Full wwPDB X-ray Structure Validation Report ⓘ

Nov 22, 2023 – 11:53 AM JST

PDB ID	:	7VPR
Title	:	Crystal structure of the ligand-binding domain of C. glabrata Upc2 in complex with ergosterol
Authors	:	Tan, L.; Im, Y.J.
Deposited on	:	2021-10-17
Resolution	:	2.59 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

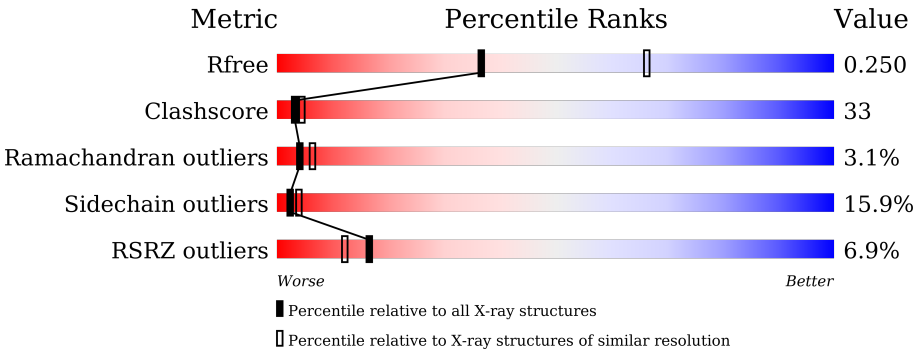
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	308	5% 56% 29% 7% 9%
1	B	308	9% 47% 34% 9% • 9%
1	C	308	5% 48% 34% 8% • 8%
1	D	308	6% 40% 29% 11% • 18%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9014 atoms, of which 176 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 Sterol uptake control protein 2 (Upc2).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	281	Total	C	N	O	S	0	0	0
			2215	1437	352	413	13			
1	B	280	Total	C	N	O	S	0	0	0
			2208	1431	351	413	13			
1	C	282	Total	C	N	O	S	0	0	0
			2223	1441	353	416	13			
1	D	253	Total	C	N	O	S	0	0	0
			2012	1313	322	366	11			

There are 24 discrepancies between the modelled and reference sequences:

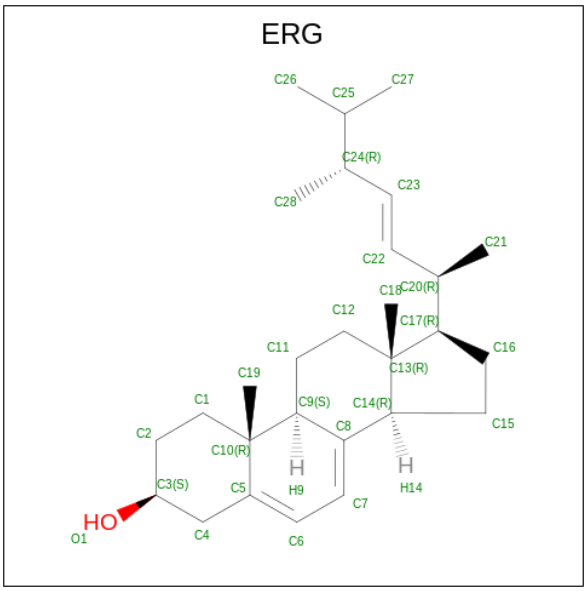
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	GLY	-	expression tag	UNP Q6FX18
A	616	SER	-	expression tag	UNP Q6FX18
A	617	ALA	-	expression tag	UNP Q6FX18
A	618	MET	-	expression tag	UNP Q6FX18
A	619	GLY	-	expression tag	UNP Q6FX18
A	620	SER	-	expression tag	UNP Q6FX18
B	615	GLY	-	expression tag	UNP Q6FX18
B	616	SER	-	expression tag	UNP Q6FX18
B	617	ALA	-	expression tag	UNP Q6FX18
B	618	MET	-	expression tag	UNP Q6FX18
B	619	GLY	-	expression tag	UNP Q6FX18
B	620	SER	-	expression tag	UNP Q6FX18
C	615	GLY	-	expression tag	UNP Q6FX18
C	616	SER	-	expression tag	UNP Q6FX18
C	617	ALA	-	expression tag	UNP Q6FX18
C	618	MET	-	expression tag	UNP Q6FX18
C	619	GLY	-	expression tag	UNP Q6FX18
C	620	SER	-	expression tag	UNP Q6FX18
D	615	GLY	-	expression tag	UNP Q6FX18
D	616	SER	-	expression tag	UNP Q6FX18
D	617	ALA	-	expression tag	UNP Q6FX18

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	618	MET	-	expression tag	UNP Q6FX18
D	619	GLY	-	expression tag	UNP Q6FX18
D	620	SER	-	expression tag	UNP Q6FX18

- Molecule 2 is ERGOSTEROL (three-letter code: ERG) (formula: $C_{28}H_{44}O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			73	28	44	1		
2	B	1	Total	C	H	O	0	0
			73	28	44	1		
2	C	1	Total	C	H	O	0	0
			73	28	44	1		
2	D	1	Total	C	H	O	0	0
			73	28	44	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	16	Total	O	0	0
			16	16		
3	B	22	Total	O	0	0
			22	22		
3	C	14	Total	O	0	0
			14	14		

Continued on next page...

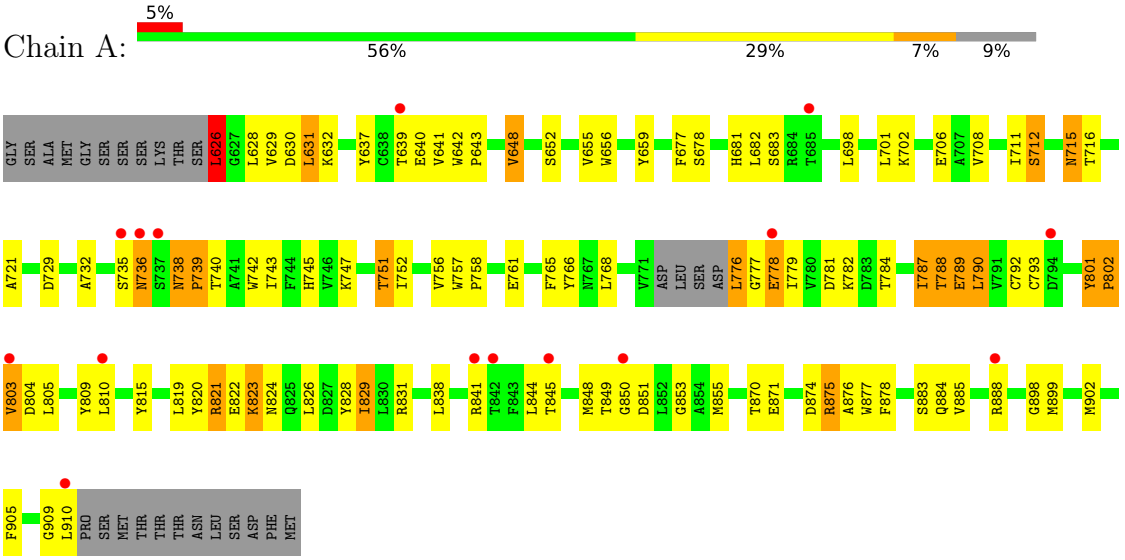
Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	12	Total O 12 12	0	0

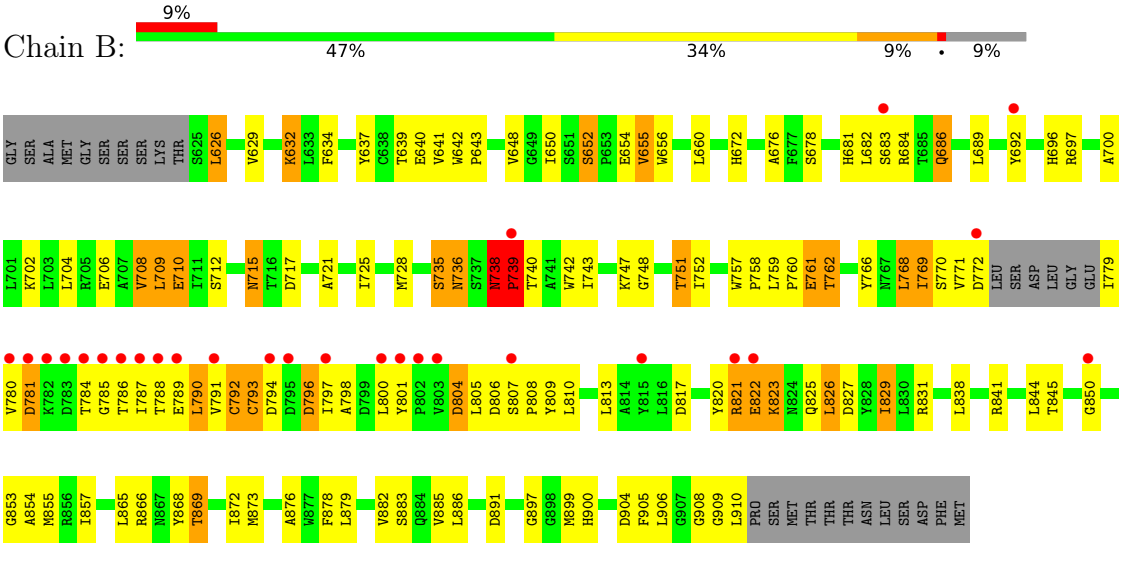
3 Residue-property plots (i)

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

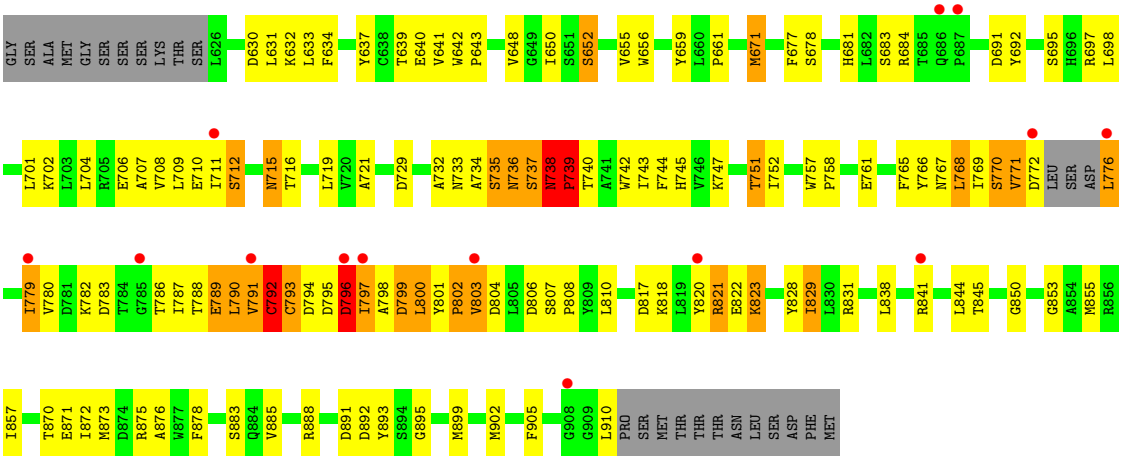
• Molecule 1: Sterol uptake control protein 2 (Upc2)



• Molecule 1: Sterol uptake control protein 2 (Upc2)

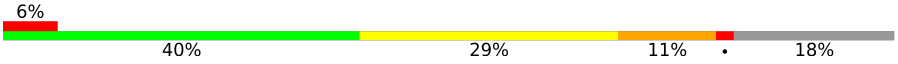


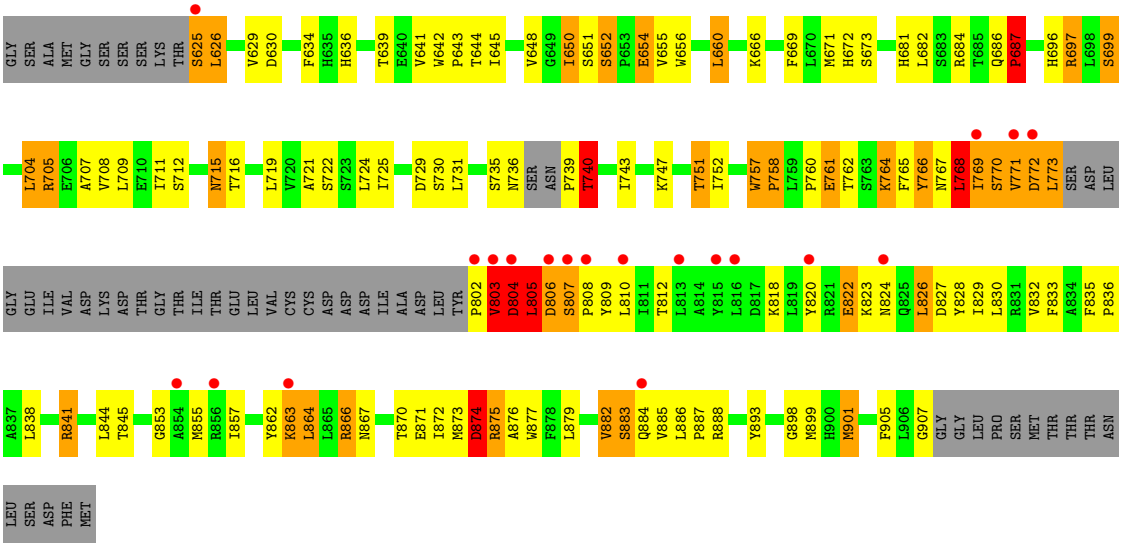
• Molecule 1: Sterol uptake control protein 2 (Upc2)



• Molecule 1: Sterol uptake control protein 2 (Upc2)

Chain D:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.42Å 105.63Å 98.87Å 90.00° 93.28° 90.00°	Depositor
Resolution (Å)	27.60 – 2.59 38.20 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.0 (27.60-2.59) 94.0 (38.20-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	-0.26 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.231 , 0.250 0.230 , 0.250	Depositor DCC
R_{free} test set	1723 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å^2)	41.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	9014	wwPDB-VP
Average B, all atoms (Å^2)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ERG

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	0.89	3/2267 (0.1%)	0.89	2/3089 (0.1%)
1	B	1.07	2/2260 (0.1%)	0.96	8/3080 (0.3%)
1	C	0.77	0/2275	0.83	4/3100 (0.1%)
1	D	1.09	1/2062 (0.0%)	0.88	2/2806 (0.1%)
All	All	0.96	6/8864 (0.1%)	0.89	16/12075 (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
1	B	0	1
All	All	0	2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	802	PRO	N-CA	12.57	1.68	1.47
1	B	739	PRO	N-CA	12.56	1.68	1.47
1	B	738	ASN	C-N	5.56	1.44	1.34
1	A	801	TYR	C-N	5.43	1.44	1.34
1	D	757	TRP	CB-CG	-5.27	1.40	1.50
1	A	871	GLU	C-O	5.09	1.33	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	739	PRO	N-CA-CB	-9.69	91.68	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	739	PRO	CA-N-CD	-8.90	99.04	111.50
1	A	802	PRO	CA-N-CD	-7.99	100.31	111.50
1	B	804	ASP	CB-CA-C	-6.66	97.08	110.40
1	C	792	CYS	CA-C-N	-6.06	103.87	117.20
1	B	807	SER	C-N-CD	5.70	140.38	128.40
1	B	735	SER	C-N-CA	5.68	135.89	121.70
1	B	736	ASN	CB-CA-C	5.42	121.25	110.40
1	B	736	ASN	N-CA-C	-5.21	96.94	111.00
1	C	799	ASP	CB-CG-OD2	5.20	122.98	118.30
1	D	687	PRO	CA-N-CD	-5.17	104.26	111.50
1	B	759	LEU	C-N-CD	5.07	139.05	128.40
1	C	793	CYS	N-CA-C	5.07	124.68	111.00
1	A	626	LEU	CA-CB-CG	5.05	126.92	115.30
1	D	807	SER	C-N-CD	5.03	138.97	128.40
1	C	807	SER	C-N-CD	5.02	138.94	128.40

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	776	LEU	Mainchain
1	B	738	ASN	Peptide

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	2215	0	2209	127	0
1	B	2208	0	2198	150	1
1	C	2223	0	2212	151	3
1	D	2012	0	2018	160	2
2	A	29	44	44	4	0
2	B	29	44	44	2	0
2	C	29	44	44	3	0
2	D	29	44	44	9	0
3	A	16	0	0	7	0
3	B	22	0	0	7	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	14	0	0	0	0
3	D	12	0	0	1	0
All	All	8838	176	8813	587	3

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 (587) 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:779:ILE:HD11	1:A:790:LEU:CD1	1.33	1.56
1:A:738:ASN:ND2	1:A:739:PRO:HD3	1.32	1.37
1:D:771:VAL:HG21	1:D:818:LYS:CE	1.53	1.37
1:A:802:PRO:N	1:A:802:PRO:CA	1.68	1.36
1:B:739:PRO:N	1:B:739:PRO:CA	1.68	1.35
1:B:850:GLY:HA2	1:B:855:MET:CE	1.57	1.34
1:A:779:ILE:CD1	1:A:790:LEU:HD11	1.64	1.28
1:A:736:ASN:HB2	1:A:884:GLN:NE2	1.50	1.26
1:D:771:VAL:CG2	1:D:818:LYS:HE3	1.67	1.22
1:B:708:VAL:CG2	1:B:752:ILE:HD12	1.72	1.17
1:C:738:ASN:HB3	1:C:739:PRO:HA	1.20	1.15
1:D:771:VAL:HG21	1:D:818:LYS:HE2	1.19	1.15
1:A:708:VAL:CG1	1:A:752:ILE:HD12	1.77	1.15
1:A:738:ASN:ND2	1:A:739:PRO:CD	2.10	1.13
1:A:779:ILE:HG13	1:A:787:ILE:HD13	1.25	1.12
1:B:708:VAL:HG23	1:B:752:ILE:HD12	1.30	1.11
1:B:760:PRO:HB2	1:B:762:THR:HG23	1.29	1.11
1:D:644:THR:HG21	1:D:877:TRP:NE1	1.65	1.11
1:B:850:GLY:HA2	1:B:855:MET:HE1	1.29	1.10
1:B:850:GLY:HA2	1:B:855:MET:HE3	1.31	1.10
1:D:771:VAL:CG2	1:D:818:LYS:CE	2.26	1.08
1:A:736:ASN:CB	1:A:884:GLN:NE2	2.18	1.07
1:D:802:PRO:HA	1:D:803:VAL:HG13	1.33	1.06
1:B:757:TRP:CG	1:B:838:LEU:HD22	1.92	1.05
1:A:757:TRP:CG	1:A:838:LEU:HD22	1.92	1.05
1:C:769:ILE:HD13	1:C:838:LEU:HD12	1.37	1.05
1:C:757:TRP:CG	1:C:838:LEU:HD22	1.92	1.04
1:D:771:VAL:HG23	1:D:818:LYS:HE3	1.36	1.04
1:A:849:THR:C	3:A:1101:HOH:O	1.94	1.03
1:A:736:ASN:CB	1:A:884:GLN:HE22	1.71	1.03
1:A:738:ASN:CG	1:A:739:PRO:HD2	1.78	1.02

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:GLY:N	3:A:1101:HOH:O	1.90	1.02
1:A:779:ILE:CD1	1:A:790:LEU:CD1	2.28	1.02
1:C:739:PRO:HB2	1:C:742:TRP:HE1	1.17	1.02
1:C:776:LEU:HD23	1:C:810:LEU:HD21	1.44	0.98
1:A:738:ASN:CG	1:A:739:PRO:CD	2.30	0.98
1:A:708:VAL:HG11	1:A:752:ILE:HD12	1.44	0.98
1:D:644:THR:HG21	1:D:877:TRP:CD1	1.98	0.98
1:A:902:MET:HG3	2:A:1001:ERG:C6	1.96	0.96
1:D:841:ARG:O	1:D:845:THR:HG23	1.66	0.96
1:A:736:ASN:HB2	1:A:884:GLN:HE22	0.80	0.95
1:A:781:ASP:HB2	1:A:788:THR:CG2	1.98	0.94
1:A:708:VAL:HG13	1:A:752:ILE:HD12	1.45	0.94
1:B:708:VAL:CG2	1:B:752:ILE:CD1	2.45	0.94
1:B:708:VAL:HG21	1:B:752:ILE:CD1	1.99	0.93
1:C:776:LEU:HD23	1:C:810:LEU:CD2	1.98	0.93
1:A:626:LEU:N	3:A:1102:HOH:O	2.01	0.93
1:B:850:GLY:CA	1:B:855:MET:CE	2.47	0.92
1:A:779:ILE:HD11	1:A:790:LEU:HD12	1.49	0.92
1:B:850:GLY:CA	1:B:855:MET:HE1	1.98	0.91
1:D:802:PRO:CA	1:D:803:VAL:HG13	2.00	0.89
1:D:644:THR:HG21	1:D:877:TRP:HE1	1.27	0.89
1:A:779:ILE:HG13	1:A:787:ILE:CD1	2.02	0.88
1:A:781:ASP:HB2	1:A:788:THR:HG22	1.56	0.88
1:A:738:ASN:HD22	1:A:739:PRO:HD3	1.35	0.87
1:D:893:TYR:CD1	1:D:901:MET:HG3	2.10	0.87
1:D:870:THR:CG2	1:D:883:SER:HB2	2.05	0.86
1:D:757:TRP:CG	1:D:838:LEU:HD22	2.09	0.86
1:C:779:ILE:HG23	1:C:790:LEU:HD11	1.58	0.86
1:D:697:ARG:HD2	1:D:729:ASP:OD2	1.77	0.85
1:B:788:THR:HG23	1:B:789:GLU:HG2	1.58	0.85
1:A:735:SER:H	1:A:738:ASN:HB2	1.41	0.85
1:D:644:THR:CG2	1:D:877:TRP:HE1	1.90	0.85
1:C:771:VAL:HG23	1:C:772:ASP:H	1.40	0.84
1:C:739:PRO:HB2	1:C:742:TRP:NE1	1.92	0.84
1:D:805:LEU:HD13	1:D:805:LEU:H	1.42	0.83
1:C:738:ASN:CB	1:C:739:PRO:HA	2.03	0.83
1:D:697:ARG:CD	1:D:729:ASP:OD2	2.26	0.83
1:C:739:PRO:HB3	1:C:885:VAL:CG2	2.09	0.83
1:C:708:VAL:HG21	1:C:752:ILE:HD12	1.61	0.83
1:D:681:HIS:O	1:D:681:HIS:ND1	2.13	0.82
1:B:712:SER:H	1:B:715:ASN:HD21	1.28	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:762:THR:OG1	3:B:1101:HOH:O	1.98	0.81
1:D:634:PHE:HD1	1:D:671:MET:HE1	1.44	0.81
1:A:648:VAL:HG22	1:A:876:ALA:HB2	1.62	0.81
1:D:644:THR:CG2	1:D:877:TRP:CD1	2.62	0.81
1:D:644:THR:CG2	1:D:877:TRP:NE1	2.43	0.81
1:C:708:VAL:CG2	1:C:752:ILE:HD12	2.10	0.80
1:B:757:TRP:CH2	1:B:769:ILE:HG12	2.16	0.80
1:A:736:ASN:HA	1:A:884:GLN:NE2	1.97	0.80
1:C:648:VAL:HA	1:C:875:ARG:HD2	1.63	0.79
1:D:645:ILE:O	1:D:648:VAL:HG12	1.82	0.79
1:D:812:THR:OG1	3:D:1101:HOH:O	2.00	0.78
1:C:712:SER:O	1:C:715:ASN:ND2	2.17	0.78
1:A:708:VAL:HG11	1:A:752:ILE:CD1	2.13	0.78
1:B:708:VAL:HG21	1:B:752:ILE:HD13	1.64	0.78
1:B:710:GLU:OE1	1:B:710:GLU:HA	1.85	0.77
1:B:757:TRP:CD1	1:B:838:LEU:HD22	2.20	0.77
1:C:850:GLY:HA2	1:C:855:MET:HE1	1.67	0.77
1:A:855:MET:HE2	1:A:899:MET:HG3	1.67	0.77
1:D:802:PRO:CB	1:D:803:VAL:HG22	2.14	0.77
1:C:757:TRP:CD1	1:C:838:LEU:HD22	2.20	0.77
1:D:870:THR:HG22	1:D:883:SER:HB2	1.67	0.77
1:C:738:ASN:HB3	1:C:739:PRO:CA	2.11	0.76
1:C:739:PRO:HB3	1:C:885:VAL:HG23	1.66	0.76
1:C:850:GLY:HA2	1:C:855:MET:CE	2.15	0.76
1:D:863:LYS:NZ	1:D:867:ASN:HD21	1.83	0.76
1:A:757:TRP:CD1	1:A:838:LEU:HD22	2.20	0.76
1:A:855:MET:CE	1:A:899:MET:HG3	2.16	0.75
1:C:769:ILE:HD13	1:C:838:LEU:CD1	2.14	0.75
1:D:769:ILE:HD12	1:D:770:SER:N	2.02	0.74
1:A:747:LYS:O	1:A:751:THR:HG22	1.87	0.74
1:A:648:VAL:CG2	1:A:876:ALA:HB2	2.17	0.74
1:D:747:LYS:O	1:D:751:THR:HG22	1.87	0.74
1:B:652:SER:HB2	1:B:655:VAL:HG22	1.68	0.74
1:B:780:VAL:HG12	1:B:790:LEU:HD11	1.69	0.74
1:C:747:LYS:O	1:C:751:THR:HG22	1.87	0.74
1:D:735:SER:O	1:D:736:ASN:ND2	2.20	0.74
1:D:712:SER:H	1:D:715:ASN:HD21	1.35	0.74
1:D:862:TYR:OH	1:D:887:PRO:O	2.02	0.74
1:A:736:ASN:CA	1:A:884:GLN:NE2	2.50	0.73
1:B:905:PHE:CE1	2:B:1001:ERG:H22	2.24	0.73
1:A:736:ASN:HA	1:A:884:GLN:CD	2.09	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:LEU:HB3	1:A:630:ASP:OD2	1.88	0.73
1:C:697:ARG:HD2	1:C:729:ASP:OD2	1.88	0.73
1:D:802:PRO:HB3	1:D:803:VAL:CG2	2.19	0.72
1:B:850:GLY:O	3:B:1102:HOH:O	2.07	0.72
1:B:855:MET:CE	1:B:899:MET:SD	2.78	0.72
1:C:787:ILE:O	1:C:802:PRO:HB3	1.88	0.72
1:D:829:ILE:HD11	1:D:833:PHE:CZ	2.24	0.72
1:B:787:ILE:HD11	1:B:810:LEU:HD12	1.71	0.72
1:D:656:TRP:HA	1:D:660:LEU:HD22	1.69	0.72
1:B:850:GLY:CA	1:B:855:MET:HE3	2.16	0.72
1:D:874:ASP:OD1	1:D:874:ASP:N	2.20	0.71
1:C:771:VAL:CG2	1:C:818:LYS:HE3	2.20	0.71
1:C:736:ASN:OD1	1:C:736:ASN:N	2.23	0.71
1:A:779:ILE:HD11	1:A:790:LEU:HD11	0.72	0.71
1:A:851:ASP:N	3:A:1101:HOH:O	2.07	0.71
1:D:651:SER:O	1:D:652:SER:OG	2.09	0.71
1:B:873:MET:CE	1:B:883:SER:H	2.04	0.70
1:D:704:LEU:HG	1:D:752:ILE:HG13	1.73	0.70
1:B:891:ASP:CG	3:B:1103:HOH:O	2.29	0.70
1:D:634:PHE:CD1	1:D:671:MET:HE1	2.25	0.70
1:A:712:SER:H	1:A:715:ASN:HD21	1.40	0.70
1:A:848:MET:SD	1:A:902:MET:CE	2.80	0.70
1:B:652:SER:HB2	1:B:655:VAL:CG2	2.21	0.70
1:B:797:ILE:HD11	1:B:801:TYR:HE1	1.55	0.70
1:A:805:LEU:HA	1:A:810:LEU:HD22	1.74	0.69
1:B:855:MET:HE1	1:B:899:MET:SD	2.32	0.69
1:D:855:MET:CE	2:D:1001:ERG:O1	2.41	0.69
1:B:891:ASP:OD1	3:B:1103:HOH:O	2.11	0.69
1:C:779:ILE:CG2	1:C:790:LEU:HD11	2.22	0.69
1:D:739:PRO:O	1:D:740:THR:HG23	1.92	0.69
1:D:855:MET:HE2	2:D:1001:ERG:O1	1.93	0.69
1:D:642:TRP:CG	1:D:643:PRO:HD3	2.28	0.68
1:A:821:ARG:HH11	1:A:821:ARG:CG	2.06	0.68
1:A:841:ARG:O	1:A:845:THR:HG23	1.94	0.68
1:D:655:VAL:HG12	1:D:764:LYS:HD2	1.76	0.68
1:A:757:TRP:CE2	1:A:838:LEU:HD13	2.28	0.68
1:A:789:GLU:O	1:A:789:GLU:HG2	1.93	0.68
1:B:757:TRP:CE2	1:B:838:LEU:HD13	2.28	0.68
1:B:771:VAL:HG22	1:B:772:ASP:N	2.09	0.68
1:C:757:TRP:CE2	1:C:838:LEU:HD13	2.28	0.68
1:D:672:HIS:HD2	1:D:696:HIS:ND1	1.91	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:769:ILE:CG1	1:D:770:SER:H	2.06	0.68
1:C:739:PRO:CB	1:C:742:TRP:HE1	2.03	0.67
1:C:739:PRO:CB	1:C:885:VAL:CG2	2.73	0.67
1:B:841:ARG:O	1:B:845:THR:HG23	1.94	0.67
1:C:841:ARG:O	1:C:845:THR:HG23	1.94	0.67
1:D:802:PRO:HB3	1:D:803:VAL:CG1	2.25	0.67
1:B:700:ALA:O	1:B:704:LEU:HB2	1.94	0.67
1:C:740:THR:HA	1:C:743:ILE:HD12	1.77	0.67
1:D:768:LEU:HD23	1:D:768:LEU:C	2.14	0.67
1:C:771:VAL:HG22	1:C:818:LYS:HE3	1.77	0.66
1:D:802:PRO:CB	1:D:803:VAL:HG13	2.25	0.66
1:D:863:LYS:HE2	1:D:867:ASN:ND2	2.11	0.66
1:C:766:TYR:O	1:C:769:ILE:HG22	1.96	0.66
1:D:757:TRP:CE2	1:D:838:LEU:HD13	2.31	0.66
1:D:642:TRP:HA	1:D:645:ILE:HD12	1.76	0.66
1:B:797:ILE:CD1	1:B:801:TYR:CE1	2.79	0.66
1:D:802:PRO:HA	1:D:803:VAL:CG1	2.19	0.66
1:C:787:ILE:HB	1:C:803:VAL:CG1	2.25	0.66
1:B:672:HIS:HD2	1:B:696:HIS:CD2	2.13	0.65
1:A:738:ASN:CB	1:A:739:PRO:CD	2.74	0.65
1:C:738:ASN:HD22	1:C:738:ASN:N	1.93	0.65
1:D:805:LEU:HA	1:D:810:LEU:HD22	1.78	0.65
1:D:802:PRO:HB3	1:D:803:VAL:HG22	1.75	0.65
1:B:676:ALA:HB2	1:B:696:HIS:HB3	1.79	0.65
1:B:865:LEU:O	1:B:869:THR:OG1	2.14	0.65
1:B:797:ILE:HD11	1:B:801:TYR:CE1	2.31	0.64
1:D:743:ILE:HG12	1:D:905:PHE:CZ	2.31	0.64
1:A:848:MET:SD	1:A:902:MET:HE3	2.37	0.64
1:B:910:LEU:HD23	1:B:910:LEU:C	2.17	0.64
1:B:652:SER:CB	1:B:655:VAL:HG22	2.27	0.64
1:D:697:ARG:HD3	1:D:729:ASP:OD2	1.96	0.64
1:D:757:TRP:CD2	1:D:758:PRO:HA	2.33	0.64
1:B:672:HIS:HD2	1:B:696:HIS:HD2	1.43	0.64
1:B:808:PRO:HD2	1:B:809:TYR:H	1.61	0.64
1:B:797:ILE:CD1	1:B:801:TYR:HE1	2.10	0.64
1:D:634:PHE:CE1	1:D:671:MET:HE3	2.32	0.63
1:A:781:ASP:CB	1:A:788:THR:HG22	2.26	0.63
1:B:708:VAL:HG21	1:B:752:ILE:HA	1.79	0.63
1:D:893:TYR:CG	1:D:901:MET:HG3	2.33	0.63
1:D:655:VAL:HG23	1:D:656:TRP:CD1	2.32	0.63
1:A:738:ASN:CB	1:A:739:PRO:HD2	2.27	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:ASN:HB2	1:B:740:THR:H	1.63	0.63
1:D:803:VAL:O	1:D:804:ASP:HB2	1.99	0.63
1:C:739:PRO:HB3	1:C:885:VAL:HG21	1.80	0.62
1:B:738:ASN:HB3	1:B:740:THR:HG23	1.81	0.62
1:D:641:VAL:O	1:D:644:THR:HB	1.98	0.62
1:B:879:LEU:O	1:B:882:VAL:HG23	1.99	0.62
1:C:802:PRO:HA	1:C:803:VAL:HB	1.80	0.62
1:C:871:GLU:HG3	1:C:872:ILE:H	1.65	0.62
1:B:655:VAL:HG23	1:B:656:TRP:CD1	2.34	0.61
1:C:648:VAL:HG21	1:C:876:ALA:HB2	1.82	0.61
1:D:634:PHE:CD1	1:D:671:MET:CE	2.82	0.61
1:B:808:PRO:CD	1:B:809:TYR:H	2.12	0.61
1:C:771:VAL:O	1:C:772:ASP:HB2	1.99	0.61
1:B:808:PRO:HD2	1:B:809:TYR:N	2.15	0.61
1:B:641:VAL:HG21	1:B:678:SER:HB2	1.82	0.61
1:C:779:ILE:HG23	1:C:790:LEU:CD1	2.28	0.60
1:C:787:ILE:HD12	1:C:803:VAL:HG11	1.83	0.60
1:D:805:LEU:H	1:D:805:LEU:CD1	2.10	0.60
1:B:747:LYS:O	1:B:751:THR:HG22	2.01	0.60
1:C:776:LEU:HD23	1:C:810:LEU:HD23	1.82	0.60
1:B:808:PRO:CD	1:B:809:TYR:N	2.64	0.60
1:A:787:ILE:HB	1:A:803:VAL:HG23	1.84	0.60
1:A:822:GLU:OE1	1:A:831:ARG:NH1	2.33	0.60
1:D:757:TRP:CG	1:D:758:PRO:HA	2.37	0.60
1:C:770:SER:O	1:C:771:VAL:HG13	2.01	0.60
1:D:731:LEU:HD22	1:D:882:VAL:HG21	1.84	0.60
1:C:633:LEU:CD1	1:C:692:TYR:CE2	2.85	0.59
1:D:626:LEU:N	1:D:626:LEU:HD22	2.17	0.59
1:D:636:HIS:O	1:D:641:VAL:HG23	2.02	0.59
1:D:873:MET:O	1:D:875:ARG:N	2.33	0.59
1:A:902:MET:HG3	2:A:1001:ERG:C7	2.33	0.59
1:B:768:LEU:HD23	1:B:769:ILE:HG13	1.85	0.59
1:A:848:MET:SD	1:A:902:MET:HE1	2.41	0.59
1:B:855:MET:HE2	1:B:899:MET:SD	2.42	0.59
1:D:669:PHE:CE1	1:D:719:LEU:HD23	2.37	0.59
1:A:757:TRP:CD2	1:A:838:LEU:HD22	2.38	0.59
1:B:757:TRP:CD2	1:B:838:LEU:HD22	2.38	0.59
1:C:770:SER:O	1:C:771:VAL:HG22	2.02	0.59
1:B:712:SER:H	1:B:715:ASN:ND2	1.98	0.59
1:C:736:ASN:HA	1:C:738:ASN:N	2.18	0.58
1:A:637:TYR:HA	1:A:641:VAL:HB	1.85	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:ASP:CB	1:A:788:THR:CG2	2.77	0.58
1:B:761:GLU:OE1	1:B:766:TYR:CE2	2.56	0.58
1:A:779:ILE:CD1	1:A:790:LEU:HD12	2.19	0.58
1:B:648:VAL:HG21	1:B:876:ALA:HB2	1.85	0.58
1:D:802:PRO:HB3	1:D:803:VAL:HG13	1.84	0.58
1:A:652:SER:HB2	1:A:655:VAL:HG22	1.85	0.58
1:D:634:PHE:HE1	1:D:671:MET:HE3	1.67	0.58
1:B:757:TRP:CG	1:B:838:LEU:CD2	2.79	0.58
1:B:804:ASP:HB3	1:B:806:ASP:H	1.67	0.58
1:C:757:TRP:CD2	1:C:838:LEU:HD22	2.38	0.57
1:C:739:PRO:CB	1:C:885:VAL:HG23	2.33	0.57
1:B:650:ILE:HD11	1:B:829:ILE:HG21	1.86	0.57
1:C:650:ILE:HD11	1:C:829:ILE:HG21	1.86	0.57
1:A:681:HIS:HD2	1:A:877:TRP:CE2	2.23	0.57
1:B:739:PRO:HG2	1:B:743:ILE:HD12	1.87	0.57
1:B:772:ASP:N	1:B:772:ASP:OD1	2.36	0.57
1:D:765:PHE:O	1:D:767:ASN:N	2.38	0.57
1:C:711:ILE:HG22	1:C:711:ILE:O	2.03	0.57
1:C:637:TYR:HA	1:C:641:VAL:HB	1.85	0.57
1:C:802:PRO:CA	1:C:803:VAL:HB	2.34	0.57
1:C:803:VAL:HG12	1:C:803:VAL:O	2.03	0.57
1:D:625:SER:C	1:D:626:LEU:HD22	2.25	0.57
1:D:715:ASN:O	1:D:719:LEU:HG	2.05	0.57
1:A:822:GLU:HG2	1:A:822:GLU:O	2.05	0.57
1:D:835:PHE:HB3	1:D:836:PRO:HD3	1.85	0.57
1:D:769:ILE:HD12	1:D:770:SER:H	1.70	0.57
1:A:821:ARG:HH11	1:A:821:ARG:HG3	1.69	0.57
1:A:849:THR:CA	3:A:1101:HOH:O	2.44	0.57
1:C:710:GLU:O	1:C:710:GLU:HG3	2.04	0.56
1:B:787:ILE:HD11	1:B:810:LEU:CD1	2.35	0.56
1:C:757:TRP:CG	1:C:838:LEU:CD2	2.79	0.56
1:D:648:VAL:O	1:D:648:VAL:HG22	2.04	0.56
1:B:626:LEU:N	1:B:626:LEU:HD23	2.20	0.56
1:B:827:ASP:OD2	3:B:1104:HOH:O	2.18	0.56
1:C:855:MET:HE1	1:C:899:MET:SD	2.45	0.56
1:A:898:GLY:O	2:A:1001:ERG:H12	2.06	0.56
1:B:897:GLY:O	1:B:900:HIS:N	2.37	0.56
1:A:757:TRP:CD2	1:A:758:PRO:HA	2.41	0.56
1:C:757:TRP:CD2	1:C:758:PRO:HA	2.41	0.56
1:A:804:ASP:OD1	1:A:804:ASP:N	2.34	0.56
1:C:797:ILE:HB	1:C:800:LEU:HD13	1.87	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:802:PRO:N	1:A:802:PRO:C	2.52	0.56
1:B:728:MET:HG2	1:B:878:PHE:CE1	2.41	0.56
1:D:652:SER:O	1:D:655:VAL:HG22	2.05	0.56
1:D:769:ILE:HG23	1:D:770:SER:N	2.21	0.56
1:D:804:ASP:O	1:D:807:SER:N	2.38	0.56
1:A:648:VAL:CG2	1:A:876:ALA:CB	2.84	0.56
1:A:702:LYS:O	1:A:706:GLU:HG3	2.06	0.56
1:A:855:MET:CE	1:A:899:MET:CG	2.84	0.56
1:A:757:TRP:CG	1:A:838:LEU:CD2	2.79	0.56
1:D:802:PRO:HB2	1:D:803:VAL:HG22	1.88	0.56
1:C:769:ILE:HG13	1:C:770:SER:N	2.20	0.55
1:D:873:MET:C	1:D:875:ARG:H	2.08	0.55
1:B:853:GLY:O	1:B:857:ILE:HG12	2.06	0.55
1:D:634:PHE:HD1	1:D:671:MET:CE	2.17	0.55
1:D:828:TYR:O	1:D:832:VAL:HG23	2.05	0.55
1:A:721:ALA:HB2	1:A:765:PHE:CZ	2.42	0.55
1:C:902:MET:HG3	2:C:1001:ERG:C6	2.36	0.55
1:A:855:MET:HE1	1:A:899:MET:CG	2.37	0.55
1:C:871:GLU:HG3	1:C:872:ILE:N	2.21	0.55
1:D:826:LEU:O	1:D:827:ASP:HB2	2.05	0.55
1:A:909:GLY:O	1:A:910:LEU:HD12	2.07	0.55
1:B:780:VAL:HB	1:B:787:ILE:HG12	1.87	0.55
1:B:873:MET:HE3	1:B:883:SER:CB	2.36	0.55
1:C:721:ALA:HB2	1:C:765:PHE:CZ	2.42	0.55
1:C:786:THR:HG22	1:C:804:ASP:OD1	2.06	0.55
1:C:817:ASP:O	1:C:821:ARG:HG3	2.07	0.55
1:C:641:VAL:HG21	1:C:678:SER:HB2	1.90	0.54
1:A:641:VAL:HG21	1:A:678:SER:HB2	1.89	0.54
1:B:751:THR:HB	1:B:908:GLY:HA2	1.88	0.54
1:D:898:GLY:O	2:D:1001:ERG:H12	2.07	0.54
1:B:769:ILE:O	1:B:831:ARG:NE	2.41	0.54
1:D:772:ASP:O	1:D:773:LEU:HB2	2.06	0.54
1:A:855:MET:HG2	2:A:1001:ERG:H41	1.88	0.54
1:B:681:HIS:O	1:B:684:ARG:HB2	2.08	0.54
1:B:721:ALA:O	1:B:725:ILE:HG12	2.08	0.54
1:C:739:PRO:C	1:C:740:THR:HG23	2.26	0.54
1:D:769:ILE:CD1	1:D:770:SER:H	2.20	0.54
1:D:769:ILE:HG13	1:D:770:SER:H	1.73	0.54
1:B:769:ILE:HG23	1:B:838:LEU:CD1	2.38	0.54
1:C:769:ILE:CG1	1:C:770:SER:H	2.20	0.54
1:C:771:VAL:CG2	1:C:818:LYS:CE	2.86	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:642:TRP:CD2	1:D:643:PRO:HD3	2.43	0.54
1:B:757:TRP:CD2	1:B:758:PRO:HA	2.43	0.53
1:C:708:VAL:HG21	1:C:752:ILE:CD1	2.34	0.53
1:C:769:ILE:HG13	1:C:770:SER:H	1.73	0.53
1:D:712:SER:O	1:D:716:THR:OG1	2.24	0.53
1:C:630:ASP:OD2	1:C:692:TYR:OH	2.22	0.53
1:C:733:ASN:O	1:C:738:ASN:OD1	2.26	0.53
1:C:769:ILE:CG1	1:C:770:SER:N	2.72	0.53
1:D:760:PRO:O	1:D:762:THR:N	2.42	0.53
1:A:875:ARG:O	1:A:875:ARG:HG3	2.07	0.53
1:C:798:ALA:O	1:C:800:LEU:N	2.41	0.53
1:A:715:ASN:HD22	1:A:715:ASN:H	1.55	0.53
1:C:706:GLU:O	1:C:709:LEU:HB2	2.09	0.53
1:B:682:LEU:CD1	1:B:686:GLN:HB2	2.39	0.53
1:C:787:ILE:HB	1:C:803:VAL:HG11	1.89	0.53
1:B:798:ALA:O	1:B:801:TYR:HB2	2.08	0.53
1:D:855:MET:HE3	2:D:1001:ERG:O1	2.09	0.53
1:B:771:VAL:CG2	1:B:772:ASP:N	2.72	0.53
1:D:708:VAL:HG21	1:D:752:ILE:HD12	1.90	0.53
1:B:697:ARG:HG2	1:B:697:ARG:HH11	1.75	0.52
1:D:707:ALA:C	1:D:709:LEU:H	2.13	0.52
1:B:781:ASP:HA	1:B:787:ILE:HA	1.90	0.52
1:D:805:LEU:HD13	1:D:805:LEU:N	2.19	0.52
1:A:823:LYS:HB3	1:A:828:TYR:CE2	2.45	0.52
1:B:906:LEU:HA	3:B:1108:HOH:O	2.10	0.52
1:D:805:LEU:CD1	1:D:805:LEU:N	2.72	0.52
1:A:821:ARG:HG3	1:A:821:ARG:NH1	2.25	0.52
1:C:634:PHE:HZ	1:C:661:PRO:HB3	1.74	0.52
1:D:626:LEU:N	1:D:626:LEU:CD2	2.72	0.52
1:C:634:PHE:HD2	1:C:671:MET:HE1	1.74	0.51
1:C:708:VAL:HG13	1:C:711:ILE:HD11	1.91	0.51
1:D:769:ILE:CD1	1:D:770:SER:N	2.73	0.51
1:C:715:ASN:HD22	1:C:715:ASN:H	1.58	0.51
1:D:820:TYR:HD2	1:D:864:LEU:CD1	2.22	0.51
1:A:776:LEU:O	1:A:778:GLU:N	2.44	0.51
1:A:909:GLY:O	1:A:910:LEU:HB2	2.10	0.51
1:B:823:LYS:HB2	1:B:823:LYS:NZ	2.24	0.51
1:C:698:LEU:HD12	1:C:701:LEU:HD23	1.92	0.51
1:A:652:SER:O	1:A:655:VAL:HG22	2.09	0.51
1:C:771:VAL:HG23	1:C:772:ASP:N	2.17	0.51
1:A:792:CYS:SG	1:A:793:CYS:N	2.84	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:872:ILE:HG13	1:D:872:ILE:O	2.09	0.51
1:A:855:MET:HE1	1:A:899:MET:HG3	1.91	0.51
1:B:873:MET:HE3	1:B:883:SER:HB3	1.93	0.51
1:C:681:HIS:O	1:C:684:ARG:HG3	2.12	0.50
1:C:767:ASN:OD1	1:C:768:LEU:N	2.44	0.50
1:D:863:LYS:CE	1:D:867:ASN:ND2	2.74	0.50
1:B:873:MET:HE1	1:B:883:SER:H	1.75	0.50
1:D:855:MET:HG2	2:D:1001:ERG:H41	1.94	0.50
1:B:797:ILE:HD12	1:B:801:TYR:CE1	2.46	0.50
1:C:634:PHE:CZ	1:C:661:PRO:HB3	2.46	0.50
1:A:711:ILE:HD13	1:A:756:VAL:HG12	1.93	0.50
1:A:781:ASP:OD2	1:A:788:THR:HG21	2.12	0.50
1:D:757:TRP:CD1	1:D:838:LEU:HD22	2.45	0.50
1:D:655:VAL:CG1	1:D:764:LYS:HD2	2.41	0.50
1:D:731:LEU:HD21	2:D:1001:ERG:H271	1.94	0.50
1:B:905:PHE:CD1	2:B:1001:ERG:H22	2.46	0.50
1:C:855:MET:CE	1:C:902:MET:CE	2.90	0.50
1:D:757:TRP:CZ2	1:D:769:ILE:HG12	2.47	0.50
1:B:637:TYR:HA	1:B:641:VAL:CG2	2.42	0.49
1:A:850:GLY:HA2	1:A:855:MET:CE	2.43	0.49
1:A:742:TRP:NE1	1:A:885:VAL:HG21	2.28	0.49
1:A:781:ASP:HB3	1:A:784:THR:OG1	2.13	0.49
1:B:697:ARG:HG2	1:B:697:ARG:NH1	2.28	0.49
1:B:792:CYS:HG	1:B:793:CYS:N	2.10	0.49
1:B:797:ILE:HB	1:B:800:LEU:HD12	1.93	0.49
1:C:786:THR:CG2	1:C:804:ASP:OD1	2.60	0.49
1:C:736:ASN:HA	1:C:737:SER:C	2.33	0.49
1:D:822:GLU:O	1:D:824:ASN:N	2.46	0.49
1:D:654:GLU:O	1:D:654:GLU:HG3	2.12	0.49
1:D:769:ILE:CG1	1:D:770:SER:N	2.73	0.49
1:C:769:ILE:CD1	1:C:770:SER:H	2.26	0.49
1:D:870:THR:HG22	1:D:883:SER:CB	2.39	0.49
1:A:743:ILE:HG12	1:A:905:PHE:CZ	2.48	0.48
1:B:771:VAL:O	1:B:772:ASP:HB3	2.12	0.48
1:A:766:TYR:CD1	1:A:766:TYR:C	2.86	0.48
1:B:689:LEU:HA	1:B:692:TYR:HD2	1.78	0.48
1:B:709:LEU:HD23	1:B:709:LEU:N	2.27	0.48
1:D:629:VAL:HG13	1:D:630:ASP:N	2.28	0.48
1:C:735:SER:H	1:C:738:ASN:HB2	1.77	0.48
1:C:776:LEU:CD2	1:C:810:LEU:HD21	2.30	0.48
1:C:853:GLY:O	1:C:857:ILE:HG12	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:781:ASP:HB2	1:A:788:THR:HG21	1.93	0.48
1:B:757:TRP:HH2	1:B:769:ILE:HG12	1.76	0.48
1:D:853:GLY:O	1:D:857:ILE:HG12	2.13	0.48
1:C:771:VAL:HG21	1:C:818:LYS:CE	2.43	0.47
1:B:751:THR:CB	1:B:908:GLY:HA2	2.44	0.47
1:C:739:PRO:CB	1:C:885:VAL:HG21	2.43	0.47
1:B:654:GLU:O	1:B:654:GLU:HG3	2.13	0.47
1:B:757:TRP:CZ2	1:B:838:LEU:HD13	2.49	0.47
1:D:634:PHE:CE1	1:D:671:MET:CE	2.97	0.47
1:D:656:TRP:HA	1:D:660:LEU:CD2	2.40	0.47
1:D:876:ALA:HB3	1:D:879:LEU:HB2	1.97	0.47
1:B:702:LYS:NZ	1:B:706:GLU:OE2	2.46	0.47
1:B:891:ASP:OD2	3:B:1103:HOH:O	2.20	0.47
1:B:738:ASN:HB2	1:B:740:THR:N	2.28	0.47
1:C:757:TRP:CZ2	1:C:838:LEU:HD13	2.49	0.47
1:D:697:ARG:NH1	1:D:730:SER:OG	2.48	0.47
1:D:757:TRP:CD2	1:D:838:LEU:HD22	2.48	0.47
1:A:677:PHE:HA	1:A:729:ASP:OD1	2.15	0.47
1:A:742:TRP:CE2	1:A:743:ILE:HG13	2.50	0.47
1:C:796:ASP:C	1:C:797:ILE:HG23	2.35	0.47
1:D:704:LEU:HD12	1:D:719:LEU:HD22	1.97	0.47
1:D:712:SER:OG	1:D:715:ASN:ND2	2.48	0.47
1:D:747:LYS:HE2	1:D:907:GLY:O	2.14	0.47
1:A:642:TRP:CG	1:A:643:PRO:HD3	2.50	0.47
1:A:708:VAL:CG1	1:A:752:ILE:CD1	2.68	0.47
1:B:817:ASP:O	1:B:821:ARG:HG3	2.15	0.47
1:D:757:TRP:CZ2	1:D:838:LEU:HD13	2.49	0.47
1:C:739:PRO:O	1:C:740:THR:OG1	2.20	0.46
1:A:732:ALA:HB2	1:A:878:PHE:HB2	1.98	0.46
1:C:677:PHE:HA	1:C:729:ASP:OD1	2.14	0.46
1:C:734:ALA:O	1:C:735:SER:HB3	2.14	0.46
1:D:862:TYR:HD1	2:D:1001:ERG:H183	1.80	0.46
1:A:757:TRP:CZ2	1:A:838:LEU:HD13	2.49	0.46
1:C:802:PRO:HB2	1:C:803:VAL:CA	2.45	0.46
1:A:631:LEU:HD21	1:B:634:PHE:HB2	1.96	0.46
1:B:642:TRP:CG	1:B:643:PRO:HD3	2.50	0.46
1:B:785:GLY:C	1:B:786:THR:HG23	2.35	0.46
1:C:780:VAL:CG1	1:C:786:THR:O	2.64	0.46
1:A:779:ILE:CG1	1:A:787:ILE:CD1	2.86	0.46
1:B:682:LEU:HD11	1:B:686:GLN:HB2	1.97	0.46
1:B:790:LEU:CD2	1:B:813:LEU:HD22	2.45	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:769:ILE:HD12	1:C:770:SER:H	1.79	0.46
1:D:651:SER:C	1:D:652:SER:OG	2.50	0.46
1:D:863:LYS:HZ1	1:D:867:ASN:HD21	1.60	0.46
1:B:632:LYS:CE	1:B:686:GLN:HE22	2.28	0.46
1:B:637:TYR:HA	1:B:641:VAL:HB	1.96	0.46
1:C:732:ALA:HB2	1:C:878:PHE:HB2	1.97	0.46
1:A:655:VAL:HG23	1:A:656:TRP:CD1	2.51	0.46
1:B:672:HIS:CD2	1:B:696:HIS:HD2	2.30	0.46
1:A:819:LEU:O	1:A:828:TYR:HE1	1.99	0.46
1:A:855:MET:HE1	1:A:899:MET:SD	2.56	0.46
1:B:704:LEU:HG	1:B:752:ILE:HG13	1.98	0.45
1:C:797:ILE:HB	1:C:800:LEU:CD1	2.46	0.45
1:D:802:PRO:CA	1:D:803:VAL:CG1	2.84	0.45
1:D:804:ASP:O	1:D:806:ASP:N	2.49	0.45
1:A:849:THR:CB	3:A:1101:HOH:O	2.63	0.45
1:D:863:LYS:CE	1:D:867:ASN:HD21	2.28	0.45
1:B:798:ALA:O	1:B:801:TYR:N	2.49	0.45
1:C:642:TRP:CG	1:C:643:PRO:HD3	2.50	0.45
1:C:655:VAL:HG23	1:C:656:TRP:CD1	2.51	0.45
1:B:689:LEU:HD23	1:B:692:TYR:CD2	2.52	0.45
1:B:747:LYS:HG3	1:B:904:ASP:O	2.15	0.45
1:B:766:TYR:O	1:B:766:TYR:CD2	2.70	0.45
1:B:821:ARG:HG3	1:B:821:ARG:H	1.65	0.45
1:C:639:THR:HG22	1:C:640:GLU:HG3	1.99	0.45
1:C:738:ASN:N	1:C:738:ASN:ND2	2.62	0.45
1:C:801:TYR:HA	1:C:802:PRO:HA	1.56	0.45
1:D:681:HIS:O	1:D:684:ARG:HG3	2.17	0.45
1:D:721:ALA:O	1:D:725:ILE:HG12	2.16	0.45
1:B:780:VAL:HB	1:B:787:ILE:CG1	2.47	0.45
1:D:766:TYR:O	1:D:766:TYR:CD2	2.70	0.45
1:C:633:LEU:HD12	1:C:692:TYR:CE2	2.51	0.45
1:A:639:THR:HG22	1:A:640:GLU:HG3	1.99	0.45
1:C:788:THR:O	1:C:789:GLU:HB3	2.17	0.45
1:C:855:MET:HG2	2:C:1001:ERG:H41	1.99	0.45
1:B:715:ASN:C	1:B:715:ASN:HD22	2.19	0.45
1:C:634:PHE:CD2	1:C:671:MET:HE1	2.51	0.45
1:A:909:GLY:C	1:A:910:LEU:HD12	2.37	0.45
1:B:910:LEU:C	1:B:910:LEU:CD2	2.85	0.44
1:C:798:ALA:C	1:C:800:LEU:H	2.19	0.44
1:D:682:LEU:O	1:D:684:ARG:N	2.50	0.44
1:C:701:LEU:HD22	1:C:745:HIS:CD2	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:787:ILE:HB	1:C:803:VAL:HG12	1.97	0.44
1:D:761:GLU:H	1:D:761:GLU:HG3	1.58	0.44
1:C:787:ILE:HD12	1:C:803:VAL:CG1	2.48	0.44
1:A:792:CYS:HB3	1:A:820:TYR:CG	2.53	0.44
1:B:829:ILE:HD13	1:B:829:ILE:HA	1.79	0.44
1:C:780:VAL:HG13	1:C:786:THR:C	2.38	0.44
1:D:898:GLY:O	2:D:1001:ERG:C1	2.66	0.44
1:B:785:GLY:C	1:B:786:THR:CG2	2.86	0.44
1:A:701:LEU:HD22	1:A:745:HIS:CD2	2.53	0.44
1:B:826:LEU:O	1:B:827:ASP:HB2	2.17	0.43
1:C:655:VAL:HA	1:C:659:TYR:HB3	2.00	0.43
1:B:748:GLY:O	1:B:752:ILE:HG12	2.18	0.43
1:B:796:ASP:OD1	1:B:796:ASP:N	2.51	0.43
1:D:682:LEU:C	1:D:684:ARG:N	2.70	0.43
1:C:798:ALA:C	1:C:800:LEU:N	2.71	0.43
1:D:743:ILE:HG23	1:D:905:PHE:CE1	2.53	0.43
1:C:780:VAL:HG13	1:C:786:THR:O	2.19	0.43
1:A:736:ASN:O	1:A:884:GLN:HB3	2.18	0.43
1:D:650:ILE:CD1	1:D:829:ILE:HG21	2.48	0.43
1:A:809:TYR:OH	1:A:853:GLY:HA3	2.19	0.43
1:B:790:LEU:HD23	1:B:813:LEU:HD22	2.01	0.43
1:A:768:LEU:N	1:A:768:LEU:HD23	2.32	0.43
1:A:779:ILE:CG1	1:A:790:LEU:HD11	2.39	0.43
1:B:715:ASN:ND2	1:B:715:ASN:C	2.72	0.43
1:C:633:LEU:HD13	1:C:692:TYR:CE2	2.54	0.43
1:C:648:VAL:CG2	1:C:876:ALA:HB2	2.48	0.43
1:D:681:HIS:O	1:D:681:HIS:CG	2.70	0.43
1:C:707:ALA:HB3	1:C:719:LEU:HD21	2.00	0.43
1:C:892:ASP:O	1:C:893:TYR:C	2.57	0.43
1:B:632:LYS:HE2	1:B:686:GLN:HE22	1.83	0.43
1:D:712:SER:H	1:D:715:ASN:ND2	2.09	0.43
1:D:715:ASN:N	1:D:715:ASN:HD22	2.16	0.43
1:D:862:TYR:O	1:D:866:ARG:HB2	2.19	0.43
1:A:822:GLU:CD	1:A:831:ARG:HH11	2.21	0.43
1:B:854:ALA:O	1:B:857:ILE:HB	2.19	0.43
1:C:765:PHE:O	1:C:768:LEU:HD22	2.19	0.43
1:B:639:THR:HG22	1:B:640:GLU:HG2	2.00	0.42
1:A:655:VAL:HA	1:A:659:TYR:HB3	2.00	0.42
1:A:848:MET:CE	1:A:902:MET:CE	2.96	0.42
1:B:879:LEU:C	1:B:882:VAL:HG23	2.39	0.42
1:C:829:ILE:HD13	1:C:829:ILE:HA	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:802:PRO:HB3	1:D:803:VAL:CB	2.49	0.42
1:A:742:TRP:HE1	1:A:885:VAL:HG21	1.83	0.42
1:C:821:ARG:HG3	1:C:821:ARG:H	1.69	0.42
1:C:870:THR:HG22	1:C:883:SER:HB3	2.00	0.42
1:D:765:PHE:C	1:D:767:ASN:N	2.73	0.42
1:B:797:ILE:O	1:B:800:LEU:HB2	2.20	0.42
1:C:769:ILE:O	1:C:831:ARG:NE	2.52	0.42
1:C:797:ILE:O	1:C:800:LEU:HB2	2.19	0.42
1:C:742:TRP:CE2	1:C:743:ILE:HG13	2.55	0.42
1:D:642:TRP:N	1:D:643:PRO:CD	2.82	0.42
1:D:715:ASN:ND2	1:D:715:ASN:C	2.73	0.42
1:B:825:GLN:HG3	1:B:826:LEU:H	1.84	0.42
1:C:715:ASN:ND2	1:C:715:ASN:C	2.72	0.42
1:D:696:HIS:HA	1:D:699:SER:HB2	2.02	0.42
1:D:681:HIS:HB2	1:D:877:TRP:CH2	2.55	0.42
1:B:769:ILE:HG23	1:B:838:LEU:HD12	2.02	0.42
1:B:868:TYR:CE2	1:B:872:ILE:HD13	2.55	0.42
1:C:652:SER:OG	1:C:655:VAL:HG22	2.19	0.42
1:C:871:GLU:C	1:C:873:MET:H	2.22	0.42
1:D:687:PRO:HD2	1:D:687:PRO:O	2.20	0.42
1:B:873:MET:CE	1:B:883:SER:OG	2.68	0.41
1:A:738:ASN:HD22	1:A:738:ASN:HA	1.55	0.41
1:C:791:VAL:HG23	1:C:820:TYR:CE1	2.56	0.41
1:C:797:ILE:O	1:C:797:ILE:HD12	2.19	0.41
1:D:707:ALA:C	1:D:709:LEU:N	2.73	0.41
1:D:898:GLY:O	2:D:1001:ERG:H21	2.20	0.41
1:D:681:HIS:ND1	1:D:681:HIS:C	2.71	0.41
1:D:802:PRO:CB	1:D:803:VAL:CG1	2.91	0.41
1:D:873:MET:C	1:D:875:ARG:N	2.72	0.41
1:D:886:LEU:HD23	1:D:886:LEU:HA	1.83	0.41
1:A:850:GLY:HA2	1:A:855:MET:HE1	2.01	0.41
1:B:757:TRP:CD2	1:B:838:LEU:CD2	3.04	0.41
1:C:742:TRP:NE1	1:C:885:VAL:HG21	2.35	0.41
1:C:739:PRO:HG2	1:C:740:THR:HG23	2.02	0.41
1:D:629:VAL:CG1	1:D:630:ASP:N	2.83	0.41
1:A:790:LEU:HB2	1:A:801:TYR:OH	2.20	0.41
1:B:866:ARG:NE	1:B:886:LEU:O	2.27	0.41
1:D:835:PHE:CD1	1:D:835:PHE:C	2.94	0.41
1:B:739:PRO:HB2	1:B:742:TRP:NE1	2.35	0.41
1:C:905:PHE:CD1	2:C:1001:ERG:H22	2.56	0.41
1:D:724:LEU:HD22	1:D:830:LEU:HD22	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:820:TYR:C	1:B:822:GLU:H	2.24	0.41
1:B:826:LEU:HA	1:B:826:LEU:HD12	1.89	0.41
1:B:910:LEU:HD23	1:B:910:LEU:O	2.21	0.41
1:C:795:ASP:O	1:C:796:ASP:CB	2.69	0.41
1:A:849:THR:OG1	3:A:1101:HOH:O	2.17	0.41
1:A:870:THR:HG22	1:A:883:SER:HB3	2.03	0.41
1:C:701:LEU:HD21	1:C:744:PHE:CE2	2.56	0.41
1:C:709:LEU:HD23	1:C:709:LEU:HA	1.84	0.41
1:C:704:LEU:HG	1:C:752:ILE:HG13	2.03	0.41
1:C:707:ALA:CB	1:C:719:LEU:HD21	2.51	0.41
1:A:829:ILE:O	1:A:829:ILE:HD12	2.21	0.40
1:B:766:TYR:CG	1:B:769:ILE:HD11	2.56	0.40
1:B:757:TRP:CZ3	1:B:769:ILE:HG12	2.56	0.40
1:C:791:VAL:CG2	1:C:792:CYS:N	2.83	0.40
1:B:650:ILE:HD11	1:B:829:ILE:CG2	2.50	0.40
1:D:809:TYR:OH	1:D:853:GLY:HA3	2.21	0.40
1:A:677:PHE:CD1	1:A:729:ASP:HB2	2.56	0.40
1:A:715:ASN:C	1:A:715:ASN:ND2	2.72	0.40
1:A:829:ILE:HD13	1:A:829:ILE:HA	1.79	0.40
1:C:757:TRP:CD2	1:C:838:LEU:CD2	3.04	0.40
1:C:823:LYS:HA	1:C:828:TYR:CD2	2.57	0.40
1:C:829:ILE:O	1:C:829:ILE:HD12	2.21	0.40
1:B:708:VAL:CG2	1:B:752:ILE:HA	2.50	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:895:GLY:O	1:D:705:ARG:NH1[2_554]	1.89	0.31
1:C:702:LYS:NZ	1:D:893:TYR:O[2_554]	1.95	0.25
1:B:629:VAL:CG1	1:C:783:ASP:O[1_556]	1.97	0.23

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	277/308 (90%)	261 (94%)	14 (5%)	2 (1%)	22 43
1	B	276/308 (90%)	252 (91%)	19 (7%)	5 (2%)	8 16
1	C	278/308 (90%)	240 (86%)	25 (9%)	13 (5%)	2 2
1	D	247/308 (80%)	221 (90%)	13 (5%)	13 (5%)	2 2
All	All	1078/1232 (88%)	974 (90%)	71 (7%)	33 (3%)	4 6

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	777	GLY
1	B	736	ASN
1	B	738	ASN
1	B	794	ASP
1	C	735	SER
1	C	771	VAL
1	C	796	ASP
1	C	803	VAL
1	D	803	VAL
1	D	805	LEU
1	D	823	LYS
1	D	874	ASP
1	C	738	ASN
1	C	794	ASP
1	D	687	PRO
1	D	761	GLU
1	D	766	TYR
1	D	804	ASP
1	A	739	PRO
1	C	737	SER
1	C	768	LEU
1	C	799	ASP
1	C	739	PRO
1	D	768	LEU
1	D	771	VAL
1	C	652	SER
1	D	740	THR
1	B	739	PRO
1	B	909	GLY
1	D	652	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	711	ILE
1	C	797	ILE
1	C	802	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	244/268 (91%)	210 (86%)	34 (14%)	3 6
1	B	244/268 (91%)	207 (85%)	37 (15%)	3 4
1	C	245/268 (91%)	210 (86%)	35 (14%)	3 5
1	D	221/268 (82%)	175 (79%)	46 (21%)	1 2
All	All	954/1072 (89%)	802 (84%)	152 (16%)	2 4

All (152) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	626	LEU
1	A	628	LEU
1	A	629	VAL
1	A	631	LEU
1	A	632	LYS
1	A	648	VAL
1	A	682	LEU
1	A	683	SER
1	A	698	LEU
1	A	712	SER
1	A	715	ASN
1	A	716	THR
1	A	736	ASN
1	A	738	ASN
1	A	740	THR
1	A	751	THR
1	A	761	GLU
1	A	778	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	782	LYS
1	A	787	ILE
1	A	788	THR
1	A	789	GLU
1	A	790	LEU
1	A	803	VAL
1	A	815	TYR
1	A	821	ARG
1	A	823	LYS
1	A	824	ASN
1	A	826	LEU
1	A	829	ILE
1	A	844	LEU
1	A	874	ASP
1	A	875	ARG
1	A	888	ARG
1	B	626	LEU
1	B	632	LYS
1	B	652	SER
1	B	655	VAL
1	B	660	LEU
1	B	683	SER
1	B	686	GLN
1	B	708	VAL
1	B	709	LEU
1	B	710	GLU
1	B	715	ASN
1	B	717	ASP
1	B	735	SER
1	B	739	PRO
1	B	751	THR
1	B	761	GLU
1	B	762	THR
1	B	768	LEU
1	B	769	ILE
1	B	770	SER
1	B	779	ILE
1	B	781	ASP
1	B	784	THR
1	B	790	LEU
1	B	791	VAL
1	B	792	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	793	CYS
1	B	796	ASP
1	B	805	LEU
1	B	821	ARG
1	B	822	GLU
1	B	823	LYS
1	B	826	LEU
1	B	829	ILE
1	B	844	LEU
1	B	869	THR
1	B	885	VAL
1	C	631	LEU
1	C	632	LYS
1	C	671	MET
1	C	683	SER
1	C	691	ASP
1	C	695	SER
1	C	712	SER
1	C	715	ASN
1	C	716	THR
1	C	736	ASN
1	C	738	ASN
1	C	739	PRO
1	C	751	THR
1	C	761	GLU
1	C	770	SER
1	C	776	LEU
1	C	779	ILE
1	C	782	LYS
1	C	789	GLU
1	C	790	LEU
1	C	791	VAL
1	C	792	CYS
1	C	793	CYS
1	C	796	ASP
1	C	800	LEU
1	C	806	ASP
1	C	808	PRO
1	C	821	ARG
1	C	822	GLU
1	C	823	LYS
1	C	829	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	844	LEU
1	C	888	ARG
1	C	891	ASP
1	C	910	LEU
1	D	625	SER
1	D	626	LEU
1	D	639	THR
1	D	650	ILE
1	D	654	GLU
1	D	660	LEU
1	D	666	LYS
1	D	673	SER
1	D	686	GLN
1	D	697	ARG
1	D	699	SER
1	D	704	LEU
1	D	705	ARG
1	D	715	ASN
1	D	722	SER
1	D	740	THR
1	D	751	THR
1	D	758	PRO
1	D	764	LYS
1	D	768	LEU
1	D	769	ILE
1	D	770	SER
1	D	772	ASP
1	D	773	LEU
1	D	803	VAL
1	D	804	ASP
1	D	805	LEU
1	D	806	ASP
1	D	808	PRO
1	D	822	GLU
1	D	826	LEU
1	D	841	ARG
1	D	844	LEU
1	D	863	LYS
1	D	864	LEU
1	D	866	ARG
1	D	871	GLU
1	D	874	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	875	ARG
1	D	882	VAL
1	D	883	SER
1	D	884	GLN
1	D	885	VAL
1	D	888	ARG
1	D	899	MET
1	D	901	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	672	HIS
1	A	715	ASN
1	A	738	ASN
1	A	884	GLN
1	B	672	HIS
1	B	686	GLN
1	B	696	HIS
1	B	715	ASN
1	B	767	ASN
1	C	715	ASN
1	C	738	ASN
1	D	636	HIS
1	D	672	HIS
1	D	715	ASN
1	D	736	ASN
1	D	867	ASN
1	D	884	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

4 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
2	ERG	A	1001	-	31,32,32	1.93	7 (22%)	47,50,50	1.49	9 (19%)
2	ERG	C	1001	-	31,32,32	1.92	7 (22%)	47,50,50	1.49	9 (19%)
2	ERG	B	1001	-	31,32,32	1.93	7 (22%)	47,50,50	1.48	9 (19%)
2	ERG	D	1001	-	31,32,32	1.94	7 (22%)	47,50,50	1.49	9 (19%)

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
2	ERG	A	1001	-	-	0/13/71/71	0/4/4/4
2	ERG	C	1001	-	-	0/13/71/71	0/4/4/4
2	ERG	B	1001	-	-	0/13/71/71	0/4/4/4
2	ERG	D	1001	-	-	0/13/71/71	0/4/4/4

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	ERG	C23-C22	5.95	1.50	1.32
2	C	1001	ERG	C23-C22	5.95	1.50	1.32
2	A	1001	ERG	C23-C22	5.94	1.50	1.32
2	B	1001	ERG	C23-C22	5.94	1.50	1.32
2	A	1001	ERG	C10-C5	-5.36	1.42	1.52
2	D	1001	ERG	C10-C5	-5.34	1.42	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1001	ERG	C10-C5	-5.31	1.42	1.52
2	C	1001	ERG	C10-C5	-5.25	1.42	1.52
2	B	1001	ERG	C4-C5	-3.54	1.44	1.51
2	C	1001	ERG	C4-C5	-3.51	1.44	1.51
2	D	1001	ERG	C4-C5	-3.51	1.44	1.51
2	A	1001	ERG	C4-C5	-3.49	1.44	1.51
2	B	1001	ERG	C9-C8	-3.27	1.43	1.51
2	D	1001	ERG	C9-C8	-3.26	1.43	1.51
2	C	1001	ERG	C9-C8	-3.25	1.43	1.51
2	A	1001	ERG	C9-C8	-3.24	1.43	1.51
2	D	1001	ERG	C11-C9	3.09	1.59	1.53
2	C	1001	ERG	C11-C9	3.03	1.59	1.53
2	A	1001	ERG	C11-C9	3.02	1.59	1.53
2	B	1001	ERG	C11-C9	3.01	1.59	1.53
2	A	1001	ERG	C14-C8	-2.42	1.45	1.51
2	B	1001	ERG	C6-C5	2.39	1.39	1.33
2	D	1001	ERG	C14-C8	-2.39	1.45	1.51
2	C	1001	ERG	C14-C8	-2.38	1.45	1.51
2	A	1001	ERG	C6-C5	2.37	1.39	1.33
2	D	1001	ERG	C6-C5	2.35	1.39	1.33
2	C	1001	ERG	C6-C5	2.35	1.39	1.33
2	B	1001	ERG	C14-C8	-2.34	1.45	1.51

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1001	ERG	C19-C10-C5	-3.39	102.86	108.34
2	D	1001	ERG	C19-C10-C5	-3.38	102.88	108.34
2	B	1001	ERG	C19-C10-C5	-3.36	102.91	108.34
2	A	1001	ERG	C19-C10-C5	-3.36	102.91	108.34
2	A	1001	ERG	C4-C5-C10	3.13	120.57	116.42
2	B	1001	ERG	C4-C5-C10	3.09	120.53	116.42
2	D	1001	ERG	C4-C5-C10	3.07	120.50	116.42
2	C	1001	ERG	C4-C5-C10	3.05	120.47	116.42
2	C	1001	ERG	C11-C12-C13	-2.73	108.10	112.78
2	B	1001	ERG	C11-C12-C13	-2.70	108.16	112.78
2	D	1001	ERG	C11-C12-C13	-2.69	108.16	112.78
2	A	1001	ERG	C15-C14-C13	-2.69	101.81	104.21
2	A	1001	ERG	C11-C12-C13	-2.68	108.19	112.78
2	B	1001	ERG	C15-C14-C13	-2.60	101.89	104.21
2	D	1001	ERG	C15-C14-C13	-2.58	101.91	104.21
2	C	1001	ERG	C15-C14-C13	-2.58	101.91	104.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	1001	ERG	C19-C10-C9	-2.51	106.82	111.03
2	A	1001	ERG	C19-C10-C9	-2.49	106.85	111.03
2	B	1001	ERG	C19-C10-C9	-2.49	106.85	111.03
2	C	1001	ERG	C19-C10-C9	-2.48	106.86	111.03
2	B	1001	ERG	C1-C2-C3	-2.44	107.34	110.47
2	C	1001	ERG	C1-C2-C3	-2.42	107.36	110.47
2	A	1001	ERG	C1-C2-C3	-2.40	107.39	110.47
2	D	1001	ERG	C1-C2-C3	-2.37	107.42	110.47
2	C	1001	ERG	C14-C8-C9	2.35	118.20	114.66
2	D	1001	ERG	C14-C8-C9	2.32	118.15	114.66
2	D	1001	ERG	C17-C20-C22	-2.30	105.90	110.27
2	A	1001	ERG	C17-C20-C22	-2.28	105.93	110.27
2	C	1001	ERG	C17-C20-C22	-2.27	105.95	110.27
2	A	1001	ERG	C14-C8-C9	2.27	118.07	114.66
2	C	1001	ERG	C18-C13-C14	2.27	113.92	110.24
2	B	1001	ERG	C14-C8-C9	2.27	118.07	114.66
2	A	1001	ERG	C18-C13-C14	2.27	113.91	110.24
2	B	1001	ERG	C17-C20-C22	-2.26	105.96	110.27
2	B	1001	ERG	C18-C13-C14	2.25	113.89	110.24
2	D	1001	ERG	C18-C13-C14	2.22	113.84	110.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

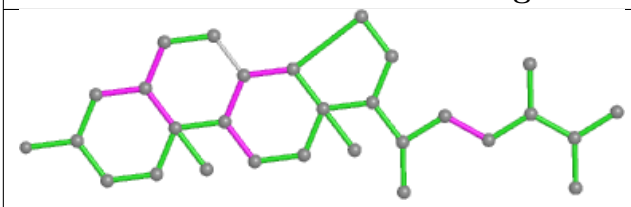
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ERG	4	0
2	C	1001	ERG	3	0
2	B	1001	ERG	2	0
2	D	1001	ERG	9	0

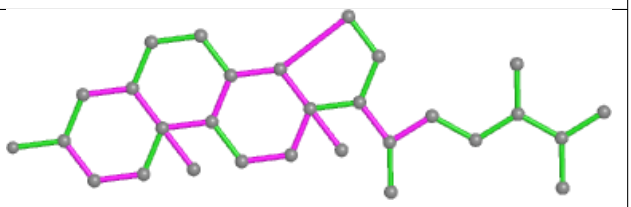
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

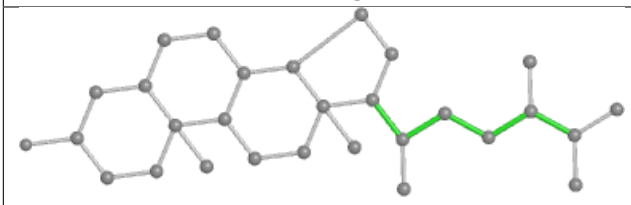
Ligand ERG A 1001



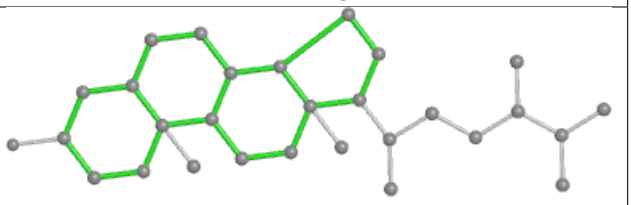
Bond lengths



Bond angles

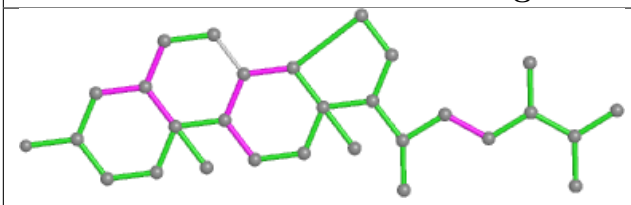


Torsions

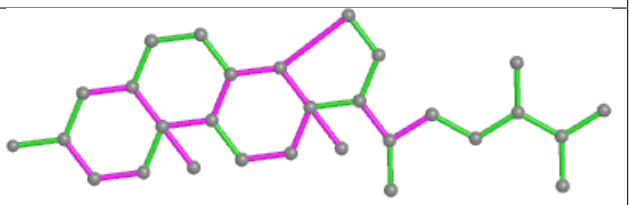


Rings

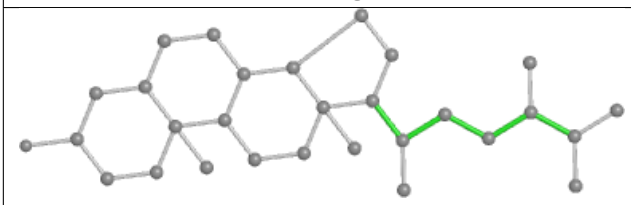
Ligand ERG C 1001



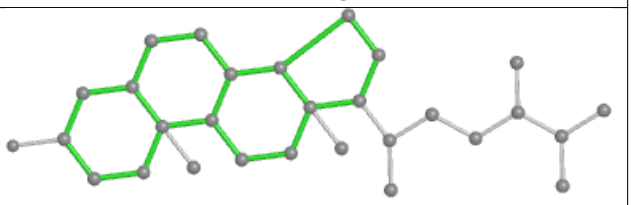
Bond lengths



Bond angles

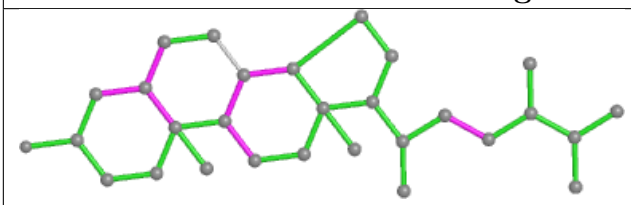


Torsions

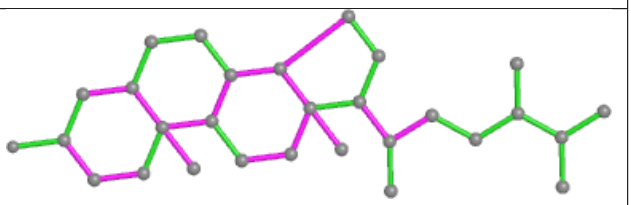


Rings

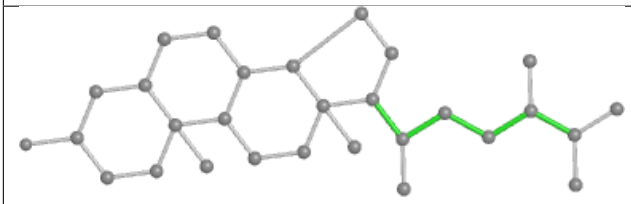
Ligand ERG B 1001



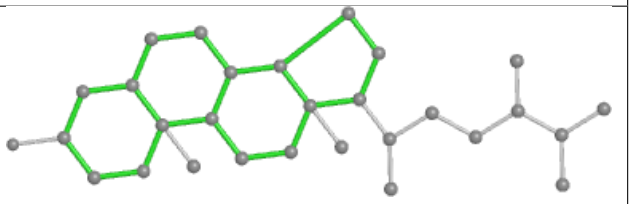
Bond lengths



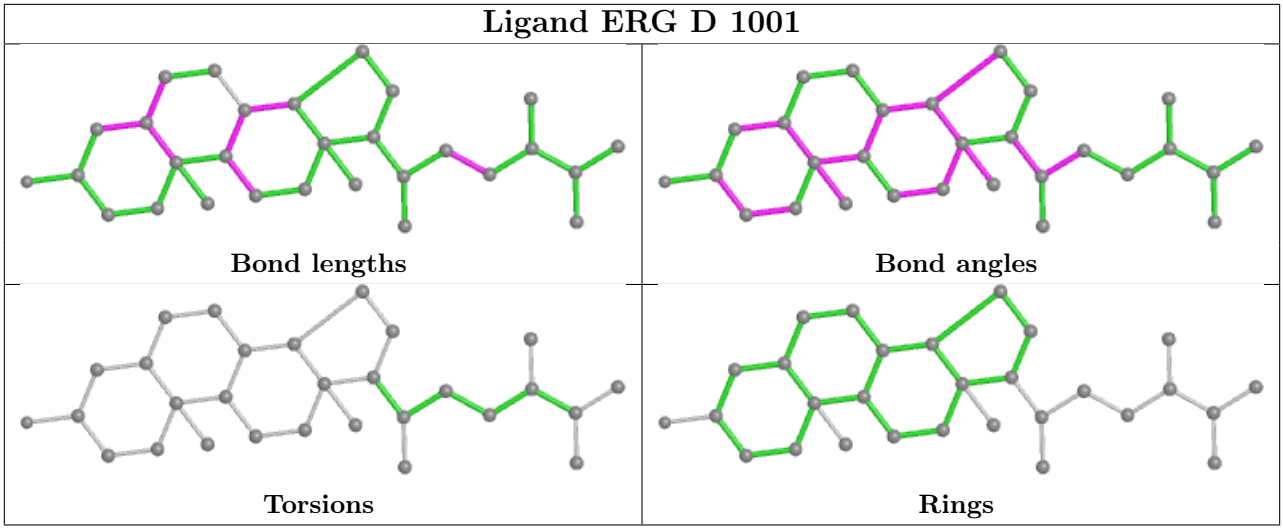
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	281/308 (91%)	0.53	15 (5%) 26 20	30, 47, 79, 95	0
1	B	280/308 (90%)	0.49	27 (9%) 8 5	29, 44, 86, 100	0
1	C	282/308 (91%)	0.40	14 (4%) 28 23	30, 47, 76, 95	0
1	D	253/308 (82%)	0.47	20 (7%) 12 9	34, 55, 84, 105	0
All	All	1096/1232 (88%)	0.47	76 (6%) 16 12	29, 49, 83, 105	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	785	GLY	5.4
1	A	910	LEU	5.1
1	D	810	LEU	4.8
1	A	735	SER	4.8
1	B	786	THR	4.5
1	B	772	ASP	4.5
1	D	771	VAL	4.4
1	A	736	ASN	4.3
1	D	854	ALA	4.2
1	B	781	ASP	3.8
1	B	797	ILE	3.6
1	B	802	PRO	3.6
1	D	769	ILE	3.6
1	D	806	ASP	3.6
1	A	737	SER	3.5
1	B	801	TYR	3.5
1	C	797	ILE	3.5
1	B	807	SER	3.5
1	C	908	GLY	3.5
1	B	787	ILE	3.4
1	D	807	SER	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	791	VAL	3.4
1	B	783	ASP	3.4
1	A	810	LEU	3.3
1	D	820	TYR	3.3
1	B	800	LEU	3.2
1	A	841	ARG	3.1
1	B	788	THR	3.1
1	C	772	ASP	3.1
1	B	850	GLY	3.0
1	B	822	GLU	3.0
1	B	739	PRO	2.9
1	A	794	ASP	2.8
1	C	785	GLY	2.8
1	D	824	ASN	2.8
1	A	888	ARG	2.8
1	D	772	ASP	2.8
1	B	692	TYR	2.8
1	A	803	VAL	2.7
1	B	780	VAL	2.7
1	B	782	LYS	2.7
1	C	796	ASP	2.7
1	D	625	SER	2.7
1	B	803	VAL	2.7
1	C	841	ARG	2.6
1	B	815	TYR	2.6
1	C	686	GLN	2.6
1	C	803	VAL	2.5
1	C	711	ILE	2.5
1	A	685	THR	2.5
1	D	815	TYR	2.5
1	B	784	THR	2.4
1	D	804	ASP	2.4
1	D	802	PRO	2.4
1	B	795	ASP	2.4
1	B	794	ASP	2.4
1	D	856	ARG	2.4
1	A	845	THR	2.4
1	A	778	GLU	2.3
1	D	884	GLN	2.3
1	A	850	GLY	2.3
1	C	791	VAL	2.2
1	D	803	VAL	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	776	LEU	2.2
1	B	683	SER	2.2
1	B	821	ARG	2.2
1	C	820	TYR	2.2
1	C	687	PRO	2.2
1	C	779	ILE	2.1
1	D	863	LYS	2.1
1	D	808	PRO	2.1
1	D	816	LEU	2.1
1	B	789	GLU	2.0
1	A	639	THR	2.0
1	A	842	THR	2.0
1	D	813	LEU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

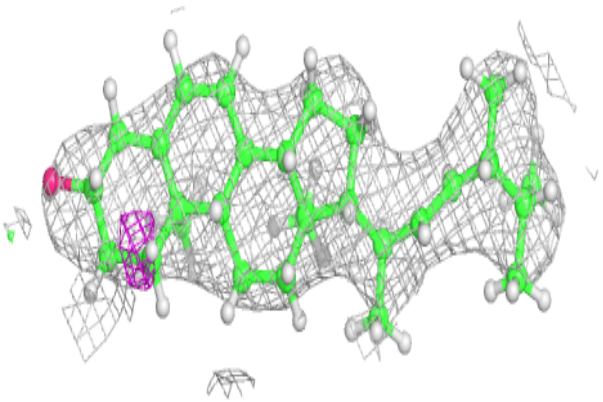
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

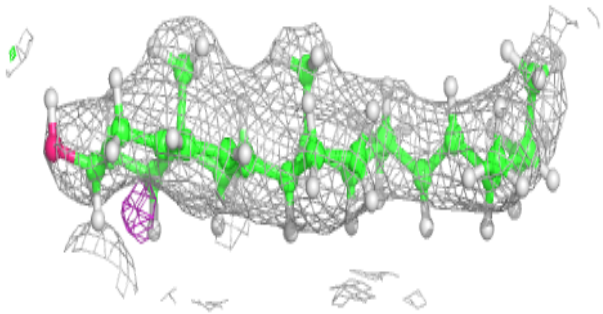
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ERG	D	1001	29/29	0.86	0.21	35,55,68,75	0
2	ERG	B	1001	29/29	0.90	0.17	26,40,47,54	0
2	ERG	C	1001	29/29	0.92	0.15	33,45,54,57	0
2	ERG	A	1001	29/29	0.92	0.17	24,41,49,52	0

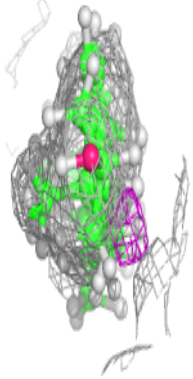
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ERG D 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

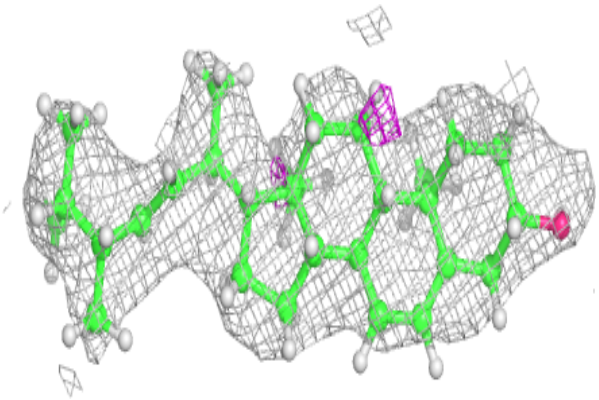


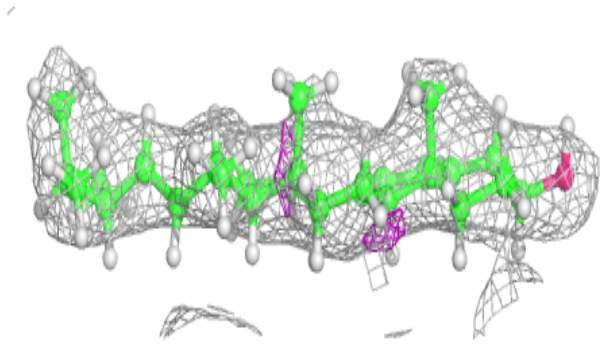


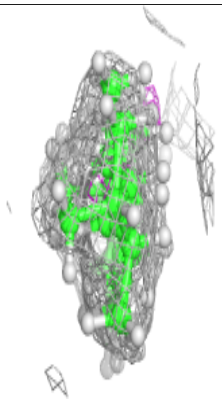


Electron density around ERG B 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

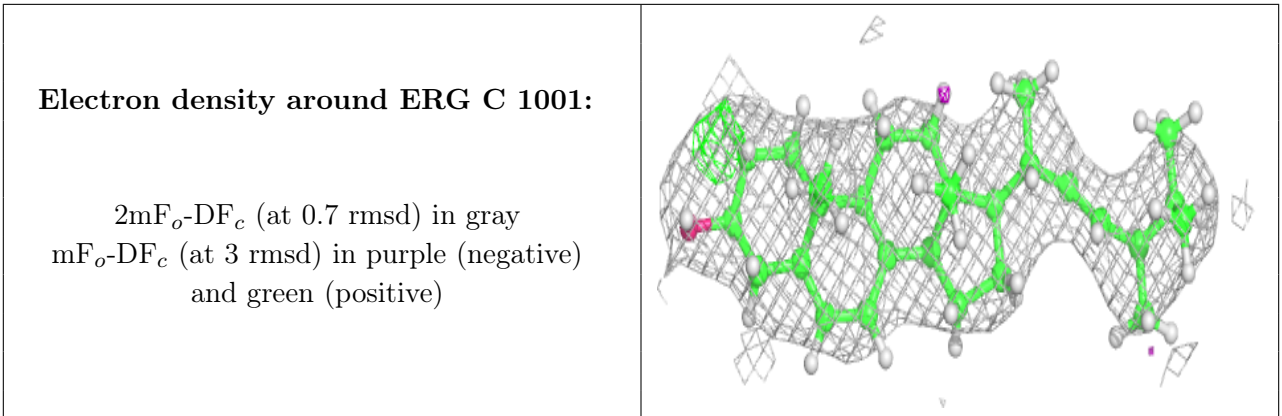


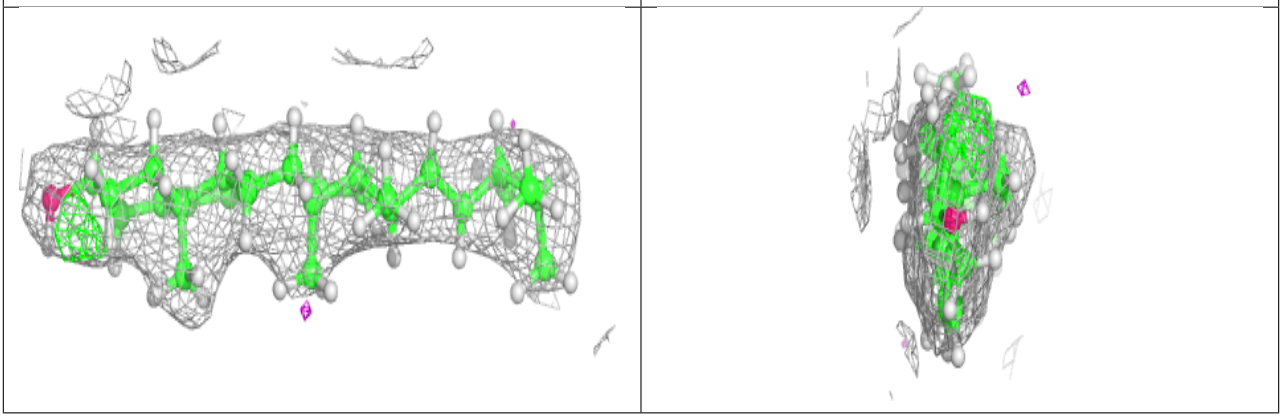




Electron density around ERG C 1001:

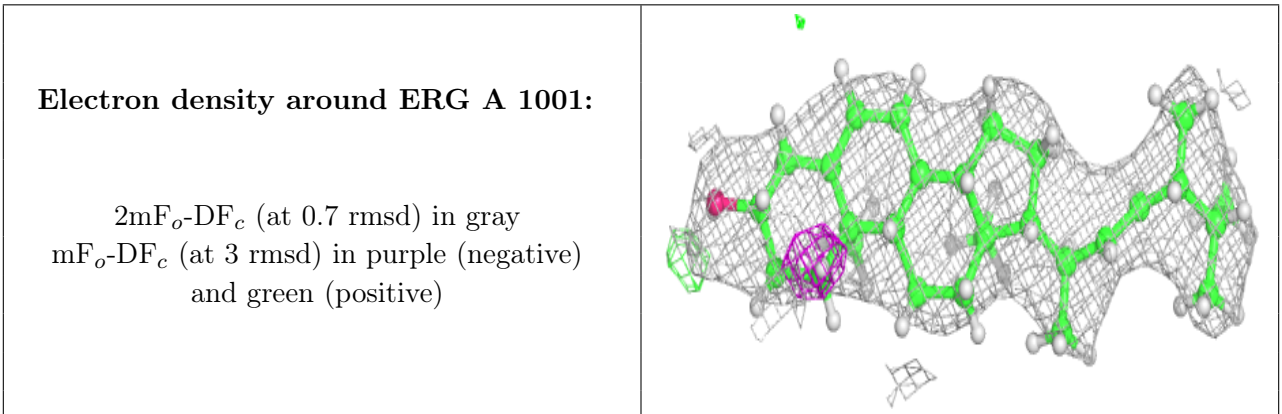
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

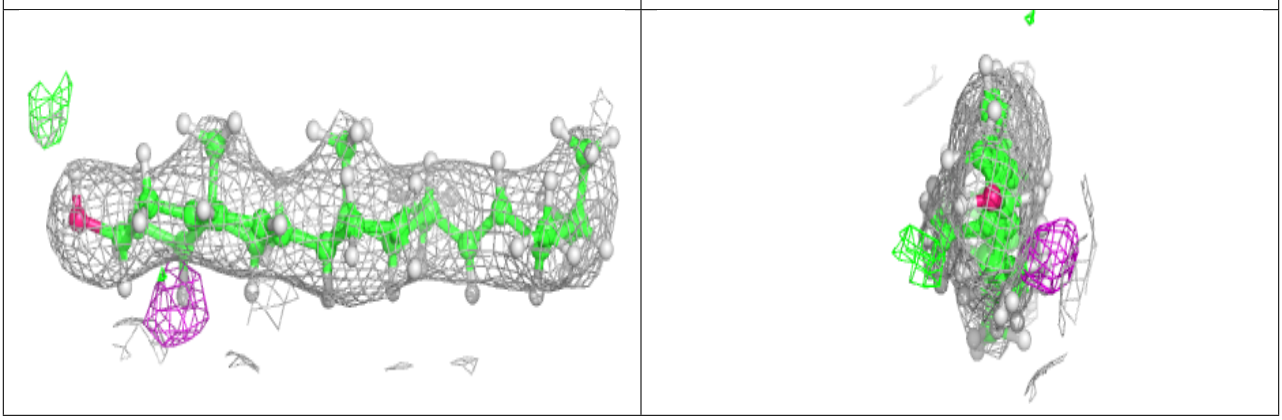




Electron density around ERG A 1001:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





6.5 Other polymers (i)

There are no such residues in this entry.