



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 17, 2017 – 08:44 AM EDT

PDB ID : 5F4Z  
Title : The crystal structure of an epoxide hydrolase from *Streptomyces carzinostaticus* subsp. *neocarzinostaticus*  
Authors : Tan, K.; Li, H.; Jedrzejczak, R.; BABNIGG, G.; BINGMAN, C.A.; YEN-NAMALLI, R.; LOHMAN, J.; Chang, C.Y.; Shen, B.; PHILLIPS JR, G.N.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG); Enzyme Discovery for Natural Product Biosynthesis (NatPro)  
Deposited on : unknown  
Resolution : 1.82 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20029824  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20029824

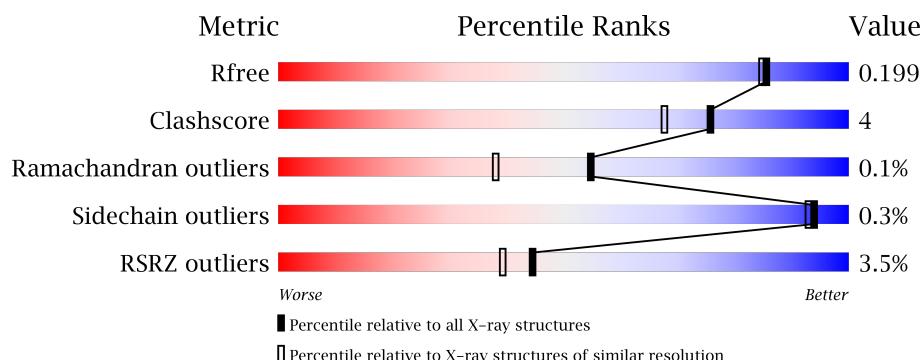
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.82 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))
$R_{free}$	100719	5868 (1.84-1.80)
Clashscore	112137	6856 (1.84-1.80)
Ramachandran outliers	110173	6780 (1.84-1.80)
Sidechain outliers	110143	6780 (1.84-1.80)
RSRZ outliers	101464	5947 (1.84-1.80)

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. 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	393	<div> <div>4%</div> <div>92%</div> <div>6%</div> <div>..</div> </div>
1	B	393	<div> <div>2%</div> <div>91%</div> <div>7%</div> <div>..</div> </div>
1	C	393	<div> <div>3%</div> <div>91%</div> <div>7%</div> <div>..</div> </div>
1	D	393	<div> <div>5%</div> <div>87%</div> <div>11%</div> <div>..</div> </div>
1	E	393	<div> <div>4%</div> <div>94%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	GOL	A	402	-	-	-	X
2	GOL	A	403	-	-	-	X
2	GOL	A	404	-	-	-	X
2	GOL	C	401	-	-	-	X
3	ACT	A	406	-	-	X	X
4	PEG	A	407	-	-	-	X
5	5V4	B	404[A]	-	-	-	X
5	5V4	B	404[B]	-	-	-	X
6	PG4	B	402	-	-	-	X
7	TRS	B	403	-	-	-	X

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 16650 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 Epoxide hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	388	Total	C	N	O	Se	0	4	0
			3052	1958	525	562	7			
1	B	390	Total	C	N	O	Se	0	1	0
			3051	1956	526	562	7			
1	C	387	Total	C	N	O	Se	0	5	0
			3047	1953	525	562	7			
1	D	391	Total	C	N	O	Se	0	4	0
			3078	1972	533	566	7			
1	E	388	Total	C	N	O	Se	0	3	0
			3040	1949	522	562	7			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	388	HIS	-	expression tag	UNP Q84HB1
A	389	HIS	-	expression tag	UNP Q84HB1
A	390	HIS	-	expression tag	UNP Q84HB1
A	391	HIS	-	expression tag	UNP Q84HB1
A	392	HIS	-	expression tag	UNP Q84HB1
A	393	HIS	-	expression tag	UNP Q84HB1
B	388	HIS	-	expression tag	UNP Q84HB1
B	389	HIS	-	expression tag	UNP Q84HB1
B	390	HIS	-	expression tag	UNP Q84HB1
B	391	HIS	-	expression tag	UNP Q84HB1
B	392	HIS	-	expression tag	UNP Q84HB1
B	393	HIS	-	expression tag	UNP Q84HB1
C	388	HIS	-	expression tag	UNP Q84HB1
C	389	HIS	-	expression tag	UNP Q84HB1
C	390	HIS	-	expression tag	UNP Q84HB1
C	391	HIS	-	expression tag	UNP Q84HB1
C	392	HIS	-	expression tag	UNP Q84HB1
C	393	HIS	-	expression tag	UNP Q84HB1
D	388	HIS	-	expression tag	UNP Q84HB1

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Chain	Residue	Modelled	Actual	Comment	Reference
D	389	HIS	-	expression tag	UNP Q84HB1
D	390	HIS	-	expression tag	UNP Q84HB1
D	391	HIS	-	expression tag	UNP Q84HB1
D	392	HIS	-	expression tag	UNP Q84HB1
D	393	HIS	-	expression tag	UNP Q84HB1
E	388	HIS	-	expression tag	UNP Q84HB1
E	389	HIS	-	expression tag	UNP Q84HB1
E	390	HIS	-	expression tag	UNP Q84HB1
E	391	HIS	-	expression tag	UNP Q84HB1
E	392	HIS	-	expression tag	UNP Q84HB1
E	393	HIS	-	expression tag	UNP Q84HB1

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



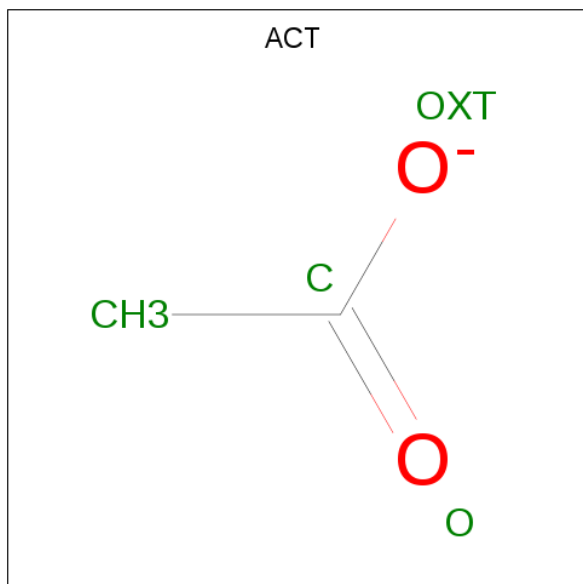
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	A	1	Total	C	O	0	0
			6	3	3		
2	C	1	Total	C	O	0	0
			6	3	3		

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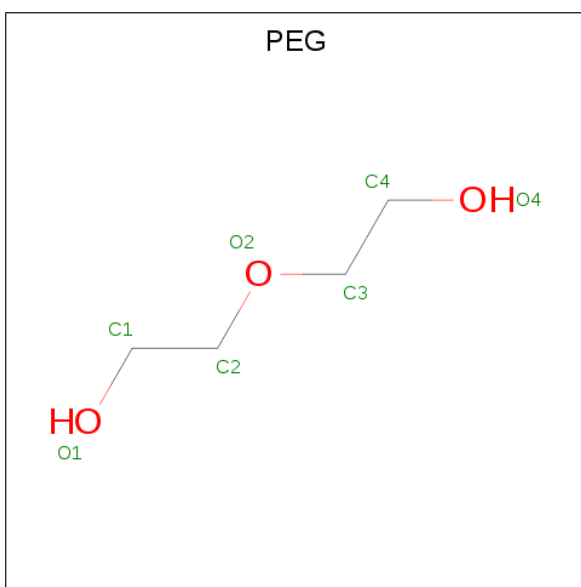
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is ACETATE ION (three-letter code: ACT) (formula:  $\text{C}_2\text{H}_3\text{O}_2$ ).



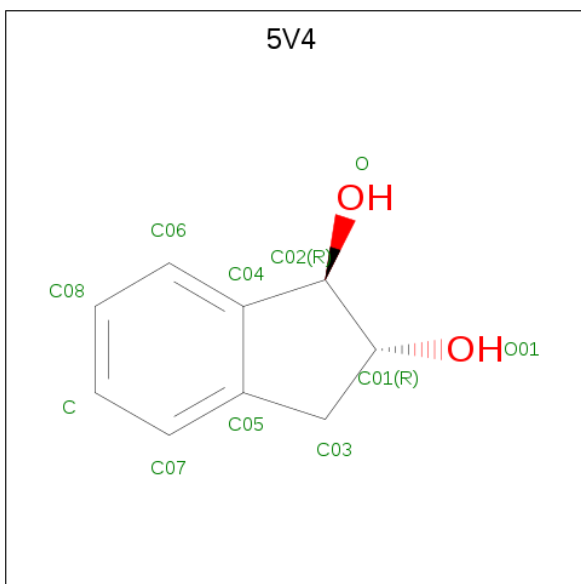
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $\text{C}_4\text{H}_{10}\text{O}_3$ ).



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

- Molecule 5 is (1 {R},2 {R})-2,3-dihydro-1 {H}-indene-1,2-diol (three-letter code: 5V4) (formula: C<sub>9</sub>H<sub>10</sub>O<sub>2</sub>).



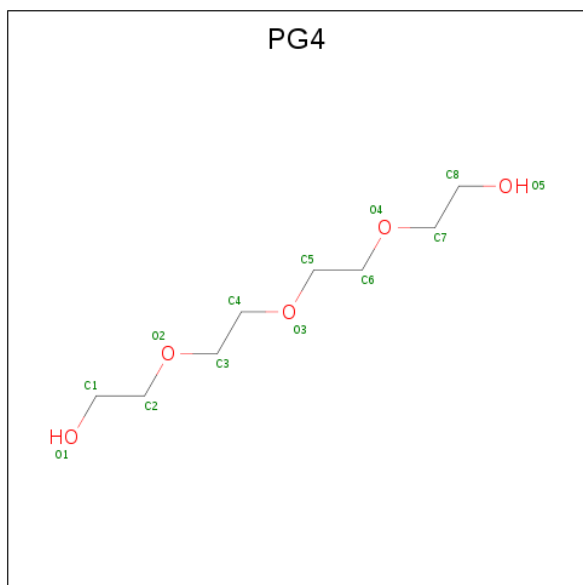
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	1
			22	18	4		
5	B	1	Total	C	O	0	1
			22	18	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	1
			22	18	4		
5	D	1	Total	C	O	0	1
			22	18	4		
5	E	1	Total	C	O	0	1
			22	18	4		

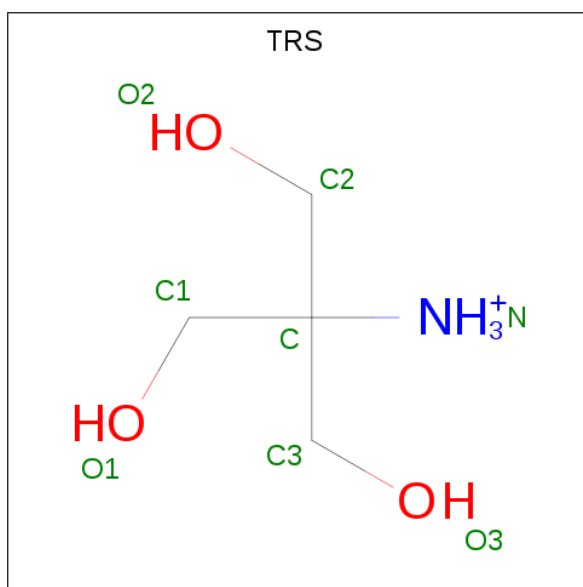
- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula:  $C_8H_{18}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 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
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

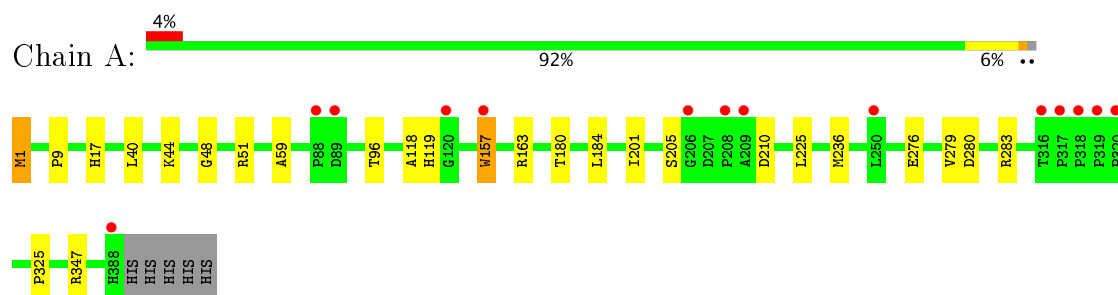
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	287	Total	O	0	1
			288	288		
8	B	256	Total	O	0	0
			256	256		
8	C	239	Total	O	0	1
			240	240		
8	D	191	Total	O	0	0
			191	191		
8	E	219	Total	O	0	0
			219	219		

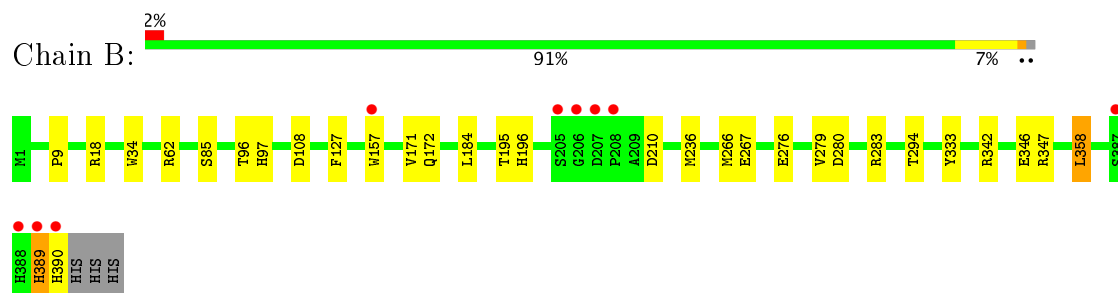
### 3 Residue-property plots

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.

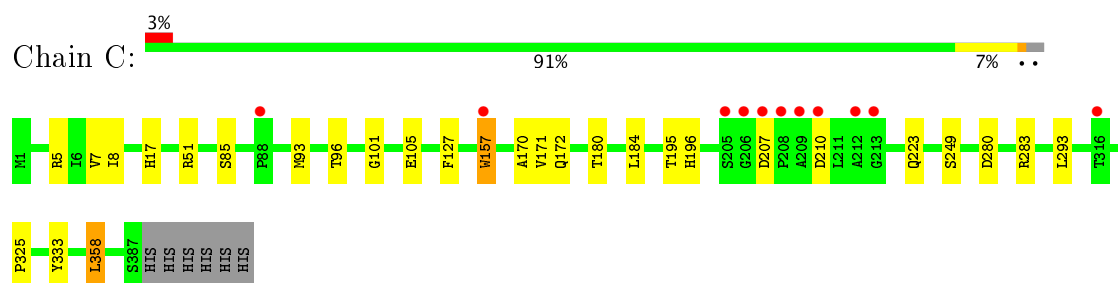
#### • Molecule 1: Epoxide hydrolase



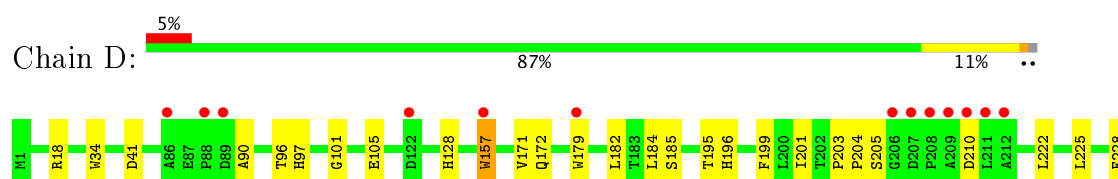
#### • Molecule 1: Epoxide hydrolase

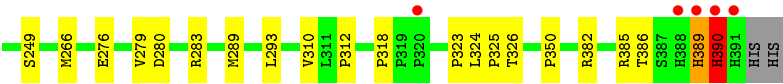


#### • Molecule 1: Epoxide hydrolase

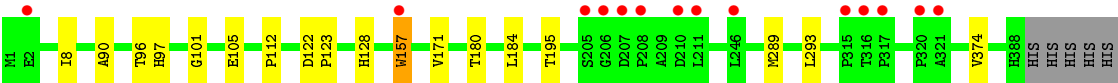


#### • Molecule 1: Epoxide hydrolase





● Molecule 1: Epoxide hydrolase



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	179.36Å 93.07Å 134.06Å 90.00° 115.33° 90.00°	Depositor
Resolution (Å)	33.27 – 1.82 43.32 – 1.82	Depositor EDS
% Data completeness (in resolution range)	99.7 (33.27-1.82) 99.5 (43.32-1.82)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 1.82Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, $R_{free}$	0.160 , 0.200 0.161 , 0.199	Depositor DCC
$R_{free}$ test set	8901 reflections (5.01%)	DCC
Wilson B-factor (Å <sup>2</sup> )	24.5	Xtriage
Anisotropy	0.343	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 49.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	16650	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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: GOL, 5V4, PG4, ACT, TRS, PEG

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	0.46	2/3158 (0.1%)	0.56	0/4320
1	B	0.41	0/3153	0.54	0/4315
1	C	0.42	2/3155 (0.1%)	0.53	1/4316 (0.0%)
1	D	0.36	1/3189 (0.0%)	0.51	0/4362
1	E	0.39	1/3145 (0.0%)	0.51	0/4303
All	All	0.41	6/15800 (0.0%)	0.53	1/21616 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	157	TRP	CB-CG	-7.16	1.37	1.50
1	C	157	TRP	CB-CG	-6.92	1.37	1.50
1	A	157	TRP	CB-CG	-6.47	1.38	1.50
1	A	157	TRP	CE3-CZ3	-6.42	1.27	1.38
1	C	157	TRP	CE3-CZ3	-5.85	1.28	1.38
1	D	157	TRP	CB-CG	-5.05	1.41	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	358	LEU	CA-CB-CG	-5.43	102.80	115.30

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	3052	0	2940	22	0
1	B	3051	0	2922	21	0
1	C	3047	0	2935	19	0
1	D	3078	0	2957	34	0
1	E	3040	0	2925	14	0
2	A	30	0	40	1	0
2	C	6	0	8	0	0
2	E	6	0	8	0	0
3	A	4	0	3	2	0
3	B	4	0	3	1	0
4	A	7	0	10	1	0
5	A	22	0	20	1	0
5	B	22	0	20	1	0
5	C	22	0	20	0	0
5	D	22	0	20	4	0
5	E	22	0	20	0	0
6	B	13	0	18	2	0
7	B	8	0	12	1	0
8	A	288	0	0	1	0
8	B	256	0	0	2	0
8	C	240	0	0	0	0
8	D	191	0	0	2	0
8	E	219	0	0	0	0
All	All	16650	0	14881	109	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 4.

All (109) 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:D:179[A]:TRP:CH2	5:D:401[A]:5V4:H9	2.14	0.82
1:B:157:TRP:HE3	1:B:184:LEU:HD22	1.48	0.77
1:A:157:TRP:HE3	1:A:184:LEU:HD22	1.50	0.75
1:A:325:PRO:HB3	1:C:325:PRO:HB3	1.78	0.66
1:A:59:ALA:HA	2:A:404:GOL:H32	1.78	0.65
1:E:96:THR:OG1	1:E:157:TRP:CH2	2.45	0.64
1:D:324:LEU:HD12	1:D:325:PRO:HD2	1.79	0.64
1:A:96:THR:OG1	1:A:157:TRP:CH2	2.42	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:283:ARG:HH11	1:A:283:ARG:HG3	1.64	0.63
1:C:96:THR:OG1	1:C:157:TRP:CH2	2.41	0.62
1:D:157:TRP:HE3	1:D:184:LEU:HD22	1.64	0.62
1:A:1:MSE:HE1	1:A:163:ARG:HB3	1.82	0.61
1:B:342:ARG:O	1:B:346:GLU:HG2	2.02	0.60
1:A:347:ARG:NH2	8:A:503:HOH:O	2.36	0.58
1:C:280:ASP:OD2	1:C:283:ARG:NH1	2.37	0.56
1:E:96:THR:HG21	1:E:157:TRP:HH2	1.71	0.56
1:B:96:THR:OG1	1:B:157:TRP:CH2	2.45	0.56
1:C:96:THR:HG21	1:C:157:TRP:HH2	1.72	0.54
1:C:157:TRP:HE3	1:C:184:LEU:HD22	1.72	0.53
1:D:90:ALA:HB3	1:D:128:HIS:CD2	2.44	0.53
1:D:179[A]:TRP:CZ2	5:D:401[A]:5V4:H9	2.43	0.52
1:B:280:ASP:OD2	1:B:283:ARG:NH1	2.40	0.52
1:D:312:PRO:HG2	5:D:401[A]:5V4:H10	1.91	0.51
1:D:205:SER:OG	1:D:210:ASP:OD2	2.25	0.51
1:A:40:LEU:HD11	1:A:44:LYS:HE3	1.94	0.50
1:A:280:ASP:OD2	1:A:283:ARG:NH1	2.44	0.50
1:B:18:ARG:HD2	8:B:541:HOH:O	2.11	0.50
1:C:96:THR:HG21	1:C:157:TRP:CH2	2.47	0.50
1:B:389:HIS:CD2	1:B:389:HIS:C	2.84	0.50
1:D:324:LEU:HG	1:D:326:THR:HG22	1.94	0.49
1:D:386:THR:O	1:D:389:HIS:HB3	2.12	0.49
1:B:276:GLU:HA	1:B:279:VAL:O	2.12	0.49
1:E:157:TRP:HE3	1:E:184:LEU:HD22	1.77	0.49
1:C:249:SER:HB2	1:D:249[B]:SER:HB3	1.95	0.48
1:B:9:PRO:HG2	6:B:402:PG4:H11	1.96	0.48
1:B:62:ARG:NH2	1:B:108:ASP:OD1	2.32	0.48
1:D:182:LEU:O	1:D:185:SER:HB2	2.14	0.47
1:A:283:ARG:HG3	1:A:283:ARG:NH1	2.29	0.47
1:A:48:GLY:HA2	3:A:406:ACT:H3	1.96	0.47
1:D:204:PRO:HD3	1:D:222:LEU:HD22	1.96	0.47
1:E:289:MSE:HE3	1:E:293:LEU:HD11	1.97	0.47
1:D:96:THR:HG22	1:D:97:HIS:O	2.15	0.47
1:C:333:TYR:CZ	1:C:358:LEU:HD13	2.50	0.46
1:E:96:THR:HG22	1:E:97:HIS:O	2.16	0.46
1:C:8:ILE:HG13	1:C:293:LEU:HD13	1.97	0.46
1:A:17:HIS:HB3	1:A:51:ARG:CZ	2.46	0.46
1:A:201[A]:ILE:HG23	1:A:225:LEU:HD11	1.97	0.46
1:C:157:TRP:CH2	1:C:180:THR:HG21	2.51	0.46
1:D:199:PHE:CZ	1:D:201:ILE:HD11	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:201:ILE:HG22	1:D:203:PRO:HD3	1.97	0.46
1:A:51:ARG:HG2	3:A:406:ACT:OXT	2.16	0.45
1:A:96:THR:HG21	1:A:157:TRP:CH2	2.51	0.45
1:D:228:PHE:CE1	5:D:401[A]:5V4:H5	2.51	0.45
1:C:5[A]:ARG:HG2	1:C:7:VAL:HG23	1.99	0.45
1:D:101:GLY:HA3	1:D:105:GLU:OE2	2.17	0.45
1:A:9:PRO:HG2	4:A:407:PEG:H11	1.99	0.45
1:B:210:ASP:OD2	1:B:347:ARG:NH1	2.45	0.45
1:B:389:HIS:HD2	1:B:390:HIS:HD2	1.64	0.45
1:D:310:VAL:HA	1:D:318:PRO:HG3	1.99	0.45
1:E:96:THR:HG21	1:E:157:TRP:CH2	2.51	0.45
1:D:185:SER:OG	1:D:195:THR:OG1	2.26	0.44
1:E:157:TRP:CH2	1:E:180:THR:HG21	2.53	0.44
1:D:382:ARG:HG2	1:D:385:ARG:NH1	2.32	0.44
1:D:41:ASP:HB2	8:D:670:HOH:O	2.17	0.44
1:B:333:TYR:CZ	1:B:358:LEU:HD13	2.52	0.44
1:C:101:GLY:HA3	1:C:105:GLU:OE2	2.18	0.44
1:A:118:ALA:O	1:A:119:HIS:HD2	2.01	0.44
3:B:401:ACT:H1	8:B:745:HOH:O	2.17	0.44
1:A:205:SER:OG	1:A:210:ASP:OD2	2.23	0.43
1:D:171:VAL:HG23	1:D:195:THR:HG23	2.00	0.43
1:D:289:MSE:HE3	1:D:293:LEU:HD11	1.99	0.43
1:E:101:GLY:HA3	1:E:105:GLU:OE2	2.18	0.43
1:E:112:PRO:HB2	1:E:374:VAL:HG21	2.01	0.43
1:B:389:HIS:HD2	1:B:390:HIS:CD2	2.36	0.43
1:E:90:ALA:HB3	1:E:128:HIS:NE2	2.33	0.43
1:B:294:THR:HA	6:B:402:PG4:H51	2.01	0.43
1:D:96:THR:OG1	1:D:157:TRP:CH2	2.52	0.43
1:D:172:GLN:HA	1:D:196:HIS:O	2.19	0.43
1:D:386:THR:O	1:D:390:HIS:CD2	2.72	0.43
1:A:157:TRP:CH2	1:A:180:THR:HG21	2.54	0.43
1:A:96:THR:HG21	1:A:157:TRP:HH2	1.84	0.42
1:B:236:MSE:HE1	5:B:404[B]:5V4:H6	2.01	0.42
1:E:171:VAL:HG23	1:E:195:THR:HG23	2.02	0.42
1:E:8:ILE:HG13	1:E:293:LEU:HD13	2.00	0.42
1:B:34:TRP:CE3	1:B:266:MSE:HG2	2.53	0.42
1:D:18:ARG:HD2	8:D:624:HOH:O	2.18	0.42
1:B:85:SER:HB2	1:B:127:PHE:O	2.20	0.42
1:D:276:GLU:HA	1:D:279:VAL:O	2.20	0.42
1:C:85:SER:HB2	1:C:127:PHE:O	2.21	0.41
1:C:93:MSE:HE3	1:C:170:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:MSE:HE1	5:A:408[B]:5V4:H6	2.01	0.41
1:B:96:THR:HG22	1:B:97:HIS:O	2.21	0.41
1:C:96:THR:CG2	1:C:157:TRP:CH2	3.03	0.41
1:D:323:PRO:HB3	1:D:350:PRO:HD3	2.03	0.41
1:D:390:HIS:CD2	1:D:390:HIS:H	2.38	0.41
1:C:172:GLN:HA	1:C:196:HIS:O	2.21	0.41
1:C:17:HIS:HB3	1:C:51:ARG:CZ	2.51	0.41
1:D:225:LEU:HD23	1:D:225:LEU:HA	1.93	0.41
1:D:280:ASP:OD2	1:D:283:ARG:HD2	2.21	0.41
1:D:96:THR:HG21	1:D:157:TRP:CH2	2.56	0.41
1:E:96:THR:CG2	1:E:157:TRP:HH2	2.34	0.41
1:A:276:GLU:HA	1:A:279:VAL:O	2.21	0.41
1:B:267:GLU:O	7:B:403:TRS:N	2.42	0.41
1:B:171:VAL:HG23	1:B:195:THR:HG23	2.03	0.40
1:B:172:GLN:HA	1:B:196:HIS:O	2.20	0.40
1:E:122:ASP:OD1	1:E:123:PRO:HD2	2.21	0.40
1:D:34:TRP:CE3	1:D:266:MSE:HG2	2.56	0.40
1:C:171:VAL:HG23	1:C:195:THR:HG23	2.04	0.40
1:C:207:ASP:O	1:C:210:ASP:HB2	2.21	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	390/393 (99%)	381 (98%)	9 (2%)	0	100	100
1	B	389/393 (99%)	375 (96%)	14 (4%)	0	100	100
1	C	390/393 (99%)	379 (97%)	11 (3%)	0	100	100
1	D	393/393 (100%)	378 (96%)	13 (3%)	2 (0%)	32	17
1	E	389/393 (99%)	379 (97%)	10 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1951/1965 (99%)	1892 (97%)	57 (3%)	2 (0%)	55 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	389	HIS
1	D	390	HIS

### 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	320/315 (102%)	319 (100%)	1 (0%)	94 93
1	B	319/315 (101%)	317 (99%)	2 (1%)	89 86
1	C	320/315 (102%)	319 (100%)	1 (0%)	94 93
1	D	323/315 (102%)	322 (100%)	1 (0%)	94 93
1	E	319/315 (101%)	319 (100%)	0	100 100
All	All	1601/1575 (102%)	1596 (100%)	5 (0%)	94 93

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	B	358	LEU
1	B	389	HIS
1	C	223	GLN
1	D	390	HIS

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

Mol	Chain	Res	Type
1	B	389	HIS
1	B	390	HIS

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Mol	Chain	Res	Type
1	D	390	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 ⓘ

22 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	GOL	A	401	-	5,5,5	0.35	0	5,5,5	0.23	0
2	GOL	A	402	-	5,5,5	0.43	0	5,5,5	0.19	0
2	GOL	A	403	-	5,5,5	0.39	0	5,5,5	0.18	0
2	GOL	A	404	-	5,5,5	0.36	0	5,5,5	0.27	0
2	GOL	A	405	-	5,5,5	0.33	0	5,5,5	0.21	0
3	ACT	A	406	-	1,3,3	1.25	0	0,3,3	0.00	-
4	PEG	A	407	-	6,6,6	0.62	0	5,5,5	0.68	0
5	5V4	A	408[A]	-	11,12,12	3.66	6 (54%)	13,17,17	1.66	4 (30%)
5	5V4	A	408[B]	-	11,12,12	3.61	5 (45%)	13,17,17	1.50	2 (15%)
3	ACT	B	401	-	1,3,3	1.23	0	0,3,3	0.00	-
6	PG4	B	402	-	12,12,12	0.94	0	11,11,11	0.25	0
7	TRS	B	403	-	7,7,7	0.34	0	9,9,9	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	5V4	B	404[A]	-	11,12,12	3.60	6 (54%)	13,17,17	1.62	4 (30%)
5	5V4	B	404[B]	-	11,12,12	3.56	5 (45%)	13,17,17	1.47	2 (15%)
2	GOL	C	401	-	5,5,5	0.37	0	5,5,5	0.12	0
5	5V4	C	402[A]	-	11,12,12	3.60	6 (54%)	13,17,17	1.58	4 (30%)
5	5V4	C	402[B]	-	11,12,12	3.63	6 (54%)	13,17,17	1.56	4 (30%)
5	5V4	D	401[A]	-	11,12,12	3.44	6 (54%)	13,17,17	1.74	4 (30%)
5	5V4	D	401[B]	-	11,12,12	3.64	6 (54%)	13,17,17	1.47	2 (15%)
2	GOL	E	401	-	5,5,5	0.34	0	5,5,5	0.17	0
5	5V4	E	402[A]	-	11,12,12	3.61	6 (54%)	13,17,17	1.61	4 (30%)
5	5V4	E	402[B]	-	11,12,12	3.57	6 (54%)	13,17,17	1.54	3 (23%)

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	A	401	-	-	0/4/4/4	0/0/0/0
2	GOL	A	402	-	-	0/4/4/4	0/0/0/0
2	GOL	A	403	-	-	0/4/4/4	0/0/0/0
2	GOL	A	404	-	-	0/4/4/4	0/0/0/0
2	GOL	A	405	-	-	0/4/4/4	0/0/0/0
3	ACT	A	406	-	-	0/0/0/0	0/0/0/0
4	PEG	A	407	-	-	0/4/4/4	0/0/0/0
5	5V4	A	408[A]	-	-	0/0/12/12	0/2/2/2
5	5V4	A	408[B]	-	-	0/0/12/12	0/2/2/2
3	ACT	B	401	-	-	0/0/0/0	0/0/0/0
6	PG4	B	402	-	-	0/10/10/10	0/0/0/0
7	TRS	B	403	-	-	0/9/9/9	0/0/0/0
5	5V4	B	404[A]	-	-	0/0/12/12	0/2/2/2
5	5V4	B	404[B]	-	-	0/0/12/12	0/2/2/2
2	GOL	C	401	-	-	0/4/4/4	0/0/0/0
5	5V4	C	402[A]	-	-	0/0/12/12	0/2/2/2
5	5V4	C	402[B]	-	-	0/0/12/12	0/2/2/2
5	5V4	D	401[A]	-	-	0/0/12/12	0/2/2/2
5	5V4	D	401[B]	-	-	0/0/12/12	0/2/2/2
2	GOL	E	401	-	-	0/4/4/4	0/0/0/0
5	5V4	E	402[A]	-	-	0/0/12/12	0/2/2/2
5	5V4	E	402[B]	-	-	0/0/12/12	0/2/2/2

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	401[A]	5V4	C04-C02	-2.91	1.46	1.50
5	D	401[B]	5V4	C03-C01	-2.53	1.49	1.53
5	E	402[B]	5V4	C03-C01	-2.51	1.49	1.53
5	A	408[B]	5V4	C03-C01	-2.46	1.49	1.53
5	C	402[B]	5V4	C03-C01	-2.40	1.49	1.53
5	D	401[A]	5V4	C03-C01	-2.40	1.49	1.53
5	E	402[A]	5V4	C03-C01	-2.36	1.49	1.53
5	B	404[B]	5V4	C03-C01	-2.36	1.49	1.53
5	A	408[A]	5V4	C03-C01	-2.33	1.49	1.53
5	A	408[A]	5V4	C04-C02	-2.32	1.47	1.50
5	C	402[A]	5V4	C04-C02	-2.30	1.47	1.50
5	E	402[A]	5V4	C04-C02	-2.30	1.47	1.50
5	C	402[A]	5V4	C03-C01	-2.27	1.49	1.53
5	B	404[A]	5V4	C04-C02	-2.23	1.47	1.50
5	B	404[A]	5V4	C03-C01	-2.17	1.50	1.53
5	E	402[B]	5V4	C04-C02	-2.06	1.47	1.50
5	C	402[B]	5V4	C04-C02	-2.03	1.47	1.50
5	D	401[B]	5V4	C-C07	2.03	1.42	1.38
5	D	401[A]	5V4	C03-C05	4.34	1.58	1.50
5	E	402[B]	5V4	C03-C05	4.58	1.58	1.50
5	A	408[B]	5V4	C03-C05	4.60	1.58	1.50
5	B	404[B]	5V4	C03-C05	4.63	1.58	1.50
5	D	401[B]	5V4	C03-C05	4.68	1.58	1.50
5	C	402[B]	5V4	C03-C05	4.68	1.58	1.50
5	B	404[A]	5V4	C03-C05	4.79	1.59	1.50
5	A	408[A]	5V4	C03-C05	4.82	1.59	1.50
5	E	402[A]	5V4	C03-C05	4.87	1.59	1.50
5	D	401[A]	5V4	C07-C05	4.91	1.47	1.39
5	E	402[A]	5V4	C07-C05	4.93	1.47	1.39
5	E	402[B]	5V4	C07-C05	4.99	1.48	1.39
5	B	404[B]	5V4	C07-C05	5.04	1.48	1.39
5	A	408[A]	5V4	C07-C05	5.04	1.48	1.39
5	C	402[A]	5V4	C03-C05	5.04	1.59	1.50
5	C	402[A]	5V4	C07-C05	5.07	1.48	1.39
5	C	402[B]	5V4	C07-C05	5.09	1.48	1.39
5	B	404[A]	5V4	C07-C05	5.11	1.48	1.39
5	A	408[B]	5V4	C07-C05	5.18	1.48	1.39
5	D	401[B]	5V4	C07-C05	5.18	1.48	1.39
5	C	402[A]	5V4	C08-C	5.53	1.51	1.38
5	D	401[A]	5V4	C08-C	5.57	1.51	1.38
5	B	404[B]	5V4	C08-C	5.69	1.51	1.38
5	E	402[B]	5V4	C08-C	5.70	1.51	1.38
5	E	402[A]	5V4	C08-C	5.75	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	404[A]	5V4	C08-C	5.76	1.51	1.38
5	A	408[A]	5V4	C08-C	5.80	1.52	1.38
5	C	402[B]	5V4	C08-C	5.83	1.52	1.38
5	D	401[A]	5V4	C06-C04	5.86	1.47	1.39
5	D	401[B]	5V4	C08-C	5.86	1.52	1.38
5	A	408[B]	5V4	C08-C	5.88	1.52	1.38
5	C	402[A]	5V4	C06-C04	6.57	1.48	1.39
5	E	402[B]	5V4	C06-C04	6.57	1.48	1.39
5	B	404[A]	5V4	C06-C04	6.64	1.48	1.39
5	A	408[B]	5V4	C06-C04	6.65	1.48	1.39
5	B	404[B]	5V4	C06-C04	6.66	1.48	1.39
5	D	401[B]	5V4	C06-C04	6.69	1.48	1.39
5	C	402[B]	5V4	C06-C04	6.70	1.48	1.39
5	E	402[A]	5V4	C06-C04	6.71	1.48	1.39
5	A	408[A]	5V4	C06-C04	6.83	1.48	1.39

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	408[A]	5V4	C05-C03-C01	-3.37	100.11	103.43
5	B	404[A]	5V4	C05-C03-C01	-3.08	100.40	103.43
5	E	402[A]	5V4	C05-C03-C01	-3.02	100.45	103.43
5	C	402[A]	5V4	C05-C03-C01	-2.87	100.61	103.43
5	C	402[B]	5V4	C05-C03-C01	-2.30	101.16	103.43
5	C	402[A]	5V4	C03-C05-C04	-2.28	108.40	111.01
5	E	402[B]	5V4	C05-C03-C01	-2.22	101.25	103.43
5	D	401[A]	5V4	C03-C05-C04	-2.21	108.48	111.01
5	B	404[A]	5V4	C03-C05-C04	-2.12	108.58	111.01
5	D	401[A]	5V4	C05-C03-C01	-2.12	101.34	103.43
5	A	408[A]	5V4	C03-C05-C04	-2.04	108.68	111.01
5	E	402[A]	5V4	C03-C05-C04	-2.02	108.69	111.01
5	C	402[B]	5V4	C03-C05-C04	-2.02	108.69	111.01
5	D	401[A]	5V4	C08-C06-C04	-2.00	118.44	121.01
5	C	402[A]	5V4	C06-C04-C02	2.15	131.03	128.44
5	A	408[B]	5V4	C06-C04-C02	2.28	131.18	128.44
5	B	404[A]	5V4	C06-C04-C02	2.43	131.36	128.44
5	A	408[A]	5V4	C06-C04-C02	2.54	131.50	128.44
5	D	401[B]	5V4	C06-C04-C02	2.55	131.51	128.44
5	E	402[A]	5V4	C06-C04-C02	2.60	131.57	128.44
5	C	402[B]	5V4	C06-C04-C02	2.63	131.60	128.44
5	C	402[A]	5V4	C03-C01-C02	2.65	106.85	102.30
5	B	404[B]	5V4	C06-C04-C02	2.69	131.68	128.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	402[B]	5V4	C06-C04-C02	2.70	131.69	128.44
5	A	408[A]	5V4	C03-C01-C02	2.71	106.95	102.30
5	E	402[A]	5V4	C03-C01-C02	2.77	107.05	102.30
5	B	404[A]	5V4	C03-C01-C02	3.00	107.44	102.30
5	B	404[B]	5V4	C03-C01-C02	3.08	107.58	102.30
5	D	401[B]	5V4	C03-C01-C02	3.26	107.90	102.30
5	C	402[B]	5V4	C03-C01-C02	3.29	107.95	102.30
5	E	402[B]	5V4	C03-C01-C02	3.40	108.14	102.30
5	D	401[A]	5V4	C03-C01-C02	3.52	108.34	102.30
5	A	408[B]	5V4	C03-C01-C02	3.57	108.43	102.30

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	404	GOL	1	0
3	A	406	ACT	2	0
4	A	407	PEG	1	0
5	A	408[B]	5V4	1	0
3	B	401	ACT	1	0
6	B	402	PG4	2	0
7	B	403	TRS	1	0
5	B	404[B]	5V4	1	0
5	D	401[A]	5V4	4	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	381/393 (96%)	-0.25	14 (3%) 42 37	16, 23, 48, 98	0
1	B	383/393 (97%)	-0.32	9 (2%) 61 57	16, 26, 54, 105	0
1	C	380/393 (96%)	-0.36	11 (2%) 52 47	19, 27, 56, 83	0
1	D	384/393 (97%)	0.05	18 (4%) 32 27	20, 34, 65, 106	0
1	E	381/393 (96%)	-0.17	14 (3%) 42 37	19, 30, 54, 84	0
All	All	1909/1965 (97%)	-0.21	66 (3%) 44 39	16, 28, 58, 106	0

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	390	HIS	9.2
1	B	389	HIS	8.8
1	B	390	HIS	6.8
1	E	205	SER	6.4
1	D	389	HIS	6.4
1	D	388	HIS	5.9
1	E	208	PRO	5.6
1	B	206	GLY	5.4
1	E	206	GLY	5.2
1	C	88	PRO	4.9
1	C	207	ASP	4.1
1	D	86	ALA	4.0
1	D	209	ALA	4.0
1	D	88	PRO	3.9
1	B	388	HIS	3.8
1	A	388	HIS	3.7
1	D	210	ASP	3.7
1	E	210	ASP	3.7
1	A	206	GLY	3.6
1	D	391	HIS	3.6

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Mol	Chain	Res	Type	RSRZ
1	E	207	ASP	3.6
1	D	206	GLY	3.6
1	E	320	PRO	3.6
1	C	209	ALA	3.5
1	D	208	PRO	3.3
1	C	208	PRO	3.3
1	A	320	PRO	3.3
1	B	208	PRO	3.2
1	D	207	ASP	3.2
1	D	89	ASP	3.1
1	A	318	PRO	3.1
1	D	211	LEU	3.1
1	E	317	PRO	3.0
1	E	321	ALA	3.0
1	A	319	PRO	3.0
1	A	89	ASP	2.9
1	C	213	GLY	2.9
1	C	157	TRP	2.8
1	B	205	SER	2.8
1	D	122	ASP	2.8
1	E	316	THR	2.7
1	D	157	TRP	2.7
1	A	157	TRP	2.7
1	A	317	PRO	2.6
1	D	320	PRO	2.6
1	A	316	THR	2.6
1	A	208	PRO	2.6
1	C	205	SER	2.5
1	C	212	ALA	2.5
1	A	209	ALA	2.5
1	D	179[A]	TRP	2.4
1	B	157	TRP	2.4
1	E	157	TRP	2.4
1	A	88	PRO	2.4
1	B	387	SER	2.4
1	D	212	ALA	2.3
1	E	2	GLU	2.3
1	C	316	THR	2.3
1	E	211	LEU	2.3
1	A	250	LEU	2.3
1	E	315	PRO	2.2
1	A	120	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	210	ASP	2.2
1	C	206	GLY	2.2
1	B	207	ASP	2.1
1	E	246	LEU	2.1

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PEG	A	407	7/7	0.63	0.27	9.62	71,72,74,76	0
6	PG4	B	402	13/13	0.76	0.23	9.31	46,73,80,81	0
2	GOL	C	401	6/6	0.85	0.23	8.43	51,64,66,72	0
2	GOL	A	404	6/6	0.86	0.26	6.77	66,69,71,73	0
7	TRS	B	403	8/8	0.81	0.24	4.80	34,49,58,60	0
2	GOL	A	402	6/6	0.97	0.21	4.35	31,45,45,53	0
5	5V4	B	404[B]	11/11	0.94	0.15	3.46	26,29,33,34	11
2	GOL	A	403	6/6	0.87	0.16	3.42	60,63,65,66	0
3	ACT	A	406	4/4	0.88	0.14	2.88	54,55,58,61	0
5	5V4	B	404[A]	11/11	0.94	0.15	2.51	24,29,31,31	11
5	5V4	D	401[B]	11/11	0.90	0.18	1.75	32,36,40,41	11
5	5V4	D	401[A]	11/11	0.90	0.18	1.69	30,36,39,42	11
5	5V4	C	402[A]	11/11	0.96	0.12	1.52	23,28,30,31	11
5	5V4	C	402[B]	11/11	0.96	0.12	1.26	26,30,32,33	11
2	GOL	E	401	6/6	0.89	0.22	1.14	50,57,64,66	0
5	5V4	A	408[B]	11/11	0.93	0.13	0.92	18,23,27,30	11
5	5V4	E	402[B]	11/11	0.96	0.11	0.70	26,30,33,33	11

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
5	5V4	A	408[A]	11/11	0.93	0.13	0.70	21,25,28,30	11
5	5V4	E	402[A]	11/11	0.96	0.11	0.56	28,30,33,33	11
3	ACT	B	401	4/4	0.91	0.11	-	50,59,59,61	0
2	GOL	A	405	6/6	0.74	0.24	-	67,69,69,70	0
2	GOL	A	401	6/6	0.81	0.24	-	41,59,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.