



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:19 PM GMT

PDB ID : 4L6D  
Title : Crystal structure of 5-carboxyvanillate decarboxylase from *Sphingomonas paucimobilis* complexed with vanillic acid  
Authors : Fedorov, A.A.; Fedorov, E.V.; Vladimirova, A.; Raushel, F.M.; Almo, S.C.  
Deposited on : 2013-06-12  
Resolution : 1.45 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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

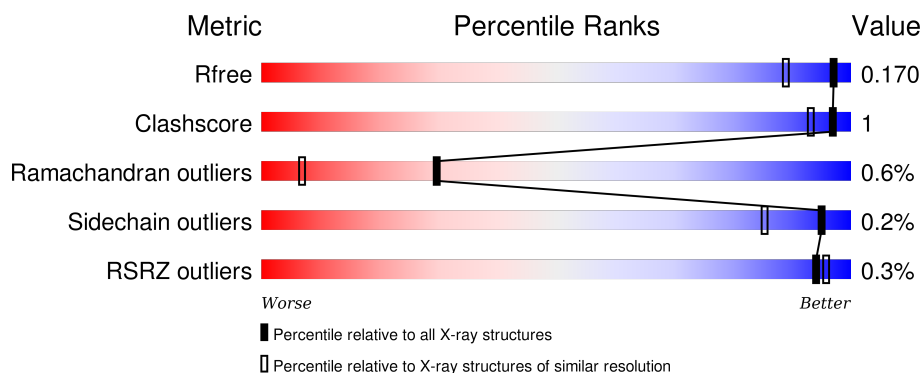
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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.




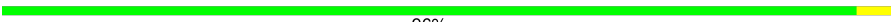

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1164 (1.46-1.42)
Clashscore	102246	1219 (1.46-1.42)
Ramachandran outliers	100387	1200 (1.46-1.42)
Sidechain outliers	100360	1200 (1.46-1.42)
RSRZ outliers	91569	1166 (1.46-1.42)

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	335	<div> <div>97%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	B	335	<div> <div>98%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	C	335	<div> <div>96%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	D	335	<div> <div>97%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>
1	E	335	<div> <div>96%</div> <div> <div></div> <div></div> <div></div> <div></div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	F	335	 96% .
1	G	335	 96% .
1	H	335	 95% 5%

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
3	VNL	A	404	-	-	-	X
3	VNL	B	403	-	-	-	X
3	VNL	B	404	-	-	-	X
3	VNL	C	403	-	-	-	X
3	VNL	D	403	-	-	-	X
3	VNL	E	403	-	-	-	X
3	VNL	E	404	-	-	-	X
3	VNL	F	403	-	-	-	X
3	VNL	G	403	-	-	-	X
3	VNL	G	404	-	-	-	X
3	VNL	H	403	-	-	-	X
4	EPE	A	405	-	-	-	X
4	EPE	B	405	-	-	-	X
4	EPE	C	404	-	-	-	X
4	EPE	D	404	-	-	-	X
4	EPE	E	405	-	-	-	X
4	EPE	F	404	-	-	-	X
4	EPE	G	405	-	-	-	X
4	EPE	H	404	-	-	-	X
5	GOL	C	405	-	-	-	X
6	PEG	E	406	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 24897 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 5-carboxyvanillate decarboxylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	4	0
			2643	1675	466	489	13			
1	B	335	Total	C	N	O	S	0	2	0
			2629	1668	464	484	13			
1	C	335	Total	C	N	O	S	0	2	0
			2623	1664	461	485	13			
1	D	335	Total	C	N	O	S	0	4	0
			2641	1674	463	491	13			
1	E	335	Total	C	N	O	S	0	2	0
			2628	1669	464	482	13			
1	F	335	Total	C	N	O	S	0	3	0
			2635	1671	463	488	13			
1	G	335	Total	C	N	O	S	0	3	0
			2637	1672	468	484	13			
1	H	335	Total	C	N	O	S	0	4	0
			2645	1676	467	489	13			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	SER	-	EXPRESSION TAG	UNP Q8RJ47
A	1	LEU	-	EXPRESSION TAG	UNP Q8RJ47
B	0	SER	-	EXPRESSION TAG	UNP Q8RJ47
B	1	LEU	-	EXPRESSION TAG	UNP Q8RJ47
C	0	SER	-	EXPRESSION TAG	UNP Q8RJ47
C	1	LEU	-	EXPRESSION TAG	UNP Q8RJ47
D	0	SER	-	EXPRESSION TAG	UNP Q8RJ47
D	1	LEU	-	EXPRESSION TAG	UNP Q8RJ47
E	0	SER	-	EXPRESSION TAG	UNP Q8RJ47
E	1	LEU	-	EXPRESSION TAG	UNP Q8RJ47
F	0	SER	-	EXPRESSION TAG	UNP Q8RJ47
F	1	LEU	-	EXPRESSION TAG	UNP Q8RJ47
G	0	SER	-	EXPRESSION TAG	UNP Q8RJ47

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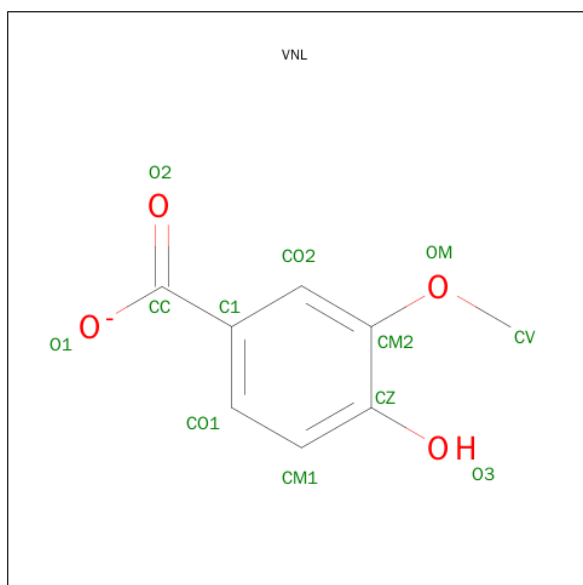
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Chain	Residue	Modelled	Actual	Comment	Reference
G	1	LEU	-	EXPRESSION TAG	UNP Q8RJ47
H	0	SER	-	EXPRESSION TAG	UNP Q8RJ47
H	1	LEU	-	EXPRESSION TAG	UNP Q8RJ47

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

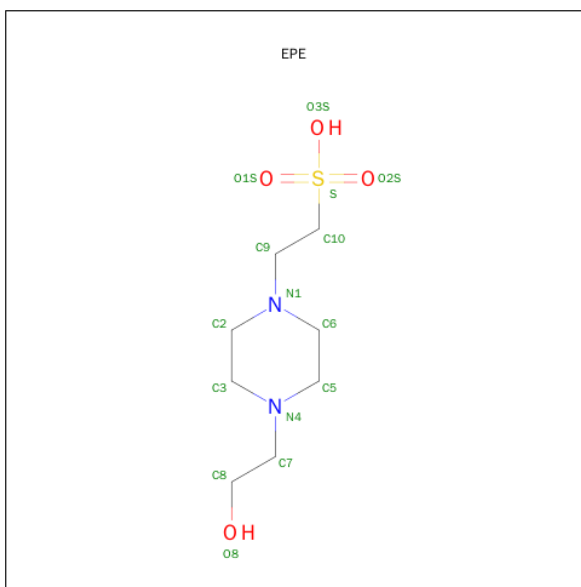
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mn 1 1	0	0
2	D	1	Total Mn 1 1	0	0
2	E	1	Total Mn 1 1	0	0
2	H	1	Total Mn 1 1	0	0
2	B	1	Total Mn 1 1	0	0
2	C	1	Total Mn 1 1	0	0
2	A	2	Total Mn 2 2	0	0
2	F	1	Total Mn 1 1	0	0

- Molecule 3 is 4-HYDROXY-3-METHOXYBENZOATE (three-letter code: VNL) (formula: C<sub>8</sub>H<sub>7</sub>O<sub>4</sub>).



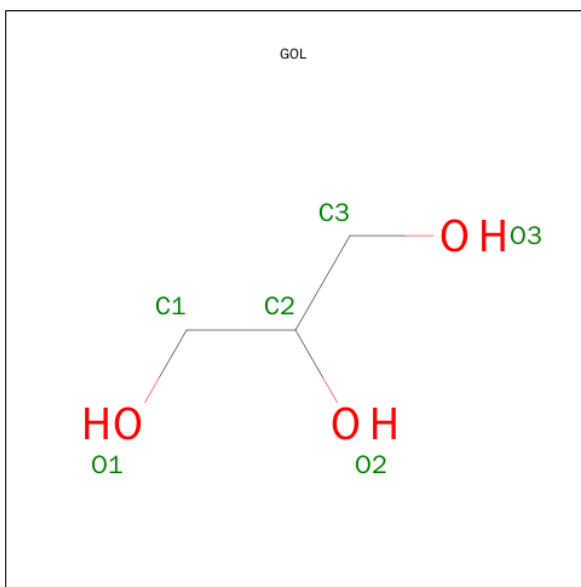
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 12 8 4	0	0
3	A	1	Total C O 12 8 4	0	0
3	A	1	Total C O 12 8 4	0	0
3	B	1	Total C O 12 8 4	0	0
3	B	1	Total C O 12 8 4	0	0
3	B	1	Total C O 12 8 4	0	0
3	C	1	Total C O 12 8 4	0	0
3	C	1	Total C O 12 8 4	0	0
3	D	1	Total C O 12 8 4	0	0
3	D	1	Total C O 12 8 4	0	0
3	E	1	Total C O 12 8 4	0	0
3	E	1	Total C O 12 8 4	0	0
3	E	1	Total C O 12 8 4	0	0
3	F	1	Total C O 12 8 4	0	0
3	F	1	Total C O 12 8 4	0	0
3	G	1	Total C O 12 8 4	0	0
3	G	1	Total C O 12 8 4	0	0
3	G	1	Total C O 12 8 4	0	0
3	H	1	Total C O 12 8 4	0	0
3	H	1	Total C O 12 8 4	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: C<sub>8</sub>H<sub>18</sub>N<sub>2</sub>O<sub>4</sub>S).



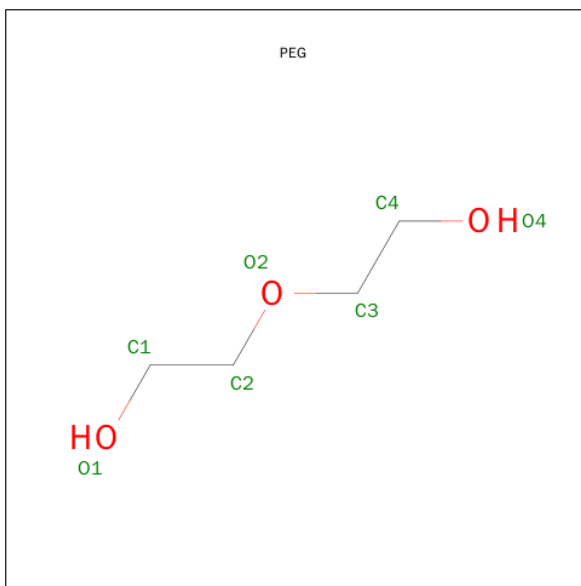
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	7	2	1		
4	B	1	Total	C	N	O	0	0
			10	7	2	1		
4	C	1	Total	C	N	O	0	0
			10	7	2	1		
4	D	1	Total	C	N	O	0	0
			10	7	2	1		
4	E	1	Total	C	N	O	0	0
			10	7	2	1		
4	F	1	Total	C	N	O	0	0
			10	7	2	1		
4	G	1	Total	C	N	O	0	0
			10	7	2	1		
4	H	1	Total	C	N	O	0	0
			10	7	2	1		

- Molecule 5 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
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



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

- Molecule 7 is water.



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	444	Total 446	O 446	0	2
7	B	467	Total 469	O 469	0	2
7	C	412	Total 416	O 416	0	4
7	D	418	Total 419	O 419	0	1
7	E	423	Total 423	O 423	0	0
7	F	420	Total 422	O 422	0	2
7	G	457	Total 460	O 460	0	3
7	H	413	Total 419	O 419	0	6

### 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 errors 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: 5-carboxyvanillate decarboxylase

Chain A:  97%



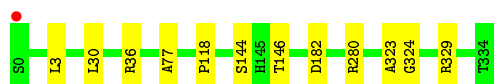
- Molecule 1: 5-carboxyvanillate decarboxylase

Chain B:  98%



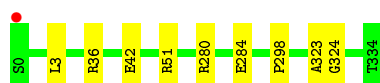
- Molecule 1: 5-carboxyvanillate decarboxylase

Chain C:  96%



- Molecule 1: 5-carboxyvanillate decarboxylase

Chain D:  97%



- Molecule 1: 5-carboxyvanillate decarboxylase

Chain E:  96%



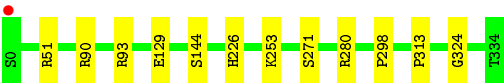
- Molecule 1: 5-carboxyvanillate decarboxylase

Chain F:  96% .



• Molecule 1: 5-carboxyvanillate decarboxylase

Chain G:  96% .



• Molecule 1: 5-carboxyvanillate decarboxylase

Chain H:  95% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	80.59 Å 96.92 Å 97.03 Å 109.71° 90.53° 111.89°	Depositor
Resolution (Å)	37.22 – 1.45 38.53 – 1.45	Depositor EDS
% Data completeness (in resolution range)	94.1 (37.22-1.45) 83.1 (38.53-1.45)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.90 (at 1.45 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.146 , 0.168 0.148 , 0.170	Depositor DCC
$R_{free}$ test set	21272 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.1	Xtriage
Anisotropy	0.160	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 43.9	EDS
Estimated twinning fraction	0.005 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 423773 reflections	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	24897	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.47% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PEG, GOL, EPE, VNL, MN

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	0.33	0/2706	0.56	0/3678
1	B	0.33	0/2692	0.56	0/3659
1	C	0.32	0/2686	0.54	0/3652
1	D	0.33	0/2704	0.55	0/3676
1	E	0.32	0/2691	0.55	0/3658
1	F	0.33	0/2698	0.54	0/3668
1	G	0.33	0/2700	0.56	0/3669
1	H	0.33	0/2708	0.55	0/3682
All	All	0.33	0/21585	0.55	0/29342

There are no bond length outliers.

There are no bond angle outliers.

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	2643	0	2601	7	0
1	B	2629	0	2594	4	0
1	C	2623	0	2584	8	0
1	D	2641	0	2594	6	0
1	E	2628	0	2599	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	2635	0	2592	8	0
1	G	2637	0	2605	8	0
1	H	2645	0	2603	10	0
2	A	2	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	36	0	20	2	0
3	B	36	0	20	0	0
3	C	24	0	13	1	0
3	D	24	0	13	1	0
3	E	36	0	20	1	0
3	F	24	0	13	1	0
3	G	36	0	20	0	0
3	H	24	0	13	0	0
4	A	10	0	13	0	0
4	B	10	0	13	0	0
4	C	10	0	13	0	0
4	D	10	0	13	0	0
4	E	10	0	13	0	0
4	F	10	0	13	0	0
4	G	10	0	13	0	0
4	H	10	0	13	0	0
5	C	6	0	8	0	0
6	E	7	0	10	0	0
7	A	446	0	0	2	0
7	B	469	0	0	1	0
7	C	416	0	0	3	0
7	D	419	0	0	3	0
7	E	423	0	0	0	0
7	F	422	0	0	3	0
7	G	460	0	0	5	0
7	H	419	0	0	4	0
All	All	24897	0	21026	55	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 1.

All (55) 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:G:51:ARG:NH2	1:G:298:PRO:O	2.23	0.72
1:G:51:ARG:NH2	7:G:947:HOH:O	2.22	0.71
1:D:280:ARG:NH2	1:E:284:GLU:OE1	2.32	0.63
1:D:36:ARG:NH2	7:D:741:HOH:O	2.33	0.61
1:F:51:ARG:NH2	1:F:298:PRO:O	2.35	0.60
3:A:404:VNL:HV1	3:E:404:VNL:HV1	1.86	0.57
1:H:56:THR:HG22	7:H:906:HOH:O	2.06	0.54
1:A:280[A]:ARG:NH1	1:H:284[A]:GLU:OE1	2.37	0.53
1:A:280[B]:ARG:HG3	7:A:924:HOH:O	2.10	0.51
1:C:36:ARG:NH2	7:C:718:HOH:O	2.43	0.50
1:H:284[B]:GLU:HG3	7:H:708:HOH:O	2.11	0.49
1:H:20[B]:ARG:HD2	1:H:39:TYR:O	2.12	0.49
1:A:180:GLN:HG2	1:H:183:ARG:HD2	1.94	0.49
1:A:239:ASP:OD2	3:A:404:VNL:O3	2.24	0.49
1:B:90:ARG:NH2	7:B:767:HOH:O	2.45	0.49
1:G:129:GLU:OE1	7:G:929:HOH:O	2.20	0.48
1:E:98:LEU:HA	1:E:101:GLN:HG2	1.95	0.48
1:G:280[B]:ARG:HD2	1:G:313:PRO:HG2	1.95	0.47
1:H:106[A]:ASN:OD1	7:H:906:HOH:O	2.20	0.47
1:F:177:PRO:HB3	1:F:181:ILE:HG13	1.97	0.46
1:G:90[B]:ARG:NH2	7:G:901:HOH:O	2.49	0.46
1:C:329:ARG:NH1	7:C:744:HOH:O	2.27	0.45
1:F:284[B]:GLU:HG3	7:F:733:HOH:O	2.16	0.45
1:F:69:ASP:HB2	7:F:621[B]:HOH:O	2.15	0.45
1:A:328:ALA:HA	1:A:333:ILE:HB	1.99	0.45
1:D:42:GLU:OE1	7:D:915:HOH:O	2.21	0.44
3:D:403:VNL:HV1	3:F:403:VNL:HV1	2.00	0.44
1:B:86:GLU:OE2	1:B:90:ARG:NH1	2.51	0.43
1:A:284[B]:GLU:HG3	7:A:664:HOH:O	2.18	0.43
1:C:30:LEU:HD22	1:C:182:ASP:HB2	2.01	0.43
1:D:3:LEU:HD23	1:D:323:ALA:HB1	2.00	0.43
1:G:93:ARG:NH1	7:G:952[B]:HOH:O	2.52	0.43
1:F:14:PRO:HG2	1:F:94:ILE:HG21	2.00	0.43
1:B:226:HIS:HA	1:B:271:SER:O	2.19	0.43
1:F:280:ARG:NH2	7:F:697:HOH:O	2.47	0.43
1:H:118:PRO:HG2	1:H:146:THR:OG1	2.18	0.43
1:H:94:ILE:HD13	7:H:701:HOH:O	2.18	0.42
1:E:14:PRO:HG2	1:E:94:ILE:HG21	2.00	0.42
1:C:77:ALA:HB3	3:C:402:VNL:HV1	2.01	0.42
1:C:118:PRO:HG2	1:C:146:THR:OG1	2.20	0.42
1:F:269:THR:HA	1:F:292:MET:O	2.19	0.42
1:D:284[B]:GLU:HG3	7:D:840:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:226:HIS:HA	1:E:271:SER:O	2.20	0.42
1:E:328:ALA:HA	1:E:333:ILE:HB	2.02	0.42
1:E:118:PRO:HG2	1:E:146:THR:OG1	2.20	0.41
1:B:142:ILE:HD12	1:B:142:ILE:HA	1.98	0.41
1:G:226:HIS:HA	1:G:271:SER:O	2.20	0.41
1:C:280:ARG:HH22	1:F:284[A]:GLU:CD	2.24	0.41
1:H:226:HIS:HA	1:H:271:SER:O	2.21	0.41
1:D:51:ARG:NH2	1:D:298:PRO:O	2.54	0.41
1:G:253:LYS:HE3	7:G:949:HOH:O	2.21	0.41
1:H:262:PHE:O	1:H:266:PHE:HB2	2.22	0.40
1:A:226:HIS:HA	1:A:271:SER:O	2.21	0.40
1:C:3:LEU:HD23	1:C:323:ALA:HB1	2.03	0.40
1:C:280:ARG:NH2	7:C:900:HOH:O	2.28	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	337/335 (101%)	329 (98%)	6 (2%)	2 (1%)	30	7
1	B	335/335 (100%)	328 (98%)	5 (2%)	2 (1%)	30	7
1	C	335/335 (100%)	327 (98%)	6 (2%)	2 (1%)	30	7
1	D	337/335 (101%)	329 (98%)	7 (2%)	1 (0%)	46	18
1	E	335/335 (100%)	326 (97%)	7 (2%)	2 (1%)	30	7
1	F	336/335 (100%)	328 (98%)	6 (2%)	2 (1%)	30	7
1	G	336/335 (100%)	329 (98%)	5 (2%)	2 (1%)	30	7
1	H	337/335 (101%)	326 (97%)	9 (3%)	2 (1%)	30	7
All	All	2688/2680 (100%)	2622 (98%)	51 (2%)	15 (1%)	30	7



All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	144	SER
1	A	324	GLY
1	B	324	GLY
1	C	144	SER
1	C	324	GLY
1	D	324	GLY
1	E	324	GLY
1	F	144	SER
1	F	324	GLY
1	G	324	GLY
1	H	324	GLY
1	B	144	SER
1	H	144	SER
1	E	144	SER
1	G	144	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	274/270 (102%)	273 (100%)	1 (0%)	93	82
1	B	272/270 (101%)	271 (100%)	1 (0%)	93	82
1	C	272/270 (101%)	272 (100%)	0	100	100
1	D	274/270 (102%)	274 (100%)	0	100	100
1	E	272/270 (101%)	271 (100%)	1 (0%)	93	82
1	F	273/270 (101%)	272 (100%)	1 (0%)	93	82
1	G	273/270 (101%)	273 (100%)	0	100	100
1	H	274/270 (102%)	273 (100%)	1 (0%)	93	82
All	All	2184/2160 (101%)	2179 (100%)	5 (0%)	95	85

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

Mol	Chain	Res	Type
1	A	296	ASP
1	B	171	TYR
1	E	161	GLU
1	F	171	TYR
1	H	171	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 39 ligands modelled in this entry, 9 are monoatomic - leaving 30 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$
3	VNL	A	402	2	9,12,12	1.55	1 (11%)	12,16,16	1.24	1 (8%)
3	VNL	A	403	-	9,12,12	1.77	1 (11%)	12,16,16	1.19	1 (8%)
3	VNL	A	404	-	9,12,12	1.73	1 (11%)	12,16,16	1.38	2 (16%)
4	EPE	A	405	-	10,10,15	0.48	0	12,12,20	1.74	1 (8%)
3	VNL	B	402	2	9,12,12	1.60	1 (11%)	12,16,16	1.15	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	VNL	B	403	-	9,12,12	1.84	1 (11%)	12,16,16	1.39	2 (16%)
3	VNL	B	404	-	9,12,12	1.85	1 (11%)	12,16,16	1.18	2 (16%)
4	EPE	B	405	-	10,10,15	0.43	0	12,12,20	1.68	1 (8%)
3	VNL	C	402	2	9,12,12	1.60	1 (11%)	12,16,16	1.45	2 (16%)
3	VNL	C	403	-	9,12,12	1.87	1 (11%)	12,16,16	1.47	2 (16%)
4	EPE	C	404	-	10,10,15	0.50	0	12,12,20	1.61	1 (8%)
5	GOL	C	405	-	5,5,5	0.37	0	5,5,5	0.44	0
3	VNL	D	402	2	9,12,12	1.55	1 (11%)	12,16,16	1.44	3 (25%)
3	VNL	D	403	-	9,12,12	1.81	1 (11%)	12,16,16	1.31	2 (16%)
4	EPE	D	404	-	10,10,15	0.46	0	12,12,20	1.61	2 (16%)
3	VNL	E	402	2	9,12,12	1.55	1 (11%)	12,16,16	1.11	0
3	VNL	E	403	-	9,12,12	1.98	1 (11%)	12,16,16	1.45	3 (25%)
3	VNL	E	404	-	9,12,12	1.80	1 (11%)	12,16,16	1.26	2 (16%)
4	EPE	E	405	-	10,10,15	0.49	0	12,12,20	1.67	1 (8%)
6	PEG	E	406	-	6,6,6	0.50	0	5,5,5	0.22	0
3	VNL	F	402	2	9,12,12	1.63	1 (11%)	12,16,16	1.20	1 (8%)
3	VNL	F	403	-	9,12,12	1.81	1 (11%)	12,16,16	1.38	3 (25%)
4	EPE	F	404	-	10,10,15	0.44	0	12,12,20	1.61	2 (16%)
3	VNL	G	402	2	9,12,12	1.54	1 (11%)	12,16,16	1.25	2 (16%)
3	VNL	G	403	-	9,12,12	1.84	1 (11%)	12,16,16	1.37	3 (25%)
3	VNL	G	404	-	9,12,12	1.85	1 (11%)	12,16,16	1.25	2 (16%)
4	EPE	G	405	-	10,10,15	0.47	0	12,12,20	1.73	1 (8%)
3	VNL	H	402	2	9,12,12	1.60	1 (11%)	12,16,16	1.22	2 (16%)
3	VNL	H	403	-	9,12,12	1.88	1 (11%)	12,16,16	1.39	3 (25%)
4	EPE	H	404	-	10,10,15	0.48	0	12,12,20	1.62	2 (16%)

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	VNL	A	402	2	-	0/2/6/6	0/1/1/1
3	VNL	A	403	-	-	0/2/6/6	0/1/1/1
3	VNL	A	404	-	-	0/2/6/6	0/1/1/1
4	EPE	A	405	-	-	0/3/13/19	0/1/1/1
3	VNL	B	402	2	-	0/2/6/6	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	VNL	B	403	-	-	0/2/6/6	0/1/1/1
3	VNL	B	404	-	-	0/2/6/6	0/1/1/1
4	EPE	B	405	-	-	0/3/13/19	0/1/1/1
3	VNL	C	402	2	-	0/2/6/6	0/1/1/1
3	VNL	C	403	-	-	0/2/6/6	0/1/1/1
4	EPE	C	404	-	-	0/3/13/19	0/1/1/1
5	GOL	C	405	-	-	0/4/4/4	0/0/0/0
3	VNL	D	402	2	-	0/2/6/6	0/1/1/1
3	VNL	D	403	-	-	0/2/6/6	0/1/1/1
4	EPE	D	404	-	-	0/3/13/19	0/1/1/1
3	VNL	E	402	2	-	0/2/6/6	0/1/1/1
3	VNL	E	403	-	-	0/2/6/6	0/1/1/1
3	VNL	E	404	-	-	0/2/6/6	0/1/1/1
4	EPE	E	405	-	-	0/3/13/19	0/1/1/1
6	PEG	E	406	-	-	0/4/4/4	0/0/0/0
3	VNL	F	402	2	-	0/2/6/6	0/1/1/1
3	VNL	F	403	-	-	0/2/6/6	0/1/1/1
4	EPE	F	404	-	-	0/3/13/19	0/1/1/1
3	VNL	G	402	2	-	0/2/6/6	0/1/1/1
3	VNL	G	403	-	-	0/2/6/6	0/1/1/1
3	VNL	G	404	-	-	0/2/6/6	0/1/1/1
4	EPE	G	405	-	-	0/3/13/19	0/1/1/1
3	VNL	H	402	2	-	0/2/6/6	0/1/1/1
3	VNL	H	403	-	-	0/2/6/6	0/1/1/1
4	EPE	H	404	-	-	0/3/13/19	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	402	VNL	CZ-CM2	3.98	1.46	1.40
3	G	402	VNL	CZ-CM2	3.99	1.46	1.40
3	B	402	VNL	CZ-CM2	4.07	1.46	1.40
3	E	402	VNL	CZ-CM2	4.14	1.46	1.40
3	F	402	VNL	CZ-CM2	4.18	1.47	1.40
3	A	402	VNL	CZ-CM2	4.22	1.47	1.40
3	C	402	VNL	CZ-CM2	4.25	1.47	1.40
3	H	402	VNL	CZ-CM2	4.28	1.47	1.40
3	A	404	VNL	CZ-CM2	4.67	1.47	1.40
3	A	403	VNL	CZ-CM2	4.76	1.47	1.40
3	D	403	VNL	CZ-CM2	4.83	1.48	1.40
3	E	404	VNL	CZ-CM2	4.86	1.48	1.40
3	B	404	VNL	CZ-CM2	4.88	1.48	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	404	VNL	CZ-CM2	4.90	1.48	1.40
3	F	403	VNL	CZ-CM2	4.91	1.48	1.40
3	G	403	VNL	CZ-CM2	4.91	1.48	1.40
3	B	403	VNL	CZ-CM2	4.94	1.48	1.40
3	C	403	VNL	CZ-CM2	4.99	1.48	1.40
3	H	403	VNL	CZ-CM2	5.05	1.48	1.40
3	E	403	VNL	CZ-CM2	5.39	1.48	1.40

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	402	VNL	O3-CZ-CM2	-2.31	114.80	120.10
3	G	402	VNL	O3-CZ-CM2	-2.30	114.80	120.10
3	B	404	VNL	CO1-C1-CO2	2.00	120.83	118.17
3	A	404	VNL	CV-OM-CM2	2.01	120.59	117.54
4	F	404	EPE	C7-N4-C3	2.01	116.42	111.27
4	D	404	EPE	C7-N4-C3	2.01	116.42	111.27
3	H	402	VNL	CO1-C1-CO2	2.02	120.85	118.17
3	F	403	VNL	OM-CM2-CZ	2.05	117.27	114.57
3	G	404	VNL	CO1-C1-CO2	2.05	120.89	118.17
3	G	403	VNL	OM-CM2-CZ	2.07	117.29	114.57
3	F	402	VNL	CO1-C1-CO2	2.07	120.92	118.17
3	E	404	VNL	OM-CM2-CZ	2.09	117.33	114.57
4	H	404	EPE	C7-N4-C3	2.11	116.66	111.27
3	F	403	VNL	CV-OM-CM2	2.13	120.77	117.54
3	D	403	VNL	OM-CM2-CZ	2.14	117.39	114.57
3	G	403	VNL	CV-OM-CM2	2.17	120.83	117.54
3	D	402	VNL	CO1-C1-CO2	2.19	121.08	118.17
3	G	402	VNL	CO1-C1-CO2	2.19	121.08	118.17
3	H	403	VNL	OM-CM2-CZ	2.20	117.46	114.57
3	H	403	VNL	CV-OM-CM2	2.20	120.88	117.54
3	E	403	VNL	CO1-C1-CO2	2.20	121.09	118.17
3	A	402	VNL	CO1-C1-CO2	2.28	121.20	118.17
3	A	403	VNL	CO1-C1-CO2	2.30	121.22	118.17
3	B	404	VNL	CV-OM-CM2	2.33	121.08	117.54
3	H	402	VNL	CV-OM-CM2	2.34	121.09	117.54
3	E	403	VNL	CV-OM-CM2	2.45	121.26	117.54
3	C	402	VNL	CO1-C1-CO2	2.46	121.44	118.17
3	D	403	VNL	CO1-C1-CO2	2.48	121.46	118.17
3	E	404	VNL	CO1-C1-CO2	2.50	121.48	118.17
3	G	403	VNL	CO1-C1-CO2	2.50	121.49	118.17
3	B	403	VNL	CV-OM-CM2	2.52	121.36	117.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	403	VNL	CV-OM-CM2	2.54	121.39	117.54
3	B	403	VNL	CO1-C1-CO2	2.62	121.64	118.17
3	H	403	VNL	CO1-C1-CO2	2.63	121.66	118.17
3	F	403	VNL	CO1-C1-CO2	2.64	121.67	118.17
3	C	403	VNL	CO1-C1-CO2	2.66	121.70	118.17
3	G	404	VNL	CV-OM-CM2	2.69	121.63	117.54
3	A	404	VNL	CO1-C1-CO2	2.76	121.83	118.17
3	D	402	VNL	CV-OM-CM2	2.91	121.95	117.54
3	C	402	VNL	CV-OM-CM2	2.94	122.01	117.54
3	E	403	VNL	OM-CM2-CZ	3.19	118.77	114.57
4	F	404	EPE	C5-N4-C3	4.03	117.63	108.90
4	H	404	EPE	C5-N4-C3	4.05	117.67	108.90
4	C	404	EPE	C5-N4-C3	4.07	117.72	108.90
4	D	404	EPE	C5-N4-C3	4.10	117.79	108.90
4	B	405	EPE	C5-N4-C3	4.11	117.79	108.90
4	A	405	EPE	C5-N4-C3	4.21	118.01	108.90
4	E	405	EPE	C5-N4-C3	4.30	118.21	108.90
4	G	405	EPE	C5-N4-C3	4.33	118.28	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	404	VNL	2	0
3	C	402	VNL	1	0
3	D	403	VNL	1	0
3	E	404	VNL	1	0
3	F	403	VNL	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 [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	335/335 (100%)	-0.52	1 (0%) 94 96	4, 8, 16, 39	0
1	B	335/335 (100%)	-0.49	1 (0%) 94 96	5, 8, 16, 40	0
1	C	335/335 (100%)	-0.41	1 (0%) 94 96	5, 10, 21, 48	0
1	D	335/335 (100%)	-0.45	1 (0%) 94 96	5, 8, 19, 34	0
1	E	335/335 (100%)	-0.41	1 (0%) 94 96	5, 10, 21, 37	0
1	F	335/335 (100%)	-0.45	1 (0%) 94 96	5, 9, 19, 34	0
1	G	335/335 (100%)	-0.43	1 (0%) 94 96	5, 8, 16, 41	0
1	H	335/335 (100%)	-0.44	1 (0%) 94 96	5, 9, 18, 33	0
All	All	2680/2680 (100%)	-0.45	8 (0%) 94 96	4, 9, 19, 48	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	0	SER	3.5
1	H	0	SER	3.5
1	E	0	SER	3.1
1	G	0	SER	3.0
1	D	0	SER	3.0
1	F	0	SER	3.0
1	C	0	SER	2.6
1	A	0	SER	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 ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å <sup>2</sup> )	Q<0.9
3	VNL	C	403	12/12	0.85	0.21	13.09	15,22,28,31	0
3	VNL	A	404	12/12	0.80	0.23	11.37	19,23,27,29	0
4	EPE	F	404	10/15	0.90	0.15	11.11	11,25,28,30	0
3	VNL	G	403	12/12	0.84	0.22	10.00	18,25,27,27	0
3	VNL	B	403	12/12	0.90	0.20	9.47	14,20,23,27	0
4	EPE	H	404	10/15	0.91	0.13	9.24	12,21,28,33	0
3	VNL	F	403	12/12	0.78	0.25	9.22	19,26,30,30	0
4	EPE	A	405	10/15	0.89	0.16	9.21	10,22,24,30	0
4	EPE	B	405	10/15	0.90	0.15	9.05	10,25,28,31	0
4	EPE	G	405	10/15	0.91	0.16	9.04	11,22,25,30	0
3	VNL	E	404	12/12	0.81	0.19	8.91	18,21,25,26	0
5	GOL	C	405	6/6	0.79	0.20	8.37	23,28,29,35	0
3	VNL	H	403	12/12	0.86	0.19	7.82	20,23,24,26	0
4	EPE	E	405	10/15	0.82	0.17	7.82	12,25,29,32	0
4	EPE	C	404	10/15	0.90	0.14	7.25	11,22,27,31	0
4	EPE	D	404	10/15	0.91	0.11	6.22	14,27,27,30	0
6	PEG	E	406	7/7	0.80	0.17	5.85	22,27,33,33	0
3	VNL	D	403	12/12	0.83	0.16	5.82	20,24,26,27	0
3	VNL	B	404	12/12	0.83	0.20	4.52	33,36,45,45	0
3	VNL	G	404	12/12	0.85	0.22	4.50	28,32,35,40	0
3	VNL	E	403	12/12	0.92	0.09	2.90	18,19,26,29	0
3	VNL	C	402	12/12	0.95	0.09	1.77	11,12,13,13	0
3	VNL	H	402	12/12	0.95	0.08	1.21	8,10,11,12	0
3	VNL	F	402	12/12	0.94	0.08	0.75	8,12,13,14	0
3	VNL	A	402	12/12	0.95	0.07	0.68	8,10,12,12	0
3	VNL	D	402	12/12	0.96	0.07	0.57	8,11,12,13	0
3	VNL	A	403	12/12	0.97	0.09	0.16	9,12,17,19	0
3	VNL	E	402	12/12	0.97	0.06	-0.75	10,12,13,14	0
3	VNL	B	402	12/12	0.98	0.06	-0.91	7,10,12,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	VNL	G	402	12/12	0.97	0.06	-1.18	7,9,10,14	0
2	MN	B	401	1/1	1.00	0.03	-	5,5,5,5	0
2	MN	A	401	1/1	1.00	0.03	-	5,5,5,5	0
2	MN	E	401	1/1	1.00	0.03	-	7,7,7,7	0
2	MN	D	401	1/1	1.00	0.03	-	5,5,5,5	0
2	MN	H	401	1/1	1.00	0.03	-	6,6,6,6	0
2	MN	G	401	1/1	1.00	0.04	-	6,6,6,6	0
2	MN	A	406	1/1	0.95	0.09	-	11,11,11,11	1
2	MN	F	401	1/1	1.00	0.03	-	6,6,6,6	0
2	MN	C	401	1/1	1.00	0.02	-	7,7,7,7	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.