



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:35 AM EDT

PDB ID : 2D0V / pdb_00002d0v
Title : Crystal structure of methanol dehydrogenase from *Hyphomicrobium denitrificans*
Authors : Nojiri, M.; Hira, D.; Yamaguchi, K.; Suzuki, S.
Deposited on : 2005-08-09
Resolution : 2.49 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

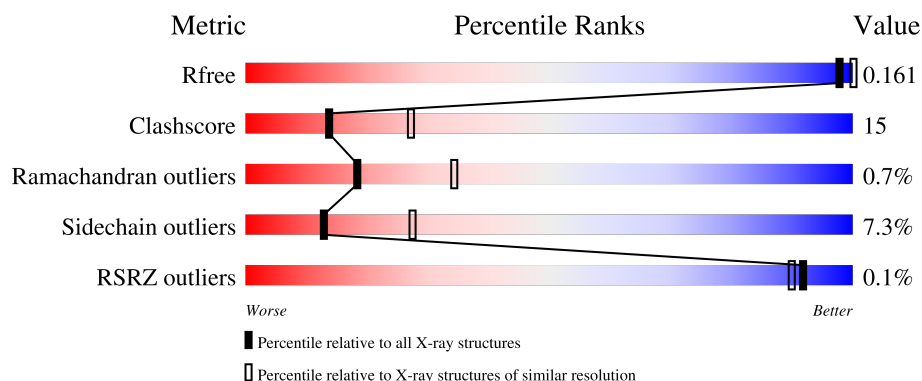
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.49 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	597	67% 28% 5%
1	D	597	64% 31% .
1	I	597	64% 29% 6%
2	B	72	65% 24% 8% .
2	E	72	% 51% 36% 7% 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	J	72	44% 40% 10%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16491 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 methanol dehydrogenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	597	Total	C	N	O	S	0	0	0
			4668	2962	797	889	20			
1	D	597	Total	C	N	O	S	0	0	0
			4668	2962	797	889	20			
1	I	595	Total	C	N	O	S	0	0	0
			4655	2954	794	887	20			

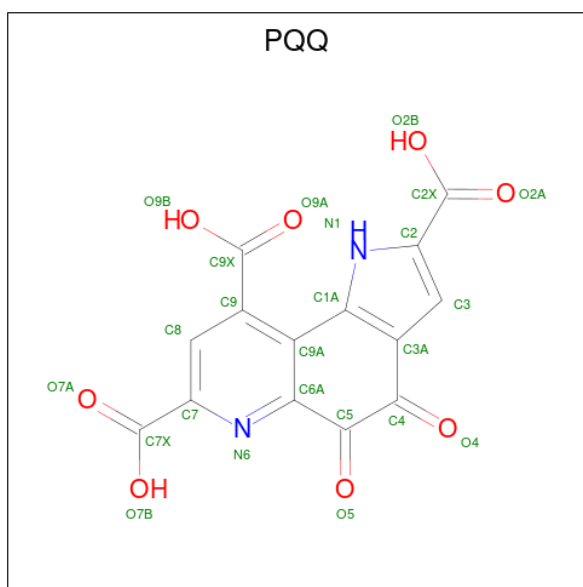
- Molecule 2 is a protein called methanol dehydrogenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	70	Total	C	N	O	S	0	0	0
			572	359	105	106	2			
2	E	68	Total	C	N	O	S	0	0	0
			554	347	101	104	2			
2	J	70	Total	C	N	O	S	0	0	0
			572	359	105	106	2			

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	I	1	Total	Ca	0	0
			1	1		

- Molecule 4 is PYRROLOQUINOLINE QUINONE (CCD ID: PQQ) (formula: C₁₄H₆N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			24	14	2	8		
4	D	1	Total	C	N	O	0	0
			24	14	2	8		
4	I	1	Total	C	N	O	0	0
			24	14	2	8		

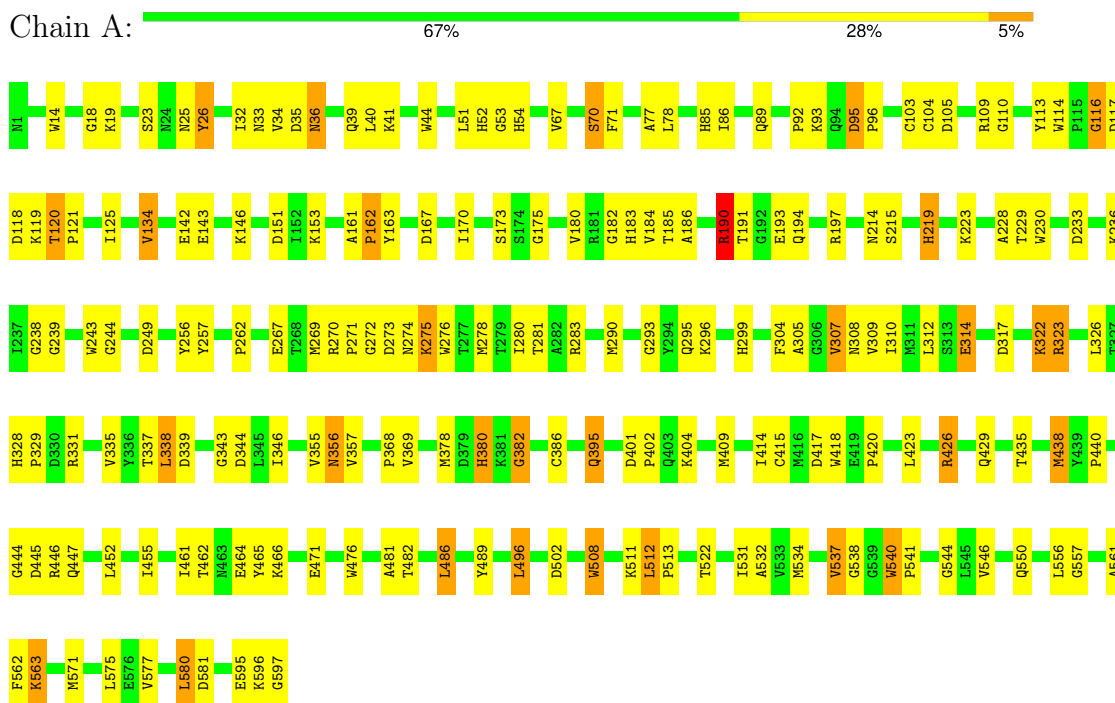
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	278	Total	O	0	0
			278	278		
5	B	31	Total	O	0	0
			31	31		
5	D	188	Total	O	0	0
			188	188		
5	E	31	Total	O	0	0
			31	31		
5	I	171	Total	O	0	0
			171	171		
5	J	28	Total	O	0	0
			28	28		

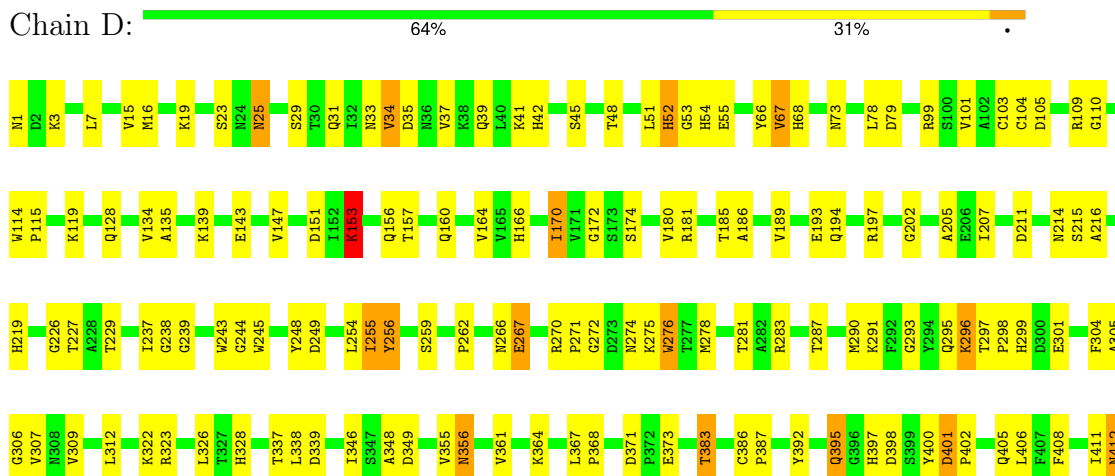
3 Residue-property plots

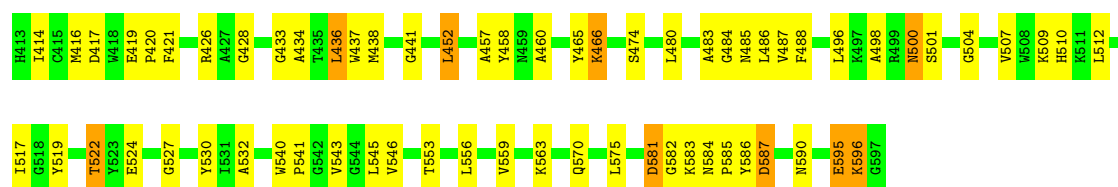
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: methanol dehydrogenase large subunit

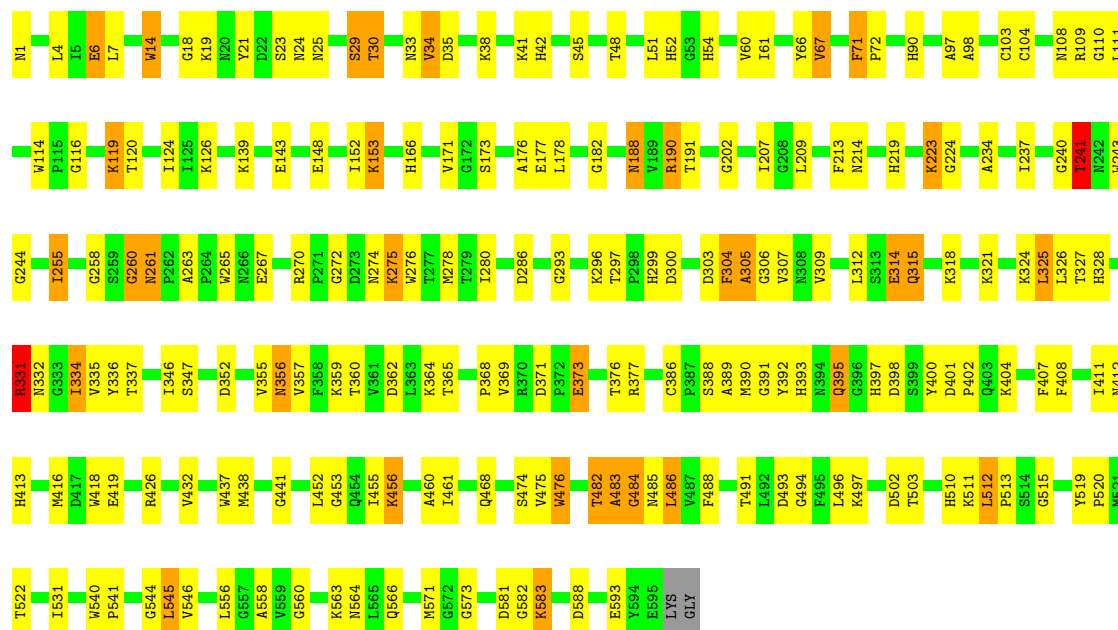


- Molecule 1: methanol dehydrogenase large subunit

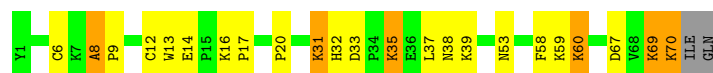




- Molecule 1: methanol dehydrogenase large subunit



- Molecule 2: methanol dehydrogenase small subunit



- Molecule 2: methanol dehydrogenase small subunit



- Molecule 2: methanol dehydrogenase small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	291.32Å 64.00Å 109.94Å 90.00° 105.74° 90.00°	Depositor
Resolution (Å)	44.60 – 2.49 44.60 – 2.49	Depositor EDS
% Data completeness (in resolution range)	99.6 (44.60-2.49) 95.4 (44.60-2.49)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 2.48Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.149 , 0.247 0.162 , 0.161	Depositor DCC
R_{free} test set	6603 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å ²)	31.6	Xtriage
Anisotropy	0.561	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16491	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.55	35/4803 (0.7%)	1.43	34/6534 (0.5%)
1	D	1.52	22/4803 (0.5%)	1.45	37/6534 (0.6%)
1	I	1.48	31/4790 (0.6%)	1.41	39/6518 (0.6%)
2	B	1.50	3/589 (0.5%)	1.50	2/789 (0.3%)
2	E	1.39	0/571	1.56	9/767 (1.2%)
2	J	1.44	4/589 (0.7%)	1.50	11/789 (1.4%)
All	All	1.51	95/16145 (0.6%)	1.44	132/21931 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	1

All (95) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	348	ALA	CA-CB	8.70	1.63	1.52
1	A	276	TRP	N-CA	-8.07	1.36	1.46
1	I	260	GLY	N-CA	7.50	1.51	1.44
1	A	32	ILE	CA-CB	7.35	1.63	1.54
1	A	116	GLY	N-CA	7.20	1.55	1.45
1	A	163	TYR	C-O	-7.15	1.15	1.23
1	A	86	ILE	C-O	6.90	1.31	1.23
1	D	39	GLN	CG-CD	6.86	1.69	1.52
1	D	164	VAL	CA-CB	6.84	1.62	1.54
1	A	113	TYR	C-O	6.74	1.31	1.23
2	J	41	VAL	CA-CB	6.62	1.61	1.54
1	A	531	ILE	C-O	6.58	1.30	1.24

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	124	ILE	CA-CB	6.55	1.62	1.54
1	D	259	SER	C-O	6.54	1.31	1.23
1	D	346	ILE	CA-C	6.49	1.61	1.52
1	A	307	VAL	CA-CB	-6.34	1.45	1.54
1	A	537	VAL	CA-CB	-6.27	1.47	1.54
1	D	67	VAL	CA-CB	6.09	1.62	1.54
1	I	331	ARG	CA-C	6.05	1.60	1.52
2	J	48	GLU	CA-C	-5.97	1.45	1.52
1	A	522	THR	C-O	5.94	1.31	1.23
1	I	369	VAL	CA-CB	5.93	1.60	1.53
1	A	85	HIS	N-CA	5.93	1.53	1.46
1	D	546	VAL	CA-CB	5.89	1.61	1.54
1	D	546	VAL	C-O	-5.84	1.17	1.24
1	I	475	VAL	CA-CB	-5.82	1.47	1.53
1	A	271	PRO	CA-C	5.82	1.59	1.52
1	A	338	LEU	C-O	5.79	1.31	1.23
1	A	508	TRP	N-CA	5.77	1.53	1.46
1	I	364	LYS	C-O	-5.75	1.18	1.23
1	A	380	HIS	CA-C	-5.74	1.45	1.52
1	A	77	ALA	N-CA	5.71	1.53	1.46
1	I	389	ALA	CA-CB	-5.67	1.44	1.53
1	D	66	TYR	C-O	5.67	1.30	1.24
1	A	382	GLY	C-O	5.63	1.29	1.23
1	D	559	VAL	C-O	-5.60	1.17	1.24
1	A	446	ARG	CG-CD	-5.59	1.35	1.52
1	A	36	ASN	CA-C	5.57	1.59	1.52
1	I	30	THR	CA-CB	5.55	1.62	1.54
2	B	58	PHE	CA-C	5.54	1.59	1.52
1	I	71	PHE	CA-C	-5.53	1.47	1.53
2	J	9	PRO	CA-C	5.50	1.59	1.52
2	B	8	ALA	N-CA	5.50	1.53	1.46
1	D	101	VAL	CA-CB	5.49	1.60	1.54
1	A	228	ALA	CA-CB	5.44	1.62	1.53
1	I	305	ALA	CA-C	5.43	1.59	1.52
1	D	412	ASN	CA-C	5.43	1.59	1.52
2	J	23	ILE	CA-CB	5.42	1.61	1.54
1	I	45	SER	CA-C	-5.39	1.46	1.52
1	A	481	ALA	N-CA	5.38	1.52	1.46
1	D	355	VAL	CA-CB	5.32	1.59	1.54
1	I	581	ASP	CA-CB	5.31	1.61	1.53
1	D	267	GLU	CA-C	5.31	1.59	1.52
1	I	297	THR	CA-CB	5.29	1.60	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	26	TYR	CA-C	5.29	1.59	1.52
1	I	419	GLU	C-N	5.28	1.40	1.33
1	I	126	LYS	C-O	5.27	1.30	1.23
1	A	314	GLU	CA-C	5.26	1.59	1.52
1	A	162	PRO	CA-C	-5.25	1.45	1.52
1	A	184	VAL	CA-CB	5.25	1.61	1.54
1	D	296	LYS	N-CA	5.25	1.52	1.46
1	I	276	TRP	N-CA	-5.23	1.40	1.46
1	D	143	GLU	CG-CD	5.23	1.65	1.52
1	I	368	PRO	N-CA	-5.22	1.41	1.47
1	I	108	ASN	CA-C	-5.21	1.46	1.52
1	I	148	GLU	CA-C	-5.18	1.46	1.52
1	A	161	ALA	CA-CB	-5.18	1.45	1.53
1	A	170	ILE	CA-CB	5.18	1.61	1.54
1	I	304	PHE	CA-C	5.17	1.59	1.52
1	I	314	GLU	CG-CD	5.17	1.65	1.52
1	I	522	THR	C-O	-5.16	1.17	1.23
1	D	355	VAL	N-CA	5.15	1.52	1.46
1	I	66	TYR	CA-C	-5.15	1.46	1.52
1	I	503	THR	N-CA	5.14	1.52	1.45
1	A	581	ASP	CB-CG	5.14	1.65	1.52
1	D	135	ALA	CA-CB	-5.14	1.46	1.53
1	I	280	ILE	N-CA	-5.13	1.40	1.46
1	D	570	GLN	CA-C	5.12	1.60	1.53
1	A	134	VAL	N-CA	-5.11	1.40	1.46
1	I	171	VAL	C-O	5.11	1.29	1.23
1	D	256	TYR	C-O	5.09	1.30	1.23
1	A	435	THR	CA-C	-5.09	1.46	1.52
1	A	369	VAL	CA-CB	5.09	1.60	1.54
1	I	360	THR	CA-CB	5.08	1.61	1.53
1	I	29	SER	C-O	5.07	1.30	1.24
1	A	540	TRP	N-CA	-5.07	1.41	1.46
1	D	522	THR	N-CA	5.06	1.52	1.46
1	I	484	GLY	C-O	-5.04	1.20	1.24
1	I	482	THR	N-CA	5.03	1.52	1.45
1	D	216	ALA	CA-C	5.02	1.59	1.52
1	A	465	TYR	CA-C	-5.02	1.46	1.52
2	B	20	PRO	CA-C	-5.02	1.47	1.52
1	A	182	GLY	C-O	5.02	1.28	1.23
1	I	346	ILE	CA-C	5.02	1.59	1.52
1	A	511	LYS	N-CA	-5.01	1.40	1.46

All (132) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	275	LYS	CA-C-N	10.85	142.25	121.54
1	D	275	LYS	C-N-CA	10.85	142.25	121.54
2	E	29	ASP	CA-C-N	10.59	130.26	119.56
2	E	29	ASP	C-N-CA	10.59	130.26	119.56
1	A	276	TRP	CB-CA-C	9.71	124.04	110.06
1	D	275	LYS	N-CA-C	9.58	122.98	110.43
1	A	275	LYS	CA-C-N	9.44	143.15	126.45
1	A	275	LYS	C-N-CA	9.44	143.15	126.45
1	I	120	THR	CA-C-N	-8.86	111.26	120.03
1	I	120	THR	C-N-CA	-8.86	111.26	120.03
2	B	14	GLU	CA-C-N	-8.32	112.22	120.21
2	B	14	GLU	C-N-CA	-8.32	112.22	120.21
1	A	346	ILE	N-CA-C	8.01	119.28	111.67
1	D	401	ASP	CA-C-N	7.91	129.73	119.84
1	D	401	ASP	C-N-CA	7.91	129.73	119.84
1	A	275	LYS	N-CA-C	7.82	120.41	110.24
1	I	419	GLU	CA-C-N	7.81	128.25	120.52
1	I	419	GLU	C-N-CA	7.81	128.25	120.52
1	D	437	TRP	N-CA-C	-7.78	95.61	108.76
1	D	466	LYS	N-CA-C	-7.10	103.47	111.14
1	A	275	LYS	O-C-N	7.05	131.85	122.82
1	I	176	ALA	N-CA-C	-7.04	103.79	112.38
1	I	476	TRP	N-CA-C	-7.01	105.26	113.88
2	E	67	ASP	N-CA-C	6.99	125.68	110.80
1	I	178	LEU	N-CA-C	-6.98	101.93	111.56
1	I	14	TRP	N-CA-C	-6.90	95.46	107.20
1	A	95	ASP	CA-C-N	-6.88	112.82	120.45
1	A	95	ASP	C-N-CA	-6.88	112.82	120.45
1	I	110	GLY	N-CA-C	6.87	120.10	111.85
1	D	275	LYS	O-C-N	6.84	130.76	122.75
1	I	564	ASN	N-CA-C	6.81	121.42	113.18
1	I	255	ILE	CB-CA-C	-6.79	101.91	111.21
1	I	67	VAL	CB-CA-C	6.77	121.52	110.69
1	D	255	ILE	CB-CA-C	-6.76	100.07	110.95
1	D	16	MET	N-CA-C	6.72	114.27	108.22
1	I	275	LYS	O-C-N	6.71	130.50	122.85
1	I	275	LYS	CA-C-N	6.68	135.00	123.91
1	I	275	LYS	C-N-CA	6.68	135.00	123.91
1	A	110	GLY	N-CA-C	6.68	119.31	111.63
1	I	276	TRP	N-CA-C	6.65	121.16	113.38
1	I	544	GLY	N-CA-C	-6.65	104.45	112.49
1	I	359	LYS	N-CA-C	-6.55	104.07	111.07
1	D	483	ALA	N-CA-C	-6.54	104.56	112.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	519	TYR	CA-C-N	-6.54	113.25	119.85
1	D	519	TYR	C-N-CA	-6.54	113.25	119.85
1	D	553	THR	N-CA-C	-6.45	105.04	113.17
1	D	287	THR	N-CA-C	-6.38	105.63	113.41
2	J	36	GLU	N-CA-C	6.36	117.90	110.97
1	A	544	GLY	N-CA-C	-6.34	104.65	112.77
2	E	38	ASN	N-CA-C	6.30	120.97	113.16
1	A	563	LYS	N-CA-C	-6.28	104.48	111.71
2	J	64	TRP	CA-C-N	-6.28	114.96	123.12
2	J	64	TRP	C-N-CA	-6.28	114.96	123.12
1	A	190	ARG	NE-CZ-NH2	-6.25	113.57	119.20
1	A	161	ALA	CA-C-N	-6.17	112.13	119.84
1	A	161	ALA	C-N-CA	-6.17	112.13	119.84
1	D	227	THR	N-CA-C	-6.16	105.67	113.43
1	I	581	ASP	N-CA-C	-6.15	104.37	112.24
1	A	446	ARG	NE-CZ-NH1	-6.11	115.39	121.50
1	D	48	THR	N-CA-C	-6.04	105.40	112.89
1	I	275	LYS	N-CA-C	6.04	118.70	110.55
1	A	415	CYS	CA-CB-SG	-6.02	100.55	114.40
1	I	519	TYR	CA-C-N	5.98	125.74	119.76
1	I	519	TYR	C-N-CA	5.98	125.74	119.76
1	I	38	LYS	N-CA-C	-5.95	105.29	112.54
1	D	441	GLY	CA-C-N	5.89	127.20	119.84
1	D	441	GLY	C-N-CA	5.89	127.20	119.84
1	I	456	LYS	N-CA-C	5.88	119.06	109.24
1	I	461	ILE	N-CA-C	5.87	117.39	111.00
1	A	409	MET	N-CA-C	5.85	118.49	109.07
1	A	307	VAL	CB-CA-C	-5.83	103.90	111.88
1	A	531	ILE	N-CA-C	-5.80	99.77	108.12
1	I	276	TRP	CB-CA-C	5.79	120.67	111.23
1	D	559	VAL	N-CA-C	5.77	116.42	110.36
1	A	215	SER	N-CA-C	-5.72	105.02	112.23
1	A	339	ASP	N-CA-C	-5.72	101.44	109.96
1	I	482	THR	N-CA-C	5.72	118.53	109.50
1	A	563	LYS	CB-CG-CD	5.59	124.15	111.30
2	E	21	GLU	N-CA-C	-5.55	106.35	113.23
1	I	324	LYS	CD-CE-NZ	5.55	129.66	111.90
2	J	8	ALA	CA-C-N	-5.55	114.07	119.90
2	J	8	ALA	C-N-CA	-5.55	114.07	119.90
2	J	66	TYR	N-CA-C	5.53	117.11	111.14
1	I	224	GLY	N-CA-C	5.53	123.26	115.30
1	D	52	HIS	CA-C-N	-5.51	114.69	120.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	52	HIS	C-N-CA	-5.51	114.69	120.31
2	J	19	PHE	CA-C-N	5.49	125.44	119.78
2	J	19	PHE	C-N-CA	5.49	125.44	119.78
1	I	437	TRP	CA-C-N	-5.48	113.22	123.03
1	I	437	TRP	C-N-CA	-5.48	113.22	123.03
1	A	269	MET	CA-C-N	-5.46	117.29	122.37
1	A	269	MET	C-N-CA	-5.46	117.29	122.37
1	A	35	ASP	N-CA-C	5.45	119.19	112.54
1	D	487	VAL	N-CA-C	-5.45	99.71	107.77
1	A	116	GLY	N-CA-C	5.43	121.43	112.30
1	A	446	ARG	N-CA-C	5.35	117.86	111.71
1	D	416	MET	N-CA-C	5.34	116.96	108.79
1	A	346	ILE	CB-CA-C	-5.32	105.52	111.80
1	D	346	ILE	N-CA-C	5.31	117.21	111.58
1	D	147	VAL	N-CA-C	5.29	117.18	108.97
1	I	21	TYR	N-CA-C	5.27	117.94	111.82
1	I	241	THR	N-CA-C	-5.26	103.09	110.50
1	D	452	LEU	CA-CB-CG	5.24	134.65	116.30
1	A	308	ASN	N-CA-C	5.22	116.83	110.41
1	I	255	ILE	N-CA-CB	5.21	117.75	110.56
1	A	423	LEU	CA-C-N	-5.20	115.21	120.31
1	A	423	LEU	C-N-CA	-5.20	115.21	120.31
1	D	156	GLN	N-CA-C	5.20	118.10	109.46
1	D	73	ASN	N-CA-C	5.20	118.80	111.52
2	E	32	HIS	N-CA-C	5.18	118.38	110.20
1	D	79	ASP	N-CA-C	5.16	116.71	108.41
1	D	504	GLY	N-CA-C	-5.16	107.93	115.72
2	J	29	ASP	CA-C-N	5.15	124.46	118.85
2	J	29	ASP	C-N-CA	5.15	124.46	118.85
2	E	7	LYS	N-CA-C	-5.12	106.14	112.38
1	I	452	LEU	CA-CB-CG	5.12	134.20	116.30
1	A	446	ARG	CA-CB-CG	-5.11	103.89	114.10
1	D	153	LYS	N-CA-C	5.10	117.57	111.71
1	A	26	TYR	N-CA-C	5.08	117.25	109.07
1	D	295	GLN	CA-C-N	5.07	127.32	120.38
1	D	295	GLN	C-N-CA	5.07	127.32	120.38
1	I	190	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	I	503	THR	N-CA-C	5.06	120.45	113.97
1	D	297	THR	CA-C-N	-5.06	114.55	119.76
1	D	297	THR	C-N-CA	-5.06	114.55	119.76
1	I	191	THR	CB-CA-C	-5.05	101.07	109.75
1	A	444	GLY	N-CA-C	-5.03	105.86	112.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	45	LYS	CB-CA-C	5.03	119.40	110.85
2	E	19	PHE	CA-C-N	5.02	125.49	120.52
2	E	19	PHE	C-N-CA	5.02	125.49	120.52
1	I	286	ASP	N-CA-C	5.00	118.54	112.23
1	D	500	ASN	N-CA-C	-5.00	101.81	109.76

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	276	TRP	CA

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ARG	Sidechain

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	4668	0	4426	123	0
1	D	4668	0	4426	116	0
1	I	4655	0	4410	151	0
2	B	572	0	553	20	0
2	E	554	0	527	24	0
2	J	572	0	553	25	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
3	I	1	0	0	0	0
4	A	24	0	3	5	0
4	D	24	0	3	5	0
4	I	24	0	3	4	0
5	A	278	0	0	15	0
5	B	31	0	0	2	0
5	D	188	0	0	10	0
5	E	31	0	0	3	0
5	I	171	0	0	13	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	J	28	0	0	1	0
All	All	16491	0	14904	446	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 15.

All (446) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:GLN:HG3	5:A:903:HOH:O	1.63	0.97
2:J:69:LYS:C	2:J:70:LYS:HD3	1.99	0.87
1:I:314:GLU:HG2	5:I:942:HOH:O	1.74	0.87
1:D:211:ASP:HB3	5:D:793:HOH:O	1.74	0.86
1:I:540:TRP:CZ3	4:I:601:PQQ:O4	2.32	0.83
1:A:278:MET:HE1	1:A:304:PHE:C	2.03	0.83
1:A:51:LEU:O	1:A:52:HIS:HB2	1.78	0.83
1:A:447:GLN:CG	5:A:903:HOH:O	2.25	0.82
1:A:143:GLU:HG3	5:A:816:HOH:O	1.79	0.81
1:D:510:HIS:HE1	1:I:42:HIS:ND1	1.79	0.80
5:A:790:HOH:O	2:B:32:HIS:HD2	1.64	0.80
1:I:540:TRP:CE3	4:I:601:PQQ:O4	2.35	0.79
1:A:356:ASN:HD21	1:A:386:CYS:H	1.29	0.79
1:D:484:GLY:O	1:D:485:ASN:HB2	1.82	0.79
1:I:482:THR:C	1:I:484:GLY:H	1.89	0.78
5:A:847:HOH:O	2:B:32:HIS:HE1	1.67	0.77
1:D:540:TRP:CZ3	4:D:601:PQQ:O4	2.37	0.77
2:J:21:GLU:HB2	5:J:118:HOH:O	1.85	0.77
1:A:52:HIS:O	1:A:54:HIS:HD2	1.67	0.76
1:I:583:LYS:HB2	1:I:583:LYS:NZ	2.01	0.76
5:D:797:HOH:O	2:E:32:HIS:HD2	1.68	0.76
1:I:314:GLU:CG	5:I:942:HOH:O	2.33	0.76
1:A:191:THR:OG1	1:A:193:GLU:HB2	1.86	0.75
1:D:109:ARG:HE	1:D:395:GLN:HE21	1.33	0.75
1:I:314:GLU:HB3	5:I:942:HOH:O	1.86	0.74
1:A:134:VAL:HG22	1:A:146:LYS:HG3	1.69	0.73
1:D:532:ALA:HB1	1:D:575:LEU:HD11	1.70	0.73
2:E:36:GLU:O	2:E:39:LYS:HG3	1.88	0.73
1:I:109:ARG:HE	1:I:395:GLN:HE21	1.37	0.73
1:D:584:ASN:HB2	1:D:585:PRO:HD2	1.71	0.72
1:I:296:LYS:NZ	1:I:328:HIS:HE1	1.88	0.72
2:J:69:LYS:C	2:J:70:LYS:CD	2.63	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:11:ASN:C	2:E:11:ASN:HD22	1.98	0.71
1:A:33:ASN:HA	1:A:486:LEU:HD22	1.72	0.71
1:I:261:ASN:H	1:I:305:ALA:HA	1.54	0.71
1:A:595:GLU:O	1:A:597:GLY:N	2.22	0.70
1:A:323:ARG:HH11	1:A:323:ARG:HG2	1.56	0.70
1:D:540:TRP:CE3	4:D:601:PQQ:O4	2.44	0.70
1:I:34:VAL:HG22	1:I:486:LEU:HD13	1.72	0.70
1:D:214:ASN:HD21	1:D:293:GLY:H	1.39	0.69
1:I:260:GLY:HA2	1:I:306:GLY:H	1.56	0.69
1:I:356:ASN:C	1:I:356:ASN:HD22	2.00	0.69
1:A:540:TRP:CE3	4:A:601:PQQ:O4	2.45	0.69
1:A:595:GLU:C	1:A:597:GLY:H	2.01	0.69
1:D:219:HIS:HE1	5:D:795:HOH:O	1.75	0.68
1:I:240:GLY:HA2	1:I:260:GLY:O	1.93	0.68
2:J:20:PRO:HB2	2:J:22:LYS:O	1.94	0.68
1:I:30:THR:HG22	1:I:483:ALA:O	1.93	0.67
1:I:371:ASP:OD2	1:I:373:GLU:HB2	1.95	0.67
1:I:152:ILE:HG23	5:I:826:HOH:O	1.94	0.67
1:A:18:GLY:HA2	1:A:25:ASN:HD21	1.60	0.66
1:A:243:TRP:CZ2	4:A:601:PQQ:C6A	2.78	0.66
1:A:356:ASN:ND2	1:A:386:CYS:H	1.93	0.66
1:I:388:SER:HA	1:I:416:MET:HE2	1.78	0.66
2:B:60:LYS:HB2	2:B:60:LYS:NZ	2.11	0.66
1:I:314:GLU:CB	5:I:942:HOH:O	2.43	0.66
1:D:595:GLU:O	1:D:596:LYS:HB2	1.95	0.65
1:A:219:HIS:H	1:A:219:HIS:CD2	2.14	0.65
1:A:426:ARG:HB3	1:A:429:GLN:HG3	1.78	0.65
1:D:510:HIS:CE1	1:I:42:HIS:ND1	2.64	0.65
1:A:438:MET:HB2	1:A:561:ALA:HB2	1.80	0.64
2:B:33:ASP:OD2	2:B:35:LYS:HG2	1.96	0.64
1:D:397:HIS:HD2	1:D:398:ASP:O	1.80	0.64
1:A:309:VAL:O	1:A:328:HIS:HD2	1.80	0.64
1:D:590:ASN:O	1:D:596:LYS:HG2	1.98	0.64
1:I:267:GLU:OE2	1:I:299:HIS:HE1	1.81	0.63
2:B:35:LYS:NZ	2:B:35:LYS:HB3	2.14	0.63
1:D:41:LYS:HB2	1:D:582:GLY:N	2.14	0.63
1:I:237:ILE:O	1:I:237:ILE:HG13	1.97	0.63
1:D:243:TRP:CZ2	4:D:601:PQQ:C6A	2.83	0.62
1:I:52:HIS:O	1:I:54:HIS:HD2	1.82	0.62
1:D:229:THR:O	1:D:272:GLY:HA3	1.99	0.62
1:D:436:LEU:CD2	1:D:438:MET:HE2	2.30	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:LYS:NZ	1:A:502:ASP:OD1	2.33	0.62
1:A:512:LEU:HB3	1:A:513:PRO:HD2	1.81	0.62
1:A:323:ARG:HH11	1:A:323:ARG:CG	2.12	0.62
1:I:188:ASN:HB2	5:I:925:HOH:O	1.98	0.61
1:A:143:GLU:CG	5:A:816:HOH:O	2.45	0.61
1:I:177:GLU:HB2	5:I:926:HOH:O	2.00	0.61
1:I:14:TRP:CH2	1:I:19:LYS:HB2	2.36	0.61
2:J:70:LYS:HD3	2:J:70:LYS:N	2.15	0.61
1:A:14:TRP:CZ2	1:A:19:LYS:HB2	2.36	0.60
1:A:238:GLY:O	1:A:262:PRO:HA	2.01	0.60
1:A:44:TRP:CZ2	1:A:577:VAL:HG21	2.36	0.60
1:D:270:ARG:HH21	1:D:274:ASN:ND2	1.99	0.60
1:A:52:HIS:O	1:A:54:HIS:CD2	2.54	0.60
1:D:326:LEU:O	1:D:337:THR:HG23	2.02	0.59
1:A:14:TRP:CE3	1:A:19:LYS:HG3	2.37	0.59
2:J:23:ILE:CD1	2:J:30:PRO:HD3	2.32	0.59
1:D:194:GLN:NE2	5:D:881:HOH:O	2.32	0.59
1:D:215:SER:HA	5:D:890:HOH:O	2.03	0.59
1:I:14:TRP:CZ2	1:I:19:LYS:HB2	2.37	0.59
1:I:391:GLY:O	1:I:412:ASN:HB2	2.02	0.59
1:I:393:HIS:NE2	1:I:398:ASP:OD2	2.30	0.59
1:A:51:LEU:O	1:A:52:HIS:CB	2.50	0.58
1:A:496:LEU:HD13	1:A:508:TRP:HZ3	1.68	0.58
1:A:19:LYS:HE3	1:A:26:TYR:O	2.03	0.58
1:I:335:VAL:O	1:I:335:VAL:HG13	2.03	0.58
1:I:390:MET:HE3	1:I:558:ALA:HB2	1.86	0.58
1:I:356:ASN:ND2	1:I:386:CYS:H	2.00	0.58
1:I:356:ASN:HD21	1:I:386:CYS:H	1.51	0.58
1:A:236:LYS:NZ	2:B:38:ASN:HD21	2.01	0.58
1:I:24:ASN:O	1:I:25:ASN:C	2.47	0.57
1:D:41:LYS:HG2	1:D:581:ASP:HA	1.86	0.57
2:E:57:HIS:HE1	2:E:63:LYS:NZ	2.03	0.57
1:A:18:GLY:HA2	1:A:25:ASN:ND2	2.19	0.57
1:D:42:HIS:ND1	1:I:510:HIS:HE1	2.01	0.57
1:D:296:LYS:HZ1	1:D:306:GLY:HA3	1.69	0.57
1:A:219:HIS:H	1:A:219:HIS:HD2	1.53	0.57
1:D:170:ILE:HD13	1:D:186:ALA:HB2	1.87	0.57
1:D:205:ALA:HA	5:D:913:HOH:O	2.04	0.57
1:D:436:LEU:HD22	1:D:438:MET:HE2	1.87	0.57
1:I:296:LYS:HZ3	1:I:328:HIS:HE1	1.52	0.56
1:I:352:ASP:O	1:I:355:VAL:HG23	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:249:ASP:OD2	1:D:249:ASP:C	2.48	0.56
1:I:583:LYS:HB2	1:I:583:LYS:HZ2	1.68	0.56
1:A:92:PRO:HA	5:A:984:HOH:O	2.04	0.56
1:A:314:GLU:HG2	1:A:322:LYS:HD2	1.86	0.56
1:D:457:ALA:O	1:D:465:TYR:HA	2.06	0.56
2:J:1:TYR:CD1	2:J:14:GLU:HG2	2.41	0.56
1:D:31:GLN:NE2	1:D:527:GLY:O	2.30	0.56
1:D:584:ASN:O	1:D:587:ASP:HB2	2.05	0.56
2:J:16:LYS:O	2:J:19:PHE:HB2	2.05	0.56
1:I:274:ASN:ND2	1:I:299:HIS:HA	2.21	0.55
1:I:173:SER:O	1:I:241:THR:HB	2.06	0.55
1:I:453:GLY:HA3	1:I:474:SER:HA	1.87	0.55
1:I:219:HIS:H	1:I:219:HIS:CD2	2.23	0.55
1:A:540:TRP:CZ3	4:A:601:PQQ:O4	2.59	0.55
1:D:128:GLN:NE2	1:D:134:VAL:HG21	2.22	0.55
1:D:356:ASN:HD21	1:D:386:CYS:H	1.54	0.55
1:I:261:ASN:OD1	1:I:303:ASP:OD2	2.25	0.55
1:D:202:GLY:O	1:D:226:GLY:HA3	2.07	0.55
1:I:258:GLY:HA3	1:I:306:GLY:O	2.06	0.55
1:A:270:ARG:HH21	1:A:274:ASN:ND2	2.04	0.54
1:D:337:THR:C	1:D:338:LEU:HD12	2.31	0.54
1:I:51:LEU:O	1:I:52:HIS:HB2	2.06	0.54
1:A:317:ASP:HA	1:A:461:ILE:HD12	1.89	0.54
1:A:546:VAL:HG22	1:A:571:MET:SD	2.48	0.54
1:I:400:TYR:CE2	1:I:402:PRO:HA	2.42	0.54
1:D:207:ILE:HD13	1:D:276:TRP:HD1	1.72	0.54
2:E:23:ILE:HD12	2:E:30:PRO:HD3	1.89	0.54
1:I:362:ASP:OD1	1:I:365:THR:N	2.39	0.54
1:A:418:TRP:C	1:A:418:TRP:CD1	2.84	0.54
1:D:420:PRO:HA	1:D:434:ALA:HA	1.90	0.54
1:A:173:SER:HB3	1:A:183:HIS:CE1	2.43	0.54
1:D:29:SER:OG	1:D:524:GLU:OE1	2.22	0.54
1:I:90:HIS:HE2	1:I:143:GLU:CD	2.16	0.54
1:A:109:ARG:HE	1:A:395:GLN:HE21	1.55	0.53
1:I:18:GLY:HA2	1:I:25:ASN:ND2	2.23	0.53
1:A:236:LYS:HZ2	2:B:38:ASN:HD21	1.56	0.53
2:B:60:LYS:HB2	2:B:60:LYS:HZ2	1.73	0.53
2:E:15:PRO:HB3	2:E:20:PRO:O	2.09	0.53
1:A:89:GLN:NE2	5:A:936:HOH:O	2.42	0.53
1:I:275:LYS:NZ	2:J:10:GLY:O	2.40	0.53
1:I:303:ASP:CG	1:I:303:ASP:O	2.52	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:HIS:HE1	5:A:814:HOH:O	1.92	0.52
1:D:583:LYS:HA	1:D:587:ASP:OD1	2.10	0.52
1:A:580:LEU:HB2	5:A:797:HOH:O	2.08	0.52
2:B:35:LYS:HB3	2:B:35:LYS:HZ3	1.72	0.52
1:I:545:LEU:C	1:I:545:LEU:HD12	2.34	0.52
2:J:33:ASP:OD2	2:J:35:LYS:HB2	2.09	0.52
1:A:496:LEU:HD13	1:A:508:TRP:CZ3	2.43	0.52
1:D:304:PHE:O	1:D:305:ALA:C	2.53	0.52
1:A:114:TRP:HZ2	1:A:190:ARG:NH2	2.08	0.52
1:A:175:GLY:N	4:A:601:PQQ:O7B	2.32	0.52
1:A:512:LEU:HB3	1:A:513:PRO:CD	2.40	0.52
2:J:23:ILE:HD12	2:J:30:PRO:HD3	1.92	0.52
1:D:509:LYS:NZ	1:I:593:GLU:OE2	2.39	0.52
1:I:33:ASN:HA	1:I:486:LEU:HD22	1.92	0.51
2:B:35:LYS:NZ	2:B:35:LYS:CB	2.73	0.51
1:I:71:PHE:CD2	1:I:72:PRO:HA	2.45	0.51
2:B:16:LYS:O	2:B:17:PRO:C	2.52	0.51
1:I:482:THR:C	1:I:484:GLY:N	2.56	0.51
1:I:390:MET:CE	1:I:558:ALA:HB2	2.40	0.51
1:A:151:ASP:OD2	1:A:153:LYS:NZ	2.41	0.51
1:D:45:SER:O	1:I:511:LYS:NZ	2.44	0.51
1:A:314:GLU:CG	1:A:322:LYS:HD2	2.40	0.51
1:A:356:ASN:C	1:A:356:ASN:HD22	2.19	0.51
1:A:382:GLY:O	1:A:417:ASP:HA	2.10	0.51
1:A:272:GLY:O	1:A:299:HIS:CD2	2.64	0.51
1:D:238:GLY:O	1:D:262:PRO:HA	2.10	0.51
1:D:488:PHE:CE2	1:D:498:ALA:HB2	2.46	0.51
1:A:595:GLU:C	1:A:597:GLY:N	2.66	0.50
1:I:223:LYS:HZ2	1:I:223:LYS:HB3	1.76	0.50
1:I:1:ASN:N	1:I:166:HIS:H	2.09	0.50
1:I:202:GLY:O	1:I:207:ILE:HD12	2.11	0.50
1:I:327:THR:HA	1:I:336:TYR:O	2.11	0.50
1:A:230:TRP:CE2	1:A:274:ASN:HA	2.46	0.50
1:I:214:ASN:HD21	1:I:293:GLY:H	1.60	0.50
1:I:296:LYS:HZ1	1:I:306:GLY:HA3	1.75	0.50
1:A:194:GLN:NE2	5:A:836:HOH:O	2.38	0.50
2:E:30:PRO:O	2:E:31:LYS:C	2.52	0.50
1:A:272:GLY:O	1:A:299:HIS:HD2	1.94	0.50
1:A:471:GLU:OE2	1:A:489:TYR:OH	2.26	0.50
1:I:173:SER:HB2	1:I:241:THR:HG22	1.94	0.50
1:I:397:HIS:HD2	1:I:398:ASP:O	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:411:ILE:CG2	1:I:412:ASN:N	2.75	0.49
1:D:408:PHE:CZ	1:D:501:SER:HB2	2.47	0.49
1:D:270:ARG:HH21	1:D:274:ASN:HD21	1.59	0.49
1:D:244:GLY:HA3	1:D:307:VAL:O	2.12	0.49
1:I:60:VAL:O	1:I:61:ILE:HD13	2.12	0.49
1:I:546:VAL:HG22	1:I:571:MET:SD	2.53	0.49
2:J:68:VAL:HG13	2:J:68:VAL:O	2.12	0.49
1:A:305:ALA:O	1:A:331:ARG:HG3	2.11	0.49
1:D:291:LYS:HD3	5:D:906:HOH:O	2.11	0.49
1:A:33:ASN:CA	1:A:486:LEU:HD22	2.40	0.49
1:A:120:THR:HG22	1:A:121:PRO:HD2	1.94	0.49
2:J:67:ASP:OD1	2:J:67:ASP:C	2.56	0.49
1:A:296:LYS:NZ	1:A:328:HIS:HE1	2.11	0.49
1:D:274:ASN:HD22	1:D:299:HIS:HA	1.77	0.49
2:E:54:ARG:HB3	2:E:64:TRP:CZ2	2.47	0.49
2:E:29:ASP:OD2	2:E:31:LYS:N	2.38	0.49
1:I:265:TRP:CD2	1:I:432:VAL:HG13	2.48	0.49
2:J:69:LYS:O	2:J:70:LYS:HD2	2.12	0.49
1:I:48:THR:OG1	1:I:54:HIS:HE1	1.96	0.48
1:D:283:ARG:NH2	1:D:290:MET:HE3	2.28	0.48
1:D:51:LEU:O	1:D:52:HIS:HB2	2.13	0.48
1:D:383:THR:HG22	1:D:417:ASP:CG	2.38	0.48
1:I:512:LEU:HB3	1:I:513:PRO:CD	2.42	0.48
1:D:356:ASN:ND2	1:D:386:CYS:H	2.11	0.48
2:E:57:HIS:HE1	2:E:63:LYS:HZ1	1.60	0.48
2:J:1:TYR:HD1	2:J:14:GLU:HG2	1.77	0.48
1:D:114:TRP:CD2	1:D:189:VAL:HG21	2.48	0.48
1:D:278:MET:HE1	1:D:304:PHE:C	2.38	0.48
2:E:57:HIS:CE1	2:E:61:THR:HG21	2.48	0.48
2:E:56:GLU:HG2	5:E:638:HOH:O	2.13	0.48
1:I:296:LYS:HZ1	1:I:306:GLY:CA	2.27	0.48
1:A:214:ASN:HD21	1:A:293:GLY:H	1.61	0.48
1:I:25:ASN:OD1	1:I:397:HIS:CD2	2.66	0.48
1:D:55:GLU:OE1	4:D:601:PQQ:O2A	2.31	0.48
2:E:63:LYS:HG3	2:E:63:LYS:O	2.14	0.48
1:I:315:GLN:HG3	1:I:325:LEU:CD1	2.44	0.48
1:D:52:HIS:O	1:D:54:HIS:HD2	1.97	0.47
1:A:185:THR:HG22	1:A:186:ALA:N	2.29	0.47
1:I:243:TRP:CZ2	4:I:601:PQQ:C6A	2.97	0.47
1:I:272:GLY:HA2	2:J:13:TRP:CB	2.44	0.47
1:I:305:ALA:O	1:I:331:ARG:HG3	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:ASP:OD1	1:A:190:ARG:CZ	2.62	0.47
1:A:440:PRO:HA	1:A:452:LEU:HD13	1.95	0.47
1:D:1:ASN:N	1:D:166:HIS:H	2.13	0.47
1:I:510:HIS:HD2	5:I:825:HOH:O	1.97	0.47
1:D:436:LEU:HD23	1:D:438:MET:HE2	1.96	0.47
1:D:584:ASN:OD1	1:D:586:TYR:HB2	2.15	0.47
1:A:146:LYS:HE3	5:A:820:HOH:O	2.14	0.47
1:D:272:GLY:O	1:D:299:HIS:CD2	2.67	0.47
1:D:298:PRO:O	1:D:299:HIS:C	2.56	0.47
1:A:337:THR:C	1:A:338:LEU:HD12	2.40	0.47
1:D:53:GLY:CA	1:D:517:ILE:HD11	2.44	0.47
1:I:304:PHE:O	1:I:305:ALA:C	2.57	0.47
1:I:219:HIS:HE1	5:I:816:HOH:O	1.97	0.47
2:B:60:LYS:NZ	2:B:60:LYS:CB	2.77	0.47
1:D:53:GLY:HA3	1:D:517:ILE:HD11	1.97	0.47
1:D:255:ILE:HG21	1:D:255:ILE:HD13	1.55	0.47
1:I:296:LYS:HZ2	1:I:328:HIS:HE1	1.62	0.46
1:A:114:TRP:CZ2	1:A:190:ARG:NH2	2.83	0.46
1:I:408:PHE:HA	1:I:456:LYS:O	2.15	0.46
1:I:491:THR:OG1	1:I:493:ASP:OD2	2.27	0.46
1:D:243:TRP:CE2	1:D:307:VAL:HG21	2.50	0.46
1:I:407:PHE:CE2	1:I:460:ALA:HB2	2.50	0.46
1:A:267:GLU:HB2	1:A:299:HIS:CE1	2.50	0.46
2:B:31:LYS:HE3	5:B:84:HOH:O	2.14	0.46
1:D:157:THR:O	1:D:174:SER:HB2	2.15	0.46
1:D:185:THR:OG1	1:D:197:ARG:HD2	2.15	0.46
1:I:545:LEU:HD12	1:I:545:LEU:O	2.16	0.46
1:I:566:GLN:H	1:I:566:GLN:HG2	1.46	0.46
1:D:397:HIS:CD2	1:D:397:HIS:C	2.94	0.46
1:D:25:ASN:O	1:D:480:LEU:HD12	2.16	0.46
2:E:29:ASP:HA	2:E:30:PRO:HD2	1.65	0.46
2:E:56:GLU:HA	5:E:638:HOH:O	2.15	0.46
1:I:234:ALA:HB2	5:I:868:HOH:O	2.14	0.46
1:A:219:HIS:CD2	1:A:219:HIS:N	2.81	0.46
1:D:400:TYR:O	1:D:402:PRO:HD3	2.16	0.46
1:I:583:LYS:HB2	1:I:583:LYS:HZ3	1.79	0.46
2:J:33:ASP:OD2	2:J:33:ASP:C	2.59	0.46
1:A:36:ASN:ND2	1:A:580:LEU:HD11	2.31	0.45
1:A:326:LEU:O	1:A:337:THR:HA	2.16	0.45
1:D:42:HIS:ND1	1:I:510:HIS:CE1	2.84	0.45
1:I:476:TRP:CD2	1:I:541:PRO:HG2	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:THR:HG23	1:A:197:ARG:HB2	1.98	0.45
1:A:267:GLU:OE2	1:A:299:HIS:HE1	1.99	0.45
1:D:267:GLU:OE2	1:D:299:HIS:HE1	1.99	0.45
1:I:272:GLY:O	1:I:299:HIS:HB2	2.16	0.45
1:I:318:LYS:HG2	5:I:821:HOH:O	2.15	0.45
1:I:390:MET:HG3	1:I:438:MET:SD	2.57	0.45
1:I:418:TRP:CD1	1:I:418:TRP:C	2.94	0.45
1:I:560:GLY:O	1:I:563:LYS:HG2	2.16	0.45
2:J:11:ASN:C	2:J:11:ASN:HD22	2.25	0.45
1:I:103:CYS:SG	1:I:104:CYS:N	2.89	0.45
1:A:540:TRP:HB2	4:A:601:PQQ:C3	2.47	0.45
2:B:12:CYS:O	2:B:13:TRP:C	2.55	0.45
1:I:304:PHE:CD2	1:I:332:ASN:HB3	2.52	0.45
1:I:390:MET:HE3	1:I:540:TRP:CE2	2.52	0.45
1:D:361:VAL:HA	1:D:368:PRO:HA	1.98	0.45
1:A:368:PRO:HG2	5:A:821:HOH:O	2.16	0.45
2:J:36:GLU:OE1	2:J:39:LYS:NZ	2.35	0.45
1:A:283:ARG:NH1	1:A:290:MET:HE2	2.32	0.45
1:A:125:ILE:HG22	1:A:162:PRO:HG2	1.98	0.45
1:D:160:GLN:OE1	1:D:172:GLY:N	2.49	0.45
1:I:356:ASN:HD22	1:I:357:VAL:N	2.14	0.44
1:D:103:CYS:C	1:D:104:CYS:SG	3.00	0.44
1:A:257:TYR:HA	1:A:310:ILE:HD12	1.99	0.44
1:A:438:MET:HG3	1:A:557:GLY:O	2.16	0.44
1:I:14:TRP:CZ3	1:I:19:LYS:HD2	2.52	0.44
1:I:209:LEU:HD22	1:I:213:PHE:CD1	2.53	0.44
1:A:317:ASP:OD2	1:A:317:ASP:C	2.61	0.44
1:A:329:PRO:HA	1:A:335:VAL:HA	1.99	0.44
1:D:33:ASN:OD1	1:D:35:ASP:HB2	2.17	0.44
1:D:458:TYR:CE2	1:D:460:ALA:HA	2.53	0.44
1:I:18:GLY:HA2	1:I:25:ASN:HD21	1.80	0.44
1:I:119:LYS:HE3	1:I:119:LYS:HB2	1.78	0.44
1:A:532:ALA:HB1	1:A:575:LEU:HD11	1.99	0.44
1:D:271:PRO:HB2	2:E:13:TRP:CH2	2.52	0.44
1:I:188:ASN:ND2	1:I:190:ARG:H	2.16	0.44
1:I:404:LYS:HD3	1:I:502:ASP:OD1	2.17	0.44
1:A:114:TRP:CZ3	1:A:116:GLY:HA2	2.53	0.44
1:A:537:VAL:HG22	1:A:538:GLY:H	1.83	0.44
1:D:197:ARG:NH2	2:E:44:ARG:HD3	2.33	0.44
1:D:428:GLY:N	5:D:783:HOH:O	2.51	0.44
1:I:401:ASP:C	1:I:401:ASP:OD1	2.61	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:34:VAL:HG11	1:D:500:ASN:ND2	2.33	0.44
1:D:401:ASP:O	1:D:405:GLN:N	2.51	0.44
1:D:414:ILE:HD11	1:D:474:SER:OG	2.18	0.44
1:I:41:LYS:HB2	1:I:582:GLY:N	2.32	0.44
1:I:267:GLU:OE1	1:I:377:ARG:HA	2.18	0.44
1:D:349:ASP:OD2	1:D:458:TYR:OH	2.30	0.43
1:D:421:PHE:CE1	1:D:433:GLY:HA2	2.53	0.43
1:D:522:THR:HA	1:D:530:TYR:O	2.17	0.43
1:I:540:TRP:HB2	4:I:601:PQQ:C3	2.48	0.43
1:D:387:PRO:HB3	1:D:392:TYR:CD2	2.53	0.43
1:I:34:VAL:HG21	1:I:485:ASN:HB2	2.00	0.43
1:D:256:TYR:HA	1:D:281:THR:O	2.18	0.43
1:D:411:ILE:CG2	1:D:412:ASN:N	2.81	0.43
1:I:412:ASN:OD1	1:I:474:SER:HB3	2.17	0.43
1:I:520:PRO:HD3	5:I:785:HOH:O	2.17	0.43
1:D:151:ASP:OD2	1:D:153:LYS:HB2	2.18	0.43
2:J:30:PRO:HG2	2:J:31:LYS:H	1.83	0.43
1:A:414:ILE:HG12	1:A:452:LEU:HD12	2.01	0.43
1:I:540:TRP:N	1:I:541:PRO:CD	2.81	0.43
2:J:68:VAL:O	2:J:68:VAL:CG1	2.66	0.43
1:A:44:TRP:CE2	1:A:577:VAL:HG21	2.53	0.43
1:D:37:VAL:HG11	1:D:507:VAL:HG21	2.00	0.43
1:D:243:TRP:CH2	4:D:601:PQQ:C9A	3.01	0.43
1:D:296:LYS:NZ	1:D:328:HIS:HE1	2.17	0.43
2:E:23:ILE:O	2:E:24:ALA:C	2.61	0.43
1:I:400:TYR:HB2	1:I:407:PHE:CD1	2.54	0.43
1:I:476:TRP:CZ2	1:I:541:PRO:HD3	2.54	0.43
1:A:229:THR:HB	1:A:273:ASP:H	1.84	0.43
1:A:233:ASP:HB3	1:A:236:LYS:HD2	2.01	0.43
1:A:537:VAL:HG22	1:A:538:GLY:N	2.34	0.43
2:E:11:ASN:C	2:E:11:ASN:ND2	2.68	0.43
2:E:40:GLN:HG3	5:E:267:HOH:O	2.19	0.43
1:I:388:SER:HA	1:I:416:MET:CE	2.48	0.43
1:A:40:LEU:O	1:A:41:LYS:HD3	2.19	0.43
2:B:32:HIS:HB3	2:B:37:LEU:CD1	2.48	0.43
2:B:69:LYS:O	2:B:70:LYS:HG3	2.19	0.43
1:D:371:ASP:OD2	1:D:373:GLU:HB2	2.18	0.43
1:I:153:LYS:HA	1:I:153:LYS:HD3	1.87	0.43
1:I:315:GLN:HG3	1:I:325:LEU:HD12	2.01	0.43
1:D:356:ASN:C	1:D:356:ASN:HD22	2.27	0.43
1:D:540:TRP:O	1:D:543:VAL:HG22	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:182:GLY:HA2	1:I:241:THR:HA	2.01	0.43
1:A:270:ARG:NH2	1:A:274:ASN:ND2	2.66	0.42
1:I:260:GLY:O	1:I:261:ASN:C	2.61	0.42
2:J:23:ILE:HD12	2:J:28:TYR:O	2.18	0.42
1:A:278:MET:HE1	1:A:304:PHE:O	2.18	0.42
1:A:466:LYS:NZ	1:A:502:ASP:O	2.51	0.42
1:I:488:PHE:HA	1:I:497:LYS:O	2.19	0.42
2:J:29:ASP:HA	2:J:30:PRO:HD2	1.79	0.42
1:A:244:GLY:HA3	1:A:307:VAL:O	2.19	0.42
1:D:99:ARG:HE	1:D:99:ARG:HB2	1.48	0.42
1:D:248:TYR:CD1	1:D:254:LEU:O	2.73	0.42
1:I:114:TRP:CZ3	1:I:116:GLY:HA2	2.54	0.42
1:I:356:ASN:C	1:I:356:ASN:ND2	2.70	0.42
1:I:456:LYS:HE2	1:I:468:GLN:HB2	2.00	0.42
1:A:180:VAL:O	1:A:239:GLY:HA2	2.18	0.42
1:A:275:LYS:HE3	1:A:295:GLN:HB2	2.02	0.42
2:B:67:ASP:OD1	2:B:67:ASP:C	2.61	0.42
1:D:7:LEU:HB3	1:D:15:VAL:HG11	2.00	0.42
1:A:167:ASP:CG	1:A:190:ARG:HH22	2.28	0.42
2:B:32:HIS:HB3	2:B:37:LEU:HD11	2.00	0.42
1:I:392:TYR:O	1:I:411:ILE:HG23	2.20	0.42
1:I:244:GLY:HA3	1:I:307:VAL:O	2.20	0.42
1:I:274:ASN:HD22	1:I:299:HIS:HA	1.83	0.42
1:I:278:MET:HE2	1:I:300:ASP:CG	2.45	0.42
1:A:296:LYS:HZ3	1:A:328:HIS:HE1	1.68	0.42
2:B:9:PRO:HD2	5:B:198:HOH:O	2.20	0.42
1:I:371:ASP:OD2	1:I:371:ASP:C	2.61	0.42
2:E:6:CYS:HB3	2:E:8:ALA:O	2.19	0.42
2:E:39:LYS:HB3	2:E:39:LYS:HE2	1.81	0.42
1:I:309:VAL:O	1:I:328:HIS:HD2	2.03	0.42
1:D:19:LYS:NZ	5:D:896:HOH:O	2.53	0.42
1:D:296:LYS:HZ1	1:D:306:GLY:CA	2.33	0.42
1:D:114:TRP:HA	1:D:115:PRO:HD3	1.83	0.42
1:D:274:ASN:ND2	1:D:299:HIS:HA	2.35	0.42
1:A:70:SER:O	1:A:71:PHE:C	2.61	0.41
1:D:245:TRP:HB2	1:D:309:VAL:HA	2.01	0.41
1:I:60:VAL:C	1:I:61:ILE:HD13	2.45	0.41
1:D:42:HIS:CB	1:I:42:HIS:HB3	2.49	0.41
2:E:54:ARG:HB3	2:E:64:TRP:CE2	2.55	0.41
1:I:334:ILE:HB	1:I:336:TYR:CE1	2.55	0.41
1:I:376:THR:O	1:I:377:ARG:HB3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLY:O	1:A:344:ASP:C	2.63	0.41
1:A:534:MET:HG2	5:A:778:HOH:O	2.20	0.41
1:I:494:GLY:HA2	1:I:515:GLY:HA2	2.03	0.41
1:A:462:THR:HG21	5:A:809:HOH:O	2.20	0.41
1:I:397:HIS:CD2	1:I:398:ASP:O	2.73	0.41
1:D:68:HIS:CE1	1:D:110:GLY:HA2	2.55	0.41
1:D:540:TRP:N	1:D:541:PRO:CD	2.84	0.41
1:I:33:ASN:C	1:I:35:ASP:N	2.77	0.41
1:I:326:LEU:O	1:I:337:THR:HA	2.21	0.41
1:A:249:ASP:OD2	1:A:249:ASP:C	2.62	0.41
1:A:256:TYR:HA	1:A:281:THR:O	2.21	0.41
1:A:309:VAL:HG22	1:A:310:ILE:N	2.36	0.41
1:A:401:ASP:HA	1:A:402:PRO:HD3	1.75	0.41
1:A:562:PHE:O	1:A:563:LYS:C	2.64	0.41
1:D:267:GLU:HG2	1:D:301:GLU:HG2	2.03	0.41
2:J:69:LYS:O	2:J:70:LYS:CD	2.67	0.41
1:D:35:ASP:HB2	5:D:867:HOH:O	2.20	0.41
1:A:36:ASN:O	1:A:39:GLN:HB2	2.20	0.41
1:A:52:HIS:O	1:A:53:GLY:C	2.62	0.41
1:A:476:TRP:CZ2	1:A:541:PRO:HD3	2.56	0.41
1:D:3:LYS:HB2	1:D:115:PRO:HG2	2.01	0.41
1:I:223:LYS:HG3	5:I:830:HOH:O	2.21	0.41
1:A:280:ILE:O	1:A:293:GLY:HA2	2.21	0.41
1:D:180:VAL:O	1:D:239:GLY:HA2	2.21	0.41
1:I:6:GLU:HG3	1:I:7:LEU:N	2.35	0.41
1:I:34:VAL:H	1:I:34:VAL:HG23	1.52	0.41
1:A:103:CYS:SG	1:A:104:CYS:N	2.94	0.40
1:I:413:HIS:CD2	1:I:441:GLY:HA3	2.56	0.40
1:A:401:ASP:OD1	1:A:401:ASP:C	2.63	0.40
1:D:181:ARG:HH11	1:D:181:ARG:HD3	1.74	0.40
1:I:263:ALA:O	1:I:270:ARG:HD3	2.21	0.40
1:A:445:ASP:C	1:A:445:ASP:OD1	2.65	0.40
1:D:296:LYS:HE3	1:D:296:LYS:HB2	1.90	0.40
2:E:23:ILE:HD12	2:E:30:PRO:CD	2.50	0.40
1:A:95:ASP:OD2	1:A:96:PRO:HD2	2.22	0.40
1:I:4:LEU:HD23	1:I:4:LEU:HA	1.89	0.40
1:I:397:HIS:CD2	1:I:397:HIS:C	2.99	0.40
1:I:411:ILE:HG22	1:I:412:ASN:N	2.36	0.40
1:I:512:LEU:HB3	1:I:513:PRO:HD2	2.04	0.40
1:A:378:MET:HA	1:A:420:PRO:HG2	2.04	0.40
2:B:6:CYS:C	2:B:8:ALA:H	2.28	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:323:ARG:NH1	1:D:339:ASP:OD2	2.53	0.40
1:I:97:ALA:O	1:I:98:ALA:C	2.65	0.40
1:I:407:PHE:HE2	1:I:460:ALA:HB2	1.87	0.40
2:J:32:HIS:O	2:J:34:PRO:HD3	2.21	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	595/597 (100%)	561 (94%)	32 (5%)	2 (0%)	36	55
1	D	595/597 (100%)	537 (90%)	53 (9%)	5 (1%)	16	31
1	I	593/597 (99%)	546 (92%)	43 (7%)	4 (1%)	18	34
2	B	68/72 (94%)	63 (93%)	5 (7%)	0	100	100
2	E	66/72 (92%)	60 (91%)	5 (8%)	1 (2%)	8	16
2	J	68/72 (94%)	60 (88%)	6 (9%)	2 (3%)	3	5
All	All	1985/2007 (99%)	1827 (92%)	144 (7%)	14 (1%)	18	34

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	266	ASN
2	E	67	ASP
1	I	261	ASN
1	I	331	ARG
1	D	587	ASP
1	D	595	GLU
1	I	483	ALA
1	A	70	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	105	ASP
1	D	105	ASP
1	D	276	TRP
2	J	35	LYS
2	J	68	VAL
1	I	573	GLY

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	487/487 (100%)	457 (94%)	30 (6%)	16	34
1	D	487/487 (100%)	455 (93%)	32 (7%)	15	32
1	I	486/487 (100%)	454 (93%)	32 (7%)	15	32
2	B	60/62 (97%)	52 (87%)	8 (13%)	4	8
2	E	58/62 (94%)	52 (90%)	6 (10%)	7	14
2	J	60/62 (97%)	49 (82%)	11 (18%)	2	3
All	All	1638/1647 (100%)	1519 (93%)	119 (7%)	13	27

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	34	VAL
1	A	67	VAL
1	A	78	LEU
1	A	93	LYS
1	A	118	ASP
1	A	119	LYS
1	A	120	THR
1	A	142	GLU
1	A	219	HIS
1	A	223	LYS
1	A	312	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	322	LYS
1	A	323	ARG
1	A	355	VAL
1	A	356	ASN
1	A	357	VAL
1	A	395	GLN
1	A	426	ARG
1	A	438	MET
1	A	455	ILE
1	A	464	GLU
1	A	482	THR
1	A	486	LEU
1	A	496	LEU
1	A	512	LEU
1	A	550	GLN
1	A	556	LEU
1	A	580	LEU
1	A	596	LYS
2	B	31	LYS
2	B	35	LYS
2	B	39	LYS
2	B	53	ASN
2	B	59	LYS
2	B	60	LYS
2	B	69	LYS
2	B	70	LYS
1	D	23	SER
1	D	25	ASN
1	D	34	VAL
1	D	67	VAL
1	D	78	LEU
1	D	119	LYS
1	D	139	LYS
1	D	153	LYS
1	D	170	ILE
1	D	193	GLU
1	D	237	ILE
1	D	312	LEU
1	D	322	LYS
1	D	356	ASN
1	D	364	LYS
1	D	367	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	383	THR
1	D	395	GLN
1	D	406	LEU
1	D	419	GLU
1	D	426	ARG
1	D	436	LEU
1	D	452	LEU
1	D	466	LYS
1	D	486	LEU
1	D	496	LEU
1	D	512	LEU
1	D	545	LEU
1	D	556	LEU
1	D	563	LYS
1	D	581	ASP
1	D	596	LYS
2	E	7	LYS
2	E	22	LYS
2	E	31	LYS
2	E	35	LYS
2	E	37	LEU
2	E	49	GLU
1	I	6	GLU
1	I	23	SER
1	I	29	SER
1	I	34	VAL
1	I	67	VAL
1	I	111	LEU
1	I	119	LYS
1	I	139	LYS
1	I	153	LYS
1	I	188	ASN
1	I	223	LYS
1	I	241	THR
1	I	255	ILE
1	I	312	LEU
1	I	315	GLN
1	I	321	LYS
1	I	325	LEU
1	I	334	ILE
1	I	347	SER
1	I	356	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	373	GLU
1	I	395	GLN
1	I	426	ARG
1	I	455	ILE
1	I	486	LEU
1	I	496	LEU
1	I	512	LEU
1	I	531	ILE
1	I	545	LEU
1	I	556	LEU
1	I	583	LYS
1	I	588	ASP
2	J	31	LYS
2	J	35	LYS
2	J	37	LEU
2	J	39	LYS
2	J	42	GLU
2	J	49	GLU
2	J	53	ASN
2	J	60	LYS
2	J	63	LYS
2	J	68	VAL
2	J	70	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (76) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	25	ASN
1	A	39	GLN
1	A	54	HIS
1	A	89	GLN
1	A	128	GLN
1	A	149	ASN
1	A	194	GLN
1	A	214	ASN
1	A	217	ASN
1	A	219	HIS
1	A	253	ASN
1	A	274	ASN
1	A	299	HIS
1	A	328	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	356	ASN
1	A	380	HIS
1	A	395	GLN
1	A	397	HIS
1	A	405	GLN
1	A	447	GLN
1	A	448	ASN
1	A	525	HIS
1	A	590	ASN
2	B	11	ASN
2	B	32	HIS
2	B	38	ASN
2	B	53	ASN
2	B	57	HIS
1	D	9	ASN
1	D	11	ASN
1	D	25	ASN
1	D	54	HIS
1	D	128	GLN
1	D	149	ASN
1	D	194	GLN
1	D	214	ASN
1	D	217	ASN
1	D	219	HIS
1	D	242	ASN
1	D	253	ASN
1	D	274	ASN
1	D	299	HIS
1	D	328	HIS
1	D	356	ASN
1	D	395	GLN
1	D	397	HIS
1	D	405	GLN
1	D	468	GLN
1	D	510	HIS
1	D	570	GLN
2	E	11	ASN
2	E	32	HIS
2	E	53	ASN
2	E	57	HIS
1	I	11	ASN
1	I	54	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	I	89	GLN
1	I	94	GLN
1	I	128	GLN
1	I	149	ASN
1	I	214	ASN
1	I	217	ASN
1	I	219	HIS
1	I	253	ASN
1	I	274	ASN
1	I	299	HIS
1	I	328	HIS
1	I	356	ASN
1	I	395	GLN
1	I	397	HIS
1	I	468	GLN
1	I	469	HIS
1	I	510	HIS
1	I	566	GLN
2	J	11	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	PQQ	D	601	3	26,26,26	3.17	10 (38%)	34,40,40	2.44	13 (38%)
4	PQQ	A	601	3	26,26,26	2.90	9 (34%)	34,40,40	2.86	21 (61%)
4	PQQ	I	601	3	26,26,26	2.65	9 (34%)	34,40,40	2.65	18 (52%)

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
4	PQQ	D	601	3	-	4/12/28/28	0/3/3/3
4	PQQ	A	601	3	-	6/12/28/28	0/3/3/3
4	PQQ	I	601	3	-	4/12/28/28	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	601	PQQ	C9-C9A	8.82	1.54	1.41
4	A	601	PQQ	C9A-C6A	8.56	1.54	1.41
4	A	601	PQQ	C9-C9A	8.39	1.53	1.41
4	D	601	PQQ	C9A-C6A	8.19	1.53	1.41
4	I	601	PQQ	C9A-C6A	7.08	1.52	1.41
4	I	601	PQQ	C9-C9A	6.20	1.50	1.41
4	D	601	PQQ	C6A-C5	5.65	1.56	1.50
4	I	601	PQQ	C3A-C1A	4.80	1.50	1.40
4	D	601	PQQ	C3A-C1A	4.80	1.50	1.40
4	A	601	PQQ	C3A-C1A	4.72	1.50	1.40
4	I	601	PQQ	C5-C4	-4.57	1.48	1.54
4	D	601	PQQ	O5-C5	3.38	1.30	1.23
4	I	601	PQQ	O2B-C2X	-2.94	1.22	1.30
4	I	601	PQQ	O5-C5	2.90	1.29	1.23
4	D	601	PQQ	C7-N6	2.86	1.38	1.34
4	A	601	PQQ	C7-N6	2.77	1.38	1.34
4	A	601	PQQ	O5-C5	2.76	1.29	1.23
4	I	601	PQQ	C3A-C4	2.68	1.53	1.46
4	D	601	PQQ	O2B-C2X	-2.58	1.23	1.30
4	A	601	PQQ	O2B-C2X	-2.55	1.23	1.30
4	I	601	PQQ	O7B-C7X	-2.49	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	601	PQQ	C7-C7X	2.44	1.55	1.50
4	D	601	PQQ	C3A-C4	2.43	1.53	1.46
4	A	601	PQQ	O7B-C7X	-2.37	1.23	1.30
4	A	601	PQQ	C6A-C5	2.23	1.52	1.50
4	D	601	PQQ	C6A-N6	2.13	1.39	1.34
4	I	601	PQQ	C6A-C5	2.13	1.52	1.50
4	A	601	PQQ	C3A-C4	2.04	1.52	1.46

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	601	PQQ	C6A-N6-C7	6.50	126.55	118.01
4	A	601	PQQ	O9A-C9X-C9	-5.18	109.61	121.97
4	A	601	PQQ	C6A-N6-C7	5.01	124.60	118.01
4	I	601	PQQ	C1A-C3A-C4	-5.01	118.11	122.33
4	A	601	PQQ	O2B-C2X-C2	4.98	125.00	114.27
4	A	601	PQQ	C3-C2-C2X	-4.92	121.19	132.53
4	I	601	PQQ	C3A-C4-C5	4.85	122.53	117.03
4	I	601	PQQ	O4-C4-C5	-4.85	112.39	118.37
4	D	601	PQQ	C9A-C6A-N6	-4.74	116.71	123.58
4	I	601	PQQ	O9A-C9X-C9	-4.71	110.71	121.97
4	A	601	PQQ	C3A-C4-C5	4.58	122.22	117.03
4	I	601	PQQ	O2B-C2X-C2	4.38	123.72	114.27
4	D	601	PQQ	C3-C2-C2X	-4.12	123.04	132.53
4	D	601	PQQ	O7B-C7X-C7	4.09	124.42	114.71
4	I	601	PQQ	O5-C5-C6A	4.02	126.34	121.76
4	A	601	PQQ	C1A-C3A-C4	-3.91	119.04	122.33
4	A	601	PQQ	C3A-C1A-N1	-3.87	102.12	107.23
4	A	601	PQQ	C3A-C3-C2	-3.78	104.05	107.94
4	I	601	PQQ	C9A-C6A-N6	-3.77	118.11	123.58
4	I	601	PQQ	C6A-N6-C7	3.64	122.79	118.01
4	D	601	PQQ	C5-C6A-N6	3.47	120.83	115.06
4	D	601	PQQ	O7B-C7X-O7A	-3.36	116.13	123.35
4	I	601	PQQ	C3-C2-C2X	-3.35	124.81	132.53
4	A	601	PQQ	O7B-C7X-C7	3.10	122.08	114.71
4	D	601	PQQ	O2B-C2X-C2	2.92	120.57	114.27
4	A	601	PQQ	C9A-C6A-N6	-2.92	119.34	123.58
4	A	601	PQQ	O5-C5-C4	2.90	121.92	118.14
4	D	601	PQQ	O9A-C9X-C9	-2.89	115.06	121.97
4	A	601	PQQ	C8-C9-C9X	-2.88	109.80	117.89
4	A	601	PQQ	O2A-C2X-C2	-2.85	115.22	121.01
4	D	601	PQQ	O9B-C9X-C9	2.72	123.03	115.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	I	601	PQQ	O2B-C2X-O2A	-2.59	117.72	123.90
4	A	601	PQQ	O7A-C7X-C7	-2.59	116.09	121.30
4	A	601	PQQ	C2X-C2-N1	2.58	127.14	120.52
4	A	601	PQQ	C9A-C9-C9X	2.55	127.09	121.49
4	A	601	PQQ	O9B-C9X-C9	2.54	122.49	115.28
4	D	601	PQQ	C8-C7-C7X	2.48	125.10	119.61
4	I	601	PQQ	C9-C8-C7	-2.47	117.91	119.93
4	I	601	PQQ	C3-C3A-C4	2.46	134.96	128.02
4	D	601	PQQ	C3A-C3-C2	-2.38	105.49	107.94
4	I	601	PQQ	C9A-C9-C9X	2.36	126.67	121.49
4	A	601	PQQ	O2B-C2X-O2A	-2.28	118.47	123.90
4	I	601	PQQ	C9A-C6A-C5	2.28	123.70	121.59
4	D	601	PQQ	C1A-C3A-C4	-2.27	120.42	122.33
4	A	601	PQQ	C3-C2-N1	2.16	111.34	107.74
4	D	601	PQQ	C3-C2-N1	2.15	111.33	107.74
4	A	601	PQQ	C8-C9-C9A	2.14	123.07	120.33
4	I	601	PQQ	C3A-C3-C2	-2.12	105.75	107.94
4	I	601	PQQ	O9B-C9X-O9A	2.08	127.83	123.35
4	A	601	PQQ	C3-C3A-C1A	2.05	110.32	107.09
4	I	601	PQQ	C8-C9-C9X	-2.05	112.12	117.89
4	I	601	PQQ	O9B-C9X-C9	2.00	120.98	115.28

There are no chirality outliers.

All (14) torsion outliers are listed below:

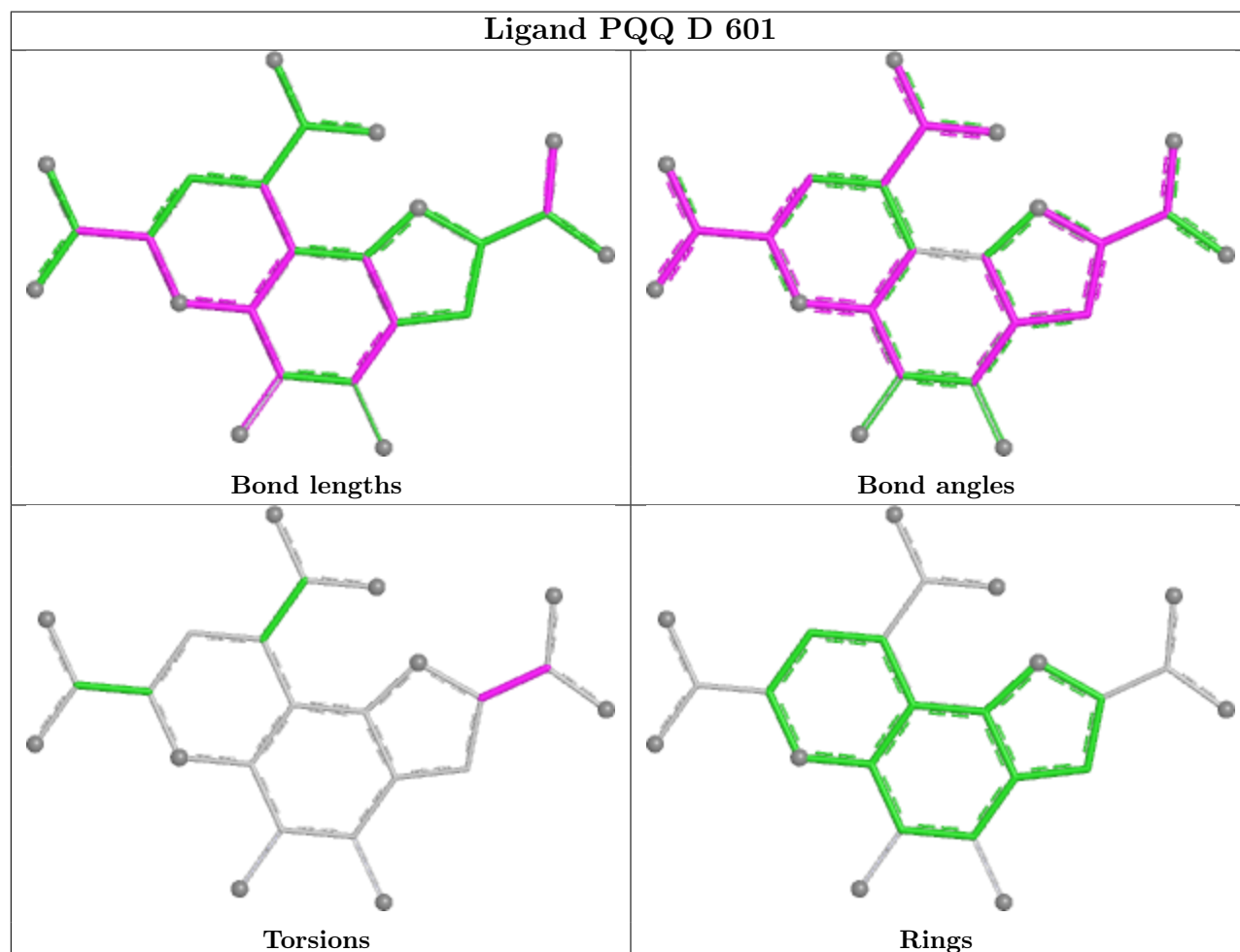
Mol	Chain	Res	Type	Atoms
4	A	601	PQQ	N1-C2-C2X-O2A
4	A	601	PQQ	C3-C2-C2X-O2A
4	I	601	PQQ	C3-C2-C2X-O2A
4	A	601	PQQ	C8-C7-C7X-O7A
4	I	601	PQQ	N1-C2-C2X-O2A
4	A	601	PQQ	N1-C2-C2X-O2B
4	D	601	PQQ	N1-C2-C2X-O2A
4	D	601	PQQ	N1-C2-C2X-O2B
4	I	601	PQQ	N1-C2-C2X-O2B
4	A	601	PQQ	C3-C2-C2X-O2B
4	D	601	PQQ	C3-C2-C2X-O2A
4	D	601	PQQ	C3-C2-C2X-O2B
4	I	601	PQQ	C3-C2-C2X-O2B
4	A	601	PQQ	N6-C7-C7X-O7A

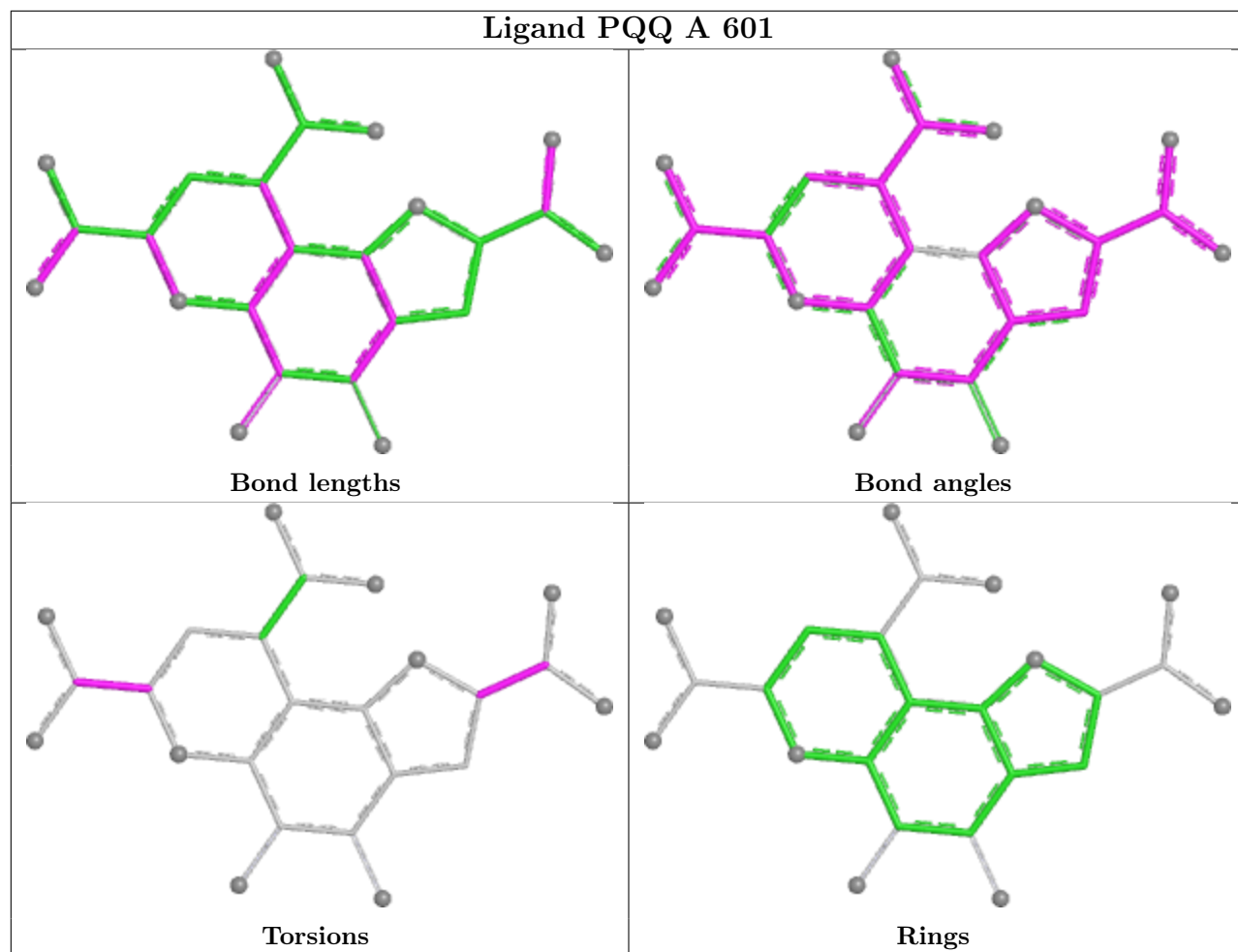
There are no ring outliers.

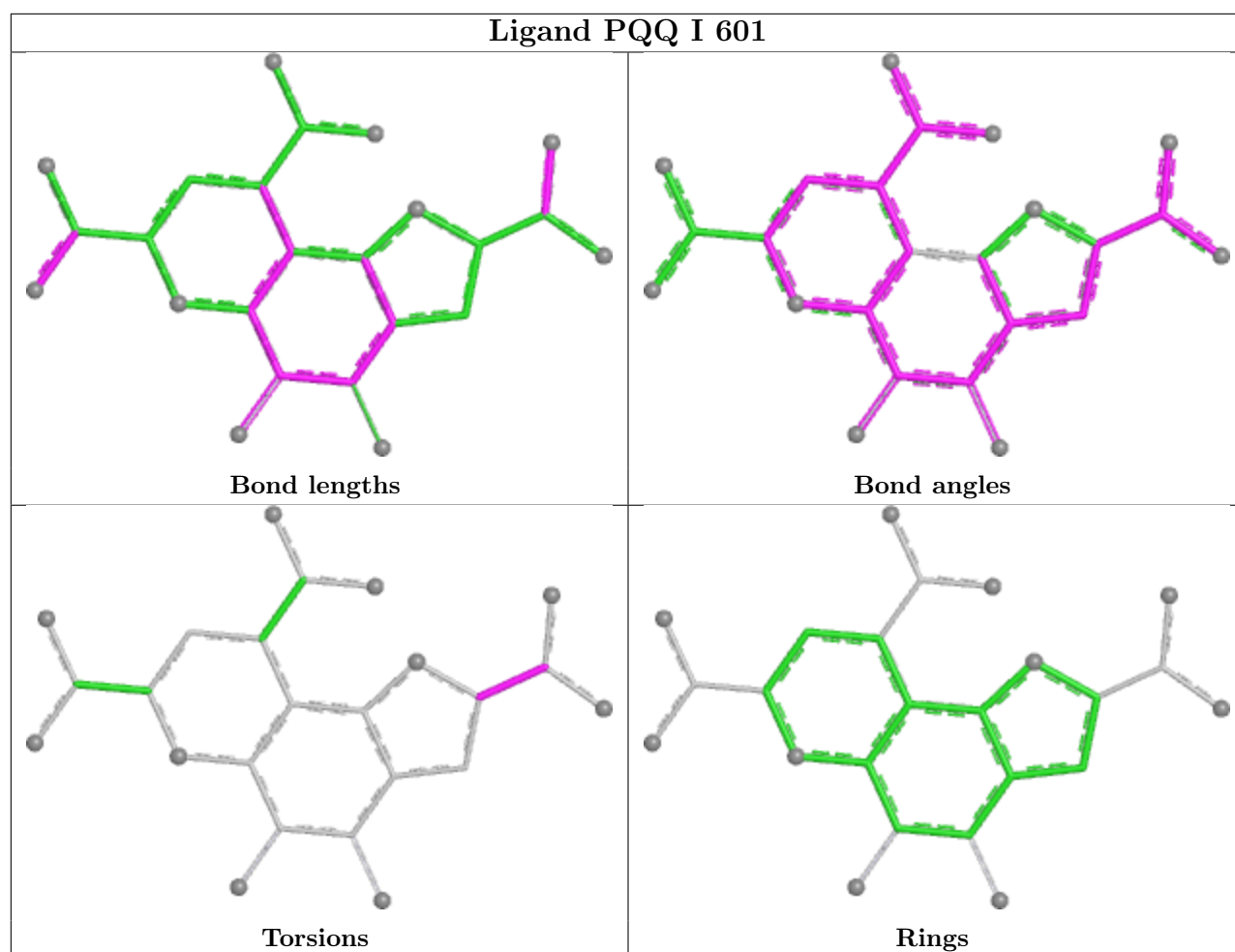
3 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	601	PQQ	5	0
4	A	601	PQQ	5	0
4	I	601	PQQ	4	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(Å²)	Q<0.9
1	A	597/597 (100%)	-0.71	0	100100	17, 28, 39, 55	0
1	D	597/597 (100%)	-0.56	0	100100	18, 32, 45, 61	0
1	I	595/597 (99%)	-0.55	0	100100	20, 34, 48, 57	0
2	B	70/72 (97%)	-0.50	0	100100	26, 36, 48, 54	0
2	E	68/72 (94%)	-0.08	1 (1%)	7268	35, 49, 58, 68	0
2	J	70/72 (97%)	-0.23	0	100100	34, 47, 59, 68	0
All	All	1997/2007 (99%)	-0.57	1 (0%)	9290	17, 32, 49, 68	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	E	68	VAL	2.9

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

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

6.3 Carbohydrates [i](#)

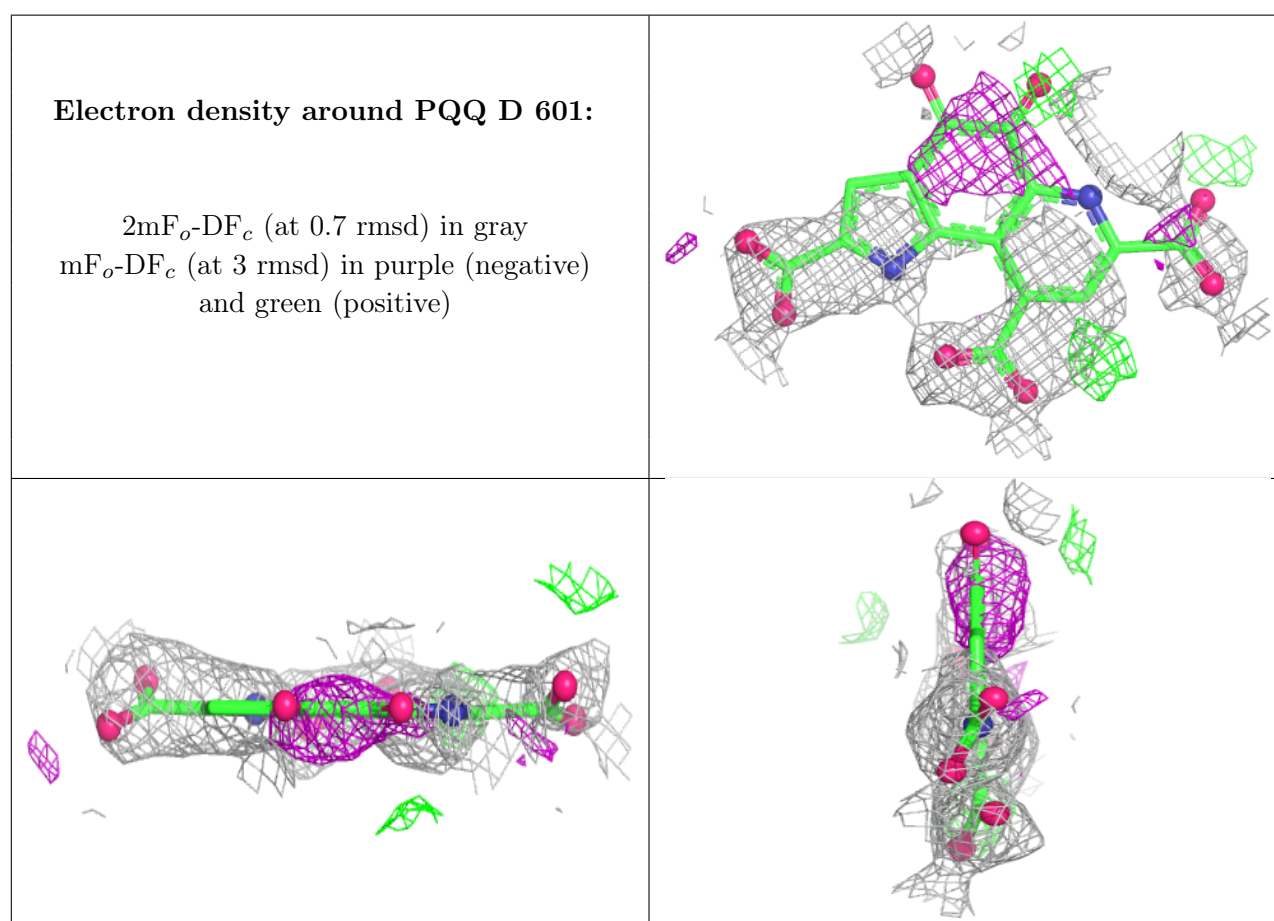
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

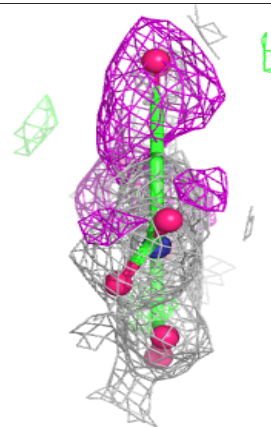
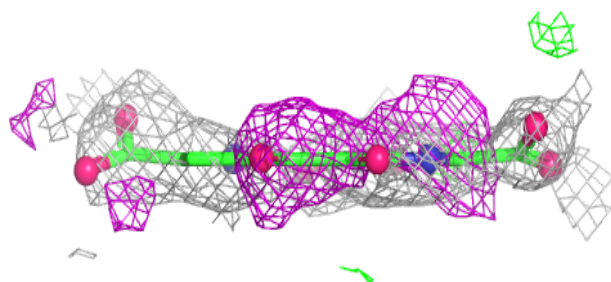
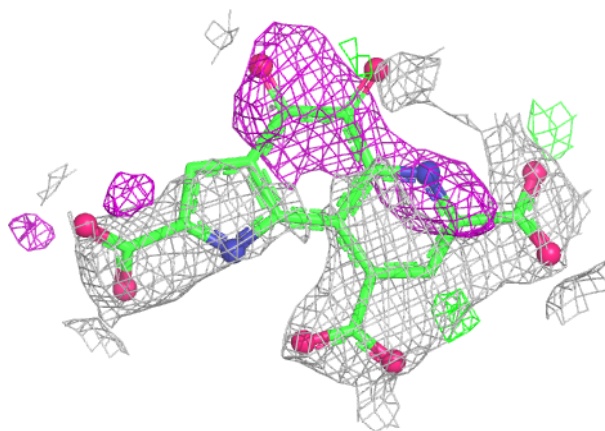
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PQQ	D	601	24/24	0.77	0.18	69,77,78,78	0
4	PQQ	A	601	24/24	0.81	0.17	59,68,69,69	0
4	PQQ	I	601	24/24	0.82	0.17	67,75,75,76	0
3	CA	I	775	1/1	0.95	0.06	49,49,49,49	1
3	CA	A	775	1/1	0.96	0.08	55,55,55,55	1
3	CA	D	775	1/1	0.98	0.04	49,49,49,49	1

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.



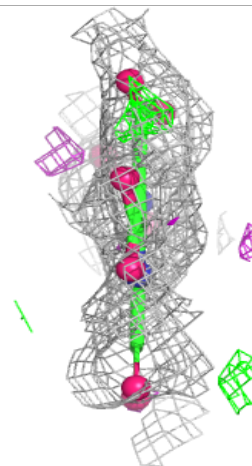
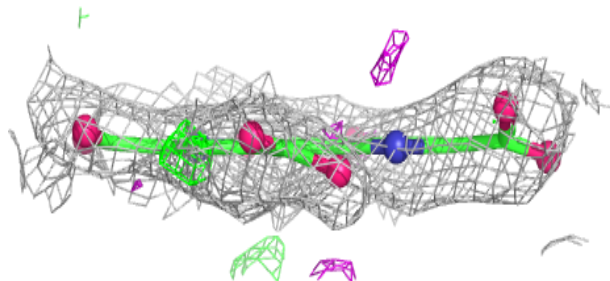
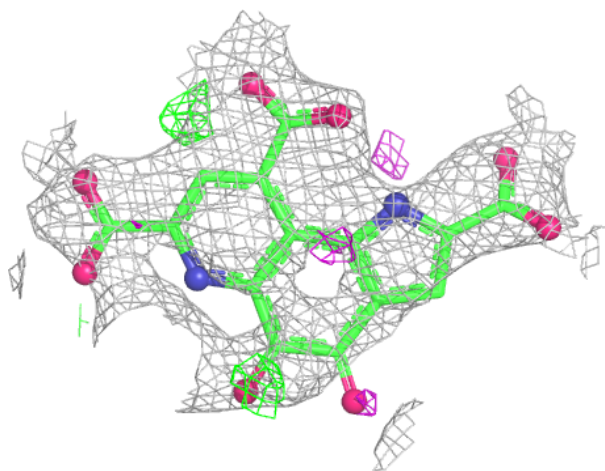
Electron density around PQQ A 601:

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



Electron density around PQQ I 601:

$2mF_o-DF_c$ (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.