



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:14 pm BST

PDB ID : 6PAI  
Title : Structure of the human DDB1-DDA1-DCAF15 E3 ubiquitin ligase bound to RBM39 and sulfonamide E7820  
Authors : Volkov, O.A.; Du, X.  
Deposited on : 2019-06-11  
Resolution : 2.90 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 ⓘ symbol.

---

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11  
buster-report : 1.1.7 (2018)  
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) : 2.11

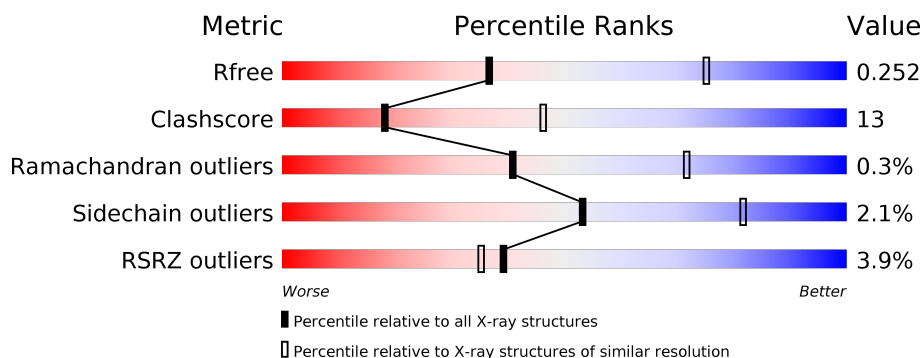
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.90 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	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 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	1140	<div> <div>2%</div> <div>73%</div> <div>22%</div> <div>• •</div> </div>
2	C	498	<div> <div>7%</div> <div>56%</div> <div>22%</div> <div>• 19%</div> </div>
3	D	109	<div> <div>60%</div> <div>14%</div> <div>27%</div> </div>
4	E	102	<div> <div>4%</div> <div>48%</div> <div>19%</div> <div>• 32%</div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13196 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 DNA damage-binding protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1099	Total	C	N	O	S	0	0	0
			8626	5478	1452	1649	47			

- Molecule 2 is a protein called DDB1- and CUL4-associated factor 15.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	401	Total	C	N	O	S	0	6	0
			3318	2139	559	604	16			

There are 7 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	MET	-	expression tag	UNP Q66K64
C	-4	HIS	-	expression tag	UNP Q66K64
C	-3	HIS	-	expression tag	UNP Q66K64
C	-2	HIS	-	expression tag	UNP Q66K64
C	-1	HIS	-	expression tag	UNP Q66K64
C	0	HIS	-	expression tag	UNP Q66K64
C	1	HIS	-	expression tag	UNP Q66K64

- Molecule 3 is a protein called RNA-binding protein 39.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	80	Total	C	N	O	S	0	0	0
			625	396	107	116	6			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	231	GLY	-	expression tag	UNP Q7Z3L0
D	232	SER	-	expression tag	UNP Q7Z3L0
D	233	HIS	-	expression tag	UNP Q7Z3L0

*Continued on next page...*

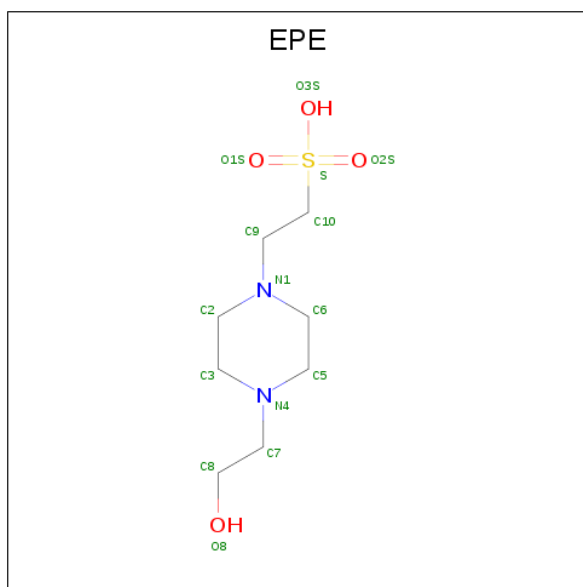
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	234	MET	-	expression tag	UNP Q7Z3L0
D	332	ASP	-	expression tag	UNP Q7Z3L0
D	333	TYR	-	expression tag	UNP Q7Z3L0
D	334	LYS	-	expression tag	UNP Q7Z3L0
D	335	ASP	-	expression tag	UNP Q7Z3L0
D	336	ASP	-	expression tag	UNP Q7Z3L0
D	337	ASP	-	expression tag	UNP Q7Z3L0
D	338	ASP	-	expression tag	UNP Q7Z3L0
D	339	LYS	-	expression tag	UNP Q7Z3L0

- Molecule 4 is a protein called DET1- and DDB1-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	69	Total	C	N	O	S	0	0	0
			571	364	104	102	1			

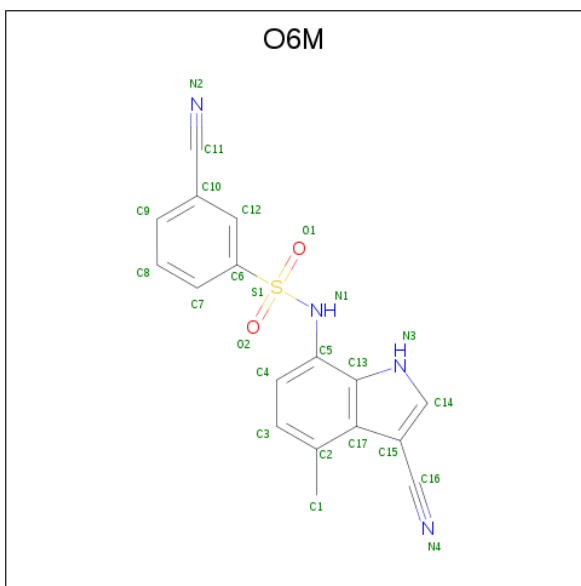
- Molecule 5 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
5	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 6 is 3-cyano-N-(3-cyano-4-methyl-1H-indol-7-yl)benzene-1-sulfonamide

(three-letter code: O6M) (formula: C<sub>17</sub>H<sub>12</sub>N<sub>4</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	S	0	0
			24	17	4	2	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total	Zn	0	0
			1	1		

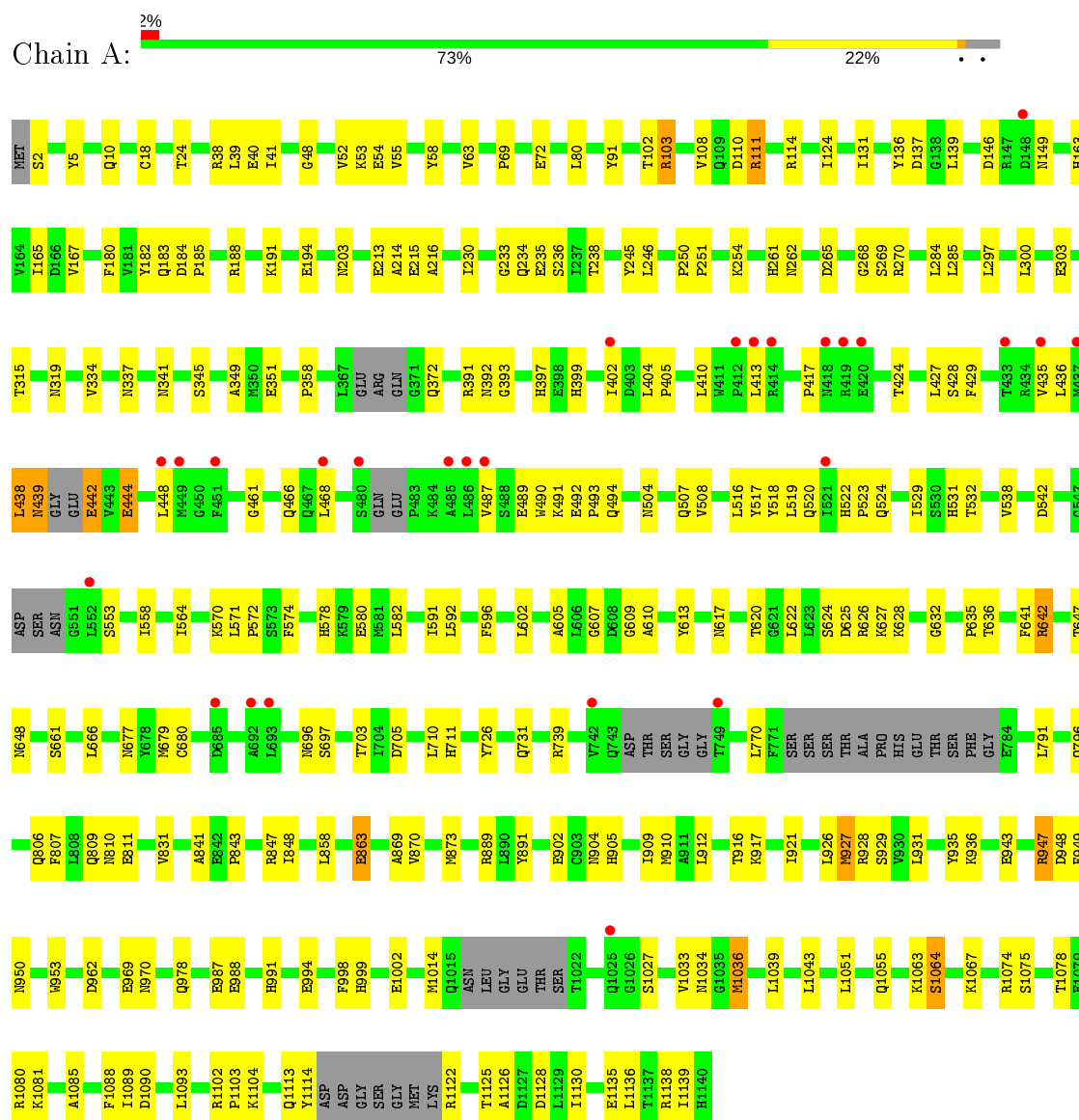
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	O	0	0
			1	1		

### 3 Residue-property plots [i](#)

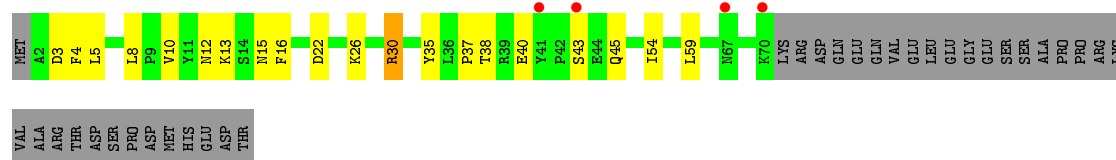
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: DNA damage-binding protein 1



- Molecule 2: DDB1- and CUL4-associated factor 15





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.51Å 94.77Å 145.71Å 90.00° 98.06° 90.00°	Depositor
Resolution (Å)	49.45 – 2.90 49.45 – 2.90	Depositor EDS
% Data completeness (in resolution range)	96.3 (49.45-2.90) 96.3 (49.45-2.90)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.84 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, $R_{free}$	0.208 , 0.252 0.208 , 0.252	Depositor DCC
$R_{free}$ test set	2310 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	70.0	Xtriage
Anisotropy	0.617	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	13196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.51% 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: ZN, EPE, O6M

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	0.29	0/8780	0.63	0/11886
2	C	0.29	0/3401	0.61	0/4615
3	D	0.32	0/637	0.55	0/851
4	E	0.29	0/585	0.67	0/790
All	All	0.29	0/13403	0.62	0/18142

There are no bond length outliers.

There are no bond angle outliers.

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	8626	0	8625	227	0
2	C	3318	0	3256	121	0
3	D	625	0	617	11	0
4	E	571	0	573	34	0
5	A	30	0	36	3	0
6	C	24	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
All	All	13196	0	13107	352	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 13.

All (352) 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:1104:LYS:HG3	4:E:38:THR:CG2	1.62	1.27
1:A:889:ARG:HG3	1:A:904:ASN:ND2	1.61	1.12
1:A:163:HIS:HD2	1:A:183:GLN:HB3	1.14	1.08
1:A:1104:LYS:HG3	4:E:38:THR:HG21	1.08	1.07
1:A:1104:LYS:HE3	4:E:38:THR:HG22	1.39	1.01
1:A:262:ASN:HD22	1:A:315:THR:HA	1.29	0.94
1:A:889:ARG:HG3	1:A:904:ASN:HD21	1.32	0.92
1:A:1055:GLN:NE2	1:A:1090:ASP:H	1.67	0.92
2:C:51:PRO:O	2:C:595[B]:TYR:OH	1.88	0.91
1:A:163:HIS:CD2	1:A:183:GLN:HB3	2.06	0.90
1:A:114:ARG:HG2	2:C:52:ARG:HH12	1.35	0.89
1:A:504:ASN:HD21	1:A:507:GLN:HE21	1.19	0.87
1:A:1125:THR:HB	1:A:1128:ASP:HB2	1.56	0.86
2:C:395:VAL:HG12	2:C:428:ARG:O	1.77	0.85
1:A:114:ARG:CG	2:C:52:ARG:HH12	1.88	0.85
1:A:53:LYS:HD2	4:E:35:TYR:HB2	1.58	0.84
1:A:1104:LYS:CG	4:E:38:THR:CG2	2.54	0.84
1:A:947:ARG:NH1	1:A:949:PHE:CD1	2.47	0.83
1:A:1104:LYS:CG	4:E:38:THR:HG21	2.03	0.82
1:A:1104:LYS:HE3	4:E:38:THR:CG2	2.10	0.81
1:A:1055:GLN:HE22	1:A:1090:ASP:H	1.28	0.81
1:A:507:GLN:HE22	1:A:553:SER:H	1.28	0.80
1:A:303:GLU:HG2	4:E:4:PHE:CZ	2.17	0.79
1:A:439:ASN:HB2	1:A:442:GLU:HB3	1.64	0.78
2:C:392:LEU:CD1	2:C:394:TYR:CE1	2.66	0.78
2:C:589:LEU:HG	2:C:600:LEU:HD21	1.64	0.77
1:A:1051:LEU:HB2	1:A:1089:ILE:HD13	1.66	0.76
1:A:1051:LEU:CB	1:A:1089:ILE:HD13	2.14	0.76
1:A:1104:LYS:CE	4:E:38:THR:HG22	2.15	0.76
1:A:285:LEU:HD23	1:A:300:LEU:HD23	1.67	0.75
1:A:504:ASN:HD21	1:A:507:GLN:NE2	1.84	0.75
1:A:889:ARG:HG3	1:A:904:ASN:HD22	1.48	0.75
1:A:1125:THR:CB	1:A:1128:ASP:HB2	2.15	0.75
2:C:392:LEU:HD11	2:C:394:TYR:CE1	2.22	0.74
2:C:515:THR:HG22	2:C:516:SER:N	2.03	0.74
1:A:1051:LEU:HB2	1:A:1089:ILE:CD1	2.18	0.74
1:A:114:ARG:NH1	1:A:137:ASP:OD2	2.20	0.73

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:193:CYS:HB3	2:C:196:CYS:HB2	1.72	0.72
1:A:1104:LYS:HG3	4:E:38:THR:HG23	1.70	0.71
1:A:40:GLU:HG2	1:A:54:GLU:HG3	1.72	0.71
2:C:51:PRO:O	2:C:595[A]:TYR:OH	2.07	0.71
2:C:206:ASP:HB2	2:C:207:PRO:HD2	1.72	0.71
1:A:285:LEU:HD23	1:A:300:LEU:CD2	2.20	0.70
1:A:870:VAL:HG11	1:A:873:MET:HE3	1.74	0.70
1:A:372:GLN:OE1	1:A:1014:MET:CG	2.41	0.69
2:C:496:LEU:O	2:C:512:THR:HA	1.93	0.68
1:A:372:GLN:OE1	1:A:1014:MET:HG2	1.92	0.68
1:A:1136:LEU:O	1:A:1139:ILE:HG12	1.93	0.68
1:A:507:GLN:NE2	1:A:553:SER:H	1.91	0.67
4:E:22:ASP:HB2	4:E:26:LYS:O	1.94	0.67
1:A:444:GLU:OE1	1:A:444:GLU:HA	1.93	0.67
1:A:18:CYS:SG	1:A:315:THR:HG23	2.34	0.67
2:C:515:THR:OG1	2:C:536:LEU:HD23	1.95	0.67
1:A:69:PRO:HD2	1:A:72:GLU:HG3	1.76	0.67
2:C:562:TRP:CZ3	4:E:54:ILE:HG22	2.29	0.67
1:A:262:ASN:ND2	1:A:315:THR:HA	2.08	0.66
1:A:439:ASN:HB2	1:A:442:GLU:CB	2.24	0.66
2:C:36:VAL:HG22	2:C:57:LEU:HD13	1.78	0.66
1:A:1113:GLN:HA	1:A:1122:ARG:HA	1.76	0.65
1:A:337:ASN:O	4:E:5:LEU:HD13	1.95	0.65
1:A:167:VAL:HG22	1:A:180:PHE:CB	2.26	0.65
1:A:351:GLU:OE2	4:E:30:ARG:NH1	2.28	0.65
1:A:902:GLU:OE2	1:A:935:TYR:OH	2.13	0.65
1:A:413:LEU:HB3	1:A:424:THR:HB	1.77	0.65
1:A:114:ARG:CG	2:C:52:ARG:NH1	2.60	0.65
1:A:518:TYR:HE2	1:A:572:PRO:HB3	1.61	0.65
2:C:213:ARG:HA	2:C:258:VAL:HG21	1.79	0.65
1:A:261:HIS:CE1	5:A:1301:EPE:H102	2.32	0.65
1:A:184:ASP:HB2	1:A:185:PRO:HD2	1.80	0.64
2:C:219:HIS:HB2	2:C:418:VAL:HG22	1.80	0.64
2:C:268:GLN:NE2	2:C:271:TYR:O	2.31	0.64
2:C:594[B]:ARG:HH21	2:C:594[B]:ARG:HG2	1.63	0.64
1:A:947:ARG:NH1	1:A:949:PHE:CE1	2.65	0.63
1:A:103:ARG:HH11	1:A:103:ARG:HG3	1.63	0.63
1:A:103:ARG:CG	1:A:103:ARG:HH11	2.11	0.63
1:A:268:GLY:O	1:A:285:LEU:HD12	1.97	0.63
1:A:285:LEU:CD2	1:A:300:LEU:CD2	2.76	0.63
2:C:390:THR:O	2:C:390:THR:HG22	1.98	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:395:VAL:HG22	2:C:396:LEU:H	1.63	0.63
2:C:571:TYR:HH	2:C:592[A]:SER:HG	1.24	0.63
1:A:518:TYR:CE2	1:A:572:PRO:HB3	2.33	0.62
1:A:841:ALA:O	2:C:36:VAL:HG23	1.98	0.62
4:E:35:TYR:CE2	4:E:37:PRO:HG3	2.33	0.62
1:A:284:LEU:HD21	4:E:4:PHE:HB3	1.81	0.62
1:A:303:GLU:HG2	4:E:4:PHE:CE2	2.34	0.61
3:D:251:ARG:HG2	3:D:297:THR:OG1	2.01	0.61
1:A:811:GLU:OE1	1:A:847:ARG:NH2	2.33	0.61
1:A:947:ARG:NH1	1:A:949:PHE:HD1	1.93	0.61
1:A:1051:LEU:HB3	1:A:1089:ILE:HD13	1.83	0.60
1:A:791:LEU:HD23	1:A:858:LEU:HD21	1.81	0.60
1:A:620:THR:HB	1:A:622:LEU:HG	1.82	0.60
1:A:811:GLU:CD	1:A:847:ARG:HH21	2.04	0.60
1:A:947:ARG:HH11	1:A:949:PHE:HE1	1.49	0.60
2:C:252:VAL:HG21	2:C:415:LEU:CD1	2.31	0.59
2:C:562:TRP:HZ3	4:E:54:ILE:HG22	1.67	0.59
1:A:926:LEU:O	1:A:953:TRP:HA	2.03	0.59
1:A:487:VAL:HG22	1:A:524:GLN:HB3	1.83	0.59
1:A:998:PHE:HB2	1:A:1088:PHE:CD2	2.37	0.59
2:C:206:ASP:HB2	2:C:207:PRO:CD	2.32	0.59
1:A:167:VAL:HG22	1:A:180:PHE:HB2	1.85	0.58
2:C:60:ARG:HG2	2:C:595[B]:TYR:HB2	1.85	0.58
2:C:205:GLY:O	2:C:206:ASP:HB3	2.03	0.58
2:C:129:PHE:O	2:C:132:GLU:HB2	2.02	0.58
1:A:230:ILE:HD11	1:A:285:LEU:HD21	1.85	0.58
2:C:560:MET:HE1	3:D:260:ASN:HB2	1.85	0.58
2:C:392:LEU:HD11	2:C:394:TYR:HE1	1.67	0.58
2:C:252:VAL:HG21	2:C:415:LEU:HD13	1.85	0.57
1:A:1027:SER:OG	1:A:1039:LEU:HD11	2.04	0.57
1:A:194:GLU:HB2	1:A:203:ASN:HB2	1.85	0.57
1:A:642:ARG:NE	1:A:647:THR:OG1	2.34	0.57
1:A:1055:GLN:NE2	1:A:1090:ASP:N	2.48	0.57
1:A:213:GLU:HG2	1:A:215:GLU:H	1.70	0.57
2:C:414:SER:O	2:C:415:LEU:HD12	2.05	0.57
1:A:39:LEU:HB3	1:A:55:VAL:HG13	1.87	0.57
2:C:255:ALA:HB2	2:C:270:LEU:HD11	1.87	0.56
1:A:564:ILE:HG22	1:A:582:LEU:HB2	1.87	0.56
2:C:395:VAL:HG22	2:C:396:LEU:N	2.21	0.56
1:A:609:GLY:HA3	1:A:632:GLY:O	2.05	0.56
1:A:889:ARG:CG	1:A:904:ASN:ND2	2.54	0.56

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASN:ND2	4:E:15:ASN:O	2.38	0.56
1:A:1104:LYS:CE	4:E:38:THR:CG2	2.81	0.56
2:C:515:THR:CG2	2:C:516:SER:N	2.68	0.56
1:A:102:THR:HB	1:A:1067:LYS:HZ2	1.70	0.55
1:A:1080:ARG:NH1	2:C:593[B]:GLU:OE2	2.39	0.55
1:A:285:LEU:CD2	1:A:300:LEU:HD21	2.36	0.55
3:D:298:PHE:HB2	3:D:304:ALA:HB2	1.88	0.55
1:A:167:VAL:HG22	1:A:180:PHE:HB3	1.87	0.55
2:C:110:TYR:CE2	2:C:125:GLN:HG3	2.42	0.55
1:A:188:ARG:HD2	1:A:214:ALA:O	2.07	0.55
1:A:517:TYR:CD1	1:A:531:HIS:HB3	2.41	0.55
2:C:70:ASP:HB2	2:C:73:PHE:HD2	1.72	0.55
1:A:24:THR:HG22	1:A:91:TYR:CE2	2.42	0.55
1:A:987:GLU:OE1	1:A:991:HIS:HE1	1.90	0.55
1:A:235:GLU:HB2	1:A:254:LYS:HG2	1.89	0.54
1:A:165:ILE:HG12	1:A:188:ARG:NH2	2.22	0.54
1:A:504:ASN:ND2	1:A:507:GLN:HE21	1.98	0.54
1:A:889:ARG:HD2	1:A:891:TYR:CZ	2.43	0.54
4:E:10:VAL:HG11	4:E:13:LYS:HD3	1.90	0.54
1:A:1080:ARG:NH1	2:C:592[A]:SER:OG	2.40	0.53
1:A:607:GLY:HA2	1:A:635:PRO:HB3	1.89	0.53
1:A:402:ILE:HG22	1:A:404:LEU:HG	1.89	0.53
2:C:560:MET:HE1	3:D:260:ASN:CB	2.38	0.53
1:A:213:GLU:OE2	1:A:234:GLN:N	2.41	0.53
2:C:594[B]:ARG:HH21	2:C:594[B]:ARG:CG	2.20	0.53
1:A:372:GLN:OE1	1:A:1014:MET:HG3	2.09	0.53
2:C:253:ALA:O	2:C:270:LEU:HD21	2.08	0.53
1:A:889:ARG:HH11	1:A:904:ASN:HD21	1.56	0.53
1:A:517:TYR:HD1	1:A:531:HIS:HB3	1.73	0.53
1:A:213:GLU:OE1	1:A:236:SER:HB3	2.09	0.53
1:A:809:GLN:O	1:A:810:ASN:HB2	2.09	0.53
2:C:414:SER:C	2:C:415:LEU:HD12	2.29	0.53
1:A:970:ASN:HB2	2:C:49:LEU:HB3	1.90	0.53
1:A:285:LEU:HD22	1:A:297:LEU:HD11	1.92	0.52
1:A:1063:LYS:HB2	4:E:37:PRO:HB2	1.89	0.52
2:C:106:ILE:HG12	2:C:108:HIS:HE1	1.75	0.52
1:A:927:MET:O	2:C:594[B]:ARG:HD2	2.09	0.52
1:A:399:HIS:HE1	1:A:703:THR:OG1	1.91	0.52
1:A:625:ASP:O	1:A:626:ARG:C	2.48	0.52
2:C:126:VAL:HG13	2:C:217:MET:SD	2.50	0.52
1:A:538:VAL:HG22	1:A:558:ILE:HD11	1.91	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:ASN:HB3	1:A:620:THR:OG1	2.10	0.52
1:A:624:SER:O	1:A:625:ASP:HB2	2.10	0.52
2:C:454:ILE:HD13	2:C:494:LEU:HD21	1.91	0.51
1:A:889:ARG:CG	1:A:904:ASN:HD21	2.13	0.51
1:A:428:SER:C	1:A:429:PHE:CD1	2.84	0.51
1:A:2:SER:HB3	1:A:978:GLN:NE2	2.25	0.51
1:A:103:ARG:NH1	1:A:103:ARG:HG3	2.25	0.51
1:A:410:LEU:HG	1:A:680:CYS:SG	2.51	0.51
1:A:397:HIS:CE1	1:A:705:ASP:OD1	2.64	0.51
1:A:905:HIS:CE1	1:A:931:LEU:HD21	2.46	0.51
2:C:219:HIS:HD2	2:C:418:VAL:HG23	1.75	0.50
3:D:267:ARG:O	3:D:271:GLU:HB2	2.11	0.50
4:E:12:ASN:HB3	4:E:15:ASN:ND2	2.26	0.50
1:A:413:LEU:HD11	1:A:468:LEU:HD22	1.92	0.50
2:C:147:SER:HB3	2:C:240:ASP:OD2	2.10	0.50
1:A:1114:TYR:H	1:A:1122:ARG:N	2.09	0.50
1:A:139:LEU:CD2	4:E:54:ILE:HD11	2.41	0.50
3:D:276:ILE:HG21	3:D:279:ILE:HG13	1.94	0.50
4:E:35:TYR:CZ	4:E:37:PRO:HG3	2.47	0.50
1:A:216:ALA:HA	1:A:233:GLY:HA2	1.92	0.50
1:A:916:THR:HG22	1:A:921:ILE:HG12	1.92	0.50
2:C:65:LEU:O	2:C:69:VAL:HG22	2.12	0.49
1:A:999:HIS:HB2	1:A:1075:SER:O	2.12	0.49
1:A:889:ARG:HH11	1:A:904:ASN:ND2	2.09	0.49
1:A:1080:ARG:HH12	2:C:592[A]:SER:CB	2.25	0.49
1:A:770:LEU:HG	1:A:863:GLU:OE1	2.13	0.49
1:A:739:ARG:HH22	1:A:806:GLN:NE2	2.11	0.49
2:C:562:TRP:HZ3	4:E:54:ILE:CG2	2.26	0.49
3:D:271:GLU:N	3:D:272:PRO:CD	2.76	0.49
1:A:41:ILE:O	1:A:52:VAL:HG12	2.13	0.49
2:C:212:LEU:HB3	2:C:439:GLN:HE21	1.78	0.49
1:A:102:THR:HB	1:A:1067:LYS:NZ	2.28	0.48
2:C:456:GLU:O	2:C:460:HIS:HB2	2.13	0.48
2:C:476:ILE:N	2:C:476:ILE:HD12	2.28	0.48
1:A:613:TYR:CD2	1:A:666:LEU:HD22	2.47	0.48
2:C:469:CYS:SG	2:C:499:PHE:CE1	3.06	0.48
1:A:909:ILE:HG12	1:A:928:ARG:HD3	1.94	0.48
2:C:212:LEU:HB3	2:C:439:GLN:NE2	2.27	0.48
1:A:931:LEU:HD12	1:A:947:ARG:HB3	1.95	0.48
1:A:1102:ARG:N	1:A:1103:PRO:HD2	2.28	0.48
1:A:427:LEU:HB3	1:A:429:PHE:HE1	1.79	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:MET:HG2	1:A:912:LEU:HD21	1.95	0.47
2:C:39:GLN:O	2:C:43:VAL:HG23	2.14	0.47
1:A:848:ILE:HG12	1:A:873:MET:CE	2.44	0.47
2:C:395:VAL:CG2	2:C:396:LEU:H	2.27	0.47
1:A:987:GLU:OE1	1:A:991:HIS:CE1	2.68	0.47
1:A:991:HIS:NE2	2:C:88:ARG:NH2	2.61	0.47
1:A:341:ASN:HD21	1:A:345:SER:HB3	1.78	0.47
1:A:1063:LYS:HG3	4:E:40:GLU:HB2	1.96	0.47
1:A:5:TYR:HB2	1:A:1043:LEU:HD11	1.96	0.47
2:C:96:SER:O	2:C:106:ILE:HG22	2.15	0.47
2:C:496:LEU:HD11	2:C:513:TYR:HB2	1.96	0.47
2:C:212:LEU:HD13	2:C:396:LEU:HD13	1.97	0.47
2:C:496:LEU:HD11	2:C:536:LEU:HD22	1.97	0.47
1:A:72:GLU:OE2	1:A:103:ARG:NH2	2.47	0.47
2:C:126:VAL:CG1	2:C:217:MET:SD	3.03	0.47
2:C:106:ILE:HG12	2:C:108:HIS:CE1	2.50	0.47
1:A:435:VAL:C	1:A:436:LEU:HD12	2.36	0.47
1:A:542:ASP:OD2	1:A:592:LEU:HD12	2.15	0.47
2:C:110:TYR:CD2	2:C:125:GLN:HG3	2.50	0.47
2:C:474:TYR:HD2	2:C:476:ILE:HD11	1.80	0.47
1:A:111:ARG:HD3	1:A:111:ARG:HA	1.67	0.47
1:A:182:TYR:HE1	1:A:191:LYS:HB2	1.79	0.47
1:A:215:GLU:HB3	1:A:234:GLN:HB2	1.96	0.47
2:C:219:HIS:HB2	2:C:418:VAL:CG2	2.45	0.47
2:C:496:LEU:CD1	2:C:513:TYR:HB2	2.45	0.46
3:D:316:LEU:O	3:D:317:ALA:HB3	2.16	0.46
2:C:419:VAL:HG12	2:C:427:LEU:HD12	1.97	0.46
2:C:518:LYS:HD3	4:E:59:LEU:HD13	1.96	0.46
1:A:1078:THR:HG23	1:A:1081:LYS:H	1.80	0.46
1:A:843:PRO:HG2	1:A:869:ALA:HB2	1.97	0.46
2:C:213:ARG:HB2	2:C:258:VAL:HG11	1.98	0.46
4:E:22:ASP:HB3	4:E:26:LYS:H	1.79	0.46
1:A:250:PRO:HA	1:A:251:PRO:HD3	1.89	0.46
1:A:410:LEU:HD23	1:A:679:MET:HA	1.97	0.46
2:C:454:ILE:HG23	2:C:494:LEU:HD11	1.98	0.46
2:C:491:ASN:HD21	2:C:516:SER:HB2	1.81	0.46
1:A:285:LEU:HD22	1:A:297:LEU:CD1	2.45	0.46
1:A:38:ARG:NE	1:A:54:GLU:OE1	2.48	0.46
1:A:1074:ARG:O	1:A:1085:ALA:HB2	2.16	0.46
1:A:1055:GLN:HG2	1:A:1093:LEU:HD23	1.98	0.46
2:C:595[B]:TYR:N	2:C:595[B]:TYR:CD1	2.84	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1135:GLU:HG2	1:A:1138:ARG:HH12	1.81	0.46
2:C:389:TYR:CZ	2:C:391:LYS:HB2	2.51	0.46
2:C:83:PHE:O	2:C:575:MET:CE	2.64	0.46
2:C:474:TYR:CD1	2:C:474:TYR:N	2.84	0.45
2:C:217:MET:HE1	2:C:219:HIS:HE1	1.81	0.45
2:C:464:TRP:O	2:C:467:GLN:HG2	2.17	0.45
1:A:522:HIS:HB3	1:A:523:PRO:HD2	1.98	0.45
1:A:726:TYR:OH	1:A:796:GLN:NE2	2.41	0.45
1:A:870:VAL:HG11	1:A:873:MET:CE	2.43	0.45
1:A:358:PRO:HA	1:A:1033:VAL:O	2.17	0.45
1:A:124:ILE:HG12	1:A:131:ILE:HG12	1.99	0.45
1:A:427:LEU:HB3	1:A:429:PHE:CE1	2.51	0.45
1:A:531:HIS:CD2	1:A:531:HIS:N	2.84	0.45
1:A:564:ILE:HG22	1:A:564:ILE:O	2.17	0.45
1:A:146:ASP:OD2	1:A:149:ASN:ND2	2.50	0.45
1:A:508:VAL:HB	1:A:519:LEU:HB2	1.98	0.44
2:C:225:VAL:HG22	2:C:226:TYR:H	1.83	0.44
2:C:268:GLN:HB3	2:C:272:ASP:OD1	2.17	0.44
1:A:677:ASN:HD21	1:A:696:ASN:ND2	2.15	0.44
3:D:279:ILE:HG12	3:D:296:ILE:HG12	2.00	0.44
1:A:494:GLN:O	1:A:494:GLN:HG2	2.17	0.44
1:A:53:LYS:CD	4:E:35:TYR:HB2	2.39	0.44
1:A:1080:ARG:NH2	2:C:85:LYS:O	2.50	0.44
1:A:988:GLU:OE1	2:C:192:ARG:HD3	2.18	0.44
1:A:438:LEU:O	1:A:439:ASN:C	2.56	0.44
1:A:641:PHE:CZ	1:A:648:ASN:HB2	2.53	0.44
1:A:858:LEU:HD12	1:A:858:LEU:HA	1.83	0.44
2:C:143:CYS:HA	2:C:573:ASN:O	2.17	0.44
2:C:82:GLY:O	2:C:90:VAL:HA	2.17	0.44
2:C:568:SER:HB2	2:C:593[B]:GLU:OE2	2.17	0.44
2:C:80:PHE:HA	2:C:92:SER:HB3	2.00	0.44
2:C:515:THR:HG22	2:C:516:SER:H	1.78	0.44
1:A:63:VAL:HB	1:A:80:LEU:HB3	2.00	0.43
1:A:948:ASP:OD2	1:A:994:GLU:OE2	2.36	0.43
2:C:106:ILE:HD11	2:C:127:ARG:HD3	1.99	0.43
1:A:1002:GLU:HG3	1:A:1036:MET:SD	2.58	0.43
2:C:560:MET:HB3	2:C:560:MET:HE2	1.94	0.43
1:A:1002:GLU:OE1	1:A:1034:ASN:HB2	2.19	0.43
1:A:625:ASP:O	1:A:627:LYS:N	2.52	0.43
1:A:917:LYS:HD3	1:A:962:ASP:OD1	2.18	0.43
2:C:224:VAL:HG22	2:C:248:SER:OG	2.18	0.43

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1301:EPE:H81	5:A:1301:EPE:H32	1.83	0.43
1:A:10:GLN:OE1	1:A:710:LEU:HD12	2.18	0.43
2:C:486:ASN:HB3	2:C:523:LEU:HB2	2.01	0.43
1:A:591:ILE:HG12	1:A:602:LEU:HD11	2.01	0.43
1:A:596:PHE:HB3	1:A:661:SER:HB2	2.01	0.43
1:A:532:THR:HG22	1:A:574:PHE:CD2	2.54	0.43
1:A:334:VAL:HG12	1:A:349:ALA:HA	2.00	0.42
2:C:93:TYR:HA	2:C:108:HIS:O	2.18	0.42
1:A:417:PRO:HB2	1:A:466:GLN:HE21	1.83	0.42
2:C:178:ARG:HH22	3:D:271:GLU:CD	2.22	0.42
2:C:193:CYS:HB3	2:C:196:CYS:CB	2.46	0.42
2:C:242:VAL:HG22	2:C:255:ALA:HB2	2.01	0.42
2:C:387:VAL:HG22	2:C:388:ASN:H	1.84	0.42
1:A:391:ARG:HG2	1:A:392:ASN:O	2.20	0.42
2:C:395:VAL:N	2:C:428:ARG:O	2.52	0.42
2:C:217:MET:HE1	2:C:219:HIS:CE1	2.53	0.42
2:C:255:ALA:HB3	2:C:270:LEU:HD13	2.00	0.42
1:A:235:GLU:CB	1:A:254:LYS:HG2	2.49	0.42
1:A:807:PHE:CZ	1:A:831:VAL:HG11	2.54	0.42
2:C:268:GLN:NE2	2:C:389:TYR:CE2	2.87	0.42
4:E:8:LEU:HA	4:E:8:LEU:HD12	1.90	0.42
1:A:929:SER:HB2	1:A:950:ASN:O	2.18	0.42
2:C:70:ASP:HB2	2:C:73:PHE:CD2	2.54	0.42
1:A:246:LEU:HD12	1:A:246:LEU:HA	1.88	0.42
1:A:262:ASN:HD22	1:A:315:THR:CA	2.16	0.42
1:A:265:ASP:OD2	1:A:270:ARG:HB2	2.20	0.42
1:A:936:LYS:HE2	1:A:943:GLU:OE2	2.19	0.42
2:C:552:ARG:O	2:C:556:VAL:HG23	2.20	0.42
1:A:405:PRO:HA	1:A:697:SER:HA	2.02	0.42
1:A:492:GLU:HG2	1:A:493:PRO:HD2	2.01	0.41
1:A:284:LEU:HD11	4:E:4:PHE:HB2	2.02	0.41
1:A:110:ASP:HB2	1:A:136:TYR:CE2	2.55	0.41
2:C:157:PHE:HD1	2:C:180:ILE:HG12	1.85	0.41
2:C:184:THR:O	2:C:217:MET:HA	2.20	0.41
1:A:215:GLU:CB	1:A:234:GLN:HB2	2.50	0.41
2:C:83:PHE:O	2:C:575:MET:HE3	2.20	0.41
1:A:165:ILE:HG12	1:A:188:ARG:CZ	2.50	0.41
1:A:448:LEU:HD12	1:A:448:LEU:HA	1.95	0.41
1:A:731:GLN:HA	1:A:796:GLN:HE21	1.84	0.41
2:C:219:HIS:CD2	2:C:418:VAL:HG23	2.54	0.41
1:A:413:LEU:HD13	1:A:461:GLY:HA2	2.01	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:489:GLU:OE2	1:A:491:LYS:HE3	2.20	0.41
1:A:610:ALA:HB1	1:A:628:LYS:HE3	2.03	0.41
2:C:255:ALA:CB	2:C:270:LEU:CD1	2.98	0.41
1:A:490:TRP:CG	1:A:519:LEU:HD21	2.56	0.41
1:A:703:THR:HG21	4:E:22:ASP:OD1	2.21	0.41
2:C:252:VAL:HG21	2:C:415:LEU:HD11	2.02	0.41
2:C:396:LEU:O	2:C:397:GLU:CB	2.69	0.41
1:A:238:THR:HG21	1:A:245:TYR:HE1	1.86	0.41
1:A:393:GLY:O	1:A:711:HIS:HB2	2.21	0.41
1:A:848:ILE:HG23	1:A:873:MET:HE2	2.02	0.41
1:A:947:ARG:HH12	1:A:949:PHE:HD1	1.68	0.41
2:C:390:THR:O	2:C:390:THR:CG2	2.65	0.41
2:C:491:ASN:O	2:C:551:TYR:OH	2.39	0.40
1:A:927:MET:HB2	2:C:594[B]:ARG:HG3	2.03	0.40
1:A:1126:ALA:O	1:A:1130:ILE:HG13	2.20	0.40
1:A:571:LEU:HA	1:A:572:PRO:HA	1.89	0.40
1:A:578:HIS:CE1	1:A:580:GLU:HG2	2.57	0.40
1:A:487:VAL:HG21	1:A:524:GLN:CG	2.52	0.40
1:A:520:GLN:HG3	1:A:529:ILE:HG13	2.04	0.40
1:A:605:ALA:HB1	1:A:636:THR:HB	2.04	0.40
2:C:272:ASP:O	2:C:273:HIS:CB	2.69	0.40
3:D:253:TYR:O	3:D:323:VAL:HA	2.22	0.40
5:A:1302:EPE:H22	5:A:1302:EPE:H101	1.84	0.40
1:A:516:LEU:HA	1:A:516:LEU:HD12	1.94	0.40
2:C:189:PRO:HA	2:C:214:HIS:CD2	2.56	0.40
2:C:78:HIS:HD2	2:C:92:SER:OG	2.04	0.40
1:A:48:GLY:HA2	4:E:16:PHE:CD1	2.56	0.40
1:A:58:TYR:CD2	1:A:1064:SER:HB2	2.56	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	1081/1140 (95%)	1036 (96%)	44 (4%)	1 (0%)	51	82
2	C	391/498 (78%)	368 (94%)	19 (5%)	4 (1%)	15	45
3	D	78/109 (72%)	76 (97%)	2 (3%)	0	100	100
4	E	67/102 (66%)	62 (92%)	5 (8%)	0	100	100
All	All	1617/1849 (88%)	1542 (95%)	70 (4%)	5 (0%)	41	71

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	206	ASP
2	C	397	GLU
1	A	444	GLU
2	C	116	VAL
2	C	248	SER

### 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	966/999 (97%)	951 (98%)	15 (2%)	62	86
2	C	373/438 (85%)	360 (96%)	13 (4%)	36	70
3	D	67/89 (75%)	67 (100%)	0	100	100
4	E	63/93 (68%)	59 (94%)	4 (6%)	18	46
All	All	1469/1619 (91%)	1437 (98%)	32 (2%)	53	81

All (32) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	103	ARG
1	A	108	VAL
1	A	111	ARG
1	A	269	SER
1	A	438	LEU
1	A	439	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	442	GLU
1	A	570	LYS
1	A	642	ARG
1	A	863	GLU
1	A	927	MET
1	A	947	ARG
1	A	969	GLU
1	A	1036	MET
1	A	1064	SER
2	C	129	PHE
2	C	151	LYS
2	C	211	CYS
2	C	256	VAL
2	C	271	TYR
2	C	272	ASP
2	C	460	HIS
2	C	472	SER
2	C	474	TYR
2	C	496	LEU
2	C	524	ASN
2	C	592[A]	SER
2	C	592[B]	SER
4	E	3	ASP
4	E	30	ARG
4	E	43	SER
4	E	45	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	109	GLN
1	A	156	ASN
1	A	163	HIS
1	A	209	GLN
1	A	262	ASN
1	A	290	GLN
1	A	399	HIS
1	A	439	ASN
1	A	456	GLN
1	A	466	GLN
1	A	507	GLN
1	A	531	HIS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	578	HIS
1	A	696	ASN
1	A	711	HIS
1	A	796	GLN
1	A	806	GLN
1	A	845	GLN
1	A	904	ASN
1	A	1025	GLN
1	A	1055	GLN
2	C	78	HIS
2	C	108	HIS
2	C	197	GLN
2	C	214	HIS
2	C	439	GLN
2	C	486	ASN
2	C	491	ASN
2	C	514	HIS
4	E	45	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 4 ligands modelled in this entry, 1 is 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	$\# Z  > 2$
5	EPE	A	1302	-	15,15,15	2.04	1 (6%)	18,20,20	1.22	2 (11%)
6	O6M	C	901	-	24,26,26	0.73	0	30,38,38	0.89	2 (6%)
5	EPE	A	1301	-	15,15,15	1.95	2 (13%)	18,20,20	6.14	5 (27%)

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
5	EPE	A	1302	-	-	6/9/19/19	0/1/1/1
6	O6M	C	901	-	-	2/13/15/15	0/3/3/3
5	EPE	A	1301	-	-	4/9/19/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1302	EPE	C10-S	-7.61	1.66	1.77
5	A	1301	EPE	C10-S	-6.85	1.67	1.77
5	A	1301	EPE	O2S-S	2.45	1.52	1.45

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1301	EPE	O1S-S-C10	-16.71	86.80	106.92
5	A	1301	EPE	O2S-S-C10	-13.65	90.48	106.92
5	A	1301	EPE	O3S-S-C10	-13.39	84.11	105.77
5	A	1301	EPE	O3S-S-O1S	4.02	121.10	111.27
5	A	1302	EPE	O3S-S-C10	3.24	111.00	105.77
5	A	1301	EPE	O3S-S-O2S	2.85	118.23	111.27
5	A	1302	EPE	O2S-S-C10	2.43	109.84	106.92
6	C	901	O6M	C13-C5-N1	2.30	118.77	115.50
6	C	901	O6M	C2-C17-C13	-2.16	119.13	122.67

There are no chirality outliers.

All (12) torsion outliers are listed below:

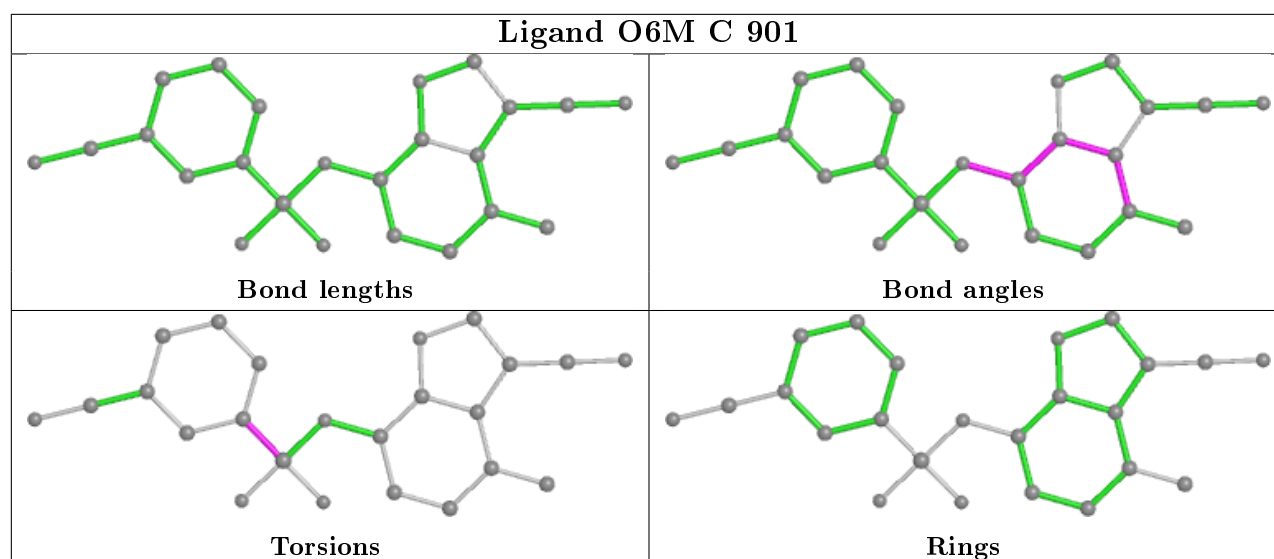
Mol	Chain	Res	Type	Atoms
5	A	1302	EPE	C10-C9-N1-C2
5	A	1302	EPE	C9-C10-S-O1S
5	A	1301	EPE	S-C10-C9-N1
5	A	1301	EPE	C9-C10-S-O1S
5	A	1301	EPE	C9-C10-S-O2S
5	A	1302	EPE	N4-C7-C8-O8
5	A	1302	EPE	C9-C10-S-O3S
5	A	1301	EPE	C9-C10-S-O3S
5	A	1302	EPE	C9-C10-S-O2S
6	C	901	O6M	C12-C6-S1-O1
6	C	901	O6M	C7-C6-S1-O1
5	A	1302	EPE	S-C10-C9-N1

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1302	EPE	1	0
5	A	1301	EPE	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 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

### 6.1 Protein, DNA and RNA chains

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	1099/1140 (96%)	0.20	27 (2%) 57 55	47, 80, 126, 158	0
2	C	401/498 (80%)	0.48	34 (8%) 10 8	59, 87, 135, 163	0
3	D	80/109 (73%)	0.18	0 100 100	66, 88, 113, 129	0
4	E	69/102 (67%)	0.29	4 (5%) 23 19	69, 89, 118, 144	0
All	All	1649/1849 (89%)	0.27	65 (3%) 39 35	47, 83, 128, 163	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	594[A]	ARG	6.6
1	A	451	PHE	5.3
1	A	413	LEU	4.9
1	A	448	LEU	4.7
2	C	75	TYR	4.5
1	A	692	ALA	4.4
2	C	100	ASP	4.2
2	C	431	ARG	4.0
1	A	419	ARG	3.9
2	C	387	VAL	3.8
2	C	101	ASP	3.8
1	A	693	LEU	3.6
1	A	742	VAL	3.6
2	C	131	ASP	3.5
2	C	130	GLN	3.4
2	C	103	SER	3.2
1	A	480	SER	3.1
4	E	70	LYS	3.0
2	C	219	HIS	3.0
2	C	135	TYR	3.0
1	A	414	ARG	3.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	392	LEU	2.9
2	C	592[A]	SER	2.9
1	A	1025	GLN	2.8
2	C	134	ILE	2.7
2	C	98	GLY	2.7
1	A	449	MET	2.7
2	C	441	LEU	2.7
1	A	486	LEU	2.6
1	A	435	VAL	2.6
2	C	221	LYS	2.6
1	A	685	ASP	2.6
2	C	527	ILE	2.5
2	C	99	ASP	2.5
2	C	443	VAL	2.5
1	A	402	ILE	2.5
2	C	568	SER	2.5
2	C	398	SER	2.5
1	A	433	THR	2.5
2	C	440	TYR	2.5
1	A	412	PRO	2.4
1	A	468	LEU	2.4
4	E	41	TYR	2.4
1	A	418	ASN	2.3
2	C	390	THR	2.2
1	A	521	ILE	2.2
1	A	485	ALA	2.2
2	C	593[A]	GLU	2.2
1	A	749	THR	2.2
2	C	133	GLU	2.2
1	A	487	VAL	2.2
1	A	148	ASP	2.1
2	C	202	ALA	2.1
1	A	420	GLU	2.1
2	C	425	ARG	2.1
4	E	67	ASN	2.1
2	C	104	PHE	2.1
2	C	203	HIS	2.1
1	A	437	MET	2.1
2	C	102	PHE	2.1
4	E	43	SER	2.0
2	C	413	ILE	2.0
1	A	552	LEU	2.0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
2	C	71	GLU	2.0
2	C	418	VAL	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](#)

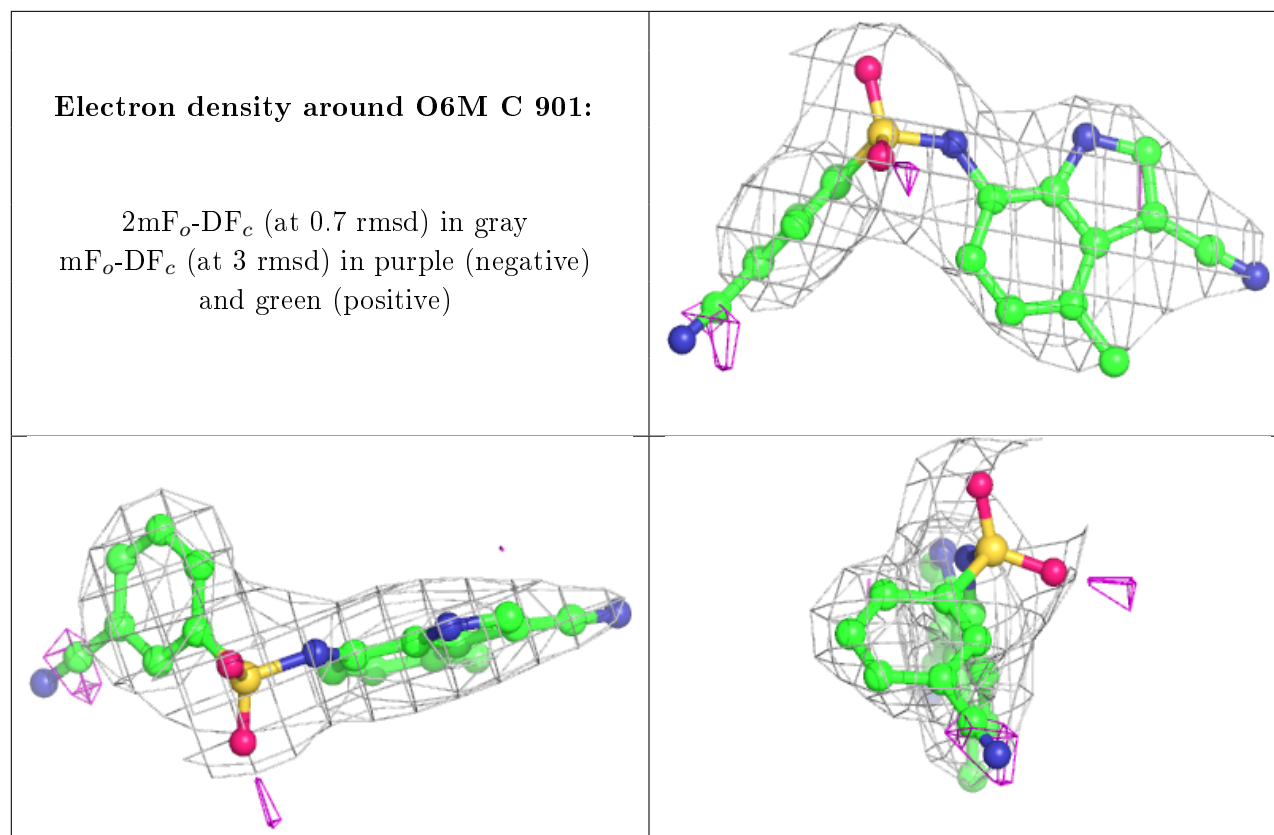
There are no carbohydrates in this entry.

## 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. 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	EPE	A	1301	15/15	0.95	0.18	63,68,72,74	0
6	O6M	C	901	24/24	0.96	0.26	56,63,78,95	0
5	EPE	A	1302	15/15	0.96	0.22	73,87,105,110	0
7	ZN	C	902	1/1	0.99	0.12	97,97,97,97	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.