



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2026 – 11:31 AM EDT

PDB ID : 6DXQ / pdb_00006dxq
Title : Crystal structure of the LigJ Hydratase product complex with 4-carboxy-4-hydroxy-2-oxoadipate
Authors : Mabanglo, M.F.; Raushel, F.M.
Deposited on : 2018-06-29
Resolution : 2.02 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 : **FAILED**
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

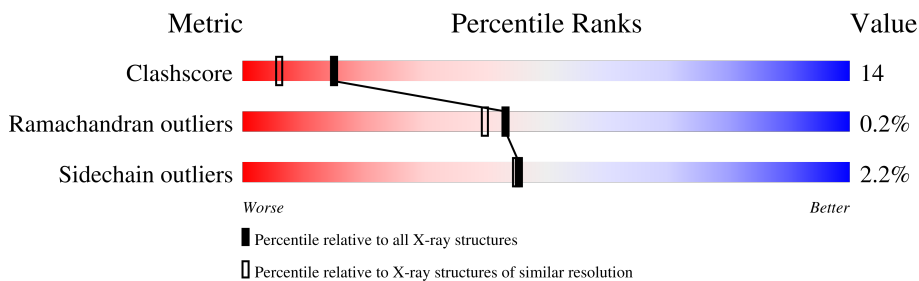
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.02 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)

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 $\leq 5\%$.

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	340	 76% 22% ..
1	B	340	 75% 24% ..
1	C	340	 69% 28% ..
1	D	340	 74% 22% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11742 atoms, of which 20 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.

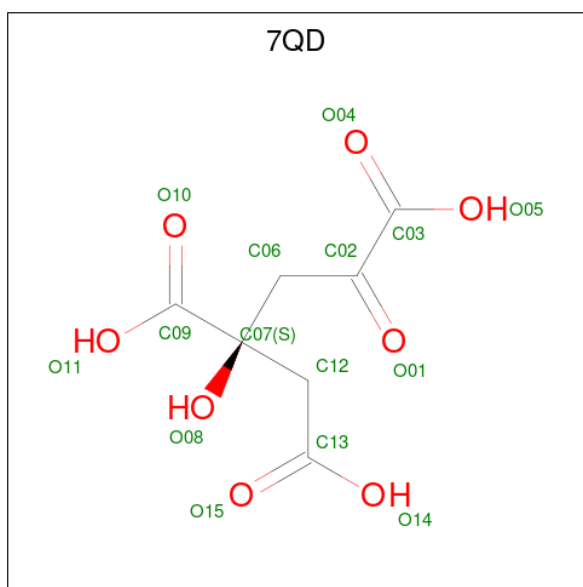
- Molecule 1 is a protein called 4-oxalomesaconate hydratase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2650	1688	459	485	18			
1	B	338	Total	C	N	O	S	0	0	0
			2650	1690	457	483	20			
1	C	334	Total	C	N	O	S	0	0	0
			2627	1673	454	480	20			
1	D	332	Total	C	N	O	S	0	0	0
			2612	1667	452	474	19			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Zn	0	0
			1	1		
2	B	1	Total	Zn	0	0
			1	1		
2	C	1	Total	Zn	0	0
			1	1		
2	D	1	Total	Zn	0	0
			1	1		

- Molecule 3 is (2S)-2-hydroxy-4-oxobutane-1,2,4-tricarboxylic acid (CCD ID: 7QD) (formula: C₇H₈O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			20	7	5	8		
3	B	1	Total	C	H	O	0	0
			20	7	5	8		
3	C	1	Total	C	H	O	0	0
			20	7	5	8		
3	D	1	Total	C	H	O	0	0
			20	7	5	8		

- Molecule 4 is water.

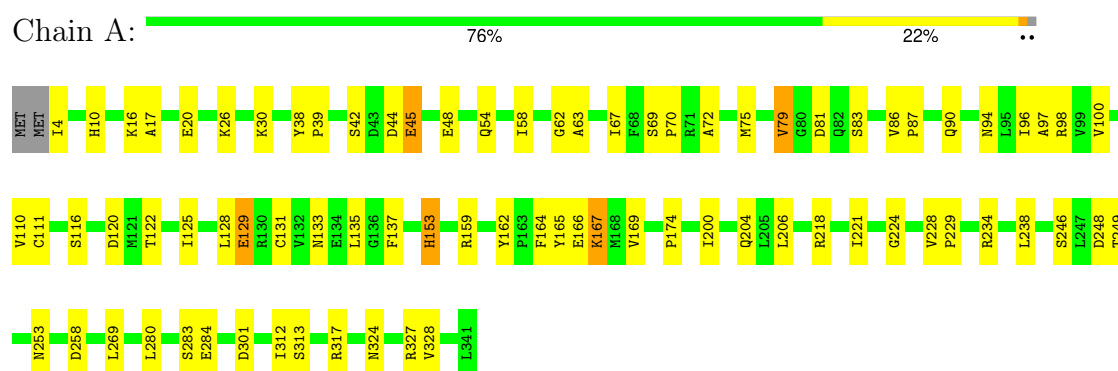
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	310	Total	O	0	0
			310	310		
4	B	284	Total	O	0	0
			284	284		
4	C	278	Total	O	0	0
			278	278		
4	D	247	Total	O	0	0
			247	247		

3 Residue-property plots [i](#)

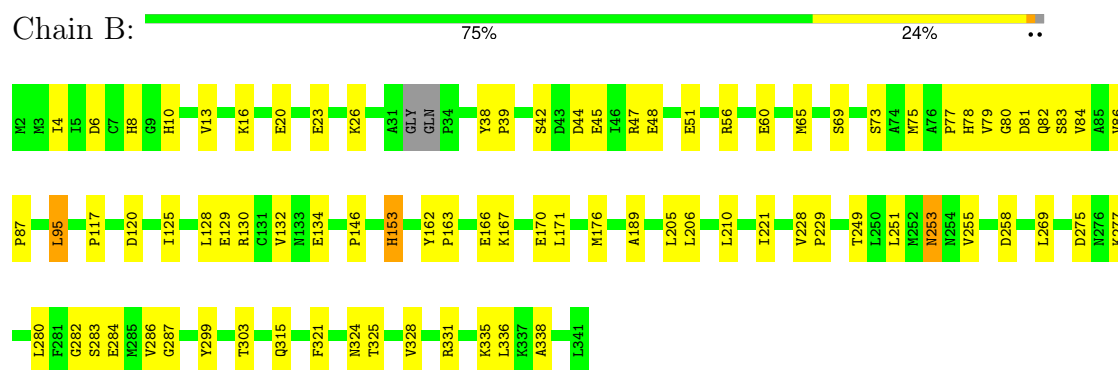
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

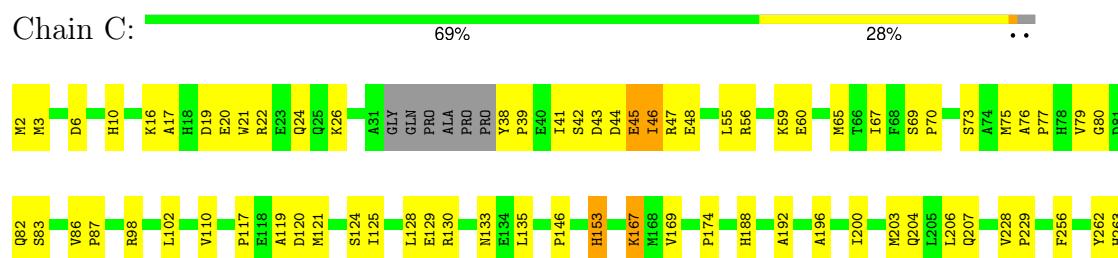
- Molecule 1: 4-oxalomesaconate hydratase



- Molecule 1: 4-oxalomesaconate hydratase

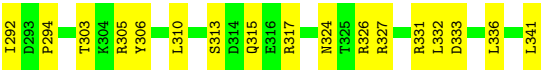
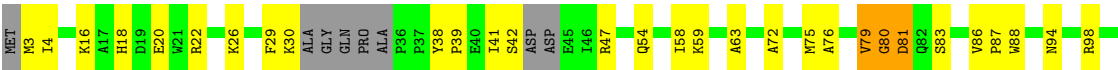


- Molecule 1: 4-oxalomesaconate hydratase





● Molecule 1: 4-oxalomesaconate hydratase



4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.52Å 78.30Å 135.64Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.80 – 2.02	Depositor
% Data completeness (in resolution range)	99.3 (27.80-2.02)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.03Å)	Xtriage
Refinement program	PHENIX dev_1108	Depositor
R, R_{free}	0.176 , 0.216	Depositor
Wilson B-factor (Å ²)	16.4	Xtriage
Anisotropy	0.485	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.438 for h,-k,-l	Xtriage
Reported twinning fraction	0.500 for h,-k,-l	Depositor
Outliers	2 of 112725 reflections (0.002%)	Xtriage
Total number of atoms	11742	wwPDB-VP
Average B, all atoms (Å ²)	46.0	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 70.03 % 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 3.3486e-06. 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 7QD, 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	0.44	0/2724	0.81	5/3705 (0.1%)
1	B	0.43	0/2723	0.79	0/3700
1	C	0.43	0/2697	0.82	1/3662 (0.0%)
1	D	0.43	0/2683	0.81	3/3643 (0.1%)
All	All	0.43	0/10827	0.81	9/14710 (0.1%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	79	VAL	CB-CA-C	-6.72	103.63	111.09
1	D	79	VAL	N-CA-C	6.55	120.22	111.44
1	D	153	HIS	CA-C-N	5.42	123.61	119.66
1	D	153	HIS	C-N-CA	5.42	123.61	119.66
1	A	116	SER	CA-C-N	5.16	124.95	119.28
1	A	116	SER	C-N-CA	5.16	124.95	119.28
1	A	153	HIS	CA-C-N	5.09	123.33	119.66
1	A	153	HIS	C-N-CA	5.09	123.33	119.66
1	C	323	GLY	N-CA-C	5.02	119.20	112.77

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	2650	0	2565	60	0
1	B	2650	0	2568	62	0
1	C	2627	0	2545	99	0
1	D	2612	0	2537	65	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
3	A	15	5	0	2	0
3	B	15	5	0	2	0
3	C	15	5	0	1	0
3	D	15	5	0	1	1
4	A	310	0	0	3	1
4	B	284	0	0	10	1
4	C	278	0	0	6	1
4	D	247	0	0	7	0
All	All	11722	20	10215	285	2

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:MET:HE1	1:C:321:PHE:CD2	1.94	1.02
1:C:41:ILE:CG2	1:C:46:ILE:HD11	2.02	0.89
1:C:2:MET:HB3	1:C:318:HIS:HD2	1.39	0.88
1:B:44:ASP:O	1:B:48:GLU:HG3	1.73	0.87
1:B:23:GLU:OE2	1:B:26:LYS:NZ	2.08	0.86
1:D:72:ALA:HA	1:D:75:MET:HE2	1.59	0.85
1:D:16:LYS:O	1:D:20:GLU:HG3	1.75	0.85
1:C:2:MET:HE1	1:C:321:PHE:HD2	1.42	0.85
1:B:167:LYS:NZ	1:B:170:GLU:OE1	2.10	0.84
1:C:128:LEU:HD23	1:C:167:LYS:HG2	1.57	0.84
1:C:2:MET:HB3	1:C:318:HIS:CD2	2.12	0.83
1:A:125:ILE:HG23	1:A:167:LYS:HD2	1.62	0.81
1:C:41:ILE:HG22	1:C:46:ILE:HD11	1.63	0.81
1:C:277:LYS:HD2	1:C:327:ARG:NH1	1.97	0.80
1:C:79:VAL:HG22	4:C:698:HOH:O	1.85	0.77
1:C:76:ALA:O	1:C:79:VAL:HG23	1.85	0.76
1:C:86:VAL:HB	1:C:87:PRO:HD3	1.68	0.76
1:A:131:CYS:HA	1:A:135:LEU:HD12	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:308:ASP:O	1:C:317:ARG:NH2	2.20	0.74
1:C:276:ASN:OD1	1:C:277:LYS:NZ	2.20	0.73
1:C:42:SER:O	1:C:46:ILE:HD13	1.89	0.72
1:C:46:ILE:HD12	1:C:46:ILE:N	2.05	0.72
1:A:44:ASP:O	1:A:48:GLU:HG3	1.90	0.72
1:B:16:LYS:HE2	1:B:20:GLU:OE2	1.90	0.72
1:C:41:ILE:HG21	1:C:46:ILE:HD11	1.72	0.70
1:C:55:LEU:O	1:C:59:LYS:HG3	1.93	0.69
1:C:41:ILE:HG22	1:C:46:ILE:CD1	2.23	0.68
1:D:38:TYR:CG	1:D:39:PRO:HD2	2.28	0.68
1:A:280:LEU:CD2	1:A:324:ASN:HB3	2.23	0.68
1:C:284:GLU:OE2	4:C:501:HOH:O	2.12	0.68
1:A:4:ILE:HD12	1:A:62:GLY:O	1.94	0.68
1:B:210:LEU:HA	4:B:651:HOH:O	1.95	0.67
1:A:204:GLN:O	4:A:502:HOH:O	2.13	0.67
1:B:269:LEU:C	1:B:269:LEU:HD23	2.20	0.67
1:A:248:ASP:OD1	1:A:249:THR:HG23	1.95	0.66
1:C:129:GLU:O	1:C:133:ASN:HB2	1.96	0.66
1:A:26:LYS:O	1:A:30:LYS:HG2	1.95	0.66
1:B:338:ALA:HB3	4:B:516:HOH:O	1.96	0.66
1:C:46:ILE:N	1:C:46:ILE:CD1	2.59	0.65
1:B:171:LEU:O	1:B:331:ARG:NH1	2.29	0.65
1:C:10:HIS:HA	1:C:69:SER:O	1.97	0.65
1:D:29:PHE:O	4:D:501:HOH:O	2.14	0.65
1:C:21:TRP:CD1	1:C:38:TYR:HA	2.32	0.64
1:A:86:VAL:O	1:A:90:GLN:HG3	1.97	0.64
1:D:280:LEU:HD22	1:D:324:ASN:HB3	1.79	0.64
1:A:128:LEU:HD23	1:A:167:LYS:HG2	1.79	0.64
1:B:8:HIS:HB2	1:B:176:MET:HE1	1.80	0.64
1:B:77:PRO:O	1:B:117:PRO:HD3	1.97	0.63
1:B:86:VAL:HB	1:B:87:PRO:HD3	1.78	0.63
1:D:54:GLN:O	1:D:58:ILE:HG13	1.98	0.63
1:C:277:LYS:HD2	1:C:327:ARG:HH12	1.62	0.62
1:D:79:VAL:N	1:D:80:GLY:HA3	2.16	0.61
1:C:69:SER:HB2	1:C:70:PRO:CD	2.30	0.61
1:C:46:ILE:CD1	1:C:46:ILE:H	2.14	0.61
1:C:196:ALA:O	1:C:200:ILE:HG13	2.00	0.61
1:D:167:LYS:O	1:D:171:LEU:HG	2.01	0.60
1:D:72:ALA:CA	1:D:75:MET:HE2	2.30	0.60
1:D:284:GLU:OE2	3:D:402:7QD:O08	2.19	0.60
1:B:125:ILE:O	1:B:129:GLU:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:81:ASP:OD1	1:D:83:SER:OG	2.18	0.59
1:D:105:GLU:OE1	1:D:105:GLU:N	2.33	0.59
1:C:323:GLY:O	1:C:327:ARG:HG3	2.03	0.59
1:C:38:TYR:CG	1:C:39:PRO:HD2	2.38	0.59
1:D:22:ARG:HH11	1:D:26:LYS:CG	2.16	0.58
1:D:29:PHE:O	1:D:30:LYS:HB2	2.04	0.58
1:A:72:ALA:HA	1:A:75:MET:HE2	1.84	0.58
1:B:23:GLU:CD	1:B:26:LYS:NZ	2.62	0.58
1:C:41:ILE:CG2	1:C:46:ILE:CD1	2.76	0.58
1:A:125:ILE:CG2	1:A:167:LYS:HD2	2.33	0.58
1:D:292:ILE:O	1:D:294:PRO:HD3	2.03	0.57
1:A:234:ARG:O	1:A:238:LEU:HG	2.04	0.57
1:C:295:THR:O	4:C:502:HOH:O	2.17	0.57
1:C:333:ASP:OD2	1:C:337:LYS:HE3	2.04	0.57
1:D:162:TYR:O	1:D:166:GLU:HG3	2.04	0.57
1:D:123:SER:OG	4:D:503:HOH:O	2.17	0.57
1:B:73:SER:HB3	3:B:402:7QD:O10	2.04	0.56
1:B:78:HIS:CD2	1:B:79:VAL:HG22	2.39	0.56
1:A:26:LYS:CD	1:A:79:VAL:HG11	2.35	0.56
1:C:200:ILE:O	1:C:204:GLN:HG3	2.05	0.56
1:C:38:TYR:CD1	1:C:39:PRO:HD2	2.41	0.56
1:D:3:MET:CE	1:D:341:LEU:HD13	2.35	0.56
1:A:42:SER:OG	1:A:45:GLU:HB2	2.06	0.55
1:D:41:ILE:HD12	1:D:41:ILE:N	2.21	0.55
1:C:69:SER:HB2	1:C:70:PRO:HD2	1.87	0.55
1:C:206:LEU:HD12	1:C:206:LEU:O	2.06	0.55
1:D:22:ARG:NH1	1:D:26:LYS:CG	2.70	0.55
1:D:127:GLU:OE1	1:D:127:GLU:HA	2.07	0.55
1:D:310:LEU:O	1:D:317:ARG:NH2	2.40	0.55
1:A:228:VAL:HB	1:A:229:PRO:HD3	1.87	0.55
1:D:22:ARG:HH12	1:D:79:VAL:HG11	1.71	0.55
1:D:22:ARG:HH11	1:D:26:LYS:HG3	1.70	0.55
1:C:128:LEU:HD23	1:C:167:LYS:CG	2.31	0.54
1:D:305:ARG:HG3	1:D:305:ARG:HH11	1.72	0.54
1:C:26:LYS:HG2	1:C:79:VAL:HG11	1.88	0.54
1:D:171:LEU:O	1:D:331:ARG:NH1	2.38	0.54
1:C:79:VAL:HB	1:C:80:GLY:HA3	1.88	0.54
1:A:86:VAL:HB	1:A:87:PRO:HD3	1.90	0.54
1:A:94:ASN:O	1:A:98:ARG:HG3	2.07	0.54
1:C:86:VAL:CB	1:C:87:PRO:HD3	2.38	0.54
1:A:16:LYS:HG2	1:A:20:GLU:OE2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:MET:HE1	4:B:595:HOH:O	2.08	0.54
1:A:111:CYS:HB3	1:A:137:PHE:CD2	2.42	0.54
1:A:26:LYS:HD2	1:A:79:VAL:HG11	1.90	0.53
1:B:81:ASP:OD2	1:B:82:GLN:N	2.41	0.53
1:B:146:PRO:HG2	1:B:153:HIS:NE2	2.23	0.53
1:C:146:PRO:HG2	1:C:153:HIS:NE2	2.24	0.53
1:C:3:MET:HE1	1:C:65:MET:SD	2.48	0.53
1:B:299:TYR:O	4:B:501:HOH:O	2.19	0.53
1:C:146:PRO:HG2	1:C:153:HIS:CE1	2.44	0.53
1:C:121:MET:HE3	1:C:124:SER:HB2	1.90	0.53
1:C:129:GLU:CG	1:C:167:LYS:HD3	2.40	0.52
1:D:258:ASP:OD1	1:D:258:ASP:C	2.53	0.52
1:C:44:ASP:OD1	1:C:47:ARG:HD2	2.10	0.52
1:A:38:TYR:CG	1:A:39:PRO:HD2	2.45	0.52
1:B:284:GLU:OE2	1:B:287:GLY:HA3	2.08	0.52
1:C:269:LEU:C	1:C:269:LEU:HD23	2.34	0.52
1:D:41:ILE:HD12	1:D:41:ILE:H	1.73	0.52
1:D:94:ASN:O	1:D:98:ARG:HG3	2.09	0.52
1:D:228:VAL:HB	1:D:229:PRO:HD3	1.90	0.52
1:D:29:PHE:CE2	1:D:30:LYS:HE3	2.44	0.52
1:B:331:ARG:O	1:B:335:LYS:HG3	2.10	0.52
1:A:218:ARG:NH1	1:A:328:VAL:O	2.43	0.52
1:D:38:TYR:CD2	1:D:39:PRO:HD2	2.45	0.52
1:C:129:GLU:HG3	1:C:167:LYS:HD3	1.92	0.52
1:B:79:VAL:N	1:B:80:GLY:HA2	2.25	0.52
1:A:313:SER:O	1:A:317:ARG:HG3	2.11	0.51
1:C:333:ASP:OD1	4:C:503:HOH:O	2.19	0.51
1:B:42:SER:OG	1:B:45:GLU:HG3	2.11	0.51
1:C:280:LEU:CD2	1:C:324:ASN:HB3	2.41	0.51
1:C:6:ASP:OD1	1:C:282:GLY:HA2	2.10	0.51
1:D:41:ILE:HG22	1:D:42:SER:N	2.25	0.51
1:B:253:ASN:HB2	4:B:555:HOH:O	2.11	0.51
1:A:280:LEU:CD2	1:A:324:ASN:CB	2.89	0.51
1:C:280:LEU:CD2	1:C:324:ASN:CB	2.89	0.51
1:A:120:ASP:OD1	1:A:120:ASP:C	2.53	0.51
1:B:56:ARG:O	1:B:60:GLU:HG3	2.11	0.51
1:A:72:ALA:CA	1:A:75:MET:HE2	2.40	0.51
1:D:47:ARG:NH2	4:D:511:HOH:O	2.37	0.50
1:C:77:PRO:O	1:C:117:PRO:HD3	2.12	0.50
1:A:128:LEU:HD22	1:A:164:PHE:CE1	2.47	0.50
1:B:73:SER:N	3:B:402:7QD:O11	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:315:GLN:CD	1:B:315:GLN:H	2.20	0.50
1:C:130:ARG:O	1:C:135:LEU:HD13	2.11	0.50
1:B:277:LYS:HE2	4:D:629:HOH:O	2.10	0.50
1:C:38:TYR:CG	1:C:39:PRO:CD	2.95	0.50
1:D:129:GLU:O	1:D:133:ASN:HB2	2.12	0.50
1:B:146:PRO:HD2	1:B:153:HIS:CG	2.47	0.49
1:B:10:HIS:HA	1:B:69:SER:O	2.13	0.49
1:C:203:MET:O	1:C:207:GLN:HG3	2.12	0.49
1:B:84:VAL:HG12	4:B:596:HOH:O	2.13	0.49
1:D:315:GLN:HG3	4:D:560:HOH:O	2.12	0.49
1:C:43:ASP:O	1:C:47:ARG:HG3	2.13	0.49
1:A:96:ILE:O	1:A:100:VAL:HG23	2.13	0.49
1:A:97:ALA:CB	1:A:135:LEU:HD22	2.43	0.48
1:C:75:MET:O	1:C:76:ALA:C	2.56	0.48
1:A:159:ARG:HA	1:A:162:TYR:CD1	2.47	0.48
1:B:81:ASP:OD2	1:B:83:SER:N	2.31	0.48
1:A:174:PRO:HB3	1:A:218:ARG:NH1	2.28	0.48
1:A:69:SER:HB2	1:A:70:PRO:CD	2.43	0.48
1:B:283:SER:HB3	1:B:303:THR:OG1	2.13	0.48
1:A:81:ASP:OD1	1:A:83:SER:OG	2.30	0.48
1:A:280:LEU:HD22	1:A:324:ASN:CB	2.44	0.48
1:C:20:GLU:O	1:C:24:GLN:HG3	2.13	0.48
1:A:10:HIS:HA	1:A:69:SER:O	2.14	0.47
1:A:129:GLU:HG3	1:A:133:ASN:OD1	2.14	0.47
1:C:45:GLU:O	1:C:48:GLU:HB3	2.14	0.47
1:C:329:PHE:HZ	4:C:617:HOH:O	1.97	0.47
1:A:327:ARG:NH1	4:A:530:HOH:O	2.46	0.47
1:B:23:GLU:HA	1:B:26:LYS:HE3	1.96	0.47
1:C:79:VAL:HB	1:C:80:GLY:CA	2.44	0.47
1:D:303:THR:HA	1:D:306:TYR:CD2	2.49	0.47
1:C:3:MET:CE	1:C:65:MET:HG3	2.45	0.47
1:D:129:GLU:OE2	1:D:167:LYS:NZ	2.42	0.47
1:A:58:ILE:HG23	1:A:63:ALA:HB3	1.96	0.47
1:A:69:SER:HB2	1:A:70:PRO:HD2	1.97	0.46
1:B:221:ILE:HD12	1:B:255:VAL:CG1	2.45	0.46
1:C:17:ALA:HB1	1:C:39:PRO:HB3	1.97	0.46
1:C:67:ILE:CG2	1:C:110:VAL:HG23	2.46	0.46
1:D:168:MET:HE2	1:D:217:LEU:CD1	2.46	0.46
1:C:125:ILE:HG23	1:C:167:LYS:HD2	1.97	0.46
1:C:228:VAL:HB	1:C:229:PRO:HD3	1.97	0.46
1:C:267:ILE:HG13	1:C:306:TYR:CB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:3:MET:HE1	1:D:341:LEU:HD13	1.98	0.46
1:C:17:ALA:HB1	1:C:39:PRO:CB	2.46	0.46
1:B:128:LEU:O	1:B:132:VAL:HG23	2.15	0.46
1:B:221:ILE:HD12	1:B:255:VAL:HG13	1.98	0.46
1:C:82:GLN:HG2	1:C:119:ALA:HB2	1.98	0.46
1:D:327:ARG:NH1	4:D:508:HOH:O	2.35	0.46
1:D:79:VAL:N	1:D:80:GLY:CA	2.79	0.46
1:A:229:PRO:O	1:A:269:LEU:HD21	2.16	0.46
1:C:121:MET:HE3	1:C:124:SER:CB	2.45	0.46
1:C:284:GLU:OE2	1:C:287:GLY:HA3	2.16	0.46
1:C:292:ILE:HG13	1:C:299:TYR:CZ	2.51	0.46
1:D:214:PHE:HB3	1:D:217:LEU:HB2	1.97	0.46
1:A:200:ILE:O	1:A:204:GLN:HG3	2.15	0.45
1:B:65:MET:HE1	1:B:336:LEU:HD21	1.98	0.45
1:B:78:HIS:NE2	1:B:79:VAL:HG22	2.31	0.45
1:C:83:SER:HB3	1:D:86:VAL:HG21	1.98	0.45
1:A:206:LEU:HD23	1:A:206:LEU:O	2.17	0.45
1:B:275:ASP:OD2	4:B:502:HOH:O	2.20	0.45
1:D:313:SER:O	1:D:317:ARG:HG3	2.17	0.45
1:B:205:LEU:HB3	1:B:251:LEU:HD21	1.98	0.45
1:C:280:LEU:HD23	1:C:324:ASN:CB	2.46	0.45
1:B:162:TYR:N	1:B:163:PRO:CD	2.80	0.45
1:D:47:ARG:HG2	1:D:103:PHE:CZ	2.52	0.45
1:A:131:CYS:HA	1:A:135:LEU:HB2	1.98	0.45
1:D:264:GLN:HB3	1:D:265:PRO:HD3	1.99	0.45
1:B:13:VAL:O	4:B:503:HOH:O	2.21	0.45
1:C:98:ARG:O	1:C:102:LEU:HG	2.17	0.45
1:C:324:ASN:O	1:C:328:VAL:HG23	2.17	0.45
1:D:4:ILE:HB	1:D:63:ALA:HA	1.98	0.45
1:A:162:TYR:O	1:A:166:GLU:HG3	2.16	0.45
1:B:78:HIS:C	1:B:80:GLY:HA2	2.41	0.45
1:C:153:HIS:HB2	4:C:549:HOH:O	2.17	0.45
1:B:81:ASP:OD2	1:B:81:ASP:C	2.60	0.45
1:A:17:ALA:N	4:A:509:HOH:O	2.34	0.44
1:D:121:MET:O	1:D:125:ILE:HG13	2.18	0.44
1:A:97:ALA:HB2	1:A:135:LEU:HD22	1.98	0.44
1:D:224:GLY:O	1:D:229:PRO:HG2	2.17	0.44
1:A:283:SER:HB2	1:A:301:ASP:O	2.17	0.44
1:A:67:ILE:CG2	1:A:110:VAL:HG23	2.48	0.44
1:D:168:MET:HE2	1:D:217:LEU:HD12	1.99	0.44
3:A:402:7QD:O01	3:A:402:7QD:C09	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:73:SER:HB3	3:C:402:7QD:O11	2.18	0.44
1:C:333:ASP:O	1:C:337:LYS:HG3	2.18	0.44
1:D:159:ARG:HA	1:D:162:TYR:CD1	2.53	0.44
1:B:249:THR:HG23	1:D:59:LYS:HE3	2.00	0.44
1:B:38:TYR:CG	1:B:39:PRO:HD2	2.53	0.44
1:A:120:ASP:CG	1:A:122:THR:HG1	2.25	0.43
1:A:229:PRO:C	1:A:269:LEU:HD21	2.43	0.43
1:B:324:ASN:O	1:B:328:VAL:HG23	2.18	0.43
1:C:16:LYS:HD2	1:C:16:LYS:N	2.33	0.43
1:B:228:VAL:HB	1:B:229:PRO:HD3	2.00	0.43
1:A:54:GLN:O	1:A:58:ILE:HG13	2.18	0.43
1:B:6:ASP:OD1	1:B:282:GLY:HA2	2.18	0.43
1:A:312:ILE:HD11	1:A:317:ARG:HG2	2.00	0.43
1:B:130:ARG:O	1:B:134:GLU:HB2	2.18	0.43
1:C:22:ARG:NH2	1:C:79:VAL:HG21	2.34	0.43
1:D:326:ARG:O	1:D:333:ASP:HB2	2.19	0.43
1:A:131:CYS:HA	1:A:135:LEU:CD1	2.45	0.43
1:B:163:PRO:HA	1:B:166:GLU:CD	2.44	0.43
1:B:167:LYS:HA	1:B:167:LYS:HE2	2.01	0.43
1:B:8:HIS:CB	1:B:176:MET:HE1	2.48	0.42
1:D:75:MET:O	1:D:76:ALA:C	2.62	0.42
1:C:56:ARG:HG2	1:C:60:GLU:OE2	2.18	0.42
1:D:200:ILE:O	1:D:204:GLN:HG3	2.19	0.42
1:C:56:ARG:O	1:C:60:GLU:HG3	2.19	0.42
1:C:120:ASP:OD1	1:C:120:ASP:C	2.62	0.42
1:C:174:PRO:HG3	1:C:328:VAL:O	2.20	0.42
1:A:284:GLU:OE2	3:A:402:7QD:O08	2.38	0.42
1:C:19:ASP:O	1:C:22:ARG:HB3	2.19	0.42
1:C:280:LEU:CD2	1:C:324:ASN:HB2	2.50	0.42
1:C:280:LEU:HD23	1:C:324:ASN:HB2	2.02	0.42
1:B:162:TYR:O	1:B:166:GLU:HG3	2.19	0.42
1:D:3:MET:HE2	1:D:341:LEU:HD13	2.02	0.42
1:B:4:ILE:HG13	1:B:321:PHE:CD1	2.55	0.42
1:C:38:TYR:CD2	1:C:39:PRO:O	2.72	0.42
1:C:256:PHE:HD1	1:C:278:ASN:HA	1.85	0.42
1:A:111:CYS:HB3	1:A:137:PHE:HD2	1.85	0.41
1:D:140:CYS:O	1:D:175:ALA:HA	2.19	0.41
1:A:72:ALA:CB	1:A:75:MET:HE2	2.50	0.41
1:A:165:TYR:O	1:A:169:VAL:HG23	2.20	0.41
1:D:3:MET:HE3	1:D:341:LEU:HB3	2.01	0.41
1:A:218:ARG:NH1	1:A:218:ARG:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:GLY:HA2	1:A:258:ASP:O	2.20	0.41
1:C:277:LYS:HA	1:C:277:LYS:HD3	1.65	0.41
1:D:39:PRO:O	1:D:41:ILE:HD12	2.20	0.41
1:C:262:TYR:O	1:C:263:HIS:HB3	2.20	0.41
1:D:269:LEU:C	1:D:269:LEU:HD23	2.46	0.41
1:B:258:ASP:OD1	1:B:258:ASP:C	2.62	0.41
1:B:277:LYS:HB2	4:B:719:HOH:O	2.21	0.41
1:C:2:MET:HE1	1:C:321:PHE:CG	2.50	0.41
1:B:47:ARG:O	1:B:51:GLU:HG3	2.20	0.41
1:C:3:MET:CE	1:C:65:MET:SD	3.08	0.41
1:D:18:HIS:CE1	1:D:88:TRP:CZ3	3.09	0.41
1:B:206:LEU:HD12	1:B:206:LEU:O	2.21	0.40
1:D:86:VAL:HB	1:D:87:PRO:HD3	2.03	0.40
1:C:46:ILE:HD13	1:C:46:ILE:H	1.86	0.40
1:C:264:GLN:N	1:C:265:PRO:CD	2.84	0.40
1:B:95:LEU:HD23	1:B:95:LEU:HA	1.93	0.40
1:C:188:HIS:O	1:C:192:ALA:HB3	2.22	0.40
1:C:292:ILE:HA	1:C:299:TYR:HA	2.03	0.40
1:D:243:LYS:NZ	4:D:527:HOH:O	2.54	0.40
1:D:332:LEU:O	1:D:336:LEU:HG	2.22	0.40
1:B:335:LYS:HD2	4:B:667:HOH:O	2.20	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:402:7QD:O05	4:B:549:HOH:O[2_757]	2.07	0.13
4:A:640:HOH:O	4:C:598:HOH:O[1_565]	2.18	0.02

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	336/340 (99%)	320 (95%)	16 (5%)	0	100	100
1	B	334/340 (98%)	317 (95%)	15 (4%)	2 (1%)	21	12
1	C	330/340 (97%)	308 (93%)	22 (7%)	0	100	100
1	D	326/340 (96%)	307 (94%)	18 (6%)	1 (0%)	36	31
All	All	1326/1360 (98%)	1252 (94%)	71 (5%)	3 (0%)	43	40

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	120	ASP
1	D	80	GLY
1	B	189	ALA

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	280/282 (99%)	273 (98%)	7 (2%)	42	40
1	B	280/282 (99%)	274 (98%)	6 (2%)	47	47
1	C	278/282 (99%)	271 (98%)	7 (2%)	42	40
1	D	277/282 (98%)	273 (99%)	4 (1%)	59	61
All	All	1115/1128 (99%)	1091 (98%)	24 (2%)	45	45

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	GLU
1	A	129	GLU
1	A	153	HIS
1	A	167	LYS
1	A	221	ILE
1	A	246	SER
1	A	253	ASN
1	B	95	LEU

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Mol	Chain	Res	Type
1	B	153	HIS
1	B	253	ASN
1	B	280	LEU
1	B	286	VAL
1	B	325	THR
1	C	45	GLU
1	C	46	ILE
1	C	153	HIS
1	C	167	LYS
1	C	169	VAL
1	C	286	VAL
1	C	325	THR
1	D	81	ASP
1	D	153	HIS
1	D	246	SER
1	D	280	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	207	GLN
1	B	82	GLN
1	C	254	ASN
1	C	318	HIS
1	D	207	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	7QD	B	402	2	14,14,14	1.92	5 (35%)	19,20,20	1.53	3 (15%)
3	7QD	A	402	2	14,14,14	1.97	5 (35%)	19,20,20	1.56	2 (10%)
3	7QD	D	402	2	14,14,14	2.00	5 (35%)	19,20,20	1.52	4 (21%)
3	7QD	C	402	2	14,14,14	2.06	5 (35%)	19,20,20	1.44	2 (10%)

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	7QD	B	402	2	-	2/20/20/20	-
3	7QD	A	402	2	-	0/20/20/20	-
3	7QD	D	402	2	-	2/20/20/20	-
3	7QD	C	402	2	-	1/20/20/20	-

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	7QD	C07-C09	-4.24	1.49	1.53
3	D	402	7QD	C07-C09	-3.94	1.49	1.53
3	D	402	7QD	C12-C07	-3.23	1.50	1.54
3	B	402	7QD	C12-C07	-3.18	1.50	1.54
3	B	402	7QD	C07-C09	-3.18	1.50	1.53
3	A	402	7QD	C07-C09	-3.07	1.50	1.53
3	A	402	7QD	C06-C07	-3.01	1.50	1.54
3	A	402	7QD	C12-C07	-2.99	1.50	1.54
3	C	402	7QD	C06-C07	-2.99	1.50	1.54
3	C	402	7QD	C12-C07	-2.95	1.50	1.54
3	B	402	7QD	C06-C07	-2.83	1.50	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	7QD	C02-C03	-2.68	1.49	1.53
3	A	402	7QD	O08-C07	-2.59	1.38	1.43
3	C	402	7QD	C02-C03	-2.54	1.49	1.53
3	D	402	7QD	O08-C07	-2.52	1.38	1.43
3	D	402	7QD	C06-C07	-2.43	1.51	1.54
3	D	402	7QD	C02-C03	-2.42	1.49	1.53
3	B	402	7QD	O08-C07	-2.41	1.38	1.43
3	C	402	7QD	O08-C07	-2.34	1.38	1.43
3	B	402	7QD	C02-C03	-2.12	1.50	1.53

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402	7QD	O11-C09-C07	3.93	120.67	113.14
3	A	402	7QD	O11-C09-C07	3.82	120.47	113.14
3	A	402	7QD	C06-C02-C03	3.35	121.53	115.95
3	C	402	7QD	O11-C09-C07	3.35	119.56	113.14
3	D	402	7QD	C06-C02-C03	3.08	121.08	115.95
3	B	402	7QD	C06-C02-C03	2.84	120.69	115.95
3	D	402	7QD	O11-C09-C07	2.66	118.24	113.14
3	D	402	7QD	O05-C03-C02	2.45	120.39	113.59
3	B	402	7QD	O05-C03-C02	2.21	119.70	113.59
3	D	402	7QD	O04-C03-C02	-2.09	119.21	121.81
3	C	402	7QD	O05-C03-C02	2.05	119.27	113.59

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	7QD	C07-C12-C13-O14
3	B	402	7QD	C07-C12-C13-O15
3	D	402	7QD	C07-C12-C13-O14
3	D	402	7QD	C07-C12-C13-O15
3	C	402	7QD	C07-C12-C13-O15

There are no ring outliers.

4 monomers are involved in 7 short contacts:

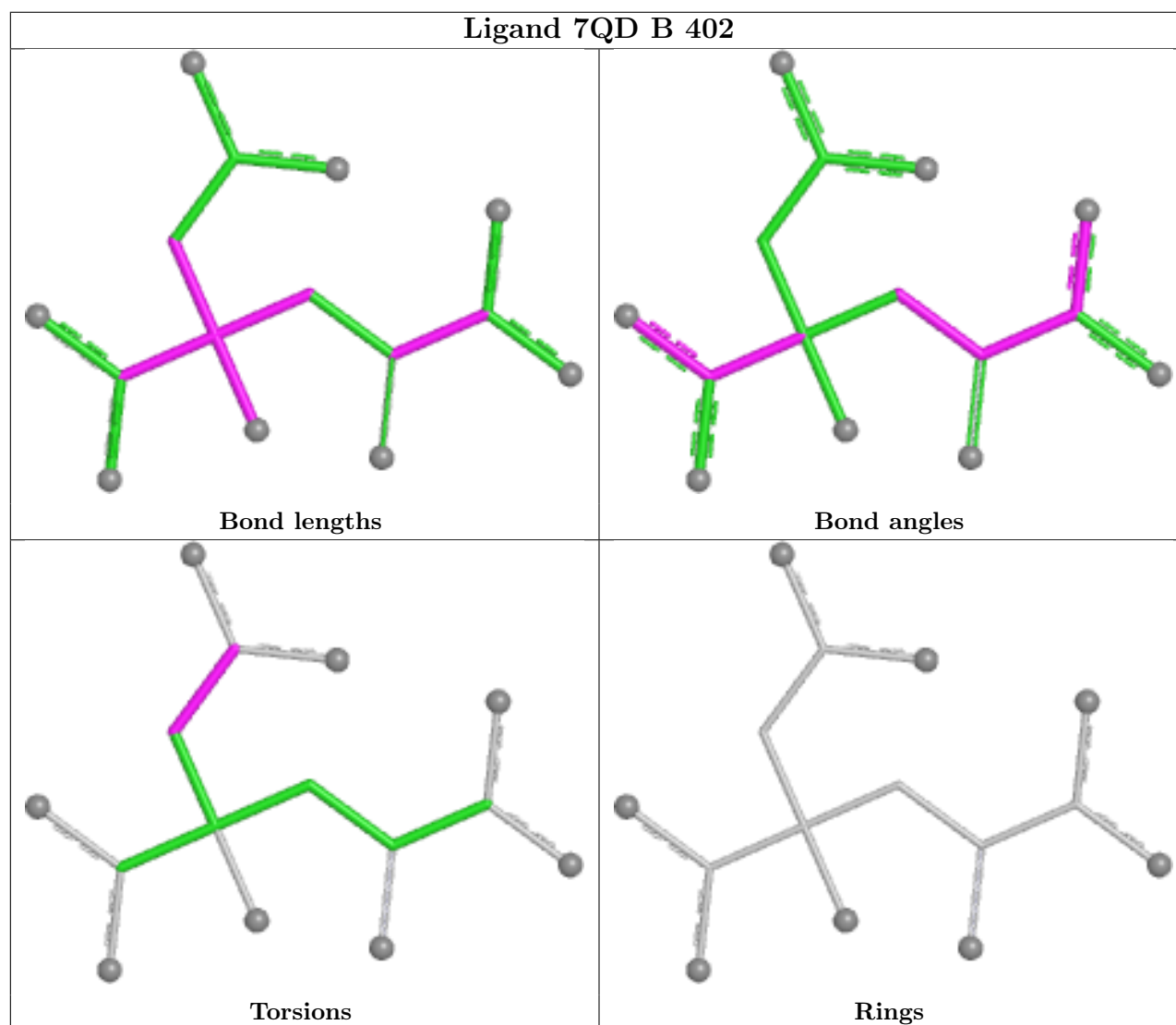
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	7QD	2	0
3	A	402	7QD	2	0

Continued on next page...

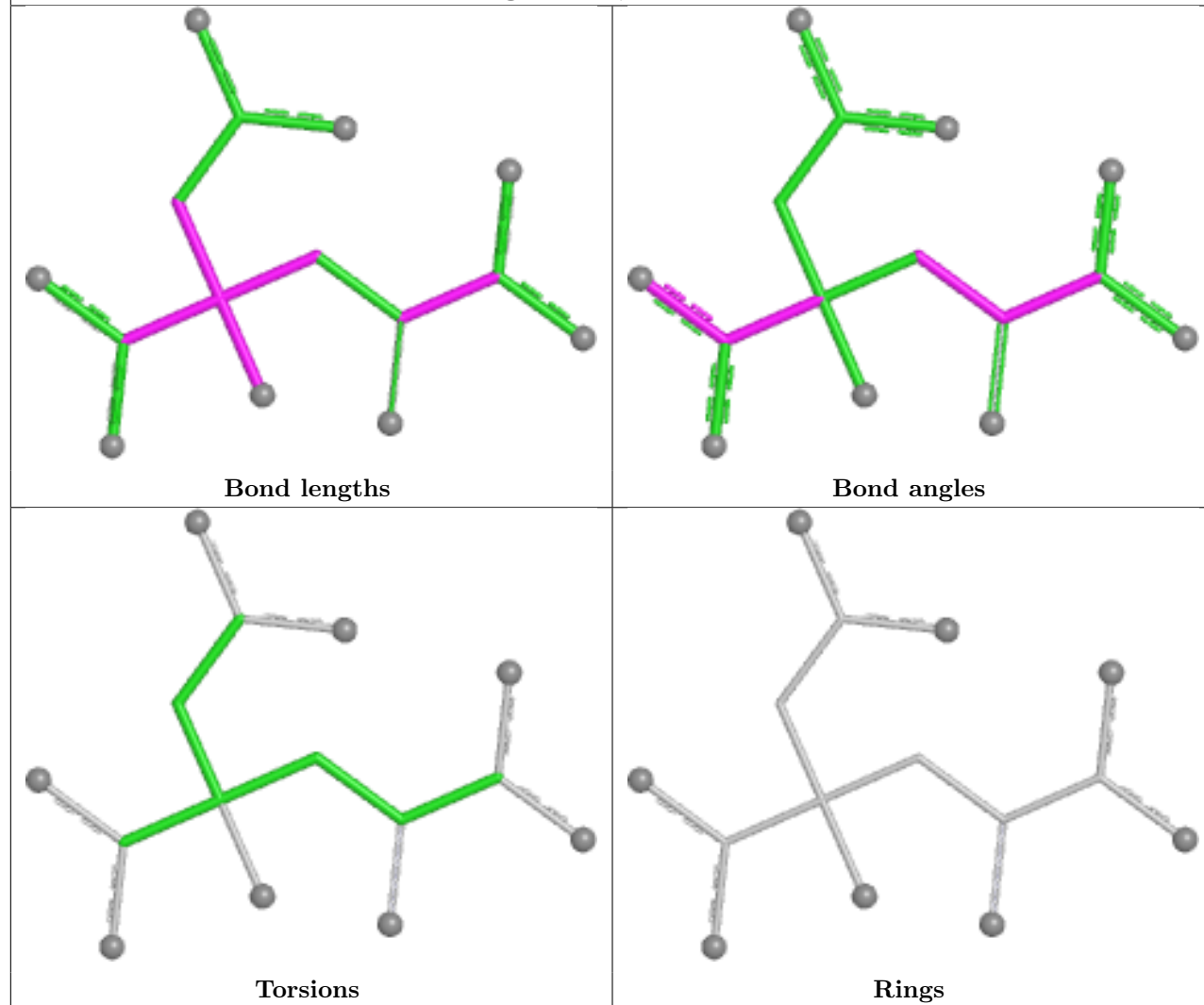
Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	402	7QD	1	1
3	C	402	7QD	1	0

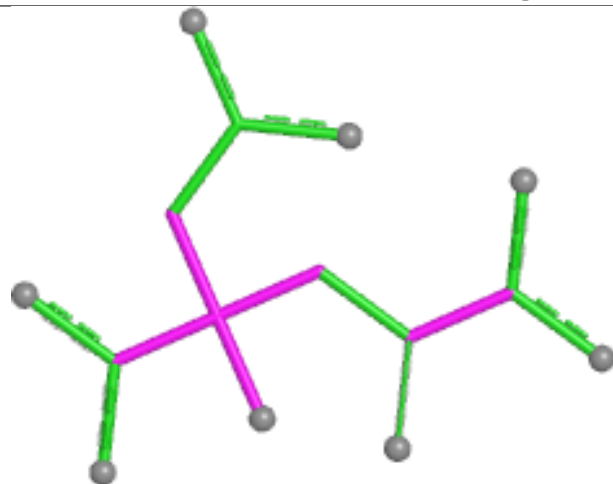
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



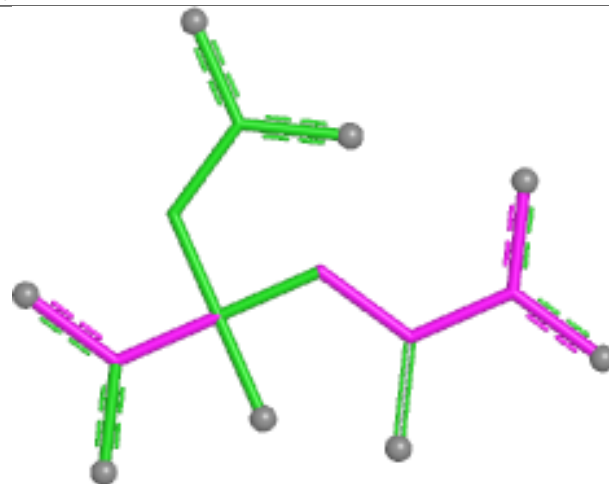
Ligand 7QD A 402



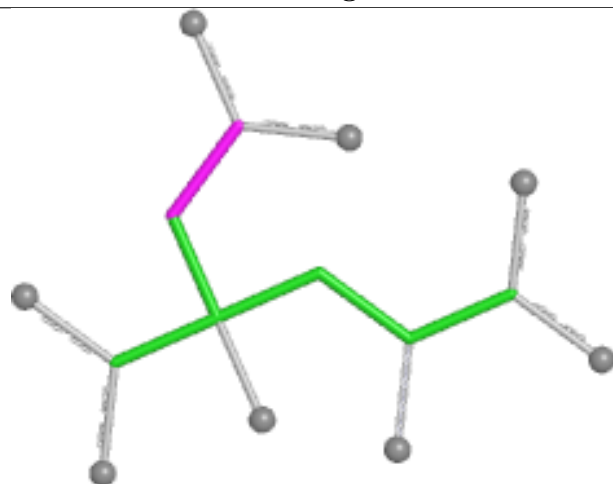
Ligand 7QD D 402



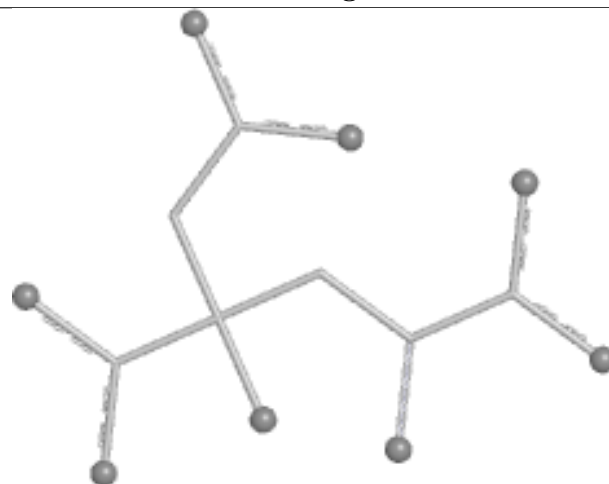
Bond lengths



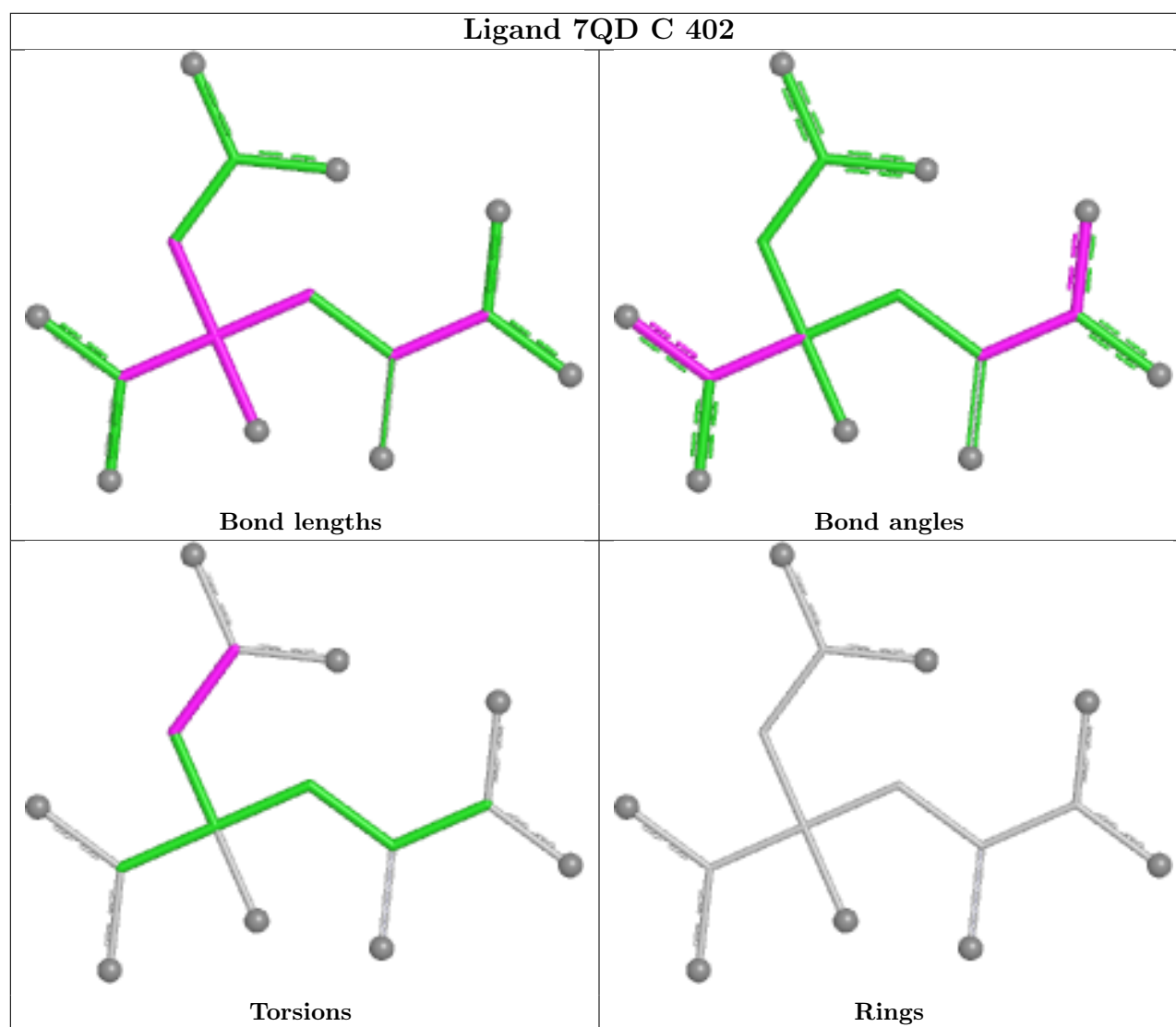
Bond angles



Torsions



Rings



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

EDS failed to run properly - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.