



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 08:07 pm BST

PDB ID : 5HC4  
Title : Structure of esterase Est22  
Authors : Li, J.; Huang, J.  
Deposited on : 2016-01-04  
Resolution : 2.00 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

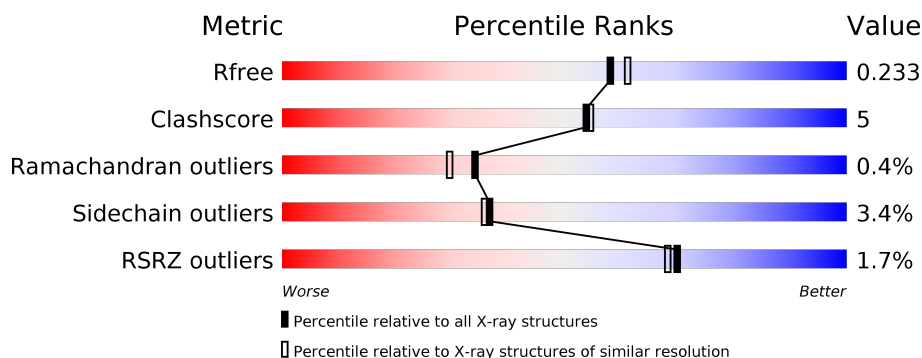
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	365	<div> <div>2%</div> <div>82% 10% 7%</div> </div>
1	B	365	<div> <div>2%</div> <div>82% 11% 7%</div> </div>
1	C	365	<div> <div>2%</div> <div>81% 12% 7%</div> </div>
1	D	365	<div> <div>2%</div> <div>82% 10% 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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	401	-	X	X	-
3	TRS	A	402	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 11334 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 Lipolytic enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	0	0	0
			2549	1596	432	505	16			
1	B	341	Total	C	N	O	S	0	0	0
			2549	1596	432	505	16			
1	C	340	Total	C	N	O	S	0	1	0
			2537	1589	431	501	16			
1	D	342	Total	C	N	O	S	0	0	0
			2553	1599	433	505	16			

There are 84 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP H6BDX1
A	-19	GLY	-	expression tag	UNP H6BDX1
A	-18	SER	-	expression tag	UNP H6BDX1
A	-17	SER	-	expression tag	UNP H6BDX1
A	-16	HIS	-	expression tag	UNP H6BDX1
A	-15	HIS	-	expression tag	UNP H6BDX1
A	-14	HIS	-	expression tag	UNP H6BDX1
A	-13	HIS	-	expression tag	UNP H6BDX1
A	-12	HIS	-	expression tag	UNP H6BDX1
A	-11	HIS	-	expression tag	UNP H6BDX1
A	-10	HIS	-	expression tag	UNP H6BDX1
A	-9	SER	-	expression tag	UNP H6BDX1
A	-8	SER	-	expression tag	UNP H6BDX1
A	-7	GLY	-	expression tag	UNP H6BDX1
A	-6	LEU	-	expression tag	UNP H6BDX1
A	-5	VAL	-	expression tag	UNP H6BDX1
A	-4	PRO	-	expression tag	UNP H6BDX1
A	-3	ARG	-	expression tag	UNP H6BDX1
A	-2	GLY	-	expression tag	UNP H6BDX1
A	-1	SER	-	expression tag	UNP H6BDX1
A	0	HIS	-	expression tag	UNP H6BDX1

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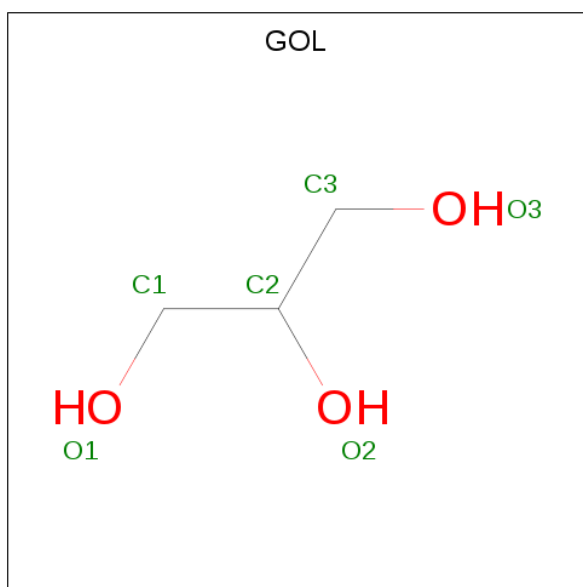
Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	MET	-	expression tag	UNP H6BDX1
B	-19	GLY	-	expression tag	UNP H6BDX1
B	-18	SER	-	expression tag	UNP H6BDX1
B	-17	SER	-	expression tag	UNP H6BDX1
B	-16	HIS	-	expression tag	UNP H6BDX1
B	-15	HIS	-	expression tag	UNP H6BDX1
B	-14	HIS	-	expression tag	UNP H6BDX1
B	-13	HIS	-	expression tag	UNP H6BDX1
B	-12	HIS	-	expression tag	UNP H6BDX1
B	-11	HIS	-	expression tag	UNP H6BDX1
B	-10	HIS	-	expression tag	UNP H6BDX1
B	-9	SER	-	expression tag	UNP H6BDX1
B	-8	SER	-	expression tag	UNP H6BDX1
B	-7	GLY	-	expression tag	UNP H6BDX1
B	-6	LEU	-	expression tag	UNP H6BDX1
B	-5	VAL	-	expression tag	UNP H6BDX1
B	-4	PRO	-	expression tag	UNP H6BDX1
B	-3	ARG	-	expression tag	UNP H6BDX1
B	-2	GLY	-	expression tag	UNP H6BDX1
B	-1	SER	-	expression tag	UNP H6BDX1
B	0	HIS	-	expression tag	UNP H6BDX1
C	-20	MET	-	expression tag	UNP H6BDX1
C	-19	GLY	-	expression tag	UNP H6BDX1
C	-18	SER	-	expression tag	UNP H6BDX1
C	-17	SER	-	expression tag	UNP H6BDX1
C	-16	HIS	-	expression tag	UNP H6BDX1
C	-15	HIS	-	expression tag	UNP H6BDX1
C	-14	HIS	-	expression tag	UNP H6BDX1
C	-13	HIS	-	expression tag	UNP H6BDX1
C	-12	HIS	-	expression tag	UNP H6BDX1
C	-11	HIS	-	expression tag	UNP H6BDX1
C	-10	HIS	-	expression tag	UNP H6BDX1
C	-9	SER	-	expression tag	UNP H6BDX1
C	-8	SER	-	expression tag	UNP H6BDX1
C	-7	GLY	-	expression tag	UNP H6BDX1
C	-6	LEU	-	expression tag	UNP H6BDX1
C	-5	VAL	-	expression tag	UNP H6BDX1
C	-4	PRO	-	expression tag	UNP H6BDX1
C	-3	ARG	-	expression tag	UNP H6BDX1
C	-2	GLY	-	expression tag	UNP H6BDX1
C	-1	SER	-	expression tag	UNP H6BDX1
C	0	HIS	-	expression tag	UNP H6BDX1

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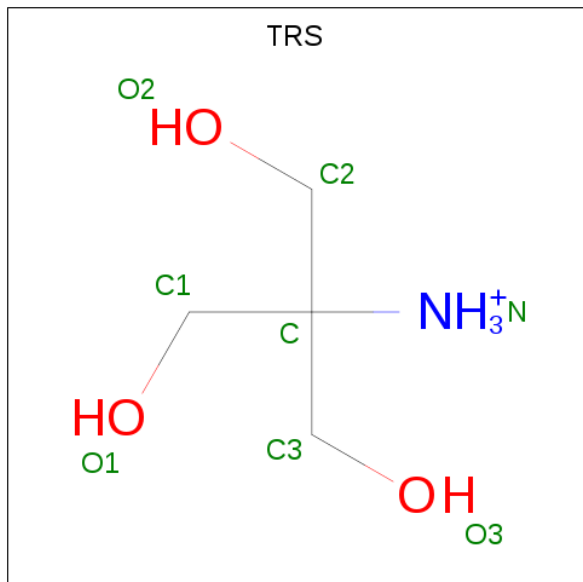
Chain	Residue	Modelled	Actual	Comment	Reference
D	-20	MET	-	expression tag	UNP H6BDX1
D	-19	GLY	-	expression tag	UNP H6BDX1
D	-18	SER	-	expression tag	UNP H6BDX1
D	-17	SER	-	expression tag	UNP H6BDX1
D	-16	HIS	-	expression tag	UNP H6BDX1
D	-15	HIS	-	expression tag	UNP H6BDX1
D	-14	HIS	-	expression tag	UNP H6BDX1
D	-13	HIS	-	expression tag	UNP H6BDX1
D	-12	HIS	-	expression tag	UNP H6BDX1
D	-11	HIS	-	expression tag	UNP H6BDX1
D	-10	HIS	-	expression tag	UNP H6BDX1
D	-9	SER	-	expression tag	UNP H6BDX1
D	-8	SER	-	expression tag	UNP H6BDX1
D	-7	GLY	-	expression tag	UNP H6BDX1
D	-6	LEU	-	expression tag	UNP H6BDX1
D	-5	VAL	-	expression tag	UNP H6BDX1
D	-4	PRO	-	expression tag	UNP H6BDX1
D	-3	ARG	-	expression tag	UNP H6BDX1
D	-2	GLY	-	expression tag	UNP H6BDX1
D	-1	SER	-	expression tag	UNP H6BDX1
D	0	HIS	-	expression tag	UNP H6BDX1

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



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


- Molecule 4 is water.

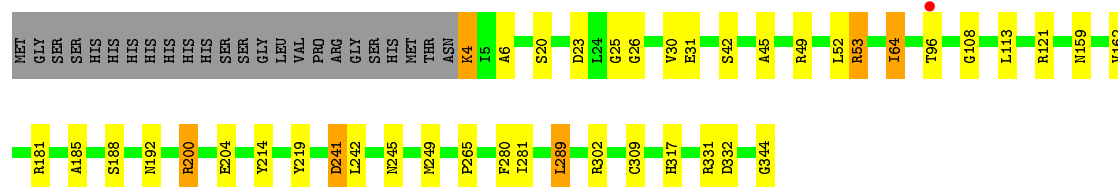
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	322	Total	O	0	0
			322	322		
4	B	264	Total	O	0	1
			265	265		
4	C	282	Total	O	0	0
			282	282		
4	D	263	Total	O	0	0
			263	263		

### 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.

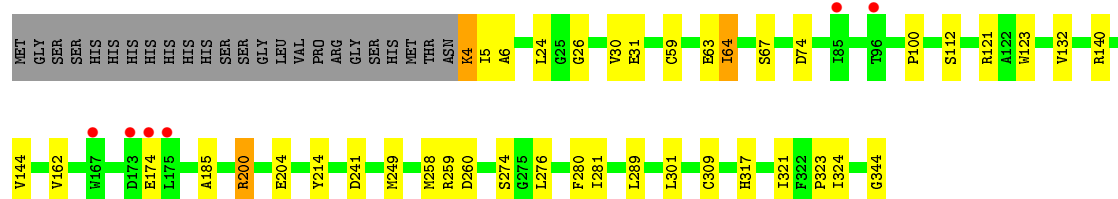
- Molecule 1: Lipolytic enzyme

Chain A: 




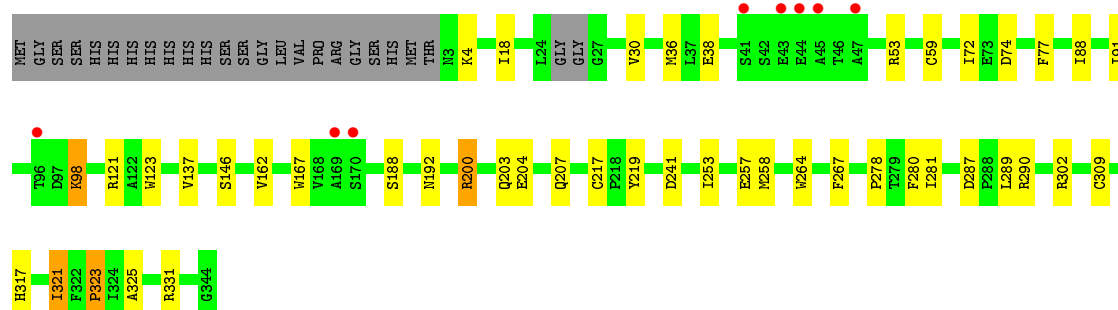
- Molecule 1: Lipolytic enzyme

Chain B: 




- Molecule 1: Lipolytic enzyme

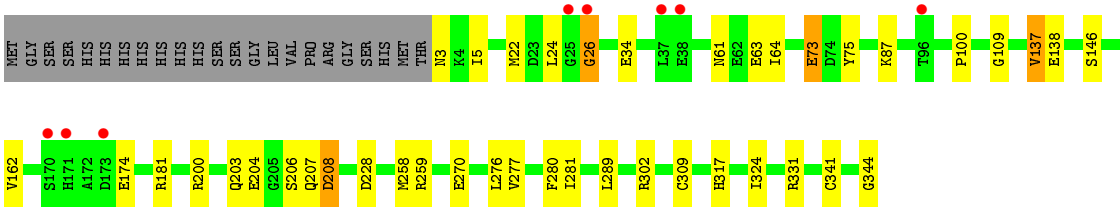
Chain C: 



- Molecule 1: Lipolytic enzyme

Chain D: 





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	81.24Å 121.81Å 150.52Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 40.91 – 2.00	Depositor EDS
% Data completeness (in resolution range)	94.7 (50.00-2.00) 94.7 (40.91-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.25 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.8.0131	Depositor
R, $R_{free}$	0.174 , 0.233 0.174 , 0.233	Depositor DCC
$R_{free}$ test set	4786 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.4	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 49.5	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	0.96	EDS
Total number of atoms	11334	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: GOL, TRS

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	1.00	0/2601	0.97	8/3532 (0.2%)
1	B	0.96	0/2601	0.94	6/3532 (0.2%)
1	C	0.91	0/2591	0.94	7/3520 (0.2%)
1	D	0.96	0/2605	0.98	5/3538 (0.1%)
All	All	0.96	0/10398	0.96	26/14122 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	D	137	VAL	CB-CA-C	-8.00	96.20	111.40
1	A	181	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	D	181	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	D	26	GLY	N-CA-C	-6.97	95.68	113.10
1	C	200	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	D	228	ASP	CB-CG-OD1	6.86	124.48	118.30
1	C	290	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	C	241	ASP	CB-CG-OD1	6.41	124.07	118.30
1	C	200	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	241	ASP	CB-CG-OD1	6.04	123.73	118.30
1	B	140	ARG	NE-CZ-NH2	-5.93	117.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	200	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	181	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	D	259	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	A	241	ASP	CB-CG-OD1	5.68	123.41	118.30
1	B	260	ASP	CB-CG-OD2	-5.63	113.23	118.30
1	A	302	ARG	NE-CZ-NH1	-5.62	117.49	120.30
1	B	260	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	332	ASP	CB-CG-OD1	5.57	123.32	118.30
1	B	200	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	C	287	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	289	LEU	CB-CG-CD1	-5.11	102.31	111.00
1	C	331	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	302	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	121	ARG	NE-CZ-NH2	-5.01	117.79	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	26	GLY	Peptide

## 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	2549	0	2463	36	0
1	B	2549	0	2463	21	0
1	C	2537	0	2438	23	0
1	D	2553	0	2462	28	1
2	A	6	0	8	5	0
3	A	8	0	12	6	0
4	A	322	0	0	13	1
4	B	265	0	0	3	0
4	C	282	0	0	6	0
4	D	263	0	0	10	0
All	All	11334	0	9846	106	1

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.

All (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:C:258:MET:SD	4:C:601:HOH:O	2.08	1.09
1:A:108:GLY:H	3:A:402:TRS:H12	1.03	1.08
1:A:4:LYS:HB3	4:A:696:HOH:O	1.63	0.97
1:A:108:GLY:N	3:A:402:TRS:H12	1.79	0.96
1:B:6:ALA:HA	4:B:538:HOH:O	1.64	0.95
1:A:113:LEU:HD23	2:A:401:GOL:H12	1.49	0.94
1:A:108:GLY:H	3:A:402:TRS:C1	1.87	0.87
1:A:121:ARG:NH1	4:A:501:HOH:O	2.13	0.82
1:B:63:GLU:HG3	4:B:591:HOH:O	1.82	0.79
1:D:61:ASN:HD21	1:D:63:GLU:HB2	1.51	0.76
1:C:200:ARG:HD2	1:C:204:GLU:OE2	1.86	0.75
1:C:30:VAL:HG11	1:C:36:MET:HG3	1.72	0.71
1:D:61:ASN:HD22	1:D:64:ILE:H	1.39	0.69
3:A:402:TRS:H22	4:A:660:HOH:O	1.92	0.69
1:D:204:GLU:OE1	4:D:402:HOH:O	2.11	0.69
1:A:49:ARG:HD2	2:A:401:GOL:H2	1.76	0.68
1:D:109:GLY:O	4:D:403:HOH:O	2.12	0.68
1:A:331:ARG:HH21	1:B:344:GLY:C	1.96	0.68
1:D:331:ARG:NH1	4:D:401:HOH:O	1.94	0.66
1:D:270:GLU:OE2	1:D:302:ARG:NH1	2.28	0.65
1:B:112:SER:HB3	1:B:144:VAL:HG22	1.77	0.65
1:D:200:ARG:HD2	1:D:204:GLU:OE2	1.97	0.65
1:D:344:GLY:C	4:D:522:HOH:O	2.36	0.65
1:D:289:LEU:HD12	1:D:317:HIS:CE1	2.31	0.63
1:B:200:ARG:HD2	1:B:204:GLU:OE2	1.98	0.63
1:C:123:TRP:CD1	1:C:321:ILE:HD11	2.33	0.63
1:D:162:VAL:HG21	1:D:200:ARG:HG2	1.83	0.61
1:A:64:ILE:HG12	4:A:741:HOH:O	2.01	0.61
1:D:64:ILE:HG13	1:D:324:ILE:HD12	1.83	0.61
1:A:204:GLU:OE1	4:A:502:HOH:O	2.16	0.60
1:A:4:LYS:CB	4:A:696:HOH:O	2.36	0.59
1:A:53:ARG:NH1	4:A:503:HOH:O	2.35	0.59
1:A:4:LYS:HG2	4:A:696:HOH:O	2.03	0.58
1:A:281:ILE:O	1:A:309:CYS:HA	2.03	0.58
1:D:207:GLN:HE22	1:D:276:LEU:HA	1.68	0.57
1:A:25:GLY:HA3	1:A:241:ASP:H	1.69	0.56
1:C:72:ILE:HG13	1:C:91:ILE:HG12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:ARG:HD2	1:A:204:GLU:OE2	2.06	0.56
1:B:112:SER:HB3	1:B:144:VAL:CG2	2.34	0.56
1:D:22:MET:CE	1:D:24:LEU:HD11	2.36	0.56
1:A:42:SER:HB2	1:A:45:ALA:H	1.70	0.56
1:B:289:LEU:HD12	1:B:317:HIS:CE1	2.42	0.55
1:D:207:GLN:NE2	1:D:277:VAL:H	2.05	0.55
1:A:52:LEU:HD23	2:A:401:GOL:H31	1.89	0.54
1:A:30:VAL:HG23	1:A:249:MET:HG2	1.88	0.54
1:C:98:LYS:HD2	4:C:597:HOH:O	2.08	0.53
1:C:162:VAL:HG21	1:C:200:ARG:HG2	1.90	0.53
1:A:162:VAL:HG21	1:A:200:ARG:HG2	1.90	0.53
1:A:289:LEU:HD12	1:A:317:HIS:CE1	2.44	0.53
1:C:204:GLU:OE1	4:C:401:HOH:O	2.18	0.52
1:C:289:LEU:HD12	1:C:317:HIS:CE1	2.45	0.52
1:D:281:ILE:O	1:D:309:CYS:HA	2.10	0.52
1:C:123:TRP:NE1	1:C:321:ILE:HD11	2.25	0.52
1:A:4:LYS:CG	4:A:696:HOH:O	2.58	0.52
1:D:61:ASN:ND2	1:D:63:GLU:H	2.09	0.51
1:C:121:ARG:NH1	4:C:407:HOH:O	2.43	0.51
1:A:188:SER:HB3	3:A:402:TRS:H11	1.92	0.51
1:D:26:GLY:HA2	4:D:585:HOH:O	2.10	0.51
1:A:159:ASN:OD1	1:A:200:ARG:NH2	2.43	0.51
1:A:113:LEU:HD23	2:A:401:GOL:C1	2.33	0.50
1:A:4:LYS:HG3	4:A:731:HOH:O	2.12	0.50
1:D:138:GLU:OE1	1:D:146:SER:HB2	2.12	0.50
1:C:4:LYS:CB	4:C:618:HOH:O	2.61	0.49
1:D:302:ARG:NE	4:D:404:HOH:O	2.31	0.49
1:D:302:ARG:NH2	4:D:404:HOH:O	2.29	0.49
1:A:49:ARG:HA	2:A:401:GOL:H32	1.94	0.48
1:A:331:ARG:NE	1:B:344:GLY:O	2.44	0.48
1:C:30:VAL:HG11	1:C:36:MET:CG	2.40	0.48
1:B:162:VAL:HG21	1:B:200:ARG:HG2	1.97	0.47
1:C:59:CYS:HB3	1:C:323:PRO:HD2	1.96	0.47
1:B:4:LYS:HD2	4:B:621:HOH:O	2.15	0.46
1:C:203:GLN:NE2	4:C:411:HOH:O	2.48	0.46
1:B:4:LYS:HE3	1:B:5:ILE:HB	1.97	0.46
1:D:331:ARG:NH2	4:D:401:HOH:O	2.48	0.46
1:C:192:ASN:HB2	1:C:219:TYR:O	2.16	0.46
1:A:108:GLY:CA	3:A:402:TRS:H12	2.45	0.45
1:D:3:ASN:N	4:D:415:HOH:O	2.47	0.45
1:D:73:GLU:HG3	1:D:75:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ILE:O	1:C:309:CYS:HA	2.16	0.45
1:A:6:ALA:HB2	1:A:20:SER:HB3	1.99	0.45
1:A:185:ALA:HA	1:A:214:TYR:O	2.17	0.45
1:C:77:PHE:HB2	1:C:167:TRP:CD1	2.52	0.44
1:B:185:ALA:HA	1:B:214:TYR:O	2.18	0.44
1:D:87:LYS:HB2	1:D:138:GLU:HB3	1.99	0.44
1:A:242:LEU:HB2	4:A:670:HOH:O	2.18	0.44
1:D:258:MET:HE2	4:D:597:HOH:O	2.17	0.44
1:B:123:TRP:CD1	1:B:321:ILE:HG22	2.52	0.43
1:C:188:SER:HA	1:C:217:CYS:O	2.18	0.43
1:B:64:ILE:HG12	1:B:324:ILE:HD12	1.99	0.43
4:A:536:HOH:O	1:B:301:LEU:HD12	2.19	0.43
1:D:100:PRO:HB2	1:D:341:CYS:SG	2.58	0.43
1:D:22:MET:HE3	1:D:24:LEU:HD11	2.01	0.42
1:B:281:ILE:O	1:B:309:CYS:HA	2.19	0.42
1:D:22:MET:HE2	1:D:24:LEU:HD11	2.00	0.42
1:A:192:ASN:HB2	1:A:219:TYR:O	2.19	0.42
1:B:59:CYS:HB3	1:B:323:PRO:HD2	2.01	0.42
1:B:30:VAL:HG23	1:B:249:MET:HG2	2.01	0.42
1:A:245:ASN:O	1:A:249:MET:HB2	2.20	0.42
1:B:100:PRO:HG2	1:B:132:VAL:HG12	2.01	0.41
1:C:264:TRP:HB2	1:C:267:PHE:CD2	2.55	0.41
1:C:18:ILE:HD12	1:C:325:ALA:HA	2.01	0.41
1:B:4:LYS:HD3	1:B:6:ALA:H	1.85	0.41
1:A:344:GLY:C	4:A:713:HOH:O	2.59	0.41
1:C:88:ILE:HD13	1:C:137:VAL:HA	2.03	0.41
1:C:253:ILE:O	1:C:257:GLU:HG3	2.21	0.41
1:A:331:ARG:NH2	1:B:344:GLY:C	2.69	0.40

All (1) 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:258:MET:SD	4:A:747:HOH:O[3_545]	2.08	0.12

## 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	339/365 (93%)	319 (94%)	19 (6%)	1 (0%)	41	37
1	B	339/365 (93%)	323 (95%)	15 (4%)	1 (0%)	41	37
1	C	337/365 (92%)	322 (96%)	14 (4%)	1 (0%)	41	37
1	D	340/365 (93%)	320 (94%)	18 (5%)	2 (1%)	25	19
All	All	1355/1460 (93%)	1284 (95%)	66 (5%)	5 (0%)	34	30

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	5	ILE
1	D	208	ASP
1	A	26	GLY
1	B	24	LEU
1	C	146	SER

### 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	266/288 (92%)	258 (97%)	8 (3%)	41	41
1	B	266/288 (92%)	255 (96%)	11 (4%)	30	28
1	C	263/288 (91%)	254 (97%)	9 (3%)	37	36
1	D	265/288 (92%)	257 (97%)	8 (3%)	41	41
All	All	1060/1152 (92%)	1024 (97%)	36 (3%)	37	36



All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LYS
1	A	23	ASP
1	A	31	GLU
1	A	53	ARG
1	A	64	ILE
1	A	96	THR
1	A	265	PRO
1	A	280	PHE
1	B	4	LYS
1	B	31	GLU
1	B	64	ILE
1	B	67	SER
1	B	74	ASP
1	B	174	GLU
1	B	258	MET
1	B	259	ARG
1	B	274	SER
1	B	276	LEU
1	B	280	PHE
1	C	38	GLU
1	C	53	ARG
1	C	74	ASP
1	C	98	LYS
1	C	207	GLN
1	C	278	PRO
1	C	280	PHE
1	C	321	ILE
1	C	323	PRO
1	D	34	GLU
1	D	73	GLU
1	D	137	VAL
1	D	174	GLU
1	D	203	GLN
1	D	206	SER
1	D	208	ASP
1	D	280	PHE

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

Mol	Chain	Res	Type
1	C	89	GLN

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Mol	Chain	Res	Type
1	D	61	ASN
1	D	207	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 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	$\# Z  > 2$
3	TRS	A	402	-	7,7,7	0.64	0	9,9,9	1.65	2 (22%)
2	GOL	A	401	-	5,5,5	1.36	1 (20%)	5,5,5	1.78	2 (40%)

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	TRS	A	402	-	-	3/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	A	401	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	GOL	O2-C2	2.34	1.50	1.43

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402	TRS	C3-C-C2	2.78	119.42	110.81
2	A	401	GOL	O1-C1-C2	2.56	122.49	110.20
2	A	401	GOL	O2-C2-C1	2.24	119.01	109.12
3	A	402	TRS	C2-C-N	-2.23	101.31	107.98

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	402	TRS	C2-C-C1-O1
3	A	402	TRS	C3-C-C1-O1
3	A	402	TRS	N-C-C1-O1
2	A	401	GOL	O1-C1-C2-C3
2	A	401	GOL	O1-C1-C2-O2
2	A	401	GOL	C1-C2-C3-O3

There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402	TRS	6	0
2	A	401	GOL	5	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, 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	341/365 (93%)	-0.38	1 (0%) 94 93	16, 25, 50, 86	0
1	B	341/365 (93%)	-0.21	6 (1%) 68 66	18, 30, 56, 95	0
1	C	340/365 (93%)	-0.24	8 (2%) 59 57	18, 32, 58, 91	0
1	D	342/365 (93%)	-0.28	8 (2%) 60 59	19, 29, 57, 78	0
All	All	1364/1460 (93%)	-0.28	23 (1%) 70 68	16, 29, 57, 95	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	96	THR	4.1
1	C	41	SER	3.8
1	D	25	GLY	3.5
1	C	169	ALA	3.3
1	B	96	THR	3.3
1	B	175	LEU	3.2
1	D	26	GLY	3.2
1	A	96	THR	3.1
1	B	167	TRP	2.9
1	C	96	THR	2.9
1	C	47	ALA	2.9
1	C	43	GLU	2.7
1	B	174	GLU	2.6
1	C	170	SER	2.6
1	D	173	ASP	2.5
1	D	170	SER	2.4
1	C	44	GLU	2.4
1	D	38	GLU	2.3
1	C	45	ALA	2.2
1	D	171	HIS	2.2
1	B	85	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	37	LEU	2.1
1	B	173	ASP	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates 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, 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( $\text{\AA}^2$ )	Q<0.9
3	TRS	A	402	8/8	0.76	0.28	37,63,68,69	0
2	GOL	A	401	6/6	0.86	0.33	27,41,51,53	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.