



# Full wwPDB X-ray Structure Validation Report ⓘ

May 18, 2020 – 09:55 pm BST

PDB ID : 4PGP  
Title : CRYSTAL STRUCTURE OF A TRAP PERIPLASMIC SOLUTE BINDING PROTEIN FROM DESULFOVIBRIO ALASKENSIS G20 (Dde\_0634, TARGET EFI-510120) WITH BOUND 3-INDOLE ACETIC ACID  
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Deposited on : 2014-05-02  
Resolution : 2.25 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](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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

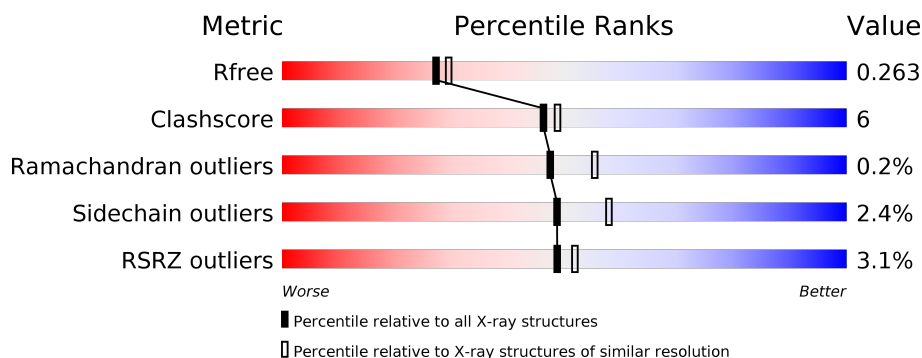
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.25 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))
$R_{free}$	130704	1377 (2.26-2.26)
Clashscore	141614	1487 (2.26-2.26)
Ramachandran outliers	138981	1449 (2.26-2.26)
Sidechain outliers	138945	1450 (2.26-2.26)
RSRZ outliers	127900	1356 (2.26-2.26)

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 on 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	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 11%, green 80%, grey 8%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>80%</span> <span>11%</span> <span>• 8%</span> </div> </div>
1	B	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 15%, green 76%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>%</span> <span>76%</span> <span>15%</span> <span>• 7%</span> </div> </div>
1	C	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 4%, orange 1%, yellow 11%, green 81%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>4%</span> <span>81%</span> <span>11%</span> <span>• 7%</span> </div> </div>
1	D	334	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 6%, orange 1%, yellow 14%, green 78%, grey 7%);"></div> <div style="display: flex; justify-content: space-between; font-size: 0.8em;"> <span>6%</span> <span>78%</span> <span>14%</span> <span>• 7%</span> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 18869 atoms, of which 8931 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 Extracellular solute-binding protein, family 7.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	308	Total	C	H	N	O	S	0	0	0
			4582	1498	2219	412	435	18			
1	B	309	Total	C	H	N	O	S	0	0	0
			4619	1504	2245	413	439	18			
1	C	310	Total	C	H	N	O	S	0	0	0
			4585	1497	2222	407	441	18			
1	D	310	Total	C	H	N	O	S	0	0	0
			4573	1494	2213	407	441	18			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	MET	-	expression tag	UNP Q315G1
A	9	HIS	-	expression tag	UNP Q315G1
A	10	HIS	-	expression tag	UNP Q315G1
A	11	HIS	-	expression tag	UNP Q315G1
A	12	HIS	-	expression tag	UNP Q315G1
A	13	HIS	-	expression tag	UNP Q315G1
A	14	HIS	-	expression tag	UNP Q315G1
A	15	SER	-	expression tag	UNP Q315G1
A	16	SER	-	expression tag	UNP Q315G1
A	17	GLY	-	expression tag	UNP Q315G1
A	18	VAL	-	expression tag	UNP Q315G1
A	19	ASP	-	expression tag	UNP Q315G1
A	20	LEU	-	expression tag	UNP Q315G1
A	21	GLY	-	expression tag	UNP Q315G1
A	22	THR	-	expression tag	UNP Q315G1
A	23	GLU	-	expression tag	UNP Q315G1
A	24	ASN	-	expression tag	UNP Q315G1
A	25	LEU	-	expression tag	UNP Q315G1
A	26	TYR	-	expression tag	UNP Q315G1
A	27	PHE	-	expression tag	UNP Q315G1
A	28	GLN	-	expression tag	UNP Q315G1

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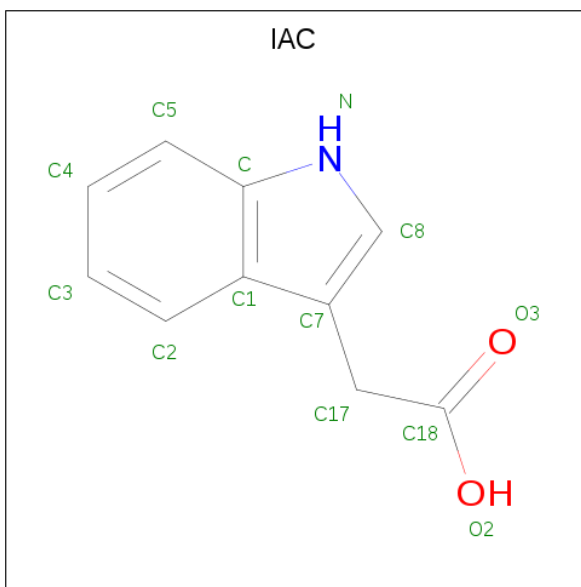
Chain	Residue	Modelled	Actual	Comment	Reference
A	29	SER	-	expression tag	UNP Q315G1
A	30	MET	-	expression tag	UNP Q315G1
B	8	MET	-	expression tag	UNP Q315G1
B	9	HIS	-	expression tag	UNP Q315G1
B	10	HIS	-	expression tag	UNP Q315G1
B	11	HIS	-	expression tag	UNP Q315G1
B	12	HIS	-	expression tag	UNP Q315G1
B	13	HIS	-	expression tag	UNP Q315G1
B	14	HIS	-	expression tag	UNP Q315G1
B	15	SER	-	expression tag	UNP Q315G1
B	16	SER	-	expression tag	UNP Q315G1
B	17	GLY	-	expression tag	UNP Q315G1
B	18	VAL	-	expression tag	UNP Q315G1
B	19	ASP	-	expression tag	UNP Q315G1
B	20	LEU	-	expression tag	UNP Q315G1
B	21	GLY	-	expression tag	UNP Q315G1
B	22	THR	-	expression tag	UNP Q315G1
B	23	GLU	-	expression tag	UNP Q315G1
B	24	ASN	-	expression tag	UNP Q315G1
B	25	LEU	-	expression tag	UNP Q315G1
B	26	TYR	-	expression tag	UNP Q315G1
B	27	PHE	-	expression tag	UNP Q315G1
B	28	GLN	-	expression tag	UNP Q315G1
B	29	SER	-	expression tag	UNP Q315G1
B	30	MET	-	expression tag	UNP Q315G1
C	8	MET	-	expression tag	UNP Q315G1
C	9	HIS	-	expression tag	UNP Q315G1
C	10	HIS	-	expression tag	UNP Q315G1
C	11	HIS	-	expression tag	UNP Q315G1
C	12	HIS	-	expression tag	UNP Q315G1
C	13	HIS	-	expression tag	UNP Q315G1
C	14	HIS	-	expression tag	UNP Q315G1
C	15	SER	-	expression tag	UNP Q315G1
C	16	SER	-	expression tag	UNP Q315G1
C	17	GLY	-	expression tag	UNP Q315G1
C	18	VAL	-	expression tag	UNP Q315G1
C	19	ASP	-	expression tag	UNP Q315G1
C	20	LEU	-	expression tag	UNP Q315G1
C	21	GLY	-	expression tag	UNP Q315G1
C	22	THR	-	expression tag	UNP Q315G1
C	23	GLU	-	expression tag	UNP Q315G1
C	24	ASN	-	expression tag	UNP Q315G1

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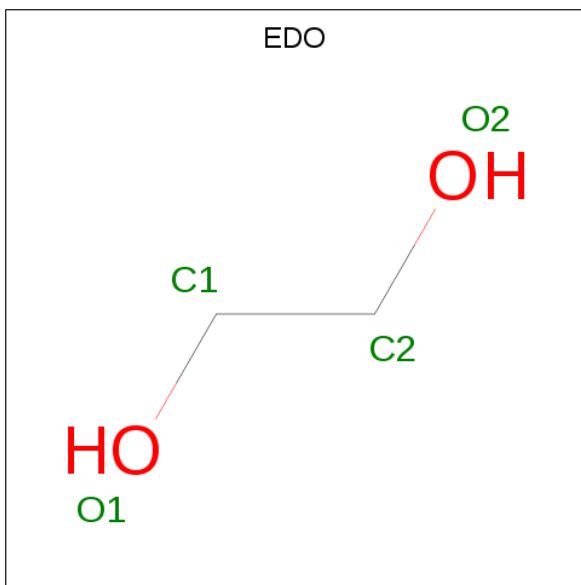
Chain	Residue	Modelled	Actual	Comment	Reference
C	25	LEU	-	expression tag	UNP Q315G1
C	26	TYR	-	expression tag	UNP Q315G1
C	27	PHE	-	expression tag	UNP Q315G1
C	28	GLN	-	expression tag	UNP Q315G1
C	29	SER	-	expression tag	UNP Q315G1
C	30	MET	-	expression tag	UNP Q315G1
D	8	MET	-	expression tag	UNP Q315G1
D	9	HIS	-	expression tag	UNP Q315G1
D	10	HIS	-	expression tag	UNP Q315G1
D	11	HIS	-	expression tag	UNP Q315G1
D	12	HIS	-	expression tag	UNP Q315G1
D	13	HIS	-	expression tag	UNP Q315G1
D	14	HIS	-	expression tag	UNP Q315G1
D	15	SER	-	expression tag	UNP Q315G1
D	16	SER	-	expression tag	UNP Q315G1
D	17	GLY	-	expression tag	UNP Q315G1
D	18	VAL	-	expression tag	UNP Q315G1
D	19	ASP	-	expression tag	UNP Q315G1
D	20	LEU	-	expression tag	UNP Q315G1
D	21	GLY	-	expression tag	UNP Q315G1
D	22	THR	-	expression tag	UNP Q315G1
D	23	GLU	-	expression tag	UNP Q315G1
D	24	ASN	-	expression tag	UNP Q315G1
D	25	LEU	-	expression tag	UNP Q315G1
D	26	TYR	-	expression tag	UNP Q315G1
D	27	PHE	-	expression tag	UNP Q315G1
D	28	GLN	-	expression tag	UNP Q315G1
D	29	SER	-	expression tag	UNP Q315G1
D	30	MET	-	expression tag	UNP Q315G1

- Molecule 2 is 1H-INDOL-3-YLACETIC ACID (three-letter code: IAC) (formula: C<sub>10</sub>H<sub>9</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	0	0
			21	10	8	1	2		
2	B	1	Total	C	H	N	O	0	0
			21	10	8	1	2		
2	C	1	Total	C	H	N	O	0	0
			21	10	8	1	2		
2	D	1	Total	C	H	N	O	0	0
			21	10	8	1	2		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

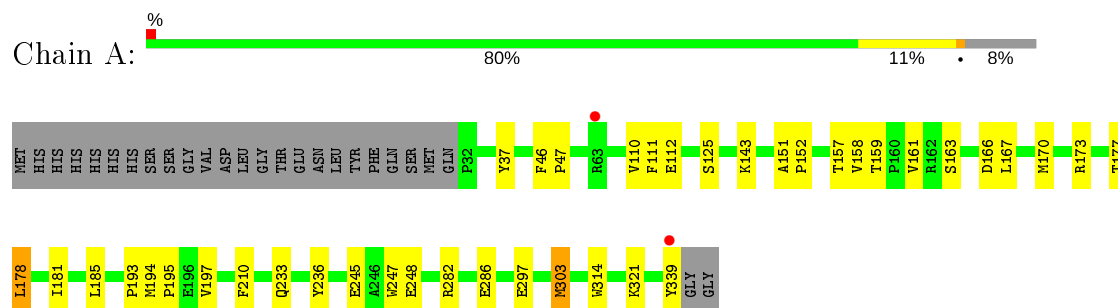
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	105	Total	O	0	0
			105	105		
4	B	103	Total	O	0	0
			103	103		
4	C	94	Total	O	0	0
			94	94		
4	D	120	Total	O	0	0
			120	120		

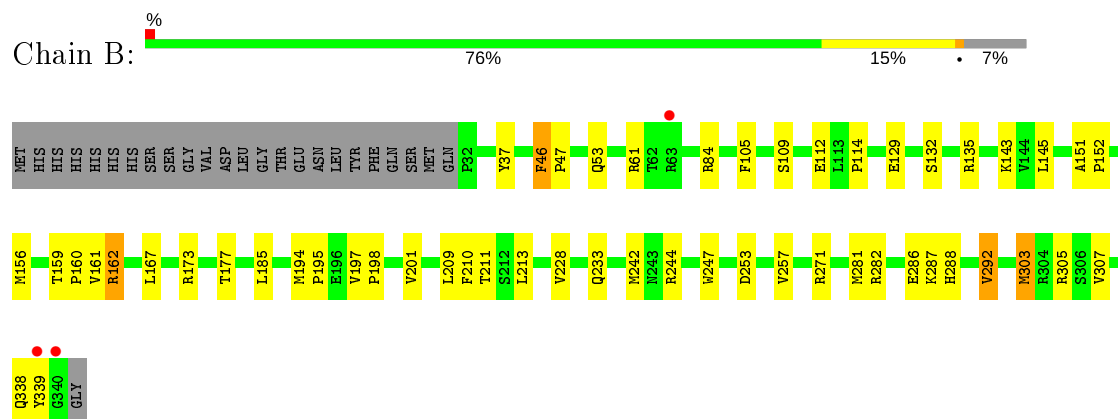
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

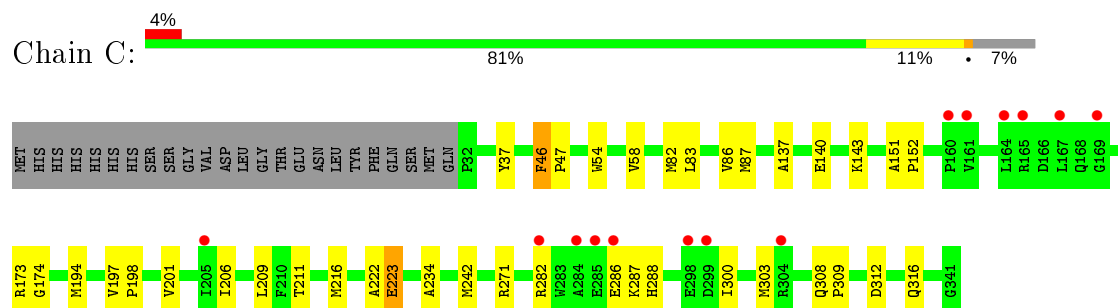
- Molecule 1: Extracellular solute-binding protein, family 7



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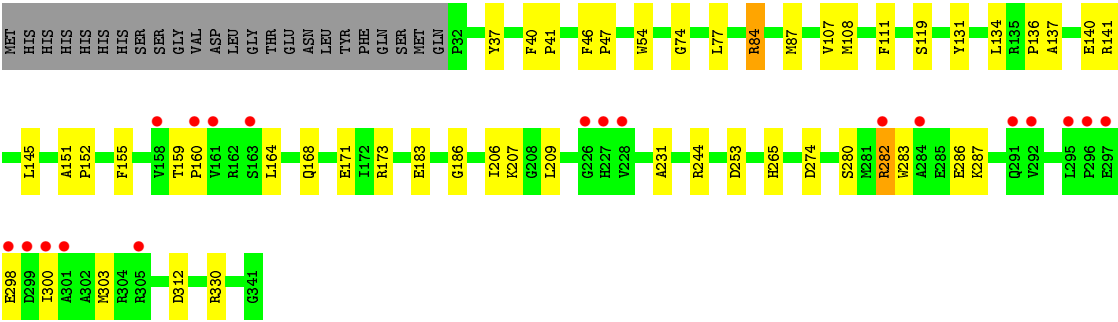
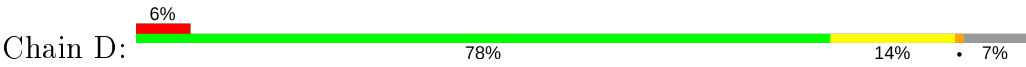


- Molecule 1: Extracellular solute-binding protein, family 7



- Molecule 1: Extracellular solute-binding protein, family 7





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	50.29Å 145.54Å 97.92Å 90.00° 92.19° 90.00°	Depositor
Resolution (Å)	35.74 – 2.25 43.46 – 2.25	Depositor EDS
% Data completeness (in resolution range)	92.3 (35.74-2.25) 92.5 (43.46-2.25)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.63 (at 2.24Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, $R_{free}$	0.202 , 0.262 0.209 , 0.263	Depositor DCC
$R_{free}$ test set	3133 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.7	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.41 , 48.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.53$ , $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	0.039 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	18869	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	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 56.03 % 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 2.9018e-05. 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 ⓘ

### 5.1 Standard geometry ⓘ

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

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	0.69	0/2420	0.71	0/3294
1	B	0.75	0/2431	0.81	5/3307 (0.2%)
1	C	0.60	0/2420	0.68	0/3294
1	D	0.70	0/2417	0.73	1/3290 (0.0%)
All	All	0.69	0/9688	0.74	6/13185 (0.0%)

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	162	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	B	162	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	B	135	ARG	NE-CZ-NH2	-5.83	117.38	120.30
1	B	61	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	D	330	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	303	MET	CA-CB-CG	5.24	122.22	113.30

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	2363	2219	2329	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2374	2245	2343	34	0
1	C	2363	2222	2313	25	0
1	D	2360	2213	2304	31	0
2	A	13	8	8	0	0
2	B	13	8	8	0	0
2	C	13	8	8	0	0
2	D	13	8	8	0	0
3	B	4	0	6	1	0
4	A	105	0	0	2	0
4	B	103	0	0	3	0
4	C	94	0	0	1	0
4	D	120	0	0	3	0
All	All	9938	8931	9327	118	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 6.

All (118) 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:297:GLU:OE2	4:A:551:HOH:O	2.09	0.71
1:B:305:ARG:NH1	4:B:543:HOH:O	2.29	0.66
1:A:321:LYS:O	4:A:578:HOH:O	2.13	0.66
3:B:402:EDO:H22	4:B:548:HOH:O	1.94	0.66
1:D:164:LEU:O	1:D:168:GLN:NE2	2.29	0.65
1:B:84:ARG:HD2	1:C:287:LYS:O	1.97	0.65
1:A:185:LEU:CD2	1:A:303:MET:HB2	2.27	0.64
1:B:287:LYS:O	1:B:288:HIS:CD2	2.51	0.63
1:A:46:PHE:CD2	1:A:47:PRO:HD3	2.35	0.61
1:C:223:GLU:OE2	1:C:288:HIS:NE2	2.35	0.60
1:D:283:TRP:NE1	1:D:287:LYS:HD3	2.17	0.60
1:A:185:LEU:HD22	1:A:303:MET:HB2	1.84	0.59
1:C:83:LEU:O	1:C:87:MET:HG3	2.03	0.59
1:B:145:LEU:HD11	1:B:242:MET:HE2	1.85	0.58
1:D:283:TRP:CD1	1:D:287:LYS:HD3	2.38	0.57
1:B:129:GLU:HG3	1:B:339:TYR:CZ	2.41	0.56
1:B:287:LYS:O	1:B:288:HIS:CG	2.59	0.56
1:B:143:LYS:HE2	1:B:247:TRP:CZ2	2.41	0.55
1:B:271:ARG:NH1	4:B:545:HOH:O	2.38	0.55
1:B:213:LEU:HD13	1:B:281:MET:SD	2.46	0.55
1:C:300:ILE:O	1:C:303:MET:HB3	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:PHE:CD2	1:C:47:PRO:HD3	2.42	0.54
1:B:210:PHE:HZ	1:B:233:GLN:HG3	1.73	0.54
1:D:46:PHE:CD2	1:D:47:PRO:HD3	2.43	0.53
1:D:108:MET:HE1	1:D:134:LEU:HD23	1.91	0.53
1:A:112:GLU:HB3	1:A:177:THR:HB	1.90	0.53
1:D:108:MET:HE2	1:D:136:PRO:HG3	1.90	0.52
1:A:161:VAL:HG11	1:A:167:LEU:HD13	1.90	0.52
1:A:143:LYS:HE2	1:A:247:TRP:CZ2	2.43	0.52
1:C:137:ALA:O	1:C:140:GLU:HG2	2.10	0.52
1:D:84:ARG:HG2	4:D:586:HOH:O	2.10	0.52
1:B:197:VAL:O	1:B:201:VAL:HG23	2.09	0.51
1:B:228:VAL:HG11	1:B:281:MET:HE1	1.92	0.51
1:B:129:GLU:HG3	1:B:339:TYR:OH	2.12	0.50
1:B:129:GLU:HG3	1:B:339:TYR:CE1	2.46	0.50
1:D:171:GLU:HB3	1:D:206:ILE:HA	1.94	0.49
1:A:210:PHE:HZ	1:A:233:GLN:HG3	1.77	0.49
1:B:161:VAL:HG11	1:B:167:LEU:HD13	1.94	0.49
1:B:105:PHE:O	1:B:109:SER:HB3	2.12	0.49
1:B:197:VAL:N	1:B:198:PRO:CD	2.76	0.49
1:D:168:GLN:HA	1:D:186:GLY:O	2.13	0.49
1:A:177:THR:O	1:A:181:ILE:HG13	2.13	0.49
1:A:245:GLU:HA	1:A:248:GLU:HG2	1.94	0.48
1:A:151:ALA:HB1	1:A:152:PRO:CD	2.43	0.48
1:C:82:MET:O	1:C:86:VAL:HG23	2.14	0.48
1:D:173:ARG:C	1:D:173:ARG:HD3	2.33	0.48
1:A:157:THR:HB	1:A:170:MET:HE1	1.96	0.48
1:D:137:ALA:HA	1:D:140:GLU:HG3	1.96	0.47
1:C:308:GLN:HB2	1:C:309:PRO:HD3	1.95	0.47
1:B:84:ARG:CD	1:C:287:LYS:O	2.61	0.47
1:D:87:MET:HE1	1:D:141:ARG:HE	1.79	0.47
1:C:194:MET:HE1	1:C:211:THR:HG21	1.95	0.47
1:B:156:MET:HE1	1:B:211:THR:HG23	1.95	0.47
1:A:143:LYS:HE2	1:A:247:TRP:CH2	2.50	0.47
1:D:74:GLY:HA2	1:D:77:LEU:O	2.15	0.47
1:B:53:GLN:HA	1:B:53:GLN:OE1	2.15	0.46
1:B:194:MET:N	1:B:195:PRO:CD	2.78	0.46
1:C:271:ARG:NH1	4:C:561:HOH:O	2.38	0.46
1:C:54:TRP:O	1:C:58:VAL:HG23	2.16	0.46
1:D:298:GLU:O	1:D:298:GLU:OE2	2.34	0.46
1:B:253:ASP:O	1:B:257:VAL:HG23	2.15	0.46
1:B:282:ARG:O	1:B:286:GLU:HG2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:PRO:HG3	1:B:307:VAL:HG11	1.97	0.45
1:A:178:LEU:N	1:A:178:LEU:HD22	2.31	0.45
1:D:300:ILE:O	1:D:303:MET:HB3	2.17	0.45
1:B:185:LEU:CD2	1:B:303:MET:HG3	2.46	0.45
1:B:151:ALA:HB1	1:B:152:PRO:HD2	1.99	0.45
1:D:119:SER:HB2	1:D:274:ASP:OD2	2.16	0.45
1:D:155:PHE:CE2	1:D:231:ALA:HB2	2.51	0.45
1:C:46:PHE:N	1:C:47:PRO:CD	2.80	0.45
1:D:159:THR:HB	1:D:160:PRO:CD	2.46	0.45
1:B:228:VAL:HB	1:B:292:VAL:HG13	1.98	0.45
1:C:312:ASP:O	1:C:316:GLN:HG2	2.17	0.45
1:A:282:ARG:O	1:A:286:GLU:HG2	2.16	0.45
1:D:40:PHE:CG	1:D:41:PRO:HD3	2.52	0.45
1:D:282:ARG:O	1:D:286:GLU:HG2	2.17	0.44
1:C:173:ARG:HG3	1:C:197:VAL:HG22	1.98	0.44
1:C:151:ALA:HB1	1:C:152:PRO:CD	2.47	0.44
1:B:151:ALA:HB1	1:B:152:PRO:CD	2.48	0.44
1:C:173:ARG:HD2	1:C:174:GLY:O	2.17	0.44
1:A:339:TYR:CD1	1:A:339:TYR:N	2.85	0.43
1:B:173:ARG:HG3	1:B:197:VAL:HG22	1.99	0.43
1:A:193:PRO:HB2	1:A:195:PRO:HD2	2.00	0.43
1:A:173:ARG:C	1:A:173:ARG:HD3	2.39	0.43
1:D:107:VAL:HG12	1:D:108:MET:HE2	2.00	0.43
1:A:151:ALA:HB1	1:A:152:PRO:HD2	2.00	0.43
1:C:201:VAL:HG23	1:C:206:ILE:HD11	2.01	0.43
1:A:173:ARG:HG3	1:A:197:VAL:HG22	1.99	0.43
1:A:125:SER:HB3	1:A:339:TYR:CD2	2.54	0.43
1:A:125:SER:HB3	1:A:339:TYR:HD2	1.83	0.43
1:C:282:ARG:O	1:C:286:GLU:HG2	2.19	0.43
1:C:197:VAL:N	1:C:198:PRO:CD	2.82	0.43
1:D:159:THR:HB	1:D:160:PRO:HD2	2.00	0.42
1:A:158:VAL:HG23	1:A:159:THR:HG23	2.01	0.42
1:A:194:MET:N	1:A:195:PRO:CD	2.82	0.42
1:D:108:MET:CE	1:D:136:PRO:HG3	2.48	0.42
1:D:145:LEU:HD23	1:D:145:LEU:HA	1.80	0.42
1:B:145:LEU:HD21	1:B:242:MET:HE3	2.00	0.42
1:D:183:GLU:OE2	4:D:595:HOH:O	2.22	0.42
1:B:46:PHE:CD2	1:B:47:PRO:HD3	2.55	0.42
1:C:216:MET:HE1	1:C:222:ALA:HA	2.02	0.41
1:D:207:LYS:NZ	4:D:504:HOH:O	2.52	0.41
1:D:244:ARG:HD3	1:D:244:ARG:HA	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:VAL:HG13	1:A:166:ASP:HB2	2.02	0.41
1:A:110:VAL:HB	1:A:314:TRP:CZ2	2.55	0.41
1:C:143:LYS:HB3	1:C:242:MET:HB3	2.02	0.41
1:D:151:ALA:HB1	1:D:152:PRO:CD	2.50	0.41
1:B:173:ARG:HD3	1:B:173:ARG:C	2.41	0.41
1:C:151:ALA:HB1	1:C:152:PRO:HD2	2.02	0.41
1:A:339:TYR:N	1:A:339:TYR:HD1	2.18	0.41
1:C:216:MET:CE	1:C:222:ALA:HA	2.50	0.41
1:B:112:GLU:HB3	1:B:177:THR:HB	2.02	0.41
1:B:159:THR:HB	1:B:160:PRO:HD2	2.02	0.41
1:A:178:LEU:HG	1:A:236:TYR:CZ	2.56	0.41
1:D:131:TYR:C	1:D:131:TYR:CD2	2.95	0.41
1:C:46:PHE:CG	1:C:47:PRO:HD3	2.55	0.41
1:D:54:TRP:HB2	1:D:265:HIS:CE1	2.57	0.40
1:D:151:ALA:HB1	1:D:152:PRO:HD2	2.03	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	306/334 (92%)	299 (98%)	7 (2%)	0	100	100
1	B	307/334 (92%)	296 (96%)	10 (3%)	1 (0%)	41	46
1	C	308/334 (92%)	302 (98%)	5 (2%)	1 (0%)	41	46
1	D	308/334 (92%)	299 (97%)	9 (3%)	0	100	100
All	All	1229/1336 (92%)	1196 (97%)	31 (2%)	2 (0%)	47	55

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	338	GLN
1	C	234	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	247/273 (90%)	242 (98%)	5 (2%)	55	64
1	B	249/273 (91%)	242 (97%)	7 (3%)	43	52
1	C	246/273 (90%)	242 (98%)	4 (2%)	62	73
1	D	245/273 (90%)	237 (97%)	8 (3%)	38	46
All	All	987/1092 (90%)	963 (98%)	24 (2%)	49	58

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

Mol	Chain	Res	Type
1	A	37	TYR
1	A	111	PHE
1	A	163	SER
1	A	178	LEU
1	A	303	MET
1	B	37	TYR
1	B	46	PHE
1	B	132	SER
1	B	162	ARG
1	B	209	LEU
1	B	244	ARG
1	B	292	VAL
1	C	37	TYR
1	C	46	PHE
1	C	209	LEU
1	C	223	GLU
1	D	37	TYR
1	D	84	ARG
1	D	111	PHE
1	D	209	LEU

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Mol	Chain	Res	Type
1	D	253	ASP
1	D	280	SER
1	D	282	ARG
1	D	312	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	HIS
1	B	288	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

5 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	IAC	D	401	-	10,14,14	1.20	0	11,19,19	0.99	1 (9%)
2	IAC	C	401	-	10,14,14	1.13	1 (10%)	11,19,19	0.57	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	B	402	-	3,3,3	1.08	0	2,2,2	0.94	0
2	IAC	B	401	-	10,14,14	1.53	1 (10%)	11,19,19	0.79	0
2	IAC	A	401	-	10,14,14	1.45	1 (10%)	11,19,19	1.28	1 (9%)

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	IAC	D	401	-	-	0/2/4/4	0/2/2/2
2	IAC	C	401	-	-	0/2/4/4	0/2/2/2
3	EDO	B	402	-	-	0/1/1/1	-
2	IAC	B	401	-	-	0/2/4/4	0/2/2/2
2	IAC	A	401	-	-	0/2/4/4	0/2/2/2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	IAC	C5-C	-3.63	1.35	1.41
2	A	401	IAC	C5-C	-3.27	1.36	1.41
2	C	401	IAC	C3-C2	2.06	1.41	1.36

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	IAC	C18-C17-C7	-2.90	107.98	114.71
2	D	401	IAC	C18-C17-C7	-2.32	109.31	114.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	EDO	1	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 ⓘ

### 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, 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	308/334 (92%)	-0.25	2 (0%) 89 89	24, 36, 55, 76	0
1	B	309/334 (92%)	-0.28	3 (0%) 82 84	18, 29, 50, 72	0
1	C	310/334 (92%)	0.16	14 (4%) 33 36	27, 42, 71, 97	0
1	D	310/334 (92%)	0.10	19 (6%) 21 23	19, 33, 60, 82	0
All	All	1237/1336 (92%)	-0.07	38 (3%) 49 52	18, 36, 62, 97	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	169	GLY	3.7
1	C	205	ILE	3.3
1	D	160	PRO	3.3
1	D	227	HIS	3.1
1	D	299	ASP	3.1
1	D	158	VAL	3.0
1	D	297	GLU	3.0
1	D	298	GLU	3.0
1	C	160	PRO	3.0
1	D	305	ARG	2.9
1	C	286	GLU	2.9
1	C	282	ARG	2.8
1	D	300	ILE	2.8
1	C	299	ASP	2.7
1	C	161	VAL	2.7
1	A	63	ARG	2.7
1	D	226	GLY	2.7
1	C	165	ARG	2.6
1	C	164	LEU	2.6
1	C	285	GLU	2.6
1	B	339	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	296	PRO	2.6
1	B	340	GLY	2.5
1	D	163	SER	2.5
1	A	339	TYR	2.5
1	D	282	ARG	2.5
1	D	301	ALA	2.4
1	D	228	VAL	2.4
1	D	295	LEU	2.3
1	D	284	ALA	2.3
1	C	304	ARG	2.2
1	C	298	GLU	2.2
1	B	63	ARG	2.2
1	C	167	LEU	2.2
1	D	161	VAL	2.1
1	D	292	VAL	2.1
1	D	291	GLN	2.1
1	C	284	ALA	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 carbohydrates 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
3	EDO	B	402	4/4	0.91	0.14	20,20,20,20	0
2	IAC	C	401	13/13	0.97	0.11	25,32,37,41	0
2	IAC	D	401	13/13	0.97	0.15	17,25,30,36	0
2	IAC	B	401	13/13	0.97	0.11	14,21,27,32	0
2	IAC	A	401	13/13	0.98	0.10	17,24,29,31	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.