



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jul 7, 2025 – 10:14 am BST

PDB ID : 9QCZ / pdb\_00009qcz  
Title : Crystal structure of Rhizobium etli L-asparaginase ReAV K263A mutant  
Authors : Pokrywka, K.; Grzechowiak, M.; Loch, J.I.; Ruszkowski, M.; Gilski, M.; Jaskolski, M.  
Deposited on : 2025-03-05  
Resolution : 1.60 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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>.

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

MolProbity : 4-5-2 with Phenix2.0rc1  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 2.0rc1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.44

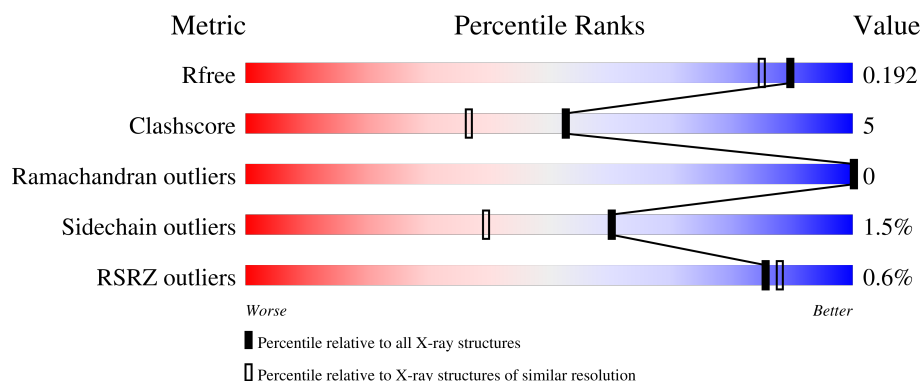
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.60 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))
$R_{free}$	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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  $\geq 3$ , 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	373	<div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div>
1	B	373	<div> <div>%</div> <div>87%</div> <div>6%</div> <div>6%</div> </div>
1	C	373	<div> <div>%</div> <div>88%</div> <div>5%</div> <div>6%</div> </div>
1	D	373	<div> <div>87%</div> <div>7%</div> <div>6%</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	EDO	A	409	-	-	X	-
6	TRS	A	410	-	-	X	-

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 12447 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 L-asparaginase II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	16	0
			2665	1653	482	507	23			
1	B	350	Total	C	N	O	S	0	12	0
			2648	1638	486	501	23			
1	C	350	Total	C	N	O	S	0	15	0
			2663	1649	482	509	23			
1	D	349	Total	C	N	O	S	0	21	0
			2688	1667	489	508	24			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	expression tag	UNP Q9RFN5
A	-4	ILE	-	expression tag	UNP Q9RFN5
A	-3	ASP	-	expression tag	UNP Q9RFN5
A	-2	PRO	-	expression tag	UNP Q9RFN5
A	-1	PHE	-	expression tag	UNP Q9RFN5
A	0	THR	-	expression tag	UNP Q9RFN5
A	263	ALA	LYS	engineered mutation	UNP Q9RFN5
B	-5	GLY	-	expression tag	UNP Q9RFN5
B	-4	ILE	-	expression tag	UNP Q9RFN5
B	-3	ASP	-	expression tag	UNP Q9RFN5
B	-2	PRO	-	expression tag	UNP Q9RFN5
B	-1	PHE	-	expression tag	UNP Q9RFN5
B	0	THR	-	expression tag	UNP Q9RFN5
B	263	ALA	LYS	engineered mutation	UNP Q9RFN5
C	-5	GLY	-	expression tag	UNP Q9RFN5
C	-4	ILE	-	expression tag	UNP Q9RFN5
C	-3	ASP	-	expression tag	UNP Q9RFN5
C	-2	PRO	-	expression tag	UNP Q9RFN5
C	-1	PHE	-	expression tag	UNP Q9RFN5
C	0	THR	-	expression tag	UNP Q9RFN5
C	263	ALA	LYS	engineered mutation	UNP Q9RFN5

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	GLY	-	expression tag	UNP Q9RFN5
D	-4	ILE	-	expression tag	UNP Q9RFN5
D	-3	ASP	-	expression tag	UNP Q9RFN5
D	-2	PRO	-	expression tag	UNP Q9RFN5
D	-1	PHE	-	expression tag	UNP Q9RFN5
D	0	THR	-	expression tag	UNP Q9RFN5
D	263	ALA	LYS	engineered mutation	UNP Q9RFN5

- 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	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0

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

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O<sub>4</sub>S).



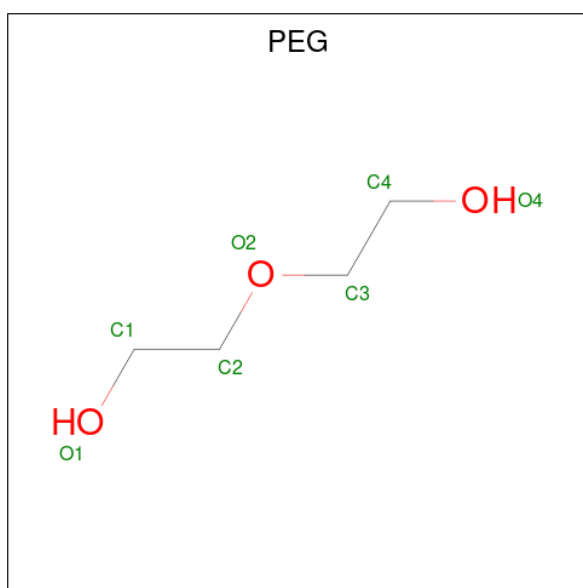
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	1
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 5 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

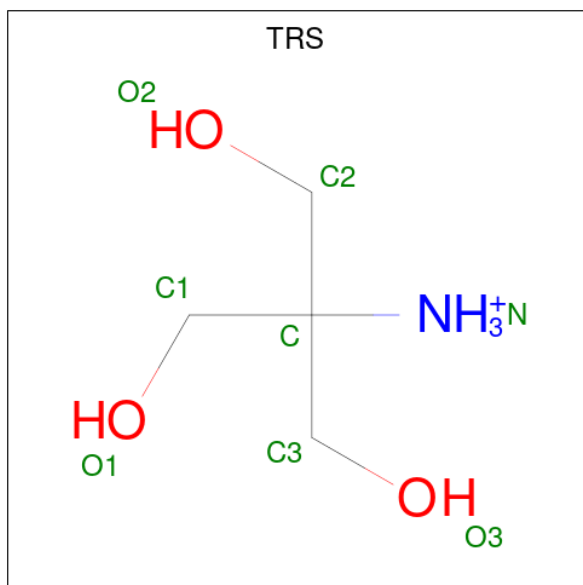
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			8	4	1	3		
6	B	1	Total	C	N	O	0	0
			8	4	1	3		
6	C	1	Total	C	N	O	0	0
			8	4	1	3		
6	D	1	Total	C	N	O	0	0
			8	4	1	3		

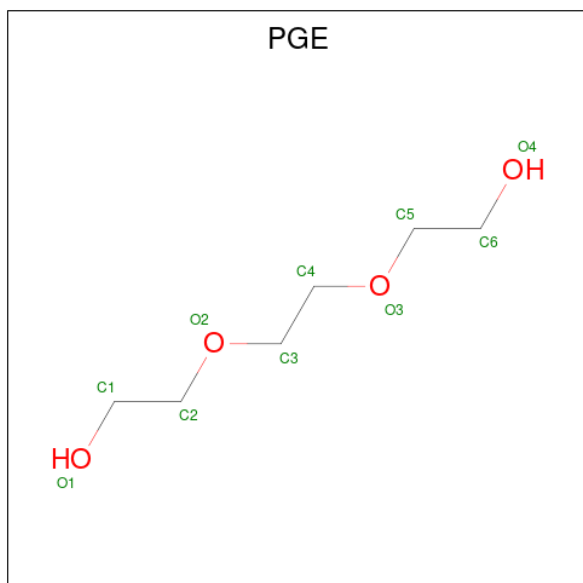
- Molecule 7 is ZINC ION (CCD ID: ZN) (formula:  $Zn$ ).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	D	1	Total	Cl	0	0
			1	1		

- Molecule 9 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	1
			20	12	8		


- Molecule 10 is water.

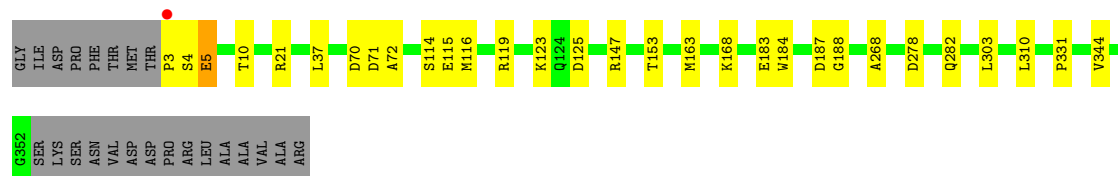
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	383	Total	O	0	0
			383	383		
10	B	373	Total	O	0	0
			373	373		
10	C	413	Total	O	0	0
			413	413		
10	D	380	Total	O	0	0
			380	380		

### 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.

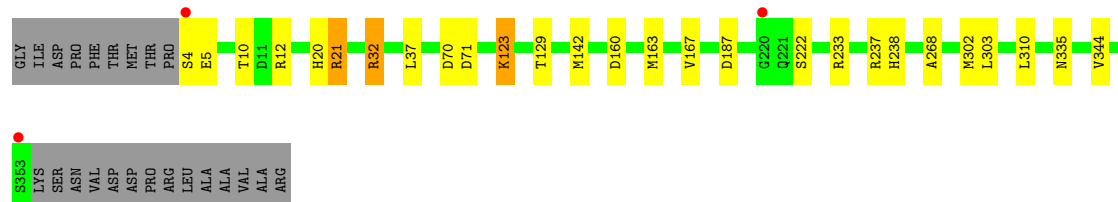
#### • Molecule 1: L-asparaginase II

Chain A: 




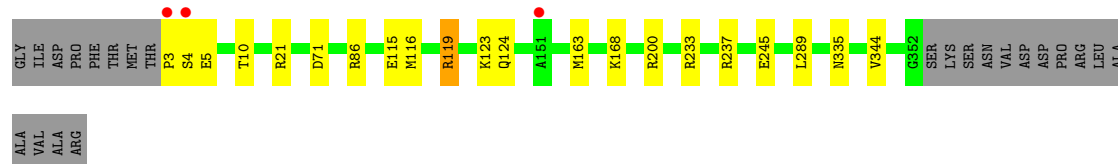
#### • Molecule 1: L-asparaginase II

Chain B: 




#### • Molecule 1: L-asparaginase II

Chain C: 



#### • Molecule 1: L-asparaginase II

Chain D: 



ASP  
ASP  
PRO  
ARG  
LEU  
ALA  
ALA  
VAL  
ALA  
ARG

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.89Å 91.51Å 114.34Å 90.00° 97.08° 90.00°	Depositor
Resolution (Å)	48.69 – 1.60 48.69 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (48.69-1.60) 99.3 (48.69-1.60)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 1.60Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.160 , 0.192 0.161 , 0.192	Depositor DCC
$R_{free}$ test set	2518 reflections (0.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	17.8	Xtriage
Anisotropy	0.273	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12447	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	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 39.82 % 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 2.9996e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: PGE, CL, EDO, TRS, PEG, GOL, SO4, ZN, CSO

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	0.59	2/2750 (0.1%)	0.65	2/3711 (0.1%)
1	B	0.53	0/2721	0.61	0/3673
1	C	0.57	0/2745	0.63	0/3705
1	D	0.56	2/2788 (0.1%)	0.63	0/3762
All	All	0.56	4/11004 (0.0%)	0.63	2/14851 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	183[A]	GLU	C-O	5.70	1.30	1.23
1	A	183[B]	GLU	C-O	5.70	1.30	1.23
1	D	183[A]	GLU	C-O	5.66	1.31	1.23
1	D	183[B]	GLU	C-O	5.66	1.31	1.23

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	183[A]	GLU	CA-C-O	5.12	127.50	121.36
1	A	183[B]	GLU	CA-C-O	5.12	127.50	121.36

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	2665	0	2671	36	0
1	B	2648	0	2643	23	0
1	C	2663	0	2656	21	0
1	D	2688	0	2703	20	0
2	A	16	0	24	13	0
2	B	20	0	30	3	0
2	C	32	0	48	2	0
2	D	20	0	30	4	0
3	A	10	0	0	0	0
3	B	15	0	0	0	0
3	C	20	0	0	0	0
3	D	10	0	0	0	0
4	A	12	0	16	1	0
5	A	7	0	10	1	0
5	C	7	0	10	1	0
5	D	7	0	10	1	0
6	A	8	0	12	6	0
6	B	8	0	12	4	0
6	C	8	0	12	4	0
6	D	8	0	12	5	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	C	20	0	28	3	0
10	A	383	0	0	7	0
10	B	373	0	0	3	0
10	C	413	0	0	5	0
10	D	380	0	0	4	0
All	All	12447	0	10927	106	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 5.

The worst 5 of 106 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:A:71:ASP:H	6:A:410:TRS:H11	1.21	1.00
1:B:12:ARG:HH22	2:B:407:EDO:H11	1.30	0.97
1:D:70:ASP:HB2	6:D:408:TRS:H21	1.56	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:ASP:HB2	6:C:407:TRS:H31	1.59	0.84
1:D:10:THR:HG22	1:D:344[B]:VAL:HG12	1.64	0.79

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	363/373 (97%)	354 (98%)	9 (2%)	0	100	100
1	B	359/373 (96%)	350 (98%)	9 (2%)	0	100	100
1	C	362/373 (97%)	353 (98%)	9 (2%)	0	100	100
1	D	367/373 (98%)	358 (98%)	9 (2%)	0	100	100
All	All	1451/1492 (97%)	1415 (98%)	36 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	278/281 (99%)	274 (99%)	4 (1%)	62	43
1	B	274/281 (98%)	268 (98%)	6 (2%)	47	23
1	C	277/281 (99%)	274 (99%)	3 (1%)	70	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	282/281 (100%)	277 (98%)	5 (2%)	54 31
All	All	1111/1124 (99%)	1093 (98%)	18 (2%)	60 37

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	116	MET
1	D	332	GLN
1	D	187	ASP
1	B	160	ASP
1	D	5	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	124	GLN
1	A	282	GLN
1	C	124	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	CSO	C	249	1	3,6,7	0.84	0	0,6,8	-	-
1	CSO	D	249	1	3,6,7	0.67	0	0,6,8	-	-
1	CSO	B	249	1	3,6,7	0.84	0	0,6,8	-	-
1	CSO	A	249	1	3,6,7	0.84	0	0,6,8	-	-

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
1	CSO	C	249	1	-	0/1/5/7	-
1	CSO	D	249	1	-	0/1/5/7	-
1	CSO	B	249	1	-	0/1/5/7	-
1	CSO	A	249	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 6 are monoatomic - leaving 44 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	$\# Z  > 2$
2	EDO	A	402	-	3,3,3	0.34	0	2,2,2	0.48	0
2	EDO	B	407	-	3,3,3	0.61	0	2,2,2	0.27	0
2	EDO	A	401	-	3,3,3	0.65	0	2,2,2	0.22	0
2	EDO	A	403	-	3,3,3	0.09	0	2,2,2	0.23	0
2	EDO	D	407	-	3,3,3	0.16	0	2,2,2	1.59	0
2	EDO	D	409	-	3,3,3	0.59	0	2,2,2	0.17	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	SO4	D	402	-	4,4,4	0.15	0	6,6,6	0.25	0
3	SO4	C	404	-	4,4,4	0.34	0	6,6,6	0.30	0
2	EDO	C	406	-	3,3,3	0.27	0	2,2,2	0.64	0
2	EDO	C	402	-	3,3,3	0.40	0	2,2,2	0.40	0
9	PGE	C	415[A]	-	9,9,9	0.37	0	8,8,8	0.27	0
6	TRS	A	410	-	7,7,7	0.19	0	9,9,9	0.32	0
6	TRS	C	407	-	7,7,7	0.63	0	9,9,9	1.02	0
3	SO4	A	408	-	4,4,4	0.25	0	6,6,6	0.21	0
3	SO4	C	405	-	4,4,4	0.20	0	6,6,6	0.52	0
2	EDO	D	401	-	3,3,3	0.27	0	2,2,2	0.68	0
2	EDO	B	405	-	3,3,3	0.13	0	2,2,2	0.08	0
5	PEG	C	414	-	6,6,6	0.21	0	5,5,5	0.32	0
4	GOL	A	405	-	5,5,5	0.09	0	5,5,5	0.35	0
6	TRS	B	404	-	7,7,7	0.54	0	9,9,9	1.02	0
2	EDO	A	409	-	3,3,3	0.46	0	2,2,2	0.88	0
5	PEG	D	405	-	6,6,6	0.16	0	5,5,5	0.21	0
3	SO4	B	403	-	4,4,4	0.30	0	6,6,6	0.54	0
2	EDO	C	408	-	3,3,3	0.35	0	2,2,2	0.49	0
3	SO4	C	412[B]	-	4,4,4	0.19	0	6,6,6	0.27	0
3	SO4	D	404	-	4,4,4	0.29	0	6,6,6	0.63	0
3	SO4	C	413	-	4,4,4	0.20	0	6,6,6	0.55	0
3	SO4	B	409	-	4,4,4	0.17	0	6,6,6	0.22	0
2	EDO	C	411	-	3,3,3	0.54	0	2,2,2	0.22	0
2	EDO	C	409	-	3,3,3	0.67	0	2,2,2	0.18	0
5	PEG	A	407	-	6,6,6	0.12	0	5,5,5	0.11	0
9	PGE	C	415[B]	-	9,9,9	0.46	0	8,8,8	0.41	0
2	EDO	C	410	-	3,3,3	0.13	0	2,2,2	0.30	0
2	EDO	C	401	-	3,3,3	0.42	0	2,2,2	0.36	0
2	EDO	D	403	-	3,3,3	0.16	0	2,2,2	0.06	0
2	EDO	D	406	-	3,3,3	0.46	0	2,2,2	0.56	0
2	EDO	B	401	-	3,3,3	0.69	0	2,2,2	0.61	0
4	GOL	A	406	-	5,5,5	0.68	0	5,5,5	1.25	0
2	EDO	C	403	-	3,3,3	0.34	0	2,2,2	0.89	0
2	EDO	B	402	-	3,3,3	0.52	0	2,2,2	0.36	0
3	SO4	B	406	-	4,4,4	0.20	0	6,6,6	0.41	0
2	EDO	B	408	-	3,3,3	0.37	0	2,2,2	0.46	0
3	SO4	A	404	-	4,4,4	0.21	0	6,6,6	0.42	0
6	TRS	D	408	-	7,7,7	0.15	0	9,9,9	0.26	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	402	-	-	0/1/1/1	-
2	EDO	B	407	-	-	0/1/1/1	-
2	EDO	A	401	-	-	0/1/1/1	-
2	EDO	A	403	-	-	0/1/1/1	-
2	EDO	D	407	-	-	0/1/1/1	-
2	EDO	D	409	-	-	0/1/1/1	-
2	EDO	C	406	-	-	0/1/1/1	-
2	EDO	C	402	-	-	0/1/1/1	-
9	PGE	C	415[A]	-	-	3/7/7/7	-
6	TRS	A	410	-	-	9/9/9/9	-
6	TRS	C	407	-	-	6/9/9/9	-
2	EDO	D	401	-	-	0/1/1/1	-
2	EDO	B	405	-	-	1/1/1/1	-
5	PEG	C	414	-	-	2/4/4/4	-
4	GOL	A	405	-	-	2/4/4/4	-
6	TRS	B	404	-	-	8/9/9/9	-
2	EDO	A	409	-	-	0/1/1/1	-
5	PEG	D	405	-	-	3/4/4/4	-
2	EDO	C	408	-	-	0/1/1/1	-
2	EDO	C	411	-	-	0/1/1/1	-
2	EDO	C	409	-	-	0/1/1/1	-
5	PEG	A	407	-	-	4/4/4/4	-
9	PGE	C	415[B]	-	-	3/7/7/7	-
2	EDO	C	410	-	-	1/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-
2	EDO	D	403	-	-	0/1/1/1	-
2	EDO	D	406	-	-	0/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-
4	GOL	A	406	-	-	0/4/4/4	-
2	EDO	C	403	-	-	0/1/1/1	-
2	EDO	B	402	-	-	0/1/1/1	-
2	EDO	B	408	-	-	0/1/1/1	-
6	TRS	D	408	-	-	6/9/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 48 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	410	TRS	C2-C-C1-O1
6	B	404	TRS	C2-C-C3-O3
6	B	404	TRS	N-C-C3-O3
6	C	407	TRS	C2-C-C1-O1
6	C	407	TRS	C3-C-C1-O1

There are no ring outliers.

19 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	402	EDO	3	0
2	B	407	EDO	2	0
2	D	407	EDO	1	0
2	C	402	EDO	1	0
9	C	415[A]	PGE	2	0
6	A	410	TRS	6	0
6	C	407	TRS	4	0
2	D	401	EDO	2	0
5	C	414	PEG	1	0
6	B	404	TRS	4	0
2	A	409	EDO	10	0
5	D	405	PEG	1	0
2	C	409	EDO	1	0
5	A	407	PEG	1	0
9	C	415[B]	PGE	1	0
2	D	403	EDO	1	0
2	B	401	EDO	1	0
4	A	406	GOL	1	0
6	D	408	TRS	5	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	349/373 (93%)	-0.43	1 (0%) 90 91	10, 19, 35, 61	16 (4%)
1	B	349/373 (93%)	-0.32	3 (0%) 81 83	10, 21, 42, 67	12 (3%)
1	C	349/373 (93%)	-0.46	3 (0%) 81 83	10, 18, 33, 70	15 (4%)
1	D	348/373 (93%)	-0.38	1 (0%) 90 91	10, 20, 36, 64	21 (6%)
All	All	1395/1492 (93%)	-0.40	8 (0%) 85 88	10, 20, 37, 70	64 (4%)

The worst 5 of 8 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	3	PRO	4.3
1	A	3	PRO	3.5
1	B	353	SER	3.3
1	B	220	GLY	3.1
1	D	4	SER	2.8

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	CSO	A	249	7/8	0.97	0.06	17,17,24,32	0
1	CSO	C	249	7/8	0.97	0.06	16,17,23,31	0
1	CSO	B	249	7/8	0.98	0.06	16,17,24,31	0
1	CSO	D	249	7/8	0.98	0.05	17,17,23,29	0

## 6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

## 6.4 Ligands ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
5	PEG	A	407	7/7	0.67	0.20	43,44,48,52	0
6	TRS	A	410	8/8	0.68	0.20	23,34,43,46	8
3	SO4	A	408	5/5	0.69	0.17	34,37,40,47	5
3	SO4	C	413	5/5	0.72	0.16	33,39,40,44	5
6	TRS	D	408	8/8	0.73	0.18	25,35,41,44	8
2	EDO	C	410	4/4	0.75	0.17	42,43,44,47	0
2	EDO	B	405	4/4	0.76	0.16	41,41,44,49	0
5	PEG	C	414	7/7	0.76	0.16	40,43,49,51	0
4	GOL	A	405	6/6	0.77	0.19	30,34,46,46	0
2	EDO	A	403	4/4	0.78	0.17	37,47,47,48	0
3	SO4	C	412[B]	5/5	0.78	0.17	31,37,38,40	5
2	EDO	B	402	4/4	0.80	0.16	43,45,49,49	0
2	EDO	D	406	4/4	0.81	0.16	42,48,51,53	0
9	PGE	C	415[A]	10/10	0.82	0.15	17,20,22,27	10
9	PGE	C	415[B]	10/10	0.82	0.15	9,23,24,31	10
2	EDO	D	409	4/4	0.83	0.12	40,41,46,48	0
2	EDO	A	402	4/4	0.83	0.15	37,38,43,50	0
3	SO4	C	405	5/5	0.83	0.14	26,29,38,40	5
2	EDO	C	408	4/4	0.83	0.15	31,40,41,44	0
6	TRS	B	404	8/8	0.84	0.16	27,31,37,41	8
2	EDO	D	403	4/4	0.84	0.15	32,34,35,39	4
3	SO4	D	402	5/5	0.85	0.09	40,41,49,50	5
3	SO4	B	409	5/5	0.85	0.09	36,38,49,50	5
2	EDO	D	407	4/4	0.85	0.17	35,36,39,40	0
4	GOL	A	406	6/6	0.86	0.12	28,30,32,33	0
6	TRS	C	407	8/8	0.86	0.15	23,34,40,42	8
2	EDO	D	401	4/4	0.86	0.15	30,30,35,37	0
2	EDO	B	401	4/4	0.86	0.13	35,36,38,38	0
2	EDO	C	402	4/4	0.86	0.15	28,30,30,34	4
2	EDO	B	408	4/4	0.87	0.14	36,38,41,45	0
2	EDO	A	409	4/4	0.87	0.11	35,35,36,39	0
3	SO4	B	406	5/5	0.87	0.10	35,39,45,47	5

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	EDO	B	407	4/4	0.89	0.15	22,29,40,40	0
5	PEG	D	405	7/7	0.89	0.12	28,34,38,42	0
2	EDO	C	403	4/4	0.90	0.14	22,28,39,40	0
2	EDO	C	409	4/4	0.90	0.12	26,33,36,40	0
2	EDO	C	411	4/4	0.91	0.13	22,31,35,39	4
2	EDO	C	406	4/4	0.92	0.12	29,32,34,37	0
3	SO4	A	404	5/5	0.92	0.12	26,26,29,34	5
8	CL	A	412	1/1	0.93	0.10	40,40,40,40	0
3	SO4	D	404	5/5	0.93	0.11	22,24,25,35	5
2	EDO	A	401	4/4	0.93	0.10	27,29,32,39	0
2	EDO	C	401	4/4	0.94	0.08	27,28,34,38	0
8	CL	D	411	1/1	0.96	0.10	37,37,37,37	0
3	SO4	C	404	5/5	0.96	0.09	21,23,27,34	5
3	SO4	B	403	5/5	0.96	0.07	22,24,28,35	5
7	ZN	A	411	1/1	1.00	0.02	17,17,17,17	1
7	ZN	B	410	1/1	1.00	0.01	17,17,17,17	1
7	ZN	C	416	1/1	1.00	0.02	16,16,16,16	1
7	ZN	D	410	1/1	1.00	0.01	16,16,16,16	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.