



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:46 AM UTC

PDB ID : 9G2I / pdb_00009g2i
Title : 25-phosphosteroid lyase + phosphate
Authors : Ermler, U.; Boll, M.; Demmer, U.; Jacoby, C.
Deposited on : 2024-07-11
Resolution : 2.00 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

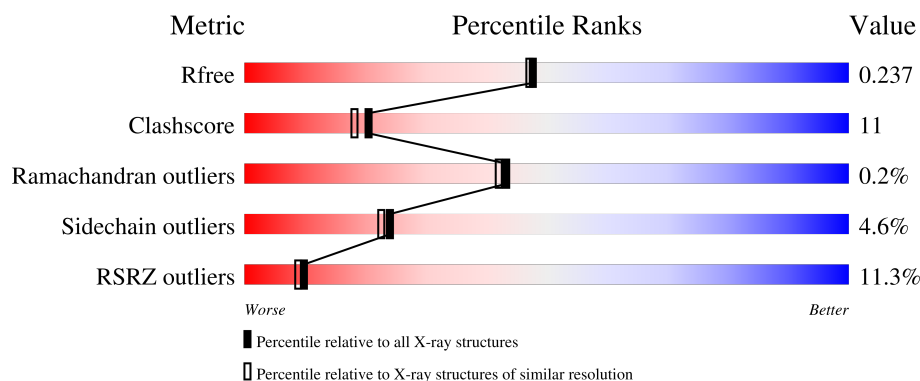
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
R_{free}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	362	<div> <div>6%</div> <div>82%</div> <div>18%</div> </div>
1	B	362	<div> <div>22%</div> <div>66%</div> <div>31%</div> </div>
1	C	362	<div> <div>7%</div> <div>78%</div> <div>20%</div> </div>
1	D	362	<div> <div>10%</div> <div>82%</div> <div>17%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	B	402	-	X	-	-

2 Entry composition [i](#)

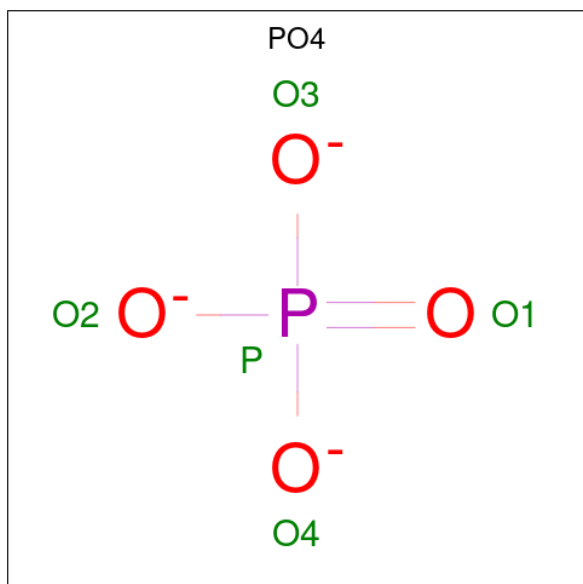
There are 6 unique types of molecules in this entry. The entry contains 12347 atoms, of which 82 are hydrogens and 0 are deuteriums.

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 25-phosphosteroid lyase (25-PSL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	362	Total	C	N	O	S	0	6	0
			2978	1898	514	552	14			
1	B	361	Total	C	N	O	S	0	4	0
			2955	1886	509	546	14			
1	C	361	Total	C	N	O	S	0	4	0
			2957	1885	511	548	13			
1	D	361	Total	C	N	O	S	0	5	0
			2966	1890	514	548	14			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



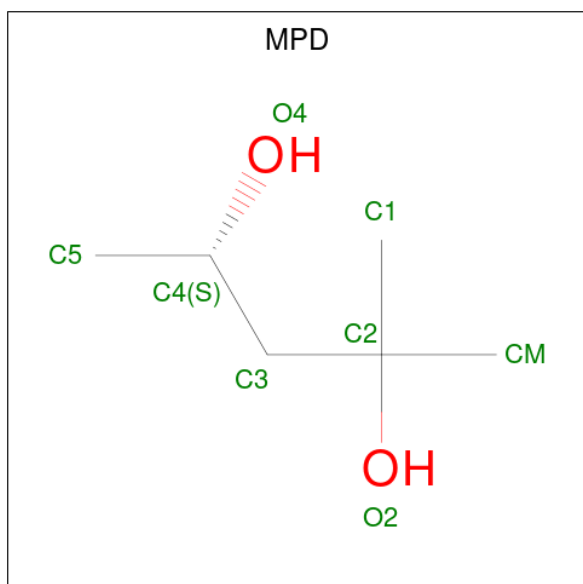
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



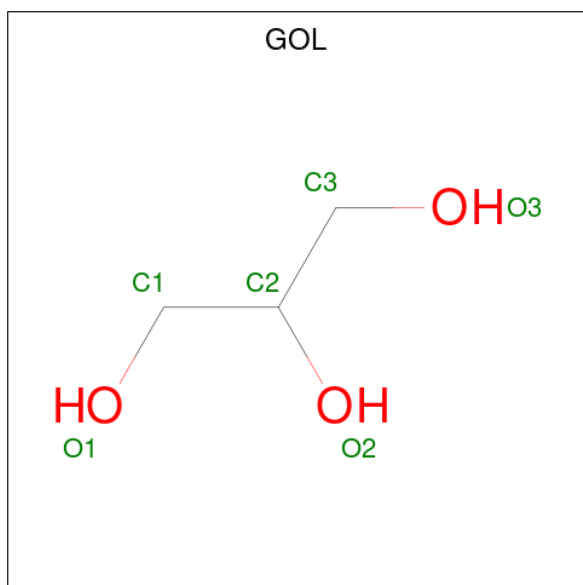
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	A	1	Total	C	H	O	0	0
			22	6	14	2		
3	D	1	Total	C	H	O	0	0
			22	6	14	2		

- Molecule 4 is IMIDAZOLE (CCD ID: IMD) (formula: C₃H₅N₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	N	0	0
			9	3	4	2		
4	A	1	Total	C	H	N	0	0
			9	3	4	2		
4	C	1	Total	C	H	N	0	0
			9	3	4	2		
4	D	1	Total	C	H	N	0	0
			9	3	4	2		

- Molecule 5 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			14	3	8	3		
5	B	1	Total	C	H	O	0	0
			14	3	8	3		
5	C	1	Total	C	H	O	0	0
			14	3	8	3		

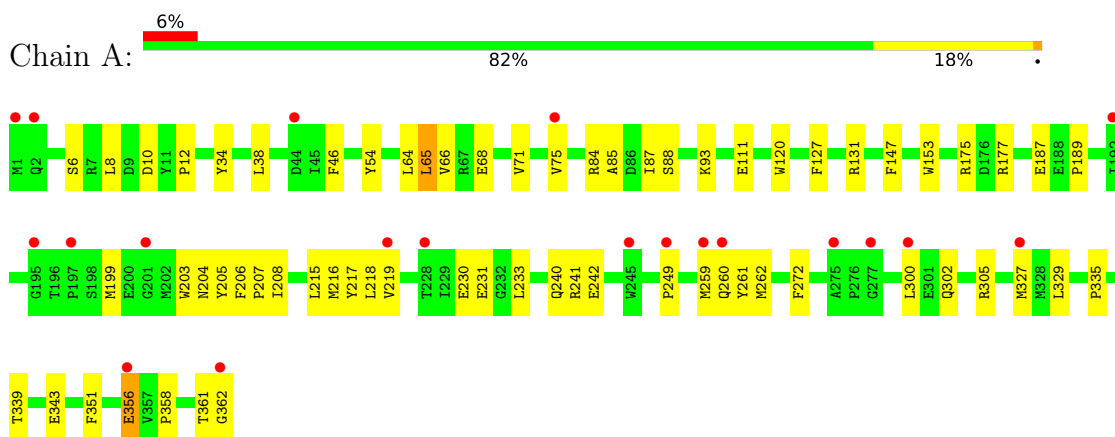
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	73	Total	O	0	1
			74	74		
6	B	69	Total	O	0	2
			71	71		
6	C	72	Total	O	0	1
			73	73		
6	D	88	Total	O	0	1
			89	89		

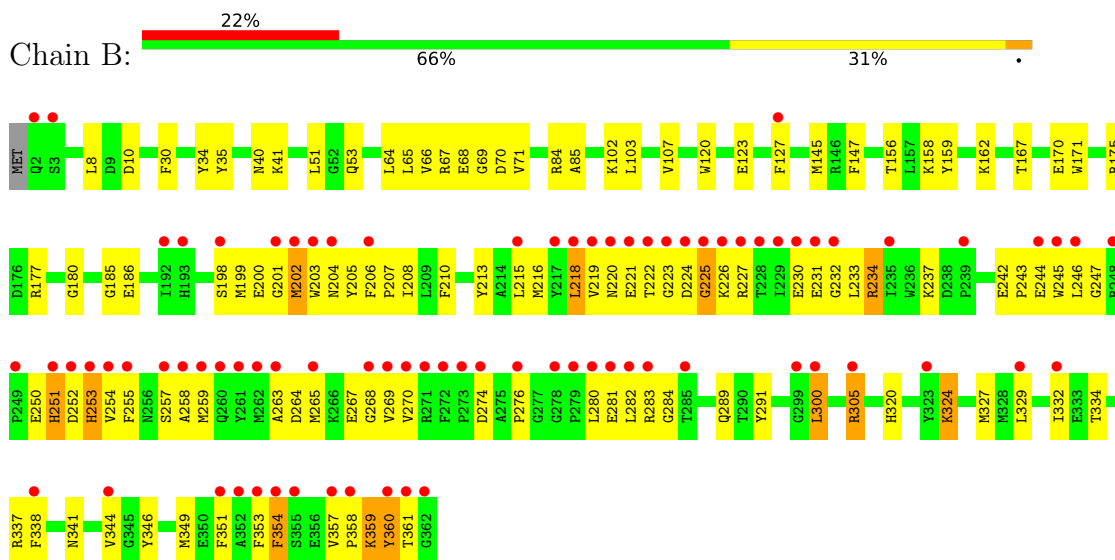
3 Residue-property plots [i](#)

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.

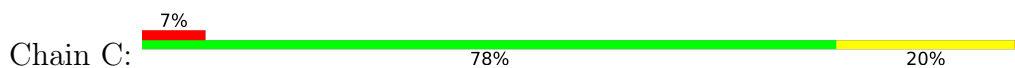
- Molecule 1: 25-phosphosteroid lyase (25-PSL)

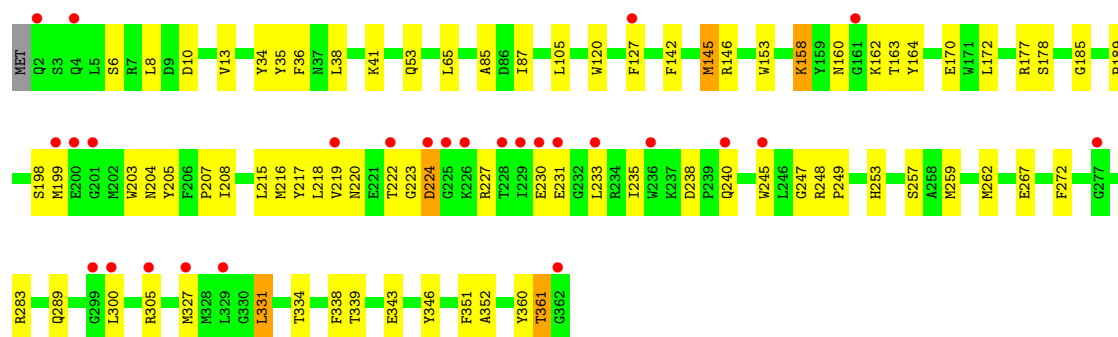


- Molecule 1: 25-phosphosteroid lyase (25-PSL)

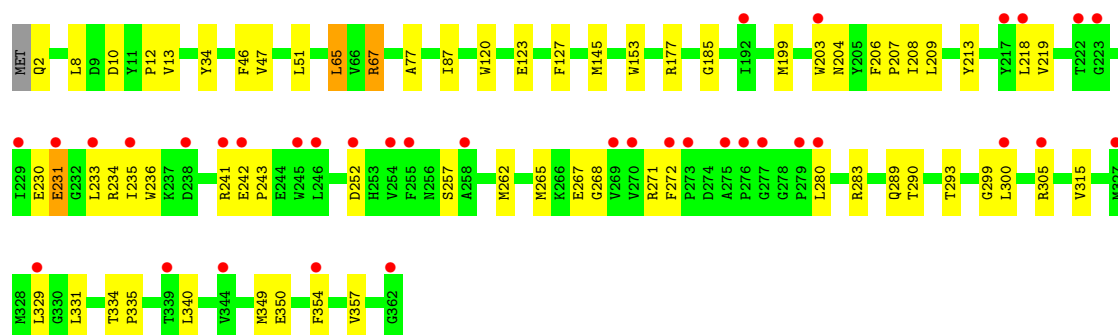
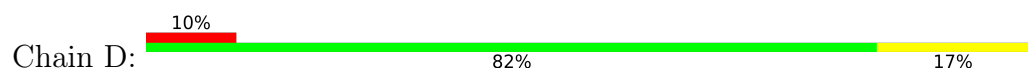


- Molecule 1: 25-phosphosteroid lyase (25-PSL)





● Molecule 1: 25-phosphosteroid lyase (25-PSL)



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	141.70Å 143.57Å 96.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.89 – 2.00 45.89 – 2.00	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.89-2.00) 98.6 (45.89-2.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.45 (at 2.00Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.237 , 0.282 0.239 , 0.237	Depositor DCC
R_{free} test set	6710 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	35.8	Xtriage
Anisotropy	0.152	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12347	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 49.33 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 7.5723e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, IMD, MPD, PO4

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	0.32	0/3060	0.53	0/4144
1	B	0.35	0/3037	0.53	0/4113
1	C	0.36	0/3039	0.54	0/4116
1	D	0.33	0/3048	0.53	0/4127
All	All	0.34	0/12184	0.53	0/16500

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	305[A]	ARG	Sidechain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2978	0	2862	53	0
1	B	2955	0	2842	103	0
1	C	2957	0	2838	56	0
1	D	2966	0	2849	51	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0
3	A	16	28	28	5	0
3	D	8	14	14	2	0
4	A	10	8	10	1	0
4	C	5	4	5	0	0
4	D	5	4	5	0	0
5	A	6	8	8	0	0
5	B	6	8	8	0	0
5	C	6	8	6	0	0
6	A	74	0	0	3	0
6	B	71	0	0	1	0
6	C	73	0	0	1	0
6	D	89	0	0	0	0
All	All	12265	82	11475	262	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 11.

All (262) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ASN:HB2	1:B:219:VAL:HG12	1.40	1.00
3:A:403:MPD:H11	3:A:403:MPD:H52	1.41	0.99
1:B:234:ARG:HG2	1:B:234:ARG:HH21	1.28	0.97
1:C:218:LEU:HD13	1:C:231:GLU:OE1	1.71	0.90
1:D:265:MET:HE1	1:D:349:MET:SD	2.19	0.83
1:B:253:HIS:HD1	1:B:269:VAL:H	1.29	0.81
1:A:187:GLU:HB2	1:A:305[B]:ARG:HH12	1.48	0.79
1:C:199:MET:HE1	1:C:203:TRP:CE3	2.19	0.78
1:B:202:MET:HG3	1:B:353:PHE:CE1	2.20	0.77
1:B:242:GLU:HG3	1:B:243:PRO:HD2	1.67	0.77
1:B:234:ARG:HG2	1:B:234:ARG:NH2	2.00	0.77
1:B:244[B]:GLU:OE2	1:B:276:PRO:HG2	1.84	0.76
1:B:201:GLY:HA3	1:B:222:THR:HG22	1.68	0.76
1:C:230:GLU:OE2	1:C:249:PRO:HD2	1.87	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:238:ASP:OD1	1:C:240[A]:GLN:HG2	1.86	0.75
1:B:70:ASP:OD2	1:B:324:LYS:HD2	1.87	0.74
1:B:255:PHE:CD2	1:B:258:ALA:HB2	2.23	0.74
3:A:403:MPD:H11	3:A:403:MPD:C5	2.17	0.73
1:B:202:MET:HE3	1:B:360:TYR:CE1	2.23	0.73
1:A:131:ARG:HE	3:A:403:MPD:H13	1.53	0.73
1:B:225:GLY:O	1:B:227:ARG:HG3	1.87	0.73
1:D:265:MET:HE1	1:D:349:MET:CE	2.19	0.73
1:C:245:TRP:CZ2	1:C:247:GLY:HA2	2.25	0.72
1:D:242:GLU:HG3	1:D:243:PRO:HD2	1.69	0.72
1:C:224:ASP:N	1:C:224:ASP:OD1	2.24	0.70
1:C:259:MET:HA	1:C:361:THR:HG22	1.73	0.70
1:B:221:GLU:HB2	1:B:227:ARG:HE	1.57	0.70
1:C:289:GLN:HA	1:C:334:THR:HB	1.74	0.70
1:A:260[B]:GLN:HG2	1:A:261:TYR:CD2	2.27	0.69
1:A:356:GLU:HG2	1:A:361:THR:OG1	1.93	0.69
1:D:267:GLU:OE2	1:D:283:ARG:NH1	2.26	0.69
1:C:222:THR:HG22	1:C:223:GLY:H	1.58	0.68
1:A:260[A]:GLN:HE22	1:A:356:GLU:HG3	1.58	0.68
1:B:201:GLY:HA3	1:B:222:THR:CG2	2.24	0.68
1:C:199:MET:HE1	1:C:203:TRP:HE3	1.57	0.68
1:A:260[A]:GLN:NE2	1:A:356:GLU:HG3	2.09	0.67
1:D:204:ASN:HB2	1:D:219:VAL:HG12	1.76	0.67
1:C:218:LEU:HB2	1:C:231:GLU:HB3	1.78	0.66
1:B:242:GLU:HG3	1:B:243:PRO:CD	2.26	0.66
1:A:217:TYR:O	1:A:218:LEU:HD12	1.96	0.65
1:D:233:LEU:CD2	1:D:235:ILE:HG13	2.26	0.65
1:B:203:TRP:HH2	1:B:218:LEU:HD13	1.61	0.65
1:A:65:LEU:HD23	1:A:65:LEU:C	2.22	0.65
1:D:65:LEU:HD23	1:D:65:LEU:C	2.21	0.65
1:D:213:TYR:OH	1:D:340:LEU:HD22	1.96	0.65
1:C:331:LEU:HD12	1:C:352:ALA:HB2	1.77	0.64
1:B:199:MET:HE3	1:B:354:PHE:HE2	1.62	0.64
1:A:217:TYR:C	1:A:218:LEU:HD12	2.23	0.64
1:B:218:LEU:HD21	1:B:231:GLU:CD	2.23	0.64
1:D:233:LEU:HD23	1:D:235:ILE:HG13	1.79	0.64
1:D:242:GLU:HG3	1:D:243:PRO:CD	2.27	0.64
1:B:327:MET:HE3	1:B:327:MET:HA	1.81	0.63
1:D:67:ARG:HH11	1:D:67:ARG:HG3	1.63	0.63
1:A:249:PRO:HB3	1:A:272:PHE:CE1	2.33	0.63
1:D:300:LEU:HG	1:D:305[A]:ARG:NH1	2.14	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:204:ASN:HB2	1:B:219:VAL:CG1	2.25	0.61
1:D:300:LEU:HG	1:D:305[A]:ARG:HH12	1.65	0.61
1:B:203:TRP:CZ2	1:B:205:TYR:HB2	2.37	0.60
1:C:170:GLU:HG3	6:C:565:HOH:O	2.01	0.60
1:B:234:ARG:HH22	1:B:244[B]:GLU:CD	2.10	0.59
1:C:199:MET:HE3	1:C:220:ASN:ND2	2.16	0.59
1:B:203:TRP:O	1:B:351:PHE:HA	2.02	0.59
1:C:142:PHE:HE1	1:C:198:SER:HB3	1.67	0.59
1:C:127:PHE:CE1	1:C:233:LEU:HD22	2.38	0.58
1:D:127:PHE:HE2	1:D:231:GLU:OE1	1.86	0.58
1:D:340:LEU:O	1:D:340:LEU:HD23	2.04	0.58
3:D:403:MPD:O4	3:D:403:MPD:H13	2.03	0.58
1:B:64:LEU:HD22	1:B:107:VAL:HG21	1.85	0.58
1:D:34:TYR:CE2	1:D:177:ARG:HD3	2.39	0.58
1:C:238:ASP:CG	1:C:240[A]:GLN:HG2	2.29	0.58
1:C:222:THR:HG22	1:C:223:GLY:N	2.18	0.57
1:C:267:GLU:OE2	1:C:283:ARG:NE	2.32	0.57
1:A:120:TRP:HB2	1:A:153:TRP:CZ3	2.40	0.57
1:D:67:ARG:HD3	1:D:290:THR:HG23	1.85	0.56
1:B:220:ASN:O	1:B:227:ARG:HG2	2.05	0.56
1:D:242:GLU:CG	1:D:243:PRO:HD2	2.35	0.56
1:C:230:GLU:HG2	1:C:231:GLU:N	2.20	0.55
1:C:233:LEU:HD23	1:C:235:ILE:HD11	1.86	0.55
1:B:204:ASN:CB	1:B:219:VAL:HG12	2.27	0.55
1:C:65:LEU:C	1:C:65:LEU:HD23	2.31	0.55
1:C:203:TRP:O	1:C:351:PHE:HA	2.06	0.55
1:D:236:TRP:CD1	1:D:241[B]:ARG:HG2	2.41	0.55
1:C:217:TYR:O	1:C:218:LEU:HD12	2.07	0.55
3:A:403:MPD:C5	3:A:403:MPD:C1	2.84	0.55
1:B:234:ARG:O	1:B:234:ARG:HG3	2.07	0.55
1:C:41:LYS:HD3	1:C:346:TYR:CD1	2.42	0.55
1:B:210:PHE:O	1:B:237:LYS:NZ	2.41	0.54
1:B:354:PHE:N	1:B:354:PHE:CD1	2.74	0.54
1:B:270:VAL:HB	1:B:282:LEU:HD23	1.89	0.54
1:B:250:GLU:O	1:B:270:VAL:HA	2.07	0.54
1:A:259:MET:HG2	1:A:260[A]:GLN:N	2.22	0.54
1:B:34:TYR:CE2	1:B:177:ARG:HD3	2.43	0.54
1:B:255:PHE:HE2	1:B:263:ALA:HB1	1.72	0.54
1:A:358:PRO:HA	1:A:362:GLY:OXT	2.07	0.54
1:B:123:GLU:OE1	1:B:237:LYS:HE2	2.08	0.54
1:A:189:PRO:HD3	1:C:189:PRO:HD3	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:ASP:OD1	1:B:226:LYS:HD2	2.08	0.53
1:A:259:MET:HG2	1:A:260[B]:GLN:N	2.22	0.53
1:A:203:TRP:C	1:A:204:ASN:HD22	2.18	0.52
1:C:253:HIS:HB2	1:C:360:TYR:CE1	2.44	0.52
1:C:34:TYR:CE2	1:C:177:ARG:HD3	2.45	0.52
1:C:38:LEU:C	1:C:38:LEU:HD23	2.35	0.52
1:B:218:LEU:HG	1:B:231:GLU:HB3	1.91	0.52
1:C:127:PHE:CE2	1:C:231:GLU:OE2	2.64	0.51
4:A:406:IMD:H4	6:A:542:HOH:O	2.10	0.51
1:A:127:PHE:CZ	1:A:233:LEU:HD22	2.45	0.51
1:B:204:ASN:O	1:B:218:LEU:HA	2.11	0.51
1:C:220:ASN:O	1:C:227:ARG:HA	2.10	0.51
1:B:268:GLY:N	1:B:284:GLY:O	2.32	0.50
1:B:300:LEU:HD12	1:B:300:LEU:O	2.11	0.50
1:B:65:LEU:C	1:B:65:LEU:HD23	2.36	0.50
1:D:199:MET:HG2	1:D:354:PHE:CD2	2.46	0.50
1:A:215:LEU:C	1:A:215:LEU:HD23	2.36	0.50
1:A:218:LEU:HD13	1:A:231:GLU:OE2	2.12	0.50
1:B:234:ARG:NH2	1:B:234:ARG:CG	2.73	0.50
1:B:280:LEU:HD23	1:B:341:ASN:ND2	2.27	0.50
1:B:354:PHE:N	1:B:354:PHE:HD1	2.10	0.50
1:B:253:HIS:HB3	1:B:267:GLU:O	2.12	0.49
1:D:299:GLY:C	1:D:300:LEU:HD12	2.36	0.49
1:C:217:TYR:C	1:C:218:LEU:HD12	2.36	0.49
1:D:272:PHE:HB2	1:D:280:LEU:HB2	1.94	0.49
1:B:221:GLU:HB2	1:B:227:ARG:HH21	1.77	0.49
1:A:34:TYR:CE2	1:A:177:ARG:HD3	2.48	0.49
1:D:293:THR:CG2	1:D:331:LEU:H	2.26	0.49
1:B:337:ARG:HG3	1:B:346:TYR:CE1	2.48	0.49
1:C:339:THR:HA	1:C:343:GLU:O	2.13	0.49
1:A:147:PHE:CZ	1:A:177:ARG:HG3	2.48	0.48
1:B:34:TYR:CD2	1:B:177:ARG:HD3	2.48	0.48
1:A:215:LEU:HD23	1:A:216:MET:N	2.28	0.48
1:B:227:ARG:NH1	6:B:501:HOH:O	2.32	0.48
1:B:41:LYS:HD2	1:B:170:GLU:OE1	2.14	0.48
1:B:255:PHE:HA	1:B:265:MET:HA	1.95	0.48
1:C:208:ILE:HG12	1:C:338:PHE:CE1	2.49	0.48
1:C:215:LEU:C	1:C:215:LEU:HD23	2.38	0.48
1:B:66[A]:VAL:HG21	1:B:159:TYR:CE1	2.48	0.48
1:B:289:GLN:HA	1:B:334:THR:HB	1.95	0.48
1:D:123:GLU:HG3	1:D:209:LEU:HD21	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:LEU:HD13	1:A:231:GLU:CD	2.39	0.48
1:B:230:GLU:HG2	1:B:231:GLU:H	1.79	0.48
1:A:199:MET:HE1	3:A:404:MPD:H12	1.96	0.47
1:A:88:SER:HB3	1:A:93:LYS:HZ3	1.78	0.47
1:B:213:TYR:CD2	1:B:234:ARG:HD3	2.49	0.47
1:B:255:PHE:HD2	1:B:258:ALA:HB2	1.75	0.47
1:C:158:LYS:HD2	1:C:163:THR:OG1	2.15	0.47
1:A:120:TRP:CE2	1:A:175:ARG:HD3	2.50	0.47
1:B:185:GLY:O	1:B:305[A]:ARG:HD3	2.15	0.47
1:D:252:ASP:OD2	1:D:271:ARG:NH2	2.48	0.47
1:A:205:TYR:C	1:A:206:PHE:HD1	2.23	0.47
1:A:46:PHE:CD1	1:A:335:PRO:HD3	2.49	0.47
1:D:265:MET:HE1	1:D:349:MET:HE1	1.95	0.47
1:B:167:THR:H	1:B:171:TRP:CD1	2.33	0.46
1:D:331:LEU:HD21	1:D:350:GLU:HG3	1.97	0.46
1:C:215:LEU:HD23	1:C:216:MET:N	2.29	0.46
1:A:302[B]:GLN:O	1:A:302[B]:GLN:HG2	2.15	0.46
1:B:291:TYR:CE1	1:B:332:ILE:HD11	2.50	0.46
1:D:262:MET:HE2	1:D:262:MET:HB3	1.79	0.46
1:B:201:GLY:CA	1:B:222:THR:HG22	2.43	0.46
1:B:251:HIS:O	1:B:251:HIS:ND1	2.49	0.46
1:C:8:LEU:HG	1:C:85:ALA:HB2	1.98	0.46
1:C:127:PHE:HE2	1:C:231:GLU:CD	2.24	0.46
1:B:8:LEU:HG	1:B:85:ALA:HB2	1.97	0.46
1:B:224:ASP:CG	1:B:226:LYS:HD2	2.41	0.45
1:A:84:ARG:HG3	6:A:546:HOH:O	2.16	0.45
1:C:13:VAL:HG12	1:D:8:LEU:HD13	1.97	0.45
1:B:207:PRO:C	1:B:208:ILE:HG13	2.40	0.45
1:B:221:GLU:HB2	1:B:227:ARG:NE	2.30	0.45
1:B:234:ARG:HB3	1:B:246:LEU:HD21	1.98	0.45
1:B:265:MET:HE3	1:B:267:GLU:C	2.41	0.45
1:B:120:TRP:CE2	1:B:175:ARG:HD3	2.51	0.45
1:C:185:GLY:O	1:C:305[A]:ARG:NH1	2.47	0.45
1:D:203:TRP:C	1:D:204:ASN:HD22	2.24	0.45
1:D:145[A]:MET:HE3	1:D:145[A]:MET:HB3	1.74	0.45
1:B:222:THR:O	1:B:224:ASP:N	2.50	0.45
1:C:145:MET:HA	1:C:145:MET:HE2	1.99	0.45
1:A:111:GLU:HG2	6:A:519:HOH:O	2.17	0.44
1:A:208:ILE:HD12	1:A:215:LEU:HD22	1.98	0.44
1:A:205:TYR:CE1	1:A:218:LEU:HD11	2.52	0.44
1:B:208:ILE:HD13	1:B:282:LEU:HD11	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:77:ALA:HA	1:D:315:VAL:O	2.18	0.44
1:B:30:PHE:HA	1:B:180:GLY:O	2.17	0.44
1:C:259:MET:HE3	1:C:262:MET:HE2	2.00	0.44
1:B:156:THR:HG21	1:B:158:LYS:HE2	1.99	0.44
1:C:207:PRO:C	1:C:208:ILE:HG13	2.42	0.44
1:B:234:ARG:NH2	1:B:244[B]:GLU:CD	2.76	0.44
1:A:64:LEU:HB3	1:A:75[A]:VAL:CG1	2.48	0.44
1:B:208:ILE:HD12	1:B:215:LEU:HD22	2.00	0.44
1:B:251:HIS:O	1:B:251:HIS:CG	2.70	0.43
1:C:127:PHE:CZ	1:C:233:LEU:HD22	2.53	0.43
1:C:203:TRP:C	1:C:204:ASN:HD22	2.26	0.43
1:B:71:VAL:HG13	1:B:320:HIS:CE1	2.53	0.43
1:C:249:PRO:HB3	1:C:272:PHE:CE2	2.53	0.43
1:B:205:TYR:C	1:B:206:PHE:HD1	2.27	0.43
1:D:213:TYR:CD2	1:D:234:ARG:HG3	2.52	0.43
1:B:222:THR:OG1	1:B:226:LYS:HG2	2.18	0.43
1:B:242:GLU:HG3	1:B:243:PRO:N	2.33	0.43
1:C:162:LYS:HD3	1:C:164:TYR:CZ	2.53	0.43
1:B:357:VAL:C	1:B:361:THR:HG1	2.17	0.43
1:B:102:LYS:C	1:B:103:LEU:HD12	2.43	0.43
1:B:245:TRP:CZ2	1:B:247:GLY:HA2	2.54	0.43
1:B:103:LEU:HD12	1:B:103:LEU:N	2.34	0.43
1:A:12:PRO:HB2	1:B:53:GLN:OE1	2.19	0.43
1:A:65:LEU:C	1:A:65:LEU:CD2	2.91	0.43
1:C:120:TRP:HB2	1:C:153:TRP:CZ3	2.53	0.43
1:B:66[A]:VAL:HG23	1:B:66[A]:VAL:O	2.19	0.43
1:B:218:LEU:CD2	1:B:231:GLU:OE2	2.67	0.43
1:B:274:ASP:OD1	1:B:274:ASP:N	2.36	0.43
1:A:64:LEU:HB3	1:A:75[A]:VAL:HG12	2.01	0.42
1:B:40:ASN:HA	1:B:170:GLU:O	2.20	0.42
1:A:339:THR:HA	1:A:343:GLU:O	2.19	0.42
1:D:67:ARG:HG3	1:D:67:ARG:NH1	2.33	0.42
1:A:12:PRO:HG2	1:B:84:ARG:O	2.20	0.42
1:A:218:LEU:HD13	1:A:231:GLU:HG2	2.02	0.42
1:D:357:VAL:HG12	1:D:357:VAL:O	2.19	0.42
1:B:281:GLU:OE1	1:B:283:ARG:HD2	2.18	0.42
1:D:199:MET:HE1	3:D:403:MPD:HM2	2.02	0.42
1:B:202:MET:CE	1:B:360:TYR:CE1	3.00	0.42
1:B:230:GLU:HG2	1:B:231:GLU:N	2.35	0.42
1:C:146:ARG:HD3	1:C:178:SER:HB3	2.02	0.42
1:A:300:LEU:HD23	1:A:305[B]:ARG:NH1	2.35	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:TYR:CD1	1:A:54:TYR:N	2.88	0.41
1:B:145:MET:HE3	1:B:145:MET:HB3	1.93	0.41
1:D:218:LEU:C	1:D:218:LEU:HD12	2.45	0.41
1:A:68:GLU:O	1:A:71:VAL:HG22	2.20	0.41
1:A:204:ASN:HB2	1:A:219:VAL:HG12	2.02	0.41
1:C:35:TYR:CD1	1:C:35:TYR:C	2.97	0.41
1:D:34:TYR:CD2	1:D:177:ARG:HD3	2.56	0.41
1:A:203:TRP:O	1:A:351:PHE:HA	2.20	0.41
1:A:207:PRO:C	1:A:208:ILE:HG13	2.46	0.41
1:D:120:TRP:HB2	1:D:153:TRP:CZ3	2.55	0.41
1:D:185:GLY:O	1:D:305[B]:ARG:HD3	2.19	0.41
1:D:206:PHE:CD1	1:D:349:MET:HA	2.56	0.41
1:A:8:LEU:HG	1:A:85:ALA:HB2	2.01	0.41
1:B:127:PHE:HE2	1:B:231:GLU:CD	2.28	0.41
1:B:147:PHE:CZ	1:B:177:ARG:HG3	2.55	0.41
1:A:260[A]:GLN:NE2	1:A:356:GLU:CG	2.79	0.41
1:C:53:GLN:OE1	1:D:12:PRO:HB2	2.19	0.41
1:D:46:PHE:CD1	1:D:335:PRO:HD3	2.56	0.41
1:D:51:LEU:C	1:D:51:LEU:HD23	2.45	0.41
1:A:205:TYR:CD1	1:A:218:LEU:HD11	2.55	0.41
1:B:216:MET:O	1:B:232:GLY:HA2	2.20	0.41
1:B:244[B]:GLU:CD	1:B:276:PRO:HG2	2.43	0.41
1:D:265:MET:HE3	1:D:268:GLY:N	2.36	0.41
1:D:293:THR:OG1	1:D:329:LEU:O	2.39	0.41
1:A:65:LEU:HD23	1:A:66:VAL:N	2.35	0.41
1:C:8:LEU:HD13	1:D:13:VAL:HG12	2.03	0.41
1:C:205:TYR:CD1	1:C:218:LEU:HD11	2.56	0.41
1:C:283:ARG:O	1:C:338:PHE:HA	2.21	0.41
1:D:47:VAL:HA	1:D:65:LEU:O	2.21	0.41
1:D:207:PRO:C	1:D:208:ILE:HG13	2.46	0.41
1:B:51:LEU:HD23	1:B:51:LEU:C	2.46	0.41
1:D:65:LEU:C	1:D:65:LEU:CD2	2.93	0.41
1:A:147:PHE:CE2	1:A:177:ARG:HB2	2.56	0.40
1:A:187:GLU:HB2	1:A:305[B]:ARG:NH1	2.26	0.40
1:B:35:TYR:CD1	1:B:35:TYR:C	3.00	0.40
1:B:67:ARG:NH1	1:B:69:GLY:O	2.54	0.40
1:B:205:TYR:O	1:B:206:PHE:HD1	2.03	0.40
1:B:338:PHE:HZ	1:B:349:MET:HG3	1.87	0.40
1:C:36:PHE:CZ	1:C:105:LEU:HD21	2.56	0.40
1:A:327:MET:HA	1:A:327:MET:HE2	2.03	0.40
1:B:186:GLU:H	1:B:186:GLU:CD	2.30	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:358:PRO:O	1:B:359:LYS:C	2.65	0.40
1:D:289:GLN:HA	1:D:334:THR:HB	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	366/362 (101%)	352 (96%)	14 (4%)	0	100	100
1	B	363/362 (100%)	340 (94%)	21 (6%)	2 (1%)	21	17
1	C	363/362 (100%)	349 (96%)	14 (4%)	0	100	100
1	D	364/362 (101%)	348 (96%)	15 (4%)	1 (0%)	36	35
All	All	1456/1448 (101%)	1389 (95%)	64 (4%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	225	GLY
1	B	223	GLY
1	D	87	ILE

5.3.2 Protein sidechains [i](#)

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	314/308 (102%)	302 (96%)	12 (4%)	29	29
1	B	311/308 (101%)	288 (93%)	23 (7%)	13	9
1	C	311/308 (101%)	296 (95%)	15 (5%)	23	21
1	D	312/308 (101%)	305 (98%)	7 (2%)	45	50
All	All	1248/1232 (101%)	1191 (95%)	57 (5%)	24	22

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	10	ASP
1	A	38	LEU
1	A	65	LEU
1	A	87	ILE
1	A	230	GLU
1	A	240	GLN
1	A	241	ARG
1	A	242	GLU
1	A	262	MET
1	A	329	LEU
1	A	356	GLU
1	B	10	ASP
1	B	68	GLU
1	B	162	LYS
1	B	198	SER
1	B	200	GLU
1	B	202	MET
1	B	218	LEU
1	B	233	LEU
1	B	234	ARG
1	B	251	HIS
1	B	252	ASP
1	B	253	HIS
1	B	254	VAL
1	B	257	SER
1	B	259	MET
1	B	264	ASP
1	B	300	LEU
1	B	324	LYS
1	B	329	LEU
1	B	344	VAL
1	B	354	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	359	LYS
1	B	360	TYR
1	C	6	SER
1	C	10	ASP
1	C	87	ILE
1	C	145	MET
1	C	158	LYS
1	C	160	ASN
1	C	172	LEU
1	C	219	VAL
1	C	224	ASP
1	C	248	ARG
1	C	257	SER
1	C	300	LEU
1	C	327	MET
1	C	331	LEU
1	C	361	THR
1	D	2	GLN
1	D	10	ASP
1	D	65	LEU
1	D	67	ARG
1	D	230	GLU
1	D	231	GLU
1	D	257	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	B	204	ASN
1	C	137	HIS
1	C	193	HIS
1	C	220	ASN
1	D	128	GLN
1	D	137	HIS
1	D	220	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 ⓘ

18 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	IMD	C	403	-	5,5,5	0.72	0	5,5,5	0.39	0
2	PO4	A	401	-	4,4,4	1.02	0	6,6,6	0.47	0
5	GOL	C	404	-	5,5,5	1.56	1 (20%)	5,5,5	1.43	1 (20%)
2	PO4	C	402	-	4,4,4	0.91	0	6,6,6	0.71	0
3	MPD	D	403	-	7,7,7	0.44	0	9,10,10	0.54	0
3	MPD	A	403	-	7,7,7	0.40	0	9,10,10	0.85	0
2	PO4	B	402	-	4,4,4	2.34	4 (100%)	6,6,6	0.32	0
3	MPD	A	404	-	7,7,7	0.34	0	9,10,10	0.50	0
2	PO4	C	401	-	4,4,4	0.76	0	6,6,6	0.50	0
2	PO4	D	401	-	4,4,4	0.91	0	6,6,6	0.90	0
4	IMD	A	405	-	5,5,5	0.79	0	5,5,5	0.48	0
5	GOL	A	407	-	5,5,5	0.10	0	5,5,5	0.45	0
4	IMD	A	406	-	5,5,5	0.76	0	5,5,5	0.45	0
4	IMD	D	404	-	5,5,5	0.81	0	5,5,5	0.39	0
5	GOL	B	403	-	5,5,5	0.86	0	5,5,5	1.30	1 (20%)
2	PO4	B	401	-	4,4,4	0.97	0	6,6,6	0.48	0
2	PO4	D	402	-	4,4,4	0.65	0	6,6,6	0.48	0
2	PO4	A	402	-	4,4,4	0.86	0	6,6,6	0.66	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
4	IMD	C	403	-	-	-	0/1/1/1
5	GOL	C	404	-	-	2/4/4/4	-
3	MPD	D	403	-	-	0/5/5/5	-
3	MPD	A	403	-	-	1/5/5/5	-
3	MPD	A	404	-	-	0/5/5/5	-
5	GOL	A	407	-	-	2/4/4/4	-
4	IMD	A	405	-	-	-	0/1/1/1
4	IMD	A	406	-	-	-	0/1/1/1
4	IMD	D	404	-	-	-	0/1/1/1
5	GOL	B	403	-	-	0/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	402	PO4	P-O4	-2.88	1.46	1.54
5	C	404	GOL	O2-C2	-2.60	1.35	1.43
2	B	402	PO4	P-O2	-2.19	1.48	1.54
2	B	402	PO4	P-O3	-2.16	1.48	1.54
2	B	402	PO4	P-O1	-2.02	1.46	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	404	GOL	C3-C2-C1	-2.98	100.86	111.80
5	B	403	GOL	C3-C2-C1	-2.47	102.74	111.80

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	404	GOL	C1-C2-C3-O3
5	C	404	GOL	O2-C2-C3-O3
5	A	407	GOL	O2-C2-C3-O3
5	A	407	GOL	C1-C2-C3-O3
3	A	403	MPD	O2-C2-C3-C4

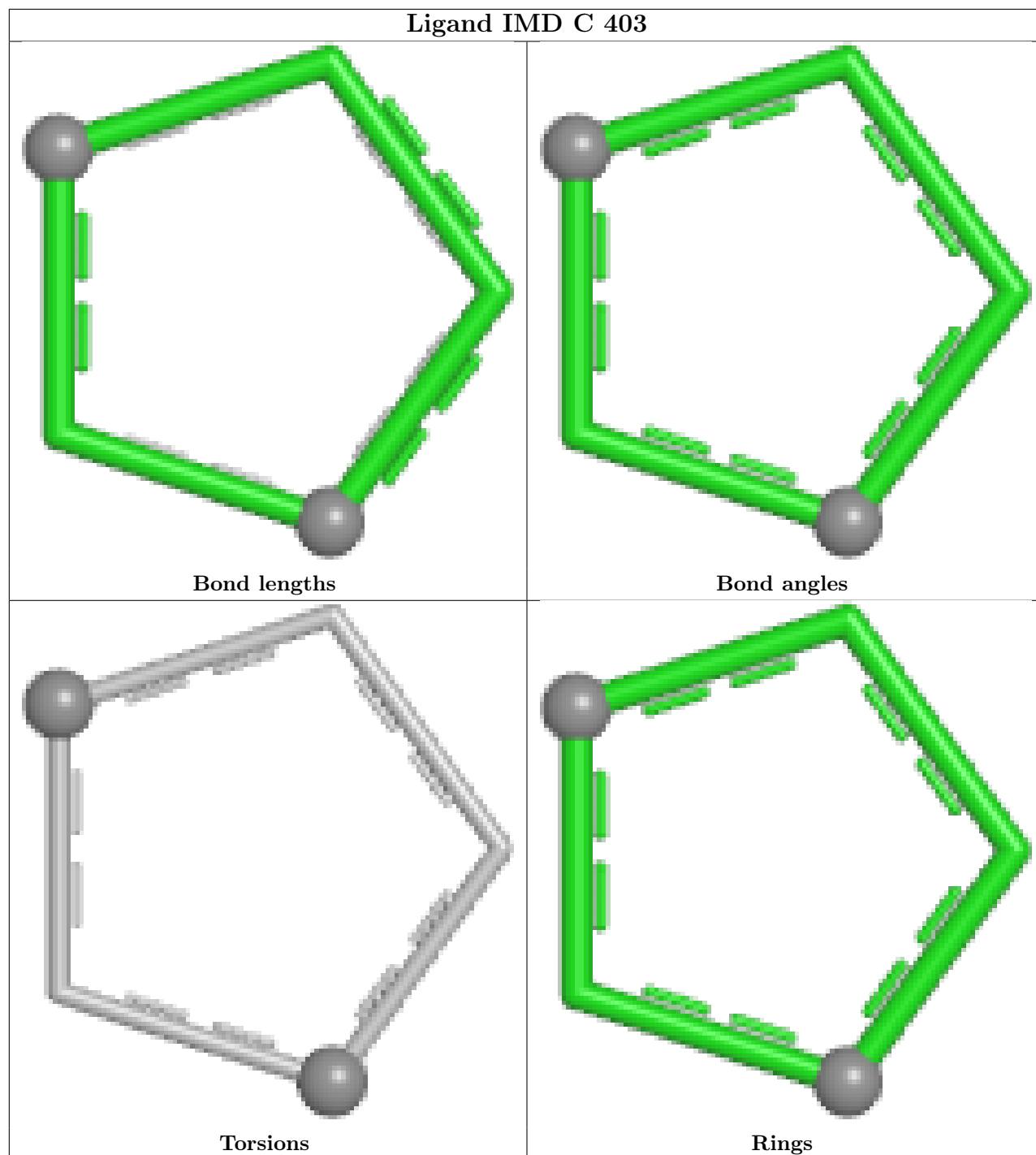
There are no ring outliers.

4 monomers are involved in 8 short contacts:

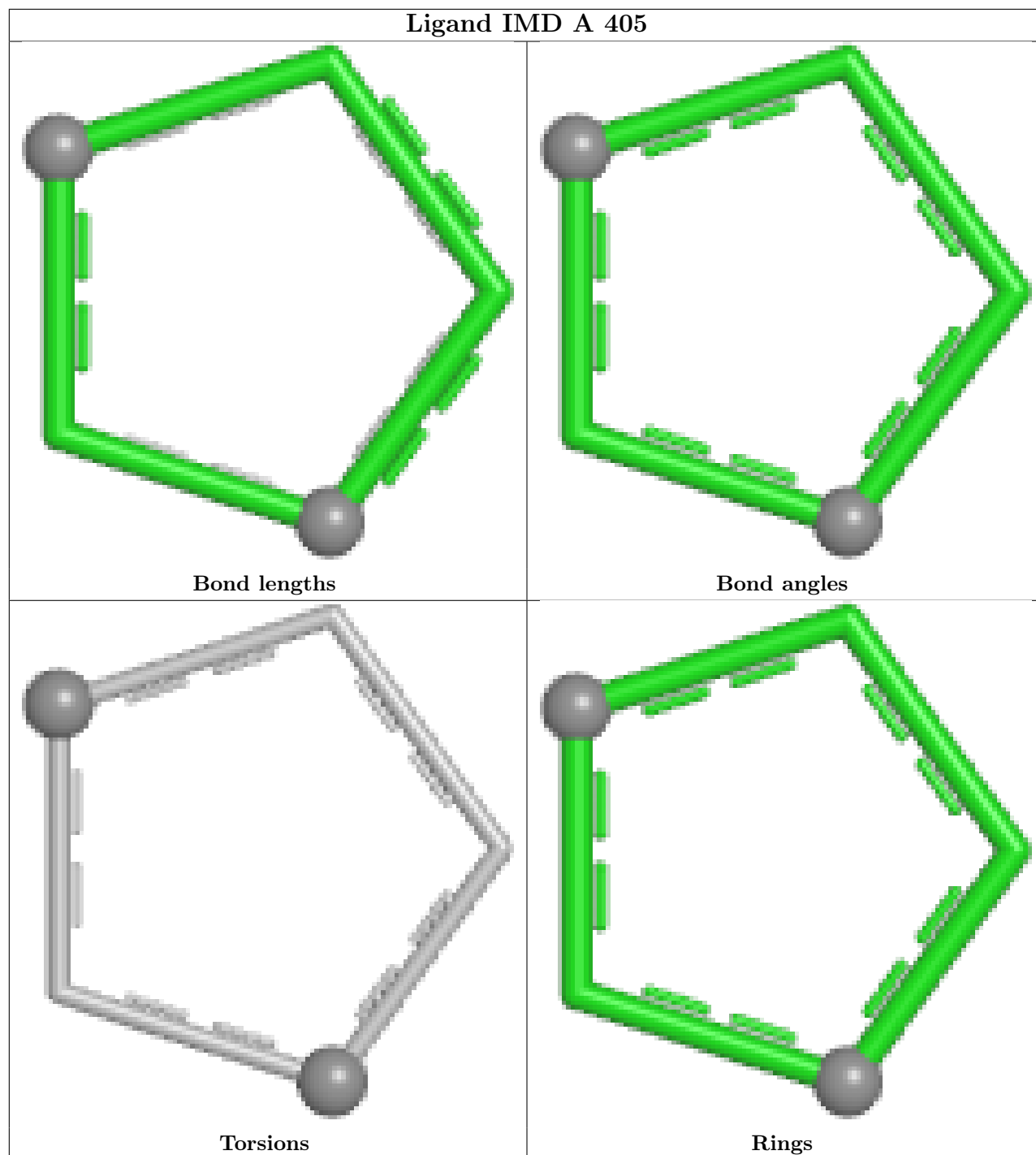
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	403	MPD	2	0
3	A	403	MPD	4	0
3	A	404	MPD	1	0
4	A	406	IMD	1	0

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.

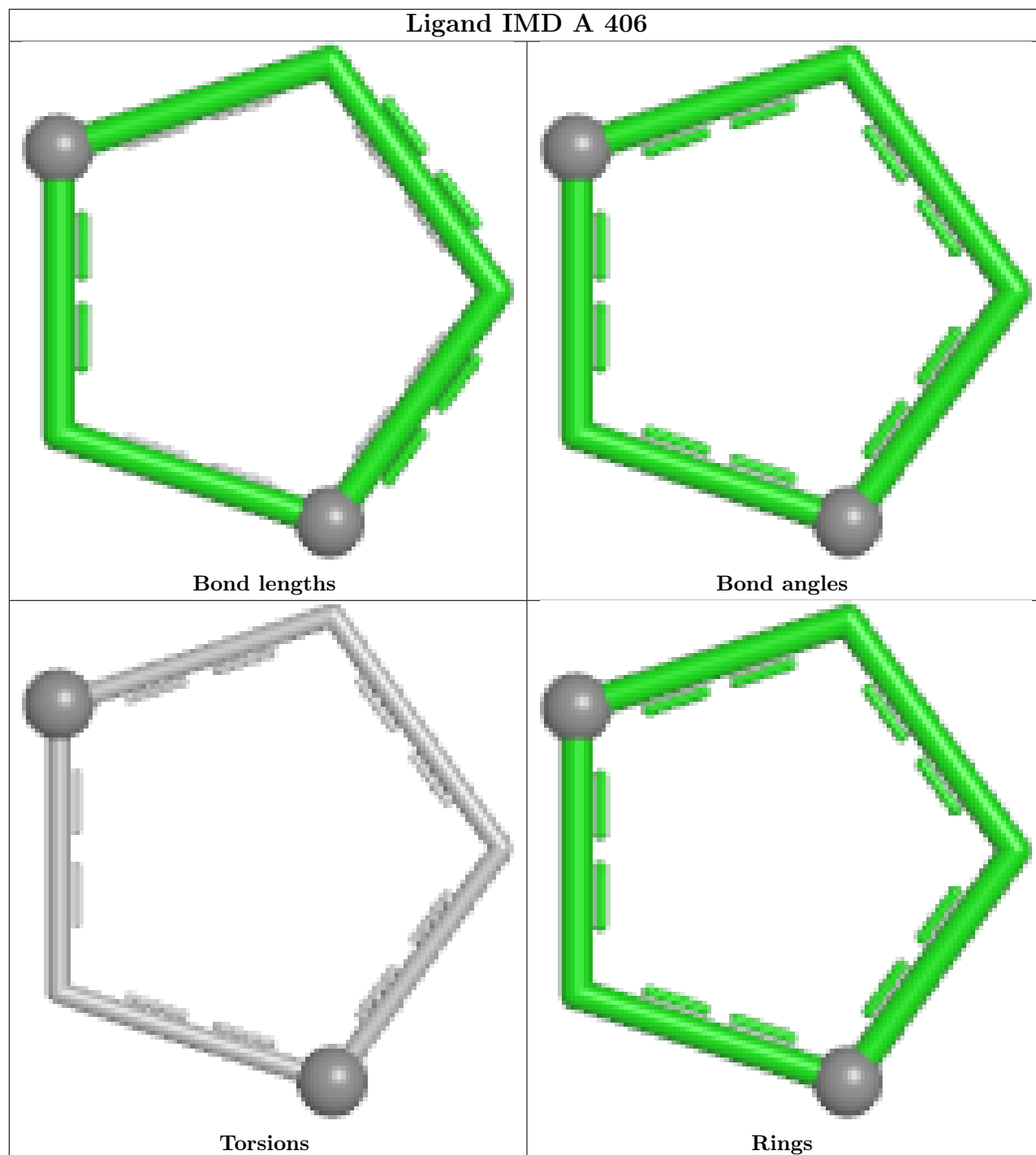
Ligand IMD C 403

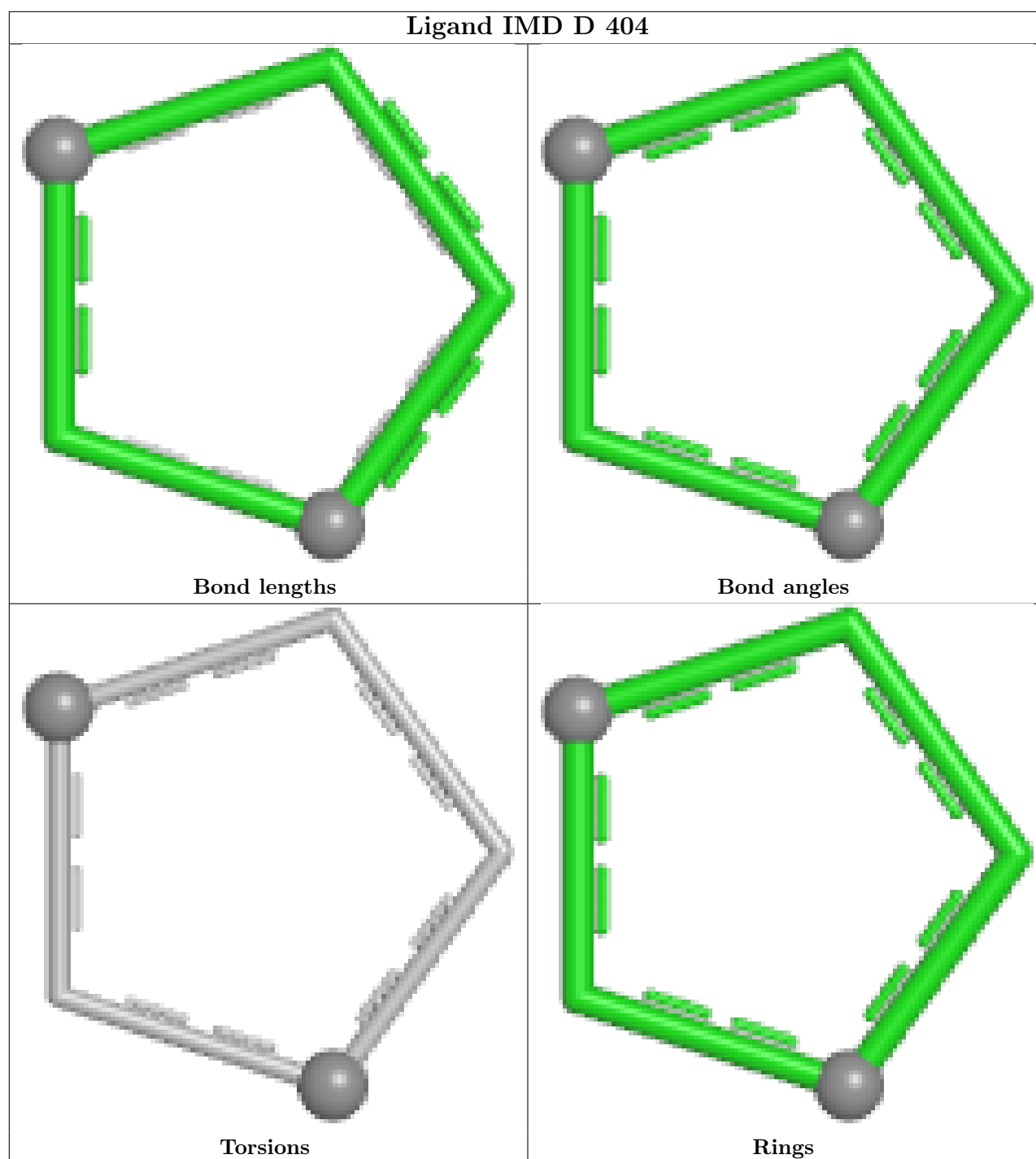


Ligand IMD A 405



Ligand IMD A 406





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	362/362 (100%)	0.57	20 (5%) 30 29	18, 40, 59, 77	6 (1%)
1	B	361/362 (99%)	1.17	81 (22%) 2 2	21, 48, 85, 104	4 (1%)
1	C	361/362 (99%)	0.80	27 (7%) 20 19	16, 39, 70, 84	4 (1%)
1	D	361/362 (99%)	0.66	36 (9%) 12 11	16, 38, 68, 80	5 (1%)
All	All	1445/1448 (99%)	0.80	164 (11%) 10 9	16, 41, 74, 104	19 (1%)

All (164) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	225	GLY	6.4
1	B	360	TYR	5.9
1	B	246	LEU	5.8
1	B	245	TRP	5.6
1	D	245	TRP	5.4
1	B	255	PHE	5.3
1	B	229	ILE	5.2
1	B	202	MET	4.9
1	B	228	THR	4.8
1	B	282	LEU	4.7
1	B	354	PHE	4.7
1	B	219	VAL	4.6
1	C	362	GLY	4.5
1	B	231	GLU	4.5
1	B	223	GLY	4.4
1	C	300	LEU	4.3
1	B	203	TRP	4.3
1	B	222	THR	4.3
1	C	245	TRP	4.1
1	B	357	VAL	4.1
1	B	279	PRO	4.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	201	GLY	3.9
1	B	221	GLU	3.9
1	D	233	LEU	3.9
1	A	1	MET	3.9
1	B	224	ASP	3.9
1	C	299	GLY	3.8
1	C	228	THR	3.8
1	B	254	VAL	3.8
1	D	300	LEU	3.8
1	B	259	MET	3.7
1	C	225	GLY	3.7
1	B	217	TYR	3.7
1	C	4[A]	GLN	3.6
1	B	300	LEU	3.5
1	B	261	TYR	3.5
1	D	222	THR	3.5
1	B	353	PHE	3.5
1	B	273	PRO	3.5
1	C	222	THR	3.5
1	D	362	GLY	3.4
1	B	358	PRO	3.4
1	A	228	THR	3.4
1	B	280	LEU	3.4
1	D	272	PHE	3.4
1	C	236	TRP	3.3
1	D	276	PRO	3.3
1	B	272	PHE	3.3
1	B	226	LYS	3.3
1	C	231	GLU	3.3
1	A	260[A]	GLN	3.3
1	C	329	LEU	3.3
1	B	232	GLY	3.2
1	A	192	ILE	3.2
1	C	233	LEU	3.1
1	B	274	ASP	3.1
1	B	329	LEU	3.1
1	B	265	MET	3.1
1	B	260	GLN	3.1
1	B	258	ALA	3.0
1	B	352	ALA	3.0
1	B	269	VAL	3.0
1	D	229	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	305[A]	ARG	3.0
1	D	305[A]	ARG	2.9
1	B	220	ASN	2.9
1	B	270	VAL	2.9
1	A	362	GLY	2.9
1	C	327	MET	2.9
1	B	271	ARG	2.9
1	A	245	TRP	2.9
1	B	276	PRO	2.9
1	D	279	PRO	2.9
1	B	218	LEU	2.9
1	D	217	TYR	2.9
1	B	362	GLY	2.9
1	A	2	GLN	2.8
1	D	269	VAL	2.8
1	D	344	VAL	2.8
1	D	192	ILE	2.8
1	D	327	MET	2.7
1	B	249	PRO	2.7
1	B	263	ALA	2.7
1	B	344	VAL	2.7
1	B	299	GLY	2.7
1	B	283	ARG	2.7
1	D	255	PHE	2.7
1	A	277	GLY	2.7
1	C	277	GLY	2.7
1	D	241[A]	ARG	2.7
1	B	351	PHE	2.6
1	B	253	HIS	2.6
1	B	198	SER	2.6
1	B	355	SER	2.6
1	D	277	GLY	2.6
1	A	249	PRO	2.6
1	C	127	PHE	2.6
1	C	240[A]	GLN	2.6
1	B	239	PRO	2.6
1	B	2	GLN	2.5
1	D	242	GLU	2.5
1	B	192	ILE	2.5
1	B	252	ASP	2.5
1	B	206	PHE	2.5
1	B	338	PHE	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	278	GLY	2.5
1	C	219	VAL	2.5
1	D	235	ILE	2.5
1	C	226	LYS	2.5
1	B	251	HIS	2.5
1	B	361	THR	2.5
1	C	200	GLU	2.4
1	A	219	VAL	2.4
1	B	285	THR	2.4
1	B	230	GLU	2.4
1	C	229	ILE	2.4
1	D	270	VAL	2.4
1	D	218	LEU	2.3
1	C	161	GLY	2.3
1	C	305[A]	ARG	2.3
1	B	323	TYR	2.3
1	C	199	MET	2.3
1	A	300	LEU	2.3
1	B	268	GLY	2.3
1	D	329	LEU	2.3
1	B	262[A]	MET	2.3
1	A	327	MET	2.3
1	D	339	THR	2.2
1	B	227	ARG	2.2
1	A	195	GLY	2.2
1	A	259	MET	2.2
1	D	280	LEU	2.2
1	B	281	GLU	2.2
1	D	273	PRO	2.2
1	C	224	ASP	2.2
1	D	238	ASP	2.2
1	A	356	GLU	2.2
1	B	204	ASN	2.2
1	A	201	GLY	2.2
1	D	231	GLU	2.2
1	D	275	ALA	2.2
1	B	257	SER	2.2
1	B	127	PHE	2.1
1	B	235	ILE	2.1
1	D	354	PHE	2.1
1	C	201	GLY	2.1
1	A	275	ALA	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	3	SER	2.1
1	D	246	LEU	2.1
1	D	252	ASP	2.1
1	B	248	ARG	2.1
1	D	203	TRP	2.1
1	D	258	ALA	2.1
1	A	197	PRO	2.1
1	B	193	HIS	2.1
1	B	332	ILE	2.1
1	A	75[A]	VAL	2.1
1	B	244[A]	GLU	2.0
1	C	230	GLU	2.0
1	B	215	LEU	2.0
1	C	2	GLN	2.0
1	D	223	GLY	2.0
1	D	254	VAL	2.0
1	A	44	ASP	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(Å ²)	Q<0.9
5	GOL	A	407	6/6	0.64	0.19	42,53,64,67	0
3	MPD	A	403	8/8	0.65	0.19	41,54,58,74	0
5	GOL	C	404	6/6	0.77	0.15	58,69,77,77	0
3	MPD	A	404	8/8	0.78	0.31	20,20,20,20	0
5	GOL	B	403	6/6	0.78	0.15	49,60,71,78	0
3	MPD	D	403	8/8	0.78	0.13	38,48,50,58	0

Continued on next page...

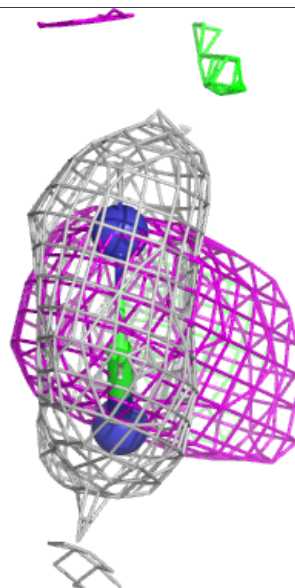
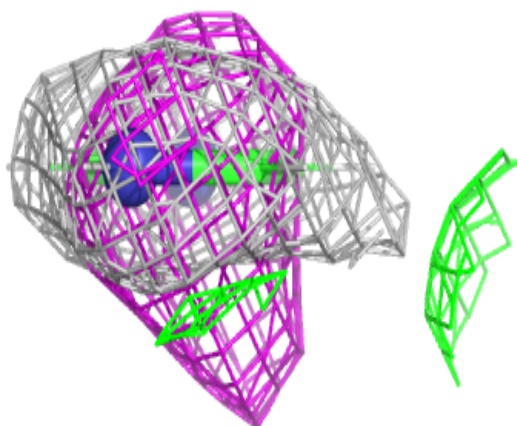
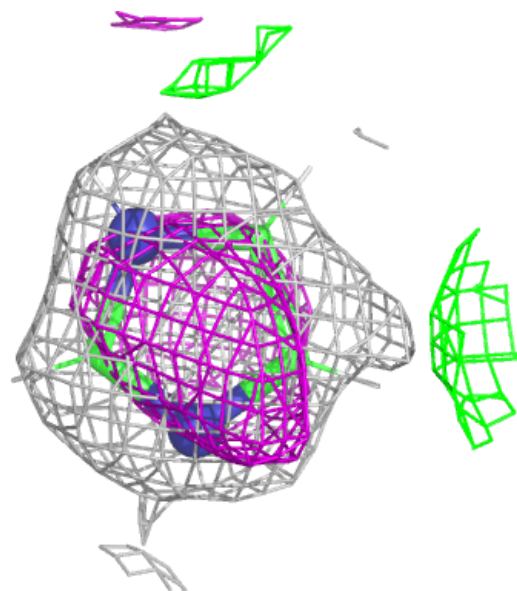
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	PO4	B	402	5/5	0.83	0.17	41,46,52,52	0
4	IMD	A	406	5/5	0.87	0.28	39,42,50,51	0
2	PO4	D	402	5/5	0.87	0.22	37,41,48,50	0
2	PO4	C	402	5/5	0.88	0.17	38,44,52,56	0
4	IMD	D	404	5/5	0.91	0.17	37,39,47,49	0
2	PO4	A	402	5/5	0.91	0.14	40,43,50,50	0
4	IMD	A	405	5/5	0.93	0.09	38,39,47,47	0
4	IMD	C	403	5/5	0.94	0.08	37,37,44,45	0
2	PO4	C	401	5/5	0.96	0.09	32,33,35,35	0
2	PO4	D	401	5/5	0.98	0.06	24,27,31,31	0
2	PO4	B	401	5/5	0.98	0.08	30,35,36,40	0
2	PO4	A	401	5/5	0.99	0.05	27,30,33,35	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.

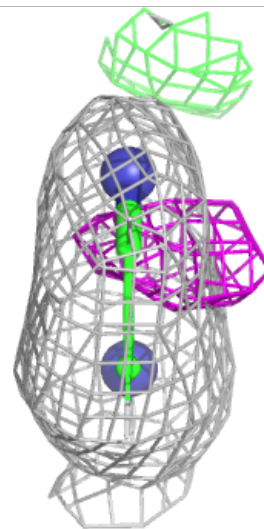
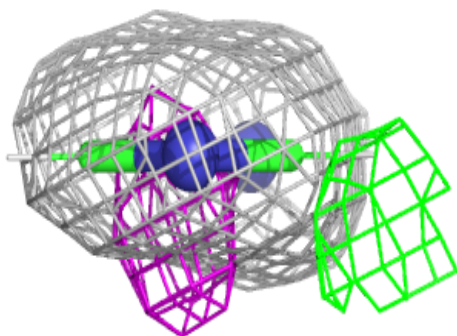
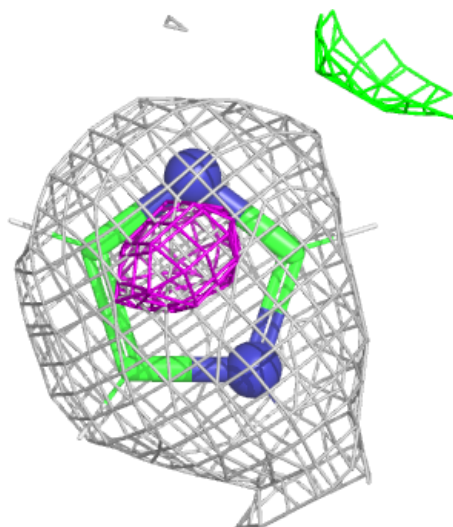
Electron density around IMD A 406:

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



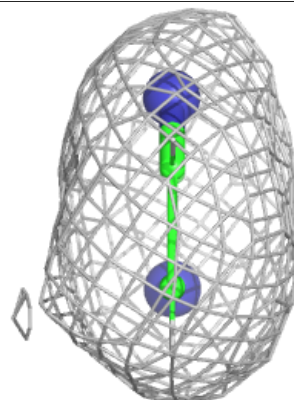
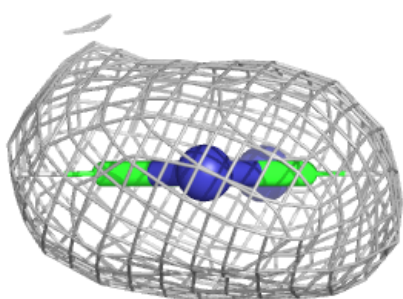
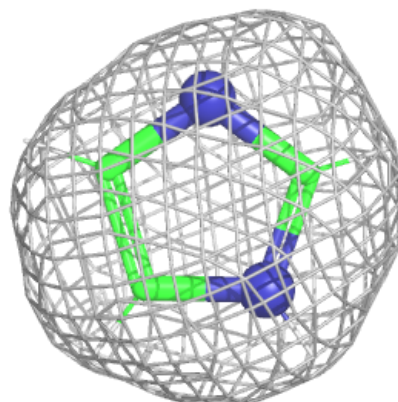
Electron density around IMD D 404:

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

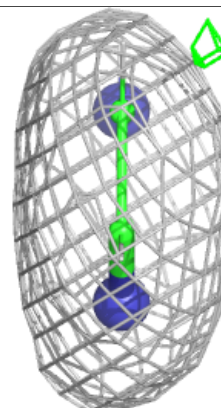
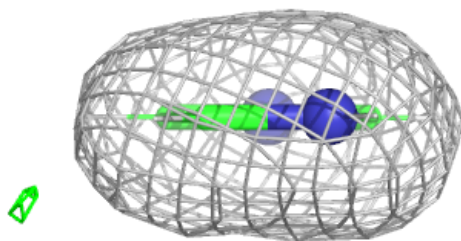
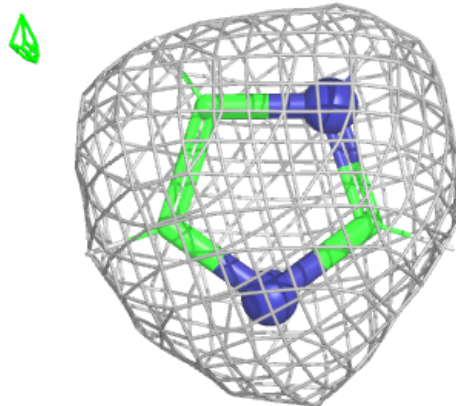


Electron density around IMD A 405:

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

**Electron density around IMD C 403:**

$2mF_o-DF_c$ (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.