



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:02 AM UTC

PDB ID : 6OP5 / pdb_00006op5
Title : Crystal Structure of Piper methysticum Styrylpyrone Synthase 1 in complex with p-coumaroyl-CoA
Authors : Pluskal, T.; Weng, J.K.
Deposited on : 2019-04-24
Resolution : 2.70 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

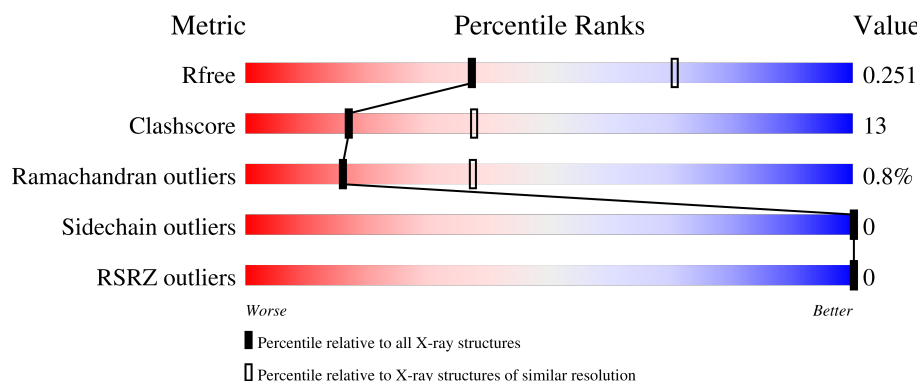
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	3538 (2.70-2.70)
Clashscore	190562	3843 (2.70-2.70)
Ramachandran outliers	187476	3778 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)
RSRZ outliers	180081	3538 (2.70-2.70)

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	397	 74% 21% . .
1	B	397	 68% 28% .
1	D	397	 70% 26% .
1	E	397	 67% 28% . .
1	F	397	 67% 28% . .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	C	397	73% 23% . .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17920 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.

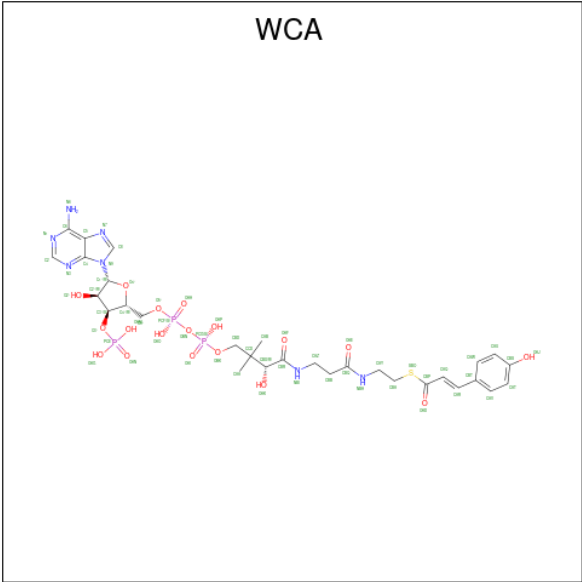
- Molecule 1 is a protein called Styrylpyrone synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2939	1867	502	550	20			
1	B	382	Total	C	N	O	S	0	0	0
			2934	1864	501	549	20			
1	D	382	Total	C	N	O	S	0	0	0
			2934	1864	501	549	20			
1	E	382	Total	C	N	O	S	0	0	0
			2934	1864	501	549	20			
1	F	382	Total	C	N	O	S	0	0	0
			2934	1864	501	549	20			

- Molecule 2 is a protein called Styrylpyrone synthase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	382	Total	C	N	O	S	0	0	0
			2945	1873	501	551	20			

- Molecule 3 is p-coumaroyl-CoA (CCD ID: WCA) (formula: $C_{30}H_{42}N_7O_{18}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			59	30	7	18	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			59	30	7	18	3	1		

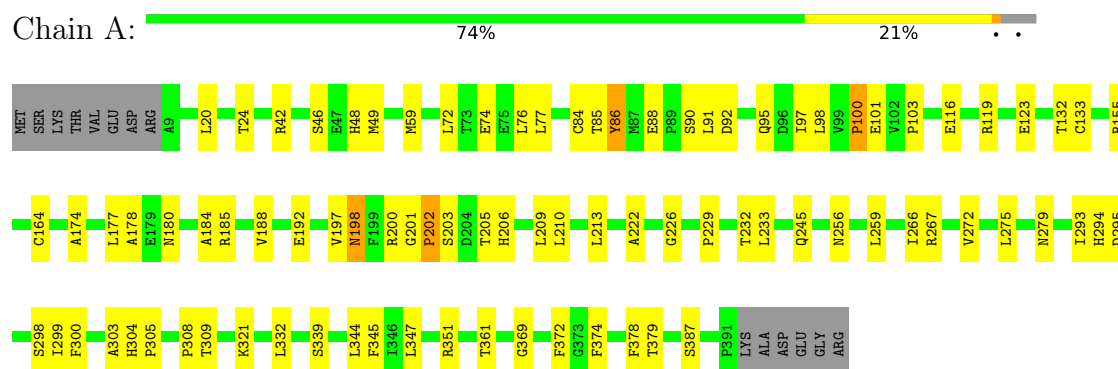
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	39	Total	O	0	0
			39	39		
4	B	36	Total	O	0	0
			36	36		
4	C	33	Total	O	0	0
			33	33		
4	D	32	Total	O	0	0
			32	32		
4	E	21	Total	O	0	0
			21	21		
4	F	21	Total	O	0	0
			21	21		

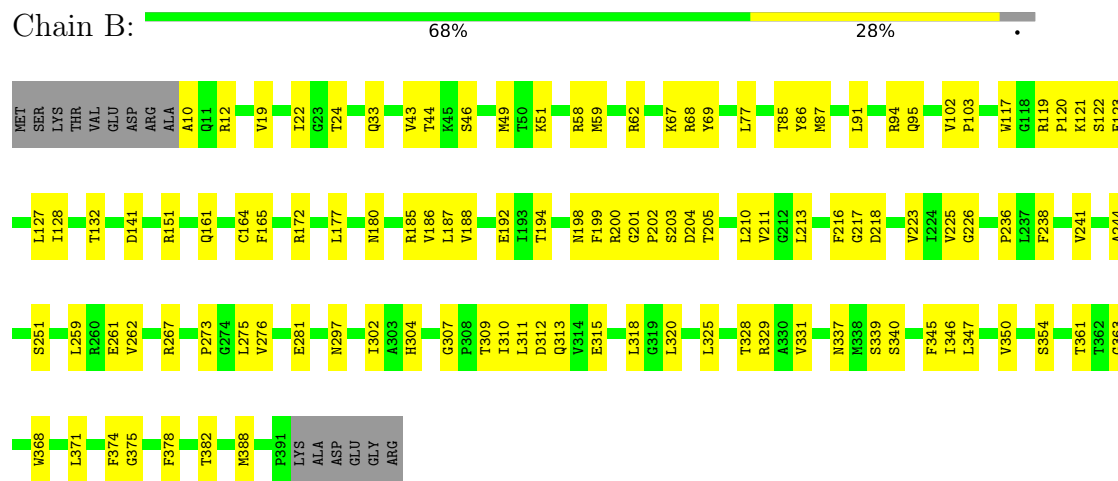
3 Residue-property plots

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.

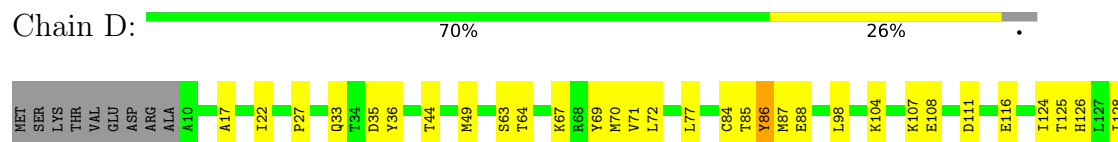
• Molecule 1: Styrylpyrone synthase 1

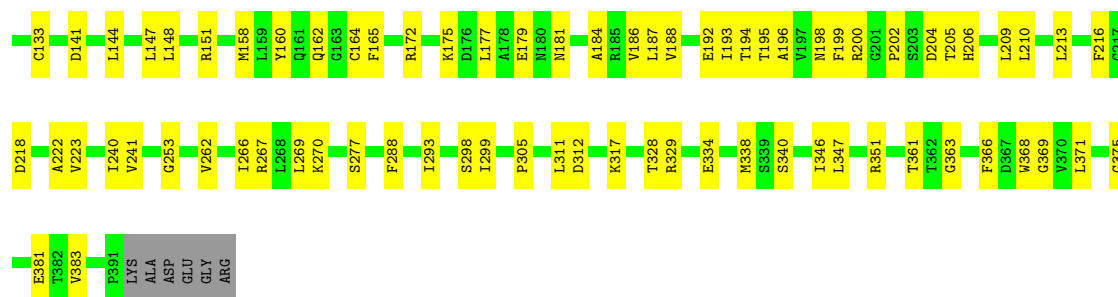


• Molecule 1: Styrylpyrone synthase 1



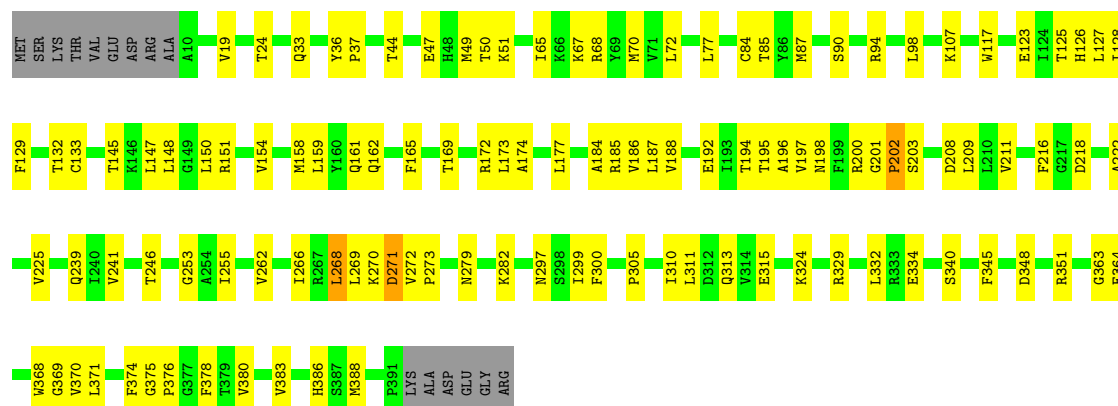
• Molecule 1: Styrylpyrone synthase 1





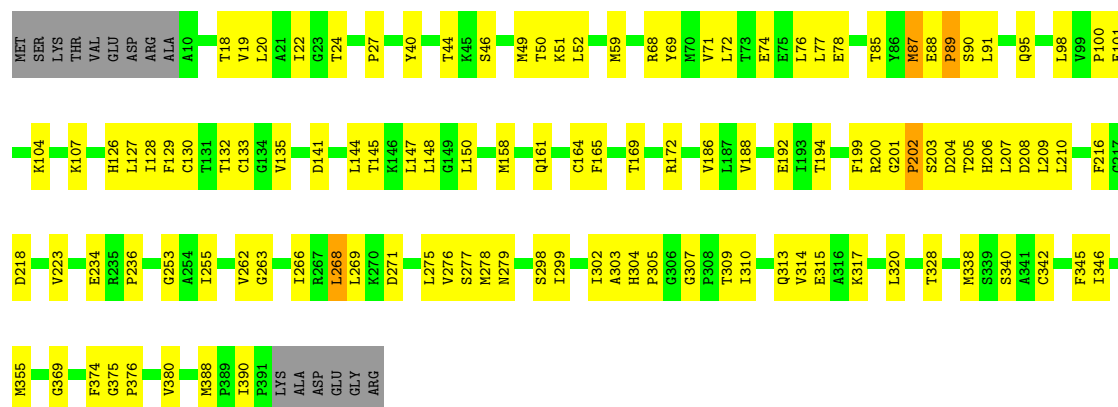
• Molecule 1: Styrylpyrone synthase 1

Chain E: 67% 28% ..



• Molecule 1: Styrylpyrone synthase 1

Chain F: 67% 28% ..



• Molecule 2: Styrylpyrone synthase 1

Chain C: 73% 23% ..



L127	I128	C133	L148	R151	V154	R155	R156	60F164	F165	T169	R172	L177	M181	V186	L187	V188	S191	E192	I193	T194	T195	A196	V197	N198	F199	R200	G201	P202	S203	D204	T205	H206	L207	L213	D218	G219	V223	D230	P231	T232	P236	I255
I266	R267	L268	V276	F300	H304	I310	E315	L320	E323	K326	G336	N337	M338	S339	F345	D348	R351	T361	G369	V370	L371	F372	G373	F374	G375	F378	E381	T382	V383	P389	I390	P391	LYS	ALA	ASP	GLU	GLY	ARG				

4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	164.40Å 164.40Å 87.12Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	82.20 – 2.70 82.20 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.8 (82.20-2.70) 98.7 (82.20-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.204 , 0.261 0.191 , 0.251	Depositor DCC
R_{free} test set	1987 reflections (2.75%)	wwPDB-VP
Wilson B-factor (Å ²)	44.0	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 11.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.439 for -h,-k,l 0.039 for h,-h-k,-l 0.039 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	17920	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: 60F, WCA

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	0.18	0/2996	0.40	1/4060 (0.0%)
1	B	0.19	0/2991	0.41	1/4053 (0.0%)
1	D	0.18	0/2991	0.38	0/4053
1	E	0.20	0/2991	0.40	0/4053
1	F	0.20	0/2991	0.42	0/4053
2	C	0.18	0/2984	0.38	0/4042
All	All	0.19	0/17944	0.40	2/24314 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	SER	CB-CA-C	-6.26	109.37	116.63
1	A	339	SER	CB-CA-C	-5.53	110.21	116.63

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2939	0	2978	66	0
1	B	2934	0	2973	95	0
1	D	2934	0	2973	74	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2934	0	2973	77	0
1	F	2934	0	2973	90	0
2	C	2945	0	2968	62	0
3	A	59	0	38	3	0
3	B	59	0	38	2	0
4	A	39	0	0	3	0
4	B	36	0	0	5	0
4	C	33	0	0	2	0
4	D	32	0	0	2	0
4	E	21	0	0	3	0
4	F	21	0	0	1	0
All	All	17920	0	17914	451	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 (451) 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:F:255:ILE:HD13	1:F:268:LEU:HG	1.25	1.10
1:B:86:TYR:H	1:B:200:ARG:NE	1.53	1.04
1:B:86:TYR:HB3	1:B:200:ARG:CZ	1.89	1.02
1:B:86:TYR:H	1:B:200:ARG:HE	1.02	0.99
1:A:86:TYR:H	1:A:200:ARG:HE	1.03	0.98
1:D:194:THR:HG21	1:D:216:PHE:HB3	1.46	0.98
1:B:86:TYR:HB2	1:B:200:ARG:HG2	1.48	0.94
1:E:200:ARG:HD3	1:E:202:PRO:HG2	1.54	0.87
1:F:255:ILE:CD1	1:F:268:LEU:HG	2.04	0.87
1:F:255:ILE:HD13	1:F:268:LEU:CG	2.06	0.84
1:D:200:ARG:HB3	1:D:202:PRO:HG3	1.59	0.83
1:D:361:THR:HG22	1:D:363:GLY:H	1.45	0.79
1:E:50:THR:HG1	1:F:271:ASP:H	1.30	0.79
1:B:309:THR:HA	1:B:312:ASP:HB2	1.63	0.78
1:F:87:MET:HE2	1:F:262:VAL:HA	1.67	0.77
1:E:50:THR:OG1	1:F:271:ASP:N	2.18	0.77
1:F:44:THR:HG23	1:F:200:ARG:HG2	1.67	0.76
1:F:206:HIS:NE2	1:F:266:ILE:O	2.17	0.76
1:A:86:TYR:N	1:A:200:ARG:HE	1.83	0.74
1:E:174:ALA:HB1	1:E:225:VAL:HG21	1.70	0.74
1:F:278:MET:HE3	1:F:317:LYS:HD3	1.69	0.73
1:A:259:LEU:O	1:B:95:GLN:NE2	2.21	0.73

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:194:THR:O	1:D:196:ALA:N	2.21	0.72
1:D:85:THR:HG21	1:D:88:GLU:HB2	1.72	0.72
1:E:297:ASN:O	1:E:324:LYS:NZ	2.22	0.72
1:B:51:LYS:NZ	1:B:204:ASP:OD2	2.22	0.72
2:C:348:ASP:OD1	2:C:351:ARG:NH2	2.22	0.72
1:B:87:MET:H	1:B:200:ARG:NH1	1.88	0.71
1:A:205:THR:O	1:A:267:ARG:NH2	2.23	0.71
1:B:205:THR:O	1:B:267:ARG:NH2	2.23	0.71
1:E:315:GLU:OE2	1:E:329:ARG:NH2	2.24	0.71
1:F:148:LEU:HD23	1:F:150:LEU:HD21	1.73	0.70
1:B:33:GLN:OE1	1:B:68:ARG:NH2	2.26	0.69
1:D:86:TYR:HB2	1:D:202:PRO:HG2	1.75	0.69
2:C:230:ASP:OD2	2:C:232:THR:OG1	2.09	0.69
1:F:355:MET:HE1	1:F:390:ILE:HG13	1.76	0.68
1:F:51:LYS:NZ	1:F:204:ASP:OD2	2.25	0.68
1:E:200:ARG:HG2	1:E:202:PRO:HD2	1.76	0.68
1:F:165:PHE:HD2	1:F:375:GLY:HA3	1.59	0.68
2:C:49:MET:HE1	2:C:202:PRO:HA	1.76	0.67
1:B:86:TYR:N	1:B:200:ARG:HE	1.84	0.67
1:F:201:GLY:O	1:F:203:SER:N	2.26	0.67
1:B:315:GLU:OE1	1:B:329:ARG:NH2	2.28	0.67
2:C:72:LEU:HG	2:C:195:THR:HG22	1.76	0.67
1:E:348:ASP:OD1	1:E:351:ARG:NH1	2.28	0.67
1:F:127:LEU:HD11	1:F:144:LEU:HD23	1.77	0.67
1:A:59:MET:HE1	1:A:210:LEU:HB3	1.76	0.66
1:B:10:ALA:N	4:B:902:HOH:O	2.27	0.66
1:D:164:CYS:SG	4:D:414:HOH:O	2.43	0.66
2:C:198:ASN:HA	2:C:213:LEU:HD21	1.77	0.66
1:A:95:GLN:NE2	1:B:259:LEU:O	2.24	0.66
1:B:87:MET:HA	1:B:262:VAL:HG11	1.76	0.66
2:C:194:THR:N	2:C:218:ASP:OD2	2.29	0.66
1:B:87:MET:N	1:B:200:ARG:NH1	2.44	0.66
1:F:203:SER:OG	1:F:205:THR:OG1	2.10	0.65
2:C:127:LEU:HB3	2:C:156:ARG:HG2	1.77	0.65
1:B:86:TYR:N	1:B:200:ARG:NE	2.37	0.65
1:A:184:ALA:O	1:A:185:ARG:NH1	2.29	0.65
1:E:165:PHE:HD2	1:E:375:GLY:HA3	1.61	0.65
1:D:87:MET:HG2	1:D:262:VAL:HG11	1.79	0.65
1:A:275:LEU:O	1:A:279:ASN:ND2	2.29	0.64
1:E:98:LEU:HD22	1:E:133:CYS:HB3	1.80	0.64
1:E:87:MET:HG3	1:E:262:VAL:HG21	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:145:THR:HA	1:E:150:LEU:HD23	1.79	0.64
1:F:130:CYS:SG	4:F:421:HOH:O	2.55	0.64
1:A:86:TYR:H	1:A:200:ARG:NE	1.87	0.64
1:E:194:THR:N	1:E:218:ASP:OD1	2.32	0.63
1:F:200:ARG:HD3	1:F:202:PRO:HG2	1.80	0.63
1:E:208:ASP:O	1:E:211:VAL:HG12	1.97	0.63
1:E:305:PRO:HA	1:E:311:LEU:HD21	1.80	0.63
1:D:200:ARG:O	1:D:202:PRO:HD3	1.99	0.63
1:A:86:TYR:N	1:A:200:ARG:HB3	2.13	0.63
1:D:67:LYS:NZ	1:D:334:GLU:OE2	2.30	0.62
1:F:95:GLN:HE22	1:F:135:VAL:H	1.48	0.62
1:D:371:LEU:HB3	1:D:383:VAL:HB	1.81	0.62
1:F:192:GLU:OE1	1:F:340:SER:OG	2.18	0.62
1:E:194:THR:O	1:E:196:ALA:N	2.32	0.62
2:C:126:HIS:HB2	2:C:186:VAL:HG22	1.80	0.62
1:F:374:PHE:HD1	1:F:380:VAL:HG12	1.65	0.61
1:B:165:PHE:HD2	1:B:375:GLY:HA3	1.64	0.61
1:B:192:GLU:OE2	1:B:340:SER:OG	2.10	0.61
1:E:132:THR:HG23	1:E:161:GLN:HA	1.81	0.61
1:F:194:THR:N	1:F:218:ASP:OD2	2.33	0.61
1:D:72:LEU:HD21	1:D:77:LEU:HD21	1.82	0.61
1:D:312:ASP:OD1	1:D:329:ARG:NH2	2.31	0.61
1:F:22:ILE:HG12	1:F:223:VAL:HG22	1.83	0.61
1:F:194:THR:HG23	1:F:218:ASP:OD2	2.01	0.61
1:A:155:ARG:HD2	1:B:172:ARG:HD2	1.82	0.61
1:D:86:TYR:CB	1:D:202:PRO:HG2	2.31	0.61
1:B:59:MET:HE2	1:B:211:VAL:HB	1.83	0.61
1:B:201:GLY:O	1:B:203:SER:N	2.34	0.61
1:B:307:GLY:HA3	3:B:801:WCA:H17	1.82	0.61
2:C:194:THR:O	2:C:196:ALA:N	2.33	0.60
1:B:350:VAL:O	1:B:354:SER:OG	2.17	0.60
1:B:361:THR:HG23	1:B:363:GLY:H	1.67	0.59
1:A:293:ILE:HG21	1:A:299:ILE:HD11	1.83	0.59
1:D:71:VAL:HG21	1:D:193:ILE:HD13	1.85	0.59
1:B:122:SER:O	1:B:151:ARG:NH2	2.35	0.59
2:C:164:60F:SG	2:C:304:HIS:NE2	2.75	0.59
1:E:313:GLN:HB3	4:E:402:HOH:O	2.03	0.59
1:A:49:MET:HE1	1:A:202:PRO:HG3	1.85	0.59
1:A:72:LEU:HD12	1:A:76:LEU:HB3	1.83	0.58
1:E:148:LEU:HD23	1:E:150:LEU:HD21	1.83	0.58
1:E:201:GLY:O	1:E:203:SER:N	2.36	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:205:THR:HG22	1:D:205:THR:HG23	1.86	0.58
1:F:307:GLY:O	1:F:310:ILE:HG22	2.03	0.58
1:D:144:LEU:HG	1:D:148:LEU:HD13	1.86	0.58
1:B:244:ALA:HB3	1:B:382:THR:HG23	1.86	0.57
1:D:104:LYS:NZ	1:D:108:GLU:OE2	2.36	0.57
2:C:188:VAL:HB	2:C:223:VAL:HG23	1.86	0.57
2:C:165:PHE:HB2	2:C:381:GLU:HG3	1.86	0.57
2:C:276:VAL:HG21	2:C:310:ILE:HG23	1.86	0.57
1:E:70:MET:HE2	1:E:194:THR:HG21	1.85	0.57
1:A:305:PRO:HB2	1:A:332:LEU:HD13	1.86	0.57
1:B:67:LYS:NZ	1:B:69:TYR:OH	2.35	0.57
2:C:177:LEU:O	2:C:181:ASN:ND2	2.34	0.57
1:A:72:LEU:HD21	1:A:77:LEU:HD21	1.86	0.56
1:E:273:PRO:HB3	1:E:310:ILE:HG22	1.87	0.56
1:F:18:THR:HG21	1:F:236:PRO:HB3	1.87	0.56
1:F:310:ILE:O	1:F:314:VAL:HG23	2.05	0.56
1:D:126:HIS:HB2	1:D:186:VAL:HG22	1.87	0.56
1:B:382:THR:HG21	4:B:906:HOH:O	2.05	0.56
1:A:116:GLU:OE1	1:A:351:ARG:NH1	2.29	0.56
1:B:86:TYR:HB3	1:B:200:ARG:NH2	2.21	0.56
1:A:201:GLY:O	1:A:203:SER:N	2.38	0.56
1:F:20:LEU:HD22	1:F:234:GLU:HB3	1.88	0.55
1:F:85:THR:HA	1:F:200:ARG:HD2	1.87	0.55
1:B:22:ILE:HG12	1:B:223:VAL:HG12	1.87	0.55
1:B:128:ILE:HD11	1:B:177:LEU:HD12	1.89	0.55
1:D:124:ILE:O	1:D:151:ARG:NH1	2.39	0.55
1:D:194:THR:C	1:D:196:ALA:H	2.14	0.55
1:E:184:ALA:O	1:E:185:ARG:NH1	2.39	0.55
2:C:165:PHE:HD2	2:C:375:GLY:HA3	1.70	0.55
1:F:40:TYR:OH	1:F:199:PHE:O	2.20	0.55
1:F:91:LEU:HD13	1:F:263:GLY:HA2	1.89	0.55
2:C:70:MET:HE2	2:C:194:THR:HG21	1.88	0.54
1:D:253:GLY:O	1:D:269:LEU:HB3	2.08	0.54
1:F:19:VAL:HG13	1:F:223:VAL:HG13	1.88	0.54
1:B:46:SER:HB3	1:B:49:MET:HE2	1.88	0.54
1:D:188:VAL:HB	1:D:223:VAL:HG23	1.90	0.54
1:A:180:ASN:HD22	1:A:180:ASN:C	2.15	0.54
1:B:86:TYR:CB	1:B:200:ARG:CZ	2.76	0.54
1:E:51:LYS:NZ	1:F:208:ASP:OD1	2.29	0.54
1:A:90:SER:O	1:A:90:SER:OG	2.23	0.54
1:D:36:TYR:CE1	1:D:70:MET:HE1	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:71:VAL:HG11	1:F:101:GLU:HG2	1.90	0.53
1:B:86:TYR:CE1	1:B:87:MET:HG2	2.44	0.53
1:F:44:THR:HG23	1:F:200:ARG:CG	2.36	0.53
2:C:63:SER:C	2:C:65:ILE:H	2.16	0.53
1:D:288:PHE:HB3	1:D:293:ILE:HG23	1.89	0.53
1:E:151:ARG:NH1	4:E:405:HOH:O	2.42	0.53
1:D:85:THR:O	1:D:199:PHE:HB2	2.07	0.53
1:F:132:THR:HG23	1:F:161:GLN:HA	1.91	0.53
1:E:67:LYS:HE2	1:E:334:GLU:HB3	1.90	0.53
1:E:255:ILE:HA	1:E:268:LEU:HA	1.90	0.53
1:A:98:LEU:HD22	1:A:133:CYS:HB3	1.92	0.52
1:B:194:THR:HG21	1:B:216:PHE:HD2	1.73	0.52
1:B:241:VAL:HG21	1:B:368:TRP:HZ3	1.74	0.52
1:F:59:MET:HE1	1:F:210:LEU:HB3	1.91	0.52
2:C:65:ILE:HG12	2:C:336:GLY:HA2	1.91	0.52
1:D:298:SER:HA	1:D:366:PHE:CE2	2.45	0.52
1:F:40:TYR:O	1:F:44:THR:HB	2.10	0.52
1:F:87:MET:HE1	1:F:90:SER:N	2.23	0.52
1:F:277:SER:OG	1:F:278:MET:SD	2.58	0.52
1:B:198:ASN:ND2	4:B:901:HOH:O	2.39	0.52
1:B:199:PHE:HE1	1:B:262:VAL:HG12	1.74	0.52
1:E:107:LYS:HD2	1:E:147:LEU:HB3	1.91	0.52
1:B:58:ARG:NH2	4:B:908:HOH:O	2.42	0.51
2:C:117:TRP:CE2	2:C:119:ARG:HB2	2.45	0.51
2:C:151:ARG:HG3	2:C:154:VAL:HG13	1.91	0.51
2:C:172:ARG:NH1	2:C:381:GLU:OE2	2.43	0.51
1:D:192:GLU:OE2	1:D:340:SER:OG	2.25	0.51
1:B:281:GLU:HB3	4:B:935:HOH:O	2.11	0.51
1:E:169:THR:HG23	1:E:172:ARG:NH2	2.25	0.51
1:B:19:VAL:HG22	1:B:238:PHE:H	1.76	0.51
1:D:107:LYS:NZ	1:D:147:LEU:O	2.43	0.51
1:E:270:LYS:HA	1:F:50:THR:HB	1.91	0.51
1:A:295:ASP:O	1:A:298:SER:OG	2.20	0.51
2:C:51:LYS:NZ	2:C:204:ASP:OD2	2.34	0.51
2:C:255:ILE:HG12	2:C:268:LEU:HG	1.93	0.51
1:D:44:THR:HB	1:D:200:ARG:HG3	1.92	0.51
1:F:298:SER:O	1:F:298:SER:OG	2.24	0.51
1:B:68:ARG:NH1	1:B:216:PHE:O	2.42	0.50
2:C:116:GLU:CD	2:C:351:ARG:HH12	2.19	0.50
1:B:86:TYR:CD1	1:B:87:MET:HG2	2.46	0.50
1:D:361:THR:HG21	1:D:366:PHE:O	2.10	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:VAL:HG21	1:D:368:TRP:HZ3	1.77	0.50
1:F:192:GLU:HG3	1:F:338:MET:O	2.12	0.50
1:A:232:THR:HG23	1:A:233:LEU:HD12	1.92	0.50
1:A:294:HIS:O	1:A:294:HIS:ND1	2.42	0.50
1:A:100:PRO:O	1:A:103:PRO:HD2	2.12	0.50
2:C:361:THR:HG22	2:C:389:PRO:HA	1.94	0.50
1:D:107:LYS:HE3	1:D:111:ASP:OD1	2.11	0.50
1:E:126:HIS:HB2	1:E:186:VAL:HG13	1.93	0.50
1:F:132:THR:HA	1:F:161:GLN:HA	1.92	0.50
1:F:338:MET:N	1:F:342:CYS:SG	2.76	0.49
1:F:87:MET:HE2	1:F:262:VAL:CA	2.40	0.49
1:F:68:ARG:NH1	1:F:216:PHE:O	2.45	0.49
1:D:194:THR:CG2	1:D:216:PHE:HB3	2.32	0.49
1:F:255:ILE:HG23	1:F:376:PRO:HA	1.95	0.49
2:C:86:TYR:HB2	2:C:202:PRO:HB2	1.95	0.49
1:E:145:THR:HG21	1:E:154:VAL:HG11	1.93	0.49
1:E:85:THR:HA	1:E:200:ARG:HD2	1.94	0.49
1:B:217:GLY:N	1:B:337:ASN:O	2.34	0.49
1:D:128:ILE:HD11	1:D:177:LEU:HD12	1.93	0.49
1:A:97:ILE:O	1:A:101:GLU:HB2	2.13	0.49
1:B:132:THR:HA	1:B:161:GLN:HA	1.94	0.49
1:E:374:PHE:HB3	1:E:378:PHE:HZ	1.78	0.49
1:A:300:PHE:CZ	1:A:369:GLY:HA3	2.48	0.49
1:B:94:ARG:NH2	1:B:198:ASN:O	2.34	0.49
1:E:49:MET:HE1	1:E:202:PRO:HA	1.94	0.49
2:C:194:THR:HG23	2:C:218:ASP:OD2	2.13	0.48
1:F:277:SER:O	1:F:317:LYS:HG2	2.13	0.48
1:B:185:ARG:HD3	1:B:226:GLY:HA3	1.95	0.48
1:B:194:THR:N	1:B:218:ASP:OD2	2.46	0.48
2:C:172:ARG:HH12	2:C:381:GLU:CD	2.21	0.48
1:E:201:GLY:N	1:E:202:PRO:HD2	2.28	0.48
2:C:90:SER:O	2:C:94:ARG:HG3	2.12	0.48
1:B:273:PRO:HB2	1:B:313:GLN:OE1	2.13	0.48
2:C:206:HIS:NE2	2:C:266:ILE:O	2.44	0.48
1:D:116:GLU:OE1	1:D:351:ARG:NH2	2.40	0.48
1:E:128:ILE:HD11	1:E:177:LEU:HD12	1.95	0.48
1:A:372:PHE:HB3	1:A:374:PHE:CE2	2.49	0.48
1:D:160:TYR:O	1:D:162:GLN:NE2	2.47	0.48
1:F:98:LEU:HD22	1:F:133:CYS:HB3	1.95	0.48
1:F:303:ALA:H	1:F:328:THR:HG21	1.79	0.48
2:C:85:THR:N	2:C:200:ARG:HB2	2.29	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:128:ILE:HD11	2:C:177:LEU:HD12	1.96	0.47
2:C:207:LEU:N	4:C:402:HOH:O	2.37	0.47
1:B:121:LYS:HE3	1:B:121:LYS:HB2	1.75	0.47
1:E:188:VAL:O	1:E:222:ALA:HA	2.15	0.47
1:F:253:GLY:O	1:F:269:LEU:HB3	2.14	0.47
1:A:361:THR:HB	1:A:387:SER:HB3	1.97	0.47
1:B:86:TYR:H	1:B:200:ARG:CZ	2.23	0.47
1:B:297:ASN:HD21	1:B:320:LEU:HA	1.80	0.47
1:B:328:THR:HA	1:B:346:ILE:HD13	1.96	0.47
1:D:299:ILE:HG23	1:D:369:GLY:HA2	1.95	0.47
1:D:361:THR:HG22	1:D:363:GLY:N	2.24	0.47
1:E:192:GLU:OE1	1:E:340:SER:OG	2.32	0.47
1:A:198:ASN:HA	1:A:213:LEU:HD21	1.97	0.47
1:D:328:THR:HA	1:D:346:ILE:HD13	1.97	0.47
1:D:347:LEU:HD23	1:D:347:LEU:HA	1.75	0.47
1:E:90:SER:O	1:E:94:ARG:HG3	2.15	0.47
1:F:100:PRO:O	1:F:104:LYS:HD3	2.14	0.47
2:C:114:ILE:HD13	2:C:121:LYS:HG2	1.95	0.47
1:E:209:LEU:HD21	1:E:266:ILE:HB	1.96	0.47
1:D:188:VAL:O	1:D:222:ALA:HA	2.14	0.47
1:D:200:ARG:C	1:D:202:PRO:HD3	2.40	0.47
1:F:299:ILE:HG12	1:F:369:GLY:HA2	1.97	0.47
2:C:200:ARG:HG2	2:C:202:PRO:HD2	1.98	0.46
1:A:245:GLN:HE21	1:A:379:THR:HG21	1.79	0.46
1:D:210:LEU:HA	1:D:213:LEU:HD23	1.98	0.46
1:D:205:THR:HG22	1:D:267:ARG:HH22	1.80	0.46
1:E:148:LEU:HB3	1:E:150:LEU:CD2	2.46	0.46
1:E:268:LEU:HD21	1:E:271:ASP:HA	1.97	0.46
1:F:27:PRO:HD2	1:F:69:TYR:HB3	1.97	0.46
1:F:104:LYS:HD2	1:F:147:LEU:HD21	1.96	0.46
1:F:328:THR:HG22	1:F:346:ILE:HG21	1.96	0.46
1:B:43:VAL:HG11	1:B:77:LEU:HD13	1.97	0.46
1:B:62:ARG:HD3	3:B:801:WCA:OAO	2.15	0.46
1:D:209:LEU:O	1:D:213:LEU:HD22	2.15	0.46
1:F:72:LEU:HD12	1:F:76:LEU:HB3	1.98	0.46
1:B:132:THR:HG23	1:B:161:GLN:HA	1.97	0.46
2:C:82:SER:HB2	2:C:90:SER:HB3	1.98	0.46
1:F:255:ILE:CG2	1:F:376:PRO:HA	2.45	0.46
1:F:315:GLU:HA	1:F:320:LEU:HD12	1.98	0.46
2:C:84:CYS:O	2:C:200:ARG:HD2	2.15	0.46
1:B:302:ILE:HD11	1:B:350:VAL:HG21	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:272:VAL:HG23	1:E:310:ILE:HG21	1.98	0.46
1:F:51:LYS:HB3	1:F:51:LYS:HE2	1.64	0.46
2:C:85:THR:CA	2:C:200:ARG:HB2	2.46	0.46
1:D:172:ARG:NH2	1:D:381:GLU:OE1	2.48	0.46
1:E:72:LEU:HD21	1:E:77:LEU:HD21	1.98	0.46
1:A:259:LEU:HB3	1:B:95:GLN:HE22	1.81	0.46
1:B:85:THR:C	1:B:200:ARG:HB3	2.41	0.46
1:D:305:PRO:HA	1:D:311:LEU:HD21	1.98	0.46
1:F:255:ILE:HG23	1:F:255:ILE:O	2.16	0.46
1:B:86:TYR:HB3	1:B:200:ARG:NE	2.28	0.45
1:B:198:ASN:HA	1:B:213:LEU:HD21	1.98	0.45
1:E:253:GLY:O	1:E:269:LEU:HB3	2.16	0.45
1:F:309:THR:O	1:F:313:GLN:HG3	2.16	0.45
1:A:92:ASP:OD1	1:B:261:GLU:HG3	2.16	0.45
1:E:194:THR:HG23	1:E:218:ASP:OD1	2.17	0.45
1:A:48:HIS:NE2	1:A:49:MET:HE3	2.31	0.45
1:B:188:VAL:HB	1:B:223:VAL:HG22	1.98	0.45
1:F:128:ILE:HB	1:F:188:VAL:HG22	1.99	0.45
1:F:302:ILE:HG23	1:F:346:ILE:HB	1.98	0.45
1:A:119:ARG:NH2	1:A:123:GLU:OE2	2.49	0.45
1:F:107:LYS:HE3	1:F:148:LEU:HA	1.97	0.45
1:E:129:PHE:CD2	1:E:158:MET:HE1	2.52	0.45
1:F:305:PRO:HD3	1:F:346:ILE:HD11	1.98	0.45
1:B:86:TYR:CB	1:B:200:ARG:NE	2.80	0.45
2:C:192:GLU:HG3	2:C:339:SER:HB3	1.99	0.45
1:A:300:PHE:CE2	1:A:369:GLY:HA3	2.52	0.45
1:B:44:THR:HG21	1:B:201:GLY:H	1.81	0.45
2:C:98:LEU:HD22	2:C:133:CYS:HB2	1.99	0.45
1:E:47:GLU:H	1:E:47:GLU:HG2	1.57	0.45
1:F:52:LEU:HD22	1:F:207:LEU:HD11	1.99	0.45
1:E:255:ILE:HG23	1:E:376:PRO:HA	1.99	0.45
1:A:174:ALA:HA	1:A:177:LEU:HD12	1.99	0.45
1:D:49:MET:HE1	1:D:202:PRO:HA	1.98	0.45
1:D:198:ASN:ND2	4:D:405:HOH:O	2.49	0.45
1:D:165:PHE:HD2	1:D:375:GLY:HA3	1.82	0.44
1:D:17:ALA:HB2	1:D:179:GLU:HG3	1.99	0.44
1:D:63:SER:O	1:D:64:THR:HB	2.16	0.44
1:F:127:LEU:HD13	1:F:145:THR:HG22	1.99	0.44
2:C:18:THR:HG21	2:C:236:PRO:HB3	1.99	0.44
2:C:151:ARG:HG2	4:C:409:HOH:O	2.16	0.44
1:D:298:SER:HA	1:D:366:PHE:HE2	1.82	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:46:SER:HB2	1:F:49:MET:HG3	1.99	0.44
1:F:87:MET:HG3	1:F:262:VAL:O	2.17	0.44
1:F:209:LEU:HD21	1:F:266:ILE:HB	1.98	0.44
1:B:86:TYR:HB2	1:B:200:ARG:CG	2.33	0.44
2:C:75:GLU:HA	2:C:78:GLU:OE1	2.18	0.44
1:A:164:CYS:HB3	1:A:304:HIS:CE1	2.52	0.44
1:B:12:ARG:HG2	1:B:180:ASN:O	2.17	0.44
1:D:98:LEU:HD22	1:D:133:CYS:HB3	1.99	0.44
2:C:315:GLU:HG3	2:C:320:LEU:HB2	1.99	0.44
1:D:84:CYS:C	1:D:200:ARG:HB2	2.42	0.44
1:A:155:ARG:NH1	4:A:913:HOH:O	2.51	0.44
1:B:119:ARG:NH2	1:B:123:GLU:OE1	2.51	0.44
2:C:371:LEU:HB3	2:C:383:VAL:HB	1.99	0.44
1:A:42:ARG:O	4:A:901:HOH:O	2.21	0.44
2:C:102:VAL:HG13	2:C:191:SER:HB3	2.00	0.44
1:F:207:LEU:HA	1:F:207:LEU:HD12	1.75	0.44
1:A:20:LEU:HD21	1:A:229:PRO:HB3	2.00	0.43
1:A:46:SER:HA	1:A:48:HIS:CE1	2.53	0.43
1:B:276:VAL:HG21	1:B:310:ILE:HD11	1.99	0.43
2:C:300:PHE:CE2	2:C:369:GLY:HA3	2.53	0.43
1:D:253:GLY:HA3	1:D:269:LEU:HD23	1.99	0.43
1:A:85:THR:HG21	1:A:88:GLU:HB2	2.01	0.43
1:F:236:PRO:HB2	1:F:388:MET:HG3	2.00	0.43
1:A:272:VAL:HB	1:A:378:PHE:CE1	2.52	0.43
1:A:309:THR:HB	3:A:801:WCA:CBR	2.49	0.43
1:E:65:ILE:HG13	1:E:332:LEU:O	2.19	0.43
2:C:50:THR:OG1	1:D:270:LYS:HA	2.18	0.43
1:D:218:ASP:OD1	1:D:218:ASP:N	2.52	0.43
1:E:246:THR:HG22	1:E:380:VAL:HG23	2.00	0.43
1:E:300:PHE:CZ	1:E:369:GLY:HA3	2.53	0.43
1:A:293:ILE:HD13	1:A:299:ILE:HD11	2.00	0.43
1:A:308:PRO:HB2	4:A:930:HOH:O	2.17	0.43
1:B:347:LEU:HD23	1:B:347:LEU:HA	1.89	0.43
1:D:22:ILE:HG12	1:D:223:VAL:HG12	2.00	0.43
1:E:371:LEU:HB3	1:E:383:VAL:HB	2.01	0.43
1:F:88:GLU:O	1:F:89:PRO:C	2.62	0.43
1:A:132:THR:HG22	1:A:192:GLU:OE1	2.19	0.43
1:B:141:ASP:OD1	1:B:141:ASP:N	2.49	0.43
1:A:46:SER:OG	1:A:202:PRO:HD3	2.19	0.43
1:B:85:THR:CA	1:B:200:ARG:HB3	2.49	0.43
1:B:262:VAL:HG12	1:B:262:VAL:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:36:TYR:HE1	1:D:70:MET:HE1	1.83	0.43
1:F:141:ASP:O	1:F:145:THR:HG23	2.19	0.43
1:A:206:HIS:CG	1:A:209:LEU:HD23	2.54	0.43
1:B:374:PHE:HB3	1:B:378:PHE:CZ	2.54	0.43
1:D:200:ARG:CZ	1:D:202:PRO:HB3	2.48	0.43
1:E:77:LEU:HB3	1:E:84:CYS:SG	2.58	0.43
1:A:48:HIS:CE1	1:A:49:MET:HE3	2.54	0.42
1:A:197:VAL:HG11	3:A:801:WCA:H3	2.00	0.42
1:A:303:ALA:HA	1:A:372:PHE:HB2	2.01	0.42
1:B:273:PRO:HA	1:B:310:ILE:HG13	2.00	0.42
1:E:44:THR:O	1:E:200:ARG:CZ	2.67	0.42
1:A:91:LEU:HD22	1:B:91:LEU:HD22	2.01	0.42
1:E:36:TYR:N	1:E:37:PRO:HD2	2.33	0.42
1:E:117:TRP:HH2	1:E:123:GLU:HB3	1.83	0.42
1:F:164:CYS:HB3	1:F:304:HIS:CE1	2.54	0.42
2:C:201:GLY:N	2:C:202:PRO:HD2	2.35	0.42
1:D:277:SER:O	1:D:317:LYS:HG2	2.19	0.42
1:F:278:MET:SD	1:F:278:MET:N	2.92	0.42
1:A:188:VAL:O	1:A:222:ALA:HA	2.20	0.42
1:E:198:ASN:ND2	4:E:401:HOH:O	2.22	0.42
1:E:299:ILE:HD11	1:E:370:VAL:HG23	2.01	0.42
1:F:87:MET:HB3	1:F:262:VAL:HB	2.01	0.42
1:F:276:VAL:HG21	1:F:310:ILE:CG1	2.49	0.42
1:B:10:ALA:C	1:B:12:ARG:H	2.27	0.42
1:B:251:SER:HB2	1:B:275:LEU:HD21	2.01	0.42
2:C:323:GLU:HG3	2:C:326:LYS:HD2	2.01	0.42
1:F:255:ILE:HD13	1:F:268:LEU:CD1	2.50	0.42
2:C:86:TYR:CE1	2:C:87:MET:HG3	2.53	0.42
2:C:107:LYS:HA	2:C:148:LEU:HD11	2.02	0.42
1:E:374:PHE:HB3	1:E:378:PHE:CZ	2.55	0.42
1:A:256:ASN:O	1:A:266:ILE:HA	2.20	0.42
1:B:164:CYS:HB3	1:B:304:HIS:CE1	2.55	0.42
2:C:300:PHE:CZ	2:C:369:GLY:HA3	2.54	0.42
1:D:175:LYS:HD2	1:D:240:ILE:HG22	2.01	0.42
1:E:388:MET:HE2	1:E:388:MET:HA	2.00	0.42
1:F:24:THR:HB	1:F:345:PHE:CZ	2.54	0.42
1:F:169:THR:HG23	1:F:172:ARG:NH2	2.34	0.42
1:B:120:PRO:HD2	1:B:123:GLU:OE2	2.20	0.42
1:B:241:VAL:HG21	1:B:368:TRP:CZ3	2.55	0.42
1:D:206:HIS:NE2	1:D:266:ILE:O	2.52	0.42
1:D:338:MET:HE3	1:D:338:MET:HB2	1.92	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:19:VAL:HG22	1:E:225:VAL:HG12	2.02	0.42
1:B:119:ARG:HH21	1:B:123:GLU:CD	2.28	0.42
1:D:141:ASP:HB3	1:D:158:MET:HB2	2.00	0.42
1:F:72:LEU:HD21	1:F:77:LEU:HD21	2.02	0.42
1:B:59:MET:HE1	1:B:210:LEU:HB2	2.02	0.41
1:B:311:LEU:HB3	1:B:325:LEU:HD13	2.02	0.41
2:C:338:MET:HE1	2:C:345:PHE:CD2	2.55	0.41
1:E:241:VAL:HG11	1:E:368:TRP:HZ3	1.85	0.41
1:E:305:PRO:HB2	1:E:332:LEU:HD13	2.03	0.41
2:C:201:GLY:O	2:C:202:PRO:C	2.63	0.41
1:D:187:LEU:HD11	1:D:222:ALA:HB1	2.01	0.41
1:A:86:TYR:HB3	1:A:200:ARG:NH1	2.36	0.41
1:B:24:THR:HB	1:B:345:PHE:CZ	2.55	0.41
2:C:372:PHE:HB3	2:C:374:PHE:CZ	2.55	0.41
1:E:127:LEU:HD12	1:E:187:LEU:O	2.20	0.41
1:F:205:THR:O	1:F:206:HIS:C	2.63	0.41
2:C:219:GLY:HA3	2:C:338:MET:SD	2.59	0.41
2:C:267:ARG:NH1	1:D:204:ASP:HB3	2.35	0.41
1:E:279:ASN:O	1:E:282:LYS:HG3	2.20	0.41
1:F:126:HIS:HB2	1:F:186:VAL:HG22	2.03	0.41
1:B:85:THR:HA	1:B:200:ARG:HB3	2.01	0.41
1:E:24:THR:HB	1:E:345:PHE:CE2	2.55	0.41
1:E:162:GLN:HE21	1:E:162:GLN:HB3	1.64	0.41
1:E:363:GLY:C	1:E:364:GLU:HG2	2.44	0.41
1:F:275:LEU:O	1:F:279:ASN:ND2	2.35	0.41
1:B:117:TRP:CE2	1:B:119:ARG:HB2	2.56	0.41
1:B:331:VAL:HG21	1:B:346:ILE:HG12	2.03	0.41
1:A:24:THR:HB	1:A:345:PHE:CZ	2.56	0.41
2:C:169:THR:HG23	2:C:172:ARG:NH2	2.35	0.41
1:E:51:LYS:HE2	1:E:51:LYS:HB3	1.91	0.41
1:E:197:VAL:HG21	1:E:216:PHE:CE1	2.56	0.41
1:E:305:PRO:HB2	1:E:332:LEU:HD22	2.02	0.41
1:A:42:ARG:HH22	1:A:74:GLU:CD	2.28	0.41
1:A:309:THR:OG1	3:A:801:WCA:H30	2.21	0.41
1:A:321:LYS:HE3	1:A:321:LYS:HB3	1.96	0.41
1:A:344:LEU:HA	1:A:347:LEU:HB2	2.03	0.41
1:B:186:VAL:HB	1:B:225:VAL:HB	2.03	0.41
1:D:27:PRO:HD2	1:D:69:TYR:HB3	2.02	0.41
1:D:33:GLN:C	1:D:35:ASP:H	2.29	0.41
1:E:159:LEU:HD11	1:E:173:LEU:HD12	2.02	0.41
1:F:74:GLU:O	1:F:78:GLU:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:129:PHE:HB3	1:F:158:MET:SD	2.61	0.41
1:F:133:CYS:SG	1:F:192:GLU:HA	2.61	0.41
1:A:374:PHE:HB3	1:A:378:PHE:CE2	2.56	0.41
1:A:178:ALA:HB1	1:A:226:GLY:HA2	2.03	0.40
2:C:36:TYR:HA	2:C:39:TYR:HB3	2.03	0.40
1:A:49:MET:HE1	1:A:202:PRO:CG	2.51	0.40
1:A:200:ARG:HG3	1:A:202:PRO:HD2	2.03	0.40
1:B:102:VAL:HB	1:B:103:PRO:HD3	2.04	0.40
1:E:239:GLN:HB2	1:E:386:HIS:HB3	2.03	0.40
1:E:33:GLN:HE22	1:E:68:ARG:HH12	1.68	0.40
1:D:44:THR:HG22	1:D:200:ARG:HA	2.03	0.40
1:E:125:THR:N	1:E:185:ARG:O	2.48	0.40
1:B:127:LEU:HD13	1:B:187:LEU:HD23	2.03	0.40
1:B:236:PRO:HB2	1:B:388:MET:HG3	2.03	0.40
1:B:302:ILE:O	1:B:371:LEU:HA	2.22	0.40
1:B:318:LEU:HB2	1:B:320:LEU:HG	2.03	0.40
2:C:374:PHE:HB3	2:C:378:PHE:CZ	2.56	0.40
1:D:125:THR:HG21	1:D:184:ALA:HA	2.03	0.40
1:D:181:ASN:HB2	1:D:184:ALA:HB2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	381/397 (96%)	357 (94%)	19 (5%)	5 (1%)	9	25
1	B	380/397 (96%)	360 (95%)	19 (5%)	1 (0%)	36	60
1	D	380/397 (96%)	355 (93%)	23 (6%)	2 (0%)	24	48
1	E	380/397 (96%)	351 (92%)	25 (7%)	4 (1%)	11	29
1	F	380/397 (96%)	350 (92%)	26 (7%)	4 (1%)	11	29

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	379/397 (96%)	351 (93%)	26 (7%)	2 (0%)	24	48
All	All	2280/2382 (96%)	2124 (93%)	138 (6%)	18 (1%)	16	37

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	202	PRO
2	C	195	THR
1	D	195	THR
1	E	202	PRO
1	A	198	ASN
1	A	202	PRO
1	E	271	ASP
1	F	87	MET
1	F	202	PRO
1	A	86	TYR
2	C	203	SER
1	E	195	THR
1	F	89	PRO
1	F	268	LEU
1	D	86	TYR
1	E	268	LEU
1	A	84	CYS
1	A	100	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	318/330 (96%)	318 (100%)	0	100	100
1	B	318/330 (96%)	318 (100%)	0	100	100
1	D	318/330 (96%)	318 (100%)	0	100	100
1	E	318/330 (96%)	318 (100%)	0	100	100
1	F	318/330 (96%)	318 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	317/329 (96%)	317 (100%)	0	100	100
All	All	1907/1979 (96%)	1907 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	126	HIS
1	A	161	GLN
1	B	95	GLN
1	B	198	ASN
1	B	239	GLN
2	C	57	GLN
2	C	162	GLN
2	C	245	GLN
2	C	313	GLN
1	D	245	GLN
1	D	258	HIS
1	D	279	ASN
1	D	294	HIS
1	D	297	ASN
1	E	57	GLN
1	E	162	GLN
1	F	198	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	60F	C	164	2	14,17,18	0.92	1 (7%)	13,21,23	1.84	1 (7%)

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	60F	C	164	2	-	4/10/12/14	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	164	60F	C1'-C3	2.08	1.53	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	164	60F	C1'-C3-C2	-6.15	113.47	126.92

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	164	60F	SG-C1-C2-C3
2	C	164	60F	C2'-C1'-C3-C2
2	C	164	60F	C6'-C1'-C3-C2
2	C	164	60F	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	164	60F	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	$\# Z > 2$
3	WCA	B	801	-	58,62,62	2.76	18 (31%)	82,91,91	2.16	21 (25%)
3	WCA	A	801	-	58,62,62	2.77	17 (29%)	82,91,91	1.94	15 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	WCA	B	801	-	-	27/56/72/72	0/4/4/4
3	WCA	A	801	-	-	19/56/72/72	0/4/4/4

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	WCA	O4'-C1'	8.09	1.60	1.42
3	A	801	WCA	PCG-OBN	7.89	1.68	1.59
3	B	801	WCA	O4'-C1'	7.87	1.60	1.42
3	B	801	WCA	PCG-OBN	7.36	1.67	1.59
3	B	801	WCA	O4'-C4'	-6.86	1.29	1.45
3	A	801	WCA	O4'-C4'	-6.79	1.29	1.45
3	A	801	WCA	PCF-OBN	6.59	1.66	1.59
3	B	801	WCA	PCF-OBN	6.18	1.66	1.59
3	B	801	WCA	CBQ-NBH	5.88	1.47	1.33
3	A	801	WCA	CBR-NBI	5.87	1.47	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	801	WCA	CBQ-NBH	5.80	1.47	1.33
3	A	801	WCA	C2'-C1'	-5.75	1.35	1.53
3	B	801	WCA	C2'-C1'	-5.71	1.35	1.53
3	B	801	WCA	CBR-NBI	5.69	1.47	1.33
3	B	801	WCA	PCE-O3'	4.46	1.67	1.59
3	B	801	WCA	C6-N6	3.99	1.44	1.34
3	A	801	WCA	PCE-O3'	3.50	1.65	1.59
3	A	801	WCA	C6-N6	3.47	1.43	1.34
3	B	801	WCA	C5-C4	-3.27	1.33	1.39
3	A	801	WCA	CBD-CCD	3.21	1.57	1.52
3	B	801	WCA	CBD-CCD	3.04	1.57	1.52
3	A	801	WCA	O2'-C2'	2.88	1.50	1.43
3	B	801	WCA	O2'-C2'	2.86	1.50	1.43
3	B	801	WCA	CBT-CAR	2.84	1.55	1.47
3	A	801	WCA	C8-N9	-2.83	1.32	1.37
3	A	801	WCA	OAF-CBR	-2.78	1.18	1.23
3	B	801	WCA	OAF-CBR	-2.72	1.18	1.23
3	A	801	WCA	CBT-CAR	2.66	1.55	1.47
3	A	801	WCA	C4-N9	-2.48	1.32	1.37
3	B	801	WCA	C3'-C4'	2.32	1.58	1.52
3	B	801	WCA	C5-N7	-2.30	1.34	1.39
3	A	801	WCA	PCG-OBK	2.25	1.68	1.59
3	B	801	WCA	PCG-OBK	2.17	1.67	1.59
3	B	801	WCA	PCF-O5'	2.04	1.67	1.59
3	A	801	WCA	O3'-C3'	-2.04	1.37	1.44

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	801	WCA	CBA-SBO-CBP	7.38	108.55	99.85
3	B	801	WCA	CBA-SBO-CBP	7.30	108.45	99.85
3	A	801	WCA	N6-C6-N1	-6.66	103.53	118.38
3	B	801	WCA	N9-C8-N7	-6.56	104.62	113.94
3	A	801	WCA	N3-C2-N1	-6.20	119.19	128.58
3	A	801	WCA	CBT-CAR-CAQ	-5.52	114.86	126.92
3	B	801	WCA	N3-C2-N1	-5.49	120.27	128.58
3	B	801	WCA	N6-C6-N1	-5.31	106.56	118.38
3	B	801	WCA	C5-C4-N3	-5.04	119.77	126.72
3	A	801	WCA	C5-C6-N6	4.60	134.67	123.29
3	B	801	WCA	C5-N7-C8	4.31	110.22	103.45
3	B	801	WCA	C5-C6-N6	4.16	133.59	123.29
3	B	801	WCA	C4-N9-C8	3.80	109.72	105.74

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	801	WCA	CBT-CAR-CAQ	-3.74	118.75	126.92
3	A	801	WCA	C5-C4-N3	-3.47	121.94	126.72
3	B	801	WCA	CBB-CAZ-NBI	-3.43	104.70	112.00
3	A	801	WCA	C2-N3-C4	3.32	119.94	111.83
3	B	801	WCA	C2-N3-C4	3.24	119.75	111.83
3	A	801	WCA	C3'-C2'-C1'	3.19	106.89	99.89
3	B	801	WCA	O4'-C1'-N9	3.17	114.18	108.09
3	B	801	WCA	N3-C4-N9	3.04	132.34	127.17
3	B	801	WCA	C4'-O4'-C1'	-2.88	103.11	109.47
3	B	801	WCA	C4-C5-N7	-2.76	107.43	110.58
3	A	801	WCA	CAZ-CBB-CBQ	-2.71	107.88	112.39
3	B	801	WCA	C3'-C2'-C1'	2.64	105.69	99.89
3	B	801	WCA	C6-C5-C4	2.62	120.75	117.18
3	B	801	WCA	CAB-CCD-CBD	2.58	112.47	108.22
3	A	801	WCA	C2'-C1'-N9	-2.54	107.00	113.30
3	A	801	WCA	C1'-N9-C8	-2.46	121.64	127.09
3	B	801	WCA	CAZ-CBB-CBQ	-2.40	108.40	112.39
3	A	801	WCA	C4-N9-C1'	2.29	131.99	126.63
3	A	801	WCA	CAW-CBT-CAV	2.16	120.86	117.65
3	A	801	WCA	CAB-CCD-CBX	-2.09	105.20	108.77
3	B	801	WCA	CAZ-NBI-CBR	-2.08	118.81	122.55
3	A	801	WCA	N3-C4-N9	2.02	130.61	127.17
3	B	801	WCA	PCE-O3'-C3'	-2.01	118.06	123.43

There are no chirality outliers.

All (46) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	WCA	CAR-CAQ-CBP-OAD
3	A	801	WCA	CAR-CAQ-CBP-SBO
3	A	801	WCA	CAQ-CBP-SBO-CBA
3	A	801	WCA	OAD-CBP-SBO-CBA
3	A	801	WCA	CAY-CBA-SBO-CBP
3	A	801	WCA	NBI-CAZ-CBB-CBQ
3	A	801	WCA	CBD-OBK-PCG-OAP
3	A	801	WCA	CBD-OBK-PCG-OBN
3	A	801	WCA	O4'-C4'-C5'-O5'
3	A	801	WCA	C3'-C4'-C5'-O5'
3	B	801	WCA	CAR-CAQ-CBP-OAD
3	B	801	WCA	CAR-CAQ-CBP-SBO
3	B	801	WCA	CAQ-CBP-SBO-CBA
3	B	801	WCA	OAD-CBP-SBO-CBA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	B	801	WCA	CAY-CBA-SBO-CBP
3	B	801	WCA	NBI-CAZ-CBB-CBQ
3	B	801	WCA	CBR-CBX-CCD-CAA
3	B	801	WCA	CBR-CBX-CCD-CAB
3	B	801	WCA	CBR-CBX-CCD-CBD
3	B	801	WCA	OAK-CBX-CCD-CAA
3	B	801	WCA	OAK-CBX-CCD-CBD
3	B	801	WCA	OBK-CBD-CCD-CBX
3	B	801	WCA	OBK-CBD-CCD-CAA
3	B	801	WCA	OBK-CBD-CCD-CAB
3	B	801	WCA	PCF-OBN-PCG-OBK
3	A	801	WCA	CAQ-CAR-CBT-CAW
3	B	801	WCA	O4'-C4'-C5'-O5'
3	B	801	WCA	C3'-C4'-C5'-O5'
3	A	801	WCA	CAQ-CAR-CBT-CAV
3	A	801	WCA	C2'-C3'-O3'-PCE
3	B	801	WCA	C4'-C3'-O3'-PCE
3	B	801	WCA	C2'-C3'-O3'-PCE
3	B	801	WCA	CAQ-CAR-CBT-CAW
3	A	801	WCA	C4'-C3'-O3'-PCE
3	B	801	WCA	CAQ-CAR-CBT-CAV
3	A	801	WCA	C4'-C5'-O5'-PCF
3	B	801	WCA	OAK-CBX-CCD-CAB
3	A	801	WCA	OAF-CBR-CBX-CCD
3	A	801	WCA	NBI-CBR-CBX-CCD
3	A	801	WCA	PCG-OBN-PCF-OAO
3	B	801	WCA	CBD-OBK-PCG-OAI
3	B	801	WCA	C4'-C5'-O5'-PCF
3	B	801	WCA	PCG-OBN-PCF-OAH
3	A	801	WCA	C3'-O3'-PCE-OAG
3	B	801	WCA	PCG-OBN-PCF-OAO
3	B	801	WCA	CCD-CBD-OBK-PCG

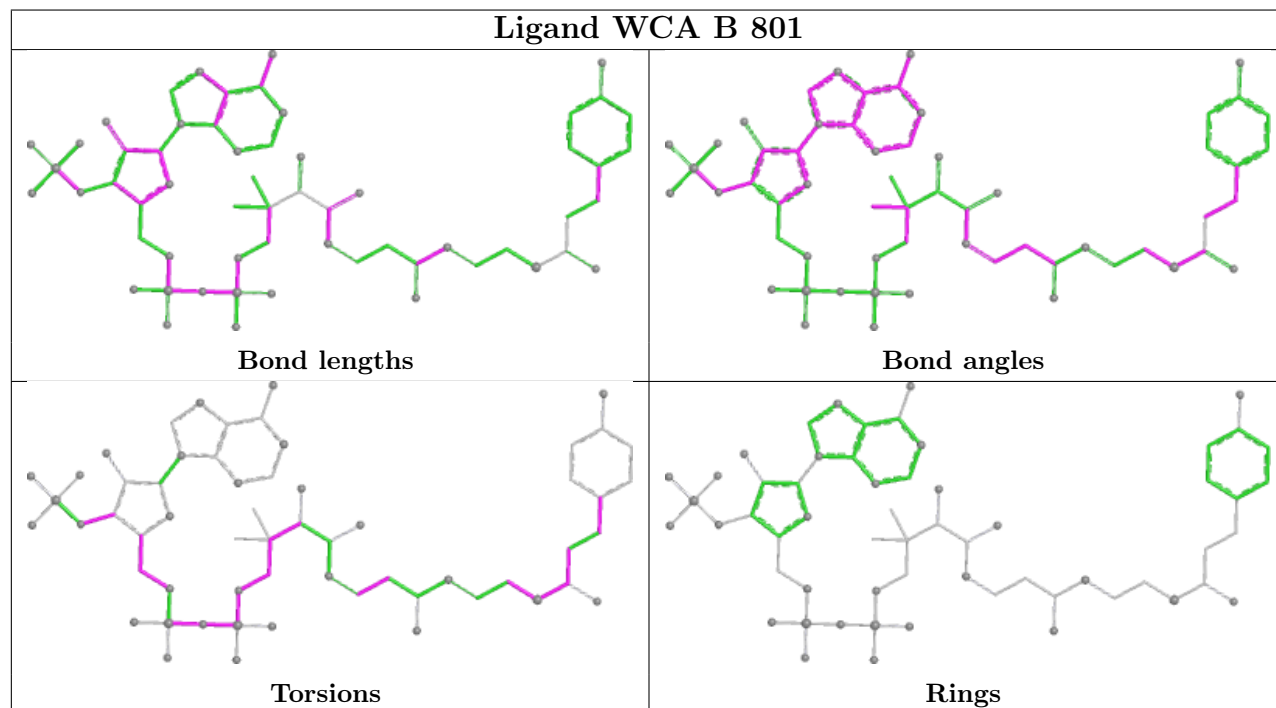
There are no ring outliers.

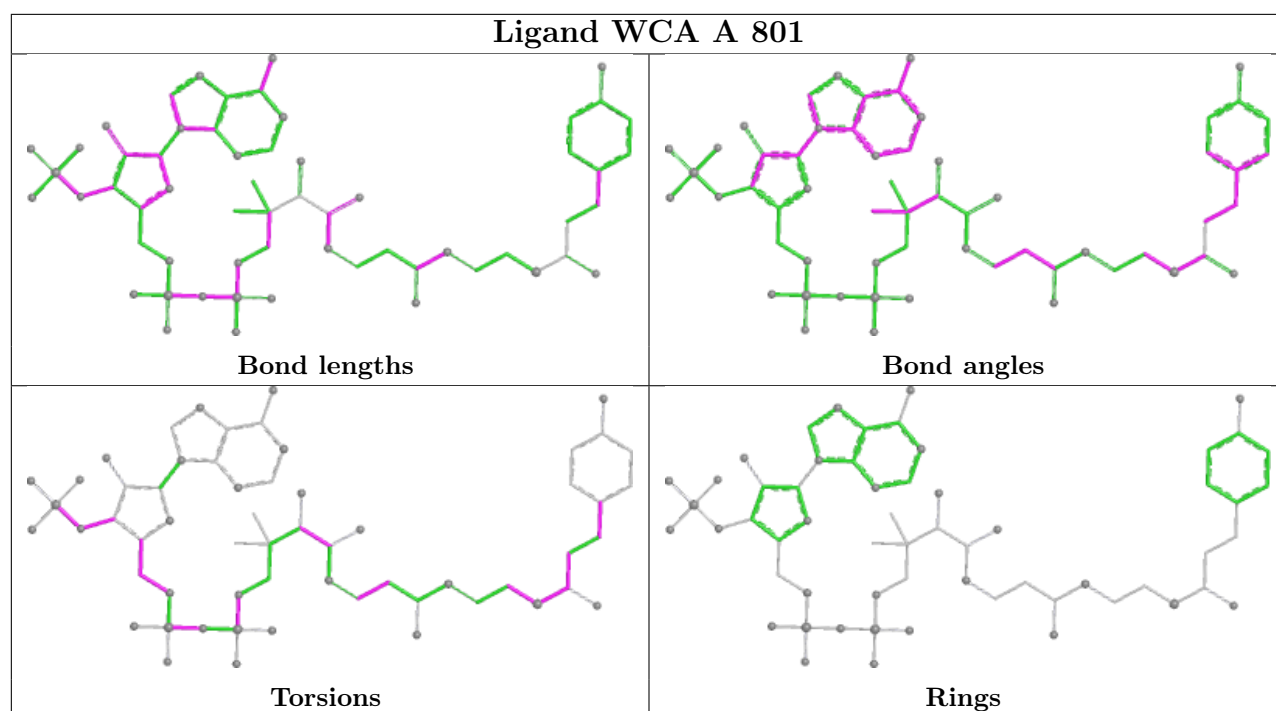
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	801	WCA	2	0
3	A	801	WCA	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	383/397 (96%)	-1.62	0 100 100	23, 35, 54, 72	0
1	B	382/397 (96%)	-1.62	0 100 100	23, 34, 47, 61	0
1	D	382/397 (96%)	-1.62	0 100 100	23, 34, 47, 67	0
1	E	382/397 (96%)	-1.59	0 100 100	26, 38, 49, 66	0
1	F	382/397 (96%)	-1.61	0 100 100	26, 36, 48, 61	0
2	C	381/397 (95%)	-1.61	0 100 100	24, 37, 56, 68	0
All	All	2292/2382 (96%)	-1.61	0 100 100	23, 36, 50, 72	0

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	60F	C	164	17/18	0.99	0.04	32,39,55,60	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

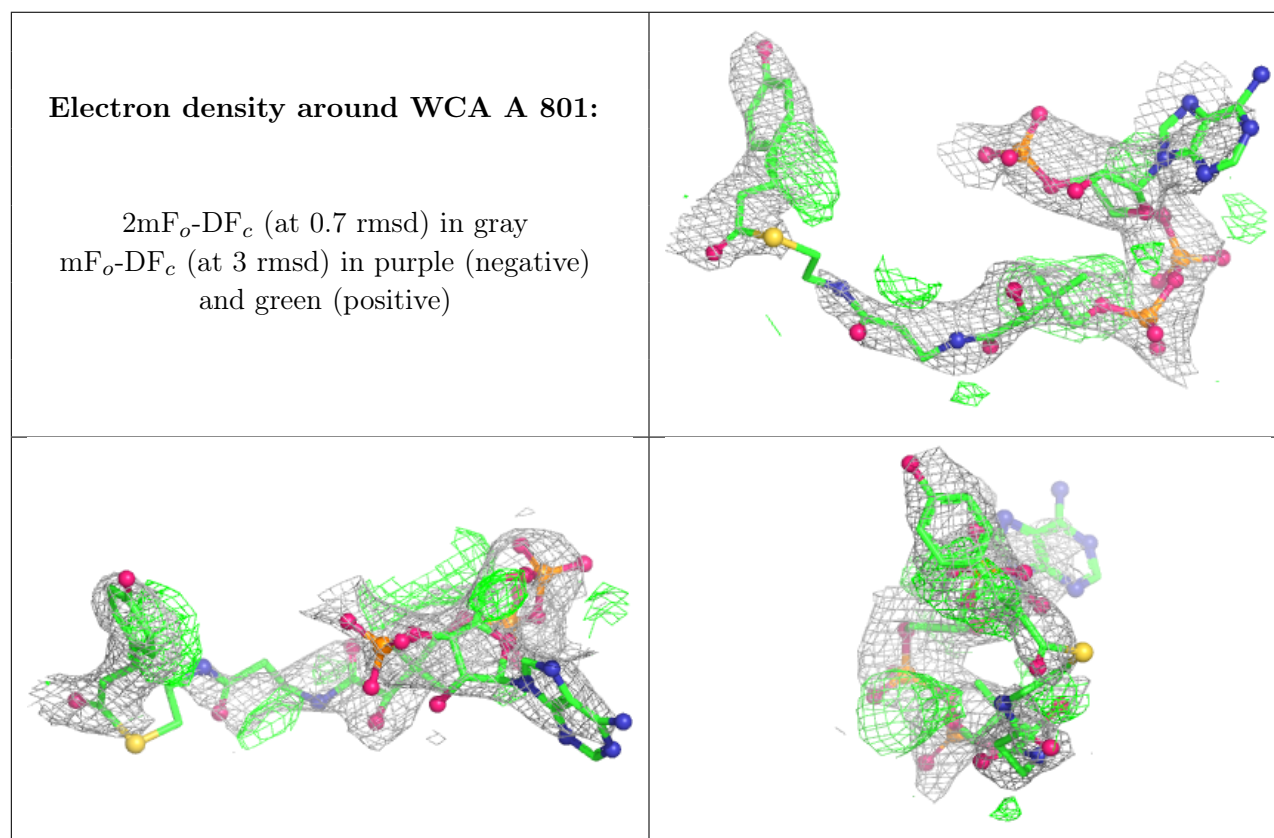
6.4 Ligands [i](#)

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.

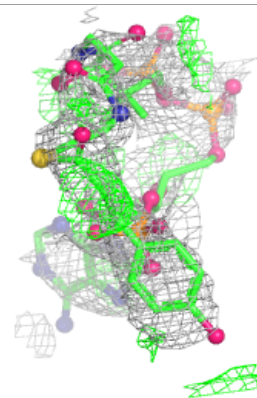
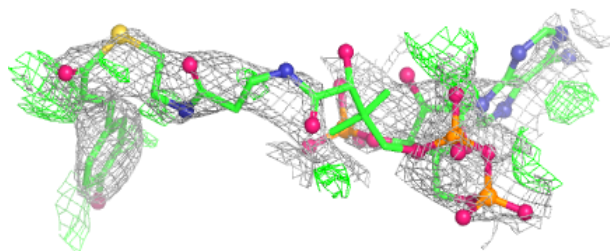
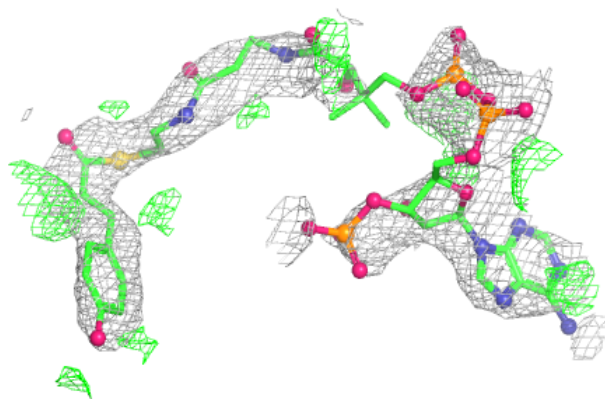
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	WCA	A	801	59/59	0.98	0.07	26,37,46,53	59
3	WCA	B	801	59/59	0.99	0.07	30,43,54,57	59

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 WCA B 801:

$2mF_o - DF_c$ (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.