



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:16 PM UTC

PDB ID : 7NCO / pdb_00007nco
Title : Glutathione-S-transferase GliG mutant K127R
Authors : Groll, M.; Huber, E.M.
Deposited on : 2021-01-29
Resolution : 1.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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<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>.

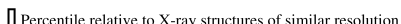
The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
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

i

X-RAY DIFFRACTION

A.



Similar resolution
(#Entries, resolution range(Å))

Quality of chain

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Mol	Chain	Length	Quality of chain
1	F	253	2% 91% 6%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12600 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 Glutathione S-transferase GliG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	237	Total	C	N	O	S	0	3	0
			1949	1250	336	357	6			
1	B	239	Total	C	N	O	S	0	1	0
			1948	1251	336	356	5			
1	C	240	Total	C	N	O	S	0	0	0
			1945	1247	336	356	6			
1	D	238	Total	C	N	O	S	0	1	0
			1939	1244	335	354	6			
1	E	240	Total	C	N	O	S	0	2	0
			1964	1261	338	358	7			
1	F	238	Total	C	N	O	S	0	1	0
			1939	1244	335	354	6			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-12	MET	-	initiating methionine	UNP B0Y813
A	-11	SER	-	expression tag	UNP B0Y813
A	-10	GLY	-	expression tag	UNP B0Y813
A	-9	SER	-	expression tag	UNP B0Y813
A	-8	HIS	-	expression tag	UNP B0Y813
A	-7	HIS	-	expression tag	UNP B0Y813
A	-6	HIS	-	expression tag	UNP B0Y813
A	-5	HIS	-	expression tag	UNP B0Y813
A	-4	HIS	-	expression tag	UNP B0Y813
A	-3	HIS	-	expression tag	UNP B0Y813
A	-2	SER	-	expression tag	UNP B0Y813
A	-1	GLY	-	expression tag	UNP B0Y813
A	0	SER	-	expression tag	UNP B0Y813
A	127	ARG	LYS	engineered mutation	UNP B0Y813
B	-12	MET	-	initiating methionine	UNP B0Y813
B	-11	SER	-	expression tag	UNP B0Y813
B	-10	GLY	-	expression tag	UNP B0Y813

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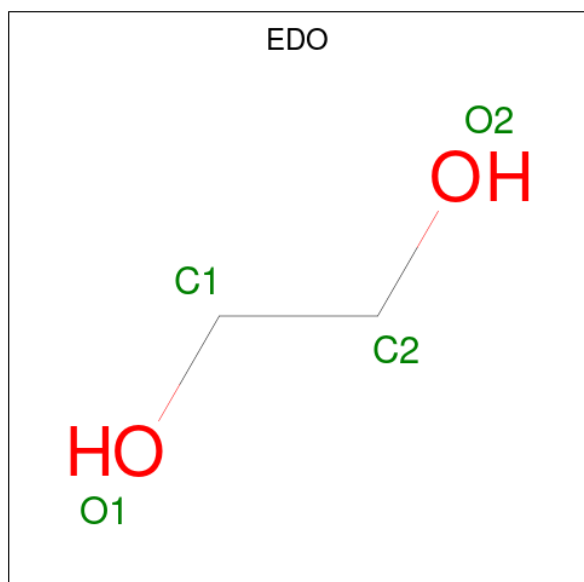
Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	SER	-	expression tag	UNP B0Y813
B	-8	HIS	-	expression tag	UNP B0Y813
B	-7	HIS	-	expression tag	UNP B0Y813
B	-6	HIS	-	expression tag	UNP B0Y813
B	-5	HIS	-	expression tag	UNP B0Y813
B	-4	HIS	-	expression tag	UNP B0Y813
B	-3	HIS	-	expression tag	UNP B0Y813
B	-2	SER	-	expression tag	UNP B0Y813
B	-1	GLY	-	expression tag	UNP B0Y813
B	0	SER	-	expression tag	UNP B0Y813
B	127	ARG	LYS	engineered mutation	UNP B0Y813
C	-12	MET	-	initiating methionine	UNP B0Y813
C	-11	SER	-	expression tag	UNP B0Y813
C	-10	GLY	-	expression tag	UNP B0Y813
C	-9	SER	-	expression tag	UNP B0Y813
C	-8	HIS	-	expression tag	UNP B0Y813
C	-7	HIS	-	expression tag	UNP B0Y813
C	-6	HIS	-	expression tag	UNP B0Y813
C	-5	HIS	-	expression tag	UNP B0Y813
C	-4	HIS	-	expression tag	UNP B0Y813
C	-3	HIS	-	expression tag	UNP B0Y813
C	-2	SER	-	expression tag	UNP B0Y813
C	-1	GLY	-	expression tag	UNP B0Y813
C	0	SER	-	expression tag	UNP B0Y813
C	127	ARG	LYS	engineered mutation	UNP B0Y813
D	-12	MET	-	initiating methionine	UNP B0Y813
D	-11	SER	-	expression tag	UNP B0Y813
D	-10	GLY	-	expression tag	UNP B0Y813
D	-9	SER	-	expression tag	UNP B0Y813
D	-8	HIS	-	expression tag	UNP B0Y813
D	-7	HIS	-	expression tag	UNP B0Y813
D	-6	HIS	-	expression tag	UNP B0Y813
D	-5	HIS	-	expression tag	UNP B0Y813
D	-4	HIS	-	expression tag	UNP B0Y813
D	-3	HIS	-	expression tag	UNP B0Y813
D	-2	SER	-	expression tag	UNP B0Y813
D	-1	GLY	-	expression tag	UNP B0Y813
D	0	SER	-	expression tag	UNP B0Y813
D	127	ARG	LYS	engineered mutation	UNP B0Y813
E	-12	MET	-	initiating methionine	UNP B0Y813
E	-11	SER	-	expression tag	UNP B0Y813
E	-10	GLY	-	expression tag	UNP B0Y813

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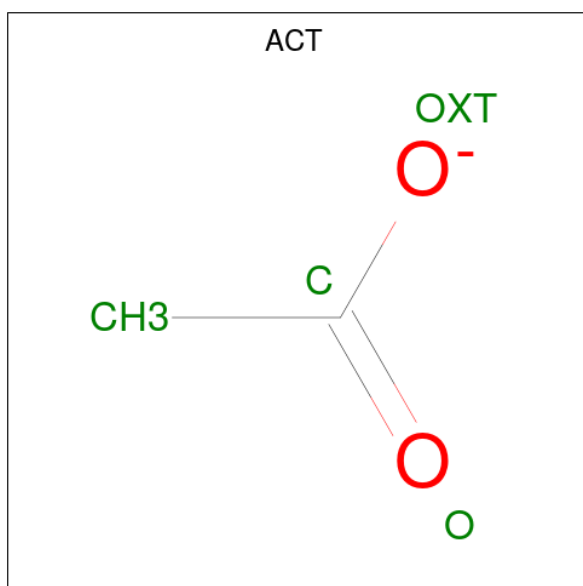
Chain	Residue	Modelled	Actual	Comment	Reference
E	-9	SER	-	expression tag	UNP B0Y813
E	-8	HIS	-	expression tag	UNP B0Y813
E	-7	HIS	-	expression tag	UNP B0Y813
E	-6	HIS	-	expression tag	UNP B0Y813
E	-5	HIS	-	expression tag	UNP B0Y813
E	-4	HIS	-	expression tag	UNP B0Y813
E	-3	HIS	-	expression tag	UNP B0Y813
E	-2	SER	-	expression tag	UNP B0Y813
E	-1	GLY	-	expression tag	UNP B0Y813
E	0	SER	-	expression tag	UNP B0Y813
E	127	ARG	LYS	engineered mutation	UNP B0Y813
F	-12	MET	-	initiating methionine	UNP B0Y813
F	-11	SER	-	expression tag	UNP B0Y813
F	-10	GLY	-	expression tag	UNP B0Y813
F	-9	SER	-	expression tag	UNP B0Y813
F	-8	HIS	-	expression tag	UNP B0Y813
F	-7	HIS	-	expression tag	UNP B0Y813
F	-6	HIS	-	expression tag	UNP B0Y813
F	-5	HIS	-	expression tag	UNP B0Y813
F	-4	HIS	-	expression tag	UNP B0Y813
F	-3	HIS	-	expression tag	UNP B0Y813
F	-2	SER	-	expression tag	UNP B0Y813
F	-1	GLY	-	expression tag	UNP B0Y813
F	0	SER	-	expression tag	UNP B0Y813
F	127	ARG	LYS	engineered mutation	UNP B0Y813

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	E	1	Total C O 4 2 2	0	0
2	F	1	Total C O 4 2 2	0	0

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: $C_2H_3O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	162	Total O 162 162	0	0

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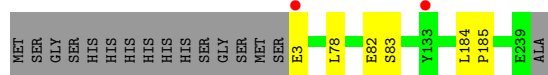
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	177	Total 177	O 177	0	0
4	C	116	Total 116	O 116	0	0
4	D	135	Total 135	O 135	0	0
4	E	152	Total 152	O 152	0	0
4	F	138	Total 138	O 138	0	0

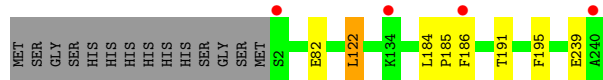
3 Residue-property plots [i](#)

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.

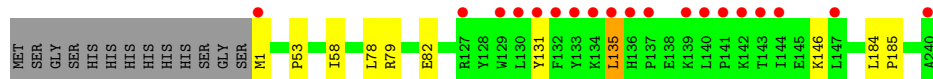
- Molecule 1: Glutathione S-transferase GliG



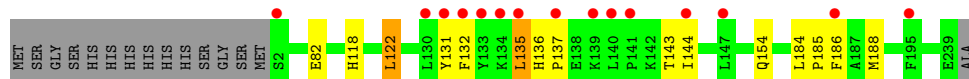
- Molecule 1: Glutathione S-transferase GliG



- Molecule 1: Glutathione S-transferase GliG



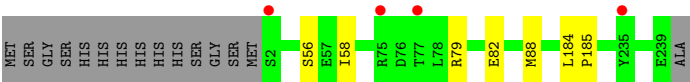
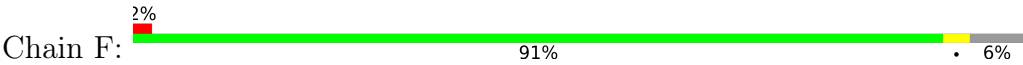
- Molecule 1: Glutathione S-transferase GliG



- Molecule 1: Glutathione S-transferase GliG



- Molecule 1: Glutathione S-transferase GliG



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.31Å 85.15Å 347.73Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.70 30.00 – 1.70	Depositor EDS
% Data completeness (in resolution range)	98.6 (30.00-1.70) 98.6 (30.00-1.70)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.75 (at 1.70Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.201 , 0.231 0.209 , 0.238	Depositor DCC
R_{free} test set	8964 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.6	Xtriage
Anisotropy	0.588	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 47.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12600	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.40% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, ACT

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	0.97	0/1999	1.35	0/2714
1	B	0.97	0/1999	1.34	0/2713
1	C	0.98	0/1995	1.39	0/2707
1	D	0.98	0/1989	1.39	0/2700
1	E	0.98	0/2015	1.36	0/2733
1	F	0.98	0/1989	1.36	0/2700
All	All	0.98	0/11986	1.36	0/16267

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 [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	1949	0	1940	4	0
1	B	1948	0	1939	4	0
1	C	1945	0	1943	7	0
1	D	1939	0	1934	13	0
1	E	1964	0	1959	9	0
1	F	1939	0	1934	4	0
2	A	12	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	4	0	6	0	0
2	E	8	0	12	0	0
2	F	4	0	6	0	0
3	A	4	0	3	1	0
3	B	4	0	3	0	0
4	A	162	0	0	0	0
4	B	177	0	0	0	0
4	C	116	0	0	0	0
4	D	135	0	0	0	0
4	E	152	0	0	0	0
4	F	138	0	0	0	0
All	All	12600	0	11697	37	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 2.

All (37) 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:131:TYR:HA	1:C:135:LEU:HD12	1.61	0.81
1:E:122:LEU:HB3	1:E:186[A]:PHE:CZ	2.19	0.78
1:A:3:GLU:O	1:A:3:GLU:HG2	1.88	0.73
1:D:118:HIS:HA	1:D:122:LEU:HG	1.72	0.70
1:E:88[A]:MET:HE1	1:F:88[A]:MET:HE1	1.75	0.68
1:D:132:PHE:CE1	1:D:143:THR:HG21	2.29	0.67
1:E:88[B]:MET:HE2	1:F:88[B]:MET:HE1	1.79	0.64
1:D:122:LEU:HB3	1:D:186:PHE:CZ	2.34	0.63
1:D:136:HIS:ND1	1:D:137:PRO:HD2	2.17	0.60
1:B:122:LEU:HG	1:B:186[B]:PHE:CE2	2.42	0.54
1:D:184:LEU:O	1:D:188:MET:HG3	2.08	0.53
1:E:122:LEU:HD22	1:E:154:GLN:HB3	1.90	0.53
1:E:122:LEU:HB3	1:E:186[A]:PHE:CE2	2.44	0.52
1:D:122:LEU:HB3	1:D:186:PHE:CE2	2.45	0.51
1:C:146:LYS:HE3	1:D:131:TYR:OH	2.10	0.51
1:E:118:HIS:HA	1:E:122:LEU:HG	1.92	0.51
1:B:186[A]:PHE:HA	1:B:191:THR:HG21	1.95	0.49
1:C:184:LEU:HB3	1:C:185:PRO:HD3	1.95	0.49
1:D:122:LEU:HD22	1:D:154:GLN:HB3	1.97	0.46
1:F:184:LEU:HB3	1:F:185:PRO:HD3	1.97	0.46
1:C:1:MET:HB3	1:C:53:PRO:HD2	1.96	0.46
1:D:131:TYR:HH	1:D:136:HIS:HD1	1.60	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:C	1:A:78:LEU:HD12	2.42	0.45
1:D:184:LEU:HB3	1:D:185:PRO:HD3	1.99	0.44
1:A:83:SER:N	3:A:304:ACT:OXT	2.49	0.44
1:C:78:LEU:C	1:C:78:LEU:HD12	2.43	0.43
1:D:131:TYR:CD1	1:D:135:LEU:HB3	2.52	0.43
1:E:186[B]:PHE:HA	1:E:191:THR:HG21	2.00	0.43
1:E:78:LEU:C	1:E:78:LEU:HD12	2.44	0.42
1:F:58:ILE:O	1:F:79:ARG:HD2	2.19	0.42
1:C:146:LYS:HE3	1:D:131:TYR:HH	1.83	0.42
1:B:184:LEU:HB3	1:B:185:PRO:HD3	2.01	0.41
1:B:191:THR:HG22	1:B:195:PHE:CE2	2.55	0.41
1:C:58:ILE:O	1:C:79:ARG:HD2	2.21	0.41
1:A:184:LEU:HB3	1:A:185:PRO:HD3	2.02	0.41
1:D:118:HIS:HD1	1:D:122:LEU:HD12	1.85	0.41
1:E:2:SER:HA	1:E:53:PRO:HB2	2.04	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	238/253 (94%)	232 (98%)	5 (2%)	1 (0%)	30	16
1	B	238/253 (94%)	233 (98%)	4 (2%)	1 (0%)	30	16
1	C	238/253 (94%)	232 (98%)	5 (2%)	1 (0%)	30	16
1	D	237/253 (94%)	232 (98%)	4 (2%)	1 (0%)	30	16
1	E	240/253 (95%)	234 (98%)	5 (2%)	1 (0%)	30	16
1	F	237/253 (94%)	232 (98%)	4 (2%)	1 (0%)	30	16
All	All	1428/1518 (94%)	1395 (98%)	27 (2%)	6 (0%)	30	16

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLU
1	B	82	GLU
1	C	82	GLU
1	E	82	GLU
1	D	82	GLU
1	F	82	GLU

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	209/219 (95%)	209 (100%)	0	100	100
1	B	208/219 (95%)	206 (99%)	2 (1%)	68	58
1	C	208/219 (95%)	207 (100%)	1 (0%)	81	76
1	D	208/219 (95%)	205 (99%)	3 (1%)	59	46
1	E	210/219 (96%)	205 (98%)	5 (2%)	43	26
1	F	208/219 (95%)	207 (100%)	1 (0%)	81	76
All	All	1251/1314 (95%)	1239 (99%)	12 (1%)	70	58

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	122	LEU
1	B	239	GLU
1	C	135	LEU
1	D	122	LEU
1	D	135	LEU
1	D	144	ILE
1	E	122	LEU
1	E	130	LEU
1	E	186[A]	PHE
1	E	186[B]	PHE
1	E	239	GLU
1	F	56	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	27	ASN
1	A	106	GLN
1	B	27	ASN
1	B	167	GLN
1	B	223	GLN
1	C	27	ASN
1	E	27	ASN
1	E	223	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
2	EDO	A	303	-	3,3,3	0.08	0	2,2,2	0.28	0
2	EDO	A	302	-	3,3,3	0.06	0	2,2,2	0.09	0
2	EDO	E	302	-	3,3,3	0.05	0	2,2,2	0.10	0
2	EDO	E	301	-	3,3,3	0.06	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	ACT	A	304	-	3,3,3	1.07	0	3,3,3	0.69	0
3	ACT	B	302	-	3,3,3	1.03	0	3,3,3	0.85	0
2	EDO	B	301	-	3,3,3	0.09	0	2,2,2	0.04	0
2	EDO	A	301	-	3,3,3	0.08	0	2,2,2	0.10	0
2	EDO	F	301	-	3,3,3	0.09	0	2,2,2	0.22	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
2	EDO	A	303	-	-	0/1/1/1	-
2	EDO	A	302	-	-	1/1/1/1	-
2	EDO	E	302	-	-	0/1/1/1	-
2	EDO	E	301	-	-	1/1/1/1	-
2	EDO	B	301	-	-	0/1/1/1	-
2	EDO	A	301	-	-	0/1/1/1	-
2	EDO	F	301	-	-	1/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	302	EDO	O1-C1-C2-O2
2	F	301	EDO	O1-C1-C2-O2
2	E	301	EDO	O1-C1-C2-O2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	304	ACT	1	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

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	237/253 (93%)	0.07	2 (0%) 82 85	14, 26, 44, 63	3 (1%)
1	B	239/253 (94%)	0.07	4 (1%) 69 73	12, 25, 42, 58	1 (0%)
1	C	240/253 (94%)	0.50	19 (7%) 18 20	21, 32, 71, 99	0
1	D	238/253 (94%)	0.40	15 (6%) 26 28	13, 31, 70, 95	1 (0%)
1	E	240/253 (94%)	0.18	4 (1%) 69 73	12, 29, 42, 62	2 (0%)
1	F	238/253 (94%)	0.07	4 (1%) 69 73	12, 28, 43, 73	1 (0%)
All	All	1432/1518 (94%)	0.22	48 (3%) 48 52	12, 29, 50, 99	8 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	186[A]	PHE	11.5
1	D	140	LEU	5.5
1	C	137	PRO	5.4
1	C	141	PRO	4.6
1	C	240	ALA	4.5
1	C	135	LEU	4.4
1	B	186[A]	PHE	4.2
1	E	240	ALA	4.0
1	D	137	PRO	4.0
1	C	140	LEU	3.9
1	C	143	THR	3.9
1	C	133	TYR	3.9
1	C	130	LEU	3.8
1	C	144	ILE	3.6
1	C	132	PHE	3.5
1	D	147	LEU	3.5
1	B	240	ALA	3.3
1	B	2	SER	3.3
1	D	133	TYR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	131	TYR	3.0
1	D	2	SER	3.0
1	D	141	PRO	3.0
1	D	134	LYS	2.9
1	D	132	PHE	2.8
1	D	130	LEU	2.8
1	E	1	MET	2.7
1	F	2	SER	2.6
1	D	186	PHE	2.6
1	E	97	ASP	2.6
1	C	142	LYS	2.6
1	F	75	ARG	2.6
1	D	195	PHE	2.5
1	A	133	TYR	2.5
1	C	139	LYS	2.4
1	D	135	LEU	2.4
1	D	139	LYS	2.4
1	C	131	TYR	2.4
1	C	147	LEU	2.3
1	C	134	LYS	2.3
1	C	129	TRP	2.2
1	B	134	LYS	2.1
1	F	77	THR	2.1
1	D	144	ILE	2.1
1	C	127	ARG	2.1
1	C	1	MET	2.1
1	A	3	GLU	2.0
1	F	235	TYR	2.0
1	C	136	HIS	2.0

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

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

6.3 Carbohydrates ⓘ

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
2	EDO	B	301	4/4	0.74	0.20	47,48,49,55	0
2	EDO	E	301	4/4	0.82	0.21	49,50,52,54	0
2	EDO	A	302	4/4	0.83	0.16	51,53,53,55	0
2	EDO	A	303	4/4	0.86	0.22	33,34,35,35	0
2	EDO	F	301	4/4	0.87	0.12	45,45,46,46	0
3	ACT	A	304	4/4	0.88	0.15	34,34,36,37	0
3	ACT	B	302	4/4	0.90	0.12	34,35,36,38	0
2	EDO	E	302	4/4	0.92	0.11	44,47,48,48	0
2	EDO	A	301	4/4	0.95	0.08	29,29,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.