



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:40 PM UTC

PDB ID : 7VPR / pdb_00007vpr
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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

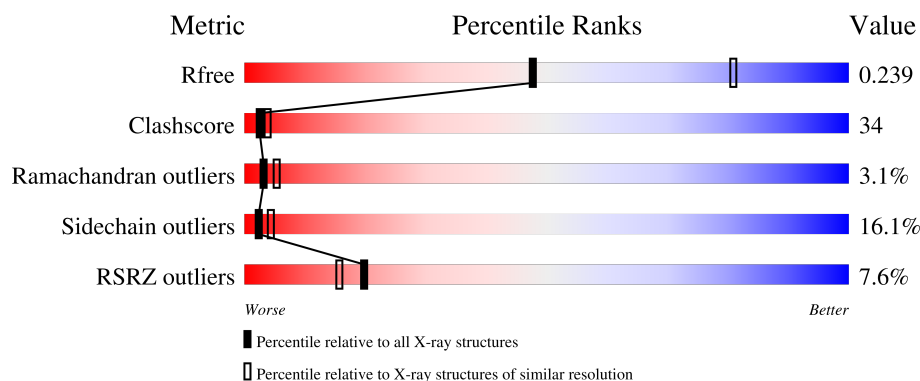
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.59 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 $\leq 5\%$. 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	308	9% 53% 28% 9% • 9%
1	B	308	7% 45% 32% 11% • 9%
1	C	308	5% 49% 32% 8% • 8%
1	D	308	6% 37% 30% 12% • 18%

2 Entry composition

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:

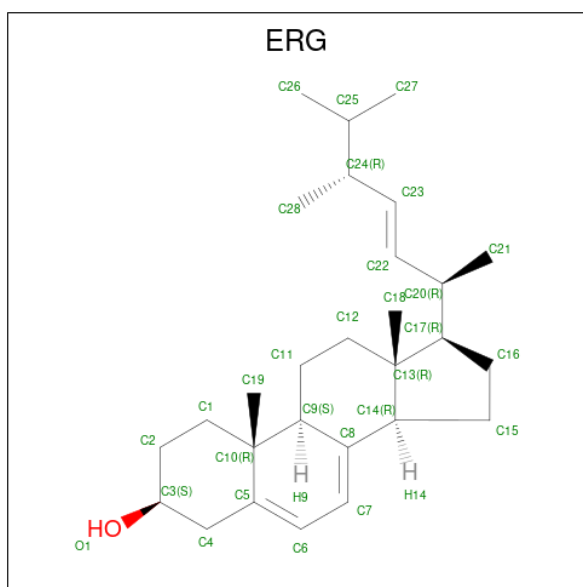
Chain	Residue	Modelled	Actual	Comment	Reference
A	615	GLY	-	expression tag	UNP Q6FX18
A	616	SER	-	expression tag	UNP Q6FX18
A	617	ALA	-	expression tag	UNP Q6FX18
A	618	MET	-	expression tag	UNP Q6FX18
A	619	GLY	-	expression tag	UNP Q6FX18
A	620	SER	-	expression tag	UNP Q6FX18
B	615	GLY	-	expression tag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

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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 (CCD ID: 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		

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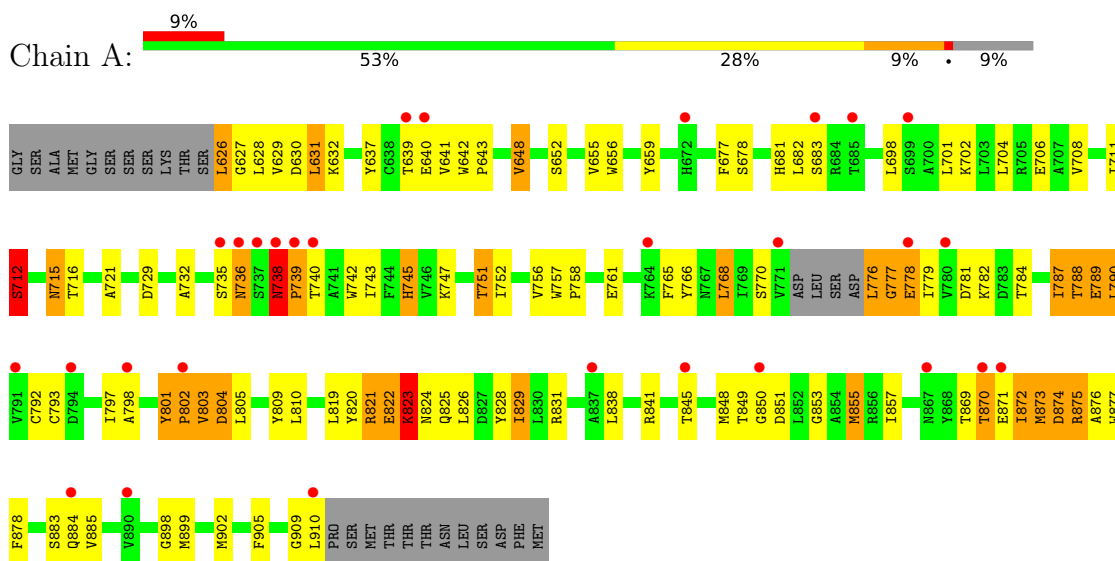
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	12	Total	O	0	0
			12	12		

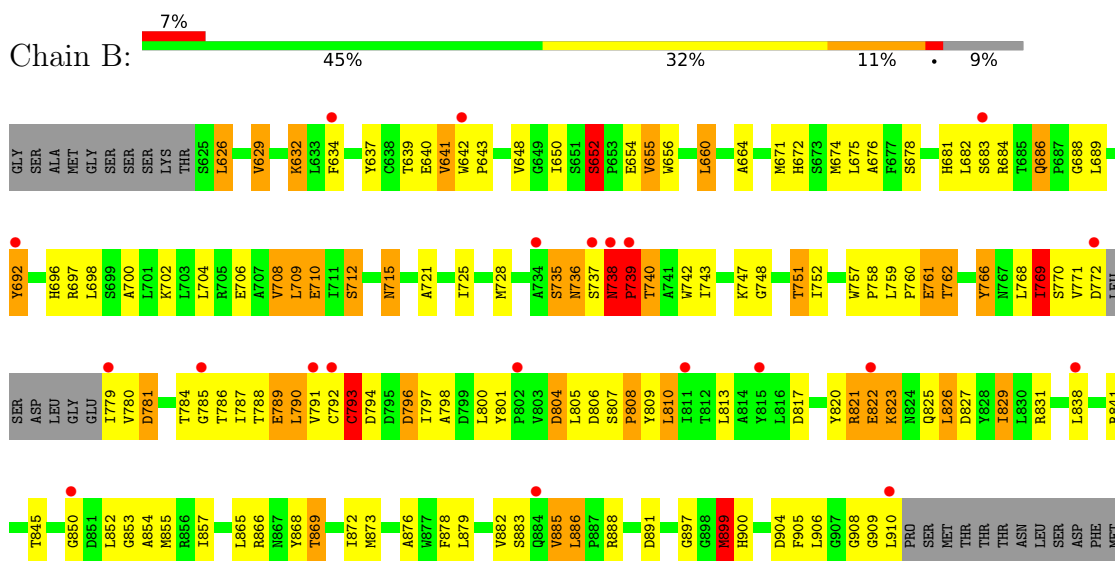
3 Residue-property plots

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

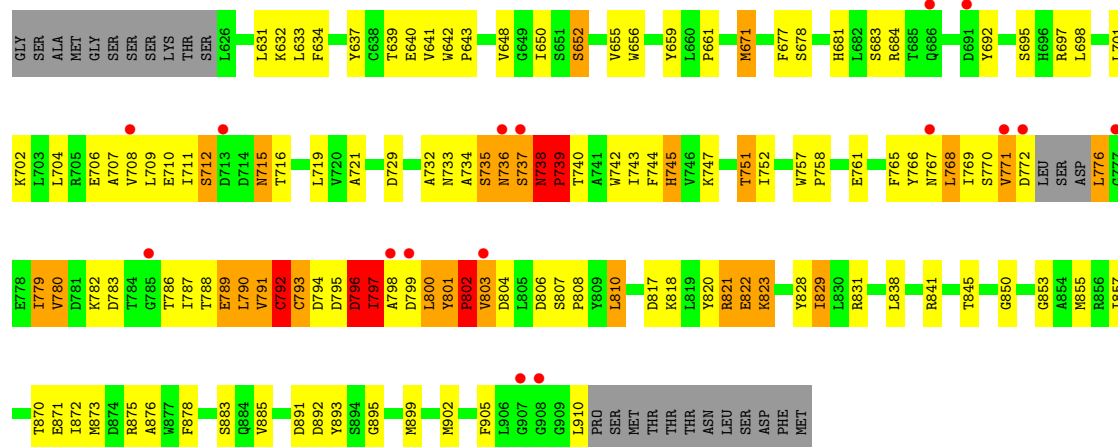
- Molecule 1: Sterol uptake control protein 2 (Upc2)



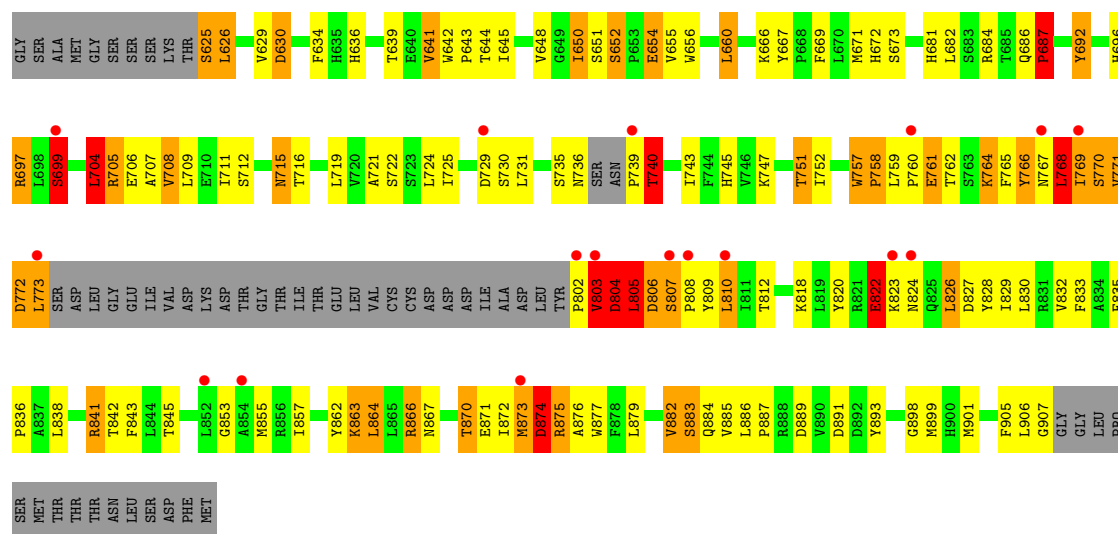
- Molecule 1: Sterol uptake control protein 2 (Upc2)



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



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



4 Data and refinement statistics

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 27.60 – 2.59	Depositor EDS
% Data completeness (in resolution range)	98.0 (27.60-2.59) 93.8 (27.60-2.59)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	-0.26 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.231 , 0.250 (Not available) , 0.239	Depositor DCC
R_{free} test set	1723 reflections (4.88%)	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 , 42.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

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	1.18	8/2267 (0.4%)	1.25	24/3089 (0.8%)
1	B	1.48	5/2260 (0.2%)	1.41	35/3080 (1.1%)
1	C	0.96	2/2275 (0.1%)	0.97	12/3100 (0.4%)
1	D	1.47	4/2062 (0.2%)	1.15	13/2806 (0.5%)
All	All	1.28	19/8864 (0.2%)	1.21	84/12075 (0.7%)

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 (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	739	PRO	N-CA	16.62	1.68	1.47
1	A	802	PRO	N-CA	12.57	1.68	1.47
1	A	871	GLU	C-O	7.50	1.33	1.24
1	A	869	THR	C-O	-6.49	1.16	1.24
1	A	870	THR	C-O	5.90	1.31	1.24
1	B	739	PRO	C-O	-5.74	1.16	1.24
1	D	807	SER	C-N	5.61	1.38	1.33
1	C	807	SER	C-N	5.60	1.38	1.33
1	D	630	ASP	C-O	-5.45	1.17	1.24
1	A	801	TYR	C-N	5.43	1.44	1.34
1	B	675	LEU	C-O	-5.40	1.17	1.24
1	A	823	LYS	N-CA	5.33	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	745	HIS	C-O	-5.32	1.18	1.24
1	A	745	HIS	C-O	-5.31	1.18	1.24
1	D	745	HIS	C-O	-5.27	1.18	1.24
1	D	667	TYR	C-O	-5.26	1.20	1.25
1	A	872	ILE	C-O	-5.24	1.18	1.24
1	B	674	MET	C-O	-5.22	1.17	1.24
1	B	885	VAL	C-O	-5.12	1.18	1.24

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	738	ASN	CA-C-N	16.73	140.75	119.84
1	B	738	ASN	C-N-CA	16.73	140.75	119.84
1	B	739	PRO	N-CA-CB	-11.02	91.68	103.25
1	B	739	PRO	CA-N-CD	-9.26	99.04	112.00
1	C	793	CYS	N-CA-C	8.43	124.68	113.72
1	B	641	VAL	N-CA-C	8.28	118.33	110.30
1	A	873	MET	N-CA-C	-8.14	102.49	111.36
1	D	699	SER	N-CA-C	-8.09	102.44	111.82
1	A	777	GLY	CA-C-N	8.09	131.92	120.28
1	A	777	GLY	C-N-CA	8.09	131.92	120.28
1	B	808	PRO	N-CA-C	-8.05	101.07	114.75
1	A	802	PRO	CA-N-CD	-7.99	100.31	111.50
1	D	641	VAL	N-CA-C	7.75	117.79	110.74
1	D	704	LEU	N-CA-C	-7.72	102.46	111.03
1	B	735	SER	CA-C-N	7.51	135.89	121.54
1	B	735	SER	C-N-CA	7.51	135.89	121.54
1	A	823	LYS	N-CA-C	7.50	123.75	111.37
1	C	792	CYS	CA-C-N	7.35	133.95	122.26
1	C	792	CYS	C-N-CA	7.35	133.95	122.26
1	C	801	TYR	N-CA-C	7.26	122.58	109.44
1	C	738	ASN	C-N-CD	7.17	136.37	120.60
1	D	757	TRP	C-N-CD	7.10	136.23	120.60
1	A	870	THR	CB-CA-C	6.90	122.24	110.79
1	B	766	TYR	CA-C-N	6.51	131.76	121.08
1	B	766	TYR	C-N-CA	6.51	131.76	121.08
1	B	736	ASN	N-CA-C	-6.51	96.94	110.80
1	B	660	LEU	O-C-N	6.50	124.75	120.27
1	B	810	LEU	N-CA-C	6.46	118.90	111.02
1	D	822	GLU	N-CA-C	6.45	120.89	112.89
1	C	810	LEU	N-CA-C	6.42	118.85	111.02
1	D	810	LEU	N-CA-C	6.38	118.80	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	871	GLU	CA-C-N	-6.26	112.50	121.52
1	A	871	GLU	C-N-CA	-6.26	112.50	121.52
1	B	804	ASP	CB-CA-C	-6.15	97.08	109.68
1	B	852	LEU	N-CA-C	6.14	118.94	111.82
1	D	906	LEU	N-CA-C	6.01	119.45	110.14
1	B	688	GLY	N-CA-C	5.97	123.60	115.30
1	B	899	MET	N-CA-C	-5.96	104.91	111.82
1	B	769	ILE	CB-CA-C	-5.87	101.67	111.29
1	B	888	ARG	CA-C-N	5.83	130.17	122.30
1	B	888	ARG	C-N-CA	5.83	130.17	122.30
1	A	712	SER	N-CA-C	-5.73	100.60	109.14
1	B	807	SER	CA-C-N	-5.67	114.40	120.47
1	B	807	SER	C-N-CA	-5.67	114.40	120.47
1	B	692	TYR	N-CA-C	-5.63	104.78	111.03
1	A	874	ASP	CA-C-N	-5.63	112.88	122.56
1	A	874	ASP	C-N-CA	-5.63	112.88	122.56
1	D	692	TYR	N-CA-C	-5.58	105.10	111.07
1	D	687	PRO	CA-N-CD	-5.53	104.26	112.00
1	A	855	MET	N-CA-C	5.52	117.30	111.28
1	B	712	SER	N-CA-C	-5.49	100.47	109.80
1	A	738	ASN	N-CA-CB	5.45	116.64	109.55
1	B	736	ASN	CB-CA-C	5.44	121.25	110.42
1	A	798	ALA	CA-C-N	5.38	128.23	120.38
1	A	798	ALA	C-N-CA	5.38	128.23	120.38
1	A	627	GLY	N-CA-C	5.37	119.31	110.77
1	C	801	TYR	C-N-CD	5.34	132.34	120.60
1	A	704	LEU	CA-C-N	5.29	127.80	120.29
1	A	704	LEU	C-N-CA	5.29	127.80	120.29
1	B	652	SER	CA-C-N	-5.27	114.39	119.87
1	B	652	SER	C-N-CA	-5.27	114.39	119.87
1	C	807	SER	CA-C-N	-5.27	114.52	120.89
1	C	807	SER	C-N-CA	-5.27	114.52	120.89
1	D	807	SER	CA-C-N	-5.24	114.55	120.89
1	D	807	SER	C-N-CA	-5.24	114.55	120.89
1	B	737	SER	CA-C-O	-5.24	116.19	122.27
1	A	770	SER	CA-C-N	5.21	131.09	121.70
1	A	770	SER	C-N-CA	5.21	131.09	121.70
1	B	740	THR	CA-C-O	-5.20	115.36	120.82
1	B	793	CYS	CA-C-N	5.15	131.38	121.54
1	B	793	CYS	C-N-CA	5.15	131.38	121.54
1	C	802	PRO	CA-C-N	5.14	130.95	121.70
1	C	802	PRO	C-N-CA	5.14	130.95	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	780	VAL	N-CA-C	5.14	116.63	109.80
1	D	759	LEU	CA-C-N	-5.09	114.38	120.13
1	D	759	LEU	C-N-CA	-5.09	114.38	120.13
1	A	768	LEU	CA-C-N	-5.09	115.11	122.69
1	A	768	LEU	C-N-CA	-5.09	115.11	122.69
1	B	759	LEU	CA-C-N	-5.05	114.51	119.92
1	B	759	LEU	C-N-CA	-5.05	114.51	119.92
1	B	886	LEU	CA-C-N	-5.02	115.06	120.03
1	B	886	LEU	C-N-CA	-5.02	115.06	120.03
1	A	801	TYR	CA-C-N	5.01	139.02	127.00
1	A	801	TYR	C-N-CA	5.01	139.02	127.00

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

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	125	0
1	B	2208	0	2198	156	1
1	C	2223	0	2212	161	3
1	D	2012	0	2018	163	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	6	0
3	B	22	0	0	7	0
3	C	14	0	0	0	0
3	D	12	0	0	1	0
All	All	8838	176	8813	604	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 34.

All (604) 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:B:850:GLY:CA	1:B:855:MET:HE3	1.78	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:D:634:PHE:CD1	1:D:671:MET:HE1	1.86	1.08
1:D:771:VAL:CG2	1:D:818:LYS:CE	2.26	1.08
1:B:855:MET:HE1	1:B:899:MET:SD	1.93	1.08
1:A:736:ASN:CB	1:A:884:GLN:NE2	2.18	1.07
1:A:738:ASN:CG	1:A:739:PRO:HD2	1.78	1.07
1:A:849:THR:C	3:A:1101:HOH:O	1.94	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:738:ASN:CG	1:A:739:PRO:CD	2.30	1.03
1:A:736:ASN:CB	1:A:884:GLN:HE22	1.71	1.03
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:850:GLY:HA2	1:B:855:MET:HE3	0.99	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:A:779:ILE:HD11	1:A:790:LEU:HD12	1.49	0.92
1:D:634:PHE:HD1	1:D:671:MET:HE1	1.33	0.90
1:D:802:PRO:CA	1:D:803:VAL:HG13	2.00	0.89
1:B:873:MET:HE1	1:B:883:SER:OG	1.72	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:D:634:PHE:CE1	1:D:671:MET:HE1	2.10	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:B:850:GLY:CA	1:B:855:MET:CE	2.47	0.84
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:A:855:MET:HE1	1:A:899:MET:HG3	1.57	0.82
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
1:A:648:VAL:HG22	1:A:876:ALA:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:848:MET:SD	1:A:902:MET:HE3	2.21	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:A:855:MET:HE1	1:A:899:MET:CG	2.12	0.78
1:B:850:GLY:HA2	1:B:855:MET:HE1	1.63	0.78
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:A:736:ASN:HA	1:A:884:GLN:CD	2.09	0.78
1:B:708:VAL:HG21	1:B:752:ILE:HD13	1.64	0.78
1:C:855:MET:HE1	1:C:899:MET:SD	2.24	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: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:C:769:ILE:HD13	1:C:838:LEU:CD1	2.14	0.75
1:B:891:ASP:CG	3:B:1103:HOH:O	2.29	0.75
1:A:855:MET:CE	1:A:899:MET:HG3	2.16	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:B:762:THR:OG1	3:B:1101:HOH:O	1.98	0.74
1:A:736:ASN:CA	1:A:884:GLN:NE2	2.50	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:PHE:CE1	2:B:1001:ERG:H22	2.24	0.73
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: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:C:634:PHE:CD2	1:C:671:MET:HE1	2.25	0.71
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:D:768:LEU:HD23	1:D:768:LEU:C	2.14	0.71
1:D:855:MET:HE3	2:D:1001:ERG:O1	1.91	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: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:CE	1:B:899:MET:SD	2.78	0.69
1:B:910:LEU:HD23	1:B:910:LEU:C	2.17	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: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: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
1:D:769:ILE:CG1	1:D:770:SER:H	2.06	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:664:ALA:HB1	1:B:671:MET:HE2	1.75	0.66
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:B:771:VAL:HG22	1:B:772:ASP:N	2.09	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:B:850:GLY:C	1:B:855:MET:HE3	2.21	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: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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:634:PHE:CE2	1:C:671:MET:HE1	2.35	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:D:625:SER:C	1:D:626:LEU:HD22	2.25	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: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:A:802:PRO:N	1:A:802:PRO:C	2.52	0.60
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:D:873:MET:C	1:D:875:ARG:H	2.08	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:HD22	1:D:626:LEU:N	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:C:739:PRO:C	1:C:740:THR:HG23	2.26	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

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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: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: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:634:PHE:HD2	1:C:671:MET:HE1	1.70	0.56
1:D:630:ASP:OD1	1:D:692:TYR:OH	2.21	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:C:850:GLY:HA2	1:C:855:MET:HE3	1.85	0.56
1:D:707:ALA:C	1:D:709:LEU:H	2.13	0.56
1:A:804:ASP:OD1	1:A:804:ASP:N	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:873:MET:HE1	1:B:883:SER:CB	2.35	0.56
1:C:797:ILE:HB	1:C:800:LEU:HD13	1.87	0.56
1:A:850:GLY:HA2	1:A:855:MET:HE3	1.88	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: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: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:739:PRO:O	1:C:740:THR:OG1	2.20	0.55
1:C:769:ILE:HG13	1:C:770:SER:N	2.20	0.55
1:C:870:THR:HA	1:C:873:MET:HE3	1.88	0.55
1:B:853:GLY:O	1:B:857:ILE:HG12	2.06	0.55
1:C:855:MET:CE	1:C:902:MET:HE1	2.35	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:D:769:ILE:HG23	1:D:770:SER:N	2.21	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: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:B:873:MET:HE1	1:B:883:SER:H	1.72	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: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:736:ASN:HA	1:C:737:SER:C	2.33	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:771:VAL:CG2	1:C:818:LYS:CE	2.86	0.54
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:A:855:MET:HE1	1:A:899:MET:SD	2.48	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: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:A:766:TYR:CD1	1:A:766:TYR:C	2.86	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: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: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:708:VAL:HG13	1:C:711:ILE:HD11	1.91	0.51
1:C:796:ASP:C	1:C:797:ILE:HG23	2.35	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:785:GLY:C	1:B:786:THR:HG23	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:651:SER:C	1:D:652:SER:OG	2.50	0.51
1:A:792:CYS:SG	1:A:793:CYS:N	2.84	0.51
1:D:872:ILE:HG13	1:D:872:ILE:O	2.09	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: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:873:MET:HE2	1:B:882:VAL:H	1.77	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:C:671:MET:HE3	1:C:671:MET:HA	1.93	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:D:855:MET:HE2	2:D:1001:ERG:O1	2.12	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:A:909:GLY:C	1:A:910:LEU:HD12	2.37	0.49
1:B:697:ARG:HG2	1:B:697:ARG:NH1	2.28	0.49
1:B:715:ASN:C	1:B:715:ASN:HD22	2.19	0.49
1:B:797:ILE:HB	1:B:800:LEU:HD12	1.93	0.49
1:B:910:LEU:C	1:B:910:LEU:CD2	2.85	0.49
1:C:786:THR:CG2	1:C:804:ASP:OD1	2.60	0.49
1:B:785:GLY:C	1:B:786:THR:CG2	2.86	0.49
1:C:798:ALA:C	1:C:800:LEU:H	2.19	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:C:780:VAL:HG13	1:C:786:THR:C	2.38	0.48
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:B:689:LEU:HA	1:B:692:TYR:HD2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:682:LEU:C	1:D:684:ARG:N	2.70	0.48
1:B:873:MET:HE2	1:B:882:VAL:N	2.28	0.48
1:C:798:ALA:C	1:C:800:LEU:N	2.71	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
1:A:781:ASP:HB2	1:A:788:THR:HG21	1.93	0.48
1:B:715:ASN:ND2	1:B:715:ASN:C	2.72	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:B:792:CYS:HG	1:B:793:CYS:N	2.10	0.47
1:C:771:VAL:HG21	1:C:818:LYS:CE	2.43	0.47
1:C:892:ASP:O	1:C:893:TYR:C	2.57	0.47
1:B:751:THR:CB	1:B:908:GLY:HA2	2.44	0.47
1:A:822:GLU:CD	1:A:831:ARG:HH11	2.21	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: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:879:LEU:C	1:B:882:VAL:HG23	2.39	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:634:PHE:HD1	1:D:671:MET:CE	2.17	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:715:ASN:ND2	1:C:715:ASN:C	2.72	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:A:732:ALA:HB2	1:A:878:PHE:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:871:GLU:C	1:C:873:MET:H	2.22	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:C:780:VAL:CG1	1:C:786:THR:O	2.64	0.46
1:D:765:PHE:C	1:D:767:ASN:N	2.73	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
1:C:769:ILE:HD12	1:C:770:SER:H	1.79	0.46
1:D:681:HIS:ND1	1:D:681:HIS:C	2.71	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:D:835:PHE:CD1	1:D:835:PHE:C	2.94	0.46
1:A:819:LEU:O	1:A:828:TYR:HE1	1.99	0.46
1:B:664:ALA:CB	1:B:671:MET:HE2	2.43	0.46
1:B:820:TYR:C	1:B:822:GLU:H	2.24	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:855:MET:HE2	1:C:902:MET:CE	2.46	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:D:765:PHE:C	1:D:767:ASN:H	2.25	0.45
1:C:796:ASP:C	1:C:797:ILE:CG2	2.90	0.45
1:D:715:ASN:ND2	1:D:715:ASN:C	2.73	0.45
1:D:873:MET:C	1:D:875:ARG:N	2.72	0.45
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
1:C:787:ILE:HB	1:C:803:VAL:HG12	1.97	0.44
1:A:715:ASN:C	1:A:715:ASN:ND2	2.72	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:D:898:GLY:O	2:D:1001:ERG:C1	2.66	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:637:TYR:CD1	1:B:637:TYR:C	2.96	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:D:889:ASP:CG	1:D:891:ASP:HB2	2.43	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: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:A:848:MET:SD	1:A:902:MET:HE1	2.58	0.43
1:C:707:ALA:HB3	1:C:719:LEU:HD21	2.00	0.43
1:B:632:LYS:HE2	1:B:686:GLN:HE22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:899:MET:HE2	1:B:899:MET:HB2	1.85	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: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:C:820:TYR:C	1:C:822:GLU:H	2.26	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:C:829:ILE:HD13	1:C:829:ILE:HA	1.79	0.42
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: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:B:825:GLN:HG3	1:B:826:LEU:H	1.84	0.42
1:C:708:VAL:C	1:C:710:GLU:N	2.77	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:D:682:LEU:C	1:D:684:ARG:H	2.26	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:767:ASN:C	1:C:769:ILE:H	2.28	0.42
1:D:681:HIS:C	1:D:681:HIS:HD1	2.26	0.42
1:D:687:PRO:HD2	1:D:687:PRO:O	2.20	0.42
1:D:842:THR:O	1:D:843:PHE:C	2.63	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:898:GLY:O	2:D:1001:ERG:H21	2.20	0.41
1:B:796:ASP:OD1	1:B:796:ASP:N	2.51	0.41
1:D:802:PRO:CB	1:D:803:VAL:CG1	2.91	0.41
1:D:886:LEU:HD23	1:D:886:LEU:HA	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:760:PRO:C	1:D:762:THR:N	2.78	0.41
1:B:739:PRO:HB2	1:B:742:TRP:NE1	2.35	0.41
1:C:855:MET:HE2	1:C:902:MET:SD	2.61	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
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: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:715:ASN:HD22	1:C:715:ASN:C	2.29	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:715:ASN:HD22	1:A:715:ASN:C	2.29	0.40
1:A:829:ILE:O	1:A:829:ILE:HD12	2.21	0.40
1:B:640:GLU:C	1:B:643:PRO:HD2	2.46	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:B:682:LEU:C	1:B:684:ARG:N	2.76	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:829:ILE:HD13	1:A:829:ILE:HA	1.79	0.40
1:C:708:VAL:C	1:C:710:GLU:H	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	18	38
1	B	276/308 (90%)	252 (91%)	19 (7%)	5 (2%)	6	14
1	C	278/308 (90%)	240 (86%)	25 (9%)	13 (5%)	2	2
1	D	247/308 (80%)	221 (90%)	13 (5%)	13 (5%)	1	1
All	All	1078/1232 (88%)	974 (90%)	71 (7%)	33 (3%)	3	5

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

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	244/268 (91%)	206 (84%)	38 (16%)	2	4
1	B	244/268 (91%)	207 (85%)	37 (15%)	3	5
1	C	245/268 (91%)	213 (87%)	32 (13%)	4	8
1	D	221/268 (82%)	174 (79%)	47 (21%)	1	2
All	All	954/1072 (89%)	800 (84%)	154 (16%)	2	4

All (154) 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

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Mol	Chain	Res	Type
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
1	A	782	LYS
1	A	787	ILE
1	A	788	THR
1	A	789	GLU
1	A	790	LEU
1	A	797	ILE
1	A	803	VAL
1	A	804	ASP
1	A	821	ARG
1	A	822	GLU
1	A	823	LYS
1	A	824	ASN
1	A	825	GLN
1	A	826	LEU
1	A	829	ILE
1	A	857	ILE
1	A	872	ILE
1	A	873	MET
1	A	874	ASP
1	A	875	ARG
1	B	626	LEU
1	B	629	VAL
1	B	632	LYS
1	B	652	SER
1	B	655	VAL
1	B	660	LEU
1	B	683	SER

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Mol	Chain	Res	Type
1	B	686	GLN
1	B	698	LEU
1	B	708	VAL
1	B	709	LEU
1	B	710	GLU
1	B	715	ASN
1	B	735	SER
1	B	739	PRO
1	B	751	THR
1	B	761	GLU
1	B	762	THR
1	B	769	ILE
1	B	770	SER
1	B	779	ILE
1	B	781	ASP
1	B	784	THR
1	B	789	GLU
1	B	790	LEU
1	B	791	VAL
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	869	THR
1	B	885	VAL
1	B	899	MET
1	C	631	LEU
1	C	632	LYS
1	C	671	MET
1	C	683	SER
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

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Mol	Chain	Res	Type
1	C	761	GLU
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	797	ILE
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
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	706	GLU
1	D	708	VAL
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

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Mol	Chain	Res	Type
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	863	LYS
1	D	864	LEU
1	D	866	ARG
1	D	870	THR
1	D	871	GLU
1	D	873	MET
1	D	874	ASP
1	D	875	ARG
1	D	882	VAL
1	D	883	SER
1	D	884	GLN
1	D	885	VAL
1	D	899	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	635	HIS
1	A	672	HIS
1	A	715	ASN
1	A	738	ASN
1	A	745	HIS
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	672	HIS
1	C	686	GLN

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Mol	Chain	Res	Type
1	C	715	ASN
1	C	738	ASN
1	C	745	HIS
1	C	884	GLN
1	D	636	HIS
1	D	672	HIS
1	D	715	ASN
1	D	736	ASN
1	D	745	HIS
1	D	867	ASN
1	D	884	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 oligosaccharides 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	C	1001	-	32,32,32	2.01	8 (25%)	45,50,50	1.60	11 (24%)
2	ERG	D	1001	-	32,32,32	2.03	8 (25%)	45,50,50	1.60	11 (24%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	ERG	A	1001	-	32,32,32	2.02	8 (25%)	45,50,50	1.60	11 (24%)
2	ERG	B	1001	-	32,32,32	2.02	8 (25%)	45,50,50	1.59	11 (24%)

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

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	ERG	C23-C22	5.97	1.50	1.32
2	C	1001	ERG	C23-C22	5.97	1.50	1.32
2	A	1001	ERG	C23-C22	5.96	1.50	1.32
2	B	1001	ERG	C23-C22	5.95	1.50	1.32
2	A	1001	ERG	C10-C5	-5.58	1.42	1.52
2	D	1001	ERG	C10-C5	-5.56	1.42	1.52
2	B	1001	ERG	C10-C5	-5.53	1.42	1.52
2	C	1001	ERG	C10-C5	-5.46	1.42	1.52
2	B	1001	ERG	C4-C5	-3.86	1.44	1.51
2	C	1001	ERG	C4-C5	-3.83	1.44	1.51
2	D	1001	ERG	C4-C5	-3.83	1.44	1.51
2	A	1001	ERG	C4-C5	-3.81	1.44	1.51
2	B	1001	ERG	C9-C8	-3.55	1.43	1.51
2	D	1001	ERG	C9-C8	-3.53	1.43	1.51
2	C	1001	ERG	C9-C8	-3.52	1.43	1.51
2	A	1001	ERG	C9-C8	-3.51	1.43	1.51
2	D	1001	ERG	C11-C9	3.24	1.59	1.53
2	C	1001	ERG	C11-C9	3.17	1.59	1.53
2	A	1001	ERG	C11-C9	3.16	1.59	1.53
2	B	1001	ERG	C11-C9	3.15	1.59	1.53
2	A	1001	ERG	C14-C8	-2.62	1.45	1.51
2	D	1001	ERG	C14-C8	-2.59	1.45	1.51
2	D	1001	ERG	C7-C8	2.59	1.40	1.34
2	A	1001	ERG	C7-C8	2.59	1.40	1.34
2	C	1001	ERG	C14-C8	-2.58	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1001	ERG	C7-C8	2.56	1.40	1.34
2	B	1001	ERG	C14-C8	-2.55	1.45	1.51
2	B	1001	ERG	C7-C8	2.52	1.40	1.34
2	B	1001	ERG	C6-C5	2.24	1.39	1.34
2	A	1001	ERG	C6-C5	2.22	1.39	1.34
2	D	1001	ERG	C6-C5	2.20	1.39	1.34
2	C	1001	ERG	C6-C5	2.20	1.39	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	ERG	C19-C10-C5	-3.62	102.86	108.38
2	D	1001	ERG	C19-C10-C5	-3.61	102.88	108.38
2	B	1001	ERG	C19-C10-C5	-3.58	102.91	108.38
2	A	1001	ERG	C19-C10-C5	-3.58	102.91	108.38
2	A	1001	ERG	C4-C5-C10	3.24	120.57	116.42
2	B	1001	ERG	C4-C5-C10	3.21	120.53	116.42
2	D	1001	ERG	C4-C5-C10	3.19	120.50	116.42
2	C	1001	ERG	C4-C5-C10	3.16	120.47	116.42
2	C	1001	ERG	C11-C12-C13	-2.75	108.10	112.74
2	B	1001	ERG	C11-C12-C13	-2.71	108.16	112.74
2	D	1001	ERG	C11-C12-C13	-2.71	108.16	112.74
2	A	1001	ERG	C9-C10-C5	2.71	113.98	109.66
2	B	1001	ERG	C9-C10-C5	2.70	113.96	109.66
2	A	1001	ERG	C11-C12-C13	-2.70	108.19	112.74
2	A	1001	ERG	C15-C14-C13	-2.68	101.81	104.21
2	D	1001	ERG	C9-C10-C5	2.68	113.93	109.66
2	C	1001	ERG	C9-C10-C5	2.64	113.87	109.66
2	B	1001	ERG	C15-C14-C13	-2.59	101.89	104.21
2	D	1001	ERG	C15-C14-C13	-2.58	101.91	104.21
2	C	1001	ERG	C15-C14-C13	-2.57	101.91	104.21
2	D	1001	ERG	C19-C10-C9	-2.51	106.82	110.98
2	A	1001	ERG	C19-C10-C9	-2.49	106.85	110.98
2	B	1001	ERG	C19-C10-C9	-2.49	106.85	110.98
2	C	1001	ERG	C19-C10-C9	-2.48	106.86	110.98
2	B	1001	ERG	C1-C2-C3	-2.37	107.34	110.48
2	C	1001	ERG	C1-C2-C3	-2.36	107.36	110.48
2	C	1001	ERG	C14-C8-C9	2.35	118.20	114.46
2	D	1001	ERG	C17-C20-C22	-2.34	105.90	110.49
2	A	1001	ERG	C1-C2-C3	-2.33	107.39	110.48
2	A	1001	ERG	C17-C20-C22	-2.32	105.93	110.49
2	D	1001	ERG	C14-C8-C9	2.32	118.15	114.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1001	ERG	C17-C20-C22	-2.31	105.95	110.49
2	D	1001	ERG	C1-C2-C3	-2.31	107.42	110.48
2	B	1001	ERG	C17-C20-C22	-2.31	105.96	110.49
2	A	1001	ERG	C14-C8-C9	2.27	118.07	114.46
2	B	1001	ERG	C14-C8-C9	2.27	118.07	114.46
2	C	1001	ERG	C18-C13-C14	2.15	113.92	110.35
2	A	1001	ERG	C18-C13-C14	2.15	113.91	110.35
2	B	1001	ERG	C18-C13-C14	2.14	113.89	110.35
2	D	1001	ERG	C18-C13-C14	2.11	113.84	110.35
2	C	1001	ERG	C24-C23-C22	-2.09	119.48	125.81
2	D	1001	ERG	C24-C23-C22	-2.09	119.48	125.81
2	B	1001	ERG	C24-C23-C22	-2.08	119.51	125.81
2	A	1001	ERG	C24-C23-C22	-2.06	119.57	125.81

There are no chirality outliers.

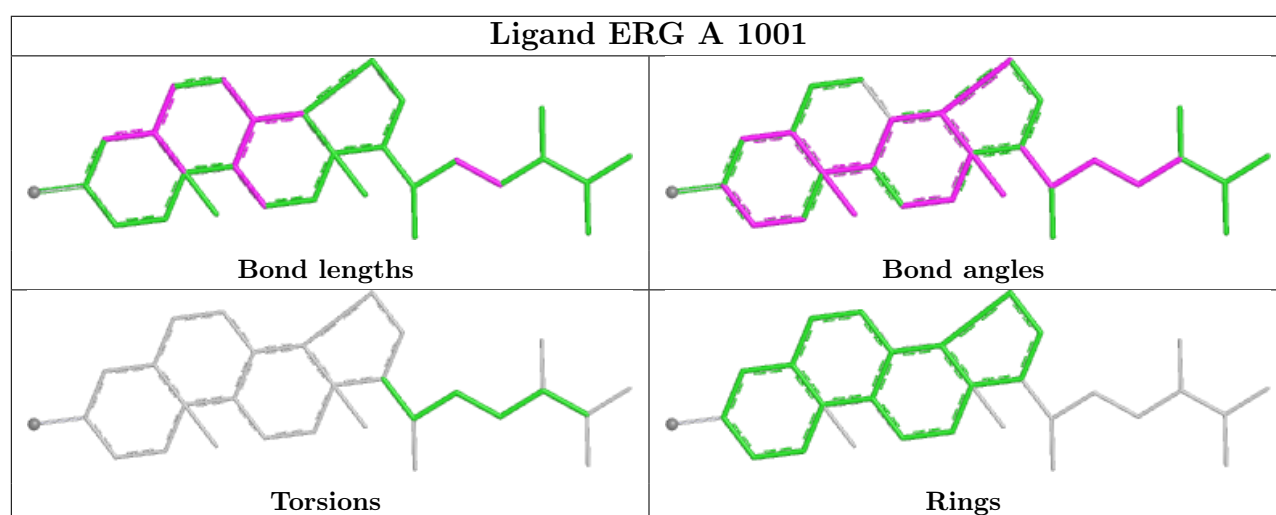
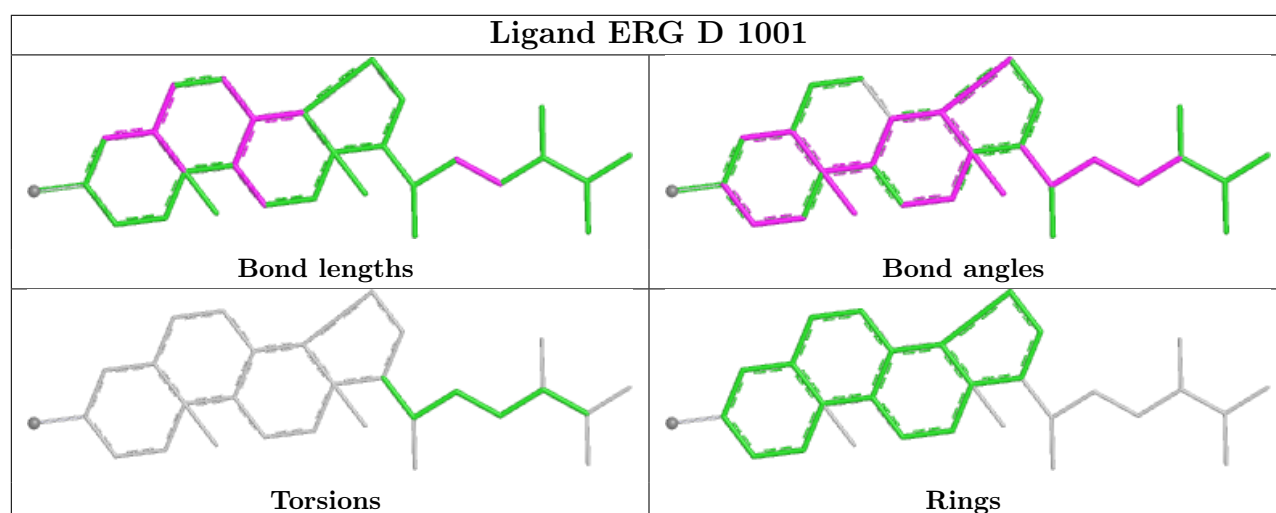
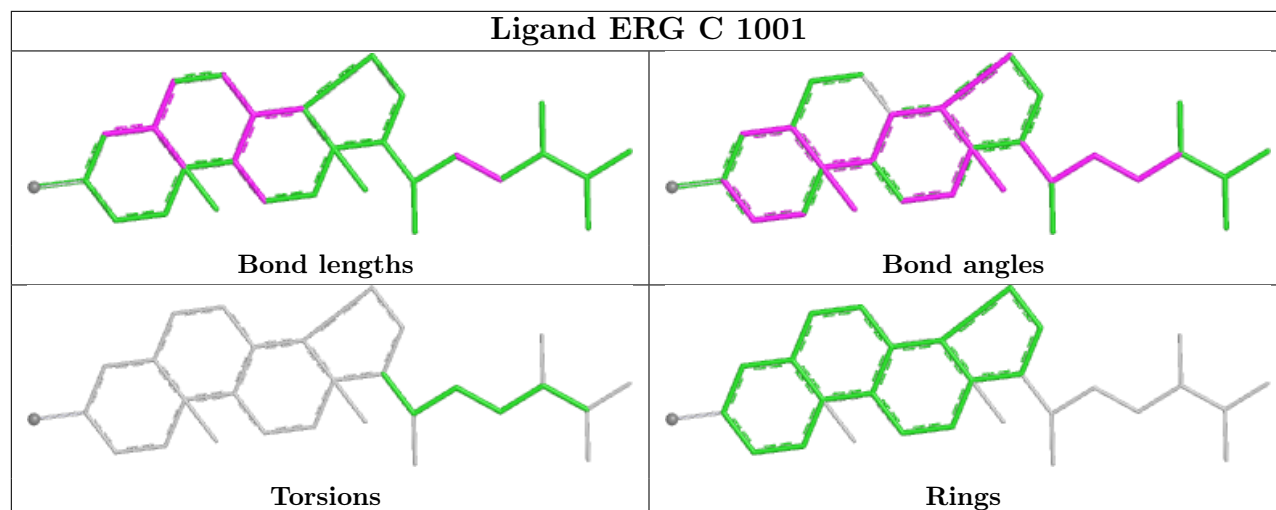
There are no torsion outliers.

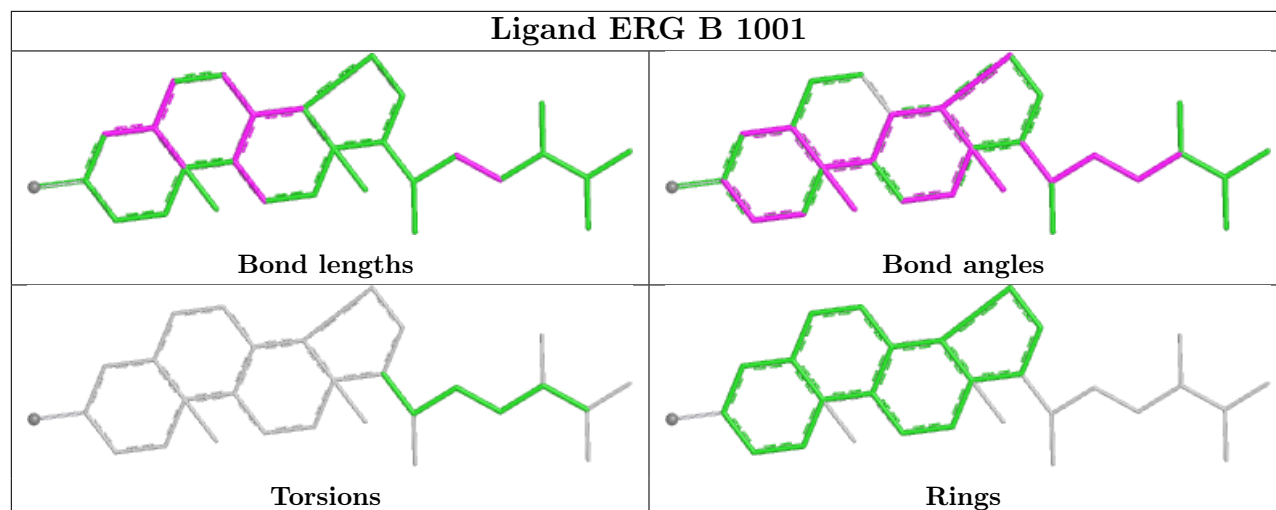
There are no ring outliers.

4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1001	ERG	3	0
2	D	1001	ERG	9	0
2	A	1001	ERG	4	0
2	B	1001	ERG	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, 95th 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%)	0.77	29 (10%) 12 9	30, 47, 79, 95	0
1	B	280/308 (90%)	0.54	21 (7%) 20 16	29, 44, 86, 100	0
1	C	282/308 (91%)	0.50	16 (5%) 29 24	30, 47, 76, 95	0
1	D	253/308 (82%)	0.66	17 (6%) 24 19	34, 55, 84, 105	0
All	All	1096/1232 (88%)	0.62	83 (7%) 20 16	29, 49, 83, 105	0

All (83) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	SER	4.8
1	A	850	GLY	4.3
1	B	850	GLY	4.3
1	A	870	THR	3.8
1	C	736	ASN	3.8
1	D	854	ALA	3.7
1	A	685	THR	3.7
1	B	739	PRO	3.6
1	C	798	ALA	3.6
1	B	822	GLU	3.4
1	D	739	PRO	3.4
1	C	908	GLY	3.3
1	A	740	THR	3.2
1	B	692	TYR	3.0
1	A	890	VAL	3.0
1	B	779	ILE	3.0
1	B	791	VAL	2.9
1	D	808	PRO	2.9
1	B	910	LEU	2.9
1	D	767	ASN	2.8
1	D	769	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	810	LEU	2.8
1	A	739	PRO	2.7
1	A	640	GLU	2.7
1	C	767	ASN	2.7
1	A	791	VAL	2.7
1	D	807	SER	2.7
1	A	837	ALA	2.6
1	C	799	ASP	2.6
1	A	736	ASN	2.6
1	A	738	ASN	2.6
1	A	867	ASN	2.6
1	B	683	SER	2.6
1	C	803	VAL	2.5
1	D	873	MET	2.5
1	A	910	LEU	2.5
1	D	803	VAL	2.5
1	C	785	GLY	2.4
1	C	708	VAL	2.4
1	C	771	VAL	2.4
1	B	734	ALA	2.4
1	B	811	ILE	2.4
1	B	642	TRP	2.4
1	B	838	LEU	2.4
1	B	792	CYS	2.4
1	A	737	SER	2.3
1	A	794	ASP	2.3
1	B	772	ASP	2.3
1	A	845	THR	2.3
1	C	772	ASP	2.3
1	B	738	ASN	2.3
1	B	884	GLN	2.3
1	C	691	ASP	2.3
1	C	907	GLY	2.3
1	A	683	SER	2.3
1	A	884	GLN	2.2
1	B	802	PRO	2.2
1	A	798	ALA	2.2
1	B	785	GLY	2.2
1	D	823	LYS	2.2
1	B	737	SER	2.2
1	A	802	PRO	2.2
1	D	773	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	699	SER	2.2
1	A	778	GLU	2.2
1	D	802	PRO	2.2
1	B	815	TYR	2.1
1	A	699	SER	2.1
1	A	639	THR	2.1
1	C	777	GLY	2.1
1	D	824	ASN	2.1
1	C	737	SER	2.1
1	D	760	PRO	2.1
1	A	672	HIS	2.1
1	C	686	GLN	2.1
1	D	852	LEU	2.1
1	A	871	GLU	2.1
1	C	713	ASP	2.1
1	A	764	LYS	2.0
1	D	729	ASP	2.0
1	A	771	VAL	2.0
1	A	780	VAL	2.0
1	B	634	PHE	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 oligosaccharides 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, 95th 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
2	ERG	D	1001	29/29	0.86	0.12	35,55,68,75	0
2	ERG	B	1001	29/29	0.87	0.10	26,40,47,54	0
2	ERG	C	1001	29/29	0.89	0.09	33,45,54,57	0

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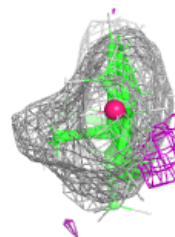
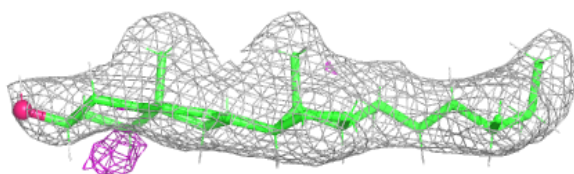
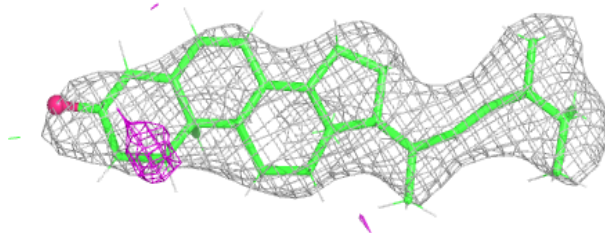
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ERG	A	1001	29/29	0.89	0.09	24,41,49,52	0

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.

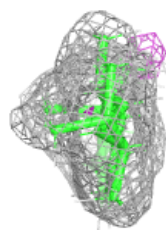
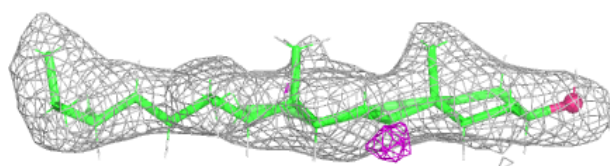
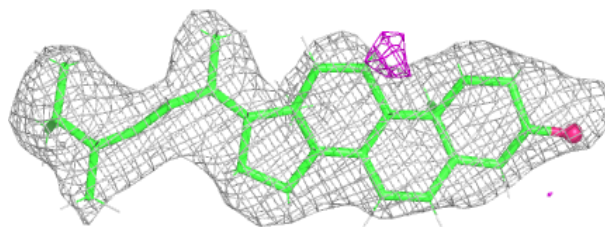
Electron density around ERG D 1001:

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

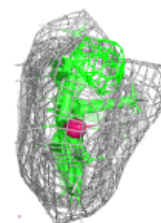
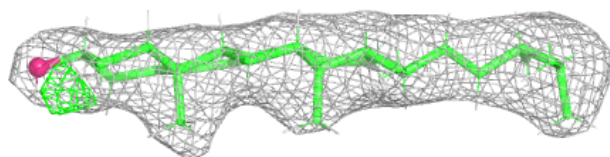
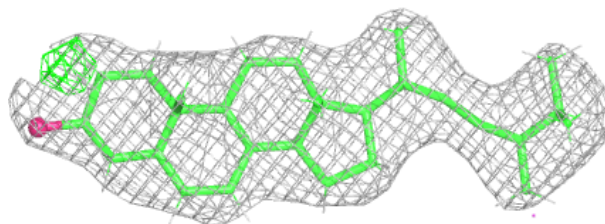


Electron density around ERG B 1001:

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

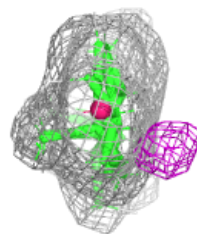
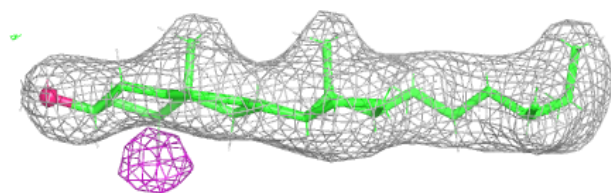
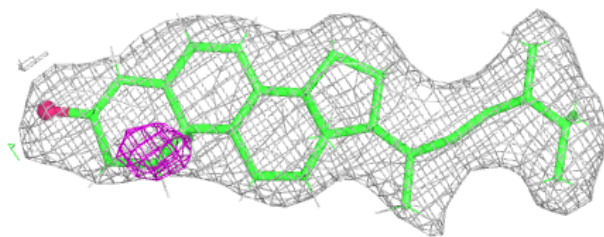
**Electron density around ERG C 1001:**

$2mF_o-DF_c$ (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.