



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 25, 2023 – 08:01 AM EDT

PDB ID : 3E5P  
Title : Crystal structure of alanine racemase from E.faecalis  
Authors : Hwang, K.Y.; Priyadarshi, A.; Lee, E.H.; Sung, M.W.  
Deposited on : 2008-08-14  
Resolution : 2.50 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>.

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

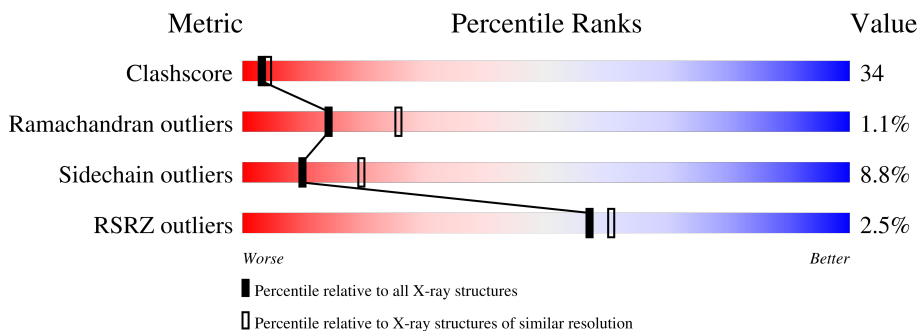
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	371	 3% 49% 41% 9%
1	B	371	 4% 55% 39% 5%
1	C	371	 % 53% 39% 8%

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	PLP	B	390	-	X	-	-
3	PPI	C	400	-	-	X	-
4	EPE	A	430	-	X	X	-

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8905 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.

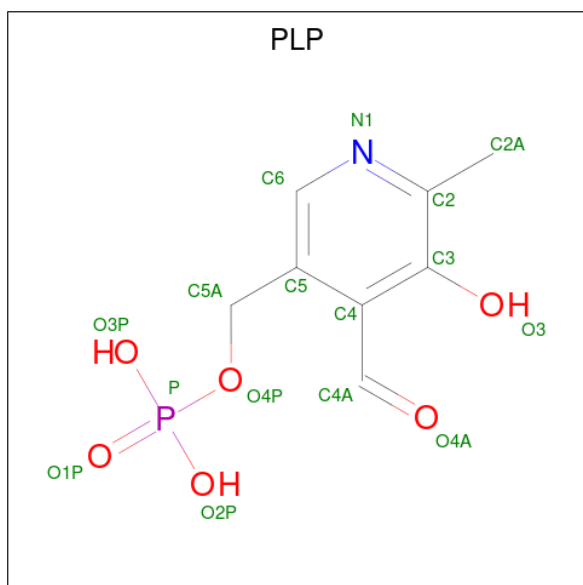
- Molecule 1 is a protein called Alanine racemase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	370	Total 2879	C 1835	N 494	O 538	S 12	0	0	0
1	B	371	Total 2887	C 1840	N 495	O 539	S 13	0	0	0
1	C	371	Total 2887	C 1840	N 495	O 539	S 13	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

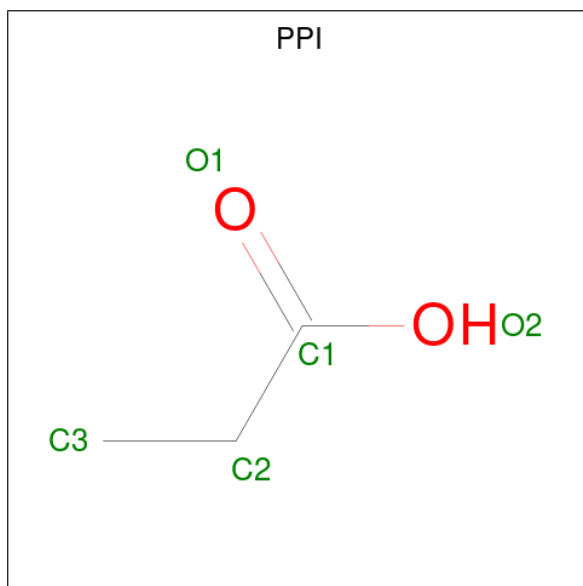
Chain	Residue	Modelled	Actual	Comment	Reference
A	329	PRO	SER	engineered mutation	UNP Q837J0
B	329	PRO	SER	engineered mutation	UNP Q837J0
C	329	PRO	SER	engineered mutation	UNP Q837J0

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (three-letter code: PLP) (formula: C<sub>8</sub>H<sub>10</sub>NO<sub>6</sub>P).



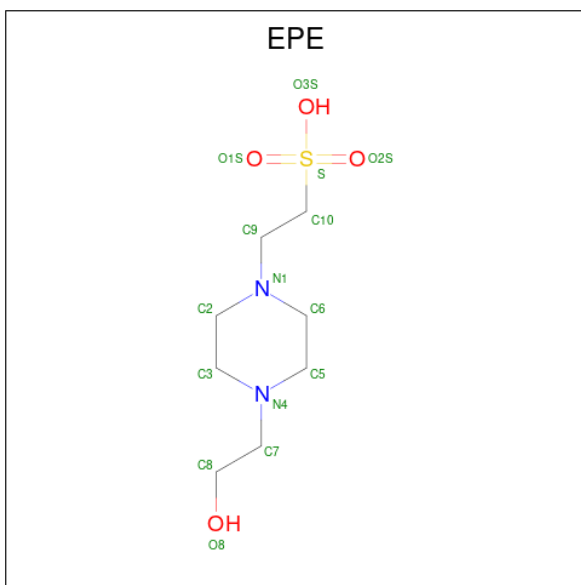
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	B	1	Total	C	N	O	P	0	0
			16	8	1	6	1		
2	C	1	Total	C	N	O	P	0	0
			16	8	1	6	1		

- Molecule 3 is PROPANOIC ACID (three-letter code: PPI) (formula: C<sub>3</sub>H<sub>6</sub>O<sub>2</sub>).



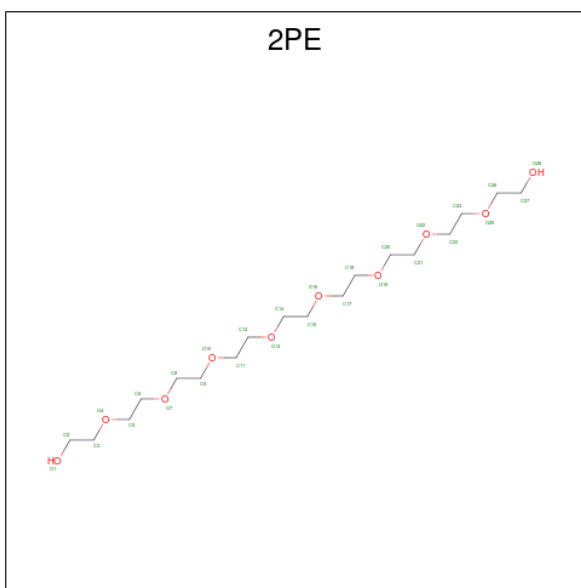
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			5	3	2		
3	B	1	Total	C	O	0	0
			5	3	2		
3	C	1	Total	C	O	0	0
			5	3	2		

- 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
			Total	C	N	O	S		
4	A	1	15	8	2	4	1	0	0

- Molecule 5 is NONAETHYLENE GLYCOL (three-letter code: 2PE) (formula:  $C_{18}H_{38}O_{10}$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
5	C	1	28	18	10	0	0

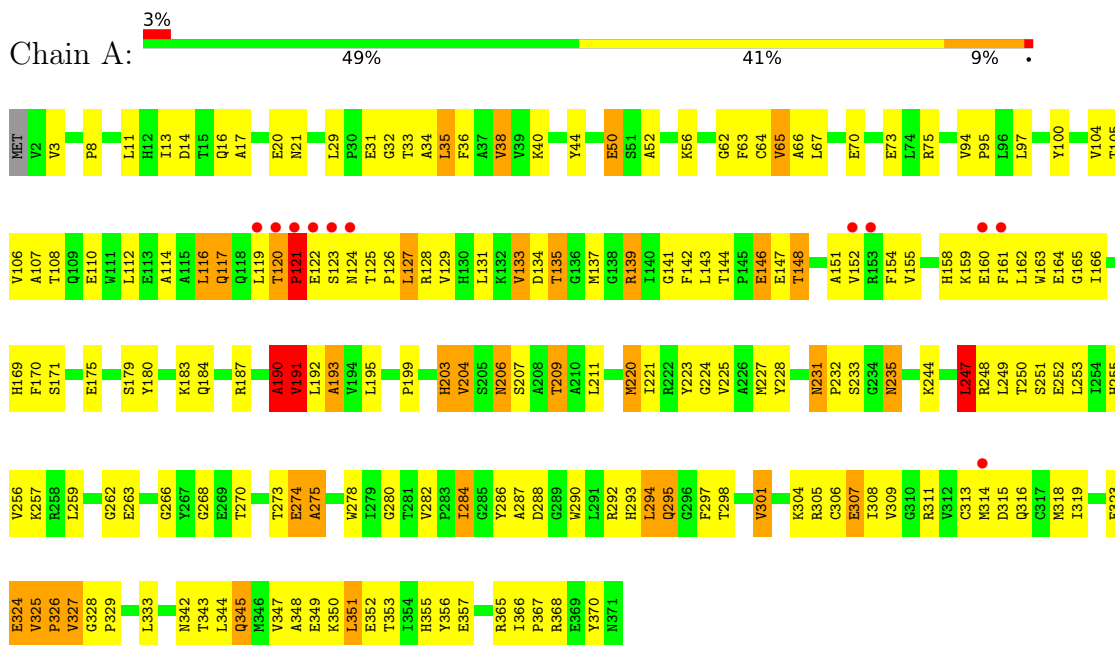
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	57	Total 57	O 57	0	0
6	B	48	Total 48	O 48	0	0
6	C	41	Total 41	O 41	0	0

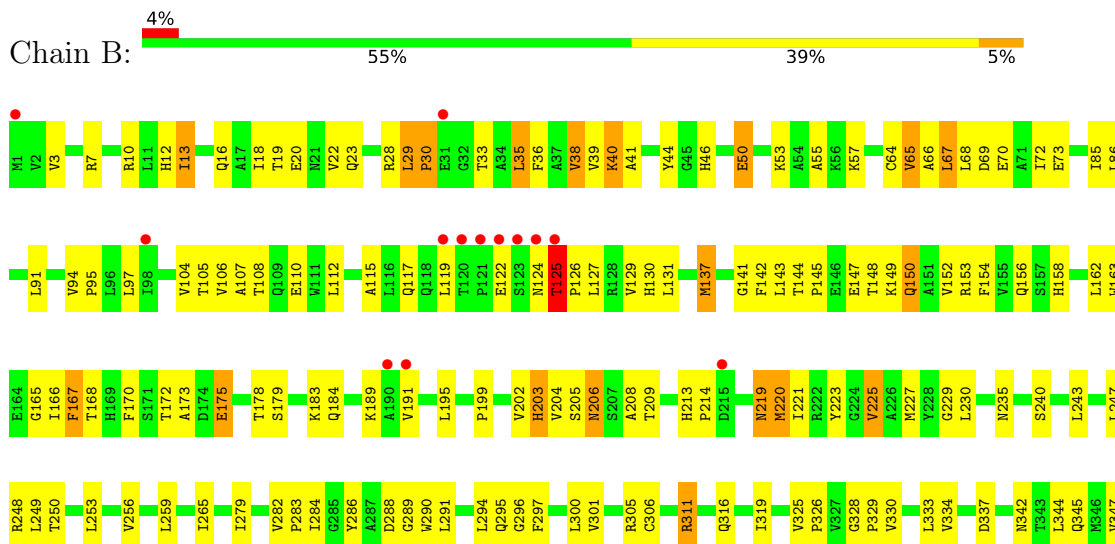
### 3 Residue-property plots

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: Alanine racemase



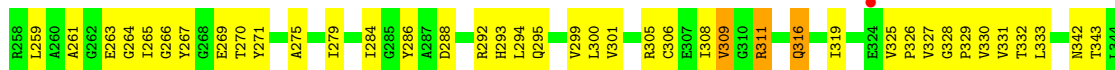
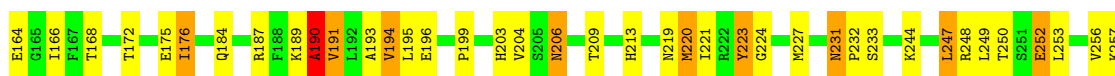
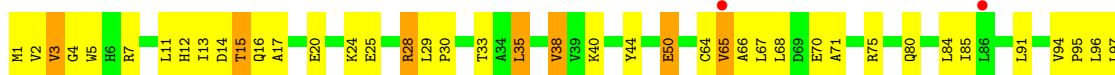
- Molecule 1: Alanine racemase







• Molecule 1: Alanine racemase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.63Å 156.52Å 147.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.50 39.05 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.7 (20.00-2.50) 98.0 (39.05-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.16 (at 2.51Å)	Xtrriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.212 , 0.281 0.216 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.3	Xtrriage
Anisotropy	0.269	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 48.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.019 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.032 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8905	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.48% 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: 2PE, PLP, PPI, EPE

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	1.01	23/2942 (0.8%)	0.89	17/4001 (0.4%)
1	B	0.38	1/2950 (0.0%)	0.71	3/4011 (0.1%)
1	C	0.55	5/2950 (0.2%)	0.73	3/4011 (0.1%)
All	All	0.70	29/8842 (0.3%)	0.78	23/12023 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	2
All	All	0	5

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	327	VAL	CB-CG2	-17.91	1.15	1.52
1	A	327	VAL	CB-CG1	-17.09	1.17	1.52
1	A	325	VAL	CA-CB	-16.88	1.19	1.54
1	A	324	GLU	CB-CG	-12.02	1.29	1.52
1	A	325	VAL	CB-CG2	-10.51	1.30	1.52
1	C	120	THR	C-N	9.78	1.52	1.34
1	A	327	VAL	CA-CB	-9.65	1.34	1.54
1	A	191	VAL	CA-CB	-9.04	1.35	1.54
1	A	327	VAL	C-O	-8.39	1.07	1.23
1	A	325	VAL	C-O	-8.20	1.07	1.23
1	A	324	GLU	C-O	-8.13	1.07	1.23
1	A	326	PRO	CA-C	-8.01	1.36	1.52

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	325	VAL	CA-C	-7.73	1.32	1.52
1	A	324	GLU	CG-CD	-7.70	1.40	1.51
1	A	326	PRO	C-O	-7.50	1.08	1.23
1	C	134	ASP	C-O	-6.93	1.10	1.23
1	C	38	VAL	C-N	6.68	1.49	1.34
1	A	295	GLN	N-CA	-6.61	1.33	1.46
1	A	325	VAL	N-CA	-6.21	1.33	1.46
1	A	307	GLU	C-N	-6.18	1.19	1.34
1	C	194	VAL	CB-CG2	-6.06	1.40	1.52
1	A	324	GLU	CD-OE2	-5.83	1.19	1.25
1	C	308	ILE	N-CA	5.83	1.58	1.46
1	A	325	VAL	CB-CG1	-5.59	1.41	1.52
1	A	326	PRO	CG-CD	-5.43	1.32	1.50
1	A	193	ALA	CA-CB	-5.41	1.41	1.52
1	B	39	VAL	C-N	-5.38	1.21	1.34
1	A	191	VAL	CB-CG1	-5.25	1.41	1.52
1	A	326	PRO	N-CD	-5.07	1.40	1.47

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	134	ASP	CB-CA-C	-18.61	73.18	110.40
1	B	124	ASN	CB-CA-C	15.35	141.10	110.40
1	A	121	PRO	N-CA-C	11.26	141.38	112.10
1	C	135	THR	N-CA-CB	-10.04	91.23	110.30
1	A	135	THR	N-CA-CB	-9.54	92.17	110.30
1	C	308	ILE	N-CA-C	-9.00	86.70	111.00
1	A	190	ALA	N-CA-C	8.23	133.22	111.00
1	A	190	ALA	C-N-CA	7.95	141.56	121.70
1	B	125	THR	N-CA-C	7.27	130.63	111.00
1	A	295	GLN	O-C-N	-6.71	111.80	123.20
1	A	120	THR	C-N-CD	-6.66	105.95	120.60
1	A	190	ALA	CB-CA-C	-6.42	100.46	110.10
1	C	309	VAL	CA-CB-CG2	-6.42	101.27	110.90
1	A	327	VAL	CG1-CB-CG2	-6.22	100.94	110.90
1	B	124	ASN	N-CA-C	-6.11	94.52	111.00
1	A	191	VAL	CB-CA-C	-6.01	99.99	111.40
1	A	294	LEU	O-C-N	5.65	131.75	122.70
1	A	295	GLN	CA-C-N	5.63	127.47	116.20
1	A	295	GLN	N-CA-CB	5.52	120.54	110.60
1	A	247	LEU	CA-CB-CG	5.31	127.51	115.30
1	A	35	LEU	CA-CB-CG	5.27	127.42	115.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	295	GLN	N-CA-C	5.20	125.03	111.00
1	A	139	ARG	N-CA-C	5.13	124.86	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	190	ALA	Peptide
1	A	323	GLU	Mainchain
1	B	29	LEU	Peptide
1	C	144	THR	Peptide
1	C	190	ALA	Peptide

## 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	2879	0	2868	226	0
1	B	2887	0	2879	163	0
1	C	2887	0	2880	212	0
2	A	16	0	7	3	0
2	B	16	0	7	0	0
2	C	16	0	6	0	0
3	A	5	0	5	0	0
3	B	5	0	5	0	0
3	C	5	0	5	5	0
4	A	15	0	16	11	0
5	C	28	0	38	9	0
6	A	57	0	0	4	0
6	B	48	0	0	6	0
6	C	41	0	0	3	0
All	All	8905	0	8716	586	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 34.

All (586) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ALA:CA	1:A:191:VAL:HG23	1.45	1.43
1:B:145:PRO:HG3	1:B:191:VAL:CG2	1.47	1.41
1:B:145:PRO:CG	1:B:191:VAL:HG22	1.51	1.41
1:A:325:VAL:CG2	1:A:326:PRO:HD2	1.65	1.26
1:A:190:ALA:N	1:A:191:VAL:HG23	1.56	1.19
1:A:325:VAL:HG22	1:A:326:PRO:N	1.54	1.19
1:C:145:PRO:HG3	1:C:191:VAL:HG22	1.17	1.15
1:A:190:ALA:O	1:A:193:ALA:HB3	1.44	1.13
1:A:325:VAL:CG2	1:A:326:PRO:CD	2.27	1.10
1:A:190:ALA:CA	1:A:191:VAL:CG2	2.30	1.09
1:B:125:THR:HG22	1:B:125:THR:O	1.54	1.07
1:A:325:VAL:HG23	1:A:326:PRO:HD2	1.11	1.06
1:B:13:ILE:HD12	1:B:46:HIS:HB3	1.37	1.06
1:A:324:GLU:HG2	1:A:325:VAL:N	1.72	1.05
1:A:325:VAL:HG22	1:A:326:PRO:CD	1.84	1.05
1:A:190:ALA:HB3	1:A:191:VAL:HG22	1.40	1.00
1:B:145:PRO:HA	1:B:191:VAL:HG13	1.42	0.99
1:B:97:LEU:HD13	1:B:104:VAL:HG21	1.45	0.98
1:A:187:ARG:O	1:A:191:VAL:HG21	1.63	0.98
1:C:176:ILE:HD12	1:C:176:ILE:H	1.29	0.97
1:C:343:THR:HG22	1:C:345:GLN:H	1.31	0.95
1:A:266:GLY:HA2	1:C:137:MET:HE3	1.48	0.95
1:A:97:LEU:HD13	1:A:104:VAL:HG21	1.44	0.95
1:A:190:ALA:N	1:A:191:VAL:CG2	2.30	0.94
1:A:206:ASN:ND2	1:A:209:THR:HG22	1.84	0.92
1:A:190:ALA:HB3	1:A:191:VAL:CG2	1.98	0.92
1:B:3:VAL:HG12	1:B:367:PRO:HG3	1.51	0.91
1:A:324:GLU:O	1:A:325:VAL:HB	1.64	0.91
1:A:288:ASP:HB3	1:A:366:ILE:HD11	1.55	0.89
1:B:295:GLN:HE22	1:B:311:ARG:HD2	1.37	0.88
1:B:205:SER:HB2	1:B:221:ILE:HG22	1.56	0.87
1:C:155:VAL:HG11	1:C:163:TRP:HB3	1.57	0.86
1:A:207:SER:OG	2:A:390:PLP:O1P	1.93	0.86
1:A:295:GLN:HE22	1:A:311:ARG:NH1	1.72	0.86
1:A:293:HIS:HD2	4:A:430:EPE:H81	1.41	0.85
1:A:190:ALA:CB	1:A:191:VAL:CG2	2.53	0.84
1:A:293:HIS:HA	4:A:430:EPE:H72	1.58	0.84
1:A:325:VAL:O	1:A:325:VAL:HG13	1.76	0.84
1:B:125:THR:O	1:B:125:THR:CG2	2.24	0.84
1:C:295:GLN:HE22	1:C:311:ARG:HH11	1.21	0.84
1:B:145:PRO:CB	1:B:191:VAL:HG22	2.08	0.84
1:A:295:GLN:HE22	1:A:311:ARG:HH11	1.24	0.83

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:GLU:HG3	1:C:223:TYR:CZ	2.13	0.83
1:A:159:LYS:H	1:A:159:LYS:HD2	1.43	0.83
1:A:293:HIS:CD2	4:A:430:EPE:H81	2.14	0.82
1:C:295:GLN:NE2	1:C:311:ARG:HD2	1.94	0.82
1:C:261:ALA:HB2	1:C:275:ALA:HA	1.61	0.81
1:A:120:THR:HG22	1:A:122:GLU:HB3	1.61	0.81
1:C:144:THR:HG23	1:C:145:PRO:HA	1.61	0.80
1:A:324:GLU:CG	1:A:325:VAL:N	2.43	0.80
1:A:295:GLN:NE2	1:A:311:ARG:HD2	1.96	0.80
1:C:295:GLN:HE22	1:C:311:ARG:NH1	1.80	0.79
1:A:231:ASN:ND2	1:A:233:SER:H	1.80	0.78
1:B:29:LEU:HD21	1:B:221:ILE:HD13	1.64	0.78
1:C:343:THR:HG22	1:C:345:GLN:N	1.98	0.78
1:B:202:VAL:H	1:B:219:ASN:HD21	1.32	0.77
1:A:343:THR:HG22	1:A:345:GLN:H	1.50	0.77
1:A:295:GLN:HG3	6:A:435:HOH:O	1.85	0.77
1:A:203:HIS:CD2	1:A:203:HIS:H	2.04	0.76
1:A:21:ASN:HD21	1:A:244:LYS:H	1.32	0.76
1:A:325:VAL:HG23	1:A:326:PRO:CD	1.98	0.76
1:C:361:THR:HB	6:C:424:HOH:O	1.85	0.76
1:B:364:GLN:HB3	6:B:425:HOH:O	1.85	0.75
1:B:144:THR:HG23	1:B:147:GLU:HB2	1.67	0.75
1:A:325:VAL:O	1:A:325:VAL:CG1	2.30	0.74
1:A:97:LEU:CD1	1:A:104:VAL:HG21	2.18	0.74
1:A:158:HIS:HB3	1:A:160:GLU:OE1	1.88	0.74
1:A:231:ASN:C	1:A:231:ASN:HD22	1.90	0.74
1:B:145:PRO:HG3	1:B:191:VAL:HG22	0.75	0.74
1:B:288:ASP:HB3	1:B:366:ILE:HD11	1.70	0.73
1:C:206:ASN:ND2	1:C:209:THR:H	1.84	0.73
1:C:267:TYR:CE2	3:C:400:PPI:H33	2.23	0.73
1:A:170:PHE:HE2	1:A:204:VAL:HG12	1.54	0.73
1:A:8:PRO:HB2	1:A:252:GLU:HG2	1.70	0.73
1:C:352:GLU:CD	5:C:401:2PE:H82	2.09	0.73
1:A:120:THR:HB	1:A:122:GLU:N	2.03	0.73
1:B:145:PRO:HA	1:B:191:VAL:CG1	2.16	0.73
1:C:85:ILE:O	1:C:105:THR:HG23	1.89	0.72
1:C:353:THR:HG21	1:C:357:GLU:OE1	1.89	0.72
1:B:301:VAL:HG12	1:B:306:CYS:SG	2.29	0.72
1:A:50:GLU:HG3	1:A:370:TYR:CZ	2.25	0.72
1:A:292:ARG:HH12	4:A:430:EPE:H92	1.54	0.72
1:C:120:THR:HG23	1:C:121:PRO:HD2	1.72	0.72

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:THR:OG1	1:C:145:PRO:C	2.28	0.71
1:A:16:GLN:O	1:A:20:GLU:HG3	1.91	0.71
1:A:120:THR:CG2	1:A:122:GLU:HB3	2.21	0.71
1:C:231:ASN:ND2	1:C:233:SER:H	1.88	0.71
1:C:299:VAL:HG11	1:C:333:LEU:HD23	1.72	0.71
1:A:206:ASN:ND2	1:A:209:THR:CG2	2.52	0.71
1:A:94:VAL:N	1:A:95:PRO:HD2	2.06	0.70
1:B:203:HIS:H	1:B:203:HIS:CD2	2.09	0.70
1:A:147:GLU:C	1:A:148:THR:HG23	2.12	0.70
1:A:224:GLY:O	1:A:227:MET:HG2	1.91	0.70
1:B:13:ILE:CD1	1:B:46:HIS:HB3	2.19	0.70
1:B:142:PHE:HB2	1:B:148:THR:HG22	1.73	0.70
1:C:109:GLN:H	1:C:109:GLN:NE2	1.89	0.70
1:B:50:GLU:HG3	1:B:370:TYR:CZ	2.26	0.70
1:A:206:ASN:HD21	1:A:209:THR:HG22	1.57	0.69
1:A:304:LYS:HZ3	1:A:304:LYS:HB3	1.57	0.69
1:B:29:LEU:CB	1:B:30:PRO:HA	2.22	0.69
1:B:152:VAL:HG11	1:B:195:LEU:HD22	1.74	0.69
1:B:206:ASN:ND2	1:B:209:THR:HG23	2.07	0.69
1:B:353:THR:HG21	1:B:357:GLU:OE1	1.92	0.69
1:A:3:VAL:HG12	1:A:367:PRO:HG3	1.74	0.69
1:A:170:PHE:CE2	1:A:204:VAL:HG12	2.27	0.69
1:A:353:THR:HG21	1:A:357:GLU:OE1	1.93	0.69
1:C:144:THR:HG23	1:C:145:PRO:CA	2.23	0.69
1:C:120:THR:HB	1:C:123:SER:HB2	1.76	0.68
1:B:345:GLN:O	1:B:349:GLU:HG3	1.92	0.68
1:A:127:LEU:O	1:A:129:VAL:HG23	1.93	0.68
1:C:128:ARG:HD3	1:C:164:GLU:OE2	1.93	0.68
1:C:145:PRO:HG3	1:C:191:VAL:CG2	2.11	0.67
1:A:165:GLY:HA2	1:A:199:PRO:CG	2.24	0.67
1:B:142:PHE:CB	1:B:148:THR:HG22	2.25	0.67
1:C:163:TRP:CH2	1:C:199:PRO:HD3	2.30	0.67
1:C:224:GLY:O	1:C:227:MET:HG2	1.95	0.67
1:A:38:VAL:HG13	1:A:224:GLY:HA2	1.77	0.67
1:C:148:THR:O	1:C:152:VAL:HG12	1.94	0.67
1:C:253:LEU:HD21	1:C:319:ILE:HD11	1.77	0.67
1:C:286:TYR:OH	3:C:400:PPI:H22	1.94	0.67
1:A:247:LEU:HD13	1:A:248:ARG:N	2.10	0.66
1:C:106:VAL:HB	1:C:131:LEU:HD23	1.76	0.66
1:C:17:ALA:HA	1:C:20:GLU:OE2	1.95	0.66
1:C:130:HIS:NE2	1:C:164:GLU:HB3	2.10	0.65

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:VAL:HG13	1:B:326:PRO:HD2	1.79	0.65
1:B:230:LEU:HD21	1:B:344:LEU:HD12	1.77	0.65
1:C:50:GLU:HG3	1:C:370:TYR:CE1	2.32	0.65
1:A:142:PHE:CB	1:A:148:THR:HG22	2.27	0.65
1:A:259:LEU:HD22	1:A:263:GLU:HG2	1.79	0.65
1:B:301:VAL:CG1	1:B:306:CYS:SG	2.85	0.65
1:A:206:ASN:H	1:A:209:THR:HG23	1.63	0.64
1:A:124:ASN:ND2	1:A:125:THR:HG22	2.13	0.64
1:A:180:TYR:HD1	1:A:183:LYS:HD2	1.61	0.64
1:C:144:THR:HB	1:C:148:THR:HG23	1.78	0.64
1:B:72:ILE:HD12	1:B:73:GLU:N	2.12	0.64
1:A:152:VAL:HG11	1:A:195:LEU:HD22	1.78	0.64
1:A:162:LEU:O	1:A:162:LEU:HD23	1.98	0.64
1:B:126:PRO:HB2	1:B:162:LEU:HB2	1.80	0.64
1:A:50:GLU:HG3	1:A:370:TYR:CE1	2.33	0.63
1:C:108:THR:HB	1:C:110:GLU:OE1	1.98	0.63
1:C:122:GLU:HG3	1:C:159:LYS:HD2	1.81	0.63
1:C:256:VAL:HG23	1:C:327:VAL:HG12	1.81	0.63
1:B:189:LYS:HB3	1:B:189:LYS:NZ	2.13	0.63
1:C:325:VAL:HG12	1:C:326:PRO:O	1.98	0.62
1:A:292:ARG:HG3	1:C:357:GLU:OE2	1.98	0.62
1:B:206:ASN:ND2	1:B:209:THR:H	1.97	0.62
1:A:190:ALA:CB	1:A:191:VAL:HG22	2.17	0.62
1:B:131:LEU:HB2	1:B:166:ILE:HG22	1.81	0.62
1:A:171:SER:H	1:A:184:GLN:HE22	1.46	0.62
1:C:144:THR:CG2	1:C:191:VAL:HG13	2.29	0.62
1:C:350:LYS:NZ	5:C:401:2PE:H122	2.15	0.62
1:A:116:LEU:HD21	1:A:160:GLU:OE1	2.00	0.62
1:A:163:TRP:CH2	1:A:199:PRO:HD3	2.34	0.62
1:A:131:LEU:HB2	1:A:166:ILE:HG22	1.81	0.61
1:A:147:GLU:O	1:A:148:THR:HG23	1.99	0.61
1:A:206:ASN:H	1:A:209:THR:CG2	2.14	0.61
1:C:38:VAL:HB	1:C:64:CYS:HB2	1.82	0.61
1:C:144:THR:HG23	1:C:145:PRO:N	2.15	0.61
1:C:176:ILE:H	1:C:176:ILE:CD1	1.95	0.61
1:B:163:TRP:CH2	1:B:199:PRO:HD3	2.36	0.61
1:B:305:ARG:NH2	1:B:342:ASN:OD1	2.34	0.61
1:C:2:VAL:HG12	1:C:3:VAL:H	1.66	0.60
1:C:305:ARG:NH2	1:C:342:ASN:OD1	2.34	0.60
1:C:144:THR:CG2	1:C:191:VAL:CG1	2.79	0.60
1:C:264:GLY:HA3	1:C:269:GLU:HG3	1.83	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:345:GLN:HE21	1:C:355:HIS:CD2	2.19	0.60
1:A:298:THR:HG22	1:A:307:GLU:HA	1.81	0.60
1:A:32:GLY:HA3	6:A:451:HOH:O	2.01	0.60
1:A:220:MET:C	1:A:220:MET:HE2	2.20	0.60
1:B:130:HIS:HA	1:B:165:GLY:O	2.02	0.60
1:A:148:THR:O	1:A:152:VAL:HG12	2.00	0.60
1:A:97:LEU:HD22	1:A:104:VAL:CG2	2.31	0.60
1:A:137:MET:HB3	6:A:484:HOH:O	2.01	0.60
1:A:250:THR:CG2	1:A:251:SER:N	2.65	0.60
1:B:203:HIS:H	1:B:203:HIS:HD2	1.50	0.60
1:C:187:ARG:O	1:C:191:VAL:CG2	2.50	0.60
1:C:247:LEU:HD13	1:C:248:ARG:N	2.17	0.60
1:C:2:VAL:HG12	1:C:3:VAL:N	2.17	0.60
1:C:176:ILE:HD12	1:C:176:ILE:N	2.08	0.59
1:B:282:VAL:HG12	1:B:284:ILE:HG22	1.82	0.59
1:A:44:TYR:HE2	1:A:225:VAL:HG13	1.68	0.59
1:A:120:THR:OG1	1:A:160:GLU:HG3	2.01	0.59
1:A:211:LEU:HD12	1:A:232:PRO:HG3	1.83	0.59
1:A:146:GLU:CD	1:A:146:GLU:H	2.05	0.59
1:C:187:ARG:O	1:C:191:VAL:HG21	2.03	0.59
1:C:295:GLN:NE2	5:C:401:2PE:H171	2.17	0.59
1:A:190:ALA:C	1:A:191:VAL:HG23	1.89	0.58
1:B:167:PHE:HB3	1:B:203:HIS:CD2	2.37	0.58
1:C:134:ASP:C	1:C:134:ASP:OD1	2.40	0.58
1:C:231:ASN:HD22	1:C:231:ASN:C	2.05	0.58
1:A:292:ARG:NH1	4:A:430:EPE:O3S	2.36	0.58
1:B:149:LYS:O	1:B:149:LYS:HD3	2.03	0.58
1:B:165:GLY:HA2	1:B:199:PRO:CG	2.33	0.58
1:B:69:ASP:O	1:B:72:ILE:HG13	2.03	0.58
1:B:179:SER:O	1:B:183:LYS:HG3	2.03	0.58
1:A:108:THR:HB	1:A:110:GLU:OE2	2.03	0.58
1:C:231:ASN:HD22	1:C:233:SER:H	1.50	0.58
1:A:231:ASN:HD22	1:A:232:PRO:N	2.01	0.57
1:B:44:TYR:CE2	1:B:225:VAL:HG13	2.39	0.57
1:B:64:CYS:HB3	1:B:86:LEU:HD11	1.86	0.57
1:B:170:PHE:HA	1:B:184:GLN:OE1	2.04	0.57
1:A:104:VAL:HG12	1:A:105:THR:O	2.04	0.57
1:A:250:THR:HG22	1:A:251:SER:N	2.19	0.57
1:C:38:VAL:HG12	1:C:223:TYR:O	2.03	0.57
1:A:206:ASN:HD22	1:A:209:THR:CG2	2.16	0.57
1:B:38:VAL:HG23	1:B:40:LYS:HD3	1.86	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:144:THR:CG2	1:C:145:PRO:HA	2.34	0.57
1:B:91:LEU:O	1:B:94:VAL:HG23	2.04	0.57
1:C:98:ILE:HD12	1:C:98:ILE:N	2.20	0.57
1:A:3:VAL:CG1	1:A:367:PRO:HG3	2.34	0.57
1:A:142:PHE:HB2	1:A:148:THR:HG22	1.86	0.57
1:B:38:VAL:HB	1:B:64:CYS:HB2	1.87	0.57
1:B:168:THR:HG22	1:B:204:VAL:HG12	1.86	0.57
1:C:68:LEU:HD21	1:C:96:LEU:HD12	1.87	0.57
1:C:144:THR:CB	1:C:148:THR:H	2.18	0.57
1:C:38:VAL:HG13	1:C:224:GLY:HA2	1.86	0.57
1:B:202:VAL:H	1:B:219:ASN:ND2	1.99	0.57
1:C:144:THR:HG23	1:C:191:VAL:HG13	1.87	0.56
1:C:213:HIS:HA	6:C:451:HOH:O	2.05	0.56
1:C:299:VAL:HG11	1:C:333:LEU:CD2	2.34	0.56
1:A:352:GLU:O	1:C:293:HIS:HE1	1.87	0.56
1:C:343:THR:CG2	1:C:345:GLN:HB2	2.34	0.56
1:A:17:ALA:CB	1:A:244:LYS:HD2	2.35	0.56
1:A:143:LEU:HD12	1:A:144:THR:HG23	1.88	0.56
1:A:315:ASP:OD2	1:C:40:LYS:HD2	2.06	0.56
1:B:115:ALA:O	1:B:119:LEU:HD13	2.05	0.56
1:B:203:HIS:CD2	1:B:203:HIS:N	2.74	0.56
1:A:107:ALA:HB1	1:A:141:GLY:H	1.70	0.56
1:A:56:LYS:HG3	1:A:63:PHE:HZ	1.69	0.56
1:B:247:LEU:HD13	1:B:248:ARG:N	2.20	0.56
1:A:34:ALA:O	1:A:220:MET:HA	2.06	0.56
1:A:120:THR:HB	1:A:122:GLU:H	1.70	0.55
1:C:325:VAL:CG1	1:C:329:PRO:HG3	2.36	0.55
1:C:328:GLY:N	1:C:329:PRO:HD2	2.21	0.55
1:B:55:ALA:HB2	1:B:227:MET:HE1	1.89	0.55
1:C:265:ILE:HD11	1:C:309:VAL:HG23	1.89	0.55
1:A:187:ARG:O	1:A:191:VAL:CG2	2.46	0.55
1:B:206:ASN:C	1:B:206:ASN:HD22	2.10	0.55
1:C:20:GLU:OE2	1:C:244:LYS:HD3	2.05	0.55
1:A:106:VAL:HG21	1:A:112:LEU:HG	1.87	0.55
1:A:256:VAL:HG23	1:A:327:VAL:HG22	1.87	0.55
1:B:18:ILE:O	1:B:22:VAL:HG23	2.06	0.55
1:C:206:ASN:HD21	1:C:209:THR:H	1.50	0.55
1:C:270:THR:HG21	1:C:311:ARG:NH1	2.21	0.55
1:B:29:LEU:HB2	1:B:30:PRO:HA	1.89	0.54
1:B:106:VAL:HG21	1:B:112:LEU:HG	1.88	0.54
1:C:11:LEU:HD22	1:C:247:LEU:HD21	1.89	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:50:GLU:HG3	1:C:370:TYR:CZ	2.42	0.54
1:C:106:VAL:HG11	1:C:112:LEU:HG	1.89	0.54
1:A:44:TYR:CE2	1:A:225:VAL:HG13	2.43	0.54
1:B:166:ILE:HD12	1:B:166:ILE:O	2.08	0.54
1:C:168:THR:HG22	1:C:204:VAL:HG12	1.90	0.54
1:C:206:ASN:HD22	1:C:206:ASN:H	1.55	0.54
1:B:33:THR:HG23	1:B:219:ASN:C	2.27	0.54
1:C:293:HIS:O	5:C:401:2PE:H141	2.06	0.54
1:B:35:LEU:HD22	1:B:221:ILE:HD11	1.89	0.54
1:C:189:LYS:C	1:C:191:VAL:H	2.11	0.54
1:B:162:LEU:HD13	1:B:162:LEU:O	2.08	0.54
1:C:220:MET:HE3	1:C:221:ILE:C	2.28	0.54
1:C:1:MET:CE	1:C:364:GLN:HB3	2.38	0.54
1:C:20:GLU:HB3	1:C:24:LYS:NZ	2.23	0.54
1:C:301:VAL:HG12	1:C:306:CYS:SG	2.48	0.54
1:A:357:GLU:OE2	1:C:292:ARG:HG3	2.08	0.53
1:B:206:ASN:HD21	1:B:209:THR:H	1.56	0.53
1:C:231:ASN:HD22	1:C:232:PRO:N	2.06	0.53
1:C:325:VAL:HG13	1:C:326:PRO:HD2	1.90	0.53
1:C:189:LYS:O	1:C:191:VAL:N	2.39	0.53
1:C:350:LYS:HZ3	5:C:401:2PE:H122	1.72	0.53
1:A:170:PHE:CE2	1:A:204:VAL:CG1	2.91	0.53
1:B:229:GLY:HA2	1:B:243:LEU:HB3	1.91	0.53
1:B:259:LEU:HD12	1:B:279:ILE:HG13	1.90	0.53
1:A:316:GLN:OE1	1:C:139:ARG:HD3	2.08	0.53
1:B:166:ILE:HD11	1:B:202:VAL:HG22	1.91	0.53
1:C:12:HIS:HE1	1:C:250:THR:HB	1.73	0.53
1:A:126:PRO:HB3	1:A:161:PHE:O	2.09	0.53
1:C:66:ALA:O	1:C:67:LEU:HD23	2.09	0.53
1:A:257:LYS:NZ	1:C:139:ARG:O	2.42	0.53
1:B:35:LEU:CD2	1:B:221:ILE:HD11	2.39	0.53
1:C:97:LEU:CD1	1:C:104:VAL:HG11	2.38	0.52
1:A:220:MET:HE3	1:A:221:ILE:C	2.28	0.52
1:C:13:ILE:N	1:C:13:ILE:HD12	2.24	0.52
1:C:98:ILE:HG23	1:C:125:THR:CG2	2.39	0.52
1:C:130:HIS:CD2	1:C:164:GLU:HB3	2.45	0.52
1:B:50:GLU:HG3	1:B:370:TYR:CE1	2.45	0.52
1:A:148:THR:HA	1:A:151:ALA:HB3	1.91	0.52
1:A:133:VAL:HG22	1:A:135:THR:HG23	1.90	0.52
1:B:364:GLN:CB	6:B:425:HOH:O	2.51	0.52
1:C:91:LEU:O	1:C:94:VAL:HG23	2.09	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:143:LEU:HD12	1:A:143:LEU:O	2.09	0.52
1:A:295:GLN:HE21	4:A:430:EPE:H52	1.75	0.52
1:B:325:VAL:CG1	1:B:329:PRO:HG2	2.40	0.52
1:A:231:ASN:HD22	1:A:233:SER:H	1.56	0.52
1:B:38:VAL:HA	1:B:64:CYS:HB2	1.91	0.52
1:B:94:VAL:N	1:B:95:PRO:HD2	2.24	0.52
1:C:144:THR:HG21	1:C:148:THR:OG1	2.10	0.52
1:C:249:LEU:HG	1:C:333:LEU:HD12	1.92	0.52
1:C:299:VAL:CG1	1:C:333:LEU:HD23	2.39	0.52
1:B:119:LEU:O	1:B:122:GLU:HB2	2.10	0.52
1:B:152:VAL:HG13	1:B:153:ARG:N	2.25	0.52
1:A:155:VAL:HG11	1:A:163:TRP:HB2	1.92	0.51
1:B:127:LEU:HD12	1:B:129:VAL:HG12	1.92	0.51
1:A:107:ALA:HB1	1:A:141:GLY:N	2.25	0.51
1:C:98:ILE:HG23	1:C:125:THR:HG21	1.92	0.51
1:A:155:VAL:HG13	1:A:161:PHE:CB	2.40	0.51
1:A:165:GLY:HA2	1:A:199:PRO:HG2	1.92	0.51
1:C:1:MET:HE1	1:C:364:GLN:HB3	1.92	0.51
1:C:33:THR:HA	1:C:219:ASN:O	2.11	0.51
1:C:144:THR:HG21	1:C:191:VAL:CG1	2.41	0.51
1:B:108:THR:HB	1:B:110:GLU:OE2	2.10	0.51
1:B:178:THR:HG22	6:B:409:HOH:O	2.11	0.51
1:C:300:LEU:HB2	1:C:332:THR:HB	1.92	0.51
1:A:52:ALA:HB1	1:A:63:PHE:CE2	2.46	0.51
1:A:255:HIS:CG	1:C:140:ILE:HG12	2.46	0.50
1:A:231:ASN:ND2	1:A:231:ASN:C	2.58	0.50
1:C:206:ASN:HD22	1:C:206:ASN:C	2.13	0.50
1:C:270:THR:HG21	1:C:311:ARG:CZ	2.42	0.50
1:C:109:GLN:H	1:C:109:GLN:CD	2.13	0.50
1:C:152:VAL:HG13	1:C:153:ARG:H	1.76	0.50
1:B:253:LEU:HD21	1:B:319:ILE:HD11	1.94	0.50
1:C:137:MET:HB3	6:C:434:HOH:O	2.10	0.50
1:A:38:VAL:HB	1:A:64:CYS:HB2	1.93	0.50
1:A:343:THR:HG22	1:A:344:LEU:N	2.27	0.50
1:B:284:ILE:HD13	1:B:333:LEU:CD2	2.42	0.50
1:C:267:TYR:HE2	3:C:400:PPI:O2	1.95	0.50
1:A:206:ASN:N	1:A:209:THR:HG23	2.25	0.50
1:A:137:MET:HE3	1:C:266:GLY:HA2	1.94	0.49
1:C:301:VAL:CG1	1:C:306:CYS:SG	3.00	0.49
1:A:284:ILE:HG23	1:A:284:ILE:O	2.12	0.49
1:B:65:VAL:CG2	1:B:70:GLU:HB3	2.42	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:HIS:HA	5:C:401:2PE:H151	1.93	0.49
1:B:28:ARG:HH21	1:B:240:SER:HB3	1.77	0.49
1:B:40:LYS:O	1:B:41:ALA:HB3	2.12	0.49
1:B:65:VAL:HG21	1:B:70:GLU:HB3	1.94	0.49
1:C:133:VAL:HG22	1:C:135:THR:HG23	1.95	0.49
1:C:120:THR:O	1:C:160:GLU:HG3	2.12	0.49
1:A:282:VAL:HG12	1:A:284:ILE:HG22	1.94	0.49
1:B:295:GLN:NE2	1:B:311:ARG:HD2	2.17	0.49
1:C:190:ALA:HB3	1:C:191:VAL:HG23	1.95	0.49
1:A:73:GLU:HB2	1:C:2:VAL:HG21	1.95	0.49
1:B:150:GLN:HE21	1:B:150:GLN:HA	1.77	0.49
1:C:120:THR:HG22	1:C:122:GLU:H	1.76	0.49
1:A:129:VAL:HG12	1:A:131:LEU:HD12	1.94	0.49
1:C:75:ARG:HG3	1:C:100:TYR:HB3	1.95	0.49
1:B:163:TRP:CZ2	1:B:199:PRO:HD3	2.48	0.49
1:A:311:ARG:NH2	4:A:430:EPE:H101	2.28	0.48
1:C:84:LEU:HD11	1:C:105:THR:HG22	1.95	0.48
1:C:94:VAL:N	1:C:95:PRO:HD2	2.28	0.48
1:A:106:VAL:CG1	1:A:131:LEU:HD12	2.43	0.48
1:A:163:TRP:CZ2	1:A:199:PRO:HD3	2.48	0.48
1:A:298:THR:HG22	1:A:307:GLU:CA	2.43	0.48
1:B:147:GLU:C	1:B:148:THR:HG23	2.34	0.48
1:B:294:LEU:HD21	1:B:347:VAL:HG13	1.95	0.48
1:A:38:VAL:HA	1:A:64:CYS:HB2	1.95	0.48
1:A:304:LYS:HB3	1:A:304:LYS:NZ	2.27	0.48
1:B:152:VAL:HG13	1:B:153:ARG:H	1.78	0.48
1:C:206:ASN:ND2	1:C:206:ASN:H	2.10	0.48
1:A:268:GLY:HA2	1:C:172:THR:HG22	1.95	0.48
1:C:252:GLU:HA	1:C:331:VAL:HG23	1.95	0.48
1:A:116:LEU:HD12	1:A:154:PHE:CZ	2.48	0.48
1:B:205:SER:HB3	1:B:209:THR:OG1	2.13	0.48
1:B:36:PHE:HB2	1:B:220:MET:HE1	1.96	0.48
1:A:270:THR:HG21	1:A:311:ARG:NH1	2.28	0.48
1:A:347:VAL:O	1:A:351:LEU:HD22	2.13	0.48
1:B:296:GLY:H	1:B:350:LYS:NZ	2.11	0.48
1:C:146:GLU:O	1:C:150:GLN:HG3	2.14	0.48
1:C:343:THR:HG22	1:C:345:GLN:HB2	1.95	0.48
1:A:29:LEU:C	1:A:31:GLU:H	2.17	0.48
1:A:292:ARG:HH11	1:C:353:THR:HG22	1.79	0.48
1:B:147:GLU:O	1:B:149:LYS:N	2.39	0.48
1:A:206:ASN:H	1:A:206:ASN:HD22	1.62	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:HB	1:A:122:GLU:O	2.14	0.47
1:A:148:THR:O	1:A:151:ALA:HB3	2.14	0.47
1:B:104:VAL:HG12	1:B:105:THR:N	2.28	0.47
1:B:36:PHE:HB2	1:B:220:MET:CE	2.44	0.47
1:C:135:THR:HB	1:C:187:ARG:HB2	1.95	0.47
1:C:189:LYS:O	1:C:193:ALA:HB2	2.14	0.47
1:C:196:GLU:OE1	1:C:196:GLU:HA	2.14	0.47
1:C:250:THR:HG23	1:C:330:VAL:HG23	1.95	0.47
1:A:120:THR:HB	1:A:122:GLU:CA	2.43	0.47
1:B:7:ARG:HD2	1:B:283:PRO:HB2	1.97	0.47
1:B:53:LYS:O	1:B:57:LYS:HG3	2.14	0.47
1:C:105:THR:HA	1:C:130:HIS:O	2.15	0.47
1:C:118:GLN:O	1:C:118:GLN:HG2	2.15	0.47
1:C:343:THR:HG21	1:C:345:GLN:HB2	1.97	0.47
1:A:8:PRO:O	1:A:251:SER:HA	2.15	0.47
1:A:94:VAL:N	1:A:95:PRO:CD	2.76	0.47
1:A:262:GLY:N	1:A:273:THR:OG1	2.48	0.47
1:B:16:GLN:HB3	6:B:408:HOH:O	2.15	0.47
1:B:38:VAL:HG23	1:B:40:LYS:CD	2.45	0.47
1:C:144:THR:HG21	1:C:191:VAL:HG13	1.97	0.47
1:A:13:ILE:HB	1:A:370:TYR:CD1	2.49	0.47
1:A:253:LEU:HD21	1:A:319:ILE:HD11	1.97	0.47
1:C:293:HIS:HA	5:C:401:2PE:C15	2.45	0.47
1:A:17:ALA:HB2	1:A:244:LYS:HD2	1.97	0.47
1:B:44:TYR:HE2	1:B:225:VAL:HG13	1.77	0.47
1:B:148:THR:O	1:B:152:VAL:HG12	2.15	0.47
1:A:324:GLU:O	1:A:325:VAL:CB	2.29	0.46
1:A:270:THR:HG21	1:A:311:ARG:CZ	2.45	0.46
1:B:12:HIS:CE1	1:B:250:THR:HG21	2.51	0.46
1:A:328:GLY:N	1:A:329:PRO:CD	2.79	0.46
1:C:135:THR:O	1:C:184:GLN:HG2	2.14	0.46
1:A:305:ARG:NH2	1:A:342:ASN:OD1	2.49	0.46
1:B:189:LYS:HB3	1:B:189:LYS:HZ2	1.80	0.46
1:B:137:MET:HB2	6:B:449:HOH:O	2.16	0.46
1:C:35:LEU:HD22	1:C:221:ILE:HD11	1.98	0.46
1:A:155:VAL:HG13	1:A:161:PHE:HB3	1.98	0.46
1:C:189:LYS:C	1:C:191:VAL:N	2.69	0.46
1:C:325:VAL:HG11	1:C:329:PRO:HG3	1.97	0.46
1:A:11:LEU:HD23	1:A:368:ARG:NE	2.31	0.46
1:B:206:ASN:ND2	1:B:206:ASN:C	2.68	0.46
1:B:300:LEU:HD13	1:B:337:ASP:HB3	1.97	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:301:VAL:O	1:B:301:VAL:HG13	2.16	0.46
1:B:66:ALA:C	1:B:67:LEU:HD23	2.36	0.46
1:B:144:THR:HG23	1:B:147:GLU:CB	2.41	0.46
1:C:121:PRO:O	1:C:160:GLU:OE2	2.33	0.46
1:B:119:LEU:HD21	1:B:127:LEU:HB2	1.98	0.46
1:A:301:VAL:CG1	1:A:306:CYS:SG	3.04	0.45
1:B:173:ALA:HB3	1:B:208:ALA:HB3	1.98	0.45
1:A:206:ASN:HD22	1:A:209:THR:HG23	1.81	0.45
1:B:152:VAL:O	1:B:156:GLN:HG2	2.15	0.45
1:C:15:THR:HG22	1:C:16:GLN:N	2.31	0.45
1:A:65:VAL:HG13	1:A:70:GLU:HB2	1.98	0.45
1:A:116:LEU:HD12	1:A:154:PHE:HZ	1.82	0.45
1:B:12:HIS:HE1	1:B:250:THR:HG21	1.81	0.45
1:C:38:VAL:HA	1:C:64:CYS:HB2	1.99	0.45
1:A:106:VAL:HG13	1:A:106:VAL:O	2.17	0.45
1:A:114:ALA:O	1:A:117:GLN:HG3	2.16	0.45
1:B:38:VAL:CG2	1:B:40:LYS:HD3	2.46	0.45
1:B:97:LEU:HD13	1:B:104:VAL:CG2	2.31	0.45
1:A:295:GLN:O	1:A:308:ILE:O	2.35	0.45
1:C:13:ILE:HB	1:C:370:TYR:CD1	2.51	0.45
1:C:144:THR:CG2	1:C:191:VAL:HG11	2.47	0.45
1:A:97:LEU:HD22	1:A:104:VAL:HG22	1.97	0.45
1:A:345:GLN:O	1:A:348:ALA:HB3	2.17	0.45
1:B:230:LEU:CD2	1:B:344:LEU:HD12	2.46	0.45
1:C:65:VAL:HG11	1:C:71:ALA:HB2	1.98	0.45
1:C:220:MET:CE	1:C:221:ILE:C	2.85	0.45
1:A:152:VAL:HG11	1:A:195:LEU:CD2	2.45	0.45
1:B:19:THR:O	1:B:23:GLN:HB2	2.16	0.45
1:C:133:VAL:HG22	1:C:135:THR:CG2	2.46	0.45
1:C:162:LEU:HD13	1:C:162:LEU:C	2.37	0.45
1:A:297:PHE:CD1	1:A:350:LYS:HG3	2.52	0.45
1:B:50:GLU:CD	1:B:50:GLU:H	2.18	0.45
1:B:219:ASN:ND2	1:B:219:ASN:C	2.70	0.45
1:C:263:GLU:OE2	1:C:263:GLU:HA	2.17	0.45
1:A:75:ARG:HG3	1:A:100:TYR:HB3	1.99	0.45
1:A:133:VAL:HG22	1:A:135:THR:CG2	2.46	0.45
1:C:35:LEU:CD2	1:C:221:ILE:HD11	2.47	0.45
1:C:259:LEU:HD12	1:C:279:ILE:HG13	1.99	0.45
1:A:169:HIS:ND1	2:A:390:PLP:H2A2	2.33	0.44
1:A:293:HIS:CD2	4:A:430:EPE:C8	2.95	0.44
1:B:3:VAL:CG1	1:B:367:PRO:HG3	2.36	0.44

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:327:VAL:C	1:C:329:PRO:HD2	2.38	0.44
1:A:307:GLU:HG2	1:A:309:VAL:HG12	1.98	0.44
1:B:28:ARG:NH2	1:B:240:SER:HB3	2.31	0.44
1:A:203:HIS:H	1:A:203:HIS:HD2	1.57	0.44
1:A:352:GLU:HG3	5:C:401:2PE:H21	1.98	0.44
1:A:274:GLU:O	1:A:275:ALA:HB2	2.17	0.44
1:B:206:ASN:HD21	1:B:209:THR:HG23	1.82	0.44
1:C:3:VAL:CG2	1:C:5:TRP:NE1	2.80	0.44
1:A:206:ASN:ND2	1:A:206:ASN:H	2.14	0.44
1:B:170:PHE:HD2	1:B:209:THR:HG21	1.83	0.44
1:A:206:ASN:HD22	1:A:206:ASN:C	2.21	0.44
1:A:247:LEU:CD1	1:A:248:ARG:N	2.78	0.44
1:A:355:HIS:O	1:A:356:TYR:C	2.55	0.44
1:C:97:LEU:HD22	1:C:104:VAL:HG13	2.00	0.44
1:C:267:TYR:HE2	3:C:400:PPI:C1	2.31	0.44
1:C:284:ILE:O	1:C:316:GLN:HA	2.17	0.44
1:A:104:VAL:HG12	1:A:105:THR:N	2.33	0.43
1:A:128:ARG:HD3	1:A:164:GLU:OE2	2.18	0.43
1:A:191:VAL:HB	1:A:192:LEU:H	1.62	0.43
1:A:278:TRP:CE2	1:A:324:GLU:HB2	2.52	0.43
1:A:290:TRP:CE2	1:A:333:LEU:HD23	2.54	0.43
1:A:65:VAL:CG1	1:A:66:ALA:N	2.81	0.43
1:A:301:VAL:HG13	1:A:306:CYS:SG	2.57	0.43
1:B:333:LEU:N	1:B:333:LEU:HD12	2.34	0.43
1:A:206:ASN:HD22	1:A:206:ASN:N	2.17	0.43
1:C:301:VAL:O	1:C:301:VAL:HG13	2.19	0.43
1:A:119:LEU:HD13	1:A:160:GLU:HB3	2.01	0.43
1:C:97:LEU:HD22	1:C:104:VAL:CG1	2.49	0.43
1:A:29:LEU:HD21	1:A:33:THR:HG22	2.00	0.43
1:B:256:VAL:HG11	1:B:325:VAL:O	2.17	0.43
1:C:120:THR:CG2	1:C:121:PRO:HD2	2.44	0.43
1:B:127:LEU:HD12	1:B:129:VAL:CG1	2.48	0.43
1:C:38:VAL:CB	1:C:64:CYS:HB2	2.47	0.43
1:C:145:PRO:CG	1:C:191:VAL:HG22	2.12	0.43
1:B:29:LEU:HD21	1:B:221:ILE:CD1	2.44	0.43
1:B:296:GLY:H	1:B:350:LYS:HZ2	1.65	0.43
1:B:328:GLY:HA2	6:B:424:HOH:O	2.18	0.43
1:C:3:VAL:HG22	1:C:5:TRP:CD1	2.54	0.43
1:C:116:LEU:O	1:C:119:LEU:HB3	2.18	0.43
1:A:14:ASP:O	1:A:17:ALA:HB3	2.19	0.43
1:B:50:GLU:HG3	1:B:370:TYR:OH	2.19	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:ALA:C	1:C:67:LEU:HD23	2.39	0.43
1:C:144:THR:HG1	1:C:148:THR:H	1.63	0.43
1:C:29:LEU:O	1:C:29:LEU:HD12	2.19	0.42
1:C:97:LEU:HD13	1:C:104:VAL:HG11	2.01	0.42
1:B:213:HIS:N	1:B:214:PRO:CD	2.82	0.42
1:A:36:PHE:CE1	1:A:62:GLY:HA3	2.54	0.42
1:A:110:GLU:CD	1:A:110:GLU:H	2.23	0.42
1:A:287:ALA:HB2	1:A:314:MET:HG3	2.02	0.42
1:B:225:VAL:HG21	1:B:356:TYR:OH	2.19	0.42
1:C:44:TYR:CD1	1:C:44:TYR:N	2.87	0.42
1:C:107:ALA:CB	1:C:140:ILE:CG2	2.97	0.42
1:A:345:GLN:NE2	6:A:455:HOH:O	2.51	0.42
1:A:295:GLN:HE21	4:A:430:EPE:C5	2.33	0.42
1:B:289:GLY:O	1:B:291:LEU:HG	2.19	0.42
1:C:65:VAL:CG2	1:C:70:GLU:HB3	2.50	0.42
1:C:117:GLN:C	1:C:119:LEU:H	2.23	0.42
5:C:401:2PE:H121	5:C:401:2PE:H91	1.81	0.42
1:A:67:LEU:CD2	1:C:7:ARG:HD3	2.50	0.42
1:A:137:MET:HE1	1:A:139:ARG:NH2	2.34	0.42
1:A:313:CYS:SG	1:C:139:ARG:NH2	2.92	0.42
1:C:38:VAL:HG12	1:C:223:TYR:C	2.39	0.42
1:C:107:ALA:CB	1:C:140:ILE:HG23	2.49	0.42
1:A:225:VAL:CG1	1:A:356:TYR:CE2	3.03	0.42
1:B:67:LEU:HD23	1:B:67:LEU:N	2.35	0.42
1:C:98:ILE:N	1:C:98:ILE:CD1	2.81	0.42
1:C:206:ASN:HD22	1:C:206:ASN:N	2.15	0.42
1:A:256:VAL:HG23	1:A:327:VAL:CG2	2.50	0.42
1:C:152:VAL:HG11	1:C:195:LEU:HD21	2.02	0.42
1:A:211:LEU:HD12	1:A:232:PRO:CG	2.49	0.42
1:C:117:GLN:C	1:C:119:LEU:N	2.73	0.42
1:A:295:GLN:HB2	4:A:430:EPE:H71	2.01	0.41
1:C:140:ILE:CG2	1:C:141:GLY:N	2.83	0.41
1:C:164:GLU:O	1:C:199:PRO:HB2	2.18	0.41
1:A:190:ALA:O	1:A:193:ALA:CB	2.38	0.41
1:B:203:HIS:HB3	1:B:220:MET:HB3	2.02	0.41
1:C:144:THR:CB	1:C:148:THR:HG23	2.48	0.41
1:C:288:ASP:HA	1:C:363:SER:HB3	2.01	0.41
1:C:206:ASN:ND2	1:C:206:ASN:C	2.73	0.41
1:A:206:ASN:ND2	1:A:209:THR:H	2.18	0.41
1:A:288:ASP:CG	1:A:365:ARG:HH21	2.23	0.41
1:B:249:LEU:H	1:B:334:VAL:HB	1.85	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:HIS:C	1:C:13:ILE:HD12	2.40	0.41
1:C:144:THR:HG21	1:C:148:THR:CG2	2.51	0.41
1:B:72:ILE:HD12	1:B:72:ILE:C	2.40	0.41
1:B:107:ALA:HB1	1:B:141:GLY:N	2.36	0.41
1:C:14:ASP:OD1	1:C:14:ASP:C	2.59	0.41
1:C:107:ALA:HB2	1:C:140:ILE:CG2	2.50	0.41
1:C:265:ILE:HG12	1:C:271:TYR:HD2	1.84	0.41
1:A:36:PHE:CZ	1:A:62:GLY:HA3	2.55	0.41
1:A:235:ASN:HD22	1:A:235:ASN:HA	1.56	0.41
1:A:295:GLN:NE2	4:A:430:EPE:H52	2.36	0.41
1:B:7:ARG:O	1:B:10:ARG:NH2	2.54	0.41
1:B:68:LEU:HA	1:B:85:ILE:HD13	2.03	0.41
1:B:148:THR:OG1	1:B:149:LYS:N	2.53	0.41
1:B:149:LYS:HA	1:B:152:VAL:HG12	2.02	0.41
1:B:247:LEU:HD13	1:B:247:LEU:C	2.41	0.41
1:C:203:HIS:CD2	1:C:203:HIS:N	2.89	0.41
1:A:139:ARG:HD3	1:C:316:GLN:OE1	2.21	0.41
1:B:110:GLU:H	1:B:110:GLU:CD	2.24	0.41
1:B:165:GLY:HA2	1:B:199:PRO:HG2	2.02	0.41
1:B:191:VAL:HG12	1:B:191:VAL:O	2.20	0.41
1:A:225:VAL:HA	1:A:228:TYR:HD2	1.85	0.41
1:A:280:GLY:O	1:A:318:MET:HA	2.20	0.41
1:B:363:SER:O	1:B:368:ARG:NH1	2.50	0.41
1:C:115:ALA:O	1:C:117:GLN:O	2.38	0.41
1:A:56:LYS:HG3	1:A:63:PHE:CZ	2.54	0.41
1:A:122:GLU:HG2	1:A:123:SER:H	1.85	0.41
1:A:286:TYR:CD1	1:C:357:GLU:HG3	2.56	0.41
1:B:300:LEU:CD1	1:B:337:ASP:HB3	2.51	0.41
1:C:65:VAL:HG13	1:C:66:ALA:N	2.35	0.41
1:C:267:TYR:CE2	3:C:400:PPI:C3	3.01	0.41
1:A:207:SER:CB	2:A:390:PLP:O1P	2.68	0.41
1:A:294:LEU:HD23	1:A:294:LEU:HA	1.91	0.41
1:B:168:THR:HG22	1:B:204:VAL:CG1	2.50	0.41
1:C:189:LYS:HB2	1:C:189:LYS:HE3	1.69	0.41
1:A:146:GLU:CD	1:A:146:GLU:N	2.73	0.40
1:A:316:GLN:HE21	1:A:316:GLN:HB3	1.58	0.40
1:B:94:VAL:HG11	1:B:119:LEU:HD11	2.03	0.40
1:C:294:LEU:CD2	1:C:351:LEU:HD13	2.51	0.40
1:B:12:HIS:HE1	1:B:250:THR:CG2	2.34	0.40
1:B:131:LEU:HD13	1:B:163:TRP:CD1	2.56	0.40
1:B:145:PRO:CA	1:B:191:VAL:HG13	2.29	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:VAL:CG1	1:C:224:GLY:HA2	2.49	0.40
1:C:163:TRP:HZ3	1:C:166:ILE:HB	1.86	0.40
1:A:11:LEU:HD13	1:A:249:LEU:HD13	2.03	0.40
1:B:147:GLU:C	1:B:149:LYS:N	2.75	0.40
1:B:147:GLU:C	1:B:149:LYS:H	2.23	0.40
1:B:286:TYR:HA	1:B:290:TRP:O	2.21	0.40
1:C:28:ARG:CZ	1:C:28:ARG:HB3	2.52	0.40
1:C:28:ARG:HH11	1:C:28:ARG:HG2	1.86	0.40
1:C:119:LEU:HD23	1:C:160:GLU:HB3	2.03	0.40
1:B:154:PHE:O	1:B:158:HIS:HD2	2.05	0.40
1:B:172:THR:HB	1:B:175:GLU:HB2	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	368/371 (99%)	320 (87%)	43 (12%)	5 (1%)	11	20
1	B	369/371 (100%)	328 (89%)	38 (10%)	3 (1%)	19	35
1	C	369/371 (100%)	332 (90%)	33 (9%)	4 (1%)	14	26
All	All	1106/1113 (99%)	980 (89%)	114 (10%)	12 (1%)	14	26

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	121	PRO
1	B	125	THR
1	B	30	PRO
1	C	4	GLY
1	C	190	ALA
1	A	179	SER

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	275	ALA
1	B	297	PHE
1	C	30	PRO
1	A	284	ILE
1	A	204	VAL
1	C	191	VAL

### 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	305/306 (100%)	278 (91%)	27 (9%)	9 19
1	B	306/306 (100%)	278 (91%)	28 (9%)	9 18
1	C	306/306 (100%)	280 (92%)	26 (8%)	10 21
All	All	917/918 (100%)	836 (91%)	81 (9%)	10 19

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	LEU
1	A	38	VAL
1	A	40	LYS
1	A	50	GLU
1	A	65	VAL
1	A	116	LEU
1	A	117	GLN
1	A	121	PRO
1	A	127	LEU
1	A	133	VAL
1	A	146	GLU
1	A	148	THR
1	A	175	GLU
1	A	191	VAL
1	A	203	HIS
1	A	206	ASN

*Continued on next page...*

*Continued from previous page...*

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	209	THR
1	A	220	MET
1	A	223	TYR
1	A	231	ASN
1	A	235	ASN
1	A	247	LEU
1	A	274	GLU
1	A	301	VAL
1	A	345	GLN
1	A	349	GLU
1	A	351	LEU
1	B	13	ILE
1	B	20	GLU
1	B	35	LEU
1	B	38	VAL
1	B	40	LYS
1	B	50	GLU
1	B	65	VAL
1	B	67	LEU
1	B	117	GLN
1	B	137	MET
1	B	143	LEU
1	B	150	GLN
1	B	167	PHE
1	B	175	GLU
1	B	203	HIS
1	B	206	ASN
1	B	219	ASN
1	B	220	MET
1	B	223	TYR
1	B	225	VAL
1	B	235	ASN
1	B	265	ILE
1	B	311	ARG
1	B	316	GLN
1	B	330	VAL
1	B	351	LEU
1	B	355	HIS
1	B	364	GLN
1	C	3	VAL
1	C	15	THR
1	C	28	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	35	LEU
1	C	50	GLU
1	C	65	VAL
1	C	80	GLN
1	C	109	GLN
1	C	116	LEU
1	C	127	LEU
1	C	133	VAL
1	C	175	GLU
1	C	176	ILE
1	C	194	VAL
1	C	206	ASN
1	C	220	MET
1	C	223	TYR
1	C	231	ASN
1	C	247	LEU
1	C	252	GLU
1	C	257	LYS
1	C	311	ARG
1	C	316	GLN
1	C	345	GLN
1	C	351	LEU
1	C	353	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	124	ASN
1	A	158	HIS
1	A	184	GLN
1	A	206	ASN
1	A	231	ASN
1	A	235	ASN
1	A	293	HIS
1	A	295	GLN
1	A	345	GLN
1	B	12	HIS
1	B	80	GLN
1	B	99	GLN
1	B	109	GLN
1	B	117	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	150	GLN
1	B	158	HIS
1	B	203	HIS
1	B	206	ASN
1	B	219	ASN
1	B	295	GLN
1	C	12	HIS
1	C	16	GLN
1	C	109	GLN
1	C	117	GLN
1	C	150	GLN
1	C	206	ASN
1	C	231	ASN
1	C	295	GLN
1	C	316	GLN
1	C	345	GLN
1	C	364	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

8 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	PLP	A	390	1	16,16,16	2.12	5 (31%)	20,23,23	3.31	7 (35%)
3	PPI	A	400	-	4,4,4	0.76	0	4,4,4	1.00	0
3	PPI	B	400	-	4,4,4	0.84	0	4,4,4	0.62	0
4	EPE	A	430	-	15,15,15	2.22	8 (53%)	18,20,20	5.02	11 (61%)
3	PPI	C	400	-	4,4,4	1.00	0	4,4,4	0.70	0
2	PLP	B	390	1	16,16,16	2.27	7 (43%)	20,23,23	2.24	9 (45%)
5	2PE	C	401	-	27,27,27	1.04	1 (3%)	26,26,26	0.58	0
2	PLP	C	390	1	16,16,16	1.72	4 (25%)	20,23,23	2.46	7 (35%)

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	PLP	A	390	1	-	2/8/8/8	0/1/1/1
3	PPI	A	400	-	-	2/2/2/2	-
3	PPI	B	400	-	-	0/2/2/2	-
4	EPE	A	430	-	-	5/9/19/19	0/1/1/1
3	PPI	C	400	-	-	2/2/2/2	-
2	PLP	B	390	1	-	5/8/8/8	0/1/1/1
5	2PE	C	401	-	-	10/25/25/25	-
2	PLP	C	390	1	-	3/8/8/8	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	390	PLP	C3-C2	-5.71	1.35	1.40
4	A	430	EPE	C5-N4	-4.55	1.34	1.46
2	A	390	PLP	C3-C2	-3.81	1.37	1.40
4	A	430	EPE	O2S-S	-3.29	1.35	1.45
2	C	390	PLP	C4-C4A	3.23	1.53	1.46
2	A	390	PLP	C4-C4A	3.23	1.53	1.46
2	A	390	PLP	P-O2P	-3.20	1.42	1.54
2	B	390	PLP	P-O1P	-3.17	1.40	1.50
2	C	390	PLP	P-O2P	-3.05	1.43	1.54
2	B	390	PLP	P-O2P	-2.95	1.43	1.54
2	B	390	PLP	C2A-C2	-2.93	1.45	1.50
2	A	390	PLP	P-O3P	-2.80	1.44	1.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	430	EPE	C2-N1	-2.79	1.39	1.46
2	A	390	PLP	C4-C3	-2.75	1.36	1.40
2	C	390	PLP	P-O1P	-2.68	1.41	1.50
2	B	390	PLP	P-O3P	-2.66	1.44	1.54
2	C	390	PLP	P-O3P	-2.50	1.45	1.54
4	A	430	EPE	O3S-S	-2.43	1.39	1.47
2	B	390	PLP	C4-C4A	2.39	1.51	1.46
4	A	430	EPE	C9-N1	-2.36	1.42	1.47
5	C	401	2PE	C24-C23	2.18	1.60	1.49
2	B	390	PLP	C4-C3	-2.12	1.37	1.40
4	A	430	EPE	C3-N4	-2.12	1.41	1.46
4	A	430	EPE	O1S-S	-2.10	1.38	1.45
4	A	430	EPE	C7-N4	-2.08	1.42	1.47

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	430	EPE	O2S-S-C10	14.58	124.48	106.92
2	A	390	PLP	C5A-C5-C6	-11.59	100.31	119.37
4	A	430	EPE	O3S-S-C10	-9.69	90.10	105.77
4	A	430	EPE	C5-C6-N1	-7.61	95.04	110.64
2	C	390	PLP	C3-C4-C5	-6.34	113.39	118.26
4	A	430	EPE	O3S-S-O1S	5.30	124.21	111.27
2	A	390	PLP	C2A-C2-C3	-4.61	115.19	120.89
2	B	390	PLP	O4P-C5A-C5	4.29	117.53	109.35
2	C	390	PLP	C4-C3-C2	4.14	122.75	120.19
2	B	390	PLP	C3-C4-C5	-3.94	115.23	118.26
2	C	390	PLP	C5A-C5-C6	-3.83	113.07	119.37
2	B	390	PLP	C5A-C5-C6	-3.81	113.11	119.37
2	A	390	PLP	C4-C3-C2	3.77	122.52	120.19
2	C	390	PLP	O4A-C4A-C4	3.73	133.05	124.91
2	A	390	PLP	C3-C4-C5	-3.42	115.63	118.26
2	C	390	PLP	O2P-P-O4P	3.19	115.22	106.73
4	A	430	EPE	C7-N4-C5	3.16	119.32	111.23
4	A	430	EPE	C5-N4-C3	3.11	115.83	108.83
2	A	390	PLP	O4A-C4A-C4	3.10	131.68	124.91
2	B	390	PLP	O4P-P-O1P	2.98	114.83	106.47
4	A	430	EPE	C7-N4-C3	2.85	118.53	111.23
2	A	390	PLP	C2A-C2-N1	2.84	123.22	117.67
2	A	390	PLP	C3-C4-C4A	-2.79	115.94	119.90
2	B	390	PLP	C5-C6-N1	-2.72	119.29	123.82
2	B	390	PLP	O2P-P-O1P	-2.71	100.08	110.68

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	390	PLP	O2P-P-O1P	-2.61	100.46	110.68
4	A	430	EPE	C9-N1-C2	-2.58	104.65	111.23
4	A	430	EPE	O3S-S-O2S	-2.46	105.26	111.27
4	A	430	EPE	C3-C2-N1	2.44	115.66	110.64
2	B	390	PLP	C6-C5-C4	2.38	122.53	118.15
2	B	390	PLP	O3P-P-O2P	2.25	116.23	107.64
4	A	430	EPE	C6-C5-N4	2.20	115.16	110.64
2	C	390	PLP	O4P-C5A-C5	2.15	113.45	109.35
2	B	390	PLP	C3-C2-N1	2.14	123.53	120.77

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	390	PLP	C3-C4-C4A-O4A
2	A	390	PLP	C5-C4-C4A-O4A
2	B	390	PLP	C3-C4-C4A-O4A
2	B	390	PLP	C5-C4-C4A-O4A
2	B	390	PLP	C5A-O4P-P-O1P
2	B	390	PLP	C5A-O4P-P-O2P
2	B	390	PLP	C5A-O4P-P-O3P
4	A	430	EPE	C8-C7-N4-C3
4	A	430	EPE	S-C10-C9-N1
4	A	430	EPE	C9-C10-S-O2S
4	A	430	EPE	C9-C10-S-O3S
5	C	401	2PE	C18-C17-O16-C15
5	C	401	2PE	O19-C20-C21-O22
5	C	401	2PE	O1-C2-C3-O4
2	C	390	PLP	C3-C4-C4A-O4A
5	C	401	2PE	O16-C17-C18-O19
5	C	401	2PE	O10-C11-C12-O13
2	C	390	PLP	C5A-O4P-P-O1P
5	C	401	2PE	C12-C11-O10-C9
5	C	401	2PE	O22-C23-C24-O25
5	C	401	2PE	C9-C8-O7-C6
2	C	390	PLP	C4-C5-C5A-O4P
4	A	430	EPE	C9-C10-S-O1S
3	C	400	PPI	O1-C1-C2-C3
3	C	400	PPI	O2-C1-C2-C3
3	A	400	PPI	O1-C1-C2-C3
3	A	400	PPI	O2-C1-C2-C3
5	C	401	2PE	O7-C8-C9-O10

*Continued on next page...*

Continued from previous page...

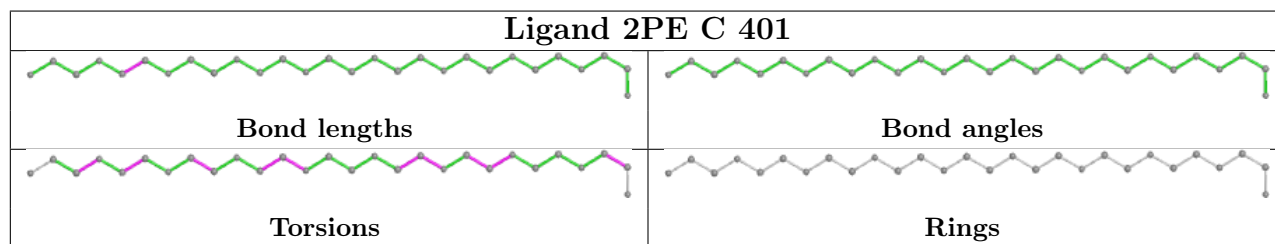
Mol	Chain	Res	Type	Atoms
5	C	401	2PE	C27-C26-O25-C24

There are no ring outliers.

4 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	390	PLP	3	0
4	A	430	EPE	11	0
3	C	400	PPI	5	0
5	C	401	2PE	9	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	307:GLU	C	308:ILE	N	1.19

## 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	370/371 (99%)	0.03	11 (2%) 50 53	15, 33, 57, 80	0
1	B	371/371 (100%)	-0.01	14 (3%) 40 43	16, 36, 59, 79	0
1	C	371/371 (100%)	-0.02	3 (0%) 86 87	18, 33, 57, 66	0
All	All	1112/1113 (99%)	0.00	28 (2%) 57 61	15, 34, 58, 80	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	121	PRO	7.0
1	B	121	PRO	6.8
1	B	120	THR	6.8
1	B	123	SER	6.5
1	B	124	ASN	4.1
1	A	123	SER	3.9
1	A	152	VAL	3.8
1	A	120	THR	3.8
1	A	160	GLU	3.1
1	B	215	ASP	3.0
1	A	153	ARG	2.9
1	B	122	GLU	2.7
1	A	119	LEU	2.7
1	A	124	ASN	2.7
1	B	191	VAL	2.5
1	B	1	MET	2.5
1	B	190	ALA	2.4
1	C	86	LEU	2.4
1	A	161	PHE	2.4
1	B	119	LEU	2.2
1	B	98	ILE	2.2
1	B	31	GLU	2.2
1	B	371	ASN	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	324	GLU	2.2
1	C	65	VAL	2.2
1	A	122	GLU	2.1
1	A	314	MET	2.0
1	B	125	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](#)

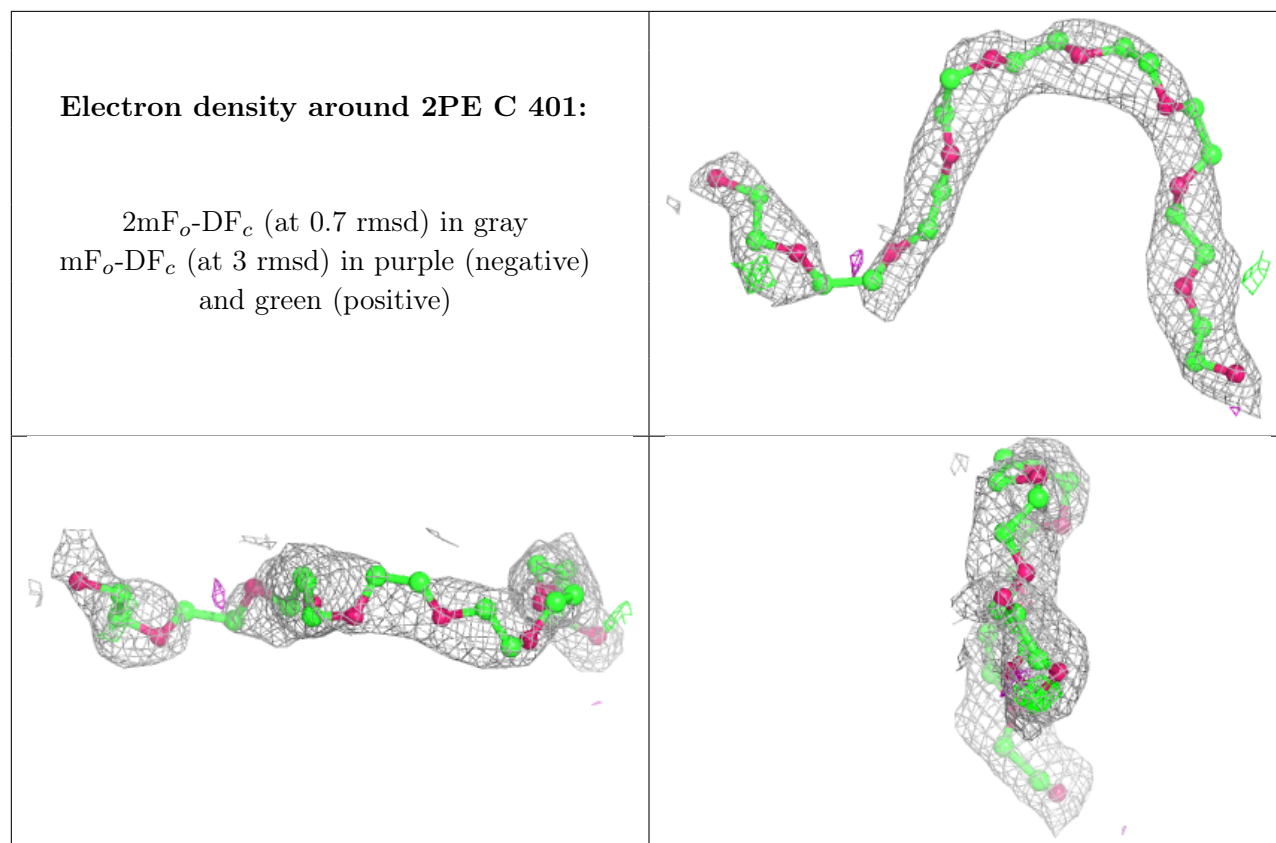
There are no monosaccharides in this entry.

## 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
3	PPI	C	400	5/5	0.63	0.40	53,55,57,59	0
3	PPI	A	400	5/5	0.75	0.38	64,65,66,67	0
3	PPI	B	400	5/5	0.79	0.36	65,66,66,69	0
5	2PE	C	401	28/28	0.80	0.30	57,61,65,65	0
4	EPE	A	430	15/15	0.87	0.41	41,47,59,61	0
2	PLP	A	390	16/16	0.94	0.13	20,20,20,20	0
2	PLP	C	390	16/16	0.95	0.15	20,20,20,20	0
2	PLP	B	390	16/16	0.96	0.12	20,20,20,20	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.