W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 7, 2023 – 11:22 PM EDT

|		
PDB ID	:	6DXS
Title	:	Crystal structure of the LigJ hydratase E284Q mutant substrate complex with (3Z)-2-keto-4-carboxy-3-hexenedioate
Authors	:	Mabanglo, M.F.; Raushel, F.M.; Hogancamp, T.N.
Deposited on	:	2018-06-29
Resolution	:	1.65 Å(reported)

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 1.65 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.
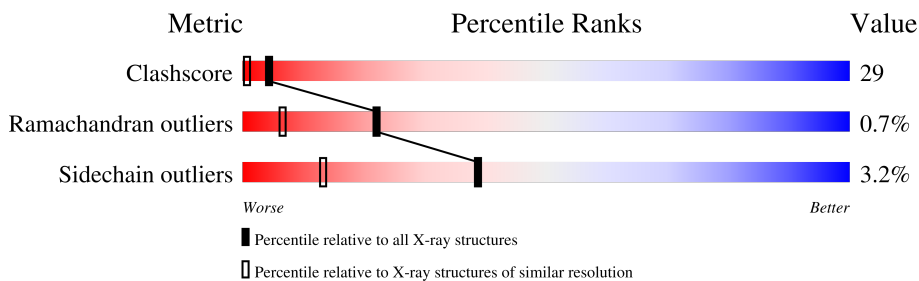
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1931 (1.66-1.66)
Ramachandran outliers	138981	1891 (1.66-1.66)
Sidechain outliers	138945	1891 (1.66-1.66)

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 <=5%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	342	51% 47% •
1	B	342	53% 44% •
1	C	342	49% 48% •
1	D	342	54% 44% •

2 Entry composition ⓘ

There are 4 unique types of molecules in this entry. The entry contains 11540 atoms, of which 11 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	342	Total	C	N	O	S	0	0	0
			2683	1709	464	490	20			
1	B	342	Total	C	N	O	S	0	0	0
			2683	1709	464	490	20			
1	C	342	Total	C	N	O	S	0	0	0
			2683	1709	464	490	20			
1	D	342	Total	C	N	O	S	0	0	0
			2683	1709	464	490	20			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	284	GLN	GLU	engineered mutation	UNP G2IQQ5
A	342	LEU	-	expression tag	UNP G2IQQ5
A	343	GLU	-	expression tag	UNP G2IQQ5
B	284	GLN	GLU	engineered mutation	UNP G2IQQ5
B	342	LEU	-	expression tag	UNP G2IQQ5
B	343	GLU	-	expression tag	UNP G2IQQ5
C	284	GLN	GLU	engineered mutation	UNP G2IQQ5
C	342	LEU	-	expression tag	UNP G2IQQ5
C	343	GLU	-	expression tag	UNP G2IQQ5
D	284	GLN	GLU	engineered mutation	UNP G2IQQ5
D	342	LEU	-	expression tag	UNP G2IQQ5
D	343	GLU	-	expression tag	UNP G2IQQ5

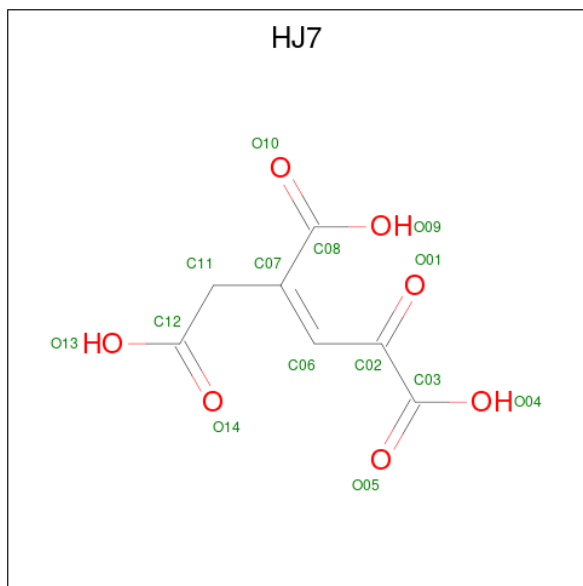- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

Continued on next page...

Continued from previous page...

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

- Molecule 3 is (2Z)-4-oxobut-2-ene-1,2,4-tricarboxylic acid (three-letter code: HJ7) (formula: $C_7H_6O_7$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 17	C 7	H 3	O 7	0	0
3	B	1	Total 17	C 7	H 3	O 7	0	0
3	C	1	Total 17	C 7	H 3	O 7	0	0
3	D	1	Total 16	C 7	H 2	O 7	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	181	Total 181	O 181	0	0
4	B	192	Total 192	O 192	0	0
4	C	169	Total 169	O 169	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	195	Total 195	O 195	0	0

3 Residue-property plots ⓘ

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

Chain A:

• Molecule 1: 4-oxalomesaconate hydratase

Chain B:

• Molecule 1: 4-oxalomesaconate hydratase

Chain C:

M2 M3 I4 I5 D6 C7 H8 G9 H10 Y11 T12 V13 L14 P15 K16 A17 H18 D19 E20 W21 R22 E23 Q24 Q25 K26 A27 A28 F29 Q33 P34 A35 P36 P37 Y38 P39 E40 I41 S42 D43 D44 E45 I46 R47 E48 T49 I50 E51 Q54 L55 R56 L57 I58 K59 E60 R61 M65 T66

I67 F68 S69 P70 R71 A72 S73 A74 M75 A76 P77 H78 V79 G80 D81 Q82 S83 V84 A85 V86 P87 W88 A89 Q90 R98 V99 V100 D101 L102 F103 P104 E105 T106 V110 C111 M112 L113 P114 Q115 S116 P117 E118 A119 D120 M121 T122 S123 S124 I125 L128 E129 R130 C131 V132 N133 E134 L135

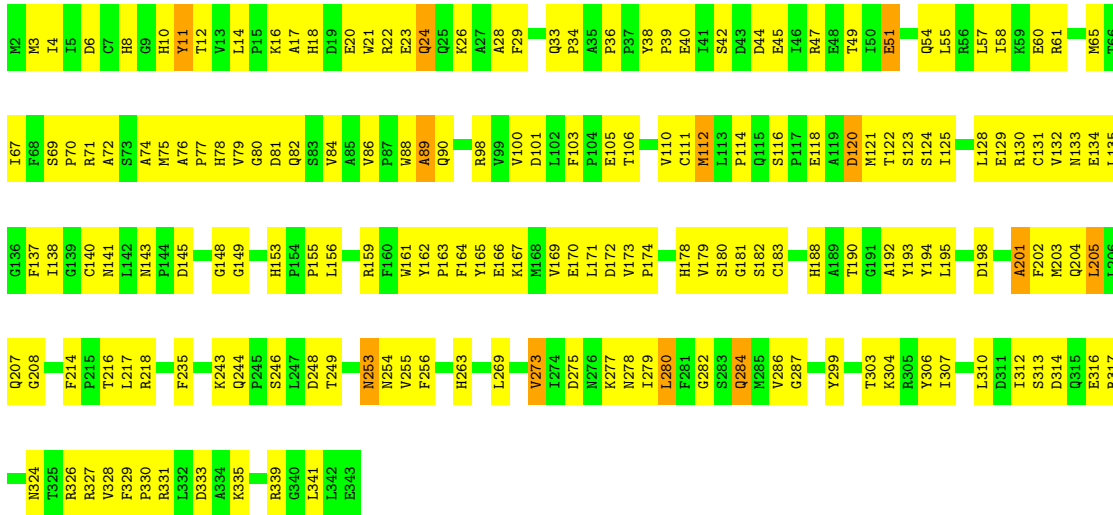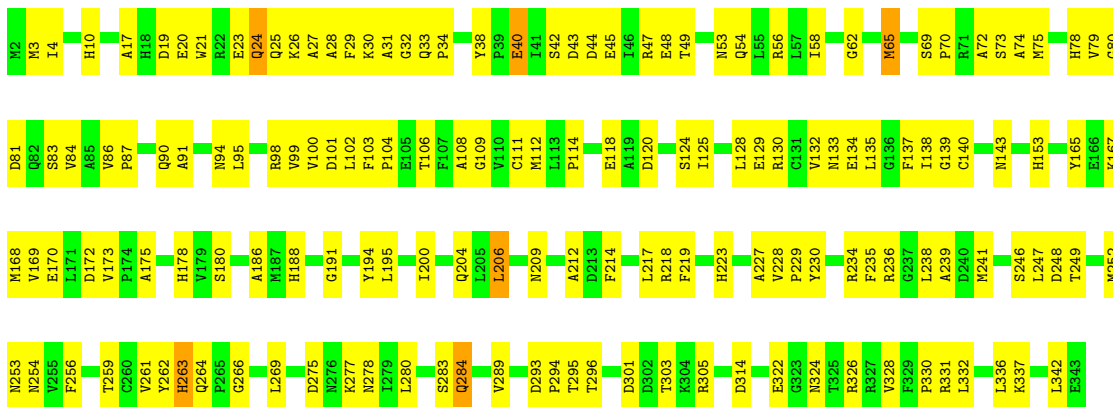G136 F137 I138 G139 C140 N141 L142 N143 P144 D145 G148 G149 H153 P154 P155 L156 R159 F160 W161 Y162 P163 F164 Y165 E166 K167 M168 V169 E170 L171 D172 V173 P174 H178 V179 S180 G181 S182 C183 H188 A189 T190 G191 A192 Y193 Y194 L195 D198 A201 F202 M203 Q204 L205 L206

Q207 G208 F214 P215 T216 L217 R218 F235 K243 Q244 P245 S246 L247 D248 T249 N253 N254 V255 F256 H263 L269 V273 I274 D275 N276 K277 N278 I279 L280 F281 G282 S283 Q284 M285 V286 G287 Y299 T303 K304 R305 Y306 I307 L310 D311 I312 S313 D314 Q315 E316 R317

N324 T325 R326 R327 V328 F329 P330 R331 L332 D333 A334 K335 R339 G340 L341 L342 E343

• Molecule 1: 4-oxalomesaconate hydratase

Chain D:

54%   44%   •

M2 M3 I4 H10 A17 H18 D19 E20 W21 R22 E23 Q24 Q25 K26 A27 A28 F29 K30 A31 G32 Q33 P34 Y38 P39 E40 I41 S42 D43 D44 E45 I46 R47 E48 T49 N53 Q54 L55 R56 L57 I58 G62 M65 S69 P70 R71 A72 S73 A74 M75 H78 V79 G80

D81 Q82 S83 V84 A85 V86 P87 Q90 A91 N94 L95 R98 V99 V100 D101 L102 F103 P104 E105 T106 F107 A108 G109 V110 C111 M112 L113 P114 E118 A119 D120 S124 I125 L128 E129 R130 C131 V132 N133 E134 L135 G136 F137 I138 G139 C140 N143 H153 Y165 E166 K167

M168 V169 E170 L171 D172 V173 P174 A175 H178 V179 S180 A186 M187 H188 G191 Y194 L195 I200 Q204 L205 L206 N209 A212 D213 F214 L217 R218 F219 H223 A227 V228 P229 Y230 R234 F235 R236 G237 L238 A239 D240 M241 S246 L247 D248 T249 M252

N253 N254 V255 F256 T259 C260 V261 Y262 H263 Q264 P265 G266 L269 D275 N276 K277 N278 I279 L280 S283 Q284 V289 D293 P294 T295 T296 D301 D302 T303 K304 R305 D314 E322 G323 N324 T325 R326 R327 V328 F329 P330 R331 L332 L336 K337 L342 E343

4 Data and refinement statistics (i)

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	82.69Å 78.25Å 136.22Å 90.00° 89.98° 90.00°	Depositor
Resolution (Å)	43.63 – 1.65	Depositor
% Data completeness (in resolution range)	97.8 (43.63-1.65)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.40 (at 1.64Å)	Xtriage
Refinement program	PHENIX (1.13_2998: ???)	Depositor
R, R_{free}	0.202 , 0.266	Depositor
Wilson B-factor (Å^2)	20.5	Xtriage
Anisotropy	0.770	Xtriage
L-test for twinning[2]	$<|L|>=0.41$, $<L^2>=0.24$	Xtriage
Estimated twinning fraction	0.479 for h,-k,-l	Xtriage
Total number of atoms	11540	wwPDB-VP
Average B, all atoms (Å^2)	25.0	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 55.95 % 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 2.9363e-05.*

---

[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ 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: HJ7, 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	0.39	0/2757	0.56	0/3748
1	B	0.40	0/2757	0.59	0/3748
1	C	0.40	0/2757	0.57	0/3748
1	D	0.39	0/2757	0.59	0/3748
All	All	0.40	0/11028	0.58	0/14992

There are no bond length outliers.

There are no bond angle outliers.

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	2683	0	2602	160	0
1	B	2683	0	2602	140	1
1	C	2683	0	2602	162	0
1	D	2683	0	2602	157	1
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	14	3	0	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	3	0	4	0
3	C	14	3	0	2	0
3	D	14	2	0	4	0
4	A	181	0	0	40	0
4	B	192	0	0	39	3
4	C	169	0	0	33	2
4	D	195	0	0	49	1
All	All	11529	11	10408	614	4

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 29.

The worst 5 of 614 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:75:MET:SD	4:C:632:HOH:O	2.08	1.11
1:C:145:ASP:OD1	4:C:501:HOH:O	1.69	1.08
1:D:195:LEU:O	4:D:501:HOH:O	1.73	1.06
1:D:112:MET:SD	4:D:629:HOH:O	2.13	1.05
1:D:40:GLU:OE1	4:D:502:HOH:O	1.73	1.04

All (4) 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)
1:D:102:LEU:O	4:B:668:HOH:O[1_655]	1.93	0.27
1:B:234:ARG:NH2	4:C:564:HOH:O[1_565]	2.11	0.09
4:B:523:HOH:O	4:C:621:HOH:O[1_565]	2.16	0.04
4:B:564:HOH:O	4:D:613:HOH:O[1_455]	2.17	0.03

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	340/342 (99%)	307 (90%)	30 (9%)	3 (1%)	17	4
1	B	340/342 (99%)	307 (90%)	31 (9%)	2 (1%)	25	8
1	C	340/342 (99%)	300 (88%)	37 (11%)	3 (1%)	17	4
1	D	340/342 (99%)	310 (91%)	29 (8%)	1 (0%)	41	22
All	All	1360/1368 (99%)	1224 (90%)	127 (9%)	9 (1%)	22	6

5 of 9 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	ASP
1	B	3	MET
1	C	201	ALA
1	A	80	GLY
1	C	89	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	284/284 (100%)	278 (98%)	6 (2%)	53	29
1	B	284/284 (100%)	274 (96%)	10 (4%)	36	11
1	C	284/284 (100%)	271 (95%)	13 (5%)	27	6
1	D	284/284 (100%)	277 (98%)	7 (2%)	47	22
All	All	1136/1136 (100%)	1100 (97%)	36 (3%)	39	13

5 of 36 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	284	GLN
1	D	284	GLN
1	D	24	GLN
1	D	153	HIS
1	B	269	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	150	HIS
1	D	133	ASN
1	D	150	HIS
1	B	284	GLN
1	A	264	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 monosaccharides 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	HJ7	C	402	2	13,13,13	1.65	3 (23%)	13,17,17	2.00	6 (46%)
3	HJ7	A	402	2	13,13,13	2.07	5 (38%)	13,17,17	1.80	4 (30%)
3	HJ7	B	402	2	13,13,13	1.74	3 (23%)	13,17,17	1.65	4 (30%)
3	HJ7	D	402	2	13,13,13	1.80	2 (15%)	13,17,17	1.43	2 (15%)

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	HJ7	C	402	2	-	7/16/16/16	-
3	HJ7	A	402	2	-	9/16/16/16	-
3	HJ7	B	402	2	-	10/16/16/16	-
3	HJ7	D	402	2	-	6/16/16/16	-

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	402	HJ7	C06-C02	4.15	1.56	1.43
3	D	402	HJ7	C06-C02	3.95	1.55	1.43
3	C	402	HJ7	C06-C02	3.56	1.54	1.43
3	B	402	HJ7	C06-C02	3.50	1.54	1.43
3	A	402	HJ7	C11-C12	3.06	1.55	1.51

The worst 5 of 16 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	402	HJ7	O04-C03-C02	3.63	122.96	113.19
3	A	402	HJ7	O04-C03-C02	3.46	122.52	113.19
3	A	402	HJ7	C11-C07-C06	-2.99	117.83	125.69
3	C	402	HJ7	O09-C08-C07	2.82	121.48	115.49
3	C	402	HJ7	C11-C07-C06	-2.76	118.44	125.69

There are no chirality outliers.

5 of 32 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	HJ7	C06-C07-C08-O09
3	A	402	HJ7	C06-C07-C08-O10
3	A	402	HJ7	C11-C07-C08-O09
3	A	402	HJ7	C11-C07-C08-O10
3	A	402	HJ7	C06-C07-C11-C12

There are no ring outliers.

4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	402	HJ7	2	0
3	A	402	HJ7	1	0
3	B	402	HJ7	4	0
3	D	402	HJ7	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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.