HB3	1:A:367:LEU:HD12	1.84	0.59
1:A:436:THR:HG21	1:A:442:SER:HA	1.85	0.59
1:A:255:LYS:NZ	1:A:660:LEU:HD13	2.18	0.58
1:A:732:ASP:HA	1:A:735:ARG:HD2	1.84	0.58
1:A:469:GLN:O	1:A:472:GLU:HG2	2.03	0.58
1:A:747:ASN:O	1:A:750:ARG:HB3	2.04	0.58
1:A:70:ARG:HD2	1:A:86:LEU:HD21	1.86	0.58
1:A:473:GLU:O	1:A:476:GLN:HG2	2.04	0.58
1:A:335:GLN:HG3	1:A:345:ILE:CG2	2.34	0.58
1:A:794:THR:HG22	1:A:795:THR:N	2.17	0.57
1:A:624:ARG:HE	1:A:696:TYR:HE2	1.50	0.57
1:A:567:THR:CG2	1:A:568:PRO:HD3	2.26	0.57
1:A:424:GLN:HG2	1:A:425:ARG:N	2.19	0.57
1:A:654:LEU:H	1:A:654:LEU:CD1	2.16	0.57
1:A:718:ARG:NH2	1:A:787:GLU:HB2	2.13	0.57
1:A:642:TYR:CG	1:A:657:LEU:HB2	2.40	0.57
1:A:283:HIS:HA	1:A:287:ASN:HB2	1.86	0.57
1:A:204:ALA:HB2	1:A:364:TYR:CE2	2.40	0.57
1:A:363:MET:HE1	5:A:1115:HOH:O	2.05	0.56
1:A:252:TYR:HB3	1:A:256:THR:H	1.69	0.56
1:A:516:ARG:NH1	1:A:583:LYS:HG2	2.20	0.56
1:A:458:VAL:HG22	1:A:482:ILE:HB	1.86	0.56
1:A:723:LYS:HG3	1:A:767:ILE:CG1	2.34	0.56
1:A:231:THR:O	1:A:235:VAL:HG23	2.05	0.56
1:A:750:ARG:O	1:A:754:MET:HG3	2.06	0.56
1:A:165:ARG:HG2	1:A:197:VAL:HA	1.88	0.56
1:A:261:LEU:HD23	1:A:663:THR:HG23	1.86	0.56
1:A:308:VAL:HG13	1:A:343:LEU:HD11	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:ARG:HH21	1:A:787:GLU:CB	2.13	0.56
1:A:749:LEU:O	1:A:753:GLN:HG3	2.06	0.55
1:A:99:GLU:HG3	1:A:372:GLY:O	2.06	0.55
1:A:633:SER:O	1:A:637:ARG:HG3	2.05	0.55
1:A:222:ILE:HG22	1:A:223:ILE:N	2.22	0.55
1:A:630:MET:CE	1:A:771:VAL:HG11	2.36	0.55
1:A:210:ASP:O	1:A:214:ILE:HB	2.06	0.55
1:A:266:MET:SD	1:A:270:GLU:OE2	2.65	0.55
1:A:516:ARG:HH12	1:A:583:LYS:HA	1.71	0.55
1:A:129:VAL:HG23	1:A:130:ASN:N	2.22	0.55
1:A:332:GLY:HA2	1:A:335:GLN:NE2	2.21	0.54
1:A:265:GLY:O	1:A:269:ALA:HB2	2.07	0.54
1:A:185:LEU:HD22	1:A:353:ALA:HB1	1.89	0.54
1:A:648:LEU:CB	1:A:651:GLU:HB2	2.35	0.54
1:A:459:LEU:HD22	1:A:467:GLU:HG2	1.89	0.54
1:A:794:THR:CG2	1:A:795:THR:N	2.70	0.54
1:A:604:ARG:O	1:A:608:GLU:HG3	2.08	0.54
1:A:631:ILE:HG12	1:A:772:ALA:HA	1.87	0.54
1:A:450:LYS:HG3	1:A:456:HIS:CE1	2.42	0.54
1:A:326:GLY:O	1:A:734:LEU:HD12	2.07	0.54
1:A:450:LYS:HE3	1:A:456:HIS:CE1	2.43	0.54
1:A:332:GLY:HA2	1:A:335:GLN:HE21	1.72	0.54
1:A:658:VAL:CG1	1:A:672:GLU:HA	2.38	0.54
1:A:734:LEU:HD22	1:A:759:MET:CE	2.38	0.54
1:A:92:LEU:HD11	1:A:370:MET:HE3	1.89	0.54
1:A:284:VAL:HG11	1:A:718:ARG:HH11	1.72	0.54
1:A:571:SER:HB3	1:A:574:VAL:CG1	2.36	0.54
1:A:260:GLN:O	1:A:262:THR:N	2.42	0.53
1:A:457:GLN:HG2	1:A:480:VAL:O	2.08	0.53
1:A:724:TRP:HA	1:A:763:MET:HE1	1.91	0.53
1:A:72:ALA:O	1:A:76:VAL:HG23	2.08	0.53
1:A:660:LEU:HD23	1:A:660:LEU:C	2.29	0.53
1:A:248:LYS:O	1:A:264:GLU:HB3	2.09	0.53
1:A:124:VAL:HG22	1:A:203:PHE:HD2	1.73	0.53
1:A:252:TYR:HB3	1:A:256:THR:N	2.24	0.53
1:A:322:ARG:HG3	1:A:323:LEU:N	2.25	0.53
1:A:429:GLY:HA3	1:A:502:LEU:HD13	1.90	0.53
1:A:277:ASN:O	1:A:279:PHE:N	2.42	0.52
1:A:50:GLU:O	1:A:54:LYS:HG3	2.08	0.52
1:A:653:LYS:C	1:A:653:LYS:HD2	2.30	0.52
1:A:739:HIS:O	1:A:740:LEU:HD23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:755:GLU:O	1:A:759:MET:HG3	2.09	0.52
1:A:268:LYS:HA	1:A:271:LYS:CD	2.39	0.52
1:A:734:LEU:HD23	1:A:752:TYR:CD1	2.44	0.52
1:A:505:LEU:O	1:A:506:ALA:HB3	2.09	0.52
1:A:293:ALA:HA	1:A:336:ALA:HB1	1.92	0.52
1:A:489:ARG:HD2	1:A:525:ARG:NH2	2.25	0.52
1:A:238:ASN:OD1	1:A:340:LYS:HA	2.09	0.52
1:A:506:ALA:HA	1:A:534:ILE:O	2.10	0.52
1:A:462:LYS:O	1:A:463:ASN:C	2.48	0.52
1:A:314:VAL:HG12	1:A:315:ILE:N	2.25	0.52
1:A:218:ARG:O	1:A:596:LEU:HD22	2.10	0.52
1:A:312:GLN:HA	1:A:343:LEU:HD13	1.92	0.51
1:A:120:THR:HG21	3:A:1003:SO4:S	2.50	0.51
1:A:468:ALA:HA	1:A:471:ILE:CG2	2.40	0.51
1:A:540:SER:O	1:A:546:MET:HG3	2.10	0.51
1:A:93:HIS:O	1:A:366:LYS:HE3	2.10	0.51
1:A:408:TYR:HB3	3:A:1006:SO4:O3	2.10	0.51
1:A:162:ASP:HA	1:A:165:ARG:NH1	2.26	0.51
1:A:268:LYS:HA	1:A:271:LYS:HD2	1.93	0.51
1:A:270:GLU:HG2	1:A:276:ASP:O	2.11	0.51
1:A:26:ILE:HG13	1:A:63:VAL:HG13	1.91	0.51
1:A:271:LYS:C	1:A:273:PHE:H	2.13	0.51
1:A:300:MET:HG3	1:A:337:ILE:HD11	1.91	0.51
1:A:106:LYS:HB3	1:A:370:MET:SD	2.51	0.51
1:A:563:MET:HA	1:A:563:MET:CE	2.37	0.51
1:A:622:ASN:HA	1:A:709:ARG:NH2	2.26	0.51
1:A:617:VAL:O	1:A:620:SER:HB3	2.11	0.51
1:A:471:ILE:HG12	1:A:493:ILE:HD11	1.91	0.51
1:A:572:LYS:HD3	1:A:576:ARG:HH21	1.76	0.50
1:A:302:LYS:HA	1:A:306:TYR:CZ	2.46	0.50
1:A:356:THR:HG23	1:A:359:ASN:H	1.76	0.50
1:A:706:GLU:HA	1:A:709:ARG:HG2	1.93	0.50
1:A:657:LEU:O	1:A:661:ILE:HD12	2.12	0.50
1:A:681:PRO:HA	1:A:684:MET:HE2	1.91	0.50
1:A:222:ILE:CG2	1:A:351:THR:HG23	2.33	0.50
1:A:649:PRO:C	1:A:651:GLU:H	2.15	0.50
1:A:358:GLN:HG2	1:A:385:TYR:OH	2.11	0.50
1:A:581:SER:O	1:A:585:VAL:HG23	2.12	0.50
1:A:458:VAL:CG2	1:A:482:ILE:HD12	2.42	0.50
1:A:600:ASP:O	1:A:603:LEU:HB2	2.11	0.50
1:A:680:GLU:O	1:A:684:MET:HG3	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:LEU:HD13	1:A:385:TYR:CE1	2.47	0.50
1:A:463:ASN:HB3	1:A:466:ARG:HD2	1.94	0.50
1:A:724:TRP:CZ2	1:A:728:ILE:HD11	2.46	0.49
1:A:112:LEU:HB2	1:A:113:PRO:HD3	1.92	0.49
1:A:684:MET:HA	1:A:687:LEU:HD12	1.94	0.49
1:A:237:ALA:O	1:A:241:VAL:HG23	2.13	0.49
1:A:275:ILE:O	1:A:278:LEU:HG	2.13	0.49
1:A:108:LEU:CA	1:A:141:MET:HE1	2.38	0.49
1:A:471:ILE:HD12	1:A:488:GLY:HA3	1.95	0.49
1:A:219:THR:HB	1:A:220:PRO:HD2	1.93	0.49
1:A:431:PRO:O	1:A:505:LEU:O	2.31	0.49
1:A:743:TYR:O	1:A:745:GLN:N	2.45	0.49
1:A:723:LYS:CG	1:A:767:ILE:HG12	2.43	0.49
1:A:183:ASP:O	1:A:187:ASP:HB2	2.11	0.49
1:A:588:ASN:O	1:A:591:ASP:HB2	2.12	0.49
1:A:758:ALA:O	1:A:761:GLU:HB2	2.13	0.49
1:A:594:LYS:O	1:A:598:GLN:HG3	2.12	0.49
1:A:637:ARG:HH12	1:A:765:GLU:CA	2.16	0.49
1:A:711:PHE:CE2	1:A:775:VAL:HA	2.47	0.49
1:A:223:ILE:HG23	1:A:794:THR:CG2	2.43	0.48
1:A:360:TYR:O	1:A:363:MET:HB2	2.13	0.48
1:A:498:GLY:HA2	1:A:500:LYS:NZ	2.28	0.48
1:A:500:LYS:HD3	1:A:500:LYS:H	1.78	0.48
1:A:255:LYS:HZ2	1:A:660:LEU:HD13	1.76	0.48
1:A:744:ALA:O	1:A:745:GLN:HG2	2.13	0.48
1:A:214:ILE:HG22	1:A:215:ASP:N	2.27	0.48
1:A:658:VAL:HG11	1:A:672:GLU:HA	1.94	0.48
1:A:750:ARG:NH1	5:A:1104:HOH:O	2.46	0.48
1:A:554:THR:O	1:A:558:LEU:HG	2.13	0.48
1:A:57:THR:HB	5:A:1106:HOH:O	2.12	0.48
1:A:165:ARG:CG	1:A:197:VAL:HA	2.42	0.48
1:A:130:ASN:C	1:A:130:ASN:OD1	2.52	0.48
1:A:206:ILE:CG2	1:A:212:ILE:HD12	2.42	0.48
1:A:99:GLU:CG	1:A:391:THR:HG22	2.44	0.48
1:A:516:ARG:NH1	1:A:583:LYS:HA	2.28	0.48
1:A:155:ASN:OD1	1:A:164:LYS:HE2	2.14	0.48
1:A:477:LYS:HE3	1:A:497:GLU:O	2.14	0.48
1:A:159:MET:HB3	1:A:163:GLU:HB2	1.96	0.47
1:A:661:ILE:HB	1:A:671:LEU:HD23	1.95	0.47
1:A:266:MET:O	1:A:269:ALA:HB3	2.14	0.47
1:A:9:PHE:CD1	1:A:9:PHE:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ASN:HB3	1:A:175:SER:HB2	1.95	0.47
1:A:248:LYS:O	1:A:262:THR:HB	2.15	0.47
1:A:734:LEU:HD22	1:A:759:MET:HE3	1.96	0.47
1:A:703:PHE:HB3	1:A:780:ILE:HD12	1.95	0.47
1:A:160:SER:O	1:A:164:LYS:HG3	2.15	0.47
1:A:355:ILE:HA	1:A:607:ARG:HH12	1.80	0.47
1:A:563:MET:C	1:A:565:ASP:H	2.18	0.47
1:A:558:LEU:HB3	1:A:563:MET:HB2	1.97	0.47
1:A:96:ASN:HB3	1:A:388:GLN:O	2.15	0.47
1:A:93:HIS:CD2	1:A:117:ASN:HD21	2.26	0.47
1:A:727:HIS:HB2	1:A:763:MET:HE3	1.97	0.47
1:A:440:GLU:O	1:A:443:GLU:HG2	2.15	0.47
1:A:264:GLU:O	1:A:268:LYS:HG3	2.14	0.47
1:A:224:SER:HA	1:A:350:MET:O	2.15	0.47
1:A:182:PHE:CZ	1:A:221:LEU:HD22	2.49	0.47
1:A:89:GLY:O	1:A:92:LEU:HB2	2.15	0.47
1:A:436:THR:HG21	1:A:442:SER:CA	2.44	0.47
1:A:563:MET:HA	1:A:563:MET:HE3	1.97	0.47
1:A:295:LYS:HG2	1:A:299:ALA:HB3	1.97	0.47
1:A:712:GLU:O	1:A:716:VAL:HG23	2.15	0.47
1:A:184:TYR:O	1:A:188:ASN:ND2	2.48	0.46
1:A:120:THR:HG21	3:A:1003:SO4:O3	2.16	0.46
1:A:128:THR:O	1:A:176:THR:HA	2.16	0.46
1:A:241:VAL:O	1:A:243:THR:N	2.49	0.46
1:A:643:THR:N	1:A:644:PRO:CD	2.78	0.46
1:A:467:GLU:O	1:A:471:ILE:HG22	2.16	0.46
1:A:97:ILE:HA	1:A:369:GLY:O	2.16	0.46
1:A:99:GLU:CD	1:A:391:THR:HG22	2.36	0.46
1:A:252:TYR:HD2	1:A:255:LYS:N	2.08	0.46
1:A:458:VAL:HG22	1:A:482:ILE:HD12	1.98	0.45
1:A:449:LEU:HD12	1:A:482:ILE:HD11	1.97	0.45
1:A:709:ARG:HA	1:A:709:ARG:HD2	1.71	0.45
1:A:719:ALA:O	1:A:723:LYS:HG2	2.16	0.45
1:A:267:THR:HA	1:A:270:GLU:OE1	2.15	0.45
1:A:323:LEU:HA	1:A:323:LEU:HD23	1.74	0.45
1:A:460:ASN:OD1	1:A:460:ASN:N	2.49	0.45
1:A:64:GLU:O	1:A:68:VAL:HG23	2.16	0.45
1:A:680:GLU:HB3	1:A:681:PRO:HD2	1.99	0.45
1:A:275:ILE:O	1:A:275:ILE:HG22	2.16	0.45
1:A:403:ARG:HA	1:A:404:PRO:HD3	1.78	0.45
1:A:19:TYR:CE1	1:A:91:ALA:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:32:ASP:HB2	1:A:33:TYR:CE1	2.52	0.45
1:A:262:THR:O	1:A:266:MET:HB2	2.16	0.45
1:A:471:ILE:HG12	1:A:493:ILE:CD1	2.47	0.45
1:A:252:TYR:CE2	1:A:642:TYR:CE1	3.01	0.44
1:A:52:LEU:HG	1:A:61:LEU:HD11	1.98	0.44
1:A:147:PHE:C	1:A:149:GLY:H	2.20	0.44
1:A:223:ILE:O	1:A:352:LEU:N	2.48	0.44
1:A:618:ILE:C	1:A:620:SER:H	2.20	0.44
1:A:129:VAL:HG23	1:A:130:ASN:H	1.82	0.44
1:A:85:GLN:O	1:A:109:THR:HG23	2.17	0.44
1:A:624:ARG:NE	1:A:696:TYR:CE2	2.86	0.44
1:A:148:LEU:HD23	1:A:148:LEU:HA	1.73	0.44
1:A:308:VAL:O	1:A:309:GLU:HG2	2.18	0.44
1:A:627:VAL:O	1:A:631:ILE:HG13	2.18	0.44
1:A:716:VAL:O	1:A:720:VAL:HG23	2.16	0.44
1:A:203:PHE:CE1	1:A:366:LYS:HE2	2.53	0.44
1:A:356:THR:CG2	1:A:359:ASN:HB2	2.46	0.44
1:A:325:LYS:HB2	1:A:325:LYS:HE2	1.40	0.44
1:A:649:PRO:O	1:A:652:TRP:CE3	2.71	0.44
1:A:192:TYR:CD2	1:A:786:ARG:HD2	2.53	0.44
1:A:734:LEU:HD22	1:A:759:MET:HE1	2.00	0.44
1:A:215:ASP:C	1:A:217:ALA:H	2.19	0.44
1:A:654:LEU:N	1:A:654:LEU:HD12	2.22	0.44
1:A:418:VAL:O	1:A:422:VAL:HG23	2.17	0.44
1:A:543:ASP:HB2	1:A:546:MET:HG2	2.00	0.44
1:A:4:ILE:O	1:A:6:ASN:N	2.50	0.44
1:A:647:GLU:HG3	1:A:647:GLU:O	2.18	0.43
1:A:414:LYS:CE	1:A:510:THR:O	2.62	0.43
1:A:406:LEU:HG	1:A:536:GLN:NE2	2.33	0.43
1:A:407:ILE:HG12	1:A:569:ILE:O	2.18	0.43
1:A:454:ILE:HA	1:A:455:PRO:HD3	1.87	0.43
1:A:468:ALA:CA	1:A:471:ILE:HG22	2.46	0.43
1:A:644:PRO:O	1:A:646:GLU:N	2.52	0.43
1:A:70:ARG:HG3	1:A:81:PRO:HB2	2.00	0.43
1:A:300:MET:O	1:A:340:LYS:NZ	2.52	0.43
1:A:672:GLU:O	1:A:675:ASP:HB2	2.19	0.43
1:A:130:ASN:OD1	1:A:132:TYR:N	2.52	0.43
1:A:498:GLY:HA2	1:A:500:LYS:HZ1	1.83	0.43
1:A:250:TYR:HE2	1:A:252:TYR:HE1	1.67	0.43
1:A:213:LEU:HD13	1:A:385:TYR:CZ	2.53	0.43
1:A:268:LYS:O	1:A:271:LYS:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:296:ALA:O	1:A:300:MET:HB2	2.18	0.43
1:A:727:HIS:O	1:A:731:MET:HG2	2.19	0.43
1:A:723:LYS:HB3	1:A:763:MET:HE2	2.00	0.43
1:A:162:ASP:HA	1:A:165:ARG:HH11	1.84	0.43
1:A:109:THR:O	1:A:113:PRO:HD2	2.19	0.43
1:A:426:TYR:CG	1:A:454:ILE:HG23	2.54	0.43
1:A:277:ASN:OD1	1:A:277:ASN:N	2.52	0.42
1:A:166:GLU:HG3	1:A:167:ALA:N	2.34	0.42
1:A:738:ILE:HD11	1:A:751:GLU:CB	2.44	0.42
1:A:631:ILE:HG12	1:A:772:ALA:CB	2.49	0.42
1:A:440:GLU:CD	1:A:440:GLU:H	2.22	0.42
1:A:74:ARG:O	1:A:78:GLY:HA2	2.19	0.42
1:A:136:ARG:HH11	1:A:140:GLN:HE22	1.66	0.42
1:A:267:THR:O	1:A:271:LYS:HG3	2.19	0.42
1:A:309:GLU:HB2	1:A:312:GLN:O	2.18	0.42
1:A:137:ASP:HB3	1:A:174:TYR:HE2	1.83	0.42
1:A:164:LYS:NZ	1:A:179:GLU:OE1	2.53	0.42
1:A:72:ALA:HB2	1:A:148:LEU:HD11	2.01	0.42
1:A:505:LEU:O	1:A:506:ALA:CB	2.68	0.42
1:A:433:LEU:HD13	1:A:481:THR:HB	2.02	0.42
1:A:469:GLN:HE21	1:A:469:GLN:HA	1.84	0.42
1:A:354:THR:CG2	1:A:355:ILE:N	2.83	0.42
1:A:214:ILE:CG2	1:A:517:ARG:HH12	2.20	0.42
1:A:264:GLU:HG2	1:A:265:GLY:N	2.35	0.42
1:A:519:ASP:O	1:A:522:LEU:HB3	2.20	0.42
1:A:734:LEU:HD23	1:A:752:TYR:CE1	2.54	0.42
1:A:45:THR:O	1:A:48:PHE:HB2	2.19	0.42
1:A:81:PRO:HA	1:A:85:GLN:OE1	2.20	0.42
1:A:467:GLU:HA	1:A:470:ILE:HD12	2.02	0.42
1:A:47:GLU:O	1:A:51:ARG:HB2	2.20	0.42
1:A:210:ASP:OD1	1:A:211:SER:N	2.53	0.41
1:A:692:ILE:HG23	1:A:776:MET:CE	2.49	0.41
1:A:489:ARG:HD2	1:A:525:ARG:HH21	1.85	0.41
1:A:708:MET:O	1:A:712:GLU:HG3	2.19	0.41
1:A:209:VAL:O	1:A:213:LEU:N	2.51	0.41
1:A:79:MET:HB3	4:A:901:ADP:C6	2.55	0.41
1:A:434:VAL:HA	1:A:508:VAL:O	2.20	0.41
1:A:425:ARG:HA	1:A:428:THR:HG22	2.02	0.41
1:A:354:THR:HG22	1:A:355:ILE:N	2.34	0.41
1:A:507:VAL:HG12	1:A:535:THR:HG22	2.02	0.41
1:A:331:GLU:HA	1:A:726:ASP:OD2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD23	1:A:61:LEU:N	2.36	0.41
1:A:161:LYS:CE	1:A:165:ARG:HH22	2.29	0.41
1:A:66:PHE:CE2	1:A:112:LEU:HB3	2.56	0.41
1:A:274:GLY:O	1:A:275:ILE:C	2.58	0.41
1:A:164:LYS:HB2	1:A:197:VAL:HG11	2.02	0.41
1:A:727:HIS:NE2	1:A:731:MET:HG3	2.36	0.41
1:A:271:LYS:C	1:A:273:PHE:N	2.74	0.41
1:A:261:LEU:HD22	1:A:777:LYS:NZ	2.36	0.41
1:A:43:HIS:O	1:A:47:GLU:HG3	2.20	0.41
1:A:394:THR:CG2	1:A:396:ARG:O	2.69	0.41
1:A:414:LYS:O	1:A:418:VAL:HG23	2.21	0.41
1:A:315:ILE:HG22	1:A:316:VAL:N	2.35	0.41
1:A:400:ARG:CD	1:A:526:SER:HB2	2.51	0.41
1:A:100:MET:HG2	1:A:392:ILE:CB	2.45	0.40
1:A:161:LYS:HG3	1:A:165:ARG:HH22	1.85	0.40
1:A:242:ARG:HH11	1:A:245:LYS:HB2	1.86	0.40
1:A:207:ASP:HA	1:A:370:MET:HG3	2.04	0.40
1:A:322:ARG:CG	1:A:323:LEU:N	2.84	0.40
1:A:27:ASP:O	1:A:30:ARG:HG2	2.21	0.40
1:A:749:LEU:O	1:A:752:TYR:HB3	2.20	0.40
1:A:512:ARG:HH21	1:A:523:ARG:NH2	2.19	0.40
1:A:79:MET:O	1:A:81:PRO:HD3	2.22	0.40
1:A:563:MET:C	1:A:565:ASP:N	2.74	0.40
1:A:642:TYR:CB	1:A:657:LEU:HD13	2.46	0.40
1:A:644:PRO:O	1:A:645:ARG:C	2.59	0.40
1:A:175:SER:OG	1:A:180:LEU:HG	2.21	0.40
1:A:444:LEU:HD12	1:A:444:LEU:O	2.21	0.40
1:A:48:PHE:CZ	1:A:68:VAL:HG21	2.56	0.40
1:A:575:SER:HA	1:A:578:VAL:HG22	2.04	0.40
1:A:282:LYS:O	1:A:286:LEU:N	2.54	0.40
1:A:9:PHE:N	1:A:9:PHE:HD1	2.18	0.40

There are no symmetry-related clashes.

## 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	800/802 (100%)	654 (82%)	102 (13%)	44 (6%)	2	13

All (44) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	LEU
1	A	278	LEU
1	A	325	LYS
1	A	528	ARG
1	A	567	THR
1	A	645	ARG
1	A	647	GLU
1	A	649	PRO
1	A	4	ILE
1	A	5	LEU
1	A	228	ALA
1	A	231	THR
1	A	241	VAL
1	A	245	LYS
1	A	312	GLN
1	A	428	THR
1	A	461	ALA
1	A	464	HIS
1	A	644	PRO
1	A	646	GLU
1	A	653	LYS
1	A	669	GLY
1	A	670	ALA
1	A	744	ALA
1	A	244	LEU
1	A	463	ASN
1	A	514	GLU
1	A	620	SER
1	A	650	GLU
1	A	673	LYS
1	A	801	GLU
1	A	276	ASP
1	A	302	LYS
1	A	506	ALA
1	A	652	TRP

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Mol	Chain	Res	Type
1	A	474	ALA
1	A	547	ARG
1	A	648	LEU
1	A	654	LEU
1	A	331	GLU
1	A	719	ALA
1	A	298	VAL
1	A	275	ILE
1	A	81	PRO

### 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	689/689 (100%)	623 (90%)	66 (10%)	10	38

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	PHE
1	A	37	SER
1	A	58	THR
1	A	81	PRO
1	A	84	VAL
1	A	102	THR
1	A	127	VAL
1	A	128	THR
1	A	133	LEU
1	A	151	THR
1	A	158	SER
1	A	165	ARG
1	A	175	SER
1	A	187	ASP
1	A	209	VAL
1	A	211	SER
1	A	224	SER

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Mol	Chain	Res	Type
1	A	249	ASP
1	A	252	TYR
1	A	262	THR
1	A	264	GLU
1	A	266	MET
1	A	277	ASN
1	A	280	ASP
1	A	318	SER
1	A	325	LYS
1	A	356	THR
1	A	363	MET
1	A	377	GLU
1	A	388	GLN
1	A	398	VAL
1	A	405	ASP
1	A	407	ILE
1	A	424	GLN
1	A	439	VAL
1	A	441	THR
1	A	457	GLN
1	A	462	LYS
1	A	465	GLU
1	A	469	GLN
1	A	481	THR
1	A	500	LYS
1	A	517	ARG
1	A	523	ARG
1	A	529	GLN
1	A	558	LEU
1	A	564	ASP
1	A	566	SER
1	A	579	GLU
1	A	614	ARG
1	A	650	GLU
1	A	652	TRP
1	A	653	LYS
1	A	654	LEU
1	A	674	SER
1	A	706	GLU
1	A	708	MET
1	A	717	LEU
1	A	741	ARG

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Mol	Chain	Res	Type
1	A	743	TYR
1	A	747	ASN
1	A	749	LEU
1	A	761	GLU
1	A	763	MET
1	A	770	GLU
1	A	787	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	HIS
1	A	140	GLN
1	A	291	ASN
1	A	335	GLN
1	A	358	GLN
1	A	424	GLN
1	A	469	GLN
1	A	753	GLN
1	A	798	GLN

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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	SO4	A	1003	-	4,4,4	0.82	0	6,6,6	0.17	0
3	SO4	A	1004	-	4,4,4	0.77	0	6,6,6	0.23	0
3	SO4	A	1005	-	4,4,4	0.81	0	6,6,6	0.19	0
3	SO4	A	1006	-	4,4,4	1.07	0	6,6,6	0.15	0
3	SO4	A	1007	-	4,4,4	0.94	0	6,6,6	0.12	0
4	ADP	A	901	2	22,29,29	1.33	3 (13%)	27,45,45	2.59	3 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1004	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1005	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1006	-	-	0/0/0/0	0/0/0/0
3	SO4	A	1007	-	-	0/0/0/0	0/0/0/0
4	ADP	A	901	2	-	0/12/32/32	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	901	ADP	PA-O2A	-2.04	1.46	1.54
4	A	901	ADP	PB-O2B	2.46	1.63	1.54
4	A	901	ADP	O4'-C1'	3.56	1.45	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	901	ADP	N3-C2-N1	-11.83	119.83	128.89
4	A	901	ADP	C4-C5-N7	-4.42	105.41	109.48
4	A	901	ADP	C2'-C3'-C4'	2.71	108.19	102.61

There are no chirality outliers.

There are no torsion outliers.



There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	SO4	2	0
3	A	1006	SO4	1	0
4	A	901	ADP	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [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	802/802 (100%)	-0.26	16 (1%) 68 39	41, 103, 170, 208	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	703	PHE	3.3
1	A	701	GLU	3.2
1	A	497	GLU	3.1
1	A	345	ILE	2.6
1	A	702	GLN	2.6
1	A	273	PHE	2.6
1	A	229	LYS	2.6
1	A	312	GLN	2.5
1	A	271	LYS	2.4
1	A	328	ARG	2.4
1	A	283	HIS	2.4
1	A	336	ALA	2.3
1	A	622	ASN	2.2
1	A	676	ILE	2.2
1	A	260	GLN	2.1
1	A	671	LEU	2.1

### 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 carbohydrates in this entry.

## 6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	SO4	A	1003	5/5	0.83	0.19	4.46	162,167,173,175	0
3	SO4	A	1007	5/5	0.79	0.27	1.88	151,152,160,167	0
3	SO4	A	1005	5/5	0.73	0.29	1.26	158,175,177,178	0
4	ADP	A	901	27/27	0.94	0.19	0.04	73,95,108,114	0
3	SO4	A	1006	5/5	0.96	0.17	-0.50	86,113,124,125	0
3	SO4	A	1004	5/5	0.96	0.09	-2.05	92,99,117,122	0
2	MG	A	902	1/1	0.94	0.13	-	86,86,86,86	0

## 6.5 Other polymers

There are no such residues in this entry.