



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 09:52 PM UTC

PDB ID : 1H4J / pdb_00001h4j
Title : Methylobacterium extorquens methanol dehydrogenase D303E mutant
Authors : Mohammed, F.; Gill, R.; Thompson, D.; Cooper, J.B.; Wood, S.P.; Afolabi, P.R.; Anthony, C.
Deposited on : 2001-05-11
Resolution : 3.00 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

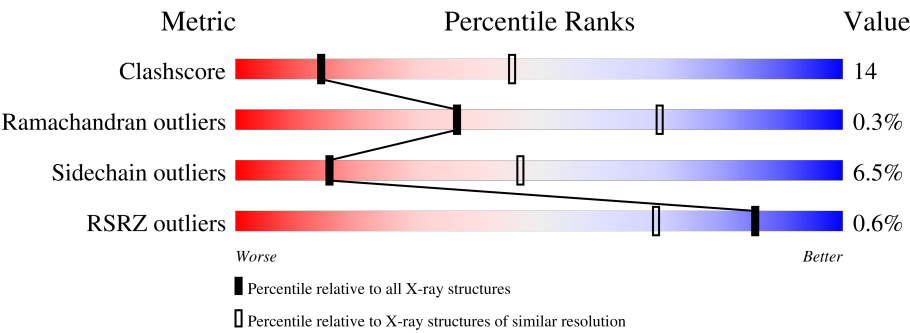
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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	599	67%28% . .
1	C	599	% 68%27% . .
1	E	599	69%27% . .
1	G	599	68%27% . .
2	B	74	% 73%19%5% .
2	D	74	3% 74%18%5% .

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Mol	Chain	Length	Quality of chain
2	F	74	% 72% 20% 5%
2	H	74	4% 74% 18% 5%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20908 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 [cytochrome c] subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	60	0	0
			4621	2948	778	875	20			
1	C	595	Total	C	N	O	S	60	0	0
			4621	2948	778	875	20			
1	E	595	Total	C	N	O	S	60	0	0
			4621	2948	778	875	20			
1	G	595	Total	C	N	O	S	60	0	0
			4621	2948	778	875	20			

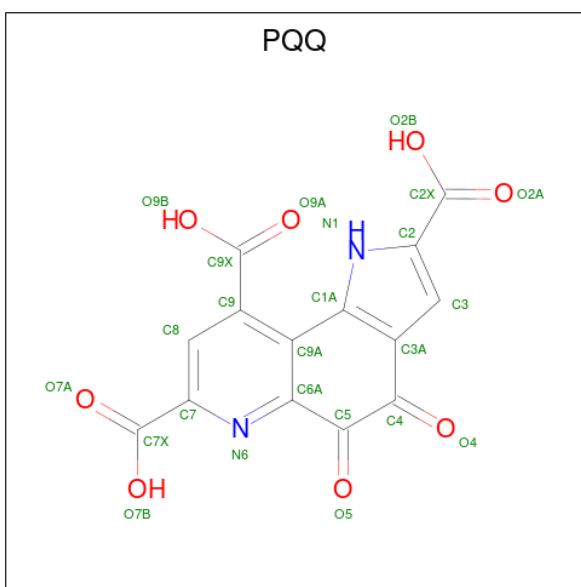
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	303	GLU	ASP	engineered mutation	UNP P16027
C	303	GLU	ASP	engineered mutation	UNP P16027
E	303	GLU	ASP	engineered mutation	UNP P16027
G	303	GLU	ASP	engineered mutation	UNP P16027

- Molecule 2 is a protein called Methanol dehydrogenase [cytochrome c] subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	72	Total	C	N	O	S	32	0	0
			581	366	102	110	3			
2	D	72	Total	C	N	O	S	32	0	0
			581	366	102	110	3			
2	F	72	Total	C	N	O	S	32	0	0
			581	366	102	110	3			
2	H	72	Total	C	N	O	S	32	0	0
			581	366	102	110	3			

- Molecule 3 is PYRROLOQUINOLINE QUINONE (CCD ID: PQQ) (formula: C₁₄H₆N₂O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			24	14	2	8		
3	C	1	Total	C	N	O	0	0
			24	14	2	8		
3	E	1	Total	C	N	O	0	0
			24	14	2	8		
3	G	1	Total	C	N	O	0	0
			24	14	2	8		

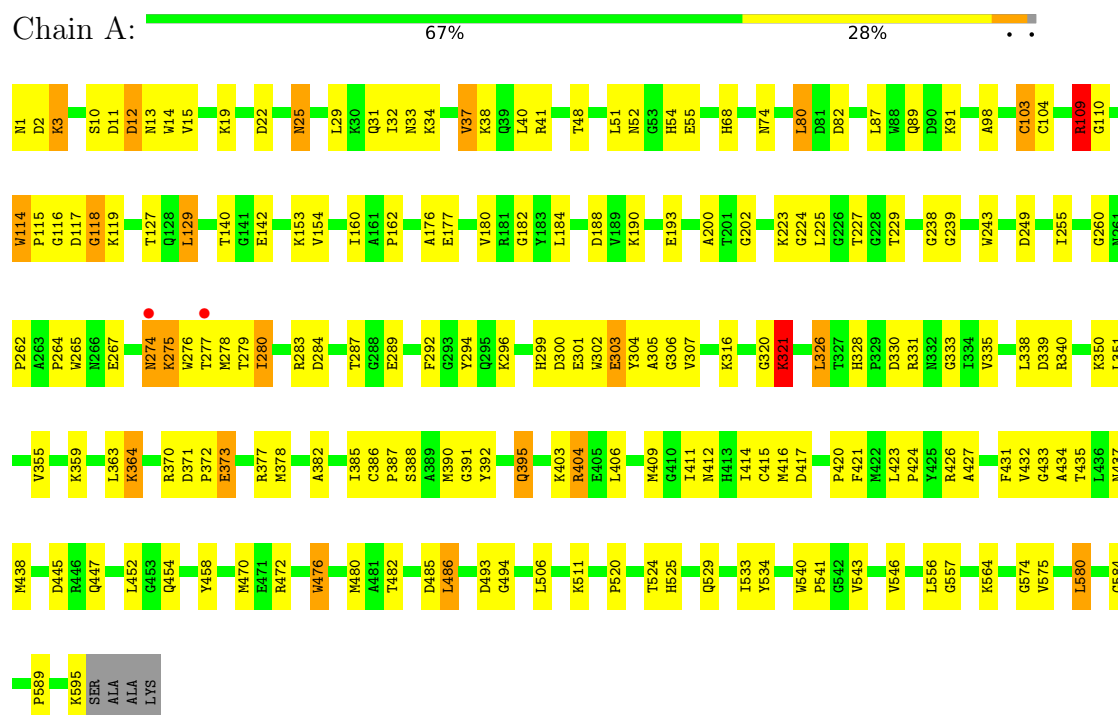
- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Ca	0	0
			1	1		
4	C	1	Total	Ca	0	0
			1	1		
4	E	1	Total	Ca	0	0
			1	1		
4	G	1	Total	Ca	0	0
			1	1		

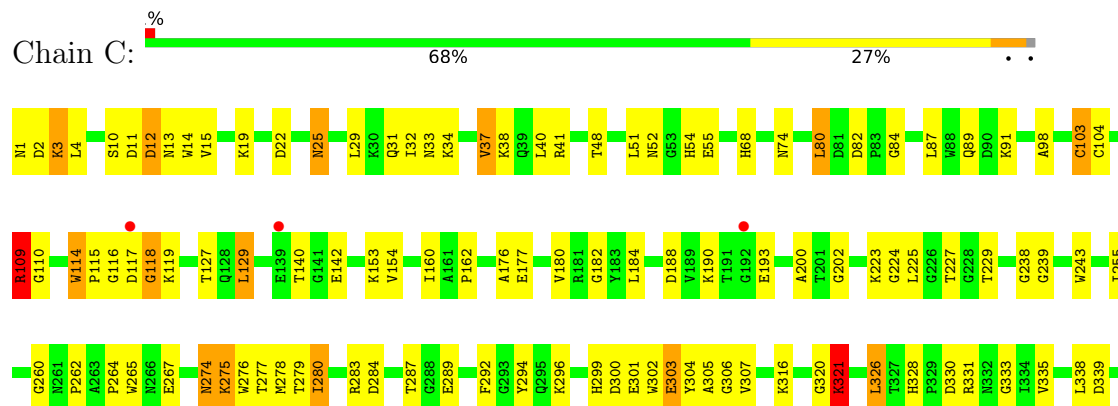
3 Residue-property plots [i](#)

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

- Molecule 1: Methanol dehydrogenase [cytochrome c] subunit 1



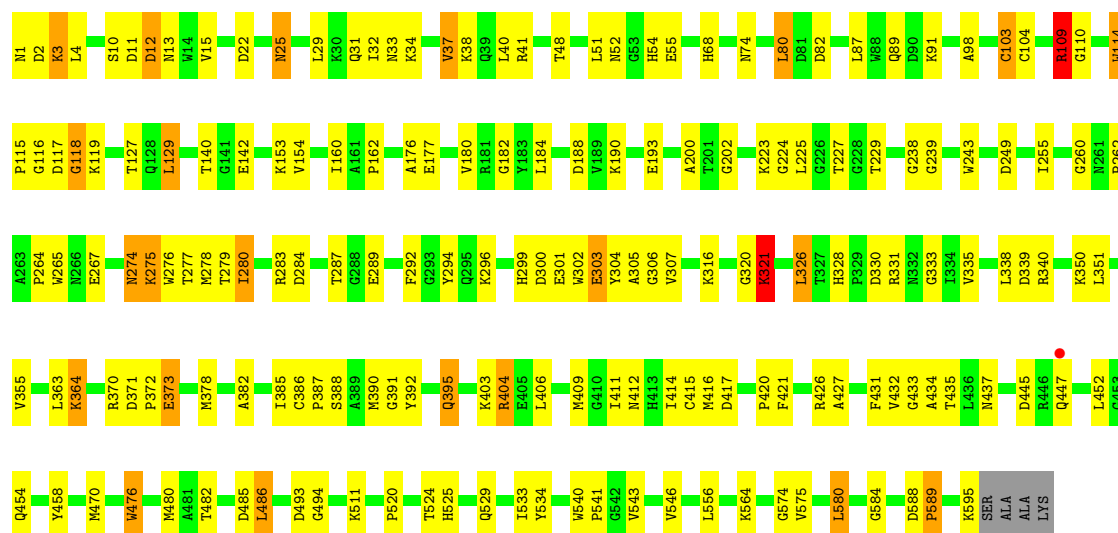
- Molecule 1: Methanol dehydrogenase [cytochrome c] subunit 1





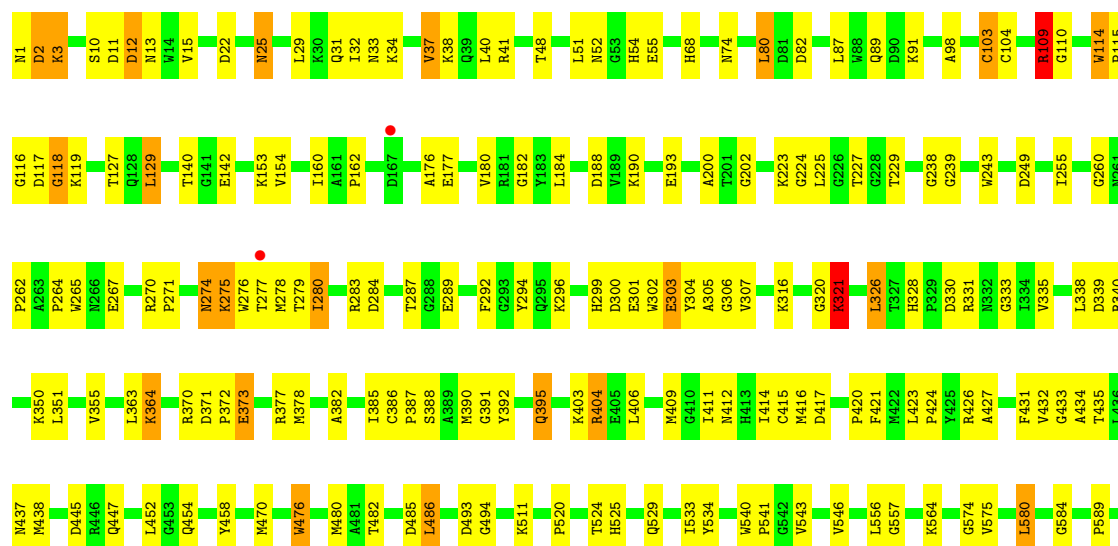
- Molecule 1: Methanol dehydrogenase [cytochrome c] subunit 1

Chain E: 69% 27%



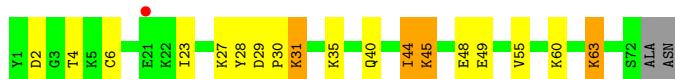
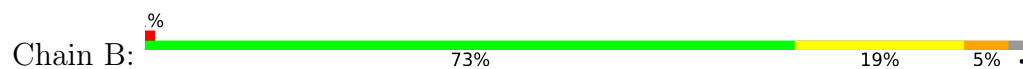
- Molecule 1: Methanol dehydrogenase [cytochrome c] subunit 1

Chain G: 68% 27%

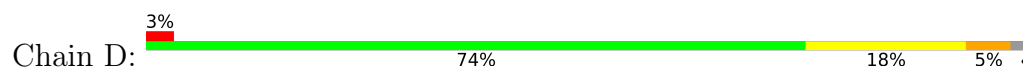




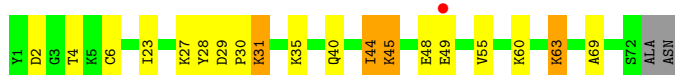
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



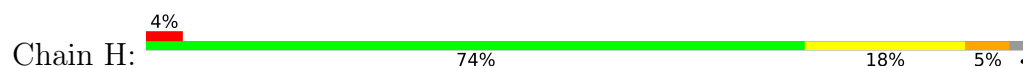
- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



- Molecule 2: Methanol dehydrogenase [cytochrome c] subunit 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.85Å 61.02Å 212.68Å 90.00° 92.83° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 20.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.5 (20.00-3.00) 90.9 (20.00-3.00)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.65 (at 3.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , 0.217 0.198 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	30.6	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 24.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.013 for h,-k,-l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	20908	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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	0.63	1/4751 (0.0%)	1.11	33/6457 (0.5%)
1	C	0.63	1/4751 (0.0%)	1.11	31/6457 (0.5%)
1	E	0.63	1/4751 (0.0%)	1.11	32/6457 (0.5%)
1	G	0.63	1/4751 (0.0%)	1.11	33/6457 (0.5%)
2	B	0.56	0/594	1.17	7/791 (0.9%)
2	D	0.56	0/594	1.17	7/791 (0.9%)
2	F	0.56	0/594	1.17	7/791 (0.9%)
2	H	0.56	0/594	1.17	7/791 (0.9%)
All	All	0.62	4/21380 (0.0%)	1.11	157/28992 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	E	0	1
1	G	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	275	LYS	C-N	5.25	1.40	1.33
1	C	275	LYS	C-N	5.23	1.40	1.33
1	G	275	LYS	C-N	5.22	1.40	1.33
1	E	275	LYS	C-N	5.21	1.40	1.33

All (157) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	476	TRP	N-CA-C	20.08	134.80	111.71
1	A	476	TRP	N-CA-C	20.06	134.78	111.71
1	G	476	TRP	N-CA-C	20.06	134.78	111.71
1	E	476	TRP	N-CA-C	20.04	134.76	111.71
1	G	2	ASP	O-C-N	-9.94	110.81	122.15
1	A	2	ASP	O-C-N	-9.94	110.82	122.15
1	E	2	ASP	O-C-N	-9.93	110.83	122.15
1	C	2	ASP	O-C-N	-9.91	110.85	122.15
2	F	44	ILE	CA-C-N	-7.86	107.60	120.72
2	F	44	ILE	C-N-CA	-7.86	107.60	120.72
2	B	44	ILE	CA-C-N	-7.85	107.61	120.72
2	B	44	ILE	C-N-CA	-7.85	107.61	120.72
2	D	44	ILE	CA-C-N	-7.84	107.62	120.72
2	D	44	ILE	C-N-CA	-7.84	107.62	120.72
2	H	44	ILE	CA-C-N	-7.83	107.65	120.72
2	H	44	ILE	C-N-CA	-7.83	107.65	120.72
2	B	4	THR	CA-C-N	-7.64	112.45	123.00
2	B	4	THR	C-N-CA	-7.64	112.45	123.00
2	D	4	THR	CA-C-N	-7.63	112.47	123.00
2	D	4	THR	C-N-CA	-7.63	112.47	123.00
2	F	4	THR	CA-C-N	-7.63	112.47	123.00
2	F	4	THR	C-N-CA	-7.63	112.47	123.00
2	H	4	THR	CA-C-N	-7.60	112.52	123.00
2	H	4	THR	C-N-CA	-7.60	112.52	123.00
2	H	6	CYS	N-CA-C	7.57	120.86	108.52
2	F	6	CYS	N-CA-C	7.56	120.84	108.52
2	B	6	CYS	N-CA-C	7.55	120.83	108.52
2	D	6	CYS	N-CA-C	7.53	120.80	108.52
1	C	321	LYS	O-C-N	-7.17	114.11	122.93
1	G	321	LYS	O-C-N	-7.16	114.12	122.93
1	A	321	LYS	O-C-N	-7.15	114.13	122.93
1	E	321	LYS	O-C-N	-7.12	114.17	122.93
1	G	114	TRP	CA-C-N	6.83	127.39	119.47
1	G	114	TRP	C-N-CA	6.83	127.39	119.47
1	A	114	TRP	CA-C-N	6.83	127.39	119.47
1	A	114	TRP	C-N-CA	6.83	127.39	119.47
1	E	328	HIS	O-C-N	-6.82	115.81	121.27
1	C	114	TRP	CA-C-N	6.82	127.38	119.47
1	C	114	TRP	C-N-CA	6.82	127.38	119.47
1	E	114	TRP	CA-C-N	6.82	127.38	119.47
1	E	114	TRP	C-N-CA	6.82	127.38	119.47
1	A	328	HIS	O-C-N	-6.79	115.83	121.27
1	G	328	HIS	O-C-N	-6.79	115.83	121.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	328	HIS	O-C-N	-6.75	115.87	121.27
1	G	82	ASP	CA-C-N	6.69	126.64	119.28
1	G	82	ASP	C-N-CA	6.69	126.64	119.28
1	C	82	ASP	CA-C-N	6.68	126.63	119.28
1	C	82	ASP	C-N-CA	6.68	126.63	119.28
1	A	82	ASP	CA-C-N	6.65	126.59	119.28
1	A	82	ASP	C-N-CA	6.65	126.59	119.28
1	E	82	ASP	CA-C-N	6.61	126.55	119.28
1	E	82	ASP	C-N-CA	6.61	126.55	119.28
1	E	320	GLY	CA-C-N	6.42	129.93	120.95
1	E	320	GLY	C-N-CA	6.42	129.93	120.95
1	A	320	GLY	CA-C-N	6.40	129.91	120.95
1	A	320	GLY	C-N-CA	6.40	129.91	120.95
1	G	320	GLY	CA-C-N	6.39	129.90	120.95
1	G	320	GLY	C-N-CA	6.39	129.90	120.95
1	C	320	GLY	CA-C-N	6.39	129.90	120.95
1	C	320	GLY	C-N-CA	6.39	129.90	120.95
1	G	363	LEU	CA-C-N	-6.37	110.89	121.92
1	G	363	LEU	C-N-CA	-6.37	110.89	121.92
1	E	363	LEU	CA-C-N	-6.37	110.90	121.92
1	E	363	LEU	C-N-CA	-6.37	110.90	121.92
1	E	109	ARG	N-CA-C	6.37	120.77	113.19
1	A	363	LEU	CA-C-N	-6.37	110.91	121.92
1	A	363	LEU	C-N-CA	-6.37	110.91	121.92
1	C	363	LEU	CA-C-N	-6.37	110.91	121.92
1	C	363	LEU	C-N-CA	-6.37	110.91	121.92
1	A	109	ARG	N-CA-C	6.36	120.76	113.19
2	F	45	LYS	O-C-N	-6.36	113.91	122.43
2	H	45	LYS	O-C-N	-6.35	113.92	122.43
1	C	109	ARG	N-CA-C	6.35	120.74	113.19
2	B	45	LYS	O-C-N	-6.34	113.93	122.43
1	G	109	ARG	N-CA-C	6.34	120.74	113.19
2	D	63	LYS	O-C-N	-6.33	115.81	123.29
2	D	45	LYS	O-C-N	-6.33	113.95	122.43
2	F	63	LYS	O-C-N	-6.32	115.83	123.29
2	B	63	LYS	O-C-N	-6.31	115.84	123.29
2	H	63	LYS	O-C-N	-6.29	115.86	123.29
1	C	182	GLY	N-CA-C	6.23	119.10	111.93
1	A	182	GLY	N-CA-C	6.22	119.08	111.93
1	E	182	GLY	N-CA-C	6.20	119.06	111.93
1	E	15	VAL	N-CA-C	5.86	121.54	109.34
1	A	15	VAL	N-CA-C	5.85	121.51	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	15	VAL	N-CA-C	5.83	121.47	109.34
1	G	15	VAL	N-CA-C	5.83	121.47	109.34
1	E	103	CYS	N-CA-C	5.79	118.06	111.11
1	C	103	CYS	N-CA-C	5.78	118.05	111.11
1	A	103	CYS	N-CA-C	5.78	118.04	111.11
1	G	103	CYS	N-CA-C	5.75	118.01	111.11
1	E	202	GLY	CA-C-N	5.65	125.66	119.90
1	E	202	GLY	C-N-CA	5.65	125.66	119.90
1	C	202	GLY	CA-C-N	5.63	125.64	119.90
1	C	202	GLY	C-N-CA	5.63	125.64	119.90
1	A	202	GLY	CA-C-N	5.61	125.63	119.90
1	A	202	GLY	C-N-CA	5.61	125.63	119.90
1	G	202	GLY	CA-C-N	5.61	125.62	119.90
1	G	202	GLY	C-N-CA	5.61	125.62	119.90
1	C	1	ASN	CA-C-N	-5.61	112.33	120.29
1	C	1	ASN	C-N-CA	-5.61	112.33	120.29
1	A	1	ASN	CA-C-N	-5.58	112.37	120.29
1	A	1	ASN	C-N-CA	-5.58	112.37	120.29
1	G	1	ASN	CA-C-N	-5.58	112.37	120.29
1	G	1	ASN	C-N-CA	-5.58	112.37	120.29
1	E	1	ASN	CA-C-N	-5.56	112.40	120.29
1	E	1	ASN	C-N-CA	-5.56	112.40	120.29
1	C	584	GLY	CA-C-N	5.45	125.53	119.32
1	C	584	GLY	C-N-CA	5.45	125.53	119.32
1	A	404	ARG	CD-NE-CZ	-5.42	116.80	124.40
1	A	584	GLY	CA-C-N	5.42	125.50	119.32
1	A	584	GLY	C-N-CA	5.42	125.50	119.32
1	E	584	GLY	CA-C-N	5.42	125.50	119.32
1	E	584	GLY	C-N-CA	5.42	125.50	119.32
1	G	404	ARG	CD-NE-CZ	-5.41	116.82	124.40
1	G	584	GLY	CA-C-N	5.40	125.48	119.32
1	G	584	GLY	C-N-CA	5.40	125.48	119.32
1	C	404	ARG	CD-NE-CZ	-5.40	116.84	124.40
1	C	280	ILE	O-C-N	-5.39	116.79	122.83
1	G	280	ILE	O-C-N	-5.39	116.79	122.83
1	E	280	ILE	O-C-N	-5.39	116.80	122.83
1	E	404	ARG	CD-NE-CZ	-5.38	116.86	124.40
1	A	280	ILE	O-C-N	-5.38	116.81	122.83
1	G	182	GLY	N-CA-C	5.34	119.03	112.14
1	E	227	THR	N-CA-C	-5.27	107.50	114.04
1	G	54	HIS	ND1-CG-CD2	5.25	111.35	106.10
1	C	54	HIS	ND1-CG-CD2	5.25	111.35	106.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	HIS	ND1-CG-CD2	5.25	111.35	106.10
1	A	227	THR	N-CA-C	-5.24	107.54	114.04
1	G	227	THR	N-CA-C	-5.24	107.54	114.04
1	C	227	THR	N-CA-C	-5.23	107.55	114.04
1	E	54	HIS	ND1-CG-CD2	5.20	111.30	106.10
1	A	339	ASP	N-CA-C	-5.17	101.99	109.59
1	C	339	ASP	N-CA-C	-5.17	102.00	109.59
1	E	339	ASP	N-CA-C	-5.16	102.01	109.59
1	G	339	ASP	N-CA-C	-5.16	102.01	109.59
1	E	224	GLY	N-CA-C	5.14	122.38	115.59
1	G	224	GLY	N-CA-C	5.13	122.37	115.59
1	A	224	GLY	N-CA-C	5.13	122.37	115.59
1	C	22	ASP	N-CA-C	-5.13	106.53	112.89
1	C	224	GLY	N-CA-C	5.12	122.36	115.59
1	E	22	ASP	N-CA-C	-5.12	106.53	112.89
1	A	22	ASP	N-CA-C	-5.12	106.55	112.89
1	G	22	ASP	N-CA-C	-5.11	106.56	112.89
1	C	364	LYS	O-C-N	-5.09	115.67	122.49
1	C	330	ASP	N-CA-C	5.07	117.07	110.53
1	A	330	ASP	N-CA-C	5.06	117.06	110.53
1	E	330	ASP	N-CA-C	5.06	117.06	110.53
1	E	364	LYS	O-C-N	-5.05	115.72	122.49
1	G	546	VAL	N-CA-C	5.05	115.28	110.53
1	G	330	ASP	N-CA-C	5.05	117.04	110.53
1	A	364	LYS	O-C-N	-5.04	115.73	122.49
1	E	546	VAL	N-CA-C	5.04	115.26	110.53
1	G	377	ARG	CD-NE-CZ	-5.03	117.36	124.40
1	A	546	VAL	N-CA-C	5.02	115.25	110.53
1	G	364	LYS	O-C-N	-5.02	115.77	122.49
1	A	377	ARG	CD-NE-CZ	-5.01	117.39	124.40

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	274	ASN	Peptide
1	C	274	ASN	Peptide
1	E	274	ASN	Peptide
1	G	274	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4621	0	4441	138	0
1	C	4621	0	4441	142	0
1	E	4621	0	4441	132	0
1	G	4621	0	4441	134	0
2	B	581	0	579	11	0
2	D	581	0	577	10	0
2	F	581	0	579	12	0
2	H	581	0	579	15	0
3	A	24	0	3	1	0
3	C	24	0	3	1	0
3	E	24	0	3	1	0
3	G	24	0	3	1	0
4	A	1	0	0	0	0
4	C	1	0	0	0	0
4	E	1	0	0	0	0
4	G	1	0	0	0	0
All	All	20908	0	20090	569	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 14.

All (569) 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:C:284:ASP:HB3	1:C:287:THR:HG22	1.56	0.87
1:E:284:ASP:HB3	1:E:287:THR:HG22	1.56	0.87
1:G:284:ASP:HB3	1:G:287:THR:HG22	1.56	0.86
1:A:284:ASP:HB3	1:A:287:THR:HG22	1.56	0.86
1:G:154:VAL:HG11	2:H:40:GLN:HG2	1.63	0.81
1:E:154:VAL:HG11	2:F:40:GLN:HG2	1.63	0.79
1:C:154:VAL:HG11	2:D:40:GLN:HG2	1.63	0.78
1:A:333:GLY:HA2	1:A:351:LEU:HD12	1.66	0.78
1:A:154:VAL:HG11	2:B:40:GLN:HG2	1.63	0.78
1:C:454:GLN:HB3	1:C:470:MET:HE2	1.66	0.78
1:G:333:GLY:HA2	1:G:351:LEU:HD12	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:TRP:CZ3	1:A:116:GLY:HA2	2.19	0.77
1:E:114:TRP:CZ3	1:E:116:GLY:HA2	2.19	0.77
1:G:114:TRP:CZ3	1:G:116:GLY:HA2	2.19	0.77
1:C:333:GLY:HA2	1:C:351:LEU:HD12	1.66	0.77
1:E:51:LEU:O	1:E:52:ASN:HB2	1.85	0.77
1:C:114:TRP:CZ3	1:C:116:GLY:HA2	2.19	0.76
1:E:333:GLY:HA2	1:E:351:LEU:HD12	1.66	0.76
1:C:51:LEU:O	1:C:52:ASN:HB2	1.85	0.76
1:A:454:GLN:HB3	1:A:470:MET:HE2	1.66	0.76
1:E:454:GLN:HB3	1:E:470:MET:HE2	1.66	0.75
1:G:51:LEU:O	1:G:52:ASN:HB2	1.85	0.75
1:C:260:GLY:O	1:C:277:THR:HB	1.87	0.75
1:A:51:LEU:O	1:A:52:ASN:HB2	1.86	0.74
1:E:260:GLY:O	1:E:277:THR:HB	1.87	0.74
1:G:454:GLN:HB3	1:G:470:MET:HE2	1.66	0.74
1:G:411:ILE:HB	1:G:454:GLN:HG3	1.69	0.74
1:E:411:ILE:HB	1:E:454:GLN:HG3	1.69	0.74
1:A:225:LEU:HB3	1:A:275:LYS:HG2	1.70	0.74
1:A:260:GLY:O	1:A:277:THR:HB	1.87	0.74
1:G:260:GLY:O	1:G:277:THR:HB	1.87	0.74
1:E:225:LEU:HB3	1:E:275:LYS:HG2	1.70	0.74
1:G:225:LEU:HB3	1:G:275:LYS:HG2	1.70	0.73
1:C:225:LEU:HB3	1:C:275:LYS:HG2	1.70	0.73
1:C:411:ILE:HB	1:C:454:GLN:HG3	1.69	0.73
1:A:411:ILE:HB	1:A:454:GLN:HG3	1.70	0.73
1:A:378:MET:HE1	1:A:421:PHE:HA	1.72	0.72
1:C:378:MET:HE1	1:C:421:PHE:HA	1.72	0.71
1:G:378:MET:HE1	1:G:421:PHE:HA	1.72	0.71
1:E:378:MET:HE1	1:E:421:PHE:HA	1.72	0.70
1:G:12:ASP:HB3	1:G:524:THR:O	1.94	0.68
1:G:284:ASP:HB3	1:G:287:THR:CG2	2.24	0.67
1:C:12:ASP:HB3	1:C:524:THR:O	1.94	0.67
1:C:37:VAL:HG22	1:C:486:LEU:HD21	1.76	0.67
1:E:284:ASP:HB3	1:E:287:THR:CG2	2.24	0.67
1:G:350:LYS:HD3	1:G:355:VAL:HB	1.76	0.67
1:C:350:LYS:HD3	1:C:355:VAL:HB	1.76	0.67
1:A:12:ASP:HB3	1:A:524:THR:O	1.94	0.67
1:A:284:ASP:HB3	1:A:287:THR:CG2	2.24	0.67
1:C:284:ASP:HB3	1:C:287:THR:CG2	2.24	0.67
1:A:350:LYS:HD3	1:A:355:VAL:HB	1.76	0.67
1:A:37:VAL:HG22	1:A:486:LEU:HD21	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:350:LYS:HD3	1:E:355:VAL:HB	1.76	0.66
1:E:12:ASP:HB3	1:E:524:THR:O	1.94	0.66
1:G:287:THR:HG23	1:G:289:GLU:H	1.61	0.65
1:E:37:VAL:HG22	1:E:486:LEU:HD21	1.77	0.65
1:G:37:VAL:HG22	1:G:486:LEU:HD21	1.76	0.65
1:E:287:THR:HG23	1:E:289:GLU:H	1.61	0.65
1:E:284:ASP:CB	1:E:287:THR:HG22	2.27	0.65
1:C:98:ALA:HB1	1:C:129:LEU:HD13	1.79	0.64
1:G:284:ASP:CB	1:G:287:THR:HG22	2.27	0.64
1:C:287:THR:HG23	1:C:289:GLU:H	1.61	0.64
1:G:98:ALA:HB1	1:G:129:LEU:HD13	1.79	0.64
1:A:287:THR:HG23	1:A:289:GLU:H	1.61	0.64
1:E:98:ALA:HB1	1:E:129:LEU:HD13	1.79	0.64
1:A:98:ALA:HB1	1:A:129:LEU:HD13	1.79	0.63
1:E:387:PRO:HB3	1:E:392:TYR:CD1	2.34	0.63
1:A:387:PRO:HB3	1:A:392:TYR:CD1	2.34	0.62
1:C:387:PRO:HB3	1:C:392:TYR:CD1	2.34	0.62
1:G:176:ALA:HB3	3:G:601:PQQ:O7B	1.99	0.62
1:A:229:THR:OG1	1:A:275:LYS:HB2	2.00	0.62
1:A:176:ALA:HB3	3:A:601:PQQ:O7B	1.99	0.62
1:C:284:ASP:CB	1:C:287:THR:HG22	2.27	0.62
1:A:284:ASP:CB	1:A:287:THR:HG22	2.28	0.62
1:G:229:THR:OG1	1:G:275:LYS:HB2	2.00	0.62
1:G:387:PRO:HB3	1:G:392:TYR:CD1	2.34	0.62
1:C:176:ALA:HB3	3:C:601:PQQ:O7B	1.99	0.62
1:E:176:ALA:HB3	3:E:601:PQQ:O7B	1.99	0.61
1:E:200:ALA:O	1:E:276:TRP:HB2	2.00	0.61
1:G:200:ALA:O	1:G:276:TRP:HB2	2.00	0.61
1:E:229:THR:OG1	1:E:275:LYS:HB2	2.00	0.61
1:C:229:THR:OG1	1:C:275:LYS:HB2	2.00	0.61
1:E:382:ALA:HB1	1:E:385:ILE:HD11	1.83	0.61
1:A:382:ALA:HB1	1:A:385:ILE:HD11	1.83	0.61
1:C:382:ALA:HB1	1:C:385:ILE:HD11	1.83	0.61
1:C:200:ALA:O	1:C:276:TRP:HB2	2.00	0.61
1:G:382:ALA:HB1	1:G:385:ILE:HD11	1.83	0.61
1:E:265:TRP:CE2	1:E:303:GLU:HG3	2.36	0.61
1:A:200:ALA:O	1:A:276:TRP:HB2	2.00	0.60
1:A:278:MET:HE1	1:A:304:TYR:C	2.26	0.60
1:G:333:GLY:CA	1:G:351:LEU:HD12	2.32	0.60
1:C:278:MET:HE1	1:C:304:TYR:C	2.26	0.60
1:C:333:GLY:CA	1:C:351:LEU:HD12	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:MET:HE1	1:E:304:TYR:C	2.26	0.60
1:G:278:MET:HE1	1:G:304:TYR:C	2.26	0.60
2:D:27:LYS:HD2	2:D:28:TYR:CE1	2.37	0.60
1:A:265:TRP:CE2	1:A:303:GLU:HG3	2.36	0.60
1:C:265:TRP:CE2	1:C:303:GLU:HG3	2.36	0.60
1:C:279:THR:HG23	1:C:294:TYR:C	2.28	0.59
1:G:154:VAL:CG1	2:H:40:GLN:HG2	2.32	0.59
1:E:279:THR:HG23	1:E:294:TYR:C	2.27	0.59
1:G:265:TRP:CE2	1:G:303:GLU:HG3	2.36	0.59
1:A:279:THR:HG23	1:A:294:TYR:C	2.27	0.59
1:E:154:VAL:CG1	2:F:40:GLN:HG2	2.32	0.59
1:G:32:ILE:HD13	1:G:40:LEU:HD11	1.85	0.59
1:G:279:THR:HG23	1:G:294:TYR:C	2.27	0.59
2:B:27:LYS:HD2	2:B:28:TYR:CE1	2.37	0.59
2:F:27:LYS:HD2	2:F:28:TYR:CE1	2.37	0.59
1:C:32:ILE:HD13	1:C:40:LEU:HD11	1.85	0.59
1:C:154:VAL:CG1	2:D:40:GLN:HG2	2.32	0.59
2:H:27:LYS:HD2	2:H:28:TYR:CE1	2.37	0.59
1:E:32:ILE:HD13	1:E:40:LEU:HD11	1.85	0.58
1:A:68:HIS:CE1	1:A:110:GLY:HA2	2.38	0.58
1:E:68:HIS:CE1	1:E:110:GLY:HA2	2.38	0.58
1:C:68:HIS:CE1	1:C:110:GLY:HA2	2.38	0.58
1:C:114:TRP:HH2	1:C:117:ASP:OD1	1.87	0.58
1:A:296:LYS:HZ1	1:A:306:GLY:CA	2.17	0.58
1:G:68:HIS:CE1	1:G:110:GLY:HA2	2.38	0.58
1:A:32:ILE:HD13	1:A:40:LEU:HD11	1.85	0.57
1:A:154:VAL:CG1	2:B:40:GLN:HG2	2.32	0.57
1:A:333:GLY:CA	1:A:351:LEU:HD12	2.32	0.57
1:C:265:TRP:CD2	1:C:432:VAL:HG13	2.40	0.57
1:E:333:GLY:CA	1:E:351:LEU:HD12	2.32	0.57
1:G:265:TRP:CD2	1:G:432:VAL:HG13	2.40	0.57
1:A:296:LYS:HZ1	1:A:306:GLY:HA3	1.69	0.57
1:E:114:TRP:HH2	1:E:117:ASP:OD1	1.87	0.57
1:A:493:ASP:OD1	1:A:493:ASP:N	2.38	0.57
1:A:506:LEU:HG	1:C:589:PRO:HB2	1.85	0.57
1:A:265:TRP:CD2	1:A:432:VAL:HG13	2.40	0.57
1:G:114:TRP:HH2	1:G:117:ASP:OD1	1.87	0.56
1:A:114:TRP:HH2	1:A:117:ASP:OD1	1.87	0.56
1:C:493:ASP:OD1	1:C:493:ASP:N	2.38	0.56
1:E:265:TRP:CD2	1:E:432:VAL:HG13	2.40	0.56
1:E:370:ARG:HB2	2:F:2:ASP:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:ARG:HB2	2:B:2:ASP:HA	1.88	0.55
1:C:370:ARG:HB2	2:D:2:ASP:HA	1.88	0.55
1:G:370:ARG:HB2	2:H:2:ASP:HA	1.88	0.55
1:A:154:VAL:HG12	1:A:154:VAL:O	2.07	0.55
1:C:154:VAL:HG12	1:C:154:VAL:O	2.07	0.55
1:E:335:VAL:HG11	1:E:458:TYR:CE2	2.42	0.54
1:G:335:VAL:HG11	1:G:458:TYR:CE2	2.42	0.54
1:C:238:GLY:O	1:C:262:PRO:HA	2.07	0.54
1:A:127:THR:HG23	1:A:162:PRO:HG3	1.90	0.54
1:C:326:LEU:C	1:C:326:LEU:HD12	2.33	0.54
1:C:335:VAL:HG11	1:C:458:TYR:CE2	2.42	0.54
1:G:301:GLU:HG3	1:G:302:TRP:CE2	2.43	0.54
1:C:140:THR:HG22	2:H:27:LYS:NZ	2.23	0.54
1:A:301:GLU:HG3	1:A:302:TRP:CE2	2.43	0.54
1:E:326:LEU:C	1:E:326:LEU:HD12	2.33	0.54
1:G:238:GLY:O	1:G:262:PRO:HA	2.07	0.54
1:C:48:THR:HG23	1:C:574:GLY:HA2	1.90	0.53
1:C:409:MET:HB2	1:C:411:ILE:HD11	1.90	0.53
1:E:238:GLY:O	1:E:262:PRO:HA	2.07	0.53
1:G:127:THR:HG23	1:G:162:PRO:HG3	1.90	0.53
1:A:238:GLY:O	1:A:262:PRO:HA	2.07	0.53
1:A:409:MET:HB2	1:A:411:ILE:HD11	1.91	0.53
1:C:127:THR:HG23	1:C:162:PRO:HG3	1.89	0.53
1:A:335:VAL:HG11	1:A:458:TYR:CE2	2.42	0.53
1:C:301:GLU:HG3	1:C:302:TRP:CE2	2.43	0.53
1:C:382:ALA:CB	1:C:385:ILE:HD11	2.39	0.53
1:E:301:GLU:HG3	1:E:302:TRP:CE2	2.43	0.53
1:E:409:MET:HB2	1:E:411:ILE:HD11	1.91	0.53
1:G:370:ARG:O	1:G:372:PRO:HD3	2.09	0.53
1:G:395:GLN:O	1:G:395:GLN:HG2	2.08	0.53
1:C:386:CYS:HB3	1:C:392:TYR:OH	2.09	0.53
1:E:386:CYS:HB3	1:E:392:TYR:OH	2.09	0.53
1:G:326:LEU:C	1:G:326:LEU:HD12	2.33	0.53
1:G:386:CYS:HB3	1:G:392:TYR:OH	2.09	0.53
1:A:255:ILE:HG22	1:A:283:ARG:HB2	1.91	0.53
1:E:127:THR:HG23	1:E:162:PRO:HG3	1.89	0.53
1:A:180:VAL:O	1:A:239:GLY:HA2	2.09	0.53
1:A:326:LEU:HD12	1:A:326:LEU:C	2.33	0.53
1:A:395:GLN:HG2	1:A:395:GLN:O	2.09	0.53
1:E:382:ALA:CB	1:E:385:ILE:HD11	2.39	0.53
1:A:48:THR:HG23	1:A:574:GLY:HA2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:180:VAL:O	1:E:239:GLY:HA2	2.09	0.53
1:G:296:LYS:HZ1	1:G:306:GLY:CA	2.21	0.53
1:A:386:CYS:HB3	1:A:392:TYR:OH	2.09	0.53
1:C:395:GLN:O	1:C:395:GLN:HG2	2.09	0.53
1:G:382:ALA:CB	1:G:385:ILE:HD11	2.39	0.53
1:G:421:PHE:CE1	1:G:433:GLY:HA2	2.44	0.53
1:C:421:PHE:CE1	1:C:433:GLY:HA2	2.44	0.53
1:E:10:SER:HB3	1:E:13:ASN:HD22	1.74	0.53
1:E:154:VAL:HG12	1:E:154:VAL:O	2.07	0.53
1:G:103:CYS:SG	1:G:104:CYS:N	2.82	0.53
1:G:154:VAL:O	1:G:154:VAL:HG12	2.07	0.53
1:C:103:CYS:SG	1:C:104:CYS:N	2.82	0.52
1:E:255:ILE:HG22	1:E:283:ARG:HB2	1.91	0.52
1:G:180:VAL:O	1:G:239:GLY:HA2	2.09	0.52
1:G:48:THR:HG23	1:G:574:GLY:HA2	1.90	0.52
1:A:382:ALA:CB	1:A:385:ILE:HD11	2.39	0.52
2:B:23:ILE:HD12	2:B:30:PRO:HD3	1.91	0.52
1:C:296:LYS:HZ1	1:C:306:GLY:CA	2.22	0.52
1:A:103:CYS:SG	1:A:104:CYS:N	2.82	0.52
1:A:370:ARG:O	1:A:372:PRO:HD3	2.09	0.52
1:A:10:SER:HB3	1:A:13:ASN:HD22	1.74	0.52
1:A:421:PHE:CE1	1:A:433:GLY:HA2	2.44	0.52
1:G:409:MET:HB2	1:G:411:ILE:HD11	1.91	0.52
1:G:493:ASP:N	1:G:493:ASP:OD1	2.38	0.52
1:E:370:ARG:O	1:E:372:PRO:HD3	2.09	0.52
1:E:395:GLN:O	1:E:395:GLN:HG2	2.09	0.52
1:C:10:SER:HB3	1:C:13:ASN:HD22	1.74	0.52
1:C:370:ARG:O	1:C:372:PRO:HD3	2.09	0.52
1:E:103:CYS:SG	1:E:104:CYS:N	2.82	0.52
1:E:421:PHE:CE1	1:E:433:GLY:HA2	2.44	0.52
2:D:23:ILE:HD12	2:D:30:PRO:HD3	1.91	0.52
2:H:23:ILE:HD12	2:H:30:PRO:HD3	1.91	0.52
1:A:74:ASN:HD22	1:A:91:LYS:HA	1.75	0.51
1:A:476:TRP:CZ2	1:A:541:PRO:HD3	2.46	0.51
1:C:74:ASN:HD22	1:C:91:LYS:HA	1.76	0.51
1:C:180:VAL:O	1:C:239:GLY:HA2	2.09	0.51
1:C:255:ILE:HG22	1:C:283:ARG:HB2	1.91	0.51
1:G:296:LYS:HZ1	1:G:306:GLY:HA3	1.75	0.51
1:G:388:SER:HB2	1:G:416:MET:HB3	1.92	0.51
1:E:48:THR:HG23	1:E:574:GLY:HA2	1.91	0.51
2:F:23:ILE:HD12	2:F:30:PRO:HD3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:371:ASP:OD1	1:G:373:GLU:HB2	2.11	0.51
1:C:388:SER:HB2	1:C:416:MET:HB3	1.92	0.51
1:A:371:ASP:OD1	1:A:373:GLU:HB2	2.11	0.51
1:E:476:TRP:CZ2	1:E:541:PRO:HD3	2.45	0.51
1:G:10:SER:HB3	1:G:13:ASN:HD22	1.74	0.51
1:G:255:ILE:HG22	1:G:283:ARG:HB2	1.91	0.51
1:E:74:ASN:HD22	1:E:91:LYS:HA	1.75	0.51
1:C:476:TRP:CZ2	1:C:541:PRO:HD3	2.46	0.51
1:C:188:ASP:OD1	1:C:190:LYS:HB2	2.11	0.51
1:E:388:SER:HB2	1:E:416:MET:HB3	1.92	0.50
1:G:476:TRP:CZ2	1:G:541:PRO:HD3	2.45	0.50
1:C:388:SER:HA	1:C:416:MET:HE2	1.93	0.50
1:G:388:SER:HA	1:G:416:MET:HE2	1.93	0.50
2:D:27:LYS:O	2:D:27:LYS:HG2	2.12	0.50
1:E:371:ASP:OD1	1:E:373:GLU:HB2	2.11	0.50
1:A:188:ASP:OD1	1:A:190:LYS:HB2	2.11	0.50
1:G:74:ASN:HD22	1:G:91:LYS:HA	1.75	0.50
1:C:296:LYS:HZ1	1:C:306:GLY:HA3	1.77	0.50
2:F:27:LYS:O	2:F:27:LYS:HG2	2.11	0.50
1:A:388:SER:HA	1:A:416:MET:HE2	1.93	0.50
1:C:371:ASP:OD1	1:C:373:GLU:HB2	2.11	0.50
1:E:388:SER:HA	1:E:416:MET:HE2	1.93	0.50
1:G:188:ASP:OD1	1:G:190:LYS:HB2	2.11	0.50
1:E:188:ASP:OD1	1:E:190:LYS:HB2	2.11	0.49
1:A:388:SER:HB2	1:A:416:MET:HB3	1.92	0.49
1:A:267:GLU:HG2	1:A:299:HIS:NE2	2.28	0.49
1:A:278:MET:HE2	1:A:300:ASP:CG	2.37	0.49
2:B:27:LYS:O	2:B:27:LYS:HG2	2.12	0.49
1:G:278:MET:HE2	1:G:300:ASP:CG	2.37	0.49
1:A:540:TRP:N	1:A:541:PRO:HD2	2.28	0.49
1:C:267:GLU:HG2	1:C:299:HIS:NE2	2.28	0.49
1:C:278:MET:HE2	1:C:300:ASP:CG	2.37	0.49
1:C:540:TRP:N	1:C:541:PRO:HD2	2.28	0.49
1:E:426:ARG:O	1:E:427:ALA:C	2.54	0.49
1:E:540:TRP:N	1:E:541:PRO:HD2	2.28	0.49
1:G:426:ARG:O	1:G:427:ALA:C	2.54	0.49
1:C:140:THR:HB	2:H:27:LYS:CE	2.43	0.49
1:C:426:ARG:O	1:C:427:ALA:C	2.54	0.49
1:E:37:VAL:HG21	1:E:486:LEU:HD11	1.95	0.49
1:E:267:GLU:HG2	1:E:299:HIS:NE2	2.28	0.49
1:E:493:ASP:OD1	1:E:493:ASP:N	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:74:ASN:ND2	1:E:91:LYS:HA	2.28	0.49
1:E:278:MET:HE2	1:E:300:ASP:CG	2.37	0.49
1:G:74:ASN:ND2	1:G:91:LYS:HA	2.28	0.49
2:H:27:LYS:O	2:H:27:LYS:HG2	2.12	0.49
1:A:37:VAL:HG21	1:A:486:LEU:HD11	1.95	0.48
1:G:32:ILE:HG12	1:G:580:LEU:HD13	1.96	0.48
1:A:74:ASN:ND2	1:A:91:LYS:HA	2.28	0.48
1:C:74:ASN:ND2	1:C:91:LYS:HA	2.28	0.48
1:G:540:TRP:N	1:G:541:PRO:HD2	2.28	0.48
1:A:32:ILE:HG12	1:A:580:LEU:HD13	1.96	0.48
1:E:264:PRO:HD3	1:E:431:PHE:CE2	2.49	0.48
1:A:316:LYS:HA	1:A:321:LYS:O	2.14	0.48
1:E:32:ILE:HG12	1:E:580:LEU:HD13	1.96	0.48
1:G:267:GLU:HG2	1:G:299:HIS:NE2	2.28	0.48
1:A:426:ARG:O	1:A:427:ALA:C	2.54	0.48
1:C:520:PRO:HG3	1:C:533:ILE:HD12	1.96	0.48
1:C:316:LYS:HA	1:C:321:LYS:O	2.14	0.47
1:E:520:PRO:HG3	1:E:533:ILE:HD12	1.96	0.47
1:G:264:PRO:HD3	1:G:431:PHE:CE2	2.49	0.47
1:A:184:LEU:HD23	1:A:184:LEU:H	1.79	0.47
1:A:264:PRO:HD3	1:A:431:PHE:CE2	2.49	0.47
1:E:184:LEU:H	1:E:184:LEU:HD23	1.79	0.47
1:E:301:GLU:HG3	1:E:302:TRP:CZ2	2.49	0.47
1:A:520:PRO:HG3	1:A:533:ILE:HD12	1.96	0.47
1:E:296:LYS:HZ1	1:E:306:GLY:CA	2.26	0.47
1:E:420:PRO:HA	1:E:434:ALA:HA	1.96	0.47
1:G:37:VAL:HG21	1:G:486:LEU:HD11	1.95	0.47
1:C:301:GLU:HG3	1:C:302:TRP:CZ2	2.49	0.47
1:C:32:ILE:HG12	1:C:580:LEU:HD13	1.96	0.47
1:C:264:PRO:HD3	1:C:431:PHE:CE2	2.49	0.47
1:E:80:LEU:HB3	1:E:525:HIS:CE1	2.50	0.47
1:E:316:LYS:HA	1:E:321:LYS:O	2.14	0.47
1:G:316:LYS:HA	1:G:321:LYS:O	2.14	0.47
1:A:80:LEU:HB3	1:A:525:HIS:CE1	2.50	0.47
1:E:304:TYR:O	1:E:305:ALA:C	2.58	0.47
1:G:301:GLU:HG3	1:G:302:TRP:CZ2	2.49	0.47
1:C:80:LEU:HB3	1:C:525:HIS:CE1	2.50	0.47
1:E:409:MET:HE2	1:E:458:TYR:HB3	1.97	0.47
1:G:184:LEU:HD23	1:G:184:LEU:H	1.79	0.47
1:A:301:GLU:HG3	1:A:302:TRP:CZ2	2.49	0.47
1:C:420:PRO:HA	1:C:434:ALA:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:80:LEU:HB3	1:G:525:HIS:CE1	2.50	0.47
1:C:31:GLN:HB3	1:C:529:GLN:OE1	2.15	0.47
1:C:184:LEU:H	1:C:184:LEU:HD23	1.79	0.47
1:C:304:TYR:O	1:C:305:ALA:C	2.58	0.47
1:G:284:ASP:OD2	1:G:287:THR:HG22	2.15	0.47
1:C:33:ASN:HA	1:C:486:LEU:HD22	1.97	0.46
1:E:89:GLN:OE1	1:E:91:LYS:HE3	2.15	0.46
1:A:31:GLN:HB3	1:A:529:GLN:OE1	2.15	0.46
1:A:409:MET:HE2	1:A:458:TYR:HB3	1.97	0.46
1:E:31:GLN:HB3	1:E:529:GLN:OE1	2.15	0.46
1:G:33:ASN:HA	1:G:486:LEU:HD22	1.97	0.46
1:C:37:VAL:HG21	1:C:486:LEU:HD11	1.95	0.46
2:D:30:PRO:O	2:D:31:LYS:HB2	2.16	0.46
1:C:89:GLN:OE1	1:C:91:LYS:HE3	2.15	0.46
1:G:520:PRO:HG3	1:G:533:ILE:HD12	1.96	0.46
1:A:284:ASP:OD2	1:A:287:THR:HG22	2.15	0.46
1:C:284:ASP:OD2	1:C:287:THR:HG22	2.15	0.46
2:B:30:PRO:O	2:B:31:LYS:HB2	2.16	0.46
1:G:420:PRO:HA	1:G:434:ALA:HA	1.96	0.46
1:G:89:GLN:OE1	1:G:91:LYS:HE3	2.15	0.46
1:A:33:ASN:HA	1:A:486:LEU:HD22	1.97	0.46
1:A:89:GLN:OE1	1:A:91:LYS:HE3	2.15	0.46
1:A:556:LEU:N	1:A:556:LEU:HD12	2.31	0.46
1:C:335:VAL:HG23	1:C:351:LEU:HG	1.98	0.46
1:G:31:GLN:HB3	1:G:529:GLN:OE1	2.15	0.46
1:G:335:VAL:HG23	1:G:351:LEU:HG	1.98	0.46
1:E:193:GLU:HB2	2:F:55:VAL:HG11	1.98	0.46
1:G:409:MET:HE2	1:G:458:TYR:HB3	1.97	0.46
1:A:333:GLY:C	1:A:351:LEU:HD12	2.41	0.46
1:A:420:PRO:HA	1:A:434:ALA:HA	1.96	0.46
1:E:32:ILE:HD13	1:E:40:LEU:CD1	2.46	0.46
1:E:284:ASP:OD2	1:E:287:THR:HG22	2.15	0.46
1:G:34:LYS:HA	1:G:37:VAL:HG23	1.98	0.46
2:H:30:PRO:O	2:H:31:LYS:HB2	2.16	0.46
1:C:556:LEU:N	1:C:556:LEU:HD12	2.31	0.45
1:E:333:GLY:C	1:E:351:LEU:HD12	2.41	0.45
1:E:335:VAL:HG23	1:E:351:LEU:HG	1.98	0.45
1:G:304:TYR:O	1:G:305:ALA:C	2.58	0.45
1:E:11:ASP:HB3	1:E:29:LEU:HD21	1.98	0.45
1:E:296:LYS:HZ1	1:E:306:GLY:HA3	1.81	0.45
1:G:193:GLU:HB2	2:H:55:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:LYS:HA	1:A:37:VAL:CG2	2.47	0.45
1:A:304:TYR:O	1:A:305:ALA:C	2.58	0.45
1:C:333:GLY:C	1:C:351:LEU:HD12	2.41	0.45
1:E:556:LEU:N	1:E:556:LEU:HD12	2.31	0.45
1:G:11:ASP:HB3	1:G:29:LEU:HD21	1.98	0.45
1:C:193:GLU:HB2	2:D:55:VAL:HG11	1.98	0.45
1:C:409:MET:HE2	1:C:458:TYR:HB3	1.97	0.45
1:E:480:MET:HE3	1:E:482:THR:HG23	1.99	0.45
1:A:335:VAL:HG23	1:A:351:LEU:HG	1.98	0.45
1:A:193:GLU:HB2	2:B:55:VAL:HG11	1.98	0.45
1:A:511:LYS:HE3	1:C:84:GLY:HA2	1.97	0.45
1:E:404:ARG:NH2	1:E:485:ASP:OD1	2.50	0.45
2:F:30:PRO:O	2:F:31:LYS:HB2	2.16	0.45
1:G:404:ARG:NH2	1:G:485:ASP:OD1	2.50	0.45
1:E:33:ASN:HA	1:E:486:LEU:HD22	1.97	0.45
1:E:34:LYS:HA	1:E:37:VAL:CG2	2.47	0.45
1:E:117:ASP:CG	1:E:118:GLY:H	2.25	0.45
1:E:388:SER:CB	1:E:416:MET:HB3	2.47	0.45
1:G:25:ASN:HD22	1:G:25:ASN:HA	1.46	0.45
1:A:117:ASP:CG	1:A:118:GLY:H	2.25	0.45
1:C:32:ILE:HD13	1:C:40:LEU:CD1	2.46	0.45
1:G:480:MET:HE3	1:G:482:THR:HG23	1.99	0.45
1:A:11:ASP:HB3	1:A:29:LEU:HD21	1.98	0.45
1:G:388:SER:CB	1:G:416:MET:HB3	2.47	0.45
1:C:117:ASP:CG	1:C:118:GLY:H	2.25	0.45
1:G:32:ILE:HD13	1:G:40:LEU:CD1	2.46	0.45
1:A:404:ARG:NH2	1:A:485:ASP:OD1	2.50	0.44
1:C:34:LYS:HA	1:C:37:VAL:CG2	2.47	0.44
1:G:333:GLY:C	1:G:351:LEU:HD12	2.41	0.44
1:A:32:ILE:HD13	1:A:40:LEU:CD1	2.46	0.44
1:A:359:LYS:HD2	2:F:69:ALA:HB3	1.98	0.44
1:A:480:MET:HE3	1:A:482:THR:HG23	1.99	0.44
1:C:385:ILE:O	1:C:415:CYS:HB3	2.18	0.44
1:C:404:ARG:NH2	1:C:485:ASP:OD1	2.50	0.44
1:C:480:MET:HE3	1:C:482:THR:HG23	1.99	0.44
1:C:534:TYR:CD1	1:C:575:VAL:HG22	2.52	0.44
1:E:417:ASP:HB2	1:E:437:ASN:HB3	1.99	0.44
1:A:34:LYS:HA	1:A:37:VAL:HG23	1.98	0.44
1:G:117:ASP:CG	1:G:118:GLY:H	2.25	0.44
1:E:534:TYR:CD1	1:E:575:VAL:HG22	2.52	0.44
1:G:55:GLU:CD	1:G:395:GLN:NE2	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:385:ILE:O	1:G:415:CYS:HB3	2.18	0.44
1:A:390:MET:HG2	1:A:540:TRP:CZ3	2.53	0.44
1:A:417:ASP:HB2	1:A:437:ASN:HB3	1.99	0.44
1:A:534:TYR:CD1	1:A:575:VAL:HG22	2.52	0.44
1:C:11:ASP:HB3	1:C:29:LEU:HD21	1.98	0.44
1:C:305:ALA:O	1:C:331:ARG:HG3	2.17	0.44
1:C:388:SER:CB	1:C:416:MET:HB3	2.47	0.44
1:C:390:MET:HG2	1:C:540:TRP:CZ3	2.53	0.44
1:E:55:GLU:CD	1:E:395:GLN:NE2	2.76	0.44
1:E:305:ALA:O	1:E:331:ARG:HG3	2.17	0.44
1:G:556:LEU:HD12	1:G:556:LEU:N	2.31	0.44
2:B:27:LYS:HD2	2:B:28:TYR:CZ	2.53	0.44
1:C:417:ASP:HB2	1:C:437:ASN:HB3	1.99	0.44
1:G:34:LYS:HA	1:G:37:VAL:CG2	2.47	0.44
1:G:305:ALA:O	1:G:331:ARG:HG3	2.17	0.44
1:G:378:MET:HE1	1:G:420:PRO:O	2.18	0.44
1:G:534:TYR:CD1	1:G:575:VAL:HG22	2.52	0.44
1:A:305:ALA:O	1:A:331:ARG:HG3	2.17	0.44
2:D:27:LYS:HD2	2:D:28:TYR:CZ	2.53	0.44
1:E:114:TRP:CH2	1:E:116:GLY:HA2	2.53	0.44
1:A:275:LYS:HG3	1:A:276:TRP:CE2	2.53	0.44
1:E:280:ILE:HG13	1:E:296:LYS:HD3	2.00	0.44
2:F:27:LYS:HD2	2:F:28:TYR:CZ	2.53	0.44
1:C:4:LEU:HD23	1:C:4:LEU:HA	1.88	0.43
1:E:34:LYS:HA	1:E:37:VAL:HG23	1.98	0.43
1:C:34:LYS:HA	1:C:37:VAL:HG23	1.98	0.43
1:E:40:LEU:O	1:E:41:ARG:HD2	2.19	0.43
1:A:25:ASN:HD22	1:A:25:ASN:HA	1.46	0.43
1:A:378:MET:HE1	1:A:420:PRO:O	2.18	0.43
1:C:109:ARG:HE	1:C:395:GLN:HG3	1.84	0.43
1:C:284:ASP:CG	1:C:287:THR:HG22	2.43	0.43
1:E:277:THR:H	1:E:277:THR:HG23	1.50	0.43
1:E:284:ASP:CG	1:E:287:THR:HG22	2.43	0.43
1:A:55:GLU:CD	1:A:395:GLN:NE2	2.76	0.43
1:C:40:LEU:O	1:C:41:ARG:CD	2.67	0.43
1:C:55:GLU:CD	1:C:395:GLN:NE2	2.76	0.43
1:E:275:LYS:HA	1:E:276:TRP:HA	1.74	0.43
1:E:385:ILE:O	1:E:415:CYS:HB3	2.18	0.43
1:G:40:LEU:O	1:G:41:ARG:CD	2.67	0.43
1:G:109:ARG:HE	1:G:395:GLN:HG3	1.84	0.43
1:A:279:THR:HG23	1:A:294:TYR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ASP:CG	1:A:287:THR:HG22	2.43	0.43
1:A:388:SER:CB	1:A:416:MET:HB3	2.47	0.43
1:C:280:ILE:HG13	1:C:296:LYS:HD3	2.00	0.43
1:G:284:ASP:CG	1:G:287:THR:HG22	2.43	0.43
2:H:27:LYS:HD2	2:H:28:TYR:CZ	2.53	0.43
1:E:249:ASP:OD2	1:E:340:ARG:NH1	2.48	0.43
1:G:445:ASP:OD1	1:G:447:GLN:HB2	2.19	0.43
1:A:280:ILE:HG13	1:A:296:LYS:HD3	2.00	0.43
1:A:385:ILE:O	1:A:415:CYS:HB3	2.18	0.43
1:C:140:THR:HG22	2:H:27:LYS:HZ1	1.83	0.43
1:E:378:MET:HE1	1:E:420:PRO:O	2.18	0.43
1:G:275:LYS:HG3	1:G:276:TRP:CD2	2.54	0.43
1:G:275:LYS:HG3	1:G:276:TRP:CE2	2.53	0.43
1:A:556:LEU:N	1:A:556:LEU:CD1	2.82	0.43
1:C:275:LYS:HG3	1:C:276:TRP:CD2	2.54	0.43
1:E:390:MET:HG2	1:E:540:TRP:CZ3	2.53	0.43
1:G:390:MET:HG2	1:G:540:TRP:CZ3	2.53	0.43
1:C:40:LEU:O	1:C:41:ARG:HD2	2.19	0.43
1:C:378:MET:HE1	1:C:420:PRO:O	2.18	0.43
1:E:556:LEU:N	1:E:556:LEU:CD1	2.82	0.43
1:A:40:LEU:O	1:A:41:ARG:CD	2.67	0.42
1:A:472:ARG:HB2	1:C:594:TRP:HB2	2.01	0.42
1:C:275:LYS:HG3	1:C:276:TRP:CE2	2.53	0.42
1:C:414:ILE:HG12	1:C:452:LEU:HD12	2.01	0.42
1:E:3:LYS:HB3	1:E:115:PRO:HG2	2.01	0.42
1:E:392:TYR:HA	1:E:412:ASN:HB2	2.01	0.42
1:G:255:ILE:HD12	1:G:255:ILE:HA	1.93	0.42
1:G:292:PHE:CD1	1:G:292:PHE:C	2.97	0.42
1:C:140:THR:HB	2:H:27:LYS:HE2	2.01	0.42
1:C:392:TYR:HA	1:C:412:ASN:HB2	2.01	0.42
1:C:556:LEU:N	1:C:556:LEU:CD1	2.82	0.42
1:E:40:LEU:O	1:E:41:ARG:CD	2.67	0.42
1:E:114:TRP:HA	1:E:115:PRO:HD3	1.85	0.42
1:E:275:LYS:HG3	1:E:276:TRP:CE2	2.53	0.42
1:E:414:ILE:HG12	1:E:452:LEU:HD12	2.01	0.42
1:G:417:ASP:HB2	1:G:437:ASN:HB3	1.99	0.42
1:A:275:LYS:HG3	1:A:276:TRP:CD2	2.54	0.42
1:A:275:LYS:HA	1:A:276:TRP:HA	1.74	0.42
1:E:109:ARG:HE	1:E:395:GLN:HG3	1.84	0.42
1:G:40:LEU:O	1:G:41:ARG:HD2	2.19	0.42
1:G:249:ASP:OD2	1:G:340:ARG:NH1	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:279:THR:HG23	1:G:294:TYR:O	2.19	0.42
1:C:3:LYS:HB3	1:C:115:PRO:HG2	2.01	0.42
1:C:480:MET:HE3	1:C:482:THR:CG2	2.49	0.42
1:E:292:PHE:CD1	1:E:292:PHE:C	2.97	0.42
1:G:3:LYS:HB3	1:G:115:PRO:HG2	2.01	0.42
1:G:480:MET:HE3	1:G:482:THR:CG2	2.50	0.42
1:A:276:TRP:O	1:A:279:THR:HB	2.20	0.42
1:C:223:LYS:O	1:C:225:LEU:HD13	2.20	0.42
1:E:279:THR:HG23	1:E:294:TYR:O	2.19	0.42
1:A:114:TRP:HA	1:A:115:PRO:HD3	1.85	0.42
1:A:445:ASP:OD1	1:A:447:GLN:HB2	2.19	0.42
1:C:279:THR:HG23	1:C:294:TYR:O	2.19	0.42
1:G:276:TRP:O	1:G:279:THR:HB	2.20	0.42
1:G:280:ILE:HG13	1:G:296:LYS:HD3	2.00	0.42
1:A:3:LYS:HB3	1:A:115:PRO:HG2	2.01	0.42
1:A:40:LEU:O	1:A:41:ARG:HD2	2.19	0.42
1:A:326:LEU:HD12	1:A:326:LEU:O	2.20	0.42
1:C:25:ASN:HD22	1:C:25:ASN:HA	1.46	0.42
1:C:277:THR:H	1:C:277:THR:HG23	1.50	0.42
1:E:275:LYS:HG3	1:E:276:TRP:CD2	2.54	0.42
1:A:109:ARG:HE	1:A:395:GLN:HG3	1.84	0.42
1:A:480:MET:HE3	1:A:482:THR:CG2	2.50	0.42
1:C:12:ASP:CB	1:C:524:THR:O	2.67	0.42
1:C:292:PHE:CD1	1:C:292:PHE:C	2.97	0.42
1:E:25:ASN:HD22	1:E:25:ASN:HA	1.46	0.42
1:G:423:LEU:HA	1:G:424:PRO:HD3	1.92	0.42
1:G:556:LEU:N	1:G:556:LEU:CD1	2.82	0.42
1:C:109:ARG:NE	1:C:395:GLN:HG3	2.35	0.42
1:C:140:THR:CG2	2:H:27:LYS:NZ	2.81	0.42
1:G:331:ARG:HD2	1:G:391:GLY:HA3	2.02	0.42
1:G:392:TYR:HA	1:G:412:ASN:HB2	2.01	0.42
1:A:109:ARG:NE	1:A:395:GLN:HG3	2.35	0.41
1:A:331:ARG:HD2	1:A:391:GLY:HA3	2.02	0.41
1:A:392:TYR:HA	1:A:412:ASN:HB2	2.01	0.41
1:C:243:TRP:CE2	1:C:307:VAL:HG21	2.55	0.41
1:C:580:LEU:HD12	1:C:580:LEU:HA	1.87	0.41
1:G:114:TRP:CH2	1:G:116:GLY:HA2	2.53	0.41
1:C:276:TRP:O	1:C:279:THR:HB	2.20	0.41
1:E:276:TRP:O	1:E:279:THR:HB	2.20	0.41
1:E:480:MET:HE3	1:E:482:THR:CG2	2.50	0.41
1:G:140:THR:OG1	1:G:142:GLU:HG2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:267:GLU:HG3	1:G:301:GLU:HB3	2.02	0.41
1:A:292:PHE:CD1	1:A:292:PHE:C	2.97	0.41
1:A:414:ILE:HG12	1:A:452:LEU:HD12	2.01	0.41
1:C:140:THR:OG1	1:C:142:GLU:HG2	2.20	0.41
1:C:445:ASP:OD1	1:C:447:GLN:HB2	2.19	0.41
1:E:243:TRP:CE2	1:E:307:VAL:HG21	2.55	0.41
1:E:494:GLY:O	1:E:511:LYS:HD2	2.20	0.41
1:G:243:TRP:CE2	1:G:307:VAL:HG21	2.55	0.41
1:G:277:THR:H	1:G:277:THR:HG23	1.50	0.41
1:G:494:GLY:O	1:G:511:LYS:HD2	2.20	0.41
1:C:114:TRP:CH2	1:C:116:GLY:HA2	2.53	0.41
1:C:423:LEU:HA	1:C:424:PRO:HD3	1.92	0.41
1:E:4:LEU:HD23	1:E:4:LEU:HA	1.88	0.41
2:B:29:ASP:HA	2:B:30:PRO:HD3	1.91	0.41
1:E:331:ARG:HD2	1:E:391:GLY:HA3	2.02	0.41
1:E:445:ASP:OD1	1:E:447:GLN:HB2	2.19	0.41
1:G:414:ILE:HG12	1:G:452:LEU:HD12	2.01	0.41
1:A:243:TRP:CE2	1:A:307:VAL:HG21	2.55	0.41
1:C:494:GLY:O	1:C:511:LYS:HD2	2.21	0.41
1:E:109:ARG:NE	1:E:395:GLN:HG3	2.35	0.41
1:G:12:ASP:CB	1:G:524:THR:O	2.67	0.41
1:G:223:LYS:O	1:G:225:LEU:HD13	2.20	0.41
1:A:296:LYS:HB2	1:A:296:LYS:HE3	1.78	0.41
1:C:37:VAL:CG2	1:C:486:LEU:HD21	2.48	0.41
1:C:267:GLU:HG3	1:C:301:GLU:HB3	2.02	0.41
1:E:371:ASP:OD1	1:E:371:ASP:C	2.64	0.41
1:A:114:TRP:CH2	1:A:116:GLY:HA2	2.53	0.41
1:A:223:LYS:O	1:A:225:LEU:HD13	2.20	0.41
1:C:326:LEU:HD12	1:C:326:LEU:O	2.20	0.41
1:C:371:ASP:OD1	1:C:371:ASP:C	2.64	0.41
1:E:223:LYS:O	1:E:225:LEU:HD13	2.20	0.41
1:A:140:THR:OG1	1:A:142:GLU:HG2	2.20	0.41
1:A:371:ASP:OD1	1:A:371:ASP:C	2.64	0.41
1:C:278:MET:HE1	1:C:304:TYR:N	2.36	0.41
2:D:44:ILE:O	2:D:48:GLU:HG3	2.21	0.41
1:E:267:GLU:HG3	1:E:301:GLU:HB3	2.02	0.41
1:E:588:ASP:HA	1:E:589:PRO:HD2	1.90	0.41
2:F:29:ASP:HA	2:F:30:PRO:HD3	1.91	0.41
2:F:44:ILE:O	2:F:48:GLU:HG3	2.20	0.41
1:G:109:ARG:NE	1:G:395:GLN:HG3	2.35	0.41
1:A:278:MET:HE1	1:A:304:TYR:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:14:TRP:CZ3	1:C:19:LYS:HD2	2.56	0.41
1:G:438:MET:HE3	1:G:557:GLY:C	2.46	0.41
2:H:44:ILE:O	2:H:48:GLU:HG3	2.20	0.41
1:G:278:MET:HE1	1:G:304:TYR:N	2.36	0.40
1:A:249:ASP:OD2	1:A:340:ARG:NH1	2.48	0.40
1:A:267:GLU:HG3	1:A:301:GLU:HB3	2.02	0.40
1:A:494:GLY:O	1:A:511:LYS:HD2	2.20	0.40
2:B:44:ILE:O	2:B:48:GLU:HG3	2.21	0.40
1:G:326:LEU:HD12	1:G:326:LEU:O	2.20	0.40
1:G:371:ASP:OD1	1:G:371:ASP:C	2.64	0.40
1:A:14:TRP:CZ3	1:A:19:LYS:HD2	2.56	0.40
1:A:423:LEU:HA	1:A:424:PRO:HD3	1.92	0.40
1:C:265:TRP:CH2	1:C:556:LEU:HD23	2.56	0.40
1:E:140:THR:OG1	1:E:142:GLU:HG2	2.20	0.40
1:E:326:LEU:HD12	1:E:326:LEU:O	2.20	0.40
1:A:12:ASP:CB	1:A:524:THR:O	2.67	0.40
1:G:270:ARG:O	1:G:271:PRO:C	2.65	0.40
1:G:275:LYS:HA	1:G:276:TRP:HA	1.74	0.40
1:A:265:TRP:CH2	1:A:556:LEU:HD23	2.56	0.40
1:A:438:MET:HE3	1:A:557:GLY:C	2.46	0.40
1:C:331:ARG:HD2	1:C:391:GLY:HA3	2.02	0.40
1:C:438:MET:HE3	1:C:557:GLY:C	2.46	0.40
1:E:12:ASP:CB	1:E:524:THR:O	2.67	0.40
1:E:265:TRP:CH2	1:E:556:LEU:HD23	2.56	0.40
1:G:2:ASP:O	1:G:3:LYS:C	2.64	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	593/599 (99%)	540 (91%)	51 (9%)	2 (0%)	36 70

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	593/599 (99%)	540 (91%)	51 (9%)	2 (0%)	36	70
1	E	593/599 (99%)	540 (91%)	51 (9%)	2 (0%)	36	70
1	G	593/599 (99%)	540 (91%)	51 (9%)	2 (0%)	36	70
2	B	70/74 (95%)	68 (97%)	2 (3%)	0	100	100
2	D	70/74 (95%)	68 (97%)	2 (3%)	0	100	100
2	F	70/74 (95%)	68 (97%)	2 (3%)	0	100	100
2	H	70/74 (95%)	68 (97%)	2 (3%)	0	100	100
All	All	2652/2692 (98%)	2432 (92%)	212 (8%)	8 (0%)	36	70

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	GLY
1	C	118	GLY
1	E	118	GLY
1	G	118	GLY
1	A	589	PRO
1	C	589	PRO
1	E	589	PRO
1	G	589	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	476/478 (100%)	447 (94%)	29 (6%)	17	49
1	C	476/478 (100%)	447 (94%)	29 (6%)	17	49
1	E	476/478 (100%)	447 (94%)	29 (6%)	17	49
1	G	476/478 (100%)	447 (94%)	29 (6%)	17	49
2	B	62/63 (98%)	56 (90%)	6 (10%)	8	30
2	D	62/63 (98%)	56 (90%)	6 (10%)	8	30

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	F	62/63 (98%)	56 (90%)	6 (10%)	8	30
2	H	62/63 (98%)	56 (90%)	6 (10%)	8	30
All	All	2152/2164 (99%)	2012 (94%)	140 (6%)	15	47

All (140) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LYS
1	A	12	ASP
1	A	25	ASN
1	A	37	VAL
1	A	38	LYS
1	A	80	LEU
1	A	87	LEU
1	A	109	ARG
1	A	119	LYS
1	A	129	LEU
1	A	153	LYS
1	A	160	ILE
1	A	177	GLU
1	A	274	ASN
1	A	303	GLU
1	A	321	LYS
1	A	326	LEU
1	A	338	LEU
1	A	364	LYS
1	A	373	GLU
1	A	395	GLN
1	A	403	LYS
1	A	406	LEU
1	A	435	THR
1	A	486	LEU
1	A	543	VAL
1	A	564	LYS
1	A	580	LEU
1	A	595	LYS
2	B	31	LYS
2	B	35	LYS
2	B	45	LYS
2	B	49	GLU
2	B	60	LYS

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Mol	Chain	Res	Type
2	B	63	LYS
1	C	3	LYS
1	C	12	ASP
1	C	25	ASN
1	C	37	VAL
1	C	38	LYS
1	C	80	LEU
1	C	87	LEU
1	C	109	ARG
1	C	119	LYS
1	C	129	LEU
1	C	153	LYS
1	C	160	ILE
1	C	177	GLU
1	C	274	ASN
1	C	303	GLU
1	C	321	LYS
1	C	326	LEU
1	C	338	LEU
1	C	364	LYS
1	C	373	GLU
1	C	395	GLN
1	C	403	LYS
1	C	406	LEU
1	C	435	THR
1	C	486	LEU
1	C	543	VAL
1	C	564	LYS
1	C	580	LEU
1	C	595	LYS
2	D	31	LYS
2	D	35	LYS
2	D	45	LYS
2	D	49	GLU
2	D	60	LYS
2	D	63	LYS
1	E	3	LYS
1	E	12	ASP
1	E	25	ASN
1	E	37	VAL
1	E	38	LYS
1	E	80	LEU

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Mol	Chain	Res	Type
1	E	87	LEU
1	E	109	ARG
1	E	119	LYS
1	E	129	LEU
1	E	153	LYS
1	E	160	ILE
1	E	177	GLU
1	E	274	ASN
1	E	303	GLU
1	E	321	LYS
1	E	326	LEU
1	E	338	LEU
1	E	364	LYS
1	E	373	GLU
1	E	395	GLN
1	E	403	LYS
1	E	406	LEU
1	E	435	THR
1	E	486	LEU
1	E	543	VAL
1	E	564	LYS
1	E	580	LEU
1	E	595	LYS
2	F	31	LYS
2	F	35	LYS
2	F	45	LYS
2	F	49	GLU
2	F	60	LYS
2	F	63	LYS
1	G	3	LYS
1	G	12	ASP
1	G	25	ASN
1	G	37	VAL
1	G	38	LYS
1	G	80	LEU
1	G	87	LEU
1	G	109	ARG
1	G	119	LYS
1	G	129	LEU
1	G	153	LYS
1	G	160	ILE
1	G	177	GLU

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Mol	Chain	Res	Type
1	G	274	ASN
1	G	303	GLU
1	G	321	LYS
1	G	326	LEU
1	G	338	LEU
1	G	364	LYS
1	G	373	GLU
1	G	395	GLN
1	G	403	LYS
1	G	406	LEU
1	G	435	THR
1	G	486	LEU
1	G	543	VAL
1	G	564	LYS
1	G	580	LEU
1	G	595	LYS
2	H	31	LYS
2	H	35	LYS
2	H	45	LYS
2	H	49	GLU
2	H	60	LYS
2	H	63	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	74	ASN
1	A	149	ASN
1	A	367	GLN
1	A	429	GLN
1	A	567	ASN
1	C	25	ASN
1	C	74	ASN
1	C	149	ASN
1	C	367	GLN
1	C	429	GLN
1	C	567	ASN
1	E	74	ASN
1	E	149	ASN
1	E	367	GLN
1	E	429	GLN

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Mol	Chain	Res	Type
1	E	567	ASN
1	G	25	ASN
1	G	74	ASN
1	G	149	ASN
1	G	367	GLN
1	G	429	GLN
1	G	567	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 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	$\# Z > 2$
3	PQQ	E	601	4	26,26,26	2.95	13 (50%)	34,40,40	2.39	9 (26%)
3	PQQ	C	601	4	26,26,26	2.94	13 (50%)	34,40,40	2.39	9 (26%)
3	PQQ	G	601	4	26,26,26	2.94	13 (50%)	34,40,40	2.40	9 (26%)
3	PQQ	A	601	4	26,26,26	2.94	13 (50%)	34,40,40	2.40	9 (26%)

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	PQQ	E	601	4	-	0/12/28/28	0/3/3/3
3	PQQ	C	601	4	-	0/12/28/28	0/3/3/3
3	PQQ	G	601	4	-	0/12/28/28	0/3/3/3
3	PQQ	A	601	4	-	0/12/28/28	0/3/3/3

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	601	PQQ	C9A-C6A	6.04	1.50	1.41
3	A	601	PQQ	C9A-C6A	6.03	1.50	1.41
3	E	601	PQQ	C9A-C6A	6.03	1.50	1.41
3	C	601	PQQ	C9A-C6A	6.00	1.50	1.41
3	E	601	PQQ	C6A-C5	5.33	1.56	1.50
3	G	601	PQQ	C6A-C5	5.33	1.56	1.50
3	C	601	PQQ	C6A-C5	5.31	1.56	1.50
3	A	601	PQQ	C6A-C5	5.30	1.56	1.50
3	A	601	PQQ	C9-C9A	5.19	1.49	1.41
3	G	601	PQQ	C9-C9A	5.19	1.49	1.41
3	C	601	PQQ	C9-C9A	5.18	1.49	1.41
3	E	601	PQQ	C9-C9A	5.17	1.49	1.41
3	E	601	PQQ	C5-C4	-4.92	1.47	1.54
3	C	601	PQQ	C5-C4	-4.90	1.47	1.54
3	A	601	PQQ	C5-C4	-4.87	1.47	1.54
3	G	601	PQQ	C5-C4	-4.87	1.47	1.54
3	C	601	PQQ	O9B-C9X	-4.41	1.17	1.30
3	G	601	PQQ	O9B-C9X	-4.41	1.17	1.30
3	A	601	PQQ	O9B-C9X	-4.40	1.17	1.30
3	E	601	PQQ	O9B-C9X	-4.39	1.17	1.30
3	C	601	PQQ	C7-N6	3.51	1.39	1.34
3	C	601	PQQ	C8-C9	3.51	1.45	1.39
3	A	601	PQQ	C8-C9	3.50	1.45	1.39
3	E	601	PQQ	C7-N6	3.50	1.39	1.34
3	E	601	PQQ	C8-C9	3.49	1.45	1.39
3	G	601	PQQ	C7-N6	3.49	1.39	1.34
3	A	601	PQQ	C7-N6	3.46	1.39	1.34
3	G	601	PQQ	C8-C9	3.46	1.45	1.39
3	E	601	PQQ	O2B-C2X	-3.24	1.21	1.30
3	C	601	PQQ	O2B-C2X	-3.23	1.21	1.30
3	E	601	PQQ	O7A-C7X	3.23	1.32	1.22
3	G	601	PQQ	O2B-C2X	-3.23	1.21	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	601	PQQ	O2B-C2X	-3.21	1.21	1.30
3	A	601	PQQ	O7A-C7X	3.20	1.32	1.22
3	G	601	PQQ	O7A-C7X	3.19	1.32	1.22
3	C	601	PQQ	O7A-C7X	3.18	1.32	1.22
3	C	601	PQQ	O2A-C2X	3.17	1.30	1.22
3	A	601	PQQ	O2A-C2X	3.17	1.30	1.22
3	G	601	PQQ	O2A-C2X	3.16	1.30	1.22
3	E	601	PQQ	O2A-C2X	3.15	1.30	1.22
3	C	601	PQQ	O7B-C7X	-3.01	1.21	1.30
3	E	601	PQQ	O7B-C7X	-3.00	1.21	1.30
3	G	601	PQQ	O7B-C7X	-2.99	1.21	1.30
3	A	601	PQQ	O7B-C7X	-2.99	1.21	1.30
3	G	601	PQQ	O4-C4	-2.79	1.17	1.23
3	A	601	PQQ	O4-C4	-2.78	1.17	1.23
3	C	601	PQQ	O4-C4	-2.78	1.17	1.23
3	E	601	PQQ	O4-C4	-2.77	1.17	1.23
3	A	601	PQQ	C9A-C1A	2.56	1.49	1.46
3	E	601	PQQ	C9A-C1A	2.55	1.49	1.46
3	C	601	PQQ	C9A-C1A	2.53	1.49	1.46
3	G	601	PQQ	C9A-C1A	2.53	1.49	1.46

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	601	PQQ	O4-C4-C5	-5.98	111.01	118.37
3	C	601	PQQ	O4-C4-C5	-5.95	111.04	118.37
3	A	601	PQQ	O4-C4-C5	-5.95	111.04	118.37
3	E	601	PQQ	O4-C4-C5	-5.92	111.08	118.37
3	A	601	PQQ	O5-C5-C6A	4.67	127.09	121.76
3	G	601	PQQ	O5-C5-C6A	4.67	127.09	121.76
3	C	601	PQQ	O5-C5-C6A	4.66	127.09	121.76
3	E	601	PQQ	O5-C5-C6A	4.65	127.07	121.76
3	E	601	PQQ	O7B-C7X-C7	4.17	124.61	114.71
3	G	601	PQQ	O7B-C7X-C7	4.15	124.57	114.71
3	A	601	PQQ	O7B-C7X-C7	4.15	124.56	114.71
3	C	601	PQQ	O7B-C7X-C7	4.14	124.55	114.71
3	E	601	PQQ	O2A-C2X-C2	-4.07	112.75	121.01
3	G	601	PQQ	O2A-C2X-C2	-4.07	112.76	121.01
3	C	601	PQQ	O2A-C2X-C2	-4.05	112.79	121.01
3	A	601	PQQ	O2A-C2X-C2	-4.05	112.79	121.01
3	G	601	PQQ	O2B-C2X-C2	3.99	122.87	114.27
3	A	601	PQQ	O2B-C2X-C2	3.99	122.86	114.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	601	PQQ	O2B-C2X-C2	3.98	122.84	114.27
3	E	601	PQQ	O2B-C2X-C2	3.96	122.81	114.27
3	G	601	PQQ	O9B-C9X-C9	3.82	126.13	115.28
3	E	601	PQQ	O9B-C9X-C9	3.82	126.13	115.28
3	C	601	PQQ	O9B-C9X-C9	3.81	126.12	115.28
3	A	601	PQQ	O9B-C9X-C9	3.81	126.12	115.28
3	A	601	PQQ	C3A-C4-C5	3.49	120.99	117.03
3	C	601	PQQ	C3A-C4-C5	3.49	120.98	117.03
3	G	601	PQQ	C3A-C4-C5	3.48	120.97	117.03
3	E	601	PQQ	C3A-C4-C5	3.48	120.97	117.03
3	E	601	PQQ	O7A-C7X-C7	-3.39	114.47	121.30
3	A	601	PQQ	O7A-C7X-C7	-3.38	114.50	121.30
3	G	601	PQQ	O7A-C7X-C7	-3.38	114.50	121.30
3	C	601	PQQ	O7A-C7X-C7	-3.37	114.52	121.30
3	C	601	PQQ	O9B-C9X-O9A	-3.26	116.35	123.35
3	A	601	PQQ	O9B-C9X-O9A	-3.25	116.37	123.35
3	E	601	PQQ	O9B-C9X-O9A	-3.25	116.37	123.35
3	G	601	PQQ	O9B-C9X-O9A	-3.24	116.39	123.35

There are no chirality outliers.

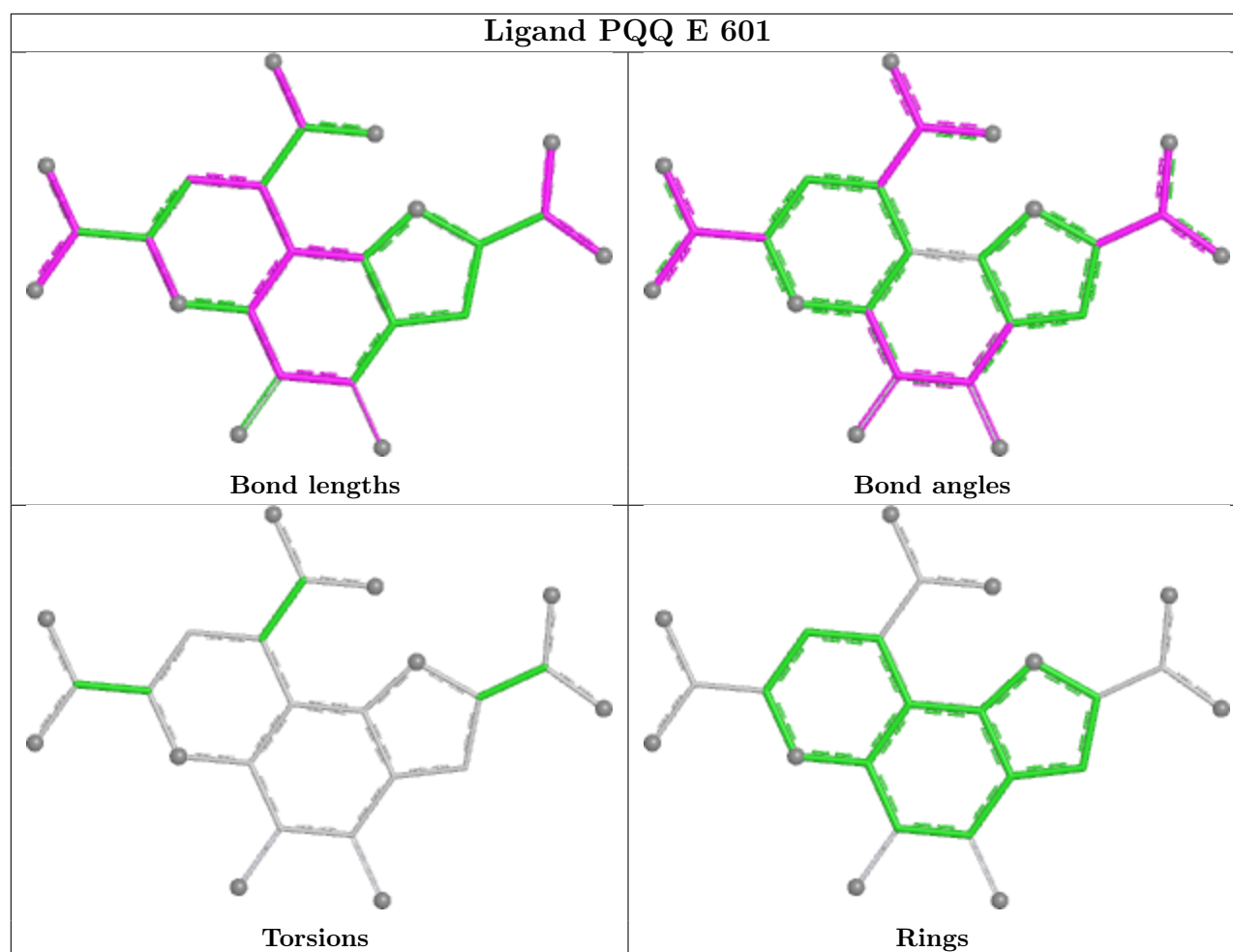
There are no torsion outliers.

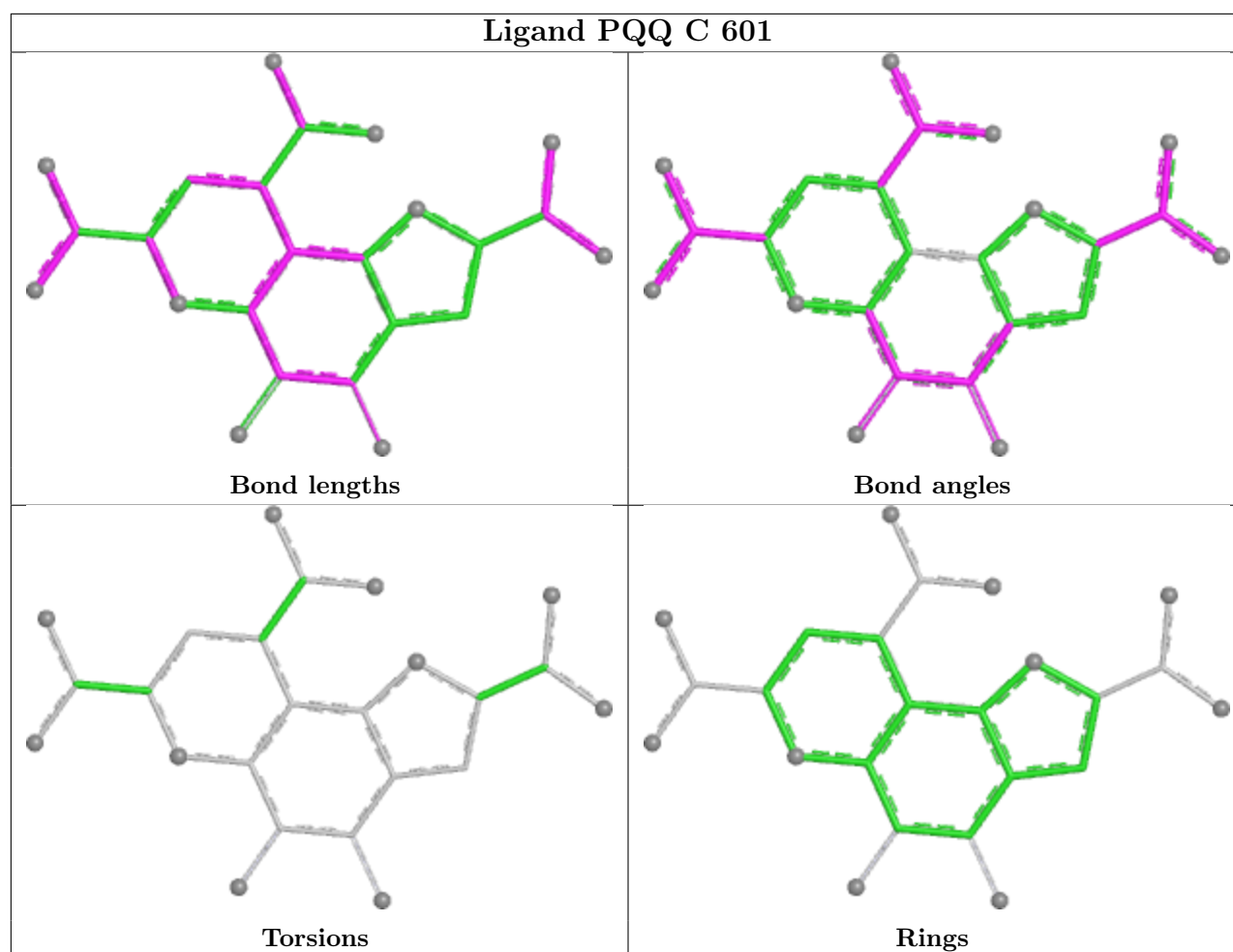
There are no ring outliers.

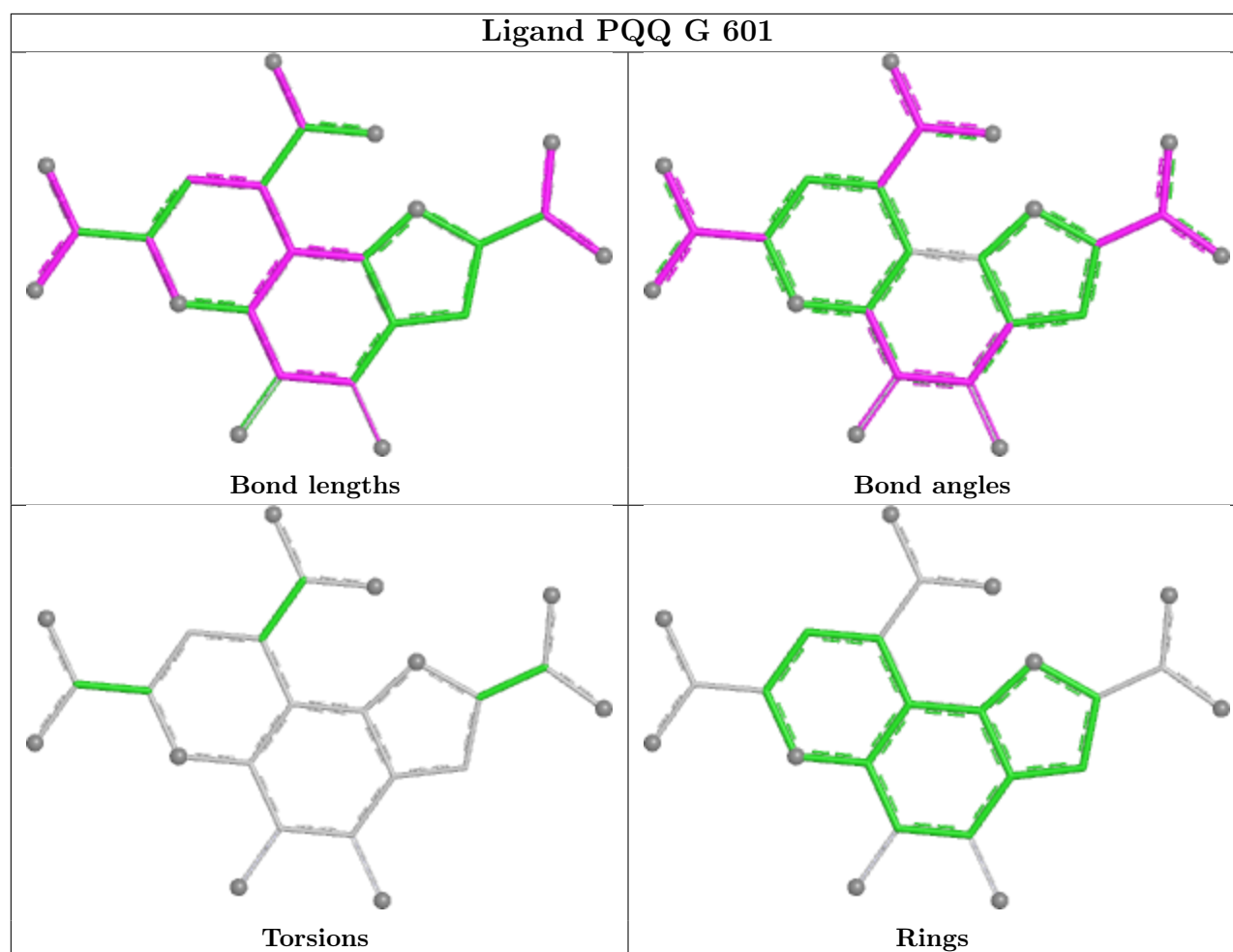
4 monomers are involved in 4 short contacts:

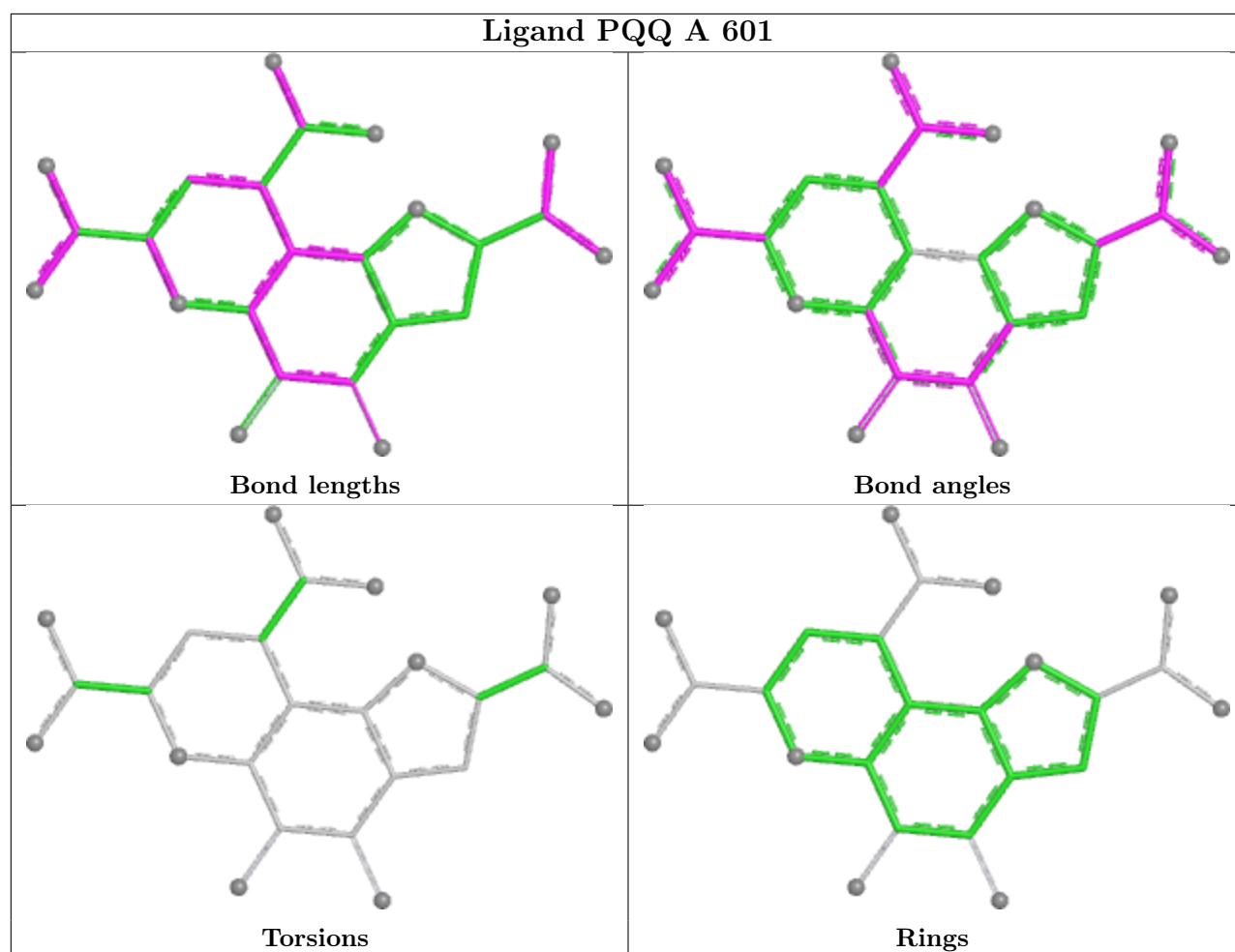
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	601	PQQ	1	0
3	C	601	PQQ	1	0
3	G	601	PQQ	1	0
3	A	601	PQQ	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	595/599 (99%)	-0.02	2 (0%) 90 79	9, 18, 29, 46	17 (2%)
1	C	595/599 (99%)	0.04	4 (0%) 84 66	9, 18, 29, 46	17 (2%)
1	E	595/599 (99%)	-0.05	1 (0%) 91 83	9, 18, 29, 46	17 (2%)
1	G	595/599 (99%)	0.08	2 (0%) 90 79	9, 18, 29, 46	17 (2%)
2	B	72/74 (97%)	0.29	1 (1%) 73 51	11, 27, 35, 45	10 (13%)
2	D	72/74 (97%)	0.24	2 (2%) 55 32	11, 27, 35, 45	10 (13%)
2	F	72/74 (97%)	0.22	1 (1%) 73 51	11, 27, 35, 45	10 (13%)
2	H	72/74 (97%)	0.52	3 (4%) 40 22	11, 27, 35, 45	10 (13%)
All	All	2668/2692 (99%)	0.04	16 (0%) 85 69	9, 18, 31, 46	108 (4%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	274	ASN	3.0
2	H	71	ILE	2.8
1	C	139	GLU	2.7
1	C	551	ASP	2.7
1	C	192	GLY	2.6
2	F	49	GLU	2.5
2	H	72	SER	2.3
2	D	72	SER	2.3
1	G	277	THR	2.2
1	E	447	GLN	2.2
2	B	21	GLU	2.2
2	H	68	VAL	2.2
1	G	167	ASP	2.1
1	C	117	ASP	2.1
1	A	277	THR	2.1
2	D	49	GLU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

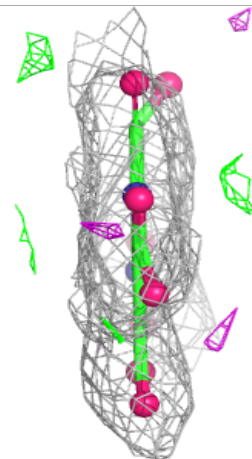
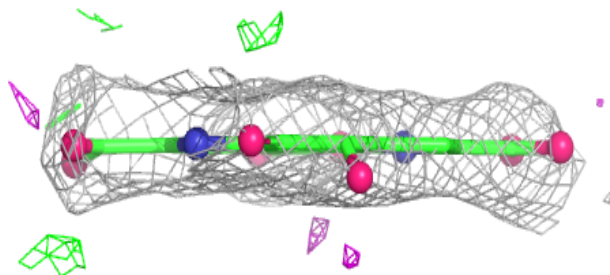
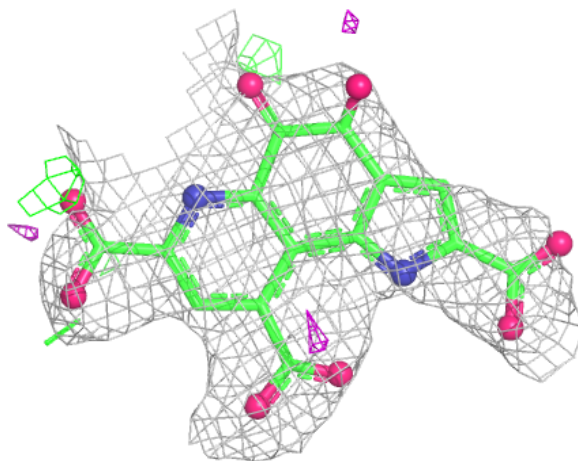
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	CA	E	701	1/1	0.87	0.13	18,18,18,18	0
4	CA	G	701	1/1	0.87	0.09	18,18,18,18	0
3	PQQ	C	601	24/24	0.88	0.12	29,29,29,29	0
3	PQQ	E	601	24/24	0.88	0.14	29,29,29,29	0
3	PQQ	G	601	24/24	0.89	0.12	29,29,29,29	0
4	CA	C	701	1/1	0.89	0.08	18,18,18,18	0
3	PQQ	A	601	24/24	0.91	0.12	29,29,29,29	0
4	CA	A	701	1/1	0.97	0.07	18,18,18,18	0

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

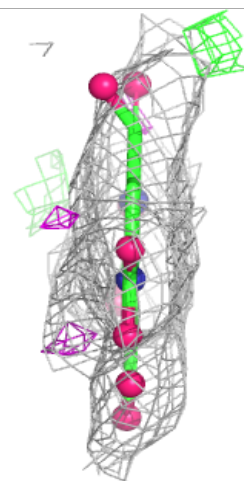
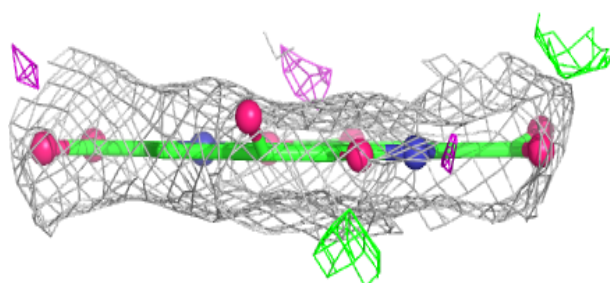
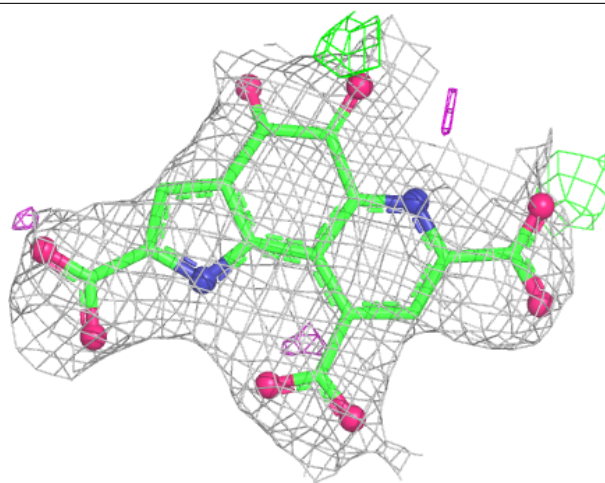
Electron density around PQQ C 601:

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



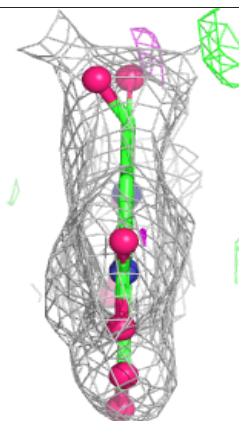
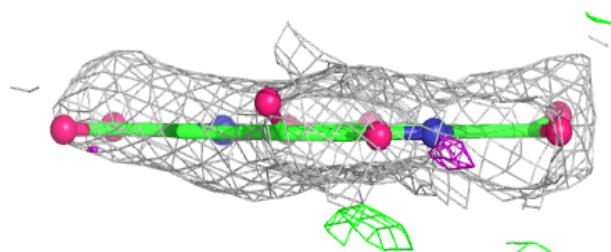
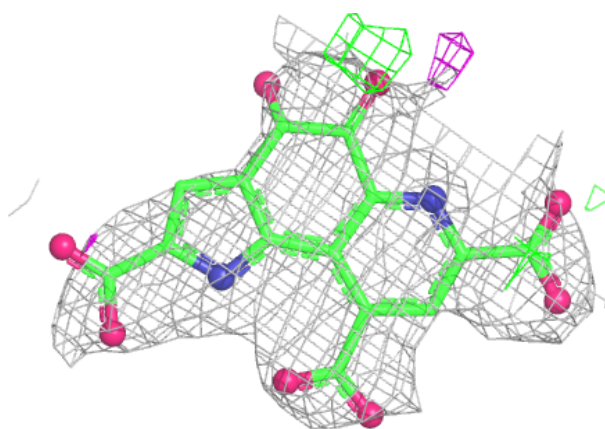
Electron density around PQQ E 601:

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



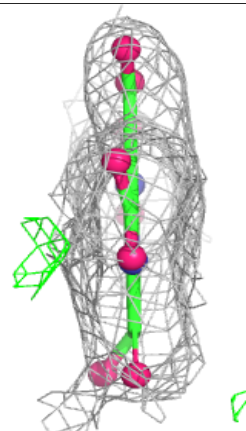
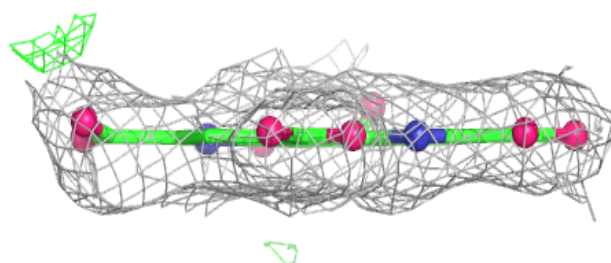
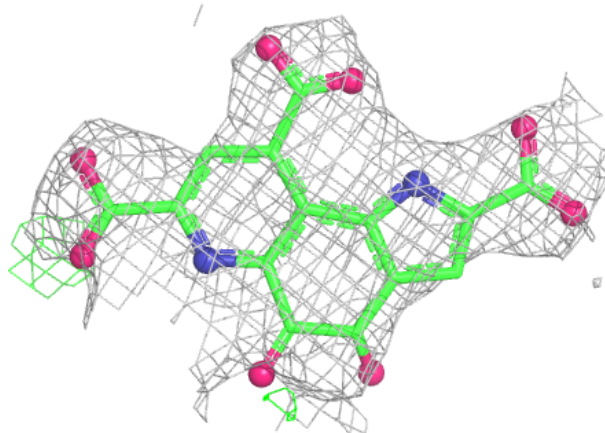
Electron density around PQQ G 601:

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



Electron density around PQQ 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.