



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:51 PM UTC

PDB ID : 4E4F / pdb\_00004e4f  
Title : Crystal structure of enolase PC1\_0802 (TARGET EFI-502240) from *Pectobacterium carotovorum* subsp. *carotovorum* PC1  
Authors : Patskovsky, Y.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Gerlt, J.A.; Almo, S.C.; Enzyme Function Initiative (EFI)  
Deposited on : 2012-03-12  
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.

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 Phenix2.0  
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

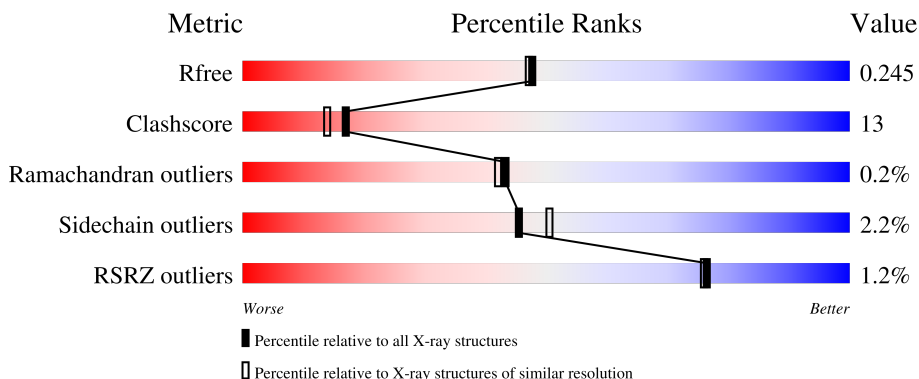
# 1 Overall quality at a glance

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))
$R_{free}$	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (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 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	426	 2% 73% 16% • 9%
1	B	426	 % 67% 21% • 11%
1	C	426	 66% 23% • 11%
1	D	426	 2% 67% 22% • 9%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	FMT	C	505	-	-	X	-

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 13154 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 MANNONATE DEHYDRATASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	386	3092	1980	524	569	19	0	1	0
1	B	381	3069	1966	521	563	19	0	3	0
1	C	381	3060	1960	519	562	19	0	1	0
1	D	388	3112	1994	527	572	19	0	1	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	expression tag	UNP C6D9S0
A	-20	HIS	-	expression tag	UNP C6D9S0
A	-19	HIS	-	expression tag	UNP C6D9S0
A	-18	HIS	-	expression tag	UNP C6D9S0
A	-17	HIS	-	expression tag	UNP C6D9S0
A	-16	HIS	-	expression tag	UNP C6D9S0
A	-15	HIS	-	expression tag	UNP C6D9S0
A	-14	SER	-	expression tag	UNP C6D9S0
A	-13	SER	-	expression tag	UNP C6D9S0
A	-12	GLY	-	expression tag	UNP C6D9S0
A	-11	VAL	-	expression tag	UNP C6D9S0
A	-10	ASP	-	expression tag	UNP C6D9S0
A	-9	LEU	-	expression tag	UNP C6D9S0
A	-8	GLY	-	expression tag	UNP C6D9S0
A	-7	THR	-	expression tag	UNP C6D9S0
A	-6	GLU	-	expression tag	UNP C6D9S0
A	-5	ASN	-	expression tag	UNP C6D9S0
A	-4	LEU	-	expression tag	UNP C6D9S0
A	-3	TYR	-	expression tag	UNP C6D9S0
A	-2	PHE	-	expression tag	UNP C6D9S0
A	-1	GLN	-	expression tag	UNP C6D9S0

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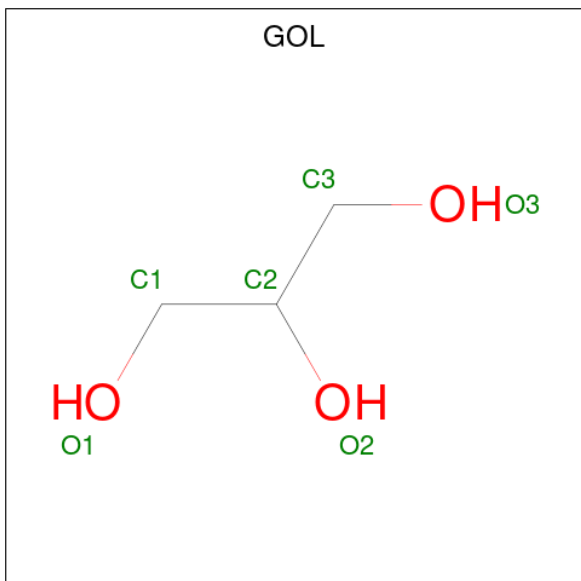
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	expression tag	UNP C6D9S0
B	-21	MET	-	expression tag	UNP C6D9S0
B	-20	HIS	-	expression tag	UNP C6D9S0
B	-19	HIS	-	expression tag	UNP C6D9S0
B	-18	HIS	-	expression tag	UNP C6D9S0
B	-17	HIS	-	expression tag	UNP C6D9S0
B	-16	HIS	-	expression tag	UNP C6D9S0
B	-15	HIS	-	expression tag	UNP C6D9S0
B	-14	SER	-	expression tag	UNP C6D9S0
B	-13	SER	-	expression tag	UNP C6D9S0
B	-12	GLY	-	expression tag	UNP C6D9S0
B	-11	VAL	-	expression tag	UNP C6D9S0
B	-10	ASP	-	expression tag	UNP C6D9S0
B	-9	LEU	-	expression tag	UNP C6D9S0
B	-8	GLY	-	expression tag	UNP C6D9S0
B	-7	THR	-	expression tag	UNP C6D9S0
B	-6	GLU	-	expression tag	UNP C6D9S0
B	-5	ASN	-	expression tag	UNP C6D9S0
B	-4	LEU	-	expression tag	UNP C6D9S0
B	-3	TYR	-	expression tag	UNP C6D9S0
B	-2	PHE	-	expression tag	UNP C6D9S0
B	-1	GLN	-	expression tag	UNP C6D9S0
B	0	SER	-	expression tag	UNP C6D9S0
C	-21	MET	-	expression tag	UNP C6D9S0
C	-20	HIS	-	expression tag	UNP C6D9S0
C	-19	HIS	-	expression tag	UNP C6D9S0
C	-18	HIS	-	expression tag	UNP C6D9S0
C	-17	HIS	-	expression tag	UNP C6D9S0
C	-16	HIS	-	expression tag	UNP C6D9S0
C	-15	HIS	-	expression tag	UNP C6D9S0
C	-14	SER	-	expression tag	UNP C6D9S0
C	-13	SER	-	expression tag	UNP C6D9S0
C	-12	GLY	-	expression tag	UNP C6D9S0
C	-11	VAL	-	expression tag	UNP C6D9S0
C	-10	ASP	-	expression tag	UNP C6D9S0
C	-9	LEU	-	expression tag	UNP C6D9S0
C	-8	GLY	-	expression tag	UNP C6D9S0
C	-7	THR	-	expression tag	UNP C6D9S0
C	-6	GLU	-	expression tag	UNP C6D9S0
C	-5	ASN	-	expression tag	UNP C6D9S0
C	-4	LEU	-	expression tag	UNP C6D9S0
C	-3	TYR	-	expression tag	UNP C6D9S0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PHE	-	expression tag	UNP C6D9S0
C	-1	GLN	-	expression tag	UNP C6D9S0
C	0	SER	-	expression tag	UNP C6D9S0
D	-21	MET	-	expression tag	UNP C6D9S0
D	-20	HIS	-	expression tag	UNP C6D9S0
D	-19	HIS	-	expression tag	UNP C6D9S0
D	-18	HIS	-	expression tag	UNP C6D9S0
D	-17	HIS	-	expression tag	UNP C6D9S0
D	-16	HIS	-	expression tag	UNP C6D9S0
D	-15	HIS	-	expression tag	UNP C6D9S0
D	-14	SER	-	expression tag	UNP C6D9S0
D	-13	SER	-	expression tag	UNP C6D9S0
D	-12	GLY	-	expression tag	UNP C6D9S0
D	-11	VAL	-	expression tag	UNP C6D9S0
D	-10	ASP	-	expression tag	UNP C6D9S0
D	-9	LEU	-	expression tag	UNP C6D9S0
D	-8	GLY	-	expression tag	UNP C6D9S0
D	-7	THR	-	expression tag	UNP C6D9S0
D	-6	GLU	-	expression tag	UNP C6D9S0
D	-5	ASN	-	expression tag	UNP C6D9S0
D	-4	LEU	-	expression tag	UNP C6D9S0
D	-3	TYR	-	expression tag	UNP C6D9S0
D	-2	PHE	-	expression tag	UNP C6D9S0
D	-1	GLN	-	expression tag	UNP C6D9S0
D	0	SER	-	expression tag	UNP C6D9S0

- Molecule 2 is GLYCEROL (CCD ID: GOL) (formula:  $C_3H_8O_3$ ).



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

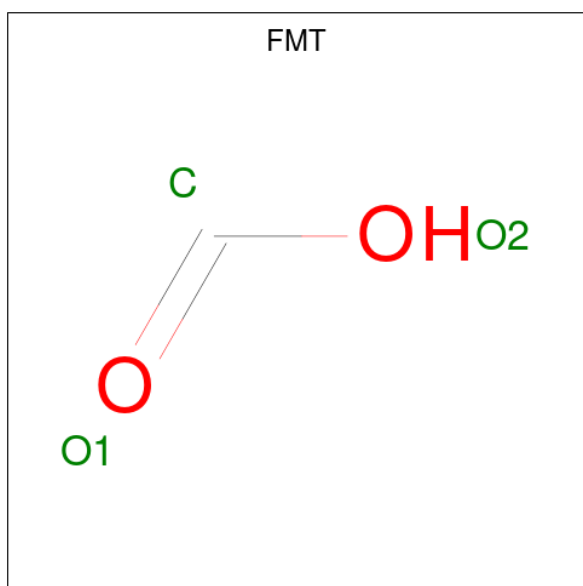
- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total Mg 1 1	0	0
4	B	1	Total Mg 1 1	0	0
4	C	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

- Molecule 5 is FORMIC ACID (CCD ID: FMT) (formula: CH<sub>2</sub>O<sub>2</sub>).



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

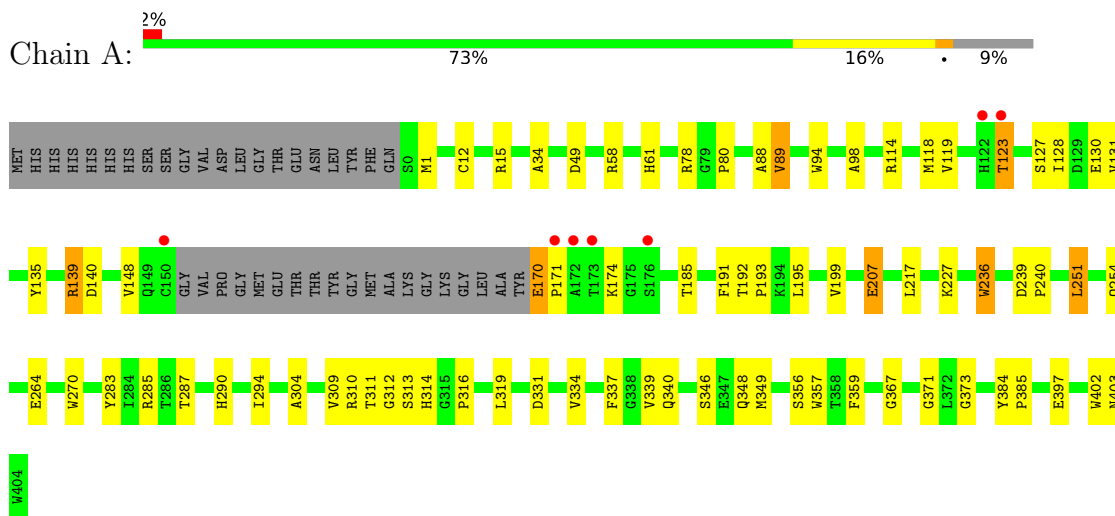
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	208	Total O 208 208	0	0
6	B	188	Total O 189 189	0	1
6	C	173	Total O 173 173	0	0
6	D	161	Total O 161 161	0	0

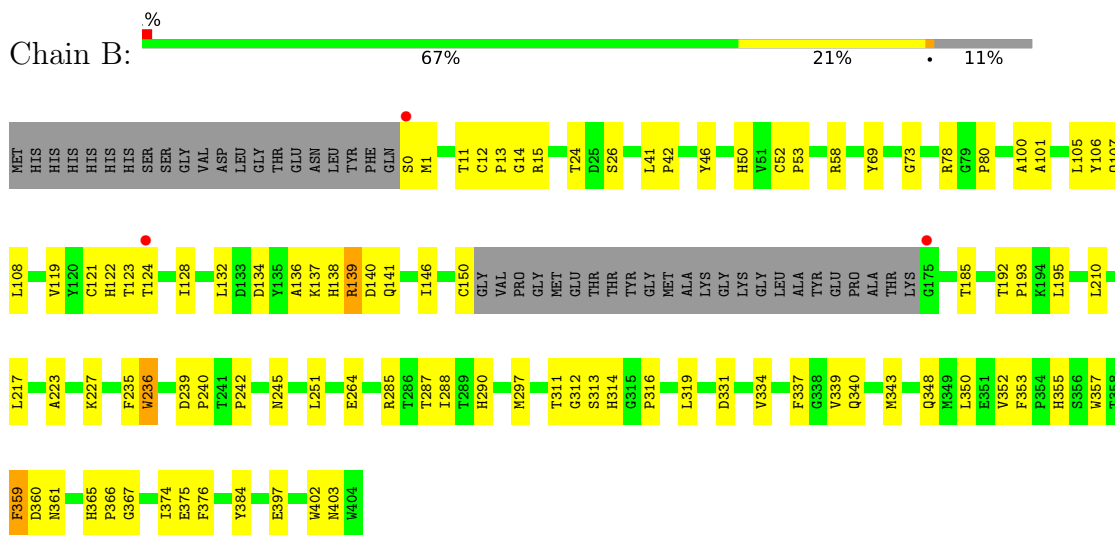
### 3 Residue-property plots [i](#)

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: MANNONATE DEHYDRATASE

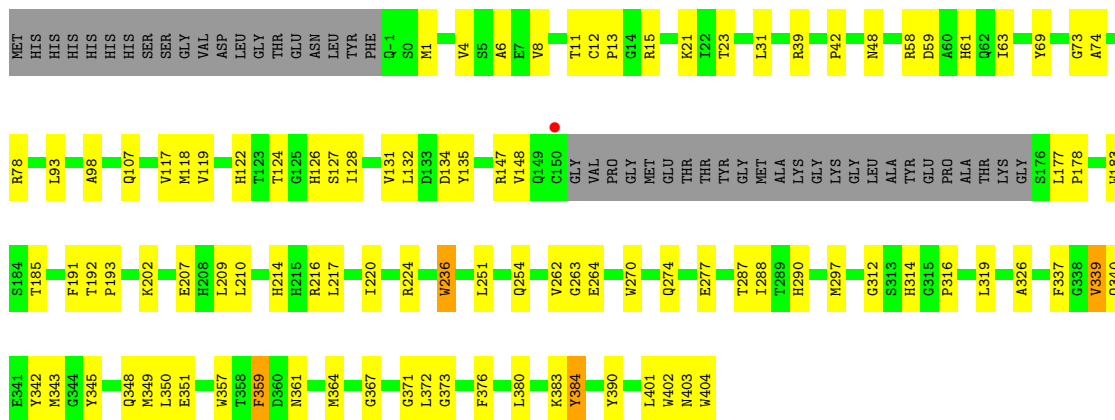


#### • Molecule 1: MANNONATE DEHYDRATASE

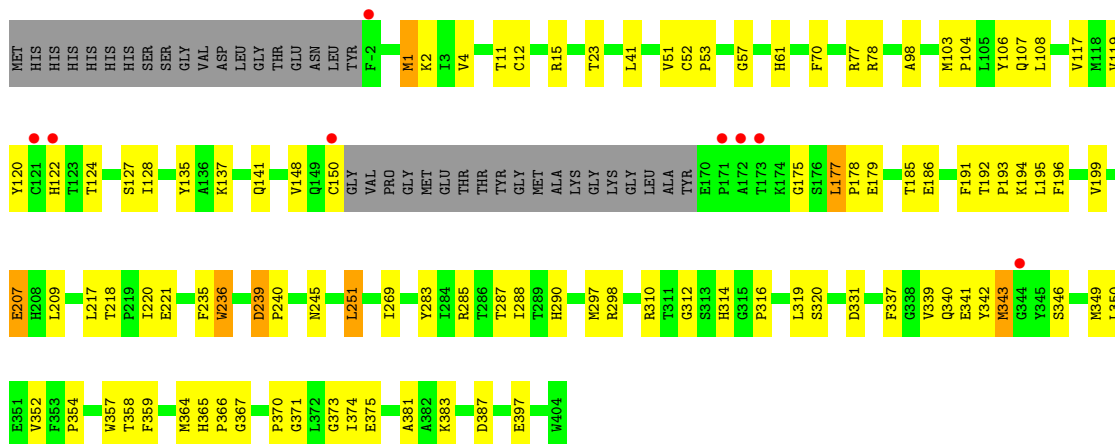


#### • Molecule 1: MANNONATE DEHYDRATASE





● Molecule 1: MANNONATE DEHYDRATASE



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.28Å 86.34Å 114.46Å 90.00° 123.07° 90.00°	Depositor
Resolution (Å)	50.00 – 2.00 50.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.00-2.00) 99.1 (50.00-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.28 (at 2.00Å)	Xtrriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.188 , 0.245 0.192 , 0.245	Depositor DCC
$R_{free}$ test set	3350 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.5	Xtrriage
Anisotropy	0.150	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 42.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	0.010 for -h-2*1,-k,l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13154	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, FMT, GOL

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	0.50	0/3184	0.78	2/4326 (0.0%)
1	B	0.50	0/3166	0.77	0/4300
1	C	0.47	0/3151	0.79	0/4281
1	D	0.48	0/3205	0.79	5/4354 (0.1%)
All	All	0.49	0/12706	0.78	7/17261 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	170	GLU	CA-C-N	7.78	127.33	119.24
1	A	170	GLU	C-N-CA	7.78	127.33	119.24
1	D	239	ASP	CA-C-N	6.80	126.60	119.05
1	D	239	ASP	C-N-CA	6.80	126.60	119.05
1	D	387	ASP	CA-C-N	5.12	126.25	119.84
1	D	387	ASP	C-N-CA	5.12	126.25	119.84
1	D	343	MET	N-CA-C	-5.12	99.90	110.80

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	3092	0	2982	62	0
1	B	3069	0	2963	80	0
1	C	3060	0	2949	90	0
1	D	3112	0	2999	80	0
2	A	18	0	24	1	0
2	B	18	0	24	1	0
2	C	18	0	24	3	0
2	D	18	0	24	1	0
3	A	1	0	0	1	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	3	0	1	1	0
5	B	3	0	1	1	0
5	C	3	0	1	2	0
5	D	3	0	1	0	0
6	A	208	0	0	9	0
6	B	189	0	0	6	0
6	C	173	0	0	16	0
6	D	161	0	0	5	0
All	All	13154	0	11993	310	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 13.

All (310) 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:15:ARG:HG2	1:C:349:MET:HE2	1.34	1.08
1:D:135:TYR:OH	1:D:207:GLU:HG2	1.60	1.00
1:B:101:ALA:HB2	1:D:103:MET:CE	1.91	0.99
1:C:359:PHE:C	1:C:359:PHE:CD2	2.52	0.87
1:C:148:VAL:HG21	1:C:209:LEU:HD11	1.59	0.85
1:C:359:PHE:C	1:C:359:PHE:HD2	1.85	0.84
1:B:101:ALA:HB2	1:D:103:MET:HE3	1.59	0.84
1:D:150:CYS:HB2	1:D:195:LEU:HD22	1.59	0.82
1:A:135:TYR:OH	1:A:207:GLU:HG2	1.80	0.82
5:C:505:FMT:H	6:C:692:HOH:O	1.80	0.82
1:B:121:CYS:HB2	6:B:652:HOH:O	1.80	0.81
1:B:1:MET:HE1	1:B:100:ALA:CB	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:HIS:CE1	1:B:319:LEU:HD21	2.20	0.77
1:B:242:PRO:HB2	2:B:502:GOL:H31	1.66	0.77
1:D:137:LYS:HG2	1:D:141:GLN:HE21	1.50	0.77
1:C:11:THR:OG1	1:C:13:PRO:HD3	1.86	0.76
1:D:148:VAL:HG21	1:D:209:LEU:HD11	1.67	0.76
1:C:191:PHE:HB2	6:C:684:HOH:O	1.85	0.76
1:C:216:ARG:HH21	1:C:404:TRP:HA	1.49	0.76
1:B:139:ARG:HG3	1:B:140:ASP:N	2.01	0.75
1:B:365:HIS:ND1	1:B:366:PRO:HD2	2.01	0.75
5:A:506:FMT:H	6:A:649:HOH:O	1.88	0.74
1:C:148:VAL:CG2	1:C:209:LEU:HD11	2.17	0.73
1:A:98:ALA:HB3	1:A:371:GLY:HA2	1.71	0.73
1:D:135:TYR:OH	1:D:207:GLU:CG	2.36	0.72
1:C:98:ALA:HB3	1:C:371:GLY:HA2	1.72	0.71
1:A:135:TYR:OH	1:A:207:GLU:CG	2.39	0.71
1:B:359:PHE:C	1:B:359:PHE:CD2	2.69	0.71
1:C:348:GLN:O	1:C:351:GLU:HB2	1.92	0.70
1:C:359:PHE:HD2	1:C:359:PHE:O	1.75	0.69
1:C:288:ILE:HD13	1:C:297:MET:HG3	1.76	0.68
1:C:128:ILE:HD11	1:C:191:PHE:CE1	2.29	0.67
1:D:98:ALA:HB3	1:D:371:GLY:HA2	1.77	0.67
2:C:502:GOL:H11	6:C:750:HOH:O	1.94	0.67
1:D:314:HIS:CE1	1:D:316:PRO:HG3	2.30	0.66
1:C:348:GLN:NE2	1:C:384:TYR:CE1	2.62	0.66
1:B:101:ALA:HB2	1:D:103:MET:HE1	1.78	0.66
1:B:1:MET:HE1	1:B:100:ALA:HB1	1.77	0.66
1:C:124:THR:HG22	1:C:134:ASP:OD1	1.96	0.65
5:B:506:FMT:H	6:B:751:HOH:O	1.95	0.65
1:D:287:THR:CG2	1:D:314:HIS:HB3	2.26	0.65
1:D:122:HIS:CE1	1:D:343:MET:HG3	2.31	0.65
1:D:236:TRP:CD1	1:D:236:TRP:C	2.74	0.64
1:D:137:LYS:HG2	1:D:141:GLN:NE2	2.12	0.64
1:B:124:THR:HG22	1:B:134:ASP:OD1	1.98	0.63
1:D:148:VAL:CG2	1:D:209:LEU:HD11	2.28	0.63
1:C:1:MET:HE2	1:C:61:HIS:CD2	2.34	0.63
1:B:122:HIS:CE1	1:B:343:MET:HG3	2.34	0.63
1:B:288:ILE:HD13	1:B:297:MET:HG3	1.81	0.62
1:C:314:HIS:CE1	1:C:316:PRO:HG3	2.33	0.62
1:C:236:TRP:C	1:C:236:TRP:CD1	2.77	0.62
1:B:375[A]:GLU:HG3	1:B:376:PHE:N	2.15	0.62
1:D:331:ASP:OD2	1:D:340:GLN:NE2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:PRO:HB3	1:B:352:VAL:HG21	1.82	0.62
1:B:361:ASN:O	1:B:361:ASN:ND2	2.33	0.61
1:A:290:HIS:CE1	1:A:319:LEU:HD21	2.34	0.61
1:A:285:ARG:HG2	1:A:312:GLY:O	2.01	0.61
1:B:314:HIS:CE1	1:B:316:PRO:HG3	2.36	0.60
1:D:359:PHE:C	1:D:359:PHE:CD2	2.79	0.60
1:C:216:ARG:NH2	1:C:404:TRP:HA	2.14	0.60
1:D:352:VAL:HG13	1:D:381:ALA:HB2	1.83	0.60
1:A:1:MET:HE2	1:A:61:HIS:CD2	2.37	0.60
1:C:216:ARG:HH21	1:C:404:TRP:CA	2.14	0.60
1:D:373:GLY:N	6:D:716:HOH:O	2.35	0.60
1:B:107:GLN:OE1	1:B:107:GLN:HA	2.02	0.59
1:A:1:MET:HE2	1:A:61:HIS:NE2	2.18	0.59
1:C:177:LEU:HG	1:C:178:PRO:HD2	1.83	0.59
1:A:348:GLN:NE2	1:A:384:TYR:CE1	2.71	0.59
1:B:12:CYS:O	1:B:14:GLY:N	2.35	0.59
1:D:288:ILE:HD13	1:D:297:MET:HG3	1.85	0.58
1:A:1:MET:HA	6:A:797:HOH:O	2.04	0.58
1:B:1:MET:HE1	1:B:100:ALA:HB2	1.84	0.58
1:C:210:LEU:N	1:C:210:LEU:HD12	2.18	0.58
5:C:505:FMT:C	6:C:692:HOH:O	2.45	0.58
1:A:236:TRP:CD1	1:A:236:TRP:C	2.81	0.58
1:B:185:THR:HG23	1:B:217:LEU:HD22	1.85	0.58
1:D:185:THR:HG23	1:D:217:LEU:HD22	1.86	0.58
1:D:367:GLY:HA3	6:D:660:HOH:O	2.04	0.58
1:C:132:LEU:HD13	1:C:202:LYS:HD2	1.86	0.58
1:B:192:THR:N	1:B:193:PRO:CD	2.67	0.57
1:A:287:THR:CG2	1:A:314:HIS:HB3	2.33	0.57
1:B:361:ASN:C	1:B:361:ASN:HD22	2.12	0.57
1:A:123:THR:HG22	1:A:148:VAL:HA	1.85	0.57
1:B:365:HIS:CG	1:B:366:PRO:HD2	2.39	0.57
1:A:139:ARG:NH1	1:A:207:GLU:OE2	2.35	0.57
1:A:123:THR:HG23	1:A:131:VAL:HG13	1.87	0.57
1:D:192:THR:N	1:D:193:PRO:CD	2.68	0.56
1:A:195:LEU:HD12	1:A:195:LEU:O	2.05	0.56
1:B:236:TRP:CD1	1:B:236:TRP:C	2.83	0.56
1:C:117:VAL:HG13	1:C:337:PHE:CZ	2.40	0.56
1:C:128:ILE:HD11	1:C:191:PHE:CZ	2.40	0.56
1:C:15:ARG:HG2	1:C:349:MET:CE	2.23	0.55
1:C:290:HIS:CE1	1:C:319:LEU:HD21	2.42	0.55
1:A:119:VAL:HA	1:A:340:GLN:O	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:ALA:CB	1:D:103:MET:HE3	2.34	0.55
1:B:287:THR:CG2	1:B:314:HIS:HB3	2.36	0.55
1:C:312:GLY:HA2	1:C:339:VAL:O	2.05	0.55
1:C:361:ASN:CG	1:C:361:ASN:O	2.47	0.55
1:D:290:HIS:CE1	1:D:319:LEU:HD21	2.42	0.55
1:A:128:ILE:HD11	1:A:191:PHE:CE1	2.41	0.55
1:D:342:TYR:C	1:D:343:MET:O	2.43	0.55
1:D:236:TRP:C	1:D:236:TRP:HD1	2.13	0.55
1:C:119:VAL:HA	1:C:340:GLN:O	2.06	0.55
1:B:123:THR:HG22	1:B:138:HIS:HD2	1.72	0.55
1:C:12:CYS:HA	1:C:15:ARG:O	2.07	0.54
1:A:127:SER:OG	1:A:130:GLU:HG3	2.07	0.54
1:C:316:PRO:HA	1:C:343:MET:HB2	1.90	0.54
1:D:120:TYR:CZ	1:D:341:GLU:HG3	2.42	0.54
1:C:254:GLN:NE2	6:C:729:HOH:O	2.40	0.54
1:B:375[A]:GLU:HG3	1:B:376:PHE:H	1.73	0.54
1:C:185:THR:HG23	1:C:217:LEU:HD22	1.89	0.53
1:A:195:LEU:O	1:A:199:VAL:HG23	2.09	0.53
1:B:339:VAL:HG22	1:B:340:GLN:H	1.73	0.53
1:A:314:HIS:CE1	1:A:316:PRO:HG3	2.44	0.53
1:C:192:THR:N	1:C:193:PRO:CD	2.72	0.53
1:D:287:THR:HG21	1:D:314:HIS:HB3	1.91	0.52
1:A:118:MET:HE3	1:A:339:VAL:HG23	1.90	0.52
1:C:31:LEU:CD1	1:C:376:PHE:HB2	2.39	0.52
1:C:236:TRP:C	1:C:236:TRP:HD1	2.18	0.52
2:C:503:GOL:C3	6:C:773:HOH:O	2.58	0.52
1:A:385:PRO:HD2	6:A:693:HOH:O	2.09	0.52
1:D:352:VAL:CG1	1:D:381:ALA:HB2	2.40	0.52
1:C:224:ARG:NH2	6:C:634:HOH:O	2.43	0.51
1:B:339:VAL:HG22	1:B:340:GLN:N	2.26	0.51
1:C:359:PHE:CD2	1:C:359:PHE:O	2.58	0.51
1:B:41:LEU:N	1:B:42:PRO:CD	2.74	0.51
1:D:239:ASP:N	1:D:240:PRO:CD	2.74	0.51
1:C:342:TYR:HD2	6:C:708:HOH:O	1.93	0.51
1:D:119:VAL:HA	1:D:340:GLN:O	2.10	0.51
1:A:192:THR:N	1:A:193:PRO:CD	2.74	0.50
1:D:283:TYR:HA	1:D:310:ARG:O	2.11	0.50
1:B:123:THR:HG23	1:B:146:ILE:CG2	2.41	0.50
1:C:126:HIS:CD2	6:C:756:HOH:O	2.63	0.50
1:A:89:VAL:HG22	6:A:633:HOH:O	2.11	0.50
1:B:367:GLY:HA3	6:B:636:HOH:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:185:THR:HG23	1:D:217:LEU:CD2	2.41	0.50
1:D:177:LEU:HD22	1:D:178:PRO:HD2	1.94	0.50
1:B:288:ILE:HG12	6:B:642:HOH:O	2.12	0.50
1:C:287:THR:CG2	1:C:314:HIS:HB3	2.42	0.50
1:B:119:VAL:HA	1:B:340:GLN:O	2.11	0.49
1:B:11:THR:OG1	1:B:13:PRO:HD3	2.13	0.49
1:A:123:THR:CG2	1:A:131:VAL:HG13	2.42	0.49
1:B:150:CYS:HB2	1:B:195:LEU:HD22	1.94	0.49
1:C:4:VAL:HG22	1:C:23:THR:O	2.13	0.49
1:D:218:THR:OG1	1:D:221:GLU:HG3	2.13	0.48
1:D:122:HIS:ND1	1:D:343:MET:HG3	2.29	0.48
1:A:346:SER:OG	1:A:349:MET:HG3	2.13	0.48
1:B:311:THR:OG1	1:B:337:PHE:HA	2.14	0.48
1:B:402:TRP:CG	1:B:403:ASN:H	2.32	0.48
1:D:12:CYS:HA	1:D:15:ARG:O	2.13	0.48
1:B:52:CYS:HB2	1:B:53:PRO:HD3	1.95	0.47
1:B:316:PRO:HA	1:B:343:MET:HB2	1.96	0.47
1:A:356:SER:OG	1:A:373:GLY:O	2.29	0.47
1:B:24:THR:C	1:B:26:SER:H	2.22	0.47
1:C:148:VAL:CG2	1:C:209:LEU:CD1	2.90	0.47
1:B:348:GLN:NE2	1:B:384:TYR:CE1	2.82	0.47
1:B:361:ASN:ND2	1:B:361:ASN:C	2.71	0.47
1:C:118:MET:HE3	1:C:339:VAL:HG23	1.96	0.47
1:A:357:TRP:C	1:A:357:TRP:CD1	2.92	0.47
1:A:254:GLN:HG3	6:A:699:HOH:O	2.15	0.47
1:B:50:HIS:HD1	1:C:390:TYR:HE1	1.63	0.47
1:B:331:ASP:OD2	1:B:340:GLN:NE2	2.38	0.47
1:C:214:HIS:O	1:C:216:ARG:HD2	2.14	0.47
1:D:1:MET:HE2	1:D:61:HIS:NE2	2.29	0.47
1:D:298:ARG:HD3	6:D:654:HOH:O	2.15	0.47
1:B:359:PHE:CD2	1:B:360:ASP:N	2.83	0.47
1:A:264:GLU:HB2	1:A:314:HIS:CG	2.51	0.46
1:D:374:ILE:HG13	1:D:375:GLU:N	2.31	0.46
1:B:359:PHE:C	1:B:359:PHE:HD2	2.18	0.46
1:B:239:ASP:N	1:B:240:PRO:CD	2.78	0.46
1:A:251:LEU:HB2	6:A:602:HOH:O	2.15	0.46
1:B:402:TRP:CD1	1:B:403:ASN:H	2.33	0.46
1:A:139:ARG:HG3	1:A:140:ASP:N	2.31	0.46
1:A:227:LYS:NZ	6:A:763:HOH:O	2.42	0.46
1:B:136:ALA:HA	1:B:139:ARG:HG2	1.98	0.46
1:C:39:ARG:O	1:C:42:PRO:HD2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:VAL:HG13	1:D:70:PHE:CZ	2.51	0.46
1:C:59:ASP:C	1:C:61:HIS:H	2.22	0.46
1:C:185:THR:HG23	1:C:217:LEU:CD2	2.46	0.46
1:A:359:PHE:C	1:A:359:PHE:CD2	2.94	0.46
1:B:121:CYS:CB	6:B:652:HOH:O	2.51	0.46
1:B:236:TRP:C	1:B:236:TRP:HD1	2.25	0.46
1:D:269:ILE:HG22	2:D:502:GOL:H32	1.97	0.46
1:D:312:GLY:HA2	1:D:339:VAL:O	2.16	0.46
1:D:354:PRO:HB2	1:D:375:GLU:HB2	1.97	0.46
1:A:58:ARG:HE	1:A:58:ARG:HB3	1.62	0.45
1:B:128:ILE:O	1:B:132:LEU:HG	2.16	0.45
1:C:367:GLY:HA3	6:C:675:HOH:O	2.15	0.45
1:D:358:THR:O	1:D:364:MET:HA	2.15	0.45
1:D:236:TRP:HD1	1:D:236:TRP:O	2.00	0.45
1:B:69:TYR:O	1:B:73:GLY:HA3	2.16	0.45
1:D:107:GLN:HA	1:D:107:GLN:OE1	2.17	0.45
1:D:381:ALA:C	1:D:383:LYS:H	2.25	0.45
1:B:264:GLU:HB2	1:B:314:HIS:CG	2.52	0.45
1:B:357:TRP:CD1	1:B:357:TRP:C	2.95	0.45
1:C:148:VAL:HG23	1:C:209:LEU:CD1	2.47	0.45
1:C:177:LEU:HG	1:C:178:PRO:CD	2.47	0.45
1:A:192:THR:O	1:A:195:LEU:HB3	2.17	0.45
1:A:236:TRP:C	1:A:236:TRP:HD1	2.23	0.45
1:A:239:ASP:N	1:A:240:PRO:CD	2.79	0.45
1:C:107:GLN:OE1	1:C:107:GLN:HA	2.17	0.45
1:D:191:PHE:O	1:D:194:LYS:HB2	2.17	0.45
1:A:367:GLY:HA3	6:A:703:HOH:O	2.17	0.44
1:B:375[A]:GLU:CG	1:B:376:PHE:N	2.80	0.44
1:D:177:LEU:HD23	1:D:177:LEU:HA	1.74	0.44
1:A:270:TRP:CH2	1:D:245:ASN:HB2	2.53	0.44
1:A:49:ASP:HB3	1:D:41:LEU:HD12	1.99	0.44
1:B:108:LEU:HD22	1:D:108:LEU:HD22	1.98	0.44
1:B:334:VAL:HG13	1:B:334:VAL:O	2.17	0.44
1:C:31:LEU:HD13	1:C:376:PHE:HB2	1.98	0.44
1:C:74:ALA:HB2	6:C:614:HOH:O	2.18	0.44
1:D:359:PHE:C	1:D:359:PHE:HD2	2.23	0.44
1:B:80:PRO:HB3	6:B:744:HOH:O	2.18	0.44
1:C:316:PRO:HD2	1:C:319:LEU:HD12	2.00	0.44
1:C:264:GLU:HB2	1:C:314:HIS:CG	2.53	0.44
1:B:123:THR:CG2	1:B:146:ILE:CG2	2.95	0.44
1:C:380:LEU:O	1:C:383:LYS:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:PRO:HD2	3:A:502:CL:CL	2.56	0.43
1:A:174:LYS:NZ	6:A:776:HOH:O	2.51	0.43
1:C:216:ARG:NH2	1:C:404:TRP:CD1	2.86	0.43
1:C:288:ILE:HG12	6:C:613:HOH:O	2.17	0.43
1:D:4:VAL:HG22	1:D:23:THR:O	2.18	0.43
1:D:320:SER:CB	6:D:641:HOH:O	2.65	0.43
1:B:223:ALA:O	1:B:227:LYS:HG3	2.18	0.43
1:D:103:MET:HB3	1:D:104:PRO:HD2	2.00	0.43
1:B:334:VAL:CG1	1:B:337:PHE:HB2	2.48	0.43
1:B:355:HIS:HA	1:B:374:ILE:HD12	1.99	0.43
1:D:175:GLY:C	1:D:177:LEU:H	2.26	0.43
1:B:285:ARG:HG2	1:B:312:GLY:O	2.18	0.43
1:D:316:PRO:HA	1:D:343:MET:HB2	2.00	0.43
1:A:127:SER:O	1:A:128:ILE:C	2.61	0.43
1:A:283:TYR:HA	1:A:310:ARG:O	2.18	0.43
1:C:262:VAL:HG22	1:C:263:GLY:N	2.34	0.43
1:D:195:LEU:O	1:D:199:VAL:HG23	2.19	0.43
1:A:304:ALA:HB1	1:A:309:VAL:HB	2.00	0.43
1:A:331:ASP:OD2	1:A:340:GLN:NE2	2.46	0.43
1:B:137:LYS:O	1:B:141:GLN:HG3	2.19	0.43
1:C:131:VAL:HG11	1:C:148:VAL:HG13	2.01	0.43
1:D:128:ILE:H	1:D:128:ILE:HG12	1.69	0.43
1:A:313:SER:HB2	1:A:340:GLN:NE2	2.34	0.43
1:C:373:GLY:N	6:C:632:HOH:O	2.41	0.43
1:D:251:LEU:HB2	6:D:609:HOH:O	2.18	0.43
1:C:6:ALA:HA	1:C:21:LYS:O	2.18	0.42
1:C:31:LEU:HD11	1:C:376:PHE:HB2	2.01	0.42
1:C:351:GLU:HB3	1:C:380:LEU:HD21	2.01	0.42
1:B:210:LEU:HG	1:B:235:PHE:HB3	2.01	0.42
1:B:313:SER:HB2	1:B:340:GLN:HE22	1.83	0.42
1:A:94:TRP:CD1	1:A:294:ILE:HB	2.53	0.42
1:B:365:HIS:CE1	1:B:366:PRO:HD2	2.53	0.42
1:C:127:SER:O	1:C:128:ILE:C	2.60	0.42
1:C:183:TRP:CE2	1:C:216:ARG:HG2	2.54	0.42
1:D:2:LYS:HZ2	1:D:57:GLY:HA2	1.85	0.42
1:C:135:TYR:OH	1:C:207:GLU:HB2	2.20	0.42
1:C:274:GLN:HA	1:C:277:GLU:HG2	2.00	0.42
1:B:245:ASN:HB2	1:C:270:TRP:CH2	2.54	0.42
1:D:52:CYS:HB2	1:D:53:PRO:HD3	2.00	0.42
1:A:334:VAL:HG13	1:A:334:VAL:O	2.19	0.42
1:C:350:LEU:HD23	1:C:350:LEU:HA	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:503:GOL:H31	6:C:773:HOH:O	2.18	0.42
1:D:346:SER:OG	1:D:349:MET:HG3	2.19	0.42
1:C:8:VAL:HB	1:C:48:ASN:ND2	2.35	0.42
1:C:236:TRP:HD1	1:C:236:TRP:O	2.01	0.42
1:B:350:LEU:O	1:B:353:PHE:N	2.50	0.42
1:D:365:HIS:ND1	1:D:366:PRO:HD2	2.35	0.42
1:B:46:TYR:O	1:B:50:HIS:HB2	2.20	0.42
1:B:58[A]:ARG:NH2	1:B:69:TYR:CE1	2.88	0.42
1:C:236:TRP:CD1	1:C:236:TRP:O	2.72	0.42
1:A:12:CYS:HA	1:A:15:ARG:O	2.20	0.41
1:D:207:GLU:N	1:D:207:GLU:CD	2.78	0.41
1:B:105:LEU:O	1:B:106:TYR:C	2.63	0.41
1:C:58:ARG:HE	1:C:58:ARG:HB3	1.61	0.41
1:D:120:TYR:CE2	1:D:341:GLU:HA	2.55	0.41
1:B:0:SER:C	1:B:1:MET:HG3	2.45	0.41
1:C:126:HIS:HD2	6:C:756:HOH:O	2.02	0.41
1:C:326:ALA:HA	1:C:372:LEU:HD22	2.02	0.41
1:D:236:TRP:CD1	1:D:236:TRP:O	2.74	0.41
1:C:122:HIS:ND1	1:C:147:ARG:CZ	2.84	0.41
1:B:12:CYS:HA	1:B:15:ARG:O	2.21	0.41
1:D:77:ARG:C	1:D:78:ARG:HG2	2.46	0.41
1:C:63:ILE:HG12	1:C:93:LEU:HB3	2.03	0.41
1:A:170:GLU:HA	1:A:171:PRO:HD2	1.84	0.41
1:D:235:PHE:O	1:D:236:TRP:HB3	2.19	0.41
1:A:195:LEU:HD12	1:A:195:LEU:C	2.45	0.41
1:C:59:ASP:C	1:C:61:HIS:N	2.79	0.41
1:C:357:TRP:CD1	1:C:364:MET:CE	3.04	0.41
1:B:375[A]:GLU:CG	1:B:376:PHE:H	2.33	0.41
1:D:103:MET:C	1:D:370:PRO:HA	2.46	0.41
1:D:186:GLU:OE1	1:D:186:GLU:N	2.40	0.41
1:D:220:ILE:HD12	1:D:220:ILE:HA	1.90	0.41
1:D:106:TYR:CD1	1:D:106:TYR:C	2.99	0.41
1:A:114:ARG:CZ	1:A:337:PHE:HB3	2.51	0.40
1:A:311:THR:OG1	1:A:337:PHE:HA	2.21	0.40
1:A:402:TRP:CG	1:A:403:ASN:H	2.39	0.40
1:A:402:TRP:CH2	2:A:505:GOL:H31	2.57	0.40
1:C:31:LEU:HD11	1:C:376:PHE:CB	2.51	0.40
1:D:350:LEU:HA	1:D:350:LEU:HD23	1.79	0.40
1:C:69:TYR:O	1:C:73:GLY:HA3	2.21	0.40
1:C:319:LEU:O	1:C:345:TYR:OH	2.32	0.40
1:D:192:THR:HG22	1:D:196:PHE:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:357:TRP:CD1	1:D:357:TRP:C	2.99	0.40
1:A:34:ALA:HB2	1:A:88:ALA:HB2	2.03	0.40
1:A:185:THR:HG23	1:A:217:LEU:CD2	2.51	0.40
1:C:128:ILE:O	1:C:132:LEU:HG	2.21	0.40
1:A:287:THR:HG21	1:A:314:HIS:HB3	2.02	0.40
1:D:117:VAL:HG13	1:D:337:PHE:CZ	2.56	0.40
1:A:135:TYR:OH	1:A:207:GLU:HG3	2.17	0.40
1:A:313:SER:HB2	1:A:340:GLN:HE22	1.86	0.40
1:C:220:ILE:HD12	1:C:220:ILE:HA	1.97	0.40
1:C:348:GLN:HG3	6:C:671:HOH:O	2.20	0.40
1:C:402:TRP:CG	1:C:403:ASN:H	2.40	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	383/426 (90%)	366 (96%)	16 (4%)	1 (0%)	36	35
1	B	380/426 (89%)	360 (95%)	19 (5%)	1 (0%)	36	35
1	C	378/426 (89%)	356 (94%)	21 (6%)	1 (0%)	36	35
1	D	385/426 (90%)	361 (94%)	24 (6%)	0	100	100
All	All	1526/1704 (90%)	1443 (95%)	80 (5%)	3 (0%)	43	42

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	B	78	ARG
1	C	78	ARG

### 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	327/357 (92%)	320 (98%)	7 (2%)	47	52
1	B	325/357 (91%)	320 (98%)	5 (2%)	57	64
1	C	324/357 (91%)	318 (98%)	6 (2%)	50	56
1	D	329/357 (92%)	318 (97%)	11 (3%)	33	34
All	All	1305/1428 (91%)	1276 (98%)	29 (2%)	45	50

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	VAL
1	A	123	THR
1	A	139	ARG
1	A	207	GLU
1	A	236	TRP
1	A	251	LEU
1	A	397	GLU
1	B	139	ARG
1	B	236	TRP
1	B	251	LEU
1	B	359	PHE
1	B	397	GLU
1	C	236	TRP
1	C	251	LEU
1	C	339	VAL
1	C	359	PHE
1	C	384	TYR
1	C	401	LEU
1	D	1	MET
1	D	11	THR
1	D	124	THR
1	D	127	SER
1	D	177	LEU
1	D	179	GLU

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Mol	Chain	Res	Type
1	D	207	GLU
1	D	236	TRP
1	D	251	LEU
1	D	285	ARG
1	D	397	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	254	GLN
1	B	138	HIS
1	B	141	GLN
1	B	279	GLN
1	B	308	GLN
1	B	361	ASN
1	C	48	ASN
1	C	206	ASN
1	C	254	GLN
1	D	102	ASN
1	D	138	HIS
1	D	141	GLN
1	D	254	GLN
1	D	279	GLN
1	D	340	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

Of 22 ligands modelled in this entry, 6 are monoatomic - leaving 16 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	GOL	C	503	-	5,5,5	0.38	0	5,5,5	0.21	0
5	FMT	D	505	4	2,2,2	0.64	0	1,1,1	0.28	0
2	GOL	B	502	-	5,5,5	0.42	0	5,5,5	0.37	0
2	GOL	A	503	-	5,5,5	0.33	0	5,5,5	0.73	0
2	GOL	D	502	-	5,5,5	0.41	0	5,5,5	0.30	0
2	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.35	0
2	GOL	D	501	-	5,5,5	0.38	0	5,5,5	0.39	0
2	GOL	C	502	-	5,5,5	0.55	0	5,5,5	0.53	0
5	FMT	B	506	4	2,2,2	0.67	0	1,1,1	0.32	0
5	FMT	C	505	4	2,2,2	0.65	0	1,1,1	0.22	0
2	GOL	C	501	-	5,5,5	0.39	0	5,5,5	0.24	0
2	GOL	D	504	-	5,5,5	0.36	0	5,5,5	0.61	0
2	GOL	B	501	-	5,5,5	0.39	0	5,5,5	0.26	0
2	GOL	B	504	-	5,5,5	0.34	0	5,5,5	0.40	0
5	FMT	A	506	4	2,2,2	0.60	0	1,1,1	0.20	0
2	GOL	A	501	-	5,5,5	0.40	0	5,5,5	0.25	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	GOL	C	503	-	-	2/4/4/4	-
2	GOL	B	502	-	-	2/4/4/4	-
2	GOL	A	503	-	-	4/4/4/4	-
2	GOL	D	502	-	-	2/4/4/4	-
2	GOL	A	505	-	-	2/4/4/4	-
2	GOL	D	501	-	-	2/4/4/4	-
2	GOL	C	502	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	C	501	-	-	0/4/4/4	-
2	GOL	D	504	-	-	2/4/4/4	-
2	GOL	B	501	-	-	1/4/4/4	-
2	GOL	B	504	-	-	3/4/4/4	-
2	GOL	A	501	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	503	GOL	C1-C2-C3-O3
2	B	502	GOL	O1-C1-C2-C3
2	B	504	GOL	O1-C1-C2-C3
2	C	502	GOL	O1-C1-C2-C3
2	C	502	GOL	C1-C2-C3-O3
2	C	503	GOL	O1-C1-C2-C3
2	D	501	GOL	O1-C1-C2-C3
2	D	504	GOL	O1-C1-C2-C3
2	C	502	GOL	O1-C1-C2-O2
2	C	502	GOL	O2-C2-C3-O3
2	A	503	GOL	O1-C1-C2-C3
2	A	505	GOL	O1-C1-C2-C3
2	B	502	GOL	O1-C1-C2-O2
2	D	504	GOL	O1-C1-C2-O2
2	A	503	GOL	O1-C1-C2-O2
2	A	503	GOL	O2-C2-C3-O3
2	A	505	GOL	O1-C1-C2-O2
2	B	504	GOL	O1-C1-C2-O2
2	C	503	GOL	O1-C1-C2-O2
2	D	501	GOL	O1-C1-C2-O2
2	D	502	GOL	O1-C1-C2-O2
2	B	504	GOL	O2-C2-C3-O3
2	D	502	GOL	O1-C1-C2-C3
2	B	501	GOL	O2-C2-C3-O3

There are no ring outliers.

8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	503	GOL	2	0
2	B	502	GOL	1	0
2	D	502	GOL	1	0
2	A	505	GOL	1	0
2	C	502	GOL	1	0
5	B	506	FMT	1	0
5	C	505	FMT	2	0
5	A	506	FMT	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	386/426 (90%)	-0.10	7 (1%) 67 67	24, 40, 67, 85	1 (0%)
1	B	381/426 (89%)	0.03	3 (0%) 82 82	25, 42, 70, 91	3 (0%)
1	C	381/426 (89%)	0.14	1 (0%) 90 89	24, 46, 74, 99	1 (0%)
1	D	388/426 (91%)	0.14	8 (2%) 63 63	23, 45, 74, 107	1 (0%)
All	All	1536/1704 (90%)	0.05	19 (1%) 76 76	23, 43, 71, 107	6 (0%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	172	ALA	4.7
1	D	171	PRO	4.3
1	D	172	ALA	4.1
1	D	-2	PHE	3.0
1	C	150	CYS	2.8
1	A	171	PRO	2.7
1	B	0	SER	2.7
1	A	150	CYS	2.7
1	B	175	GLY	2.5
1	D	150	CYS	2.4
1	A	173	THR	2.4
1	A	176	SER	2.3
1	A	122	HIS	2.2
1	D	122	HIS	2.1
1	D	121	CYS	2.1
1	D	344	GLY	2.1
1	D	173	THR	2.1
1	A	123	THR	2.0
1	B	124	THR	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 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, 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
2	GOL	C	502	6/6	0.80	0.16	44,50,57,65	0
2	GOL	D	502	6/6	0.83	0.14	54,61,72,78	0
2	GOL	A	505	6/6	0.85	0.14	45,58,66,67	0
2	GOL	C	501	6/6	0.88	0.14	46,49,63,68	0
2	GOL	B	502	6/6	0.88	0.12	39,50,56,59	0
2	GOL	B	504	6/6	0.88	0.12	50,67,74,77	0
5	FMT	A	506	3/3	0.88	0.20	39,39,43,51	0
5	FMT	C	505	3/3	0.88	0.15	37,37,50,51	0
5	FMT	D	505	3/3	0.88	0.15	52,52,54,55	0
2	GOL	B	501	6/6	0.90	0.11	42,53,58,74	0
5	FMT	B	506	3/3	0.91	0.16	37,37,52,60	0
2	GOL	D	504	6/6	0.91	0.11	34,60,64,65	0
2	GOL	C	503	6/6	0.91	0.08	52,69,72,77	0
2	GOL	A	503	6/6	0.92	0.11	28,51,59,59	0
2	GOL	A	501	6/6	0.92	0.11	39,45,59,60	0
2	GOL	D	501	6/6	0.94	0.10	46,51,58,69	0
3	CL	B	503	1/1	0.95	0.08	44,44,44,44	0
3	CL	A	502	1/1	0.96	0.06	46,46,46,46	0
4	MG	A	504	1/1	0.97	0.04	34,34,34,34	0
4	MG	B	505	1/1	0.98	0.04	38,38,38,38	0
4	MG	C	504	1/1	0.98	0.04	43,43,43,43	0
4	MG	D	503	1/1	0.99	0.04	40,40,40,40	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.