



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:13 PM UTC

PDB ID : 9LF6 / pdb_00009lf6
Title : Crystal of Glucosidase form Gelsemium sempervirens
Authors : Hao, X.L.; Kai, G.Y.
Deposited on : 2025-01-08
Resolution : 2.95 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:

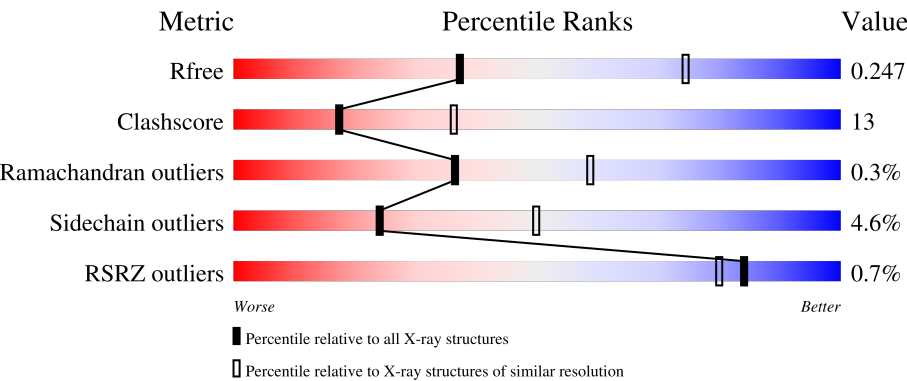
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	534	% 68%20%11%
1	B	534	% 62%25%12%
1	C	534	% 61%26%12%
1	D	534	% 49%33%5%12%
1	E	534	65%22%13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	534	 % 64% 22% • 13%
1	G	534	 % 58% 28% • 13%
1	H	534	 57% 27% • 13%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PEG	B	602	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29334 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Strictosidine glucosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	474	Total	C	N	O	S	0	0	0
			3670	2363	609	691	7			
1	B	469	Total	C	N	O	S	0	0	0
			3676	2366	609	693	8			
1	C	471	Total	C	N	O	S	0	0	0
			3687	2371	612	696	8			
1	D	469	Total	C	N	O	S	0	0	0
			3673	2364	608	693	8			
1	E	466	Total	C	N	O	S	0	0	0
			3656	2351	608	689	8			
1	F	466	Total	C	N	O	S	0	0	0
			3629	2333	597	691	8			
1	G	466	Total	C	N	O	S	0	0	0
			3625	2331	600	686	8			
1	H	464	Total	C	N	O	S	0	0	0
			3613	2321	598	686	8			

- Molecule 2 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



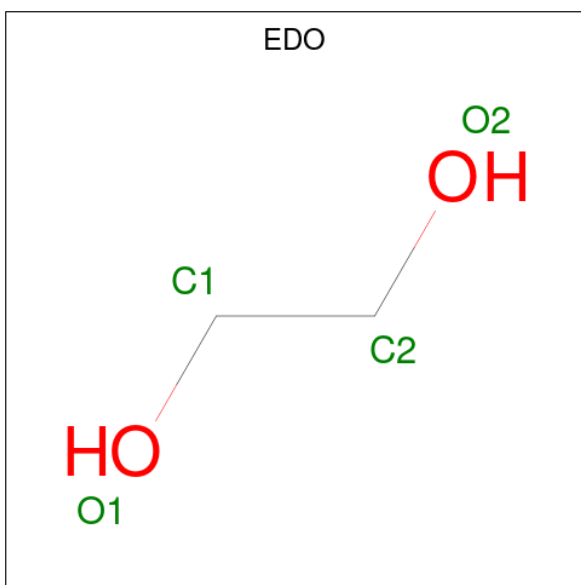
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			7	4	3		
2	A	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	B	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	C	1	Total	C	O	0	0
			7	4	3		
2	E	1	Total	C	O	0	0
			7	4	3		
2	F	1	Total	C	O	0	0
			7	4	3		
2	H	1	Total	C	O	0	0
			7	4	3		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).

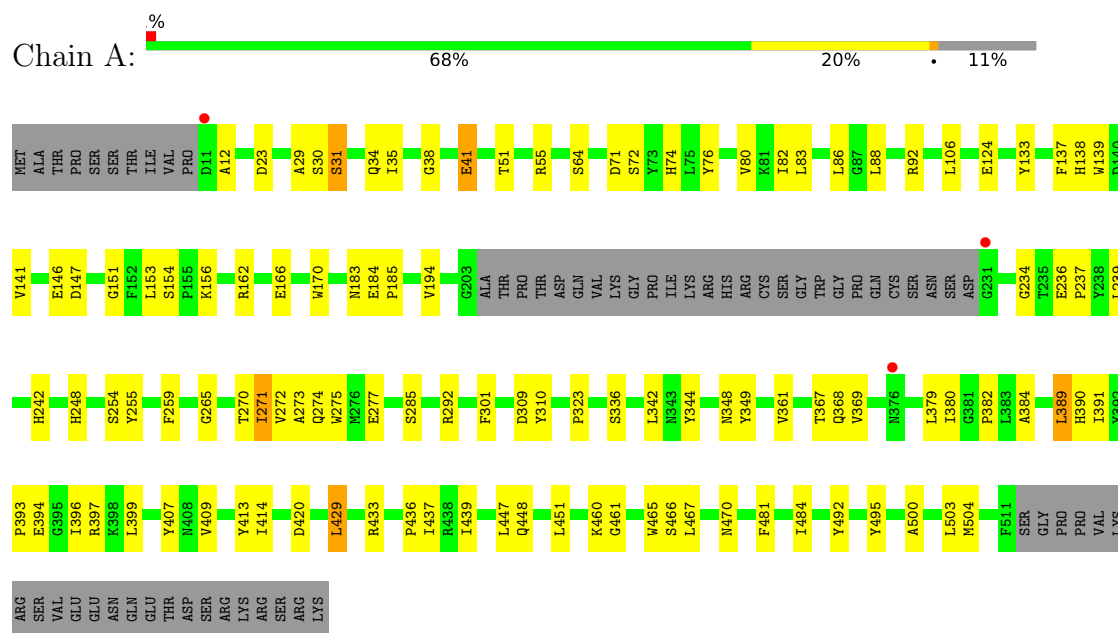


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		

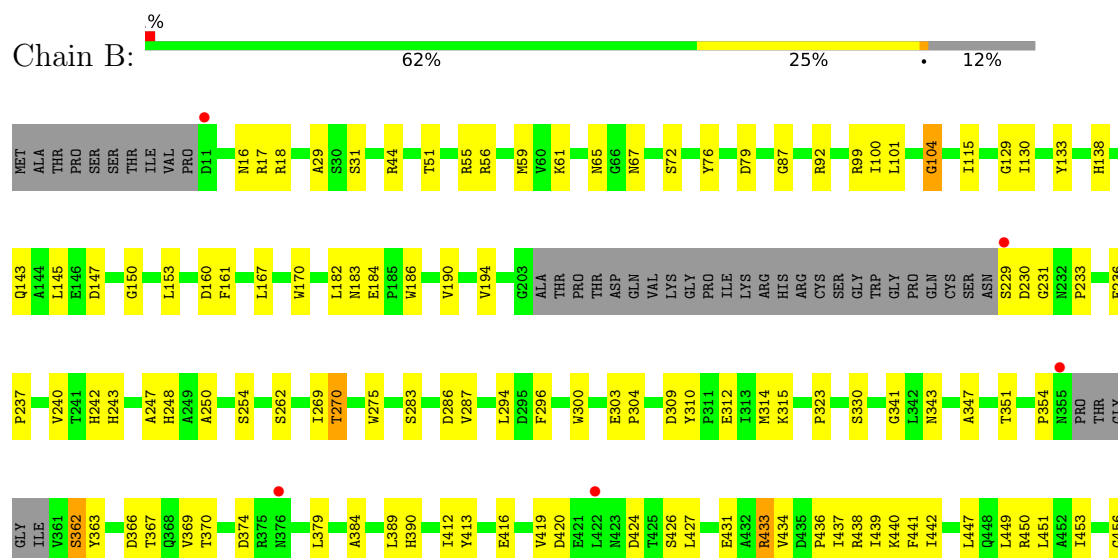
3 Residue-property plots

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: Strictosidine glucosidase

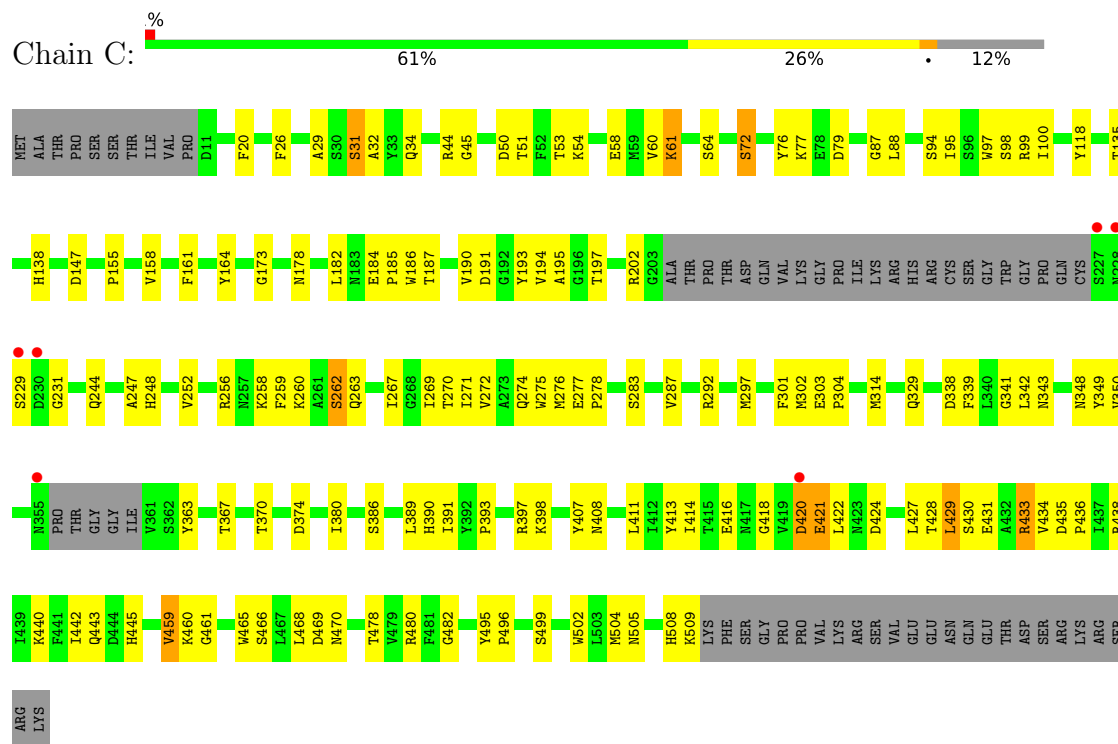


• Molecule 1: Strictosidine glucosidase

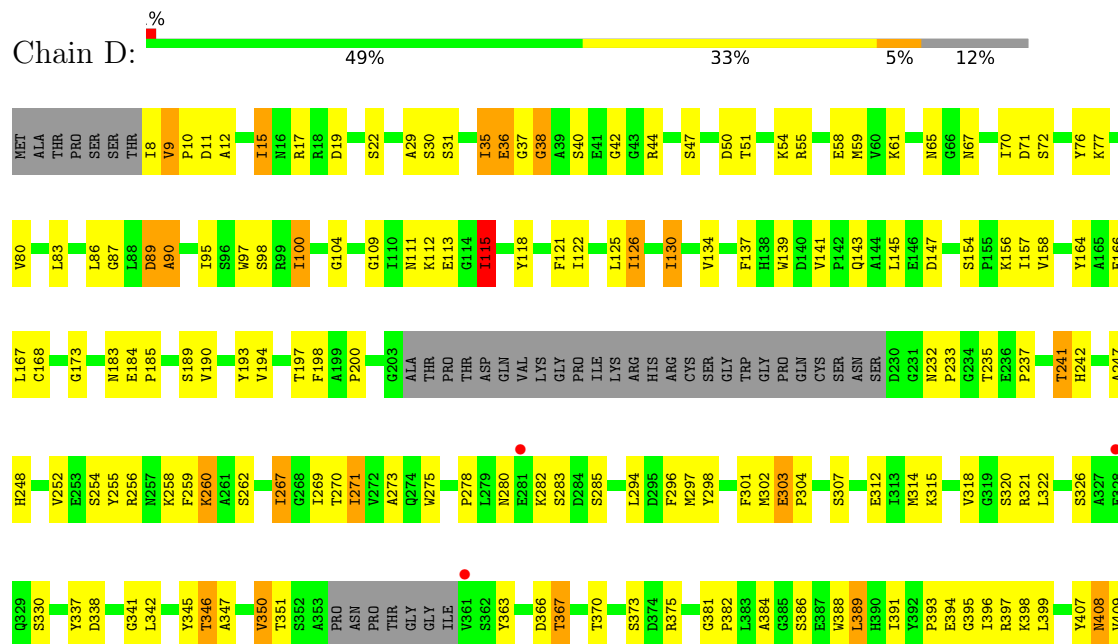


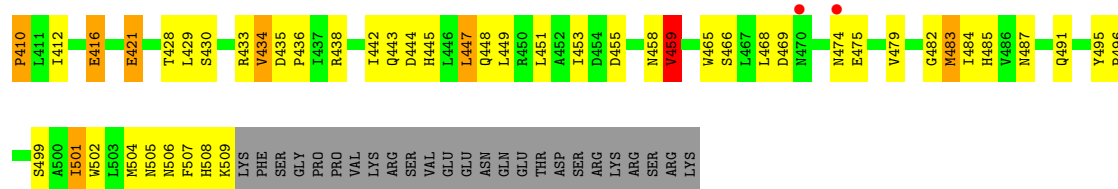


• Molecule 1: Strictosidine glucosidase

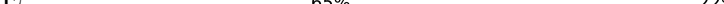


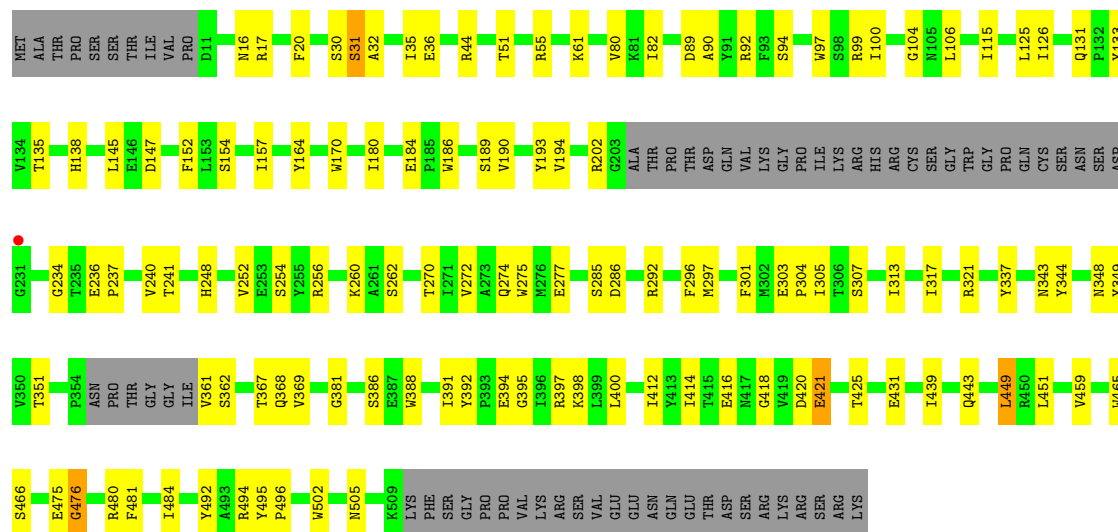
• Molecule 1: Strictosidine glucosidase



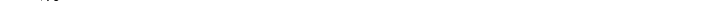


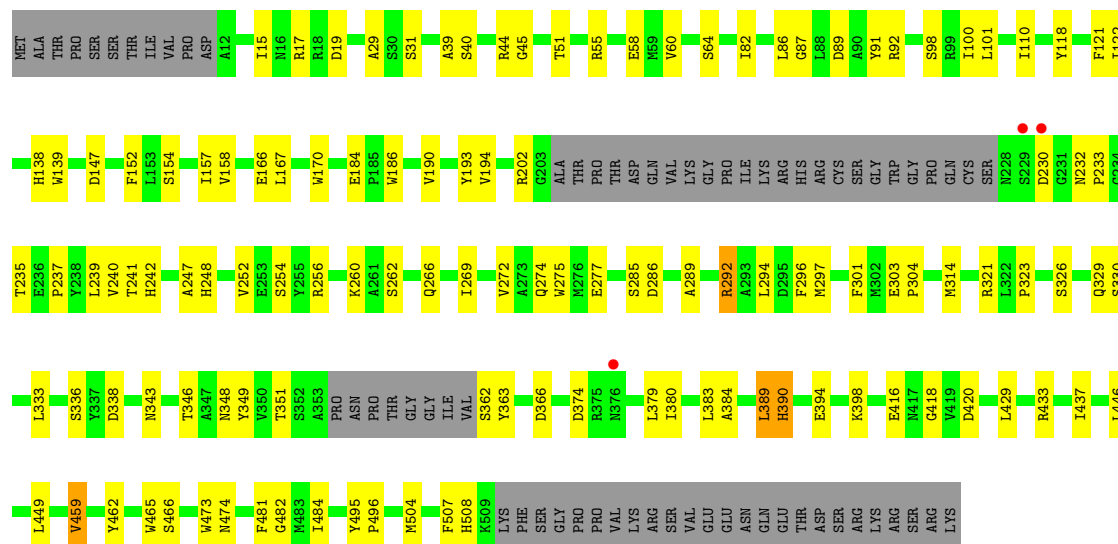
- Molecule 1: Strictosidine glucosidase

Chain E:  65% 22% • 13%



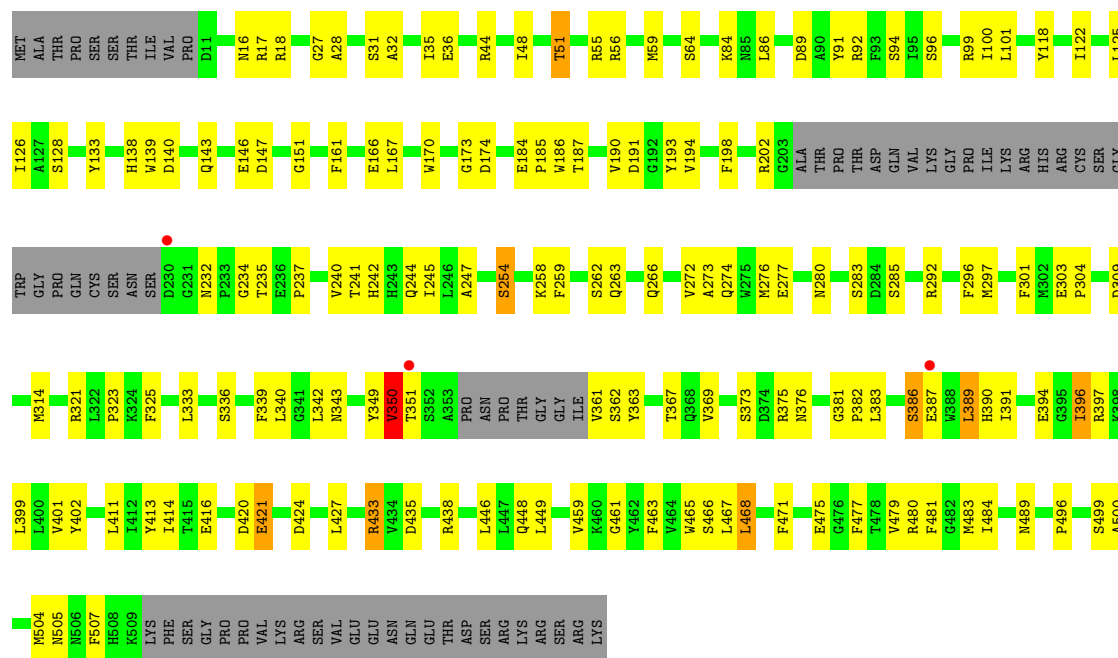
- Molecule 1: Strictosidine glucosidase

Chain F:  %



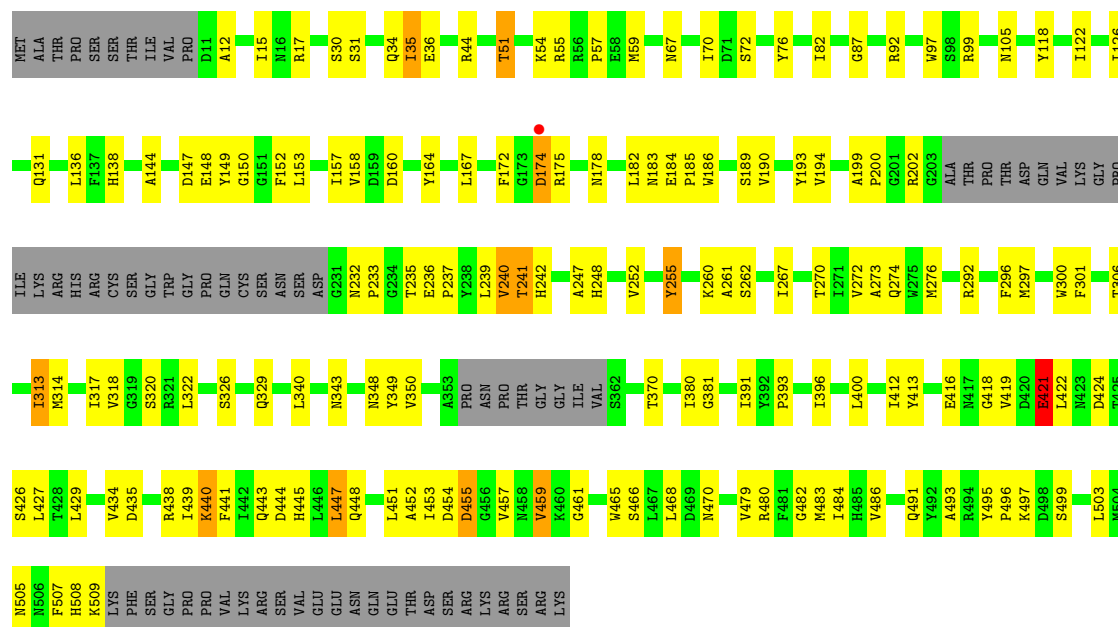
- Molecule 1: Strictosidine glucosidase

Chain G: %



• Molecule 1: Strictosidine glucosidase

Chain H: 57% 27% 13%



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	237.43Å 107.84Å 220.27Å 90.00° 118.46° 90.00°	Depositor
Resolution (Å)	48.99 – 2.95 48.99 – 2.95	Depositor EDS
% Data completeness (in resolution range)	95.8 (48.99-2.95) 95.8 (48.99-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.84 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.206 , 0.248 0.207 , 0.247	Depositor DCC
R_{free} test set	4958 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	0.484	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 35.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	29334	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.46	0/3776	0.62	0/5154
1	B	0.77	4/3780 (0.1%)	0.75	6/5150 (0.1%)
1	C	0.70	2/3791 (0.1%)	0.71	5/5166 (0.1%)
1	D	1.50	5/3777 (0.1%)	1.15	26/5145 (0.5%)
1	E	0.52	1/3760 (0.0%)	0.61	0/5124
1	F	0.53	0/3732	0.64	3/5089 (0.1%)
1	G	0.66	1/3728 (0.0%)	0.69	2/5084 (0.0%)
1	H	0.84	3/3715 (0.1%)	0.73	7/5065 (0.1%)
All	All	0.81	16/30059 (0.1%)	0.76	49/40977 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	341	GLY	CA-C	-6.96	1.47	1.52
1	D	487	ASN	CA-C	-6.50	1.44	1.52
1	B	473	TRP	CA-C	-6.24	1.47	1.53
1	C	421	GLU	N-CA	-6.05	1.38	1.45
1	B	472	GLU	CA-C	-6.00	1.44	1.52
1	H	255	TYR	CA-C	-5.81	1.44	1.52
1	B	481	PHE	CA-C	-5.71	1.45	1.52
1	D	367	THR	CA-C	-5.71	1.45	1.52
1	D	242	HIS	CA-C	-5.59	1.45	1.52
1	D	31	SER	CA-C	-5.37	1.45	1.52
1	H	340	LEU	C-N	5.21	1.36	1.33
1	C	397	ARG	CA-C	-5.14	1.46	1.52
1	H	242	HIS	CA-C	-5.12	1.46	1.52
1	E	90	ALA	CA-C	-5.11	1.46	1.52
1	G	414	ILE	CA-C	-5.11	1.47	1.53
1	B	439	ILE	CA-C	-5.02	1.46	1.52

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	421	GLU	N-CA-C	-9.68	94.53	108.96
1	C	459	VAL	N-CA-C	-9.57	94.68	108.36
1	D	260	LYS	N-CA-C	8.93	121.01	111.28
1	D	134	VAL	N-CA-C	8.74	120.48	107.80
1	B	456	GLY	N-CA-C	7.84	126.29	115.00
1	D	421	GLU	N-CA-C	-7.76	97.61	109.41
1	D	19	ASP	N-CA-C	-7.29	103.96	112.92
1	B	483	MET	N-CA-C	-7.11	104.64	113.38
1	F	346	THR	N-CA-C	7.08	118.52	108.74
1	D	350	VAL	N-CA-C	7.04	118.62	108.48
1	G	350	VAL	N-CA-C	7.03	117.96	108.11
1	H	453	ILE	N-CA-C	-6.89	102.92	112.50
1	D	482	GLY	N-CA-C	6.82	123.87	113.02
1	D	29	ALA	N-CA-C	6.74	119.96	109.52
1	D	109	GLY	N-CA-C	6.67	119.77	112.29
1	G	396	ILE	N-CA-C	-6.56	104.63	111.58
1	D	90	ALA	N-CA-C	6.52	118.86	109.14
1	D	459	VAL	N-CA-C	-6.39	99.23	108.17
1	D	491	GLN	N-CA-C	6.33	120.28	111.74
1	C	390	HIS	N-CA-C	-6.26	99.51	109.59
1	D	173	GLY	N-CA-C	6.25	121.55	114.67
1	H	174	ASP	N-CA-C	-6.21	104.59	111.36
1	B	473	TRP	CB-CA-C	-6.01	109.66	116.63
1	H	421	GLU	N-CA-C	-5.91	100.52	109.85
1	D	115	ILE	N-CA-C	-5.79	104.87	110.72
1	D	346	THR	N-CA-C	5.76	118.16	109.41
1	F	19	ASP	N-CA-C	-5.76	106.02	113.16
1	B	433	ARG	N-CA-C	5.74	119.54	112.54
1	F	390	HIS	N-CA-C	-5.71	100.09	109.40
1	B	160	ASP	N-CA-C	-5.66	104.58	112.45
1	H	418	GLY	N-CA-C	5.62	121.34	110.66
1	D	100	ILE	N-CA-C	-5.55	106.39	111.67
1	D	168	CYS	N-CA-C	-5.54	104.75	112.45
1	H	454	ASP	N-CA-C	-5.54	106.36	113.23
1	D	394	GLU	N-CA-C	5.43	119.63	112.89
1	D	338	ASP	N-CA-C	-5.41	104.93	112.45
1	D	40	SER	N-CA-C	-5.40	105.39	112.41
1	C	430	SER	N-CA-C	-5.38	105.52	111.71
1	D	428	THR	N-CA-C	-5.37	101.48	109.96
1	D	303	GLU	CA-C-N	-5.35	113.23	119.32
1	D	303	GLU	C-N-CA	-5.35	113.23	119.32
1	B	458	ASN	N-CA-C	5.29	117.92	107.98
1	C	418	GLY	N-CA-C	5.25	120.87	110.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	283	SER	N-CA-C	-5.24	100.63	109.07
1	D	38	GLY	N-CA-C	-5.22	100.80	113.18
1	D	71	ASP	N-CA-C	5.16	118.84	112.24
1	D	396	ILE	N-CA-C	-5.08	105.59	110.72
1	H	455	ASP	N-CA-C	-5.05	107.12	113.28
1	H	459	VAL	N-CA-C	-5.05	101.31	108.58

There are no chirality outliers.

There are no planarity outliers.

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	3670	0	3395	74	0
1	B	3676	0	3428	92	0
1	C	3687	0	3432	98	0
1	D	3673	0	3422	119	0
1	E	3656	0	3404	75	0
1	F	3629	0	3342	83	0
1	G	3625	0	3340	105	0
1	H	3613	0	3327	101	0
2	A	14	0	20	0	0
2	B	14	0	20	6	0
2	C	28	0	40	4	0
2	E	7	0	10	0	0
2	F	7	0	10	0	0
2	H	7	0	10	0	0
3	B	5	0	0	1	0
3	D	10	0	0	0	0
3	E	5	0	0	0	0
4	E	4	0	6	0	0
4	H	4	0	6	0	0
All	All	29334	0	27212	709	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (709) 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:B:143:GLN:HE22	2:B:602:PEG:H11	1.20	1.06
1:A:147:ASP:HB3	1:B:147:ASP:HB3	1.47	0.94
1:G:449:LEU:HD11	1:G:459:VAL:HG11	1.50	0.92
1:G:56:ARG:HE	1:G:59:MET:HE3	1.37	0.88
1:A:51:THR:HG23	1:A:55:ARG:HD2	1.56	0.87
1:H:421:GLU:HG2	1:H:480:ARG:HB2	1.56	0.85
1:G:394:GLU:HA	1:G:448:GLN:HG2	1.58	0.83
1:B:61:LYS:HD3	2:B:601:PEG:H22	1.60	0.82
1:B:65:ASN:HD22	1:B:67:ASN:H	1.25	0.81
1:H:158:VAL:HG13	1:H:247:ALA:HA	1.60	0.81
1:B:194:VAL:HG22	1:B:237:PRO:HG3	1.68	0.75
1:A:273:ALA:HB3	1:A:399:LEU:HD21	1.69	0.75
1:B:505:ASN:HA	1:C:262:SER:OG	1.87	0.74
1:D:51:THR:O	1:D:55:ARG:HB2	1.88	0.74
1:A:153:LEU:HD21	1:A:236:GLU:HG2	1.69	0.73
1:D:183:ASN:O	1:D:184:GLU:C	2.31	0.73
1:D:496:PRO:HB2	1:D:501:ILE:HD11	1.70	0.73
1:C:421:GLU:HG2	1:C:480:ARG:HB2	1.69	0.73
1:G:48:ILE:HA	1:G:143:GLN:NE2	2.03	0.72
1:C:416:GLU:HG2	1:C:465:TRP:HB2	1.71	0.72
1:B:262:SER:HB2	1:E:505:ASN:HA	1.70	0.72
1:D:189:SER:O	1:D:193:TYR:HB2	1.89	0.72
1:E:32:ALA:H	1:E:94:SER:HB3	1.54	0.71
1:E:397:ARG:NH1	1:E:451:LEU:HD13	2.06	0.71
1:C:53:THR:HG22	1:C:60:VAL:HG21	1.73	0.71
1:A:106:LEU:HD11	1:F:433:ARG:HH12	1.56	0.70
1:A:184:GLU:HG2	1:A:272:VAL:HB	1.73	0.70
1:G:147:ASP:HB3	1:H:147:ASP:HB3	1.72	0.70
1:D:30:SER:HB2	1:D:35:ILE:HG21	1.72	0.70
1:A:448:GLN:HA	1:A:451:LEU:HD12	1.73	0.70
1:B:434:VAL:O	1:B:436:PRO:HD3	1.91	0.69
1:A:275:TRP:NE1	1:A:277:GLU:OE1	2.24	0.69
1:F:277:GLU:OE2	1:F:398:LYS:NZ	2.20	0.69
1:H:413:TYR:HD2	1:H:461:GLY:HA3	1.58	0.69
1:A:309:ASP:OD1	1:A:310:TYR:N	2.24	0.69
1:H:274:GLN:HG3	1:H:297:MET:HE1	1.74	0.69
1:G:266:GLN:HG3	1:G:339:PHE:CE2	2.28	0.69
1:A:436:PRO:HA	1:A:439:ILE:HD12	1.75	0.69
1:D:17:ARG:HH22	1:D:89:ASP:CG	2.01	0.68
1:D:382:PRO:HG2	1:D:391:ILE:HB	1.76	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:30:SER:HB2	1:H:35:ILE:HG21	1.75	0.68
1:E:262:SER:HB2	1:G:505:ASN:HA	1.76	0.67
1:F:29:ALA:O	1:F:466:SER:HB2	1.93	0.67
1:E:17:ARG:HH22	1:E:89:ASP:CG	2.01	0.67
1:F:152:PHE:HA	1:F:157:ILE:HG21	1.76	0.67
1:A:437:ILE:HD12	1:A:437:ILE:H	1.58	0.67
1:C:44:ARG:HB2	1:C:99:ARG:HG3	1.78	0.66
1:H:193:TYR:CZ	1:H:200:PRO:HG3	2.29	0.66
1:A:413:TYR:HD2	1:A:461:GLY:HA3	1.59	0.66
1:B:143:GLN:NE2	2:B:602:PEG:H11	2.04	0.66
1:G:194:VAL:HG22	1:G:237:PRO:HG3	1.77	0.66
1:F:235:THR:HG22	1:F:321:ARG:HG2	1.79	0.65
1:C:274:GLN:OE1	1:C:348:ASN:ND2	2.29	0.65
1:F:190:VAL:HA	1:F:194:VAL:HG23	1.78	0.65
1:F:241:THR:HG23	1:F:301:PHE:CE1	2.32	0.65
1:D:303:GLU:HB3	1:D:304:PRO:HD3	1.79	0.65
1:A:106:LEU:CD1	1:F:433:ARG:HH12	2.09	0.64
1:D:80:VAL:HG13	1:D:125:LEU:HD23	1.79	0.64
1:D:65:ASN:HD21	1:G:489:ASN:HB3	1.63	0.64
1:E:292:ARG:NH2	1:E:368:GLN:O	2.30	0.64
1:A:12:ALA:HB2	1:A:447:LEU:HD22	1.80	0.64
1:B:16:ASN:ND2	1:B:18:ARG:H	1.96	0.63
1:D:72:SER:O	1:D:76:TYR:HB3	1.97	0.63
1:H:183:ASN:O	1:H:184:GLU:C	2.41	0.63
1:C:61:LYS:HE2	1:C:478:THR:HG21	1.81	0.63
1:A:292:ARG:NH2	1:A:368:GLN:O	2.32	0.62
1:B:426:SER:HB2	1:F:58:GLU:HB3	1.81	0.62
1:C:186:TRP:CE2	1:C:297:MET:HG3	2.35	0.62
1:D:190:VAL:HA	1:D:194:VAL:HG23	1.80	0.62
1:B:31:SER:HB2	1:B:138:HIS:CE1	2.35	0.62
1:B:233:PRO:HB2	1:B:362:SER:HB2	1.80	0.62
1:E:184:GLU:HG2	1:E:272:VAL:HB	1.81	0.62
1:B:434:VAL:HG12	1:B:436:PRO:HG3	1.82	0.61
1:G:382:PRO:HD2	1:G:391:ILE:HB	1.81	0.61
1:D:61:LYS:HD2	1:D:475:GLU:HA	1.83	0.61
1:B:242:HIS:ND1	1:B:323:PRO:HB2	2.16	0.61
1:C:147:ASP:HB3	1:F:147:ASP:HB3	1.82	0.60
1:G:44:ARG:HB2	1:G:99:ARG:HG3	1.83	0.60
1:F:17:ARG:HH22	1:F:89:ASP:CG	2.09	0.60
1:F:296:PHE:CD1	1:F:314:MET:HE3	2.36	0.60
1:G:397:ARG:HB2	1:G:448:GLN:HG3	1.84	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:HIS:CE1	1:A:323:PRO:HB2	2.36	0.60
1:B:51:THR:HG21	2:B:602:PEG:H22	1.83	0.60
1:E:51:THR:HG23	1:E:55:ARG:HD2	1.84	0.60
1:B:434:VAL:C	1:B:436:PRO:HD3	2.27	0.60
1:H:439:ILE:O	1:H:443:GLN:HG3	2.01	0.60
1:D:505:ASN:HA	1:H:262:SER:HB2	1.83	0.59
1:F:374:ASP:HB3	1:F:379:LEU:HD23	1.82	0.59
1:H:126:ILE:CD1	1:H:175:ARG:HB3	2.32	0.59
1:A:82:ILE:HG21	1:A:484:ILE:HG13	1.84	0.59
1:G:31:SER:HB2	1:G:138:HIS:CE1	2.37	0.59
1:G:51:THR:O	1:G:55:ARG:HG3	2.02	0.59
1:C:505:ASN:HA	1:G:262:SER:HB2	1.85	0.59
1:D:100:ILE:HD12	1:D:115:ILE:HG13	1.84	0.59
1:D:469:ASP:OD2	1:D:485:HIS:HA	2.03	0.59
1:C:393:PRO:HA	1:C:445:HIS:NE2	2.18	0.59
1:H:54:LYS:HE2	1:H:67:ASN:OD1	2.03	0.59
1:C:413:TYR:CD2	1:C:461:GLY:HA3	2.38	0.58
1:D:158:VAL:HG13	1:D:247:ALA:HA	1.84	0.58
1:E:92:ARG:HH12	1:E:416:GLU:HG3	1.68	0.58
1:H:118:TYR:O	1:H:122:ILE:HG13	2.02	0.58
1:C:339:PHE:HB3	1:C:411:LEU:HD23	1.86	0.58
1:G:17:ARG:HB2	1:G:507:PHE:HA	1.83	0.58
1:A:344:TYR:CD2	1:A:396:ILE:HB	2.38	0.58
1:D:193:TYR:CZ	1:D:200:PRO:HG3	2.38	0.58
1:B:229:SER:O	1:B:231:GLY:N	2.37	0.58
1:E:194:VAL:HG22	1:E:237:PRO:HG3	1.86	0.58
1:E:274:GLN:OE1	1:E:348:ASN:ND2	2.37	0.58
1:F:118:TYR:O	1:F:122:ILE:HG13	2.03	0.58
1:F:449:LEU:HD21	1:F:459:VAL:HG11	1.86	0.58
1:E:305:ILE:HD12	1:E:337:TYR:CD2	2.39	0.58
1:B:450:ARG:HH11	1:B:450:ARG:HG2	1.69	0.58
1:C:29:ALA:O	1:C:466:SER:HB2	2.04	0.57
1:C:34:GLN:O	1:C:470:ASN:HB2	2.04	0.57
1:A:384:ALA:HB3	1:A:389:LEU:HB3	1.86	0.57
1:G:16:ASN:OD1	1:G:18:ARG:N	2.32	0.57
1:G:17:ARG:HH22	1:G:89:ASP:CG	2.12	0.57
1:G:51:THR:OG1	1:G:143:GLN:NE2	2.37	0.57
1:G:375:ARG:O	1:G:376:ASN:C	2.46	0.57
1:E:421:GLU:HG2	1:E:480:ARG:HB2	1.84	0.57
1:E:400:LEU:HD21	1:E:414:ILE:HD11	1.86	0.57
1:C:413:TYR:HD2	1:C:461:GLY:HA3	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:104:GLY:HA3	1:D:145:LEU:HG	1.87	0.57
1:F:17:ARG:HD2	1:F:507:PHE:O	2.04	0.57
1:A:194:VAL:HG23	1:A:237:PRO:HG3	1.87	0.56
1:D:35:ILE:HG13	1:D:36:GLU:N	2.20	0.56
1:B:100:ILE:HG22	1:B:101:LEU:HG	1.87	0.56
1:A:34:GLN:O	1:A:470:ASN:HB2	2.06	0.56
1:C:158:VAL:HG13	1:C:247:ALA:HA	1.87	0.56
1:H:419:VAL:HG12	1:H:438:ARG:HG3	1.88	0.56
1:G:303:GLU:HB3	1:G:304:PRO:HD3	1.87	0.56
1:B:384:ALA:HB3	1:B:389:LEU:HB3	1.86	0.56
1:D:269:ILE:HD13	1:D:271:ILE:HD11	1.88	0.56
1:H:313:ILE:HD11	1:H:317:ILE:HD11	1.88	0.56
1:D:65:ASN:ND2	1:G:489:ASN:HB3	2.21	0.56
1:H:34:GLN:O	1:H:470:ASN:HB2	2.06	0.56
1:D:139:TRP:CD1	1:D:139:TRP:N	2.74	0.55
1:H:241:THR:HG23	1:H:301:PHE:CE1	2.41	0.55
1:B:87:GLY:HA3	1:B:508:HIS:CD2	2.41	0.55
1:E:32:ALA:N	1:E:94:SER:HB3	2.22	0.55
1:H:51:THR:HG22	1:H:55:ARG:HD2	1.86	0.55
1:H:150:GLY:O	1:H:153:LEU:HB2	2.07	0.55
1:E:241:THR:HG23	1:E:301:PHE:CE1	2.41	0.55
1:F:82:ILE:HG21	1:F:484:ILE:HG13	1.88	0.55
1:H:31:SER:HB2	1:H:138:HIS:CD2	2.42	0.55
1:F:275:TRP:NE1	1:F:277:GLU:HG2	2.21	0.55
1:E:31:SER:HB2	1:E:138:HIS:CE1	2.42	0.55
1:E:106:LEU:HD11	1:G:433:ARG:HH12	1.71	0.55
1:G:343:ASN:CG	1:G:416:GLU:HB2	2.32	0.55
1:H:193:TYR:CE2	1:H:240:VAL:HG21	2.41	0.55
1:B:413:TYR:HD2	1:B:461:GLY:HA3	1.72	0.55
1:H:172:PHE:HA	1:H:175:ARG:HH21	1.72	0.55
1:B:51:THR:HG23	1:B:55:ARG:HD2	1.89	0.55
1:B:72:SER:OG	1:B:79:ASP:OD2	2.22	0.55
1:B:190:VAL:HA	1:B:194:VAL:HG23	1.88	0.55
1:C:438:ARG:O	1:C:442:ILE:HG13	2.07	0.55
1:D:8:ILE:O	1:D:9:VAL:HG22	2.07	0.55
1:E:80:VAL:HG13	1:E:125:LEU:HD23	1.89	0.55
1:G:48:ILE:HA	1:G:143:GLN:HE22	1.70	0.55
1:A:393:PRO:O	1:A:396:ILE:HG22	2.07	0.55
1:C:277:GLU:OE1	1:C:278:PRO:HD2	2.06	0.55
1:B:374:ASP:HB3	1:B:379:LEU:HD22	1.89	0.54
1:D:166:GLU:HG2	1:D:259:PHE:HE2	1.71	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:92:ARG:NH1	1:F:416:GLU:HG3	2.21	0.54
1:B:167:LEU:HD13	1:E:495:TYR:HE1	1.72	0.54
1:D:194:VAL:HG22	1:D:237:PRO:HG3	1.89	0.54
1:F:194:VAL:HG22	1:F:237:PRO:HG3	1.90	0.54
1:H:440:LYS:O	1:H:441:PHE:C	2.51	0.54
1:G:280:ASN:HB3	1:G:283:SER:HB3	1.89	0.54
1:A:433:ARG:HD3	1:A:495:TYR:HE2	1.72	0.54
1:B:449:LEU:O	1:B:453:ILE:HG13	2.08	0.54
1:F:100:ILE:HG22	1:F:101:LEU:HG	1.90	0.54
1:B:65:ASN:ND2	1:B:67:ASN:H	2.01	0.54
1:B:236:GLU:O	1:B:240:VAL:HG23	2.07	0.54
1:E:44:ARG:HB2	1:E:99:ARG:HG3	1.90	0.54
1:A:170:TRP:CE2	1:F:496:PRO:HG3	2.43	0.54
1:E:82:ILE:HG21	1:E:484:ILE:HG13	1.90	0.54
1:A:29:ALA:O	1:A:466:SER:HB2	2.08	0.54
1:A:30:SER:HB2	1:A:35:ILE:HG21	1.89	0.54
1:D:273:ALA:HB3	1:D:399:LEU:HD21	1.89	0.54
1:F:166:GLU:OE2	1:F:254:SER:OG	2.21	0.54
1:H:273:ALA:HA	1:H:297:MET:HE2	1.89	0.54
1:C:424:ASP:HB3	1:C:427:LEU:HG	1.90	0.53
1:D:395:GLY:HA2	1:D:398:LYS:HB2	1.90	0.53
1:H:189:SER:O	1:H:193:TYR:HB2	2.07	0.53
1:C:187:THR:O	1:C:191:ASP:HB2	2.09	0.53
1:E:296:PHE:CG	1:E:367:THR:HG22	2.43	0.53
1:D:37:GLY:O	1:D:38:GLY:C	2.52	0.53
1:H:255:TYR:O	1:H:260:LYS:N	2.41	0.53
1:F:286:ASP:OD1	1:F:351:THR:HG22	2.08	0.53
1:F:343:ASN:CG	1:F:416:GLU:HB2	2.34	0.53
1:C:438:ARG:HG2	1:C:442:ILE:HD11	1.90	0.53
1:D:407:TYR:O	1:D:408:ASN:C	2.52	0.53
1:F:39:ALA:O	1:F:44:ARG:HD3	2.09	0.53
1:H:349:TYR:CE2	1:H:380:ILE:HB	2.44	0.53
1:A:397:ARG:HB2	1:A:448:GLN:HB3	1.91	0.53
1:B:270:THR:HA	1:B:341:GLY:O	2.09	0.53
1:A:83:LEU:HD21	1:A:467:LEU:HD22	1.91	0.53
1:B:186:TRP:CE2	1:B:190:VAL:HG21	2.44	0.52
1:C:184:GLU:HG2	1:C:272:VAL:HB	1.90	0.52
1:G:122:ILE:O	1:G:126:ILE:HG13	2.09	0.52
1:B:143:GLN:HE21	1:B:147:ASP:CG	2.17	0.52
1:E:303:GLU:HB3	1:E:304:PRO:HD3	1.91	0.52
1:G:416:GLU:HG2	1:G:465:TRP:HB2	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:PRO:HB2	1:A:301:PHE:CE1	2.44	0.52
1:G:186:TRP:CE2	1:G:297:MET:HG3	2.45	0.52
1:H:232:ASN:HB3	1:H:235:THR:OG1	2.09	0.52
1:A:137:PHE:CE1	1:A:141:VAL:HG22	2.45	0.52
1:H:194:VAL:HG22	1:H:237:PRO:HG3	1.92	0.52
1:H:12:ALA:O	1:H:15:ILE:HG22	2.10	0.52
1:B:248:HIS:ND1	1:B:269:ILE:HD12	2.25	0.52
1:C:185:PRO:HB2	1:C:301:PHE:CE2	2.45	0.52
1:D:17:ARG:NH1	1:D:507:PHE:O	2.43	0.52
1:A:31:SER:HB2	1:A:138:HIS:CD2	2.45	0.52
1:A:88:LEU:HD21	1:A:503:LEU:HD21	1.93	0.51
1:A:270:THR:C	1:A:271:ILE:HD12	2.35	0.51
1:D:248:HIS:O	1:D:252:VAL:HG23	2.10	0.51
1:C:505:ASN:ND2	1:G:258:LYS:C	2.68	0.51
1:D:252:VAL:HG12	1:D:256:ARG:HD2	1.90	0.51
1:D:449:LEU:O	1:D:453:ILE:HG13	2.10	0.51
1:G:343:ASN:OD1	1:G:416:GLU:HB2	2.11	0.51
1:C:50:ASP:O	1:C:54:LYS:HG3	2.10	0.51
1:E:303:GLU:OE2	1:E:307:SER:OG	2.22	0.51
1:E:343:ASN:CG	1:E:416:GLU:HB2	2.35	0.51
1:A:248:HIS:NE2	1:A:336:SER:O	2.43	0.51
1:C:173:GLY:HA3	1:C:263:GLN:NE2	2.25	0.51
1:D:255:TYR:O	1:D:260:LYS:N	2.42	0.51
1:C:31:SER:HB2	1:C:138:HIS:CE1	2.45	0.51
1:A:194:VAL:CG2	1:A:237:PRO:HG3	2.40	0.51
1:C:248:HIS:ND1	1:C:269:ILE:HD12	2.26	0.51
1:C:435:ASP:OD2	1:C:499:SER:OG	2.24	0.51
1:D:504:MET:O	1:D:508:HIS:HB2	2.11	0.51
1:F:329:GLN:O	1:F:333:LEU:HB2	2.10	0.51
1:A:277:GLU:O	1:A:349:TYR:HA	2.11	0.51
1:F:60:VAL:HG22	1:F:474:ASN:HA	1.93	0.51
1:G:31:SER:HB2	1:G:138:HIS:NE2	2.26	0.51
1:G:185:PRO:HA	1:G:244:GLN:HE22	1.75	0.51
1:G:424:ASP:HB3	1:G:427:LEU:HG	1.93	0.51
1:D:444:ASP:O	1:D:448:GLN:HG2	2.11	0.51
1:H:17:ARG:HB2	1:H:507:PHE:HA	1.93	0.51
1:D:143:GLN:O	1:D:147:ASP:HB2	2.11	0.51
1:G:435:ASP:OD2	1:G:438:ARG:HD2	2.11	0.51
1:H:193:TYR:CZ	1:H:240:VAL:HG21	2.46	0.51
1:H:452:ALA:HA	1:H:455:ASP:HB2	1.93	0.51
1:F:274:GLN:OE1	1:F:348:ASN:ND2	2.44	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:468:LEU:HD23	1:G:484:ILE:HB	1.92	0.51
1:H:447:LEU:O	1:H:451:LEU:HG	2.11	0.51
1:A:86:LEU:HA	1:A:504:MET:HG3	1.92	0.50
1:C:95:ILE:HG23	1:C:118:TYR:CE2	2.46	0.50
1:F:277:GLU:O	1:F:349:TYR:HA	2.11	0.50
1:G:276:MET:HB3	1:G:350:VAL:HG21	1.92	0.50
1:C:186:TRP:CE2	1:C:190:VAL:HG21	2.46	0.50
1:F:275:TRP:HE1	1:F:277:GLU:HG2	1.76	0.50
1:E:256:ARG:HA	1:E:260:LYS:HB2	1.92	0.50
1:D:296:PHE:CD2	1:D:314:MET:HE3	2.46	0.50
1:F:51:THR:HG22	1:F:55:ARG:HD2	1.94	0.50
1:F:321:ARG:NH2	1:F:366:ASP:OD2	2.44	0.50
1:H:391:ILE:HG22	1:H:393:PRO:HD3	1.93	0.50
1:E:30:SER:HB2	1:E:35:ILE:HG21	1.94	0.50
1:E:189:SER:O	1:E:193:TYR:HB2	2.11	0.50
1:G:56:ARG:NE	1:G:59:MET:HE3	2.18	0.50
1:G:483:MET:O	1:G:500:ALA:HB2	2.12	0.50
1:H:274:GLN:OE1	1:H:348:ASN:ND2	2.44	0.50
1:H:421:GLU:CG	1:H:480:ARG:HB2	2.35	0.50
1:H:400:LEU:HD13	1:H:459:VAL:HG21	1.94	0.50
1:F:262:SER:OG	1:H:505:ASN:HA	2.11	0.50
1:H:82:ILE:HG21	1:H:484:ILE:HG13	1.94	0.50
1:B:283:SER:O	1:B:287:VAL:HG23	2.12	0.50
1:C:252:VAL:HA	1:C:267:ILE:HD13	1.92	0.50
1:D:502:TRP:O	1:D:506:ASN:HB2	2.12	0.50
1:H:296:PHE:CD1	1:H:314:MET:HE3	2.47	0.50
1:H:99:ARG:HD2	1:H:118:TYR:CE2	2.46	0.49
1:B:100:ILE:HD12	1:B:115:ILE:HG12	1.94	0.49
1:F:170:TRP:CE2	1:H:496:PRO:HG3	2.47	0.49
1:A:495:TYR:CE1	1:D:167:LEU:HD13	2.47	0.49
1:C:190:VAL:HA	1:C:194:VAL:HG23	1.93	0.49
1:F:51:THR:CG2	1:F:55:ARG:HD2	2.43	0.49
1:F:91:TYR:HE2	1:F:121:PHE:HZ	1.60	0.49
1:B:286:ASP:CG	1:B:351:THR:HG22	2.37	0.49
1:D:80:VAL:HA	1:D:83:LEU:HD12	1.95	0.49
1:H:87:GLY:HA3	1:H:508:HIS:CG	2.48	0.49
1:H:200:PRO:HG2	1:H:202:ARG:HG3	1.93	0.49
1:G:259:PHE:HB3	1:G:263:GLN:OE1	2.13	0.49
1:G:383:LEU:HD11	1:G:387:GLU:HA	1.95	0.49
1:E:418:GLY:HA3	1:E:465:TRP:O	2.12	0.49
1:B:242:HIS:CE1	1:B:323:PRO:HB2	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:303:GLU:HB3	1:B:304:PRO:HD3	1.95	0.49
1:F:303:GLU:HB3	1:F:304:PRO:HD3	1.94	0.49
1:G:242:HIS:ND1	1:G:323:PRO:HB2	2.28	0.49
1:B:485:HIS:HB2	1:B:497:LYS:HE3	1.94	0.48
1:H:184:GLU:HG2	1:H:272:VAL:HB	1.95	0.48
1:B:309:ASP:OD1	1:B:310:TYR:N	2.44	0.48
1:E:344:TYR:OH	1:E:395:GLY:HA3	2.14	0.48
1:G:383:LEU:HD12	1:G:389:LEU:O	2.13	0.48
1:C:147:ASP:HB3	1:F:147:ASP:CB	2.43	0.48
1:D:433:ARG:HE	1:D:433:ARG:HB2	1.39	0.48
1:H:416:GLU:HG2	1:H:465:TRP:HB2	1.95	0.48
1:F:420:ASP:HB3	1:F:481:PHE:CD2	2.48	0.48
1:A:38:GLY:HA2	1:A:41:GLU:HG3	1.95	0.48
1:A:379:LEU:HD22	1:A:390:HIS:CD2	2.48	0.48
1:B:104:GLY:O	1:B:145:LEU:HD11	2.13	0.48
1:D:137:PHE:CE1	1:D:141:VAL:HG22	2.49	0.48
1:F:289:ALA:HA	1:F:292:ARG:NH1	2.29	0.48
1:A:154:SER:OG	1:A:156:LYS:HG3	2.14	0.48
1:B:194:VAL:HG22	1:B:237:PRO:CG	2.42	0.48
1:D:351:THR:HG22	1:D:370:THR:HB	1.95	0.48
1:E:236:GLU:O	1:E:240:VAL:HG23	2.14	0.48
1:E:465:TRP:HA	1:E:466:SER:HA	1.64	0.48
1:F:349:TYR:CE2	1:F:380:ILE:HB	2.49	0.48
1:F:383:LEU:HD13	1:F:390:HIS:NE2	2.29	0.48
1:G:383:LEU:HD13	1:G:390:HIS:CE1	2.48	0.48
1:A:495:TYR:HE1	1:D:167:LEU:HD13	1.77	0.48
1:C:443:GLN:HG3	1:C:502:TRP:CZ2	2.49	0.48
1:F:235:THR:O	1:F:239:LEU:HD12	2.14	0.48
1:G:96:SER:HA	1:G:140:ASP:OD2	2.14	0.48
1:G:241:THR:HG23	1:G:301:PHE:CE1	2.49	0.48
1:A:72:SER:O	1:A:76:TYR:HB3	2.13	0.47
1:G:27:GLY:HA3	1:G:463:PHE:CD2	2.49	0.47
1:H:292:ARG:HG3	1:H:313:ILE:HG12	1.96	0.47
1:D:97:TRP:HA	1:D:164:TYR:CE1	2.49	0.47
1:F:384:ALA:HB3	1:F:389:LEU:HB3	1.95	0.47
1:G:241:THR:O	1:G:245:ILE:HG13	2.13	0.47
1:B:182:LEU:HD12	1:B:269:ILE:HD11	1.96	0.47
1:C:58:GLU:HB3	1:H:426:SER:HB2	1.95	0.47
1:C:283:SER:O	1:C:287:VAL:HG23	2.14	0.47
1:G:17:ARG:NH2	1:G:89:ASP:OD2	2.24	0.47
1:C:496:PRO:HG3	1:G:170:TRP:CD1	2.50	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:465:TRP:HA	1:D:466:SER:HA	1.56	0.47
1:G:274:GLN:HG3	1:G:297:MET:HE1	1.96	0.47
1:C:256:ARG:HA	1:C:260:LYS:HB2	1.96	0.47
1:D:95:ILE:HG23	1:D:118:TYR:CE2	2.49	0.47
1:D:393:PRO:HA	1:D:445:HIS:CD2	2.50	0.47
1:A:274:GLN:NE2	1:A:348:ASN:OD1	2.47	0.47
1:C:72:SER:OG	1:C:79:ASP:OD2	2.29	0.47
1:C:100:ILE:HD11	1:C:118:TYR:HD2	1.79	0.47
1:C:303:GLU:HB3	1:C:304:PRO:HD3	1.96	0.47
1:C:495:TYR:CG	1:C:496:PRO:HD2	2.50	0.47
1:D:35:ILE:HG13	1:D:36:GLU:H	1.77	0.47
1:D:241:THR:HG23	1:D:301:PHE:CE2	2.50	0.47
1:D:303:GLU:O	1:D:304:PRO:C	2.52	0.47
1:D:412:ILE:HB	1:D:459:VAL:HG13	1.96	0.47
1:E:443:GLN:HG2	1:E:502:TRP:CZ2	2.49	0.47
1:F:233:PRO:HG2	1:F:362:SER:HB2	1.97	0.47
1:G:173:GLY:HA3	1:G:263:GLN:NE2	2.29	0.47
1:H:186:TRP:HD1	1:H:300:TRP:CE3	2.33	0.47
1:H:483:MET:SD	1:H:503:LEU:HD22	2.54	0.47
1:D:154:SER:OG	1:D:156:LYS:HB2	2.14	0.47
1:F:232:ASN:HB3	1:F:235:THR:OG1	2.15	0.47
1:G:273:ALA:HB3	1:G:399:LEU:HD21	1.96	0.47
1:A:413:TYR:CD2	1:A:461:GLY:HA3	2.45	0.47
1:B:161:PHE:CD2	1:B:247:ALA:HB1	2.50	0.47
1:D:318:VAL:HB	1:D:322:LEU:HB2	1.97	0.47
1:F:87:GLY:HA3	1:F:508:HIS:CG	2.49	0.47
1:G:191:ASP:HB3	1:G:198:PHE:HB2	1.96	0.47
1:H:393:PRO:HA	1:H:445:HIS:NE2	2.30	0.47
1:C:155:PRO:HB3	2:C:604:PEG:H31	1.96	0.47
1:C:193:TYR:CE2	1:C:202:ARG:HD3	2.49	0.47
1:D:337:TYR:CE1	1:D:409:VAL:HG13	2.50	0.47
1:D:429:LEU:O	1:D:433:ARG:HG2	2.14	0.47
1:A:31:SER:OG	1:A:34:GLN:HG3	2.15	0.46
1:C:495:TYR:HE1	1:G:167:LEU:HD13	1.80	0.46
1:H:497:LYS:C	1:H:499:SER:H	2.22	0.46
1:B:242:HIS:CG	1:B:323:PRO:HB2	2.49	0.46
1:D:147:ASP:HB3	1:E:147:ASP:HB3	1.96	0.46
1:E:35:ILE:HG13	1:E:36:GLU:N	2.30	0.46
1:E:186:TRP:CE2	1:E:190:VAL:HG21	2.49	0.46
1:H:194:VAL:HG22	1:H:237:PRO:CG	2.46	0.46
1:C:314:MET:HE2	1:C:314:MET:HB3	1.76	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:329:GLN:HE22	2:C:604:PEG:H22	1.80	0.46
1:C:407:TYR:O	1:C:408:ASN:C	2.57	0.46
1:E:275:TRP:NE1	1:E:277:GLU:HG2	2.31	0.46
1:E:414:ILE:HG13	1:E:449:LEU:HD11	1.97	0.46
1:F:465:TRP:CD2	1:F:466:SER:HB3	2.50	0.46
1:G:184:GLU:HG2	1:G:272:VAL:HB	1.96	0.46
1:H:276:MET:HB3	1:H:350:VAL:HG21	1.95	0.46
1:B:296:PHE:CD2	1:B:314:MET:HE3	2.50	0.46
1:C:97:TRP:HA	1:C:164:TYR:CE1	2.50	0.46
1:C:504:MET:HE2	1:C:504:MET:HB3	1.83	0.46
1:E:392:TYR:OH	1:E:398:LYS:NZ	2.49	0.46
1:G:367:THR:O	1:G:369:VAL:HG13	2.15	0.46
1:B:343:ASN:CG	1:B:416:GLU:HB2	2.41	0.46
1:C:428:THR:OG1	1:C:431:GLU:HG3	2.15	0.46
1:B:486:VAL:HA	1:B:493:ALA:O	2.16	0.46
1:D:484:ILE:HD13	1:D:496:PRO:HA	1.98	0.46
1:F:31:SER:HB2	1:F:138:HIS:CE1	2.50	0.46
1:H:31:SER:HB2	1:H:138:HIS:NE2	2.31	0.46
1:H:422:LEU:HD23	1:H:479:VAL:HG12	1.97	0.46
1:C:469:ASP:N	1:C:482:GLY:HA3	2.30	0.46
1:E:193:TYR:CE1	1:E:202:ARG:HD3	2.50	0.46
1:E:397:ARG:HH11	1:E:451:LEU:HD13	1.81	0.46
1:G:339:PHE:HB3	1:G:411:LEU:HD23	1.98	0.46
1:B:17:ARG:NH1	1:B:507:PHE:O	2.41	0.46
1:C:45:GLY:O	1:C:98:SER:HB2	2.15	0.46
1:G:35:ILE:HG13	1:G:36:GLU:N	2.30	0.46
1:H:131:GLN:OE1	1:H:178:ASN:ND2	2.46	0.46
1:H:465:TRP:HA	1:H:466:SER:HA	1.57	0.46
1:B:286:ASP:OD1	1:B:351:THR:HG22	2.15	0.46
1:B:379:LEU:HD12	1:B:390:HIS:CD2	2.51	0.46
1:E:248:HIS:O	1:E:252:VAL:HG23	2.16	0.46
1:E:286:ASP:OD1	1:E:351:THR:HG22	2.16	0.46
1:F:154:SER:O	1:F:157:ILE:HG22	2.15	0.46
1:B:243:HIS:NE2	3:B:603:SO4:O1	2.43	0.45
1:G:333:LEU:O	1:G:336:SER:OG	2.31	0.45
1:H:326:SER:OG	1:H:329:GLN:HG3	2.16	0.45
1:F:167:LEU:HD13	1:H:495:TYR:CE1	2.51	0.45
1:G:187:THR:O	1:G:191:ASP:HB2	2.17	0.45
1:A:147:ASP:HB3	1:B:147:ASP:CB	2.34	0.45
1:B:447:LEU:O	1:B:451:LEU:HG	2.16	0.45
1:C:270:THR:HA	1:C:341:GLY:O	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:SER:O	1:E:157:ILE:HG22	2.16	0.45
1:E:412:ILE:HG22	1:E:459:VAL:HG13	1.97	0.45
1:G:386:SER:OG	1:G:475:GLU:OE1	2.34	0.45
1:C:186:TRP:NE1	1:C:297:MET:HG3	2.31	0.45
1:D:15:ILE:HG22	1:D:443:GLN:HG2	1.97	0.45
1:G:193:TYR:CD1	1:G:240:VAL:HG21	2.51	0.45
1:B:367:THR:OG1	1:B:369:VAL:HG22	2.16	0.45
1:E:296:PHE:CB	1:E:367:THR:HG22	2.46	0.45
1:H:393:PRO:O	1:H:396:ILE:HG22	2.15	0.45
1:A:23:ASP:OD1	1:A:460:LYS:NZ	2.47	0.45
1:D:104:GLY:HA3	1:D:145:LEU:CG	2.45	0.45
1:D:273:ALA:HB2	1:D:298:TYR:CD1	2.51	0.45
1:E:277:GLU:O	1:E:349:TYR:HA	2.17	0.45
1:H:190:VAL:HA	1:H:194:VAL:HG23	1.98	0.45
1:A:292:ARG:NE	1:A:367:THR:O	2.46	0.45
1:B:412:ILE:O	1:B:459:VAL:HA	2.16	0.45
1:B:465:TRP:HA	1:B:466:SER:HA	1.61	0.45
1:C:260:LYS:NZ	1:C:338:ASP:OD2	2.48	0.45
1:C:343:ASN:OD1	1:C:416:GLU:HB2	2.16	0.45
1:C:363:TYR:O	1:C:367:THR:HG23	2.16	0.45
1:D:280:ASN:C	1:D:282:LYS:H	2.23	0.45
1:E:135:THR:HA	1:E:180:ILE:HB	1.99	0.45
1:A:71:ASP:OD2	1:A:74:HIS:HB2	2.16	0.45
1:C:32:ALA:HB2	1:C:94:SER:O	2.17	0.45
1:C:275:TRP:NE1	1:C:277:GLU:HG2	2.32	0.45
1:D:386:SER:HB3	1:D:388:TRP:NE1	2.32	0.45
1:F:158:VAL:HG13	1:F:247:ALA:HA	1.98	0.45
1:F:329:GLN:O	1:F:333:LEU:N	2.48	0.45
1:H:72:SER:O	1:H:76:TYR:HB3	2.17	0.45
1:H:97:TRP:HA	1:H:164:TYR:CE1	2.52	0.45
1:A:80:VAL:HG11	1:A:124:GLU:HG3	1.99	0.45
1:D:50:ASP:O	1:D:54:LYS:HD3	2.17	0.45
1:E:492:TYR:O	1:E:494:ARG:NH1	2.49	0.45
1:A:236:GLU:HA	1:A:239:LEU:HD12	1.99	0.45
1:E:274:GLN:HG3	1:E:297:MET:HE1	1.99	0.45
1:C:271:ILE:N	1:C:341:GLY:O	2.40	0.44
1:D:302:MET:HE3	1:D:302:MET:HB3	1.80	0.44
1:F:275:TRP:CD1	1:F:277:GLU:HG2	2.52	0.44
1:G:420:ASP:HB3	1:G:481:PHE:CD2	2.52	0.44
1:H:31:SER:O	1:H:35:ILE:HG23	2.17	0.44
1:C:182:LEU:HD11	1:C:244:GLN:O	2.16	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:280:ASN:C	1:D:282:LYS:N	2.75	0.44
1:E:92:ARG:NH1	1:E:416:GLU:HG3	2.32	0.44
1:E:104:GLY:HA3	1:E:145:LEU:HG	1.99	0.44
1:B:427:LEU:HB3	1:B:431:GLU:HB2	1.99	0.44
1:D:382:PRO:O	1:D:391:ILE:HG13	2.16	0.44
1:E:180:ILE:HD13	1:E:270:THR:OG1	2.18	0.44
1:E:412:ILE:O	1:E:459:VAL:HA	2.16	0.44
1:B:183:ASN:O	1:B:184:GLU:C	2.61	0.44
1:B:413:TYR:CD2	1:B:461:GLY:HA3	2.52	0.44
1:D:185:PRO:HB2	1:D:301:PHE:CE2	2.53	0.44
1:D:312:GLU:HA	1:D:315:LYS:HG3	2.00	0.44
1:B:343:ASN:OD1	1:B:416:GLU:HB2	2.16	0.44
1:B:363:TYR:O	1:B:366:ASP:HB2	2.18	0.44
1:D:386:SER:HB3	1:D:388:TRP:CD1	2.52	0.44
1:H:343:ASN:OD1	1:H:416:GLU:HB2	2.17	0.44
1:H:444:ASP:O	1:H:448:GLN:HG2	2.17	0.44
1:A:170:TRP:NE1	1:F:496:PRO:HG3	2.33	0.44
1:A:429:LEU:O	1:A:433:ARG:HG2	2.17	0.44
1:B:275:TRP:HB3	1:B:347:ALA:CB	2.48	0.44
1:E:381:GLY:HA3	1:E:391:ILE:O	2.18	0.44
1:D:342:LEU:HD12	1:D:342:LEU:HA	1.78	0.44
1:G:296:PHE:O	1:G:363:TYR:OH	2.36	0.44
1:A:259:PHE:CD2	1:F:504:MET:HE1	2.53	0.44
1:B:51:THR:HG23	1:B:55:ARG:CD	2.48	0.44
1:B:167:LEU:HD13	1:E:495:TYR:CE1	2.51	0.44
1:C:275:TRP:NE1	1:C:398:LYS:HD3	2.32	0.44
1:D:154:SER:C	1:D:156:LYS:H	2.25	0.44
1:E:439:ILE:O	1:E:443:GLN:HG3	2.18	0.44
1:G:84:LYS:HD2	1:G:128:SER:HB3	2.00	0.44
1:G:100:ILE:HD11	1:G:118:TYR:CD2	2.53	0.44
1:G:193:TYR:CE1	1:G:240:VAL:HG21	2.52	0.44
1:G:242:HIS:CE1	1:G:325:PHE:CE1	3.06	0.44
1:C:508:HIS:ND1	1:C:509:LYS:N	2.66	0.44
1:E:420:ASP:HB3	1:E:481:PHE:CD1	2.53	0.44
1:F:202:ARG:NH1	1:F:230:ASP:O	2.50	0.44
1:G:465:TRP:HA	1:G:466:SER:HA	1.59	0.44
1:H:44:ARG:HB2	1:H:99:ARG:HG3	1.99	0.44
1:H:152:PHE:HA	1:H:157:ILE:HG21	2.00	0.44
1:C:276:MET:HB3	1:C:350:VAL:HG21	2.00	0.43
1:C:302:MET:HE3	1:C:302:MET:HB3	1.51	0.43
1:D:87:GLY:HA3	1:D:508:HIS:CG	2.52	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:TRP:CE2	1:G:496:PRO:HG3	2.53	0.43
1:F:418:GLY:HA3	1:F:465:TRP:O	2.18	0.43
1:C:58:GLU:OE1	1:C:58:GLU:N	2.49	0.43
1:G:31:SER:HB2	1:G:138:HIS:CD2	2.52	0.43
1:H:185:PRO:HB2	1:H:301:PHE:CZ	2.52	0.43
1:B:491:GLN:O	1:B:492:TYR:C	2.58	0.43
1:F:194:VAL:HG13	1:F:233:PRO:HB2	2.00	0.43
1:G:292:ARG:HH11	1:G:292:ARG:HB2	1.83	0.43
1:G:314:MET:HE2	1:G:314:MET:HB3	1.93	0.43
1:G:381:GLY:HA3	1:G:391:ILE:O	2.19	0.43
1:H:424:ASP:HB3	1:H:427:LEU:HG	2.00	0.43
1:A:429:LEU:O	1:A:429:LEU:HD22	2.18	0.43
1:G:161:PHE:CD2	1:G:247:ALA:HB1	2.53	0.43
1:A:86:LEU:HD21	1:A:500:ALA:HB1	1.99	0.43
1:C:88:LEU:HD23	1:C:88:LEU:HA	1.89	0.43
1:C:505:ASN:HD22	1:G:258:LYS:C	2.26	0.43
1:D:42:GLY:O	1:D:111:ASN:ND2	2.41	0.43
1:D:65:ASN:OD1	1:D:67:ASN:HB2	2.19	0.43
1:D:397:ARG:HH21	1:D:455:ASP:CG	2.26	0.43
1:D:434:VAL:C	1:D:436:PRO:HD3	2.43	0.43
1:D:435:ASP:OD2	1:D:499:SER:OG	2.35	0.43
1:E:92:ARG:HA	1:E:133:TYR:O	2.18	0.43
1:G:32:ALA:HB2	1:G:94:SER:O	2.19	0.43
1:H:30:SER:N	1:H:92:ARG:O	2.51	0.43
1:C:229:SER:C	1:C:231:GLY:H	2.26	0.43
1:D:122:ILE:O	1:D:126:ILE:HG13	2.19	0.43
1:D:139:TRP:HZ2	1:D:184:GLU:HB2	1.84	0.43
1:G:190:VAL:HA	1:G:194:VAL:HG23	1.99	0.43
1:H:70:ILE:CD1	1:H:468:LEU:HD13	2.49	0.43
1:B:92:ARG:HA	1:B:133:TYR:O	2.18	0.43
1:B:129:GLY:C	1:B:130:ILE:HG13	2.43	0.43
1:C:161:PHE:CD2	1:C:247:ALA:HB1	2.53	0.43
1:D:11:ASP:O	1:D:12:ALA:C	2.62	0.43
1:E:313:ILE:O	1:E:317:ILE:HG13	2.18	0.43
1:F:446:LEU:HD21	1:F:462:TYR:CD2	2.54	0.43
1:B:438:ARG:O	1:B:442:ILE:HG13	2.19	0.43
1:D:278:PRO:O	1:D:375:ARG:NH2	2.48	0.43
1:G:28:ALA:HB1	1:G:467:LEU:HB2	2.00	0.43
1:A:146:GLU:HA	1:A:151:GLY:N	2.34	0.43
1:A:162:ARG:O	1:A:166:GLU:HG3	2.19	0.43
1:B:51:THR:HG22	2:B:602:PEG:H31	2.01	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:LEU:HB3	1:C:414:ILE:HD13	2.01	0.43
1:H:186:TRP:HD1	1:H:300:TRP:HE3	1.67	0.43
1:A:137:PHE:CZ	1:A:139:TRP:HA	2.54	0.43
1:C:178:ASN:OD1	2:C:602:PEG:H32	2.18	0.43
1:C:342:LEU:O	1:C:414:ILE:HA	2.19	0.43
1:E:367:THR:O	1:E:369:VAL:HG13	2.19	0.43
1:G:483:MET:HG2	1:G:499:SER:OG	2.19	0.43
1:H:97:TRP:CH2	1:H:157:ILE:HD11	2.53	0.43
1:B:51:THR:CG2	2:B:602:PEG:H22	2.48	0.42
1:C:20:PHE:CD2	1:C:26:PHE:HZ	2.36	0.42
1:E:152:PHE:HA	1:E:157:ILE:HG21	2.01	0.42
1:G:139:TRP:CD1	1:G:139:TRP:N	2.87	0.42
1:H:236:GLU:HA	1:H:239:LEU:HD12	2.01	0.42
1:A:420:ASP:HB3	1:A:481:PHE:CD2	2.55	0.42
1:C:468:LEU:C	1:C:482:GLY:HA3	2.44	0.42
1:F:242:HIS:CE1	1:F:323:PRO:HB2	2.54	0.42
1:G:146:GLU:HA	1:G:151:GLY:N	2.35	0.42
1:G:266:GLN:HG3	1:G:339:PHE:HE2	1.79	0.42
1:H:70:ILE:HD11	1:H:468:LEU:HD13	2.01	0.42
1:H:497:LYS:C	1:H:499:SER:N	2.73	0.42
1:B:56:ARG:HB3	1:B:59:MET:HG2	1.99	0.42
1:C:428:THR:O	1:C:431:GLU:N	2.50	0.42
1:D:248:HIS:CE1	1:D:269:ILE:HB	2.55	0.42
1:G:471:PHE:HB2	1:G:477:PHE:CZ	2.54	0.42
1:C:258:LYS:HB2	1:C:259:PHE:CD1	2.54	0.42
1:F:86:LEU:HA	1:F:504:MET:HB2	2.01	0.42
1:F:266:GLN:HG2	1:F:338:ASP:CB	2.49	0.42
1:G:86:LEU:HA	1:G:504:MET:HB2	2.01	0.42
1:H:241:THR:HG21	1:H:300:TRP:CE2	2.55	0.42
1:A:492:TYR:CD1	1:A:492:TYR:N	2.88	0.42
1:B:44:ARG:HG3	1:B:99:ARG:HB2	2.01	0.42
1:C:349:TYR:CE1	1:C:380:ILE:HD12	2.54	0.42
1:F:363:TYR:CD1	1:F:363:TYR:C	2.97	0.42
1:G:48:ILE:HA	1:G:143:GLN:HE21	1.82	0.42
1:G:303:GLU:HG3	1:G:309:ASP:O	2.19	0.42
1:H:235:THR:OG1	1:H:236:GLU:N	2.52	0.42
1:H:435:ASP:CG	1:H:499:SER:HB3	2.45	0.42
1:A:465:TRP:HA	1:A:466:SER:HA	1.51	0.42
1:B:449:LEU:HD11	1:B:459:VAL:HG11	2.01	0.42
1:C:386:SER:OG	1:C:420:ASP:OD2	2.37	0.42
1:D:363:TYR:O	1:D:367:THR:HG23	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:139:TRP:CZ3	1:F:473:TRP:CE2	3.08	0.42
1:H:31:SER:HB2	1:H:138:HIS:CE1	2.54	0.42
1:H:381:GLY:HA3	1:H:391:ILE:O	2.19	0.42
1:C:429:LEU:O	1:C:433:ARG:HB3	2.20	0.42
1:C:434:VAL:HG12	1:C:436:PRO:HD3	2.02	0.42
1:D:275:TRP:NE1	1:D:398:LYS:HD2	2.34	0.42
1:D:443:GLN:HG3	1:D:502:TRP:CZ2	2.54	0.42
1:A:92:ARG:HA	1:A:133:TYR:O	2.19	0.42
1:A:92:ARG:NH2	1:A:183:ASN:OD1	2.41	0.42
1:B:170:TRP:CE2	1:E:496:PRO:HG3	2.55	0.42
1:B:190:VAL:HA	1:B:194:VAL:CG2	2.50	0.42
1:C:465:TRP:CD2	1:C:466:SER:HB3	2.55	0.42
1:D:447:LEU:O	1:D:451:LEU:HG	2.20	0.42
1:E:475:GLU:O	1:E:476:GLY:C	2.63	0.42
1:G:51:THR:HG22	1:G:55:ARG:HD2	2.01	0.42
1:H:144:ALA:O	1:H:148:GLU:HB2	2.19	0.42
1:B:92:ARG:NH1	1:B:416:GLU:HG3	2.35	0.42
1:B:275:TRP:HB3	1:B:347:ALA:HB2	2.01	0.42
1:D:505:ASN:OD1	1:H:262:SER:HB2	2.20	0.42
1:E:20:PHE:HE2	1:E:449:LEU:HD23	1.85	0.42
1:F:184:GLU:HG2	1:F:272:VAL:HB	2.00	0.42
1:F:394:GLU:O	1:F:398:LYS:HG3	2.20	0.42
1:F:449:LEU:HD21	1:F:459:VAL:CG1	2.50	0.42
1:F:465:TRP:HA	1:F:466:SER:HA	1.60	0.42
1:G:421:GLU:HG2	1:G:480:ARG:HB2	2.01	0.42
1:G:446:LEU:HD23	1:G:446:LEU:HA	1.93	0.42
1:A:147:ASP:CB	1:B:147:ASP:HB3	2.34	0.42
1:B:419:VAL:HG22	1:B:420:ASP:N	2.35	0.42
1:D:54:LYS:HE3	1:D:67:ASN:OD1	2.20	0.42
1:D:505:ASN:ND2	1:H:261:ALA:HB3	2.35	0.42
1:F:326:SER:OG	1:F:329:GLN:HG3	2.20	0.42
1:F:466:SER:O	1:F:482:GLY:HA2	2.19	0.42
1:A:242:HIS:ND1	1:A:323:PRO:HB2	2.35	0.41
1:C:72:SER:O	1:C:76:TYR:N	2.53	0.41
1:D:86:LEU:HA	1:D:504:MET:HG3	2.02	0.41
1:D:90:ALA:HA	1:D:130:ILE:HG22	2.02	0.41
1:E:100:ILE:HD12	1:E:115:ILE:HG12	2.02	0.41
1:F:294:LEU:HD23	1:F:294:LEU:HA	1.84	0.41
1:G:193:TYR:CD2	1:G:202:ARG:HD3	2.55	0.41
1:D:275:TRP:HA	1:D:275:TRP:CE3	2.55	0.41
1:D:381:GLY:HA3	1:D:391:ILE:O	2.19	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:495:TYR:CG	1:D:496:PRO:HD2	2.55	0.41
1:F:186:TRP:CZ2	1:F:297:MET:HE2	2.55	0.41
1:F:248:HIS:ND1	1:F:269:ILE:HD12	2.35	0.41
1:B:72:SER:O	1:B:76:TYR:HB3	2.20	0.41
1:D:321:ARG:HH22	1:D:366:ASP:CG	2.27	0.41
1:H:149:TYR:OH	1:H:160:ASP:OD2	2.34	0.41
1:H:393:PRO:HA	1:H:445:HIS:CD2	2.56	0.41
1:C:58:GLU:CB	1:H:426:SER:HB2	2.50	0.41
1:C:87:GLY:HA3	1:C:508:HIS:CG	2.55	0.41
1:C:94:SER:HB3	1:C:135:THR:HB	2.03	0.41
1:C:195:ALA:HB1	1:C:197:THR:HG23	2.02	0.41
1:D:10:PRO:O	1:D:447:LEU:HD11	2.20	0.41
1:E:414:ILE:HG13	1:E:449:LEU:CD1	2.51	0.41
1:G:92:ARG:HA	1:G:133:TYR:O	2.20	0.41
1:G:232:ASN:ND2	1:G:235:THR:HG23	2.35	0.41
1:H:412:ILE:O	1:H:459:VAL:HA	2.20	0.41
1:A:382:PRO:HG2	1:A:391:ILE:HD12	2.02	0.41
1:A:407:TYR:HB2	1:A:409:VAL:HG23	2.02	0.41
1:D:121:PHE:HD1	1:D:121:PHE:O	2.04	0.41
1:D:294:LEU:O	1:D:298:TYR:HB3	2.20	0.41
1:E:31:SER:HB2	1:E:138:HIS:ND1	2.34	0.41
1:E:420:ASP:HB3	1:E:481:PHE:CG	2.56	0.41
1:F:256:ARG:HA	1:F:260:LYS:HB2	2.03	0.41
1:G:471:PHE:HB2	1:G:477:PHE:CE1	2.55	0.41
1:H:486:VAL:HA	1:H:493:ALA:O	2.19	0.41
1:C:248:HIS:CE1	1:C:269:ILE:HB	2.55	0.41
1:C:465:TRP:HA	1:C:466:SER:HA	1.53	0.41
1:D:346:THR:OG1	1:D:347:ALA:N	2.54	0.41
1:H:248:HIS:O	1:H:252:VAL:HG23	2.20	0.41
1:B:472:GLU:HB3	1:B:475:GLU:HB2	2.02	0.41
1:E:97:TRP:HA	1:E:164:TYR:CE1	2.55	0.41
1:E:234:GLY:O	1:E:321:ARG:HD2	2.21	0.41
1:F:17:ARG:HB2	1:F:507:PHE:HA	2.03	0.41
1:H:435:ASP:OD2	1:H:499:SER:OG	2.35	0.41
1:H:466:SER:O	1:H:482:GLY:HA2	2.20	0.41
1:D:410:PRO:O	1:D:458:ASN:HB3	2.21	0.41
1:D:483:MET:HB3	1:D:483:MET:HE3	1.67	0.41
1:D:495:TYR:CD1	1:D:496:PRO:HD2	2.56	0.41
1:H:199:ALA:HA	1:H:200:PRO:C	2.45	0.41
1:A:255:TYR:OH	1:A:265:GLY:HA3	2.20	0.41
1:B:315:LYS:HB2	1:B:315:LYS:HE3	1.82	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:438:ARG:NH2	1:C:480:ARG:O	2.54	0.41
1:D:35:ILE:HA	1:D:70:ILE:HG12	2.03	0.41
1:D:197:THR:C	1:D:198:PHE:HD1	2.29	0.41
1:D:438:ARG:O	1:D:442:ILE:HG13	2.21	0.41
1:F:45:GLY:O	1:F:98:SER:HB2	2.21	0.41
1:F:193:TYR:CE1	1:F:240:VAL:HG21	2.56	0.41
1:G:242:HIS:CE1	1:G:323:PRO:HB2	2.56	0.41
1:G:277:GLU:O	1:G:349:TYR:HA	2.21	0.41
1:G:401:VAL:O	1:G:402:TYR:C	2.64	0.41
1:A:342:LEU:O	1:A:414:ILE:HA	2.21	0.41
1:A:394:GLU:H	1:A:394:GLU:CD	2.29	0.41
1:B:419:VAL:HB	1:B:441:PHE:CD2	2.56	0.41
1:C:76:TYR:CE2	1:C:77:LYS:HG3	2.55	0.41
1:C:155:PRO:HB3	2:C:604:PEG:H12	2.02	0.41
1:D:44:ARG:HH22	1:D:47:SER:HB3	1.86	0.41
1:D:232:ASN:HB3	1:D:235:THR:OG1	2.21	0.41
1:D:384:ALA:HB3	1:D:389:LEU:HB3	2.02	0.41
1:E:394:GLU:H	1:E:394:GLU:CD	2.29	0.41
1:F:193:TYR:CD1	1:F:240:VAL:HG21	2.55	0.41
1:G:91:TYR:HD2	1:G:125:LEU:HD21	1.86	0.41
1:G:193:TYR:CE2	1:G:202:ARG:HD3	2.56	0.41
1:G:413:TYR:HD1	1:G:461:GLY:HA3	1.86	0.41
1:H:35:ILE:HG13	1:H:36:GLU:N	2.35	0.41
1:B:424:ASP:HB3	1:B:427:LEU:HG	2.02	0.40
1:C:343:ASN:CG	1:C:416:GLU:HB2	2.46	0.40
1:C:391:ILE:HG22	1:C:393:PRO:HD3	2.03	0.40
1:D:303:GLU:HB3	1:D:304:PRO:CD	2.49	0.40
1:G:101:LEU:HD21	1:G:167:LEU:HD22	2.02	0.40
1:B:29:ALA:CB	1:B:92:ARG:HB3	2.51	0.40
1:B:275:TRP:CZ3	1:B:294:LEU:HD11	2.56	0.40
1:D:337:TYR:HE1	1:D:409:VAL:HG13	1.85	0.40
1:E:386:SER:HB3	1:E:388:TRP:CD1	2.55	0.40
1:H:232:ASN:HA	1:H:233:PRO:HD3	1.86	0.40
1:A:234:GLY:HA3	1:A:361:VAL:HG23	2.02	0.40
1:D:58:GLU:HG2	1:D:59:MET:HG2	2.02	0.40
1:D:100:ILE:HD11	1:D:118:TYR:HD2	1.86	0.40
1:D:232:ASN:HA	1:D:233:PRO:HD2	1.92	0.40
1:D:345:TYR:OH	1:D:416:GLU:HG2	2.21	0.40
1:F:495:TYR:CD1	1:F:496:PRO:HD2	2.56	0.40
1:B:150:GLY:O	1:B:153:LEU:HB2	2.21	0.40
1:B:250:ALA:O	1:B:254:SER:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:252:VAL:HG13	1:D:267:ILE:HG23	2.02	0.40
1:D:508:HIS:ND1	1:D:509:LYS:N	2.70	0.40
1:F:252:VAL:HG21	1:F:336:SER:O	2.21	0.40
1:F:420:ASP:HB3	1:F:481:PHE:CG	2.57	0.40
1:G:44:ARG:HD2	1:G:99:ARG:CZ	2.51	0.40
1:H:87:GLY:O	1:H:509:LYS:HG2	2.21	0.40
1:H:318:VAL:CG1	1:H:322:LEU:HB2	2.51	0.40
1:A:349:TYR:CE2	1:A:380:ILE:HB	2.56	0.40
1:B:186:TRP:HD1	1:B:300:TRP:HE3	1.70	0.40
1:C:495:TYR:CD2	1:C:496:PRO:HD2	2.56	0.40
1:G:166:GLU:OE2	1:G:254:SER:OG	2.40	0.40
1:G:234:GLY:O	1:G:321:ARG:HD2	2.22	0.40
1:H:57:PRO:C	1:H:59:MET:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	470/534 (88%)	446 (95%)	24 (5%)	0	100	100
1	B	463/534 (87%)	434 (94%)	26 (6%)	3 (1%)	21	45
1	C	465/534 (87%)	440 (95%)	25 (5%)	0	100	100
1	D	463/534 (87%)	429 (93%)	28 (6%)	6 (1%)	9	26
1	E	460/534 (86%)	437 (95%)	21 (5%)	2 (0%)	30	53
1	F	460/534 (86%)	435 (95%)	25 (5%)	0	100	100
1	G	460/534 (86%)	421 (92%)	39 (8%)	0	100	100
1	H	458/534 (86%)	426 (93%)	31 (7%)	1 (0%)	43	66
All	All	3699/4272 (87%)	3468 (94%)	219 (6%)	12 (0%)	36	59

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	230	ASP
1	D	36	GLU
1	E	476	GLY
1	H	491	GLN
1	D	408	ASN
1	D	416	GLU
1	E	61	LYS
1	D	9	VAL
1	D	410	PRO
1	D	474	ASN
1	B	104	GLY
1	B	354	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	369/456 (81%)	360 (98%)	9 (2%)	43	67
1	B	375/456 (82%)	364 (97%)	11 (3%)	37	61
1	C	376/456 (82%)	359 (96%)	17 (4%)	24	50
1	D	374/456 (82%)	337 (90%)	37 (10%)	7	21
1	E	373/456 (82%)	361 (97%)	12 (3%)	34	59
1	F	367/456 (80%)	356 (97%)	11 (3%)	36	60
1	G	365/456 (80%)	346 (95%)	19 (5%)	21	46
1	H	364/456 (80%)	343 (94%)	21 (6%)	18	41
All	All	2963/3648 (81%)	2826 (95%)	137 (5%)	24	50

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	SER
1	A	41	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	64	SER
1	A	254	SER
1	A	271	ILE
1	A	285	SER
1	A	369	VAL
1	A	389	LEU
1	A	429	LEU
1	B	270	THR
1	B	312	GLU
1	B	330	SER
1	B	362	SER
1	B	370	THR
1	B	433	ARG
1	B	437	ILE
1	B	440	LYS
1	B	467	LEU
1	B	468	LEU
1	B	479	VAL
1	C	31	SER
1	C	51	THR
1	C	61	LYS
1	C	64	SER
1	C	72	SER
1	C	262	SER
1	C	292	ARG
1	C	370	THR
1	C	374	ASP
1	C	389	LEU
1	C	420	ASP
1	C	422	LEU
1	C	429	LEU
1	C	433	ARG
1	C	440	LYS
1	C	459	VAL
1	C	460	LYS
1	D	15	ILE
1	D	22	SER
1	D	35	ILE
1	D	77	LYS
1	D	89	ASP
1	D	98	SER
1	D	112	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	113	GLU
1	D	115	ILE
1	D	126	ILE
1	D	130	ILE
1	D	157	ILE
1	D	241	THR
1	D	254	SER
1	D	258	LYS
1	D	262	SER
1	D	267	ILE
1	D	270	THR
1	D	271	ILE
1	D	285	SER
1	D	297	MET
1	D	307	SER
1	D	320	SER
1	D	326	SER
1	D	330	SER
1	D	350	VAL
1	D	373	SER
1	D	389	LEU
1	D	421	GLU
1	D	430	SER
1	D	434	VAL
1	D	447	LEU
1	D	459	VAL
1	D	468	LEU
1	D	479	VAL
1	D	483	MET
1	D	501	ILE
1	E	16	ASN
1	E	31	SER
1	E	126	ILE
1	E	131	GLN
1	E	254	SER
1	E	285	SER
1	E	361	VAL
1	E	362	SER
1	E	421	GLU
1	E	425	THR
1	E	431	GLU
1	E	449	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	15	ILE
1	F	40	SER
1	F	64	SER
1	F	110	ILE
1	F	285	SER
1	F	292	ARG
1	F	330	SER
1	F	389	LEU
1	F	429	LEU
1	F	437	ILE
1	F	459	VAL
1	G	51	THR
1	G	64	SER
1	G	174	ASP
1	G	254	SER
1	G	285	SER
1	G	340	LEU
1	G	342	LEU
1	G	350	VAL
1	G	351	THR
1	G	361	VAL
1	G	362	SER
1	G	373	SER
1	G	386	SER
1	G	389	LEU
1	G	396	ILE
1	G	421	GLU
1	G	433	ARG
1	G	468	LEU
1	G	479	VAL
1	H	35	ILE
1	H	51	THR
1	H	105	ASN
1	H	136	LEU
1	H	167	LEU
1	H	174	ASP
1	H	182	LEU
1	H	240	VAL
1	H	241	THR
1	H	267	ILE
1	H	270	THR
1	H	306	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	H	313	ILE
1	H	320	SER
1	H	370	THR
1	H	421	GLU
1	H	429	LEU
1	H	434	VAL
1	H	440	LYS
1	H	447	LEU
1	H	457	VAL

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

Mol	Chain	Res	Type
1	A	417	ASN
1	B	16	ASN
1	B	65	ASN
1	B	143	GLN
1	B	171	ASN
1	B	390	HIS
1	B	417	ASN
1	B	448	GLN
1	B	491	GLN
1	B	508	HIS
1	C	138	HIS
1	C	348	ASN
1	C	372	HIS
1	C	487	ASN
1	C	489	ASN
1	C	491	GLN
1	D	485	HIS
1	D	489	ASN
1	E	16	ASN
1	E	266	GLN
1	E	348	ASN
1	E	372	HIS
1	E	445	HIS
1	E	470	ASN
1	E	485	HIS
1	F	417	ASN
1	F	491	GLN
1	F	506	ASN
1	G	143	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	244	GLN
1	G	390	HIS
1	H	16	ASN
1	H	65	ASN
1	H	232	ASN
1	H	348	ASN

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](#)

17 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	PEG	A	601	-	6,6,6	0.42	0	5,5,5	0.30	0
4	EDO	E	602	-	3,3,3	0.68	0	2,2,2	0.19	0
2	PEG	C	603	-	6,6,6	0.38	0	5,5,5	0.30	0
2	PEG	C	602	-	6,6,6	0.34	0	5,5,5	0.15	0
4	EDO	H	602	-	3,3,3	0.40	0	2,2,2	1.00	0
3	SO4	D	602	-	4,4,4	0.29	0	6,6,6	0.26	0
2	PEG	C	604	-	6,6,6	0.33	0	5,5,5	0.14	0
2	PEG	A	602	-	6,6,6	0.23	0	5,5,5	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PEG	C	601	-	6,6,6	0.39	0	5,5,5	0.27	0
2	PEG	H	601	-	6,6,6	0.42	0	5,5,5	0.21	0
2	PEG	B	602	-	6,6,6	0.57	0	5,5,5	0.43	0
3	SO4	E	603	-	4,4,4	0.34	0	6,6,6	0.38	0
2	PEG	F	601	-	6,6,6	0.50	0	5,5,5	0.29	0
2	PEG	B	601	-	6,6,6	0.30	0	5,5,5	0.32	0
3	SO4	B	603	-	4,4,4	0.36	0	6,6,6	0.32	0
2	PEG	E	601	-	6,6,6	0.49	0	5,5,5	0.32	0
3	SO4	D	601	-	4,4,4	0.46	0	6,6,6	0.41	0

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	PEG	A	601	-	-	1/4/4/4	-
4	EDO	E	602	-	-	1/1/1/1	-
2	PEG	C	603	-	-	4/4/4/4	-
2	PEG	C	602	-	-	1/4/4/4	-
4	EDO	H	602	-	-	0/1/1/1	-
2	PEG	C	604	-	-	1/4/4/4	-
2	PEG	A	602	-	-	2/4/4/4	-
2	PEG	C	601	-	-	1/4/4/4	-
2	PEG	H	601	-	-	1/4/4/4	-
2	PEG	B	602	-	-	1/4/4/4	-
2	PEG	F	601	-	-	2/4/4/4	-
2	PEG	B	601	-	-	3/4/4/4	-
2	PEG	E	601	-	-	1/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	601	PEG	O1-C1-C2-O2
2	C	602	PEG	O1-C1-C2-O2
2	C	604	PEG	O2-C3-C4-O4
2	B	601	PEG	O2-C3-C4-O4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	C	603	PEG	O2-C3-C4-O4
4	E	602	EDO	O1-C1-C2-O2
2	B	602	PEG	C4-C3-O2-C2
2	A	602	PEG	C1-C2-O2-C3
2	C	603	PEG	C4-C3-O2-C2
2	C	603	PEG	C1-C2-O2-C3
2	A	602	PEG	O1-C1-C2-O2
2	A	601	PEG	O1-C1-C2-O2
2	C	601	PEG	O2-C3-C4-O4
2	F	601	PEG	C4-C3-O2-C2
2	F	601	PEG	O2-C3-C4-O4
2	H	601	PEG	O2-C3-C4-O4
2	C	603	PEG	O1-C1-C2-O2
2	B	601	PEG	C1-C2-O2-C3
2	E	601	PEG	C4-C3-O2-C2

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	602	PEG	1	0
2	C	604	PEG	3	0
2	B	602	PEG	5	0
2	B	601	PEG	1	0
3	B	603	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	474/534 (88%)	-0.20	3 (0%) 85 82	5, 10, 19, 34	0
1	B	469/534 (87%)	-0.12	5 (1%) 78 73	5, 11, 22, 33	0
1	C	471/534 (88%)	-0.06	6 (1%) 75 69	8, 15, 24, 45	0
1	D	469/534 (87%)	0.30	5 (1%) 78 73	8, 16, 26, 31	0
1	E	466/534 (87%)	-0.22	1 (0%) 91 90	6, 10, 18, 32	0
1	F	466/534 (87%)	-0.05	3 (0%) 85 82	7, 13, 26, 41	0
1	G	466/534 (87%)	-0.00	3 (0%) 85 82	9, 16, 28, 40	0
1	H	464/534 (86%)	0.08	1 (0%) 91 90	9, 18, 31, 42	0
All	All	3745/4272 (87%)	-0.03	27 (0%) 84 80	5, 14, 26, 45	0

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	229	SER	4.3
1	E	231	GLY	3.8
1	C	230	ASP	3.5
1	F	376	ASN	3.4
1	A	376	ASN	3.4
1	F	230	ASP	3.4
1	B	355	ASN	3.0
1	H	174	ASP	2.8
1	D	328	GLU	2.7
1	B	376	ASN	2.7
1	B	229	SER	2.5
1	A	11	ASP	2.5
1	C	227	SER	2.4
1	D	361	VAL	2.4
1	D	474	ASN	2.3
1	F	229	SER	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	G	230	ASP	2.3
1	C	420	ASP	2.2
1	D	281	GLU	2.2
1	G	351	THR	2.2
1	G	387	GLU	2.2
1	C	228	ASN	2.1
1	C	355	ASN	2.1
1	D	470	ASN	2.1
1	A	231	GLY	2.1
1	B	422	LEU	2.1
1	B	11	ASP	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
4	EDO	H	602	4/4	0.83	0.16	22,23,27,34	0
3	SO4	D	601	5/5	0.85	0.25	37,44,49,86	0
2	PEG	C	603	7/7	0.87	0.17	14,15,25,28	0
2	PEG	C	604	7/7	0.87	0.15	12,21,36,39	0
2	PEG	A	601	7/7	0.88	0.15	15,29,31,37	0
2	PEG	B	602	7/7	0.88	0.14	9,15,24,30	0
4	EDO	E	602	4/4	0.89	0.13	11,22,24,25	0
2	PEG	C	602	7/7	0.89	0.13	21,23,29,35	0
3	SO4	E	603	5/5	0.91	0.20	27,32,48,72	0
2	PEG	E	601	7/7	0.91	0.12	7,9,14,23	0
3	SO4	D	602	5/5	0.91	0.21	34,38,50,72	0
2	PEG	B	601	7/7	0.92	0.12	11,16,19,23	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PEG	H	601	7/7	0.93	0.10	17,19,21,32	0
3	SO4	B	603	5/5	0.94	0.15	30,39,51,82	0
2	PEG	F	601	7/7	0.94	0.10	9,20,24,27	0
2	PEG	A	602	7/7	0.94	0.09	9,11,12,20	0
2	PEG	C	601	7/7	0.96	0.08	13,13,15,21	0

6.5 Other polymers [i](#)

There are no such residues in this entry.