



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:54 PM UTC

PDB ID : 4EC4 / pdb_00004ec4
Title : XIAP-BIR3 in complex with a potent divalent Smac mimetic
Authors : Mastrangelo, E.; Cossu, F.; Bolognesi, M.; Milani, M.
Deposited on : 2012-03-26
Resolution : 3.30 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

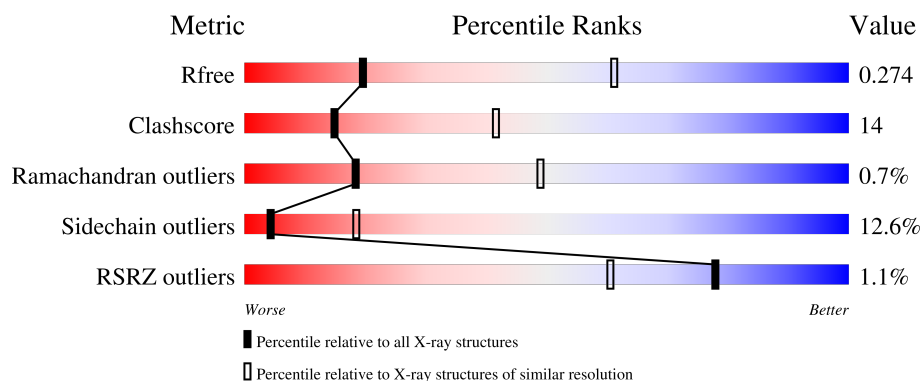
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	122	2% 69% 19% 11%
1	B	122	% 56% 28% 13%
1	C	122	% 63% 20% 14%
1	D	122	% 52% 29% 5% 14%
1	E	122	% 57% 28% 11%

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Mol	Chain	Length	Quality of chain
1	F	122	57%26%•14%
1	G	122	2% 50%32%6%12%
1	J	122	% 57%27%5%11%
1	K	122	% 61%23%•12%
1	L	122	2% 53%31%•12%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9357 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 Baculoviral IAP repeat-containing protein 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	109	Total	C	N	O	S	0	0	0
			890	566	154	165	5			
1	B	106	Total	C	N	O	S	0	0	0
			865	553	148	159	5			
1	C	105	Total	C	N	O	S	0	0	0
			854	547	144	158	5			
1	D	105	Total	C	N	O	S	0	1	0
			862	552	147	158	5			
1	E	108	Total	C	N	O	S	0	0	0
			879	560	150	164	5			
1	J	108	Total	C	N	O	S	0	0	0
			879	560	150	164	5			
1	F	105	Total	C	N	O	S	0	0	0
			858	548	147	158	5			
1	G	107	Total	C	N	O	S	0	0	0
			870	556	149	160	5			
1	K	107	Total	C	N	O	S	0	0	0
			872	555	149	163	5			
1	L	107	Total	C	N	O	S	0	0	0
			870	556	149	160	5			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	357	HIS	-	expression tag	UNP P98170
A	358	HIS	-	expression tag	UNP P98170
A	359	HIS	-	expression tag	UNP P98170
A	360	HIS	-	expression tag	UNP P98170
A	361	HIS	-	expression tag	UNP P98170
A	362	HIS	-	expression tag	UNP P98170
B	357	HIS	-	expression tag	UNP P98170
B	358	HIS	-	expression tag	UNP P98170
B	359	HIS	-	expression tag	UNP P98170

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Chain	Residue	Modelled	Actual	Comment	Reference
B	360	HIS	-	expression tag	UNP P98170
B	361	HIS	-	expression tag	UNP P98170
B	362	HIS	-	expression tag	UNP P98170
C	357	HIS	-	expression tag	UNP P98170
C	358	HIS	-	expression tag	UNP P98170
C	359	HIS	-	expression tag	UNP P98170
C	360	HIS	-	expression tag	UNP P98170
C	361	HIS	-	expression tag	UNP P98170
C	362	HIS	-	expression tag	UNP P98170
D	357	HIS	-	expression tag	UNP P98170
D	358	HIS	-	expression tag	UNP P98170
D	359	HIS	-	expression tag	UNP P98170
D	360	HIS	-	expression tag	UNP P98170
D	361	HIS	-	expression tag	UNP P98170
D	362	HIS	-	expression tag	UNP P98170
E	357	HIS	-	expression tag	UNP P98170
E	358	HIS	-	expression tag	UNP P98170
E	359	HIS	-	expression tag	UNP P98170
E	360	HIS	-	expression tag	UNP P98170
E	361	HIS	-	expression tag	UNP P98170
E	362	HIS	-	expression tag	UNP P98170
J	357	HIS	-	expression tag	UNP P98170
J	358	HIS	-	expression tag	UNP P98170
J	359	HIS	-	expression tag	UNP P98170
J	360	HIS	-	expression tag	UNP P98170
J	361	HIS	-	expression tag	UNP P98170
J	362	HIS	-	expression tag	UNP P98170
F	357	HIS	-	expression tag	UNP P98170
F	358	HIS	-	expression tag	UNP P98170
F	359	HIS	-	expression tag	UNP P98170
F	360	HIS	-	expression tag	UNP P98170
F	361	HIS	-	expression tag	UNP P98170
F	362	HIS	-	expression tag	UNP P98170
G	357	HIS	-	expression tag	UNP P98170
G	358	HIS	-	expression tag	UNP P98170
G	359	HIS	-	expression tag	UNP P98170
G	360	HIS	-	expression tag	UNP P98170
G	361	HIS	-	expression tag	UNP P98170
G	362	HIS	-	expression tag	UNP P98170
K	357	HIS	-	expression tag	UNP P98170
K	358	HIS	-	expression tag	UNP P98170
K	359	HIS	-	expression tag	UNP P98170

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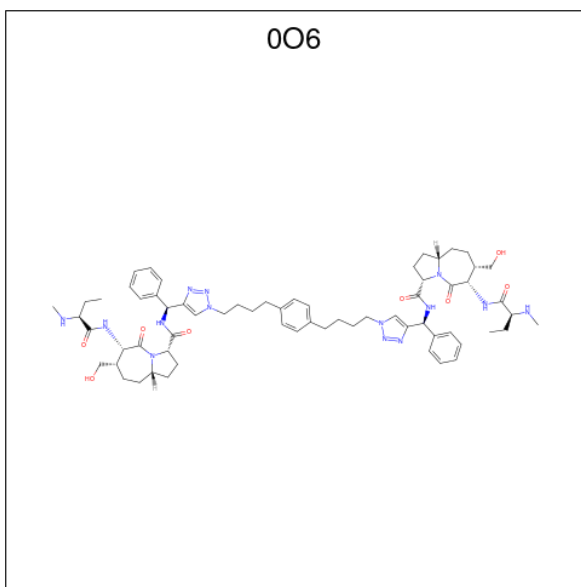
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Chain	Residue	Modelled	Actual	Comment	Reference
K	360	HIS	-	expression tag	UNP P98170
K	361	HIS	-	expression tag	UNP P98170
K	362	HIS	-	expression tag	UNP P98170
L	357	HIS	-	expression tag	UNP P98170
L	358	HIS	-	expression tag	UNP P98170
L	359	HIS	-	expression tag	UNP P98170
L	360	HIS	-	expression tag	UNP P98170
L	361	HIS	-	expression tag	UNP P98170
L	362	HIS	-	expression tag	UNP P98170

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

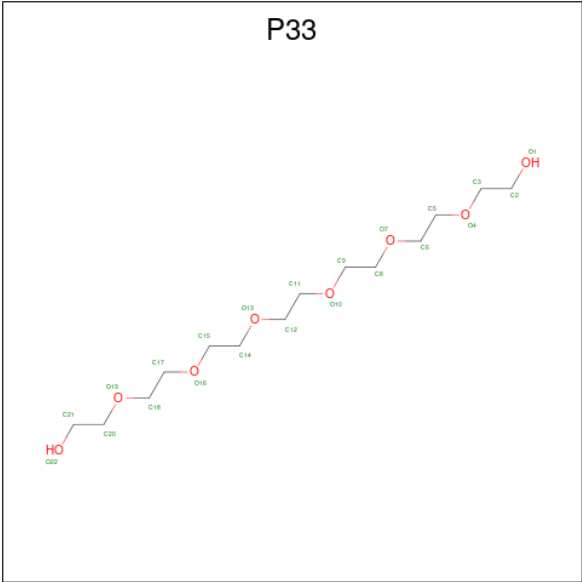
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	E	1	Total Zn 1 1	0	0
2	J	1	Total Zn 1 1	0	0
2	F	1	Total Zn 1 1	0	0
2	G	1	Total Zn 1 1	0	0
2	K	1	Total Zn 1 1	0	0
2	L	1	Total Zn 1 1	0	0

- Molecule 3 is (3S,6S,7S,9aS,3'S,6'S,7'S,9a'S)-N,N'-(benzene-1,4-diylbis{butane-4,1-diyl-1H-1,2,3-triazole-1,4-diyl[(S)-phenylmethanediyl]})bis[7-(hydroxymethyl)-6-{[(2S)-2-(methylamino)butanoyl]amino}-5-oxooctahydro-1H-pyrrolo[1,2-a]azepine-3-carboxamide] (CCD ID: 006) (formula: C₆₄H₈₈N₁₄O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			86	64	14	8		
3	B	1	Total	C	N	O	0	0
			86	64	14	8		
3	D	1	Total	C	N	O	0	0
			86	64	14	8		
3	E	1	Total	C	N	O	0	0
			86	64	14	8		
3	J	1	Total	C	N	O	0	0
			86	64	14	8		

- Molecule 4 is 3,6,9,12,15,18-HEXAOXAICOSANE-1,20-DIOL (CCD ID: P33) (formula: $C_{14}H_{30}O_8$).



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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			28	18	10		

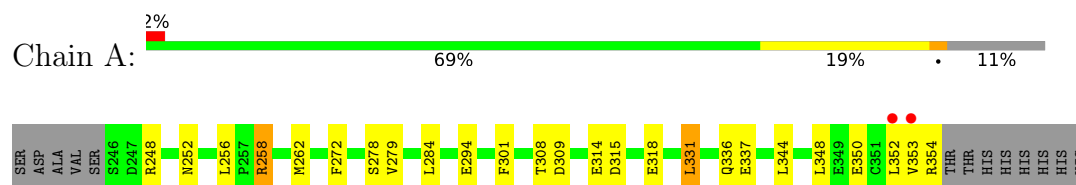
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	16	Total	O	0	0
			16	16		
6	B	6	Total	O	0	0
			6	6		
6	C	9	Total	O	0	0
			9	9		
6	D	15	Total	O	0	0
			15	15		
6	E	10	Total	O	0	0
			10	10		
6	J	8	Total	O	0	0
			8	8		
6	F	11	Total	O	0	0
			11	11		
6	G	8	Total	O	0	0
			8	8		
6	K	5	Total	O	0	0
			5	5		
6	L	8	Total	O	0	0
			8	8		

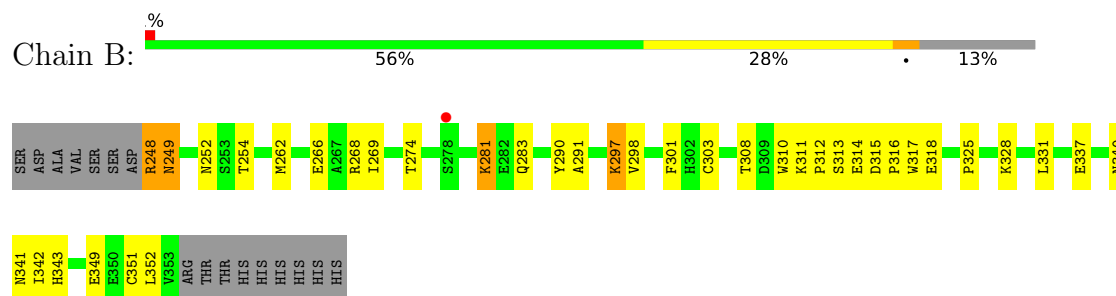
3 Residue-property plots [i](#)

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.

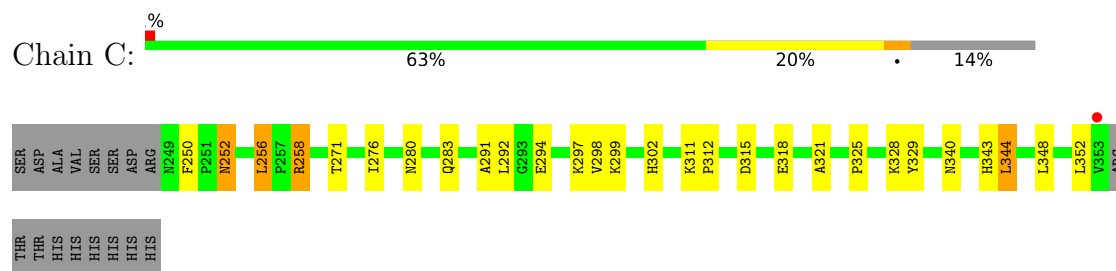
- Molecule 1: Baculoviral IAP repeat-containing protein 4



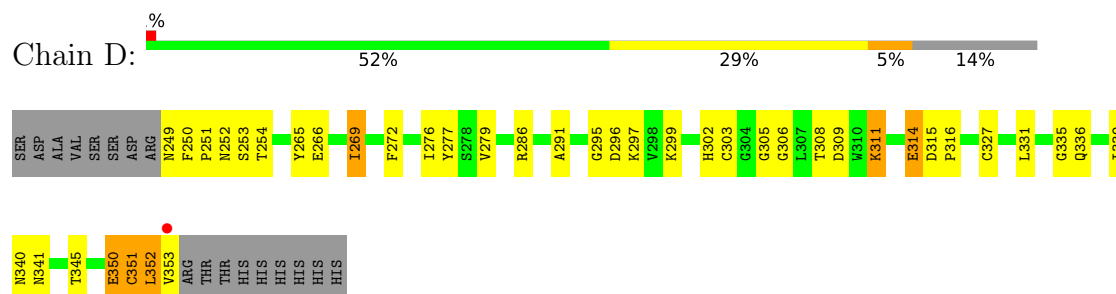
- Molecule 1: Baculoviral IAP repeat-containing protein 4



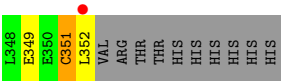
- Molecule 1: Baculoviral IAP repeat-containing protein 4



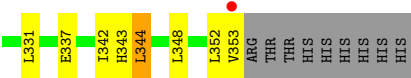
- Molecule 1: Baculoviral IAP repeat-containing protein 4



- | SER | SER |
|------|------|
| ASP | ASP |
| ALA | ALA |
| VAL | VAL |
| S246 | S246 |
| D247 | D247 |
| R248 | R248 |
| N249 | N249 |
| S252 | S252 |
| S253 | S253 |
| T254 | T254 |
| N255 | N255 |
| A263 | A263 |
| I276 | I276 |
| Y277 | Y277 |
| Z278 | Z278 |
| E282 | E282 |
| R286 | R286 |
| Y290 | Y290 |
| A291 | A291 |
| L292 | L292 |
| G295 | G295 |
| D296 | D296 |
| K297 | K297 |
| V298 | V298 |
| K299 | K299 |
| C300 | C300 |
| F301 | F301 |
| D309 | D309 |
| P312 | P312 |
| D315 | D315 |
| E318 | E318 |
| A321 | A321 |
| K322 | K322 |
| P325 | P325 |
| K328 | K328 |
| V329 | V329 |
| L330 | L330 |
| L331 | L331 |
| E332 | E332 |
| I342 | I342 |
| H346 | H346 |
| S247 | S247 |



● Molecule 1: Baculoviral IAP repeat-containing protein 4



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.42Å 130.49Å 215.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.41 – 3.30 51.41 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (51.41-3.30) 99.8 (51.41-3.30)	Depositor EDS
R_{merge}	0.26	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.210 , 0.276 0.209 , 0.274	Depositor DCC
R_{free} test set	1446 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.22$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	9357	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.94% 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: 2PE, P33, 0O6, ZN

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	0.57	0/918	0.86	0/1244
1	B	0.55	0/893	0.87	0/1211
1	C	0.50	0/882	0.94	4/1197 (0.3%)
1	D	0.55	0/893	0.86	0/1211
1	E	0.54	0/907	0.92	3/1230 (0.2%)
1	F	0.52	0/886	0.89	0/1201
1	G	0.52	0/898	0.86	0/1218
1	J	0.54	0/907	0.93	4/1230 (0.3%)
1	K	0.50	0/900	0.89	1/1220 (0.1%)
1	L	0.55	0/898	0.89	2/1218 (0.2%)
All	All	0.53	0/8982	0.89	14/12180 (0.1%)

There are no bond length outliers.

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	256	LEU	CA-C-N	6.23	126.17	119.76
1	E	256	LEU	C-N-CA	6.23	126.17	119.76
1	J	248	ARG	N-CA-C	-5.76	101.49	110.42
1	K	254	THR	CB-CA-C	-5.75	107.21	114.40
1	J	256	LEU	CA-C-N	5.73	125.68	119.78
1	J	256	LEU	C-N-CA	5.73	125.68	119.78
1	E	249	ASN	N-CA-C	-5.67	106.41	113.55
1	C	256	LEU	CA-C-N	5.42	125.34	119.76
1	C	256	LEU	C-N-CA	5.42	125.34	119.76
1	L	311	LYS	CA-C-N	5.30	126.47	119.84
1	L	311	LYS	C-N-CA	5.30	126.47	119.84
1	C	311	LYS	CA-C-N	5.29	126.46	119.84
1	C	311	LYS	C-N-CA	5.29	126.46	119.84
1	J	247	ASP	N-CA-C	5.29	117.01	108.34

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	890	0	829	14	0
1	B	865	0	808	35	0
1	C	854	0	795	15	0
1	D	862	0	808	38	0
1	E	879	0	816	21	0
1	F	858	0	799	31	0
1	G	870	0	809	28	0
1	J	879	0	816	20	0
1	K	872	0	808	21	0
1	L	870	0	810	23	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	J	1	0	0	0	0
2	K	1	0	0	0	0
2	L	1	0	0	0	0
3	A	86	0	88	4	0
3	B	86	0	88	7	0
3	D	86	0	88	10	0
3	E	86	0	88	11	0
3	J	86	0	88	1	0
4	A	22	0	30	0	0
4	D	22	0	30	1	0
4	J	22	0	30	1	0
5	E	28	0	38	0	0
5	G	28	0	38	2	0
6	A	16	0	0	0	0
6	B	6	0	0	1	0
6	C	9	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	15	0	0	0	0
6	E	10	0	0	1	0
6	F	11	0	0	0	0
6	G	8	0	0	0	0
6	J	8	0	0	0	0
6	K	5	0	0	0	0
6	L	8	0	0	0	0
All	All	9357	0	8704	248	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 (248) 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:D:286[B]:ARG:HG3	1:D:286[B]:ARG:HH11	0.97	1.12
1:G:297:LYS:HG2	1:G:308:THR:HG23	1.34	1.08
1:F:248:ARG:HB3	1:F:249:ASN:HB3	1.37	1.06
1:F:248:ARG:HB3	1:F:249:ASN:CB	1.89	1.02
1:F:248:ARG:HB3	1:F:249:ASN:CA	1.91	1.00
1:D:286[B]:ARG:HH11	1:D:286[B]:ARG:CG	1.75	0.98
1:D:286[B]:ARG:HG3	1:D:286[B]:ARG:NH1	1.71	0.95
1:F:248:ARG:HB3	1:F:249:ASN:HA	1.50	0.93
1:C:280:ASN:HD22	1:C:283:GLN:HB2	1.33	0.93
1:F:248:ARG:HG2	1:F:248:ARG:HH21	1.32	0.92
3:D:402:OO6:HBV	1:K:249:ASN:HB3	1.56	0.86
3:E:402:OO6:HAT	3:E:402:OO6:CBA	2.11	0.79
1:G:252:ASN:HB3	1:G:303:CYS:HA	1.65	0.79
1:F:248:ARG:CB	1:F:249:ASN:HB3	2.13	0.78
1:E:291:ALA:HA	1:E:298:VAL:HG12	1.66	0.77
1:B:311:LYS:HB3	1:B:312:PRO:HD2	1.67	0.76
1:D:252:ASN:HB3	1:D:303:CYS:HA	1.68	0.76
1:F:249:ASN:N	1:F:249:ASN:HD22	1.82	0.76
3:B:402:OO6:HBQ	3:B:402:OO6:HAZ	1.66	0.75
1:B:312:PRO:O	1:B:313:SER:HB2	1.87	0.74
1:B:248:ARG:HH11	1:B:248:ARG:HB3	1.52	0.74
3:B:402:OO6:HBH	1:G:249:ASN:O	1.87	0.74
1:B:248:ARG:HH11	1:B:248:ARG:CB	2.00	0.73
1:B:283:GLN:NE2	1:B:315:ASP:OD2	2.22	0.72
1:F:248:ARG:HH21	1:F:248:ARG:CG	2.04	0.70
1:L:321:ALA:HB3	1:L:342:ILE:HD12	1.72	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:ASN:HD22	1:F:249:ASN:H	1.40	0.70
3:A:402:0O6:HAV	3:A:402:0O6:NBX	2.05	0.69
1:G:292:LEU:HD21	1:G:299:LYS:HB2	1.73	0.69
1:D:350:GLU:CD	1:K:248:ARG:HH21	2.00	0.69
1:E:283:GLN:HB3	1:E:316:PRO:HG2	1.74	0.69
1:B:291:ALA:HA	1:B:298:VAL:HG12	1.74	0.68
1:G:254:THR:HG23	1:G:256:LEU:H	1.59	0.67
1:G:331:LEU:HD21	1:G:336:GLN:HG2	1.77	0.67
1:F:280:ASN:HB3	1:F:283:GLN:HB2	1.77	0.66
3:E:402:0O6:CBA	3:E:402:0O6:CAT	2.71	0.66
1:B:337:GLU:OE2	1:B:337:GLU:HA	1.96	0.66
1:B:252:ASN:HB3	1:B:303:CYS:HA	1.78	0.65
1:B:248:ARG:HH11	1:B:248:ARG:CG	2.09	0.65
1:J:306:GLY:HA3	3:J:401:0O6:CAR	2.27	0.65
1:J:297:LYS:HG2	1:J:308:THR:CG2	2.27	0.65
1:B:318:GLU:HG3	1:B:342:ILE:HD12	1.79	0.64
3:B:402:0O6:HBFA	1:G:324:TYR:HE2	1.62	0.64
1:F:248:ARG:CB	1:F:249:ASN:CA	2.70	0.63
1:C:302:HIS:CD2	1:C:329:TYR:HB2	2.33	0.63
1:F:248:ARG:CB	1:F:249:ASN:HA	2.17	0.63
1:A:262:MET:HE3	1:D:276:ILE:HD12	1.82	0.62
1:K:255:ASN:ND2	1:K:328:LYS:HG2	2.14	0.62
1:D:306:GLY:C	3:D:402:0O6:HAS	2.24	0.62
1:E:331:LEU:HD13	1:E:336:GLN:HG2	1.81	0.62
1:L:252:ASN:HB3	1:L:303:CYS:HA	1.81	0.62
1:F:252:ASN:CG	1:F:254:THR:HG22	2.25	0.62
1:D:350:GLU:HG2	1:K:252:ASN:OD1	2.01	0.61
1:A:353:VAL:O	1:A:354:ARG:HG3	2.01	0.60
1:F:284:LEU:HD23	1:F:316:PRO:HB3	1.82	0.60
1:B:325:PRO:HG3	5:G:402:2PE:H62	1.84	0.60
1:B:252:ASN:HD21	1:B:254:THR:HG22	1.67	0.60
1:F:252:ASN:ND2	1:F:254:THR:HG22	2.16	0.60
1:B:297:LYS:HD2	1:B:308:THR:HG21	1.84	0.60
3:E:402:0O6:CAT	3:E:402:0O6:HBAA	2.32	0.60
3:E:402:0O6:HCZ	3:E:402:0O6:HAU	1.82	0.60
1:B:311:LYS:HB3	1:B:312:PRO:CD	2.31	0.59
1:A:344:LEU:HD21	1:J:345:THR:HG23	1.84	0.59
1:L:305:GLY:HA3	1:L:324:TYR:CE2	2.38	0.59
6:B:505:HOH:O	1:G:353:VAL:HG11	2.03	0.58
1:G:287:ALA:HA	1:G:317:TRP:CZ2	2.38	0.58
1:E:280:ASN:HB3	1:E:283:GLN:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:325:PRO:HG3	1:C:343:HIS:CE1	2.38	0.58
1:C:340:ASN:O	1:C:344:LEU:HD12	2.04	0.58
1:F:279:VAL:HG21	1:F:310:TRP:HB3	1.86	0.58
1:B:248:ARG:HB3	1:B:248:ARG:NH1	2.17	0.57
1:K:282:GLU:O	1:K:286:ARG:HB2	2.04	0.57
1:G:259:ASN:ND2	1:G:290:TYR:OH	2.38	0.57
1:D:297:LYS:HG2	1:D:308:THR:HB	1.86	0.57
1:L:280:ASN:HD22	1:L:283:GLN:HB2	1.69	0.57
1:E:249:ASN:ND2	3:E:402:OO6:HBU	2.20	0.57
1:G:266:GLU:HA	1:G:269:ILE:HD11	1.87	0.57
1:C:291:ALA:HA	1:C:298:VAL:HG12	1.87	0.56
1:B:351:CYS:SG	1:D:351:CYS:HB3	2.45	0.56
1:B:252:ASN:ND2	1:B:254:THR:HG22	2.21	0.55
3:E:402:OO6:HBT	3:E:402:OO6:CBB	2.36	0.55
1:A:331:LEU:HD21	1:A:336:GLN:HG2	1.88	0.55
1:C:315:ASP:HB3	1:C:318:GLU:HB3	1.89	0.55
1:G:340:ASN:O	1:G:344:LEU:HG	2.07	0.55
1:B:310:TRP:HA	3:B:402:OO6:HAAB	1.89	0.55
1:A:348:LEU:HD13	1:J:348:LEU:HA	1.88	0.54
1:F:249:ASN:N	1:F:249:ASN:ND2	2.55	0.54
1:F:271:THR:HB	1:F:291:ALA:HB3	1.90	0.54
1:D:303:CYS:HB3	1:D:327:CYS:SG	2.47	0.54
3:D:402:OO6:HADB	1:K:309:ASP:O	2.08	0.54
1:B:248:ARG:O	1:B:248:ARG:HG2	2.07	0.54
1:J:278:SER:HB3	1:J:312:PRO:HA	1.90	0.53
1:D:266:GLU:HA	1:D:269:ILE:HD11	1.90	0.53
1:J:343:HIS:O	1:J:347:SER:HB2	2.08	0.53
1:D:335:GLY:O	1:D:339:ILE:HD12	2.08	0.53
3:B:402:OO6:HBFA	1:G:324:TYR:CE2	2.43	0.52
1:J:279:VAL:HG21	1:J:310:TRP:CE3	2.43	0.52
1:D:296:ASP:OD2	1:D:309:ASP:HA	2.10	0.52
1:L:321:ALA:CB	1:L:342:ILE:HD12	2.38	0.52
1:B:297:LYS:HD2	1:B:308:THR:CG2	2.38	0.52
1:D:336:GLN:OE1	1:D:340:ASN:ND2	2.42	0.52
1:D:350:GLU:CD	1:K:248:ARG:NH2	2.67	0.52
1:E:350:GLU:HG2	1:L:252:ASN:HD21	1.75	0.52
1:F:321:ALA:HA	1:F:330:LEU:HD21	1.91	0.52
1:E:308:THR:HG22	1:E:309:ASP:H	1.75	0.51
1:D:306:GLY:HA3	3:D:402:OO6:HAS	1.93	0.51
1:F:248:ARG:HG2	1:F:248:ARG:NH2	2.12	0.51
1:G:297:LYS:HG2	1:G:308:THR:CG2	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:352:LEU:N	1:D:352:LEU:HD23	2.25	0.51
1:L:280:ASN:ND2	1:L:283:GLN:HB2	2.25	0.51
1:E:263:ALA:HA	1:E:301:PHE:CE1	2.46	0.51
1:J:263:ALA:HA	1:J:301:PHE:CD1	2.45	0.51
1:L:275:TRP:CH2	1:L:296:ASP:HB2	2.46	0.51
1:E:279:VAL:HG23	1:E:284:LEU:HD11	1.93	0.50
1:L:281:LYS:HG3	1:L:282:GLU:OE1	2.11	0.50
3:A:402:OO6:HBD	1:F:310:TRP:HA	1.94	0.50
1:B:312:PRO:O	1:B:313:SER:CB	2.59	0.50
1:B:310:TRP:CE3	3:B:402:OO6:HAA	2.47	0.50
1:C:321:ALA:O	1:C:343:HIS:HE1	1.95	0.50
1:G:311:LYS:HB3	1:G:312:PRO:HD2	1.94	0.50
1:E:315:ASP:HB3	1:E:318:GLU:HB3	1.94	0.50
1:G:280:ASN:O	1:G:284:LEU:HD12	2.11	0.49
1:A:294:GLU:O	1:A:294:GLU:HG3	2.11	0.49
1:A:348:LEU:C	1:A:350:GLU:H	2.19	0.49
3:D:402:OO6:HAN	1:K:292:LEU:HD13	1.94	0.49
1:C:252:ASN:OD1	1:C:252:ASN:C	2.56	0.49
1:C:292:LEU:HD11	1:C:299:LYS:HG3	1.94	0.49
1:A:279:VAL:HG23	1:A:284:LEU:HD11	1.94	0.49
1:B:315:ASP:OD1	1:B:317:TRP:HB2	2.14	0.48
1:C:271:THR:HB	1:C:291:ALA:HB3	1.95	0.48
3:E:402:OO6:HCZ	1:L:306:GLY:O	2.13	0.48
1:K:295:GLY:C	1:K:297:LYS:H	2.21	0.48
1:D:306:GLY:HA3	3:D:402:OO6:CAS	2.43	0.48
1:E:252:ASN:HB3	1:E:303:CYS:HA	1.94	0.48
1:L:325:PRO:HG3	1:L:343:HIS:CE1	2.48	0.48
1:E:286:ARG:NH1	6:E:507:HOH:O	2.46	0.48
3:E:402:OO6:HAT	3:E:402:OO6:HBAA	1.86	0.48
1:E:350:GLU:HG2	1:L:252:ASN:ND2	2.27	0.47
1:J:252:ASN:OD1	1:J:254:THR:HG22	2.14	0.47
1:J:291:ALA:HA	1:J:298:VAL:HG12	1.96	0.47
1:L:269:ILE:HA	1:L:272:PHE:HB2	1.96	0.47
1:C:250:PHE:O	1:C:258:ARG:NH2	2.48	0.47
1:D:252:ASN:OD1	1:D:253:SER:N	2.48	0.47
1:G:262:MET:HB2	1:G:301:PHE:HB2	1.97	0.47
3:D:402:OO6:HBR	3:D:402:OO6:HAW	1.97	0.47
1:F:252:ASN:OD1	1:F:252:ASN:O	2.32	0.47
1:B:311:LYS:HB2	1:B:314:GLU:CD	2.40	0.46
1:D:299:LYS:HA	1:D:305:GLY:O	2.15	0.46
3:E:402:OO6:HBNA	3:E:402:OO6:OAH	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:402:0O6:HAN	1:G:292:LEU:HD11	1.96	0.46
1:K:321:ALA:HA	1:K:330:LEU:HD21	1.97	0.46
3:E:402:0O6:HAW	1:L:323:TRP:CE3	2.51	0.46
1:D:311:LYS:O	1:D:314:GLU:HB2	2.15	0.46
1:D:351:CYS:HB3	1:D:352:LEU:HD23	1.98	0.46
1:D:286[B]:ARG:CG	1:D:286[B]:ARG:NH1	2.47	0.46
1:A:252:ASN:ND2	1:A:256:LEU:O	2.49	0.45
1:D:306:GLY:CA	3:D:402:0O6:HAS	2.46	0.45
1:G:287:ALA:HA	1:G:317:TRP:CH2	2.51	0.45
1:E:280:ASN:HB3	1:E:283:GLN:HG3	1.98	0.45
1:B:351:CYS:SG	1:D:352:LEU:CD2	3.05	0.45
1:D:311:LYS:HB2	1:D:314:GLU:OE2	2.17	0.45
1:J:264:ASP:N	1:J:264:ASP:OD1	2.49	0.45
1:D:315:ASP:HA	1:D:316:PRO:HD2	1.85	0.45
1:D:277:TYR:OH	1:D:295:GLY:HA2	2.17	0.45
1:A:348:LEU:C	1:A:350:GLU:N	2.75	0.45
1:C:294:GLU:O	1:C:297:LYS:HB2	2.17	0.45
1:L:344:LEU:HD12	1:L:344:LEU:HA	1.78	0.45
1:K:292:LEU:HD12	1:K:299:LYS:HB2	1.99	0.45
1:A:315:ASP:HB3	1:A:318:GLU:HB3	1.99	0.45
3:E:402:0O6:HBT	3:E:402:0O6:CCR	2.47	0.45
3:A:402:0O6:NBX	3:A:402:0O6:CAV	2.77	0.44
1:K:315:ASP:HB3	1:K:318:GLU:HB2	1.99	0.44
1:B:262:MET:O	1:B:268:ARG:NH1	2.50	0.44
1:A:301:PHE:CD1	1:A:301:PHE:C	2.96	0.44
1:D:254:THR:O	1:D:302:HIS:HE1	2.00	0.44
1:K:263:ALA:HA	1:K:301:PHE:CD1	2.53	0.44
1:K:351:CYS:HA	1:K:352:LEU:HA	1.74	0.44
1:K:278:SER:OG	1:K:312:PRO:HA	2.18	0.44
1:L:256:LEU:HA	1:L:257:PRO:HD3	1.85	0.44
1:B:248:ARG:HH11	1:B:248:ARG:HG2	1.80	0.44
1:G:269:ILE:H	1:G:269:ILE:HG13	1.56	0.44
1:L:269:ILE:H	1:L:269:ILE:HG13	1.55	0.44
1:B:290:TYR:HE2	1:B:301:PHE:HA	1.82	0.44
1:C:252:ASN:HD22	1:C:258:ARG:HG3	1.83	0.44
1:K:290:TYR:HE2	1:K:301:PHE:HA	1.82	0.44
1:L:280:ASN:HB3	1:L:283:GLN:HB2	2.00	0.44
1:G:344:LEU:HA	1:G:347:SER:HB3	2.00	0.44
1:L:311:LYS:N	1:L:314:GLU:OE1	2.51	0.43
1:B:311:LYS:CB	1:B:312:PRO:CD	2.95	0.43
1:J:352:LEU:HA	1:J:353:VAL:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258:ARG:O	1:E:258:ARG:HG2	2.18	0.43
1:J:297:LYS:HE2	1:J:308:THR:HG21	1.99	0.43
1:D:351:CYS:O	1:D:353:VAL:HA	2.19	0.43
1:G:256:LEU:HA	1:G:257:PRO:HD3	1.79	0.43
1:F:292:LEU:HD12	1:F:297:LYS:C	2.43	0.43
1:C:302:HIS:HD2	1:C:329:TYR:HB2	1.82	0.43
1:D:309:ASP:O	3:D:402:O06:HA	2.19	0.43
1:J:326:GLY:O	1:J:328:LYS:HD2	2.18	0.43
1:J:262:MET:HG3	1:J:290:TYR:CD2	2.54	0.43
1:B:281:LYS:H	1:B:281:LYS:HG3	1.57	0.42
1:F:305:GLY:HA3	1:F:324:TYR:CE1	2.53	0.42
1:G:290:TYR:HE2	1:G:301:PHE:HA	1.83	0.42
1:J:297:LYS:HG2	1:J:308:THR:HG21	2.00	0.42
1:G:250:PHE:HA	1:G:251:PRO:HD3	1.83	0.42
1:K:255:ASN:HD21	1:K:328:LYS:HG2	1.81	0.42
1:L:322:LYS:HD3	1:L:323:TRP:NE1	2.34	0.42
1:L:352:LEU:HA	1:L:353:VAL:HA	1.84	0.42
1:B:249:ASN:HD22	1:B:249:ASN:HA	1.53	0.42
1:D:269:ILE:H	1:D:269:ILE:HG13	1.64	0.42
1:J:252:ASN:HB3	1:J:303:CYS:HA	2.02	0.42
1:E:337:GLU:O	1:E:341:ASN:ND2	2.53	0.42
1:L:315:ASP:HB3	1:L:318:GLU:HB3	2.01	0.42
1:B:315:ASP:OD2	1:B:316:PRO:HD2	2.20	0.42
4:D:403:P33:H111	1:K:325:PRO:HG3	2.02	0.42
1:G:271:THR:HG21	1:G:291:ALA:O	2.19	0.42
1:E:250:PHE:HA	1:E:251:PRO:HD3	1.91	0.42
1:F:252:ASN:ND2	1:F:254:THR:CG2	2.81	0.42
1:D:266:GLU:HA	1:D:269:ILE:CD1	2.49	0.42
1:F:257:PRO:HG3	1:F:302:HIS:CD2	2.55	0.42
1:K:249:ASN:ND2	1:K:249:ASN:H	2.18	0.42
1:K:322:LYS:HE3	1:K:346:HIS:CE1	2.55	0.42
1:G:257:PRO:HG3	1:G:302:HIS:CD2	2.55	0.42
3:A:402:O06:HBFA	1:F:324:TYR:HE2	1.84	0.41
1:B:343:HIS:CE1	5:G:402:2PE:H81	2.54	0.41
1:C:292:LEU:HD12	1:C:297:LYS:HB3	2.02	0.41
1:D:272:PHE:CE2	1:D:291:ALA:HB2	2.55	0.41
1:E:280:ASN:HB3	1:E:283:GLN:CG	2.50	0.41
1:F:283:GLN:HB3	1:F:316:PRO:HG2	2.01	0.41
1:F:311:LYS:HB2	1:F:314:GLU:OE1	2.20	0.41
1:A:252:ASN:HD22	1:A:258:ARG:HG2	1.84	0.41
1:J:325:PRO:HG2	4:J:403:P33:H81	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:346:HIS:O	1:E:349:GLU:HG2	2.21	0.41
1:F:248:ARG:CG	1:F:248:ARG:NH2	2.72	0.41
1:G:254:THR:HG23	1:G:256:LEU:N	2.31	0.41
1:K:332:GLU:O	1:K:332:GLU:HG2	2.20	0.41
1:B:341:ASN:HA	1:D:341:ASN:OD1	2.21	0.41
1:J:265:TYR:O	1:J:269:ILE:HG13	2.20	0.41
1:A:272:PHE:CE2	1:A:284:LEU:HD13	2.55	0.41
1:E:269:ILE:H	1:E:269:ILE:HG13	1.79	0.41
1:G:252:ASN:CB	1:G:303:CYS:HA	2.44	0.41
1:D:250:PHE:HA	1:D:251:PRO:HD3	1.94	0.41
1:F:256:LEU:HA	1:F:257:PRO:HD3	1.83	0.40
1:D:265:TYR:CZ	1:D:269:ILE:HG12	2.56	0.40
3:D:402:OO6:HAX	3:D:402:OO6:HBF	1.94	0.40
1:B:349:GLU:HA	1:B:352:LEU:HD12	2.03	0.40
1:E:287:ALA:HA	1:E:317:TRP:CZ2	2.56	0.40
1:J:269:ILE:HG13	1:J:269:ILE:H	1.54	0.40
1:L:279:VAL:HG23	1:L:284:LEU:HD11	2.04	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	107/122 (88%)	98 (92%)	9 (8%)	0	100	100
1	B	104/122 (85%)	100 (96%)	4 (4%)	0	100	100
1	C	103/122 (84%)	98 (95%)	4 (4%)	1 (1%)	12	40
1	D	104/122 (85%)	93 (89%)	11 (11%)	0	100	100
1	E	106/122 (87%)	95 (90%)	10 (9%)	1 (1%)	14	43
1	F	103/122 (84%)	95 (92%)	8 (8%)	0	100	100
1	G	105/122 (86%)	98 (93%)	5 (5%)	2 (2%)	6	28

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	106/122 (87%)	102 (96%)	4 (4%)	0	100	100
1	K	105/122 (86%)	96 (91%)	8 (8%)	1 (1%)	12	40
1	L	105/122 (86%)	97 (92%)	6 (6%)	2 (2%)	6	28
All	All	1048/1220 (86%)	972 (93%)	69 (7%)	7 (1%)	18	49

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	312	PRO
1	K	322	LYS
1	L	312	PRO
1	G	313	SER
1	L	275	TRP
1	E	295	GLY
1	G	295	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	94/106 (89%)	85 (90%)	9 (10%)	8	29
1	B	91/106 (86%)	81 (89%)	10 (11%)	6	23
1	C	90/106 (85%)	82 (91%)	8 (9%)	9	32
1	D	91/106 (86%)	81 (89%)	10 (11%)	6	23
1	E	93/106 (88%)	83 (89%)	10 (11%)	6	23
1	F	90/106 (85%)	75 (83%)	15 (17%)	2	11
1	G	91/106 (86%)	74 (81%)	17 (19%)	1	7
1	J	93/106 (88%)	79 (85%)	14 (15%)	3	13
1	K	92/106 (87%)	83 (90%)	9 (10%)	7	28
1	L	91/106 (86%)	78 (86%)	13 (14%)	3	14
All	All	916/1060 (86%)	801 (87%)	115 (13%)	4	18

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	248	ARG
1	A	258	ARG
1	A	278	SER
1	A	308	THR
1	A	309	ASP
1	A	314	GLU
1	A	331	LEU
1	A	337	GLU
1	A	352	LEU
1	B	248	ARG
1	B	249	ASN
1	B	266	GLU
1	B	269	ILE
1	B	274	THR
1	B	281	LYS
1	B	297	LYS
1	B	328	LYS
1	B	331	LEU
1	B	340	ASN
1	C	252	ASN
1	C	256	LEU
1	C	258	ARG
1	C	276	ILE
1	C	328	LYS
1	C	344	LEU
1	C	348	LEU
1	C	352	LEU
1	D	249	ASN
1	D	269	ILE
1	D	279	VAL
1	D	311	LYS
1	D	314	GLU
1	D	331	LEU
1	D	345	THR
1	D	350	GLU
1	D	351	CYS
1	D	352	LEU
1	E	249	ASN
1	E	255	ASN
1	E	261	SER
1	E	266	GLU
1	E	269	ILE

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Mol	Chain	Res	Type
1	E	294	GLU
1	E	308	THR
1	E	318	GLU
1	E	348	LEU
1	E	352	LEU
1	J	248	ARG
1	J	253	SER
1	J	264	ASP
1	J	269	ILE
1	J	279	VAL
1	J	283	GLN
1	J	294	GLU
1	J	308	THR
1	J	322	LYS
1	J	332	GLU
1	J	336	GLN
1	J	337	GLU
1	J	344	LEU
1	J	345	THR
1	F	248	ARG
1	F	249	ASN
1	F	253	SER
1	F	255	ASN
1	F	256	LEU
1	F	258	ARG
1	F	266	GLU
1	F	269	ILE
1	F	276	ILE
1	F	282	GLU
1	F	286	ARG
1	F	322	LYS
1	F	331	LEU
1	F	337	GLU
1	F	352	LEU
1	G	253	SER
1	G	254	THR
1	G	255	ASN
1	G	256	LEU
1	G	258	ARG
1	G	266	GLU
1	G	269	ILE
1	G	271	THR

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Mol	Chain	Res	Type
1	G	274	THR
1	G	279	VAL
1	G	282	GLU
1	G	308	THR
1	G	328	LYS
1	G	331	LEU
1	G	342	ILE
1	G	345	THR
1	G	352	LEU
1	K	246	SER
1	K	249	ASN
1	K	276	ILE
1	K	292	LEU
1	K	309	ASP
1	K	342	ILE
1	K	347	SER
1	K	349	GLU
1	K	351	CYS
1	L	248	ARG
1	L	249	ASN
1	L	261	SER
1	L	269	ILE
1	L	286	ARG
1	L	298	VAL
1	L	307	LEU
1	L	309	ASP
1	L	328	LYS
1	L	331	LEU
1	L	337	GLU
1	L	344	LEU
1	L	348	LEU

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

Mol	Chain	Res	Type
1	A	249	ASN
1	A	341	ASN
1	B	249	ASN
1	B	302	HIS
1	C	249	ASN
1	C	255	ASN
1	C	280	ASN

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Mol	Chain	Res	Type
1	C	343	HIS
1	D	249	ASN
1	D	280	ASN
1	D	302	HIS
1	D	346	HIS
1	E	249	ASN
1	E	319	GLN
1	J	319	GLN
1	J	341	ASN
1	J	346	HIS
1	F	249	ASN
1	F	255	ASN
1	F	319	GLN
1	F	333	GLN
1	G	255	ASN
1	G	259	ASN
1	G	283	GLN
1	G	346	HIS
1	K	249	ASN
1	K	252	ASN
1	K	255	ASN
1	K	283	GLN
1	K	346	HIS
1	L	252	ASN
1	L	255	ASN
1	L	280	ASN
1	L	319	GLN
1	L	346	HIS

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 20 ligands modelled in this entry, 10 are monoatomic - leaving 10 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	0O6	A	402	-	88,94,94	1.50	8 (9%)	100,130,130	1.35	14 (14%)
4	P33	D	403	-	21,21,21	0.62	0	20,20,20	0.30	0
4	P33	J	403	-	21,21,21	0.55	0	20,20,20	0.25	0
5	2PE	G	402	-	27,27,27	0.68	0	26,26,26	0.46	0
3	0O6	E	402	-	88,94,94	1.42	6 (6%)	100,130,130	1.75	18 (18%)
4	P33	A	403	-	21,21,21	0.51	0	20,20,20	0.32	0
3	0O6	J	401	-	88,94,94	1.47	8 (9%)	100,130,130	1.33	11 (11%)
3	0O6	B	402	-	88,94,94	1.49	9 (10%)	100,130,130	1.42	14 (14%)
3	0O6	D	402	-	88,94,94	1.47	9 (10%)	100,130,130	1.38	14 (14%)
5	2PE	E	403	-	27,27,27	0.76	0	26,26,26	0.33	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	0O6	A	402	-	-	20/74/134/134	0/9/9/9
4	P33	D	403	-	-	15/19/19/19	-
4	P33	J	403	-	-	10/19/19/19	-
5	2PE	G	402	-	-	16/25/25/25	-
3	0O6	E	402	-	-	23/74/134/134	0/9/9/9
4	P33	A	403	-	-	11/19/19/19	-
3	0O6	J	401	-	-	19/74/134/134	0/9/9/9
3	0O6	B	402	-	-	17/74/134/134	0/9/9/9
3	0O6	D	402	-	-	13/74/134/134	0/9/9/9
5	2PE	E	403	-	-	16/25/25/25	-

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	401	0O6	NDH-NBZ	-7.14	1.23	1.34
3	A	402	0O6	NDG-NBY	-6.98	1.23	1.34
3	D	402	0O6	NDG-NBY	-6.88	1.23	1.34
3	A	402	0O6	NDH-NBZ	-6.80	1.23	1.34
3	B	402	0O6	NDH-NBZ	-6.66	1.24	1.34
3	D	402	0O6	NDH-NBZ	-6.65	1.24	1.34
3	B	402	0O6	NDG-NBY	-6.60	1.24	1.34
3	E	402	0O6	NDH-NBZ	-6.46	1.24	1.34
3	J	401	0O6	NDG-NBY	-6.33	1.24	1.34
3	E	402	0O6	NDG-NBY	-6.29	1.24	1.34
3	J	401	0O6	NBX-NBZ	-5.01	1.23	1.32
3	B	402	0O6	NBW-NBY	-4.93	1.23	1.32
3	A	402	0O6	NBW-NBY	-4.92	1.23	1.32
3	A	402	0O6	NBX-NBZ	-4.89	1.24	1.32
3	D	402	0O6	NBX-NBZ	-4.87	1.24	1.32
3	E	402	0O6	NBX-NBZ	-4.84	1.24	1.32
3	B	402	0O6	NBX-NBZ	-4.69	1.24	1.32
3	E	402	0O6	NBW-NBY	-4.65	1.24	1.32
3	D	402	0O6	NBW-NBY	-4.65	1.24	1.32
3	J	401	0O6	NBW-NBY	-4.44	1.24	1.32
3	A	402	0O6	CBB-CCR	-3.14	1.32	1.36
3	J	401	0O6	CBB-CCR	-3.11	1.32	1.36
3	B	402	0O6	CBB-CCR	-3.11	1.32	1.36
3	E	402	0O6	CBA-CCQ	-2.76	1.32	1.36
3	D	402	0O6	CBB-CCR	-2.74	1.32	1.36
3	J	401	0O6	CCR-NBX	-2.52	1.32	1.36
3	A	402	0O6	CBA-CCQ	-2.46	1.33	1.36
3	E	402	0O6	CBB-CCR	-2.45	1.33	1.36
3	B	402	0O6	CBA-CCQ	-2.43	1.33	1.36
3	A	402	0O6	CCQ-NBW	-2.37	1.32	1.36
3	B	402	0O6	CCK-NDE	-2.34	1.32	1.35
3	D	402	0O6	CCQ-NBW	-2.24	1.32	1.36
3	D	402	0O6	CBA-CCQ	-2.24	1.33	1.36
3	A	402	0O6	CCR-NBX	-2.17	1.33	1.36
3	B	402	0O6	CCQ-NBW	-2.14	1.33	1.36
3	J	401	0O6	CBA-CCQ	-2.13	1.33	1.36
3	D	402	0O6	CCW-NDE	2.13	1.50	1.47
3	B	402	0O6	CCR-NBX	-2.06	1.33	1.36
3	D	402	0O6	CCR-NBX	-2.03	1.33	1.36
3	J	401	0O6	CCK-NDE	-2.03	1.33	1.35

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	0O6	CDB-NCD-CCJ	7.83	137.24	121.18
3	J	401	0O6	NDG-NBY-NBW	4.23	110.82	107.02
3	D	402	0O6	NDG-NBY-NBW	4.17	110.77	107.02
3	B	402	0O6	NDG-NBY-NBW	4.15	110.75	107.02
3	J	401	0O6	OAI-CCK-NDE	-4.15	117.23	121.78
3	A	402	0O6	NDG-NBY-NBW	4.11	110.72	107.02
3	B	402	0O6	CCZ-NDF-CCL	4.00	124.00	118.64
3	B	402	0O6	CCQ-CBA-NDG	-3.98	101.59	105.33
3	E	402	0O6	CCR-CBB-NDH	-3.89	101.67	105.33
3	E	402	0O6	CCZ-NDF-CCL	3.74	123.65	118.64
3	E	402	0O6	CCZ-CCJ-NCD	3.59	124.39	116.52
3	J	401	0O6	CBQ-CCW-NDE	3.58	105.57	101.68
3	B	402	0O6	OAJ-CCL-NDF	-3.57	117.87	121.78
3	B	402	0O6	NDH-NBZ-NBX	3.56	110.22	107.02
3	D	402	0O6	CCR-CBB-NDH	-3.52	102.03	105.33
3	J	401	0O6	CBR-CCX-NDF	3.51	105.49	101.68
3	J	401	0O6	NDH-NBZ-NBX	3.50	110.17	107.02
3	D	402	0O6	NDH-NBZ-NBX	3.50	110.17	107.02
3	B	402	0O6	CCQ-NBW-NBY	-3.48	106.45	109.32
3	E	402	0O6	CBQ-CCW-NDE	3.46	105.44	101.68
3	E	402	0O6	NDH-NBZ-NBX	3.41	110.09	107.02
3	D	402	0O6	CBR-CCX-NDF	3.40	105.37	101.68
3	E	402	0O6	CBU-NDG-CBA	-3.37	122.55	128.83
3	D	402	0O6	CCZ-NDF-CCL	3.33	123.10	118.64
3	A	402	0O6	NDH-NBZ-NBX	3.33	110.02	107.02
3	J	401	0O6	CCY-NDE-CCK	3.30	123.06	118.64
3	A	402	0O6	CCY-NDE-CCK	3.20	122.93	118.64
3	E	402	0O6	CCQ-CBA-NDG	-3.19	102.34	105.33
3	J	401	0O6	CCZ-NDF-CCL	3.15	122.86	118.64
3	A	402	0O6	OAI-CCK-NDE	-3.08	118.40	121.78
3	A	402	0O6	CBR-CCX-NDF	3.03	104.98	101.68
3	E	402	0O6	CCJ-CCZ-NDF	-3.03	106.24	112.36
3	A	402	0O6	CCQ-CBA-NDG	-3.01	102.50	105.33
3	E	402	0O6	CBR-CCX-NDF	2.98	104.92	101.68
3	A	402	0O6	OAJ-CCL-NDF	-2.96	118.54	121.78
3	A	402	0O6	CCZ-NDF-CCL	2.92	122.55	118.64
3	B	402	0O6	CCY-NDE-CCK	2.91	122.54	118.64
3	E	402	0O6	CCR-NBX-NBZ	-2.88	106.94	109.32
3	D	402	0O6	CCQ-CBA-NDG	-2.86	102.64	105.33
3	E	402	0O6	OAH-CCJ-NCD	-2.85	117.86	122.96
3	D	402	0O6	CBQ-CCW-NDE	2.80	104.72	101.68
3	E	402	0O6	NDG-NBY-NBW	2.79	109.53	107.02
3	A	402	0O6	CBV-NDH-CBB	-2.76	123.68	128.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	402	0O6	CBV-NDH-CBB	-2.73	123.73	128.83
3	E	402	0O6	CAV-CCP-CDB	-2.67	116.50	120.78
3	A	402	0O6	CBS-CBQ-CCW	-2.63	100.17	104.08
3	A	402	0O6	CBV-NDH-NBZ	2.63	126.05	120.78
3	D	402	0O6	CBV-NDH-CBB	-2.63	123.93	128.83
3	D	402	0O6	OAJ-CCL-NDF	-2.62	118.90	121.78
3	J	401	0O6	CCR-CBB-NDH	-2.62	102.87	105.33
3	E	402	0O6	OAI-CCK-NDE	-2.59	118.94	121.78
3	D	402	0O6	CCY-NDE-CCK	2.54	122.04	118.64
3	D	402	0O6	CBS-CBQ-CCW	-2.52	100.32	104.08
3	D	402	0O6	CCR-NBX-NBZ	-2.52	107.25	109.32
3	E	402	0O6	CCY-NDE-CCK	2.50	121.98	118.64
3	A	402	0O6	CBS-CCY-CCI	-2.45	106.00	111.21
3	B	402	0O6	OAI-CCK-NDE	-2.35	119.20	121.78
3	B	402	0O6	CBQ-CCW-NDE	2.33	104.22	101.68
3	E	402	0O6	CBU-NDG-NBY	2.32	125.43	120.78
3	B	402	0O6	CCR-CBB-NDH	-2.27	103.19	105.33
3	D	402	0O6	CBM-CCS-CBI	-2.27	106.90	110.49
3	B	402	0O6	CBV-NDH-CBB	-2.25	124.63	128.83
3	J	401	0O6	CBU-NDG-CBA	-2.25	124.63	128.83
3	A	402	0O6	CCQ-NBW-NBY	-2.25	107.47	109.32
3	J	401	0O6	CCQ-NBW-NBY	-2.24	107.47	109.32
3	J	401	0O6	CCQ-CBA-NDG	-2.21	103.25	105.33
3	D	402	0O6	CCQ-NBW-NBY	-2.19	107.52	109.32
3	A	402	0O6	CBQ-CCW-NDE	2.16	104.03	101.68
3	B	402	0O6	CBT-CBR-CCX	-2.14	100.89	104.08
3	B	402	0O6	CBU-NDG-CBA	-2.13	124.85	128.83
3	B	402	0O6	CBR-CCX-NDF	2.04	103.90	101.68

There are no chirality outliers.

All (160) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	0O6	N-CA-CB-CAA
3	A	402	0O6	CAB-CBD-CCV-NCB
3	A	402	0O6	CAB-CBD-CCV-CCH
3	A	402	0O6	OAK-CBI-CCS-CDC
3	A	402	0O6	NBW-CCQ-CDA-NCC
3	A	402	0O6	NBX-CCR-CDB-NCD
3	B	402	0O6	OAL-CBJ-CCT-CBN
3	B	402	0O6	OAL-CBJ-CCT-CDD
3	B	402	0O6	NBW-CCQ-CDA-NCC

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Mol	Chain	Res	Type	Atoms
3	B	402	006	NBX-CCR-CDB-NCD
3	D	402	006	OAK-CBI-CCS-CBM
3	D	402	006	OAK-CBI-CCS-CDC
3	D	402	006	OAL-CBJ-CCT-CBN
3	D	402	006	OAL-CBJ-CCT-CDD
3	D	402	006	NBW-CCQ-CDA-NCC
3	D	402	006	NBX-CCR-CDB-NCD
3	E	402	006	N-CA-CB-CAA
3	E	402	006	OAL-CBJ-CCT-CBN
3	E	402	006	OAL-CBJ-CCT-CDD
3	E	402	006	NBX-CCR-CDB-NCD
3	J	401	006	N-CA-CB-CAA
3	J	401	006	OAK-CBI-CCS-CDC
3	J	401	006	OAL-CBJ-CCT-CBN
3	J	401	006	OAL-CBJ-CCT-CDD
3	J	401	006	NBW-CCQ-CDA-NCC
3	J	401	006	CBB-CCR-CDB-NCD
3	J	401	006	NBX-CCR-CDB-NCD
4	D	403	P33	O4-C5-C6-O7
4	J	403	P33	O7-C8-C9-O10
5	G	402	2PE	O16-C17-C18-O19
4	A	403	P33	O10-C11-C12-O13
4	A	403	P33	O7-C8-C9-O10
4	J	403	P33	O19-C20-C21-O22
3	A	402	006	CBH-CBF-CBL-CCN
3	J	401	006	CBE-CBG-CBU-NDG
5	E	403	2PE	O10-C11-C12-O13
3	B	402	006	CBG-CBE-CBK-CCM
4	D	403	P33	O10-C11-C12-O13
5	E	403	2PE	O13-C14-C15-O16
3	J	401	006	CBH-CBF-CBL-CCN
5	G	402	2PE	O19-C20-C21-O22
4	A	403	P33	O16-C17-C18-O19
4	A	403	P33	O4-C5-C6-O7
5	G	402	2PE	O10-C11-C12-O13
5	E	403	2PE	O7-C8-C9-O10
4	D	403	P33	O13-C14-C15-O16
3	E	402	006	OAH-CCJ-NCD-CDB
3	B	402	006	OAH-CCJ-CCZ-CBT
4	J	403	P33	O16-C17-C18-O19
3	E	402	006	CCZ-CCJ-NCD-CDB
4	A	403	P33	O19-C20-C21-O22

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Mol	Chain	Res	Type	Atoms
5	E	403	2PE	O25-C26-C27-O28
5	E	403	2PE	O16-C17-C18-O19
3	E	402	0O6	CBH-CBF-CBL-CCN
3	B	402	0O6	CBH-CBF-CBL-CCN
3	B	402	0O6	NCD-CCJ-CCZ-CBT
4	J	403	P33	O1-C2-C3-O4
4	A	403	P33	O1-C2-C3-O4
3	E	402	0O6	CBG-CBE-CBK-CCM
4	D	403	P33	O19-C20-C21-O22
3	E	402	0O6	CBL-CBF-CBH-CBV
5	G	402	2PE	O7-C8-C9-O10
5	G	402	2PE	O13-C14-C15-O16
3	A	402	0O6	CBL-CBF-CBH-CBV
5	G	402	2PE	O25-C26-C27-O28
3	A	402	0O6	CBF-CBH-CBV-NDH
3	J	401	0O6	CBF-CBH-CBV-NDH
3	B	402	0O6	CBF-CBH-CBV-NDH
4	D	403	P33	O1-C2-C3-O4
3	J	401	0O6	CBL-CBF-CBH-CBV
3	E	402	0O6	OAF-CCH-CCV-NCB
3	A	402	0O6	C-CA-CB-CAA
3	E	402	0O6	C-CA-CB-CAA
3	J	401	0O6	C-CA-CB-CAA
3	E	402	0O6	CBH-CBV-NDH-CBB
3	A	402	0O6	CBE-CBG-CBU-NDG
4	D	403	P33	C6-C5-O4-C3
4	D	403	P33	C18-C17-O16-C15
4	D	403	P33	C15-C14-O13-C12
4	A	403	P33	C15-C14-O13-C12
4	D	403	P33	C21-C20-O19-C18
4	D	403	P33	C11-C12-O13-C14
5	E	403	2PE	C6-C5-O4-C3
4	J	403	P33	C6-C5-O4-C3
5	E	403	2PE	C5-C6-O7-C8
5	E	403	2PE	C9-C8-O7-C6
5	E	403	2PE	C27-C26-O25-C24
4	J	403	P33	C8-C9-O10-C11
5	G	402	2PE	C21-C20-O19-C18
4	A	403	P33	C6-C5-O4-C3
4	D	403	P33	C17-C18-O19-C20
5	E	403	2PE	C8-C9-O10-C11
3	E	402	0O6	NCF-CCH-CCV-NCB

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Mol	Chain	Res	Type	Atoms
4	J	403	P33	C17-C18-O19-C20
5	E	403	2PE	C23-C24-O25-C26
5	G	402	2PE	C9-C8-O7-C6
4	A	403	P33	C21-C20-O19-C18
3	D	402	0O6	CBF-CBH-CBV-NDH
4	A	403	P33	C2-C3-O4-C5
3	A	402	0O6	CCK-CDC-NCE-C
3	A	402	0O6	CBB-CCR-CDB-CCP
3	B	402	0O6	CCL-CDD-NCF-CCH
3	J	401	0O6	CCL-CDD-NCF-CCH
3	J	401	0O6	CBK-CBE-CBG-CBU
5	G	402	2PE	C23-C24-O25-C26
4	J	403	P33	O13-C14-C15-O16
3	B	402	0O6	CAT-CCO-CDA-CCQ
3	J	401	0O6	CAV-CCP-CDB-CCR
3	A	402	0O6	OAK-CBI-CCS-CBM
3	E	402	0O6	OAK-CBI-CCS-CBM
4	J	403	P33	C21-C20-O19-C18
4	D	403	P33	C14-C15-O16-C17
5	G	402	2PE	C17-C18-O19-C20
3	A	402	0O6	CBG-CBE-CBK-CCM
4	D	403	P33	C8-C9-O10-C11
4	D	403	P33	C2-C3-O4-C5
5	G	402	2PE	C14-C15-O16-C17
3	A	402	0O6	CCQ-CDA-NCC-CCI
5	E	403	2PE	C21-C20-O19-C18
5	E	403	2PE	O4-C5-C6-O7
5	E	403	2PE	C24-C23-O22-C21
3	E	402	0O6	OAH-CCJ-CCZ-NDF
3	D	402	0O6	CBF-CBL-CCN-CAX
3	D	402	0O6	OAH-CCJ-CCZ-NDF
3	D	402	0O6	CBF-CBL-CCN-CAZ
3	J	401	0O6	CBF-CBL-CCN-CAX
3	E	402	0O6	CBH-CBV-NDH-NBZ
4	J	403	P33	C2-C3-O4-C5
5	E	403	2PE	C12-C11-O10-C9
3	J	401	0O6	CBF-CBL-CCN-CAZ
5	G	402	2PE	C5-C6-O7-C8
3	A	402	0O6	CBK-CBE-CBG-CBU
5	G	402	2PE	O4-C5-C6-O7
3	A	402	0O6	NBX-CCR-CDB-CCP
3	E	402	0O6	NBW-CCQ-CDA-CCO

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Mol	Chain	Res	Type	Atoms
3	E	402	0O6	NBX-CCR-CDB-CCP
3	D	402	0O6	NCD-CCJ-CCZ-NDF
3	E	402	0O6	OAF-CCH-CCV-CBD
4	D	403	P33	O16-C17-C18-O19
3	D	402	0O6	CBB-CCR-CDB-CCP
3	E	402	0O6	CCK-CDC-NCE-C
3	E	402	0O6	CBB-CCR-CDB-CCP
5	G	402	2PE	C15-C14-O13-C12
5	G	402	2PE	O22-C23-C24-O25
5	E	403	2PE	O22-C23-C24-O25
3	B	402	0O6	CBE-CBK-CCM-CAW
3	A	402	0O6	CAU-CCP-CDB-CCR
3	A	402	0O6	CAV-CCP-CDB-CCR
3	B	402	0O6	CAS-CCO-CDA-CCQ
3	B	402	0O6	CAU-CCP-CDB-CCR
3	B	402	0O6	CAV-CCP-CDB-CCR
3	D	402	0O6	CAU-CCP-CDB-CCR
3	E	402	0O6	NBW-CCQ-CDA-NCC
3	J	401	0O6	CAU-CCP-CDB-CCR
4	A	403	P33	C14-C15-O16-C17
3	B	402	0O6	CBE-CBK-CCM-CAY
5	G	402	2PE	C20-C21-O22-C23
3	B	402	0O6	CCQ-CDA-NCC-CCI
3	E	402	0O6	CCQ-CDA-NCC-CCI
3	J	401	0O6	CCQ-CDA-NCC-CCI

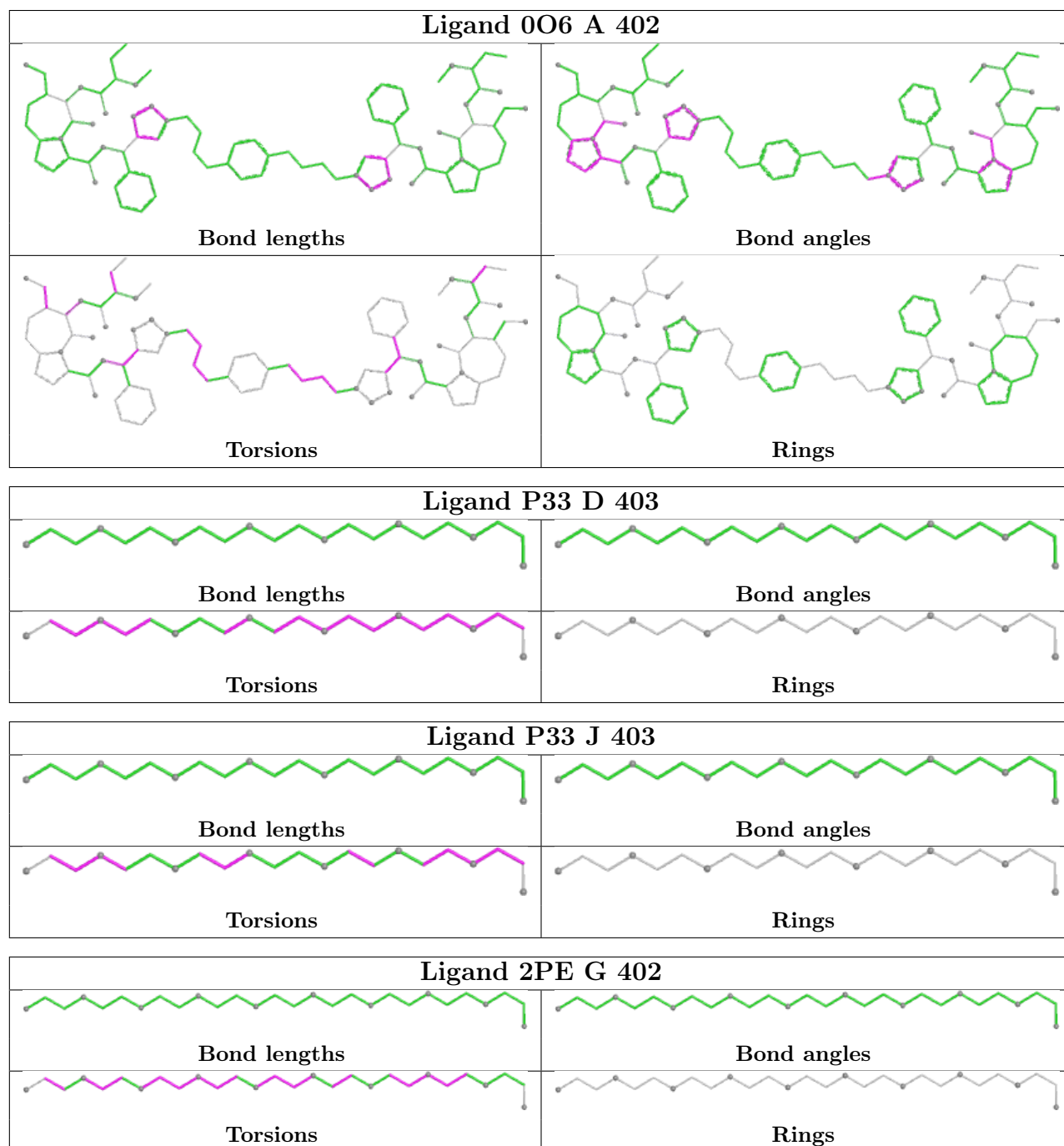
There are no ring outliers.

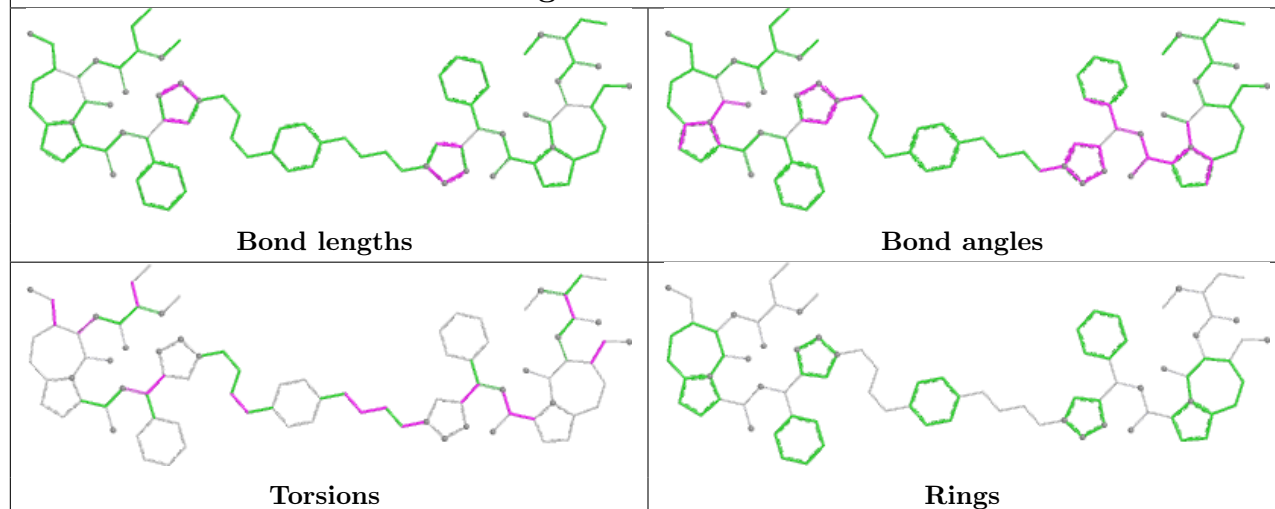
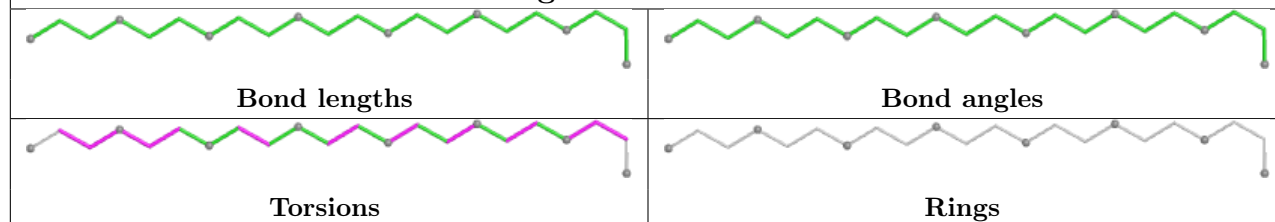
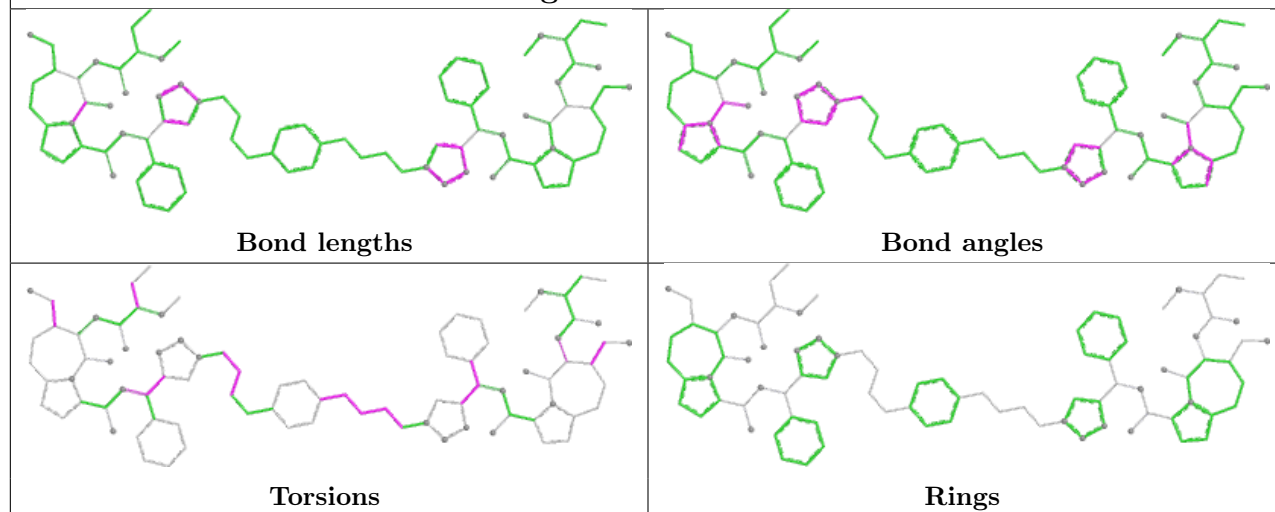
8 monomers are involved in 37 short contacts:

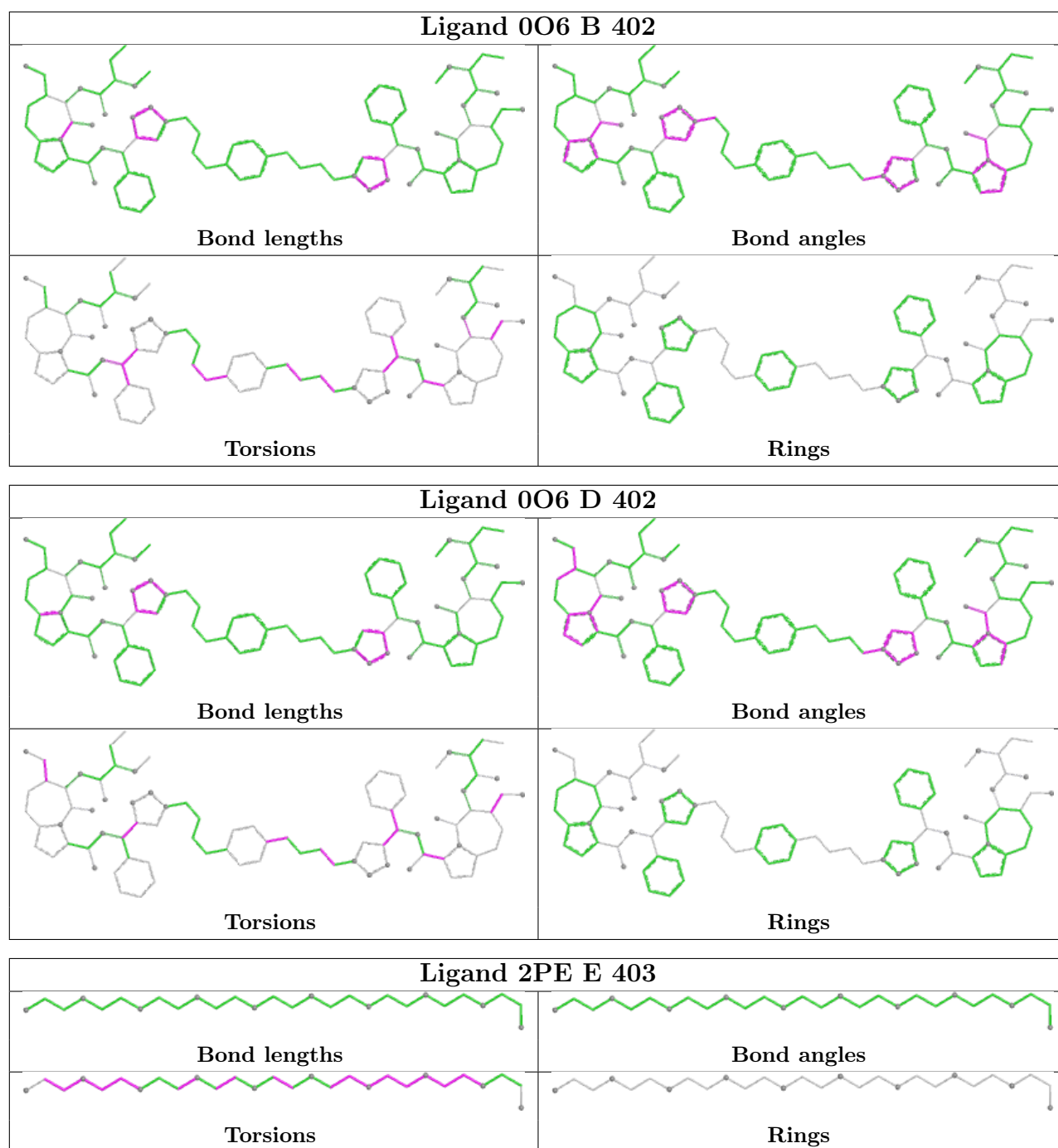
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	0O6	4	0
4	D	403	P33	1	0
4	J	403	P33	1	0
5	G	402	2PE	2	0
3	E	402	0O6	11	0
3	J	401	0O6	1	0
3	B	402	0O6	7	0
3	D	402	0O6	10	0

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.



Ligand 006 E 402**Ligand P33 A 403****Ligand 006 J 401**



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	109/122 (89%)	-0.33	2 (1%) 67 49	8, 16, 54, 75	0
1	B	106/122 (86%)	0.05	1 (0%) 81 65	22, 35, 52, 59	0
1	C	105/122 (86%)	-0.10	1 (0%) 79 63	19, 36, 56, 63	0
1	D	105/122 (86%)	-0.33	1 (0%) 79 63	10, 20, 33, 59	1 (0%)
1	E	108/122 (88%)	-0.33	0 100 100	12, 23, 40, 67	0
1	F	105/122 (86%)	-0.19	0 100 100	12, 28, 48, 59	0
1	G	107/122 (87%)	-0.13	2 (1%) 66 48	14, 31, 49, 80	0
1	J	108/122 (88%)	-0.42	1 (0%) 81 65	9, 19, 38, 57	0
1	K	107/122 (87%)	-0.09	1 (0%) 81 65	19, 35, 56, 64	0
1	L	107/122 (87%)	-0.06	3 (2%) 55 36	16, 37, 71, 79	0
All	All	1067/1220 (87%)	-0.19	12 (1%) 78 60	8, 27, 55, 80	1 (0%)

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	353	VAL	4.2
1	C	353	VAL	3.6
1	L	247	ASP	3.4
1	D	353	VAL	3.2
1	L	353	VAL	3.1
1	G	353	VAL	2.6
1	G	247	ASP	2.5
1	K	352	LEU	2.4
1	A	352	LEU	2.3
1	J	353	VAL	2.2
1	B	278	SER	2.1
1	L	270	PHE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

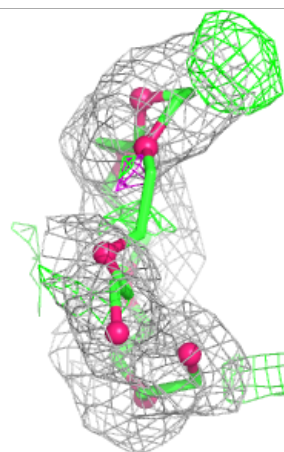
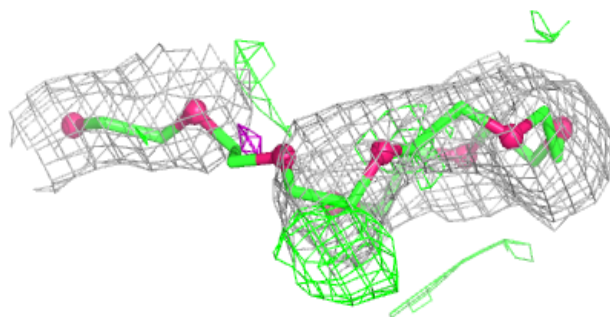
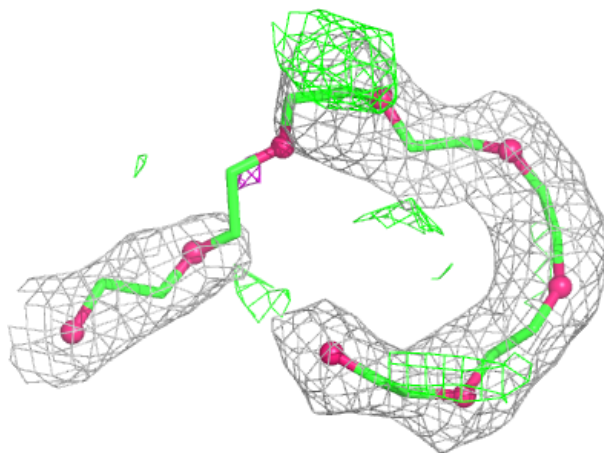
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	P33	D	403	22/22	0.83	0.17	24,29,45,47	0
5	2PE	E	403	28/28	0.89	0.14	24,24,28,29	0
4	P33	J	403	22/22	0.92	0.12	24,24,28,29	0
4	P33	A	403	22/22	0.93	0.12	24,24,30,32	0
5	2PE	G	402	28/28	0.93	0.11	24,24,27,29	0
3	0O6	E	402	86/86	0.94	0.10	15,21,35,40	0
3	0O6	B	402	86/86	0.95	0.12	23,29,38,44	0
3	0O6	J	401	86/86	0.96	0.10	17,25,32,39	0
3	0O6	D	402	86/86	0.96	0.09	12,18,34,40	0
3	0O6	A	402	86/86	0.96	0.09	11,15,33,36	0
2	ZN	B	401	1/1	0.98	0.03	25,25,25,25	0
2	ZN	D	401	1/1	0.99	0.02	11,11,11,11	0
2	ZN	E	401	1/1	1.00	0.03	13,13,13,13	0
2	ZN	J	402	1/1	1.00	0.06	9,9,9,9	0
2	ZN	F	401	1/1	1.00	0.04	14,14,14,14	0
2	ZN	G	401	1/1	1.00	0.01	16,16,16,16	0
2	ZN	K	401	1/1	1.00	0.02	22,22,22,22	0
2	ZN	L	401	1/1	1.00	0.02	21,21,21,21	0
2	ZN	C	401	1/1	1.00	0.05	23,23,23,23	0
2	ZN	A	401	1/1	1.00	0.02	8,8,8,8	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.

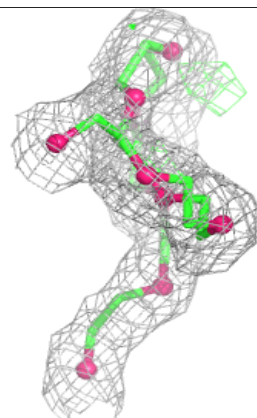
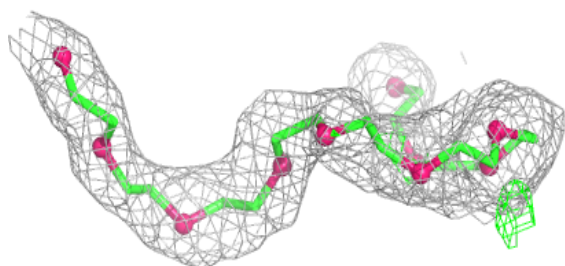
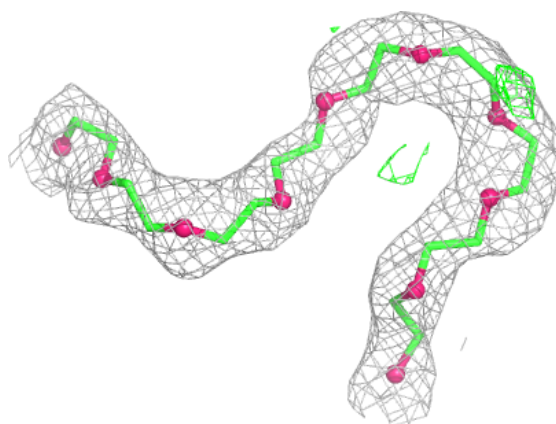
Electron density around P33 D 403:

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

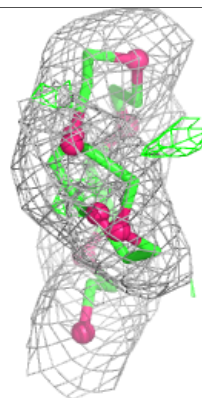
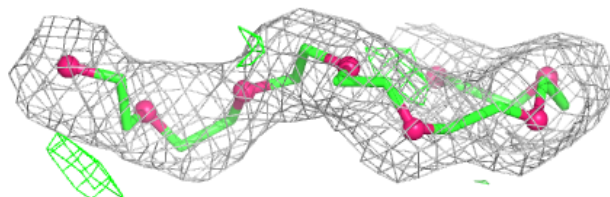
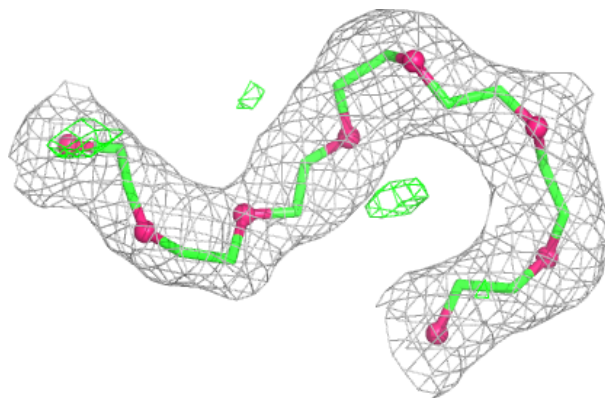


Electron density around 2PE E 403:

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

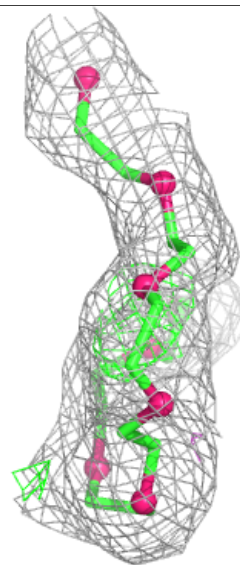
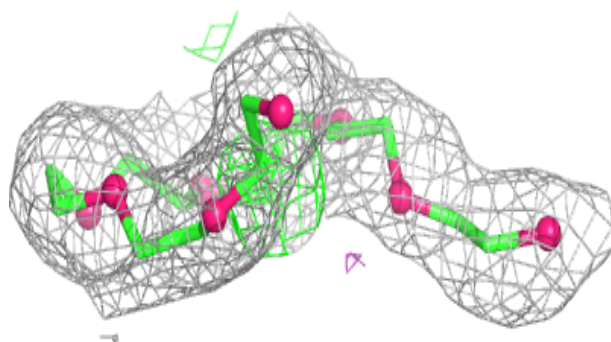
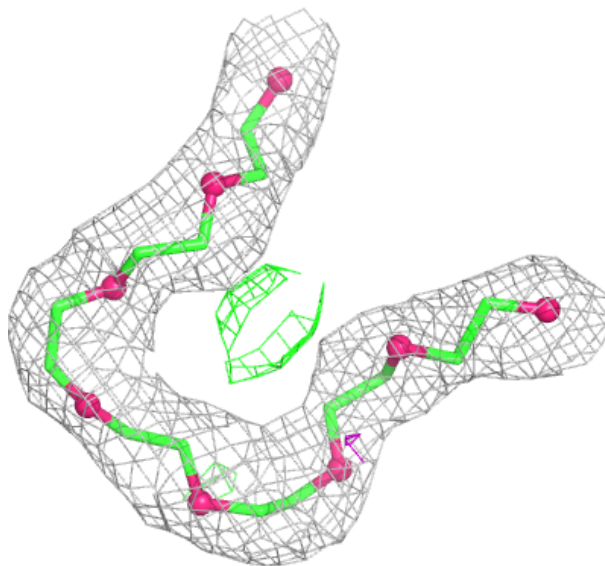
**Electron density around P33 J 403:**

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



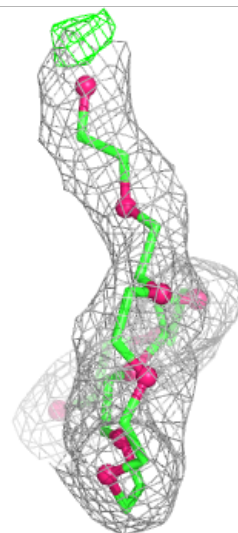
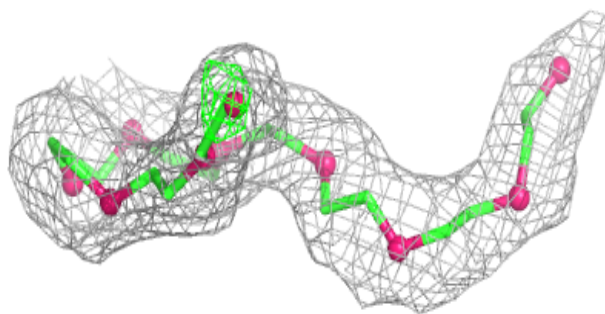
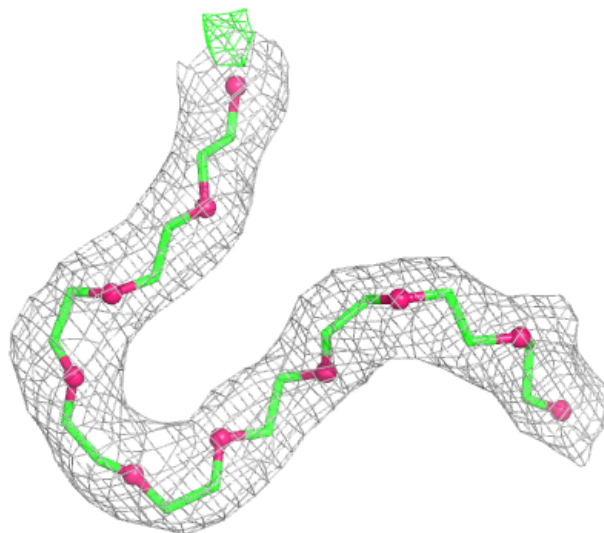
Electron density around P33 A 403:

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



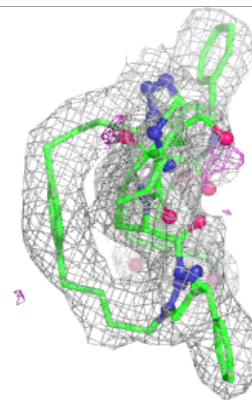
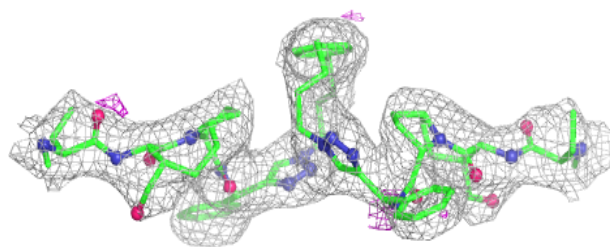
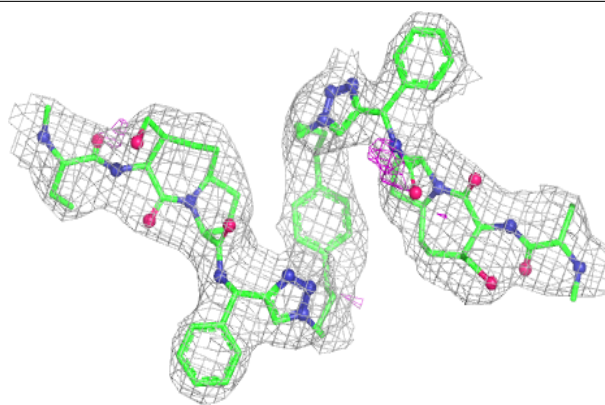
Electron density around 2PE G 402:

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

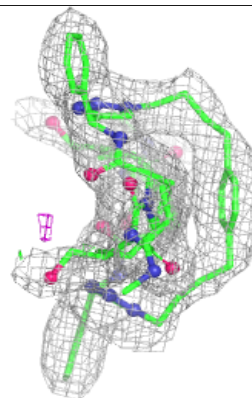
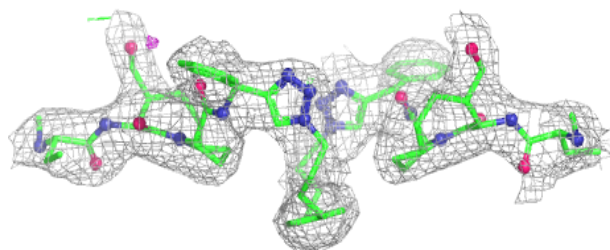
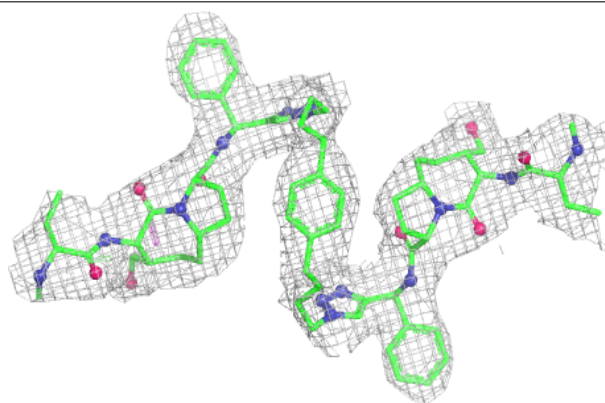


Electron density around 0O6 E 402:

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

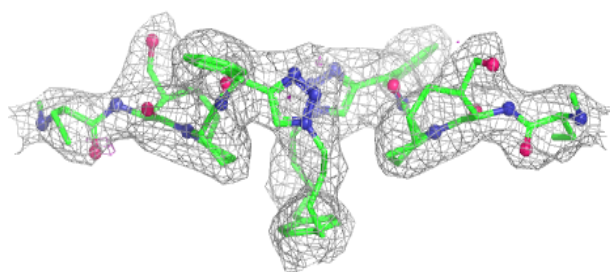
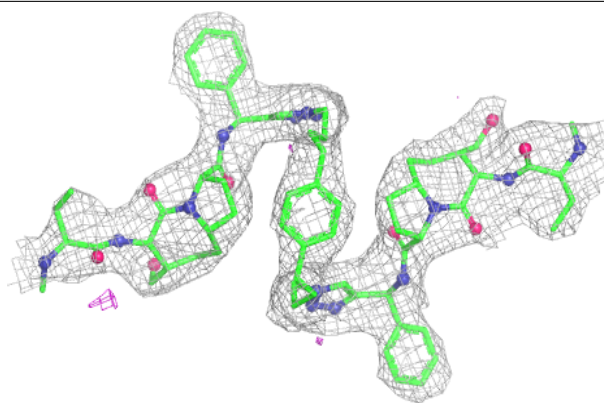
**Electron density around 0O6 B 402:**

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

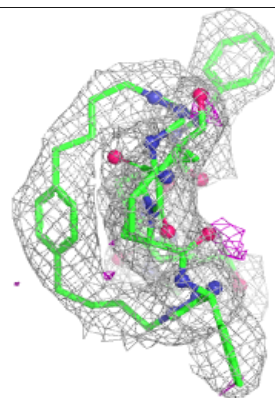
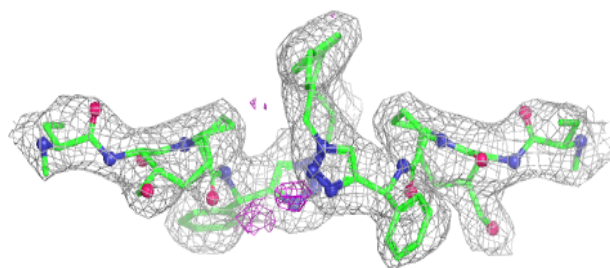
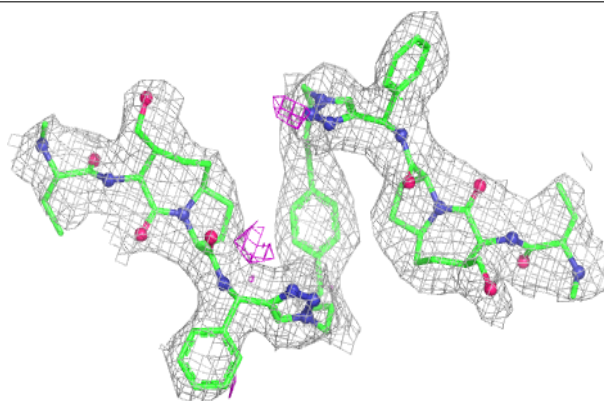


Electron density around 0O6 J 401:

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

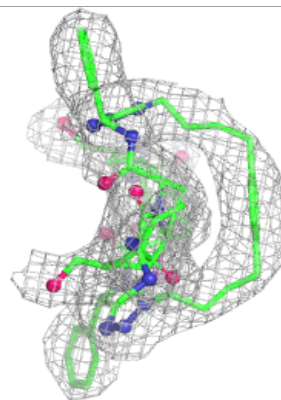
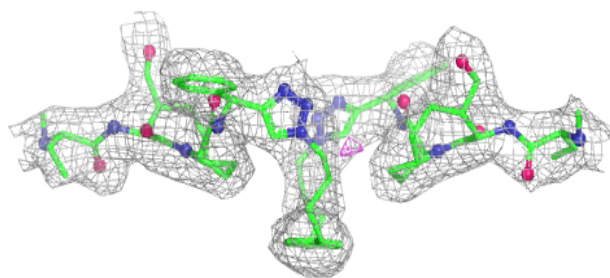
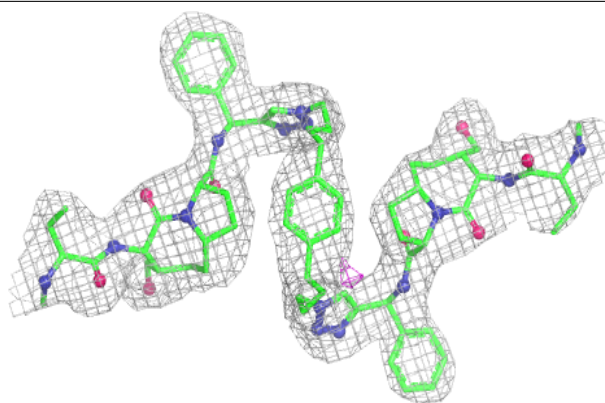
**Electron density around 0O6 D 402:**

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



Electron density around 0O6 A 402:

$2mF_o-DF_c$ (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.