



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2017 – 02:11 PM EDT

PDB ID : 3O98  
Title : Glutathionylspermidine synthetase/amidase C59A complex with ADP and Gsp  
Authors : Pai, C.H.; Lin, C.H.; Wang, A.H.-J.  
Deposited on : unknown  
Resolution : 2.80 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
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) : rb-20030345

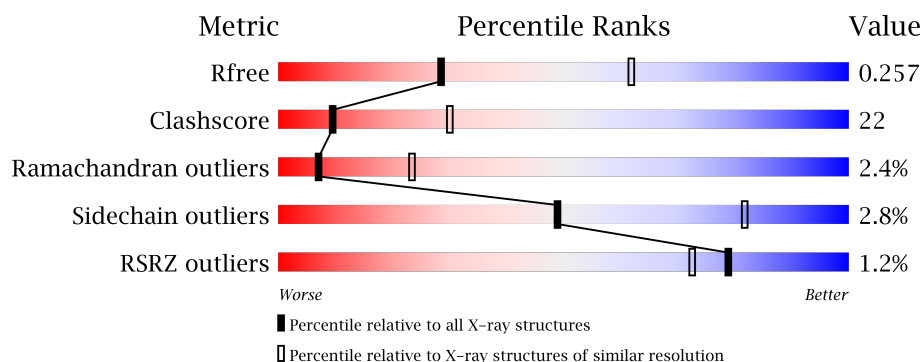
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*



The reported resolution of this entry is 2.80 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))
$R_{free}$	100719	2583 (2.80-2.80)
Clashscore	112137	3033 (2.80-2.80)
Ramachandran outliers	110173	2983 (2.80-2.80)
Sidechain outliers	110143	2985 (2.80-2.80)
RSRZ outliers	101464	2610 (2.80-2.80)

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	619	
1	B	619	

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
2	TS5	A	620	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9968 atoms, of which 3 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.

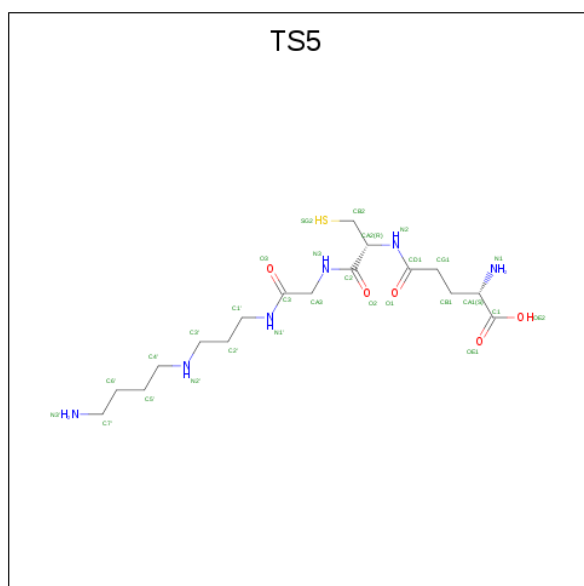
- Molecule 1 is a protein called Bifunctional glutathionylspermidine synthetase/amidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	599	Total	C	H	N	O	S	0	0	0
			4823	3087	2	826	890	18			
1	B	603	Total	C	H	N	O	S	0	0	0
			4852	3104	1	830	899	18			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	59	ALA	CYS	ENGINEERED MUTATION	UNP P0AES0
B	59	ALA	CYS	ENGINEERED MUTATION	UNP P0AES0

- Molecule 2 is GLUTATHIONYLSPERMIDINE (three-letter code: TS5) (formula: C<sub>17</sub>H<sub>34</sub>N<sub>6</sub>O<sub>5</sub>S).



- 

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

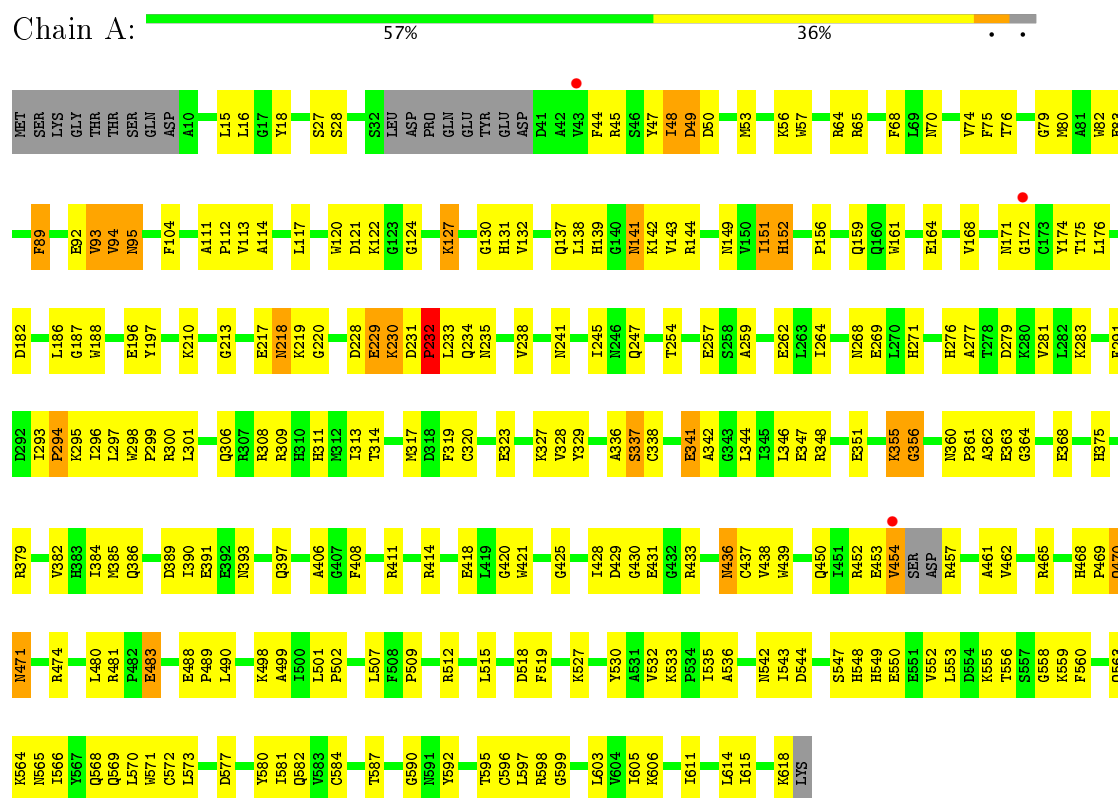
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	113	Total O 113 113	0	0
5	B	93	Total O 93 93	0	0

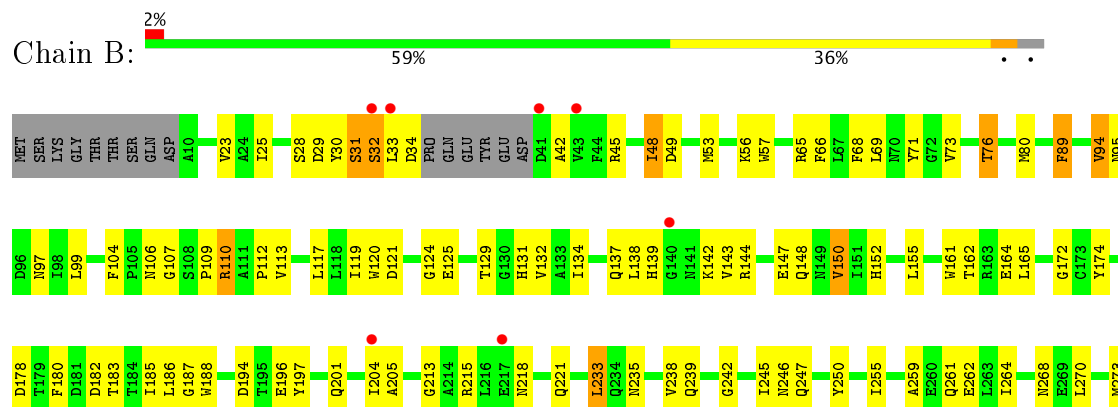
### 3 Residue-property plots

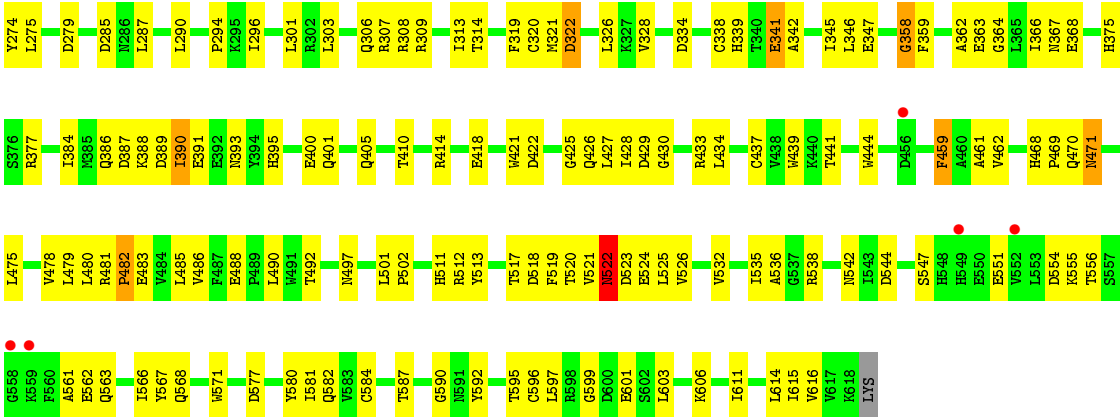
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Bifunctional glutathionylspermidine synthetase/amidase



- Molecule 1: Bifunctional glutathionylspermidine synthetase/amidase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.38Å 76.20Å 84.22Å 70.81° 74.37° 78.64°	Depositor
Resolution (Å)	30.00 – 2.80 29.57 – 2.82	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-2.80) 83.0 (29.57-2.82)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.54 (at 2.80Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.220 , 0.262 0.211 , 0.257	Depositor DCC
$R_{free}$ test set	1463 reflections (4.94%)	DCC
Wilson B-factor (Å <sup>2</sup> )	49.5	Xtriage
Anisotropy	0.580	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 48.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9968	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.47% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, TS5, 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	0.47	1/4944 (0.0%)	0.60	2/6713 (0.0%)
1	B	0.44	0/4975	0.58	1/6757 (0.0%)
All	All	0.46	1/9919 (0.0%)	0.59	3/13470 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	454	VAL	C-O	10.34	1.43	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	453	GLU	O-C-N	-6.34	112.55	122.70
1	B	48	ILE	N-CA-C	-5.32	96.65	111.00
1	A	48	ILE	N-CA-C	-5.15	97.11	111.00

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	4821	2	4697	232	0
1	B	4851	1	4722	189	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	29	0	31	5	0
3	A	27	0	12	2	0
3	B	27	0	12	1	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	113	0	0	1	0
5	B	93	0	0	3	0
All	All	9965	3	9474	417	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 (417) 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:536:ALA:H	1:A:563:GLN:NE2	1.55	1.02
1:A:355:LYS:HD2	1:A:356:GLY:N	1.75	1.02
1:B:342:ALA:HA	1:B:346:LEU:HD12	1.46	0.97
1:A:89:PHE:HE1	1:A:269:GLU:HG3	1.32	0.94
1:A:355:LYS:HD2	1:A:356:GLY:H	1.29	0.91
1:A:341:GLU:HG2	1:A:611:ILE:HG21	1.54	0.89
1:A:421:TRP:H	1:A:471:ASN:HD21	1.20	0.88
1:A:536:ALA:H	1:A:563:GLN:HE22	1.20	0.88
1:A:149:ASN:O	2:A:620:TS5:H2'2	1.77	0.84
1:A:28:SER:HB3	1:A:57:TRP:HB2	1.62	0.81
1:A:28:SER:OG	1:A:149:ASN:OD1	1.97	0.81
1:B:110:ARG:HA	1:B:110:ARG:HH11	1.45	0.81
1:B:268:ASN:HD21	1:B:592:TYR:H	1.29	0.80
1:A:536:ALA:N	1:A:563:GLN:HE22	1.79	0.80
1:A:296:ILE:HD11	1:A:461:ALA:HA	1.64	0.79
1:B:389:ASP:HB3	1:B:391:GLU:HG2	1.67	0.77
1:B:462:VAL:HG11	1:B:480:LEU:HD13	1.65	0.77
1:A:436:ASN:H	1:A:436:ASN:HD22	1.30	0.76
1:A:138:LEU:HD12	1:A:143:VAL:HG12	1.68	0.74
1:A:151:ILE:HD13	1:A:151:ILE:H	1.52	0.73
1:A:89:PHE:CE1	1:A:269:GLU:HG3	2.22	0.73
1:B:121:ASP:HB2	1:B:186:LEU:HD21	1.70	0.72
1:A:363:GLU:HG3	1:A:364:GLY:H	1.54	0.72
1:B:590:GLY:N	5:B:8220:HOH:O	2.16	0.72
1:B:213:GLY:HA3	1:B:577:ASP:OD2	1.89	0.72
1:A:245:ILE:HB	1:A:611:ILE:HD11	1.70	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:ILE:O	1:A:611:ILE:HD12	1.90	0.71
1:A:122:LYS:HB2	1:A:127:LYS:O	1.90	0.71
1:A:598:ARG:HH11	1:A:598:ARG:HG3	1.57	0.69
1:A:498:LYS:HB2	1:A:535:ILE:HA	1.74	0.69
1:A:64:ARG:NH1	2:A:620:TS5:OE2	2.20	0.69
1:A:347:GLU:OE1	1:A:363:GLU:HB3	1.92	0.68
1:A:137:GLN:HE21	1:A:139:HIS:HE1	1.40	0.68
1:A:141:ASN:ND2	1:A:142:LYS:HG2	2.09	0.68
1:A:390:ILE:HD12	1:A:391:GLU:HG3	1.76	0.68
1:A:48:ILE:O	1:A:49:ASP:HB2	1.94	0.67
1:B:131:HIS:HE1	1:B:147:GLU:OE1	1.76	0.67
1:A:229:GLU:O	1:A:235:ASN:HB2	1.95	0.66
1:B:245:ILE:HG13	1:B:246:ASN:N	2.10	0.66
1:B:31:SER:C	1:B:33:LEU:H	1.98	0.66
1:B:421:TRP:H	1:B:471:ASN:HD21	1.44	0.66
1:A:342:ALA:HA	1:A:346:LEU:HD12	1.78	0.66
1:B:542:ASN:ND2	1:B:561:ALA:HB2	2.11	0.66
1:B:338:CYS:HA	1:B:341:GLU:OE1	1.97	0.65
1:B:110:ARG:HA	1:B:110:ARG:NH1	2.12	0.65
1:A:483:GLU:CD	1:A:483:GLU:H	2.00	0.64
1:B:522:ASN:HD22	1:B:523:ASP:N	1.95	0.64
1:B:522:ASN:O	1:B:526:VAL:HG23	1.96	0.64
1:B:367:ASN:ND2	1:B:405:GLN:HE22	1.96	0.64
1:A:137:GLN:NE2	1:A:144:ARG:HD2	2.13	0.63
1:B:544:ASP:OD1	1:B:555:LYS:HG3	1.98	0.63
1:B:121:ASP:HB2	1:B:186:LEU:CD2	2.28	0.63
1:A:501:LEU:HB2	1:A:502:PRO:HD3	1.80	0.63
1:B:109:PRO:HA	1:B:172:GLY:O	1.98	0.63
1:B:427:LEU:HD21	1:B:478:VAL:HG22	1.80	0.63
1:A:465:ARG:HD3	1:A:474:ARG:NH2	2.14	0.62
1:B:296:ILE:HD11	1:B:461:ALA:HA	1.81	0.62
1:A:436:ASN:N	1:A:436:ASN:HD22	1.95	0.62
1:A:64:ARG:HG3	1:A:74:VAL:HG23	1.80	0.62
1:A:393:ASN:O	1:A:397:GLN:HG3	1.99	0.62
1:A:536:ALA:HB3	1:A:563:GLN:HE22	1.64	0.62
1:A:268:ASN:HD21	1:A:592:TYR:H	1.47	0.62
1:A:121:ASP:HB2	1:A:186:LEU:HD21	1.80	0.62
1:B:31:SER:HB3	1:B:34:ASP:OD2	2.00	0.62
2:A:620:TS5:O3	2:A:620:TS5:H2'1	2.00	0.62
1:A:542:ASN:OD1	1:A:558:GLY:HA3	2.00	0.62
1:B:131:HIS:CD2	1:B:132:VAL:H	2.18	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:ASP:HB2	1:B:152:HIS:CD2	2.35	0.61
1:A:210:LYS:HD3	1:A:323:GLU:HB3	1.82	0.61
1:A:230:LYS:HB3	1:A:230:LYS:NZ	2.15	0.61
1:A:462:VAL:HG11	1:A:480:LEU:HD13	1.84	0.60
1:A:89:PHE:C	1:A:89:PHE:HD2	2.05	0.60
1:A:196:GLU:HG2	1:A:197:TYR:CD2	2.37	0.60
1:A:64:ARG:CG	1:A:74:VAL:HG23	2.31	0.60
1:A:141:ASN:HD22	1:A:141:ASN:H	1.50	0.60
1:A:213:GLY:HA3	1:A:577:ASP:OD2	2.02	0.59
1:A:418:GLU:HG2	1:A:430:GLY:H	1.67	0.59
1:A:536:ALA:CA	1:A:563:GLN:HE22	2.14	0.59
1:A:68:PHE:CE1	1:A:93:VAL:HG21	2.37	0.59
1:B:501:LEU:HB2	1:B:502:PRO:HD3	1.84	0.59
1:A:499:ALA:O	1:A:502:PRO:HD2	2.02	0.59
1:A:89:PHE:CD2	1:A:89:PHE:C	2.75	0.59
1:B:328:VAL:HG12	1:B:513:TYR:O	2.02	0.59
1:A:92:GLU:HB3	1:A:95:ASN:HD21	1.66	0.59
1:A:151:ILE:H	1:A:151:ILE:CD1	2.16	0.58
1:A:168:VAL:CG2	1:A:175:THR:HB	2.32	0.58
1:A:390:ILE:HD12	1:A:391:GLU:N	2.17	0.58
1:B:536:ALA:H	1:B:563:GLN:NE2	2.01	0.58
1:B:536:ALA:H	1:B:563:GLN:HE22	1.50	0.58
1:A:113:VAL:HG22	1:A:114:ALA:N	2.18	0.58
1:A:411:ARG:HH11	1:A:411:ARG:HG3	1.68	0.58
1:A:598:ARG:NH1	1:A:598:ARG:HG3	2.17	0.58
1:B:95:ASN:OD1	1:B:97:ASN:HB3	2.03	0.58
1:A:457:ARG:HG2	1:A:457:ARG:HH11	1.68	0.58
1:B:428:ILE:HG22	1:B:434:LEU:HD23	1.84	0.58
1:B:518:ASP:OD2	1:B:519:PHE:N	2.36	0.58
1:A:418:GLU:HG3	1:A:430:GLY:HA3	1.84	0.58
1:B:475:LEU:HD11	1:B:479:LEU:HD11	1.85	0.58
1:B:314:THR:HA	1:B:587:THR:O	2.04	0.58
1:B:301:LEU:HD23	1:B:490:LEU:HG	1.86	0.58
1:B:341:GLU:HG2	1:B:611:ILE:HG13	1.85	0.58
1:B:139:HIS:HB2	1:B:142:LYS:O	2.02	0.57
1:B:23:VAL:HG13	1:B:69:LEU:HD12	1.86	0.57
1:B:400:GLU:HG3	1:B:410:THR:OG1	2.04	0.57
1:A:301:LEU:HD23	1:A:490:LEU:HG	1.87	0.57
1:B:367:ASN:HD22	1:B:405:GLN:HE22	1.51	0.57
1:A:314:THR:HA	1:A:587:THR:O	2.04	0.57
1:A:536:ALA:N	1:A:563:GLN:NE2	2.35	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:554:ASP:OD2	1:B:555:LYS:N	2.37	0.57
1:A:421:TRP:N	1:A:471:ASN:HD21	1.99	0.57
1:B:120:TRP:HB2	1:B:131:HIS:HB3	1.87	0.57
1:B:524:GLU:N	1:B:524:GLU:OE1	2.38	0.56
1:A:549:HIS:O	1:A:550:GLU:HB2	2.05	0.56
1:B:45:ARG:HD2	1:B:375:HIS:NE2	2.20	0.56
1:B:580:TYR:O	1:B:599:GLY:HA2	2.05	0.56
1:A:542:ASN:HA	1:A:556:THR:O	2.04	0.56
1:A:536:ALA:CB	1:A:563:GLN:HE22	2.18	0.56
1:B:147:GLU:HG3	1:B:150:VAL:HG11	1.87	0.56
1:B:42:ALA:HB1	1:B:375:HIS:CE1	2.40	0.56
1:B:520:THR:O	1:B:522:ASN:N	2.39	0.55
1:A:15:LEU:HD21	1:A:18:TYR:CZ	2.41	0.55
1:A:336:ALA:O	1:A:337:SER:HB2	2.06	0.55
1:A:418:GLU:HG2	1:A:430:GLY:N	2.21	0.55
1:A:559:LYS:HE2	1:A:560:PHE:CZ	2.42	0.55
1:B:319:PHE:CD2	1:B:326:LEU:HD11	2.42	0.55
1:A:95:ASN:HD22	1:A:95:ASN:H	1.55	0.55
1:A:306:GLN:OE1	1:B:94:VAL:HA	2.07	0.55
1:A:342:ALA:HB2	1:A:596:CYS:HB3	1.87	0.55
1:B:120:TRP:NE1	1:B:185:ILE:HG12	2.22	0.55
1:A:382:VAL:HG22	1:A:437:CYS:SG	2.46	0.55
1:B:30:TYR:O	1:B:31:SER:HB2	2.07	0.54
1:A:279:ASP:O	1:A:283:LYS:HG3	2.08	0.54
1:A:597:LEU:HD11	1:A:614:LEU:HD13	1.87	0.54
1:A:124:GLY:HA3	1:A:182:ASP:O	2.07	0.54
1:A:16:LEU:HD21	1:A:27:SER:HB2	1.88	0.54
1:B:89:PHE:HB2	1:B:99:LEU:O	2.07	0.54
1:B:233:LEU:HD12	1:B:401:GLN:OE1	2.08	0.54
1:A:535:ILE:HG22	1:A:566:ILE:HG23	1.89	0.54
1:B:309:ARG:HG3	1:B:309:ARG:HH11	1.72	0.54
1:B:42:ALA:HB1	1:B:375:HIS:HE1	1.71	0.54
1:A:298:TRP:HB2	1:A:299:PRO:HD3	1.89	0.54
1:A:454:VAL:CG1	1:A:457:ARG:HG3	2.37	0.54
1:A:572:CYS:HB3	1:A:603:LEU:HD22	1.90	0.53
1:A:308:ARG:NE	1:A:311:HIS:ND1	2.50	0.53
1:A:112:PRO:HB3	1:A:188:TRP:CD2	2.43	0.53
1:A:175:THR:O	1:A:176:LEU:HD23	2.09	0.53
1:B:194:ASP:OD1	1:B:196:GLU:HB3	2.08	0.53
1:A:229:GLU:HG2	1:A:235:ASN:HD22	1.72	0.53
1:A:556:THR:HG21	1:A:606:LYS:HE3	1.91	0.53

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:341:GLU:CG	1:B:611:ILE:HG13	2.39	0.53
1:B:532:VAL:HG22	1:B:567:TYR:CE1	2.44	0.53
1:A:568:GLN:HG2	3:A:3001:ADP:HN61	1.74	0.53
1:A:420:GLY:O	1:A:428:ILE:HG12	2.09	0.53
1:B:562:GLU:HB2	5:B:8151:HOH:O	2.08	0.53
1:A:512:ARG:HH11	1:A:512:ARG:HG2	1.74	0.52
1:B:512:ARG:HG2	1:B:512:ARG:HH11	1.74	0.52
1:A:308:ARG:HH11	1:A:308:ARG:HG3	1.73	0.52
1:A:361:PRO:HG3	1:A:614:LEU:HD23	1.92	0.52
1:A:389:ASP:HB3	1:A:391:GLU:OE1	2.09	0.52
1:B:459:PHE:HD2	1:B:459:PHE:O	1.91	0.52
1:A:469:PRO:HG2	1:A:470:GLN:NE2	2.25	0.52
1:A:48:ILE:HG12	1:A:53:MET:HG3	1.90	0.52
1:A:436:ASN:H	1:A:436:ASN:ND2	2.04	0.52
1:A:341:GLU:CG	1:A:611:ILE:HG21	2.34	0.52
1:B:28:SER:HB2	1:B:57:TRP:HB2	1.92	0.52
1:B:319:PHE:CE2	1:B:328:VAL:HB	2.45	0.52
1:B:427:LEU:HD21	1:B:478:VAL:HG13	1.92	0.52
1:B:547:SER:OG	1:B:551:GLU:HG2	2.10	0.52
1:B:601:GLU:H	1:B:601:GLU:CD	2.14	0.51
1:A:120:TRP:HB2	1:A:131:HIS:HB3	1.91	0.51
1:A:117:LEU:O	1:A:188:TRP:HA	2.10	0.51
1:B:366:ILE:HG23	1:B:367:ASN:N	2.26	0.51
1:B:522:ASN:ND2	1:B:525:LEU:H	2.08	0.51
1:B:287:LEU:O	1:B:290:LEU:HG	2.10	0.51
1:A:348:ARG:HD2	1:A:351:GLU:OE1	2.11	0.51
1:B:104:PHE:O	1:B:187:GLY:HA3	2.10	0.51
1:B:523:ASP:HB2	1:B:524:GLU:OE1	2.10	0.51
1:B:556:THR:CG2	1:B:606:LYS:HE3	2.41	0.51
1:A:276:HIS:HE1	5:A:8102:HOH:O	1.94	0.51
1:B:235:ASN:O	1:B:239:GLN:HG2	2.11	0.51
1:B:319:PHE:O	1:B:582:GLN:HG3	2.11	0.51
1:A:247:GLN:HA	1:A:247:GLN:OE1	2.12	0.50
1:B:480:LEU:O	1:B:482:PRO:HD3	2.11	0.50
1:B:117:LEU:O	1:B:188:TRP:HA	2.11	0.50
1:B:204:ILE:HG12	1:B:205:ALA:N	2.27	0.50
1:B:342:ALA:O	1:B:362:ALA:HB3	2.12	0.50
1:B:125:GLU:HB3	1:B:183:THR:CG2	2.42	0.50
1:A:210:LYS:NZ	1:A:323:GLU:HG2	2.27	0.50
1:A:532:VAL:HB	1:A:544:ASP:HB2	1.92	0.50
1:A:468:HIS:CE1	1:A:470:GLN:HE21	2.30	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:MET:SD	1:B:65:ARG:HA	2.51	0.50
1:B:124:GLY:HA3	1:B:182:ASP:O	2.12	0.49
1:B:137:GLN:CG	1:B:144:ARG:HB2	2.42	0.49
1:A:465:ARG:HD3	1:A:474:ARG:HH21	1.77	0.49
1:B:48:ILE:O	1:B:49:ASP:HB2	2.12	0.49
1:A:74:VAL:HG22	1:A:75:PHE:N	2.27	0.49
1:A:137:GLN:HG2	1:A:144:ARG:HB2	1.94	0.49
1:A:436:ASN:N	1:A:436:ASN:ND2	2.59	0.49
1:B:25:ILE:HG23	1:B:148:GLN:HG3	1.95	0.49
1:B:581:ILE:CG2	1:B:597:LEU:HD22	2.43	0.49
1:B:268:ASN:ND2	1:B:592:TYR:H	2.04	0.49
1:A:527:LYS:O	1:A:548:HIS:HB2	2.13	0.49
1:B:178:ASP:HB2	1:B:185:ILE:HD11	1.94	0.49
1:B:462:VAL:HG11	1:B:480:LEU:CD1	2.40	0.49
1:B:71:TYR:O	1:B:73:VAL:HG13	2.13	0.49
1:B:89:PHE:C	1:B:89:PHE:CD1	2.86	0.49
1:A:141:ASN:HD21	1:A:142:LYS:HG2	1.78	0.49
1:B:468:HIS:HE1	1:B:470:GLN:HB2	1.78	0.49
1:B:255:ILE:HG23	1:B:614:LEU:HD11	1.95	0.49
1:A:80:MET:H	1:A:83:GLU:CD	2.17	0.48
1:A:257:GLU:OE2	1:A:618:LYS:HD3	2.12	0.48
1:B:359:PHE:CE2	1:B:616:VAL:HB	2.48	0.48
1:B:393:ASN:OD1	1:B:414:ARG:NH1	2.46	0.48
1:A:121:ASP:HB2	1:A:186:LEU:CD2	2.42	0.48
1:A:552:VAL:HG11	1:A:555:LYS:HE3	1.95	0.48
1:B:164:GLU:O	1:B:165:LEU:HD23	2.13	0.48
1:B:538:ARG:HB3	5:B:6001:HOH:O	2.13	0.48
1:A:218:ASN:C	1:A:220:GLY:H	2.16	0.48
1:A:45:ARG:HB3	1:A:47:TYR:CE1	2.49	0.48
1:A:64:ARG:NH2	1:A:75:PHE:CE1	2.82	0.48
1:B:80:MET:CE	1:B:129:THR:HA	2.43	0.48
1:A:327:LYS:HG3	1:A:515:LEU:HD21	1.94	0.48
1:A:15:LEU:HD21	1:A:18:TYR:CE1	2.48	0.48
1:B:347:GLU:OE2	1:B:363:GLU:HB2	2.13	0.48
1:B:481:ARG:NH1	1:B:483:GLU:OE1	2.47	0.48
1:A:294:PRO:HD3	1:A:452:ARG:HH12	1.78	0.48
1:A:363:GLU:HG3	1:A:364:GLY:N	2.27	0.48
1:A:507:LEU:C	1:A:509:PRO:HD3	2.33	0.48
1:B:386:GLN:NE2	1:B:414:ARG:HD2	2.29	0.48
1:A:139:HIS:HB2	1:A:142:LYS:O	2.14	0.48
1:A:533:LYS:HG2	1:A:543:ILE:HD12	1.96	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:GLY:N	1:A:83:GLU:OE1	2.47	0.48
1:A:95:ASN:N	1:A:95:ASN:HD22	2.10	0.47
1:B:31:SER:C	1:B:33:LEU:N	2.65	0.47
1:A:329:TYR:HE2	1:A:573:LEU:HD21	1.80	0.47
1:A:94:VAL:CG1	1:B:303:LEU:HD23	2.45	0.47
1:B:523:ASP:O	1:B:526:VAL:HB	2.13	0.47
1:A:144:ARG:HG2	1:A:164:GLU:HG2	1.96	0.47
1:B:522:ASN:HD21	1:B:525:LEU:H	1.59	0.47
1:B:497:ASN:OD1	1:B:535:ILE:HB	2.15	0.47
1:A:295:LYS:HA	1:A:298:TRP:CD1	2.49	0.47
1:B:245:ILE:HG13	1:B:246:ASN:OD1	2.14	0.47
1:B:31:SER:O	1:B:33:LEU:N	2.48	0.47
1:B:321:MET:O	1:B:322:ASP:HB3	2.14	0.47
1:A:411:ARG:NH1	1:A:411:ARG:HG3	2.28	0.47
1:A:425:GLY:O	1:A:481:ARG:NH2	2.47	0.47
1:B:264:ILE:HG12	1:B:592:TYR:CD2	2.49	0.47
1:A:342:ALA:HB1	1:A:362:ALA:CB	2.45	0.47
1:B:215:ARG:HG3	1:B:215:ARG:HH11	1.80	0.47
1:B:259:ALA:O	1:B:262:GLU:HB3	2.15	0.47
1:B:390:ILE:HD13	1:B:390:ILE:N	2.29	0.47
1:B:109:PRO:HB2	1:B:197:TYR:CD1	2.50	0.47
1:B:270:LEU:HD23	1:B:273:MET:SD	2.55	0.47
1:A:231:ASP:O	1:A:233:LEU:N	2.48	0.47
1:A:151:ILE:HD13	1:A:151:ILE:N	2.27	0.46
1:A:544:ASP:OD1	1:A:555:LYS:HG2	2.15	0.46
1:B:104:PHE:CE2	1:B:110:ARG:HG2	2.50	0.46
1:A:418:GLU:HG2	1:A:418:GLU:O	2.15	0.46
1:A:137:GLN:CD	1:A:144:ARG:HD2	2.35	0.46
1:A:141:ASN:HD22	1:A:141:ASN:N	2.11	0.46
1:B:147:GLU:HG3	1:B:150:VAL:CG1	2.45	0.46
1:B:137:GLN:HG3	1:B:144:ARG:HB2	1.96	0.46
1:A:210:LYS:HZ2	1:A:323:GLU:HG2	1.81	0.46
1:B:155:LEU:HD11	1:B:162:THR:HG22	1.97	0.46
1:A:342:ALA:HB1	1:A:362:ALA:HB3	1.97	0.46
1:A:535:ILE:HG13	1:A:536:ALA:N	2.30	0.46
1:B:245:ILE:HG13	1:B:246:ASN:H	1.81	0.46
1:B:429:ASP:OD2	1:B:433:ARG:HB3	2.15	0.46
1:A:137:GLN:HE21	1:A:139:HIS:CE1	2.28	0.46
1:A:168:VAL:HG22	1:A:175:THR:HB	1.98	0.45
1:A:53:MET:SD	1:A:65:ARG:HA	2.57	0.45
1:A:113:VAL:CG2	1:A:114:ALA:N	2.79	0.45

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:GLN:NE2	1:A:414:ARG:HE	2.13	0.45
1:A:556:THR:CG2	1:A:606:LYS:HE3	2.46	0.45
1:B:425:GLY:O	1:B:481:ARG:NH2	2.40	0.45
1:B:56:LYS:HA	1:B:57:TRP:HA	1.62	0.45
1:A:406:ALA:HB1	1:A:408:PHE:HE1	1.82	0.45
1:A:104:PHE:O	1:A:187:GLY:HA3	2.16	0.45
1:A:141:ASN:HD22	1:A:142:LYS:N	2.13	0.45
1:A:138:LEU:CD1	1:A:143:VAL:HG12	2.43	0.45
1:A:44:PHE:O	1:A:56:LYS:HG3	2.17	0.45
1:B:468:HIS:CE1	1:B:470:GLN:HB2	2.51	0.45
1:A:297:LEU:O	1:A:300:ARG:N	2.50	0.45
1:A:320:CYS:HG	1:A:571:TRP:HD1	1.61	0.45
1:B:80:MET:HE1	1:B:129:THR:HG22	1.98	0.45
1:A:151:ILE:O	1:A:152:HIS:CG	2.70	0.45
1:A:566:ILE:HD12	1:A:566:ILE:C	2.36	0.45
1:B:386:GLN:HG3	1:B:387:ASP:O	2.16	0.45
1:B:387:ASP:CG	1:B:388:LYS:H	2.20	0.45
1:B:418:GLU:HG2	1:B:430:GLY:N	2.32	0.45
1:B:488:GLU:HB3	1:B:492:THR:HG21	1.99	0.45
1:B:313:ILE:HB	1:B:488:GLU:OE1	2.17	0.45
1:A:344:LEU:O	1:A:347:GLU:N	2.46	0.44
1:A:564:LYS:HG2	1:A:565:ASN:N	2.31	0.44
1:B:512:ARG:HG2	1:B:512:ARG:NH1	2.32	0.44
1:A:277:ALA:O	1:A:281:VAL:HG23	2.18	0.44
1:A:512:ARG:NH1	1:A:512:ARG:HG2	2.32	0.44
1:B:66:PHE:CE2	1:B:134:ILE:HG21	2.52	0.44
1:B:106:ASN:HD22	1:B:185:ILE:HB	1.82	0.44
1:A:308:ARG:NH1	1:A:489:PRO:HB3	2.33	0.44
1:A:259:ALA:O	1:A:262:GLU:HB3	2.17	0.44
1:A:580:TYR:O	1:A:599:GLY:HA2	2.18	0.44
1:B:178:ASP:OD2	1:B:180:PHE:HD1	2.00	0.44
1:A:291:PHE:CD1	1:A:291:PHE:N	2.85	0.44
1:B:112:PRO:HB3	1:B:188:TRP:CD2	2.52	0.44
1:B:307:ARG:HG3	1:B:308:ARG:HG3	2.00	0.44
1:B:566:ILE:C	1:B:566:ILE:HD12	2.38	0.44
1:B:320:CYS:SG	1:B:571:TRP:HD1	2.41	0.44
1:A:131:HIS:CG	1:A:132:VAL:N	2.86	0.44
1:A:462:VAL:HG11	1:A:480:LEU:CD1	2.48	0.44
1:B:196:GLU:O	1:B:197:TYR:HB2	2.17	0.44
1:B:238:VAL:HG13	1:B:242:GLY:HA2	1.98	0.44
1:B:368:GLU:HA	1:B:368:GLU:OE1	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:ILE:HG12	1:A:592:TYR:CD2	2.52	0.44
1:A:295:LYS:HA	1:A:298:TRP:NE1	2.32	0.44
1:A:568:GLN:HG2	3:A:3001:ADP:N6	2.33	0.44
1:A:530:TYR:HA	1:A:570:LEU:N	2.33	0.44
1:A:111:ALA:HB2	1:A:174:TYR:CZ	2.53	0.43
1:A:384:ILE:HG23	1:A:439:TRP:HE3	1.83	0.43
1:B:119:ILE:HD13	1:B:132:VAL:HG23	2.00	0.43
1:A:94:VAL:HA	1:B:306:GLN:NE2	2.33	0.43
1:B:320:CYS:HG	1:B:571:TRP:HD1	1.61	0.43
1:B:342:ALA:HB2	1:B:596:CYS:HB3	2.00	0.43
1:B:418:GLU:HG2	1:B:430:GLY:H	1.83	0.43
1:B:517:THR:OG1	1:B:568:GLN:HG3	2.17	0.43
1:A:320:CYS:HB2	1:A:329:TYR:CZ	2.53	0.43
1:A:56:LYS:HA	1:A:57:TRP:HA	1.61	0.43
1:A:470:GLN:N	1:A:470:GLN:NE2	2.66	0.43
1:A:595:THR:HG22	1:A:596:CYS:N	2.32	0.43
1:B:542:ASN:HD21	1:B:561:ALA:HB2	1.82	0.43
1:B:580:TYR:CE2	1:B:603:LEU:HD23	2.53	0.43
1:B:556:THR:HG21	1:B:606:LYS:HE3	1.98	0.43
1:B:426:GLN:HA	1:B:481:ARG:NH2	2.34	0.43
1:B:308:ARG:NH1	1:B:486:VAL:O	2.47	0.43
1:A:80:MET:HB2	1:A:82:TRP:NE1	2.32	0.43
1:B:481:ARG:HG2	1:B:481:ARG:HH11	1.83	0.43
1:B:437:CYS:HA	1:B:485:LEU:O	2.17	0.43
1:B:384:ILE:HG23	1:B:439:TRP:HE3	1.82	0.43
1:B:584:CYS:HB2	1:B:596:CYS:SG	2.59	0.43
1:A:389:ASP:C	1:A:391:GLU:H	2.21	0.43
1:A:144:ARG:HD3	1:A:161:TRP:CD1	2.54	0.43
1:A:80:MET:CE	2:A:620:TS5:HB22	2.48	0.43
1:B:107:GLY:HA2	1:B:174:TYR:O	2.18	0.43
1:A:94:VAL:HG13	1:B:303:LEU:HD23	2.01	0.42
1:B:358:GLY:HA3	1:B:615:ILE:CG2	2.49	0.42
1:A:234:GLN:O	1:A:238:VAL:HG23	2.19	0.42
1:A:313:ILE:HB	1:A:488:GLU:OE1	2.19	0.42
1:B:389:ASP:HB3	1:B:391:GLU:CG	2.44	0.42
1:A:271:HIS:CE1	1:A:590:GLY:HA2	2.55	0.42
1:A:45:ARG:HD2	1:A:375:HIS:NE2	2.33	0.42
1:B:386:GLN:HA	1:B:441:THR:OG1	2.19	0.42
1:A:294:PRO:HD3	1:A:452:ARG:NH1	2.34	0.42
1:A:566:ILE:HD12	1:A:566:ILE:O	2.19	0.42
1:B:275:LEU:HD23	1:B:275:LEU:N	2.33	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:TRP:HA	1:B:426:GLN:O	2.20	0.42
1:B:532:VAL:HG22	1:B:567:TYR:HE1	1.82	0.42
1:B:536:ALA:N	1:B:563:GLN:HE22	2.14	0.42
1:A:229:GLU:HG2	1:A:235:ASN:ND2	2.33	0.42
1:A:389:ASP:C	1:A:391:GLU:N	2.72	0.42
1:A:518:ASP:OD1	1:A:519:PHE:N	2.52	0.42
1:B:138:LEU:HD12	1:B:143:VAL:HG12	2.00	0.42
1:A:293:ILE:O	1:A:294:PRO:C	2.57	0.42
1:A:418:GLU:CG	1:A:430:GLY:HA3	2.48	0.42
1:B:468:HIS:CG	1:B:469:PRO:HD2	2.54	0.42
1:B:48:ILE:CG2	1:B:68:PHE:HE2	2.33	0.42
1:A:317:MET:O	1:A:584:CYS:HA	2.19	0.42
1:A:581:ILE:CG2	1:A:597:LEU:HD22	2.50	0.42
1:A:582:GLN:OE1	1:A:605:ILE:HG13	2.19	0.42
1:A:130:GLY:O	1:A:131:HIS:HB2	2.20	0.42
1:A:122:LYS:HA	1:A:130:GLY:HA2	2.00	0.42
1:A:254:THR:HA	1:A:615:ILE:O	2.20	0.42
1:A:319:PHE:CE2	1:A:328:VAL:HB	2.55	0.42
1:B:32:SER:O	1:B:33:LEU:HD23	2.19	0.42
1:B:334:ASP:OD2	1:B:444:TRP:HB2	2.19	0.42
1:A:429:ASP:OD2	1:A:433:ARG:N	2.52	0.42
1:A:418:GLU:CG	1:A:430:GLY:H	2.32	0.42
1:B:245:ILE:HG22	1:B:345:ILE:HG21	2.02	0.42
1:B:511:HIS:HE1	1:B:513:TYR:CD2	2.37	0.42
1:A:230:LYS:CB	1:A:230:LYS:NZ	2.82	0.41
1:A:298:TRP:CD1	1:A:298:TRP:N	2.88	0.41
1:A:368:GLU:OE1	1:A:368:GLU:HA	2.20	0.41
1:B:215:ARG:NH1	1:B:215:ARG:HG3	2.35	0.41
1:B:221:GLN:OE1	1:B:250:TYR:HE2	2.04	0.41
1:B:270:LEU:O	1:B:274:TYR:HD1	2.03	0.41
1:A:450:GLN:HE22	1:A:474:ARG:HB3	1.85	0.41
1:B:471:ASN:HA	1:B:471:ASN:HD22	1.61	0.41
1:A:45:ARG:HB3	1:A:47:TYR:HE1	1.85	0.41
1:A:547:SER:HB3	1:A:553:LEU:HD21	2.02	0.41
1:A:70:ASN:ND2	1:B:461:ALA:HB1	2.35	0.41
1:A:231:ASP:O	1:A:232:PRO:C	2.59	0.41
1:A:309:ARG:HG3	1:A:309:ARG:HH11	1.84	0.41
1:A:217:GLU:O	1:A:219:LYS:N	2.48	0.41
1:A:429:ASP:C	1:A:431:GLU:H	2.23	0.41
1:A:347:GLU:OE1	1:A:360:ASN:HB3	2.21	0.41
1:B:595:THR:HG22	1:B:596:CYS:N	2.35	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ALA:HB2	1:A:596:CYS:CB	2.51	0.41
1:B:245:ILE:CG1	1:B:246:ASN:N	2.80	0.41
1:B:601:GLU:N	1:B:601:GLU:CD	2.74	0.41
1:A:15:LEU:HD21	1:A:18:TYR:OH	2.21	0.41
1:A:295:LYS:HB3	1:A:295:LYS:HE2	1.89	0.41
1:B:538:ARG:HA	3:B:3002:ADP:O2B	2.21	0.41
1:A:156:PRO:HB2	1:A:159:GLN:HB2	2.02	0.41
1:A:379:ARG:HB2	1:A:437:CYS:HB2	2.03	0.41
1:B:427:LEU:CD2	1:B:478:VAL:HG13	2.51	0.41
1:A:338:CYS:HA	1:A:341:GLU:OE2	2.20	0.40
1:B:161:TRP:CZ3	1:B:164:GLU:HG3	2.56	0.40
1:B:422:ASP:OD1	1:B:426:GLN:N	2.45	0.40
1:A:385:MET:HG3	1:A:438:VAL:HG13	2.03	0.40
1:B:339:HIS:CD2	1:B:395:HIS:HE1	2.39	0.40
1:A:49:ASP:HB3	1:A:50:ASP:H	1.66	0.40
1:B:121:ASP:HB2	1:B:186:LEU:CG	2.51	0.40
1:A:469:PRO:HG2	1:A:470:GLN:HE22	1.87	0.40
1:A:131:HIS:HD2	2:A:620:TS5:HN1'	1.67	0.40
1:B:366:ILE:CG2	1:B:367:ASN:N	2.85	0.40
1:A:48:ILE:HG12	1:A:53:MET:CG	2.51	0.40
1:A:92:GLU:O	1:A:95:ASN:ND2	2.55	0.40
1:B:538:ARG:HH11	1:B:538:ARG:HG3	1.87	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	593/619 (96%)	525 (88%)	54 (9%)	14 (2%)	7	23
1	B	599/619 (97%)	540 (90%)	44 (7%)	15 (2%)	6	22
All	All	1192/1238 (96%)	1065 (89%)	98 (8%)	29 (2%)	7	23

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	LYS
1	A	341	GLU
1	B	150	VAL
1	A	94	VAL
1	A	356	GLY
1	B	32	SER
1	B	94	VAL
1	B	218	ASN
1	B	247	GLN
1	B	521	VAL
1	A	49	ASP
1	A	228	ASP
1	A	232	PRO
1	B	31	SER
1	B	341	GLU
1	B	522	ASN
1	B	76	THR
1	B	322	ASP
1	A	152	HIS
1	A	171	ASN
1	A	337	SER
1	A	218	ASN
1	B	482	PRO
1	A	93	VAL
1	A	294	PRO
1	A	172	GLY
1	B	364	GLY
1	B	358	GLY
1	B	294	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	510/529 (96%)	495 (97%)	15 (3%)	48 81

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	514/529 (97%)	500 (97%)	14 (3%)	50	83
All	All	1024/1058 (97%)	995 (97%)	29 (3%)	49	82

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	76	THR
1	A	89	PHE
1	A	95	ASN
1	A	141	ASN
1	A	151	ILE
1	A	229	GLU
1	A	230	LYS
1	A	232	PRO
1	A	241	ASN
1	A	355	LYS
1	A	436	ASN
1	A	470	GLN
1	A	471	ASN
1	A	483	GLU
1	A	569	GLN
1	B	76	THR
1	B	89	PHE
1	B	110	ARG
1	B	113	VAL
1	B	201	GLN
1	B	233	LEU
1	B	261	GLN
1	B	279	ASP
1	B	285	ASP
1	B	377	ARG
1	B	390	ILE
1	B	459	PHE
1	B	471	ASN
1	B	522	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	HIS
1	A	70	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	95	ASN
1	A	137	GLN
1	A	139	HIS
1	A	141	ASN
1	A	235	ASN
1	A	268	ASN
1	A	276	HIS
1	A	352	GLN
1	A	395	HIS
1	A	397	GLN
1	A	405	GLN
1	A	436	ASN
1	A	470	GLN
1	A	471	ASN
1	A	563	GLN
1	A	568	GLN
1	B	70	ASN
1	B	102	GLN
1	B	131	HIS
1	B	152	HIS
1	B	157	GLN
1	B	159	GLN
1	B	201	GLN
1	B	268	ASN
1	B	286	ASN
1	B	306	GLN
1	B	339	HIS
1	B	367	ASN
1	B	395	HIS
1	B	471	ASN
1	B	522	ASN
1	B	563	GLN
1	B	568	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	ADP	A	3001	4	25,29,29	0.97	1 (4%)	24,45,45	1.74	4 (16%)
2	TS5	A	620	-	23,28,28	4.80	14 (60%)	27,33,33	5.58	12 (44%)
3	ADP	B	3002	4	25,29,29	1.00	1 (4%)	24,45,45	1.79	4 (16%)

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	ADP	A	3001	4	-	0/12/32/32	0/3/3/3
2	TS5	A	620	-	1/1/6/10	0/30/34/34	0/0/0/0
3	ADP	B	3002	4	-	0/12/32/32	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	620	TS5	CB2-CA2	-11.47	1.40	1.53
2	A	620	TS5	CA2-C2	-5.21	1.38	1.52
2	A	620	TS5	C2'-C1'	-3.67	1.36	1.51
2	A	620	TS5	CA3-C3	-2.06	1.45	1.52
2	A	620	TS5	C2'-C3'	2.98	1.63	1.51
3	A	3001	ADP	C2-N1	3.13	1.39	1.33
3	B	3002	ADP	C2-N1	3.17	1.39	1.33
2	A	620	TS5	CB2-SG2	3.57	1.89	1.81
2	A	620	TS5	CA2-N2	3.77	1.54	1.45

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	620	TS5	C3'-N2'	4.37	1.61	1.47
2	A	620	TS5	C2-N3	4.44	1.42	1.33
2	A	620	TS5	CA3-N3	4.46	1.57	1.45
2	A	620	TS5	O1-CD1	4.93	1.33	1.23
2	A	620	TS5	O3-C3	5.97	1.35	1.23
2	A	620	TS5	CD1-N2	6.96	1.48	1.34
2	A	620	TS5	C3-N1'	11.75	1.61	1.33

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	620	TS5	C1'-N1'-C3	-10.38	102.90	122.84
2	A	620	TS5	CB2-CA2-N2	-10.15	96.69	111.39
3	A	3001	ADP	N3-C2-N1	-5.65	123.94	128.86
3	B	3002	ADP	N3-C2-N1	-5.56	124.01	128.86
2	A	620	TS5	CG1-CB1-CA1	-5.18	101.75	113.84
2	A	620	TS5	C2'-C3'-N2'	-4.87	99.64	112.06
2	A	620	TS5	O2-C2-CA2	-4.43	110.90	120.43
2	A	620	TS5	O1-CD1-N2	-4.19	115.74	122.97
2	A	620	TS5	O3-C3-CA3	-3.58	113.19	120.72
3	A	3001	ADP	C2-N1-C6	2.10	122.44	118.77
3	B	3002	ADP	C5-C6-N6	2.50	125.57	120.47
3	B	3002	ADP	C2-N1-C6	2.52	123.18	118.77
3	A	3001	ADP	C5-C6-N6	2.56	125.68	120.47
3	A	3001	ADP	C4'-O4'-C1'	2.96	112.92	109.77
3	B	3002	ADP	C4'-O4'-C1'	3.30	113.28	109.77
2	A	620	TS5	CA2-N2-CD1	3.67	131.32	121.62
2	A	620	TS5	C2-CA2-N2	4.16	122.66	111.20
2	A	620	TS5	C2'-C1'-N1'	9.66	139.96	112.18
2	A	620	TS5	CB2-CA2-C2	13.44	139.28	109.60
2	A	620	TS5	CA2-CB2-SG2	14.07	130.56	114.15

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	620	TS5	CA2

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	3001	ADP	2	0
2	A	620	TS5	5	0
3	B	3002	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	599/619 (96%)	-0.37	3 (0%) 90 88	18, 43, 65, 84	0
1	B	603/619 (97%)	-0.28	12 (1%) 65 56	20, 46, 69, 86	0
All	All	1202/1238 (97%)	-0.33	15 (1%) 79 72	18, 44, 67, 86	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	SER	6.0
1	B	33	LEU	3.8
1	B	456	ASP	3.7
1	A	43	VAL	3.1
1	B	558	GLY	2.6
1	B	43	VAL	2.5
1	B	217	GLU	2.5
1	B	140	GLY	2.3
1	A	454	VAL	2.3
1	B	549	HIS	2.3
1	B	559	LYS	2.2
1	B	41	ASP	2.1
1	B	204	ILE	2.1
1	B	552	VAL	2.0
1	A	172	GLY	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

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
2	TS5	A	620	29/29	0.86	0.23	1.50	39,45,75,78	0
3	ADP	B	3002	27/27	0.98	0.15	-0.51	32,39,40,42	0
3	ADP	A	3001	27/27	0.97	0.13	-1.25	30,33,34,36	0
4	MG	A	4000	1/1	0.95	0.11	-1.54	37,37,37,37	0
4	MG	B	6000	1/1	0.95	0.11	-1.58	39,39,39,39	0
4	MG	B	7000	1/1	0.95	0.11	-	34,34,34,34	0
4	MG	A	5000	1/1	0.97	0.15	-	32,32,32,32	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.