



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:10 PM GMT

PDB ID : 3VQI  
Title : Crystal structure of Kluyveromyces marxianus Atg5  
Authors : Yamaguchi, M.; Noda, N.N.; Yamamoto, H.; Shima, T.; Kumeta, H.;  
Kobashigawa, Y.; Akada, R.; Ohsumi, Y.; Inagaki, F.  
Deposited on : 2012-03-24  
Resolution : 2.50 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

---

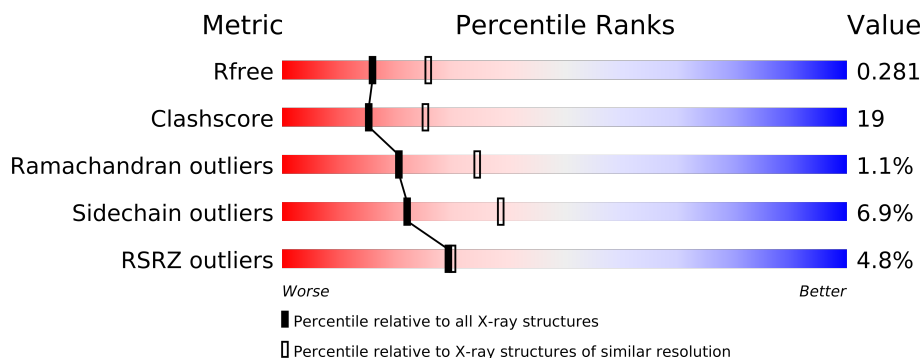
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

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))
$R_{free}$	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	274	
1	B	274	
1	C	274	
1	D	274	
1	E	274	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	EPE	A	301	-	X
2	EPE	B	301	-	X
2	EPE	E	301	-	X

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Geometry	Electron density
3	SO4	A	303	-	X
3	SO4	A	304	-	X
3	SO4	B	302	-	X
3	SO4	C	302	-	X

## 2 Entry composition i

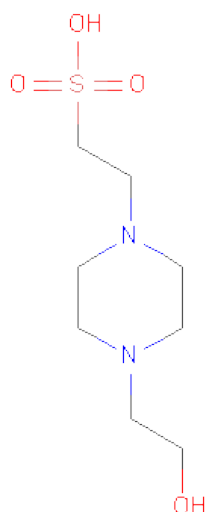
There are 4 unique types of molecules in this entry. The entry contains 10041 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Atg5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	252	Total	C	N	O	S	0	0	0
			1977	1291	326	352	8			
1	B	257	Total	C	N	O	S	0	0	0
			2027	1319	332	368	8			
1	C	241	Total	C	N	O	S	0	0	0
			1843	1201	298	336	8			
1	D	256	Total	C	N	O	S	0	0	0
			1982	1291	324	358	9			
1	E	256	Total	C	N	O	S	0	0	0
			2015	1312	335	359	9			

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



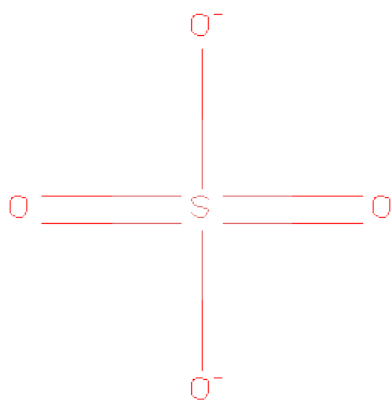
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
2	E	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	D	1	Total	O	S	0	0
			5	4	1		
3	D	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is water.

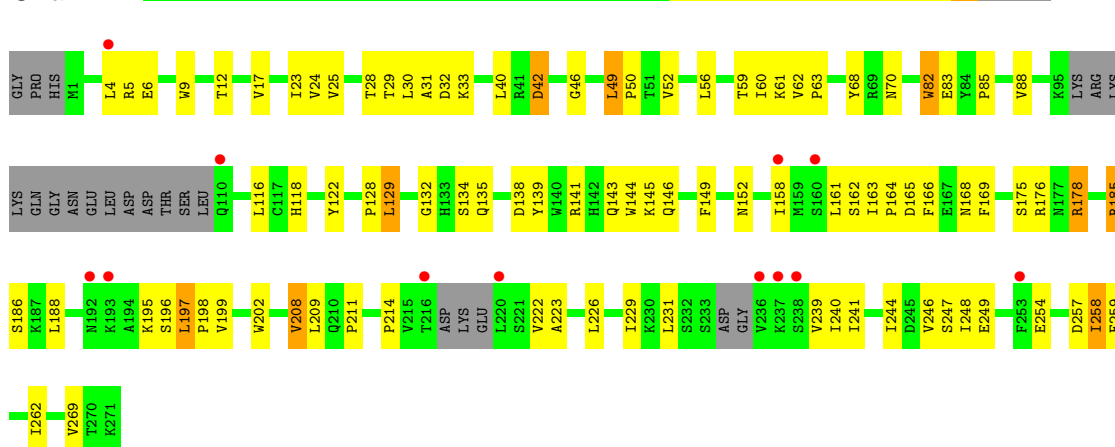
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	14	Total	O	0	0
			14	14		
4	B	22	Total	O	0	0
			22	22		
4	C	10	Total	O	0	0
			10	10		
4	D	10	Total	O	0	0
			10	10		
4	E	21	Total	O	0	0
			21	21		

### 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.

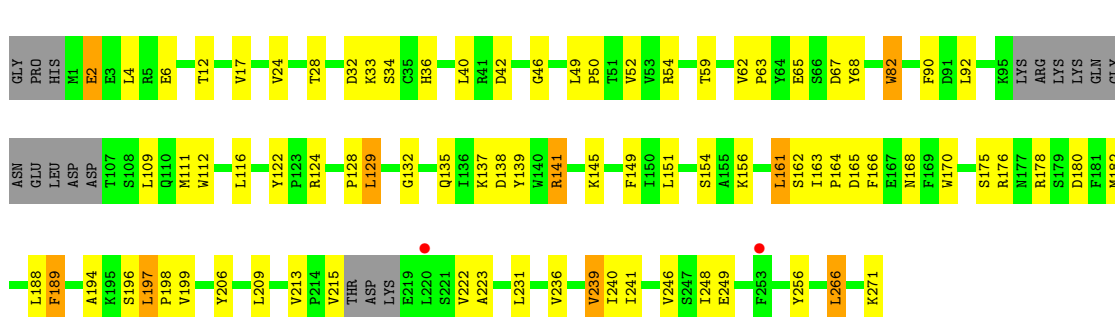
#### • Molecule 1: Atg5

Chain A:



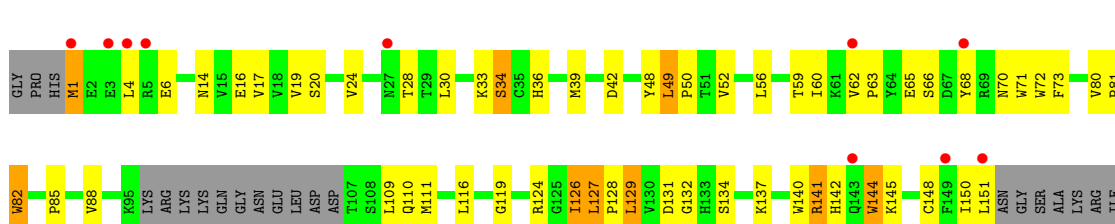
#### • Molecule 1: Atg5

Chain B:



#### • Molecule 1: Atg5

Chain C:







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	165.70Å 81.90Å 158.52Å 90.00° 92.39° 90.00°	Depositor
Resolution (Å)	35.15 – 2.50 35.15 – 2.39	Depositor EDS
% Data completeness (in resolution range)	94.8 (35.15-2.50) 92.7 (35.15-2.39)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.57 (at 2.39Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.238 , 0.268 0.254 , 0.281	Depositor DCC
$R_{free}$ test set	7022 reflections (10.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	53.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 44.0	EDS
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 83071 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	10041	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, SO4

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	0.39	0/2028	0.63	0/2771
1	B	0.41	0/2079	0.66	0/2839
1	C	0.38	0/1889	0.63	1/2589 (0.0%)
1	D	0.41	0/2034	0.63	0/2784
1	E	0.42	0/2067	0.64	0/2822
All	All	0.40	0/10097	0.64	1/13805 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	164	PRO	N-CA-CB	5.29	109.65	103.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1977	0	1888	86	0
1	B	2027	0	1948	78	0
1	C	1843	0	1677	94	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1982	0	1866	61	0
1	E	2015	0	1933	53	0
2	A	15	0	18	9	0
2	B	15	0	18	9	0
2	E	15	0	18	7	0
3	A	15	0	0	0	0
3	B	20	0	0	1	0
3	C	10	0	0	0	0
3	D	10	0	0	1	0
3	E	20	0	0	0	0
4	A	14	0	0	2	0
4	B	22	0	0	0	0
4	C	10	0	0	0	0
4	D	10	0	0	1	0
4	E	21	0	0	0	0
All	All	10041	0	9366	363	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 19.

All (363) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:135:GLN:HE21	2:A:301:EPE:H102	1.19	1.06
1:C:151:LEU:HG	1:C:198:PRO:HD3	1.47	0.96
1:C:24:VAL:HG23	1:C:59:THR:HG22	1.48	0.94
1:C:213:VAL:HG21	1:C:225:LEU:HD11	1.51	0.93
1:C:33:LYS:HB3	1:C:59:THR:HG21	1.52	0.90
1:B:40:LEU:HD11	1:B:176:ARG:HD2	1.53	0.90
1:C:150:ILE:HB	1:C:198:PRO:HG3	1.60	0.82
1:C:209:LEU:HD22	1:C:231:LEU:HD11	1.61	0.82
1:A:135:GLN:NE2	2:A:301:EPE:H102	1.95	0.82
1:D:29:THR:HG23	1:D:32:ASP:H	1.43	0.81
1:C:60:ILE:HD13	1:C:71:TRP:HH2	1.47	0.80
1:C:258:ILE:HG12	1:C:259:PHE:N	1.96	0.80
1:D:239:VAL:HG12	1:D:246:VAL:HG22	1.63	0.79
1:D:17:VAL:HG11	1:D:52:VAL:HG11	1.64	0.79
1:A:141:ARG:HG3	1:A:166:PHE:CZ	2.18	0.77
1:A:9:TRP:CD2	1:A:178:ARG:HG3	2.19	0.77
1:A:185:ARG:HH11	1:A:185:ARG:HB3	1.49	0.77
1:B:40:LEU:CD1	1:B:176:ARG:HD2	2.13	0.77
1:E:135:GLN:HE21	2:E:301:EPE:H102	1.49	0.77
1:D:82:TRP:CZ2	1:D:129:LEU:HB2	2.19	0.77

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:109:LEU:HD13	1:C:111:MET:HE1	1.66	0.76
1:A:24:VAL:HG23	1:A:59:THR:HG22	1.65	0.76
1:C:203:THR:HG22	1:C:204:SER:N	2.01	0.75
1:E:251:ASN:HD21	1:E:253:PHE:HB3	1.51	0.75
1:B:17:VAL:HG11	1:B:52:VAL:HG11	1.70	0.73
1:B:24:VAL:HG23	1:B:59:THR:HG22	1.71	0.72
1:D:65:GLU:H	1:D:65:GLU:CD	1.93	0.72
1:A:254:GLU:O	1:A:258:ILE:HG22	1.89	0.72
1:B:54:ARG:HH11	1:B:54:ARG:HG3	1.55	0.71
1:C:145:LYS:O	1:C:148:CYS:HB3	1.89	0.71
1:A:17:VAL:HG11	1:A:52:VAL:HG11	1.74	0.70
1:C:209:LEU:CD2	1:C:231:LEU:HD11	2.21	0.70
1:A:9:TRP:CG	1:A:178:ARG:HG3	2.26	0.70
1:D:251:ASN:HD21	1:D:253:PHE:HB3	1.56	0.70
1:C:85:PRO:HG2	1:C:88:VAL:CG2	2.22	0.70
1:A:83:GLU:HA	2:A:301:EPE:H31	1.75	0.69
1:D:13:ILE:HD11	1:D:87:GLY:HA2	1.74	0.69
1:C:82:TRP:CZ2	1:C:129:LEU:HB2	2.29	0.68
1:A:141:ARG:HG2	1:A:141:ARG:HH11	1.59	0.68
1:B:52:VAL:HG12	1:B:116:LEU:HD22	1.77	0.67
1:E:251:ASN:ND2	1:E:253:PHE:HB3	2.09	0.67
1:B:209:LEU:HD12	1:B:231:LEU:HD11	1.77	0.66
1:C:239:VAL:HG11	1:C:268:LEU:HD23	1.78	0.65
1:E:254:GLU:O	1:E:258:ILE:HG22	1.97	0.65
1:A:222:VAL:HG11	1:A:239:VAL:HG21	1.79	0.65
1:D:251:ASN:ND2	1:D:253:PHE:HB3	2.11	0.64
1:E:23:ILE:HB	1:E:62:VAL:HG22	1.79	0.64
1:B:197:LEU:HD13	1:B:199:VAL:CG2	2.27	0.64
1:A:33:LYS:HB3	1:A:59:THR:HG21	1.79	0.64
1:C:17:VAL:HG11	1:C:52:VAL:HG11	1.79	0.64
1:A:122:TYR:CE2	1:A:128:PRO:HB3	2.33	0.63
1:C:24:VAL:HG23	1:C:59:THR:CG2	2.25	0.63
1:B:62:VAL:HG13	1:B:63:PRO:HD2	1.80	0.63
1:B:50:PRO:O	1:B:54:ARG:HG2	1.99	0.62
1:C:60:ILE:HD13	1:C:71:TRP:CH2	2.31	0.62
1:C:203:THR:HG22	1:C:204:SER:H	1.64	0.62
1:C:49:LEU:HD12	1:C:73:PHE:CE1	2.35	0.62
1:C:71:TRP:O	1:C:82:TRP:HH2	1.82	0.62
1:A:23:ILE:O	1:A:61:LYS:HG2	2.00	0.62
1:D:24:VAL:HG23	1:D:59:THR:CG2	2.29	0.62
1:B:141:ARG:NH1	1:B:141:ARG:HG3	2.15	0.62
1:E:135:GLN:NE2	2:E:301:EPE:H102	2.13	0.62

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:122:TYR:CE2	1:D:128:PRO:HB3	2.35	0.61
1:A:85:PRO:HG2	1:A:88:VAL:CG2	2.30	0.61
1:A:17:VAL:HG11	1:A:52:VAL:CG1	2.31	0.60
1:A:9:TRP:CE2	1:A:178:ARG:HG3	2.37	0.60
1:C:14:ASN:HB2	1:C:110:GLN:O	2.02	0.60
1:A:135:GLN:HE21	2:A:301:EPE:C10	2.03	0.60
1:E:83:GLU:HA	2:E:301:EPE:H31	1.84	0.60
1:C:49:LEU:HD21	1:C:71:TRP:HB2	1.84	0.60
1:C:42:ASP:O	1:C:262:ILE:HG12	2.02	0.60
1:A:241:ILE:O	1:A:244:ILE:HG12	2.02	0.60
1:D:85:PRO:HG2	1:D:88:VAL:CG2	2.32	0.59
1:A:145:LYS:NZ	4:A:407:HOH:O	2.35	0.59
1:B:197:LEU:HD13	1:B:199:VAL:HG23	1.83	0.59
1:E:112:TRP:CE2	1:E:114:LEU:HD21	2.35	0.59
1:B:139:TYR:CB	2:B:301:EPE:H21	2.33	0.58
1:D:25:VAL:HG22	1:D:28:THR:OG1	2.03	0.58
1:C:208:VAL:HG13	1:C:208:VAL:O	2.03	0.58
1:C:151:LEU:HG	1:C:198:PRO:CD	2.28	0.58
1:A:68:TYR:CE1	1:A:132:GLY:HA2	2.39	0.58
1:B:109:LEU:CD1	1:C:111:MET:HE1	2.34	0.58
1:E:241:ILE:HD11	1:E:268:LEU:HD22	1.86	0.58
1:C:237:LYS:C	1:C:248:ILE:HG13	2.24	0.57
1:E:139:TYR:CG	2:E:301:EPE:H21	2.39	0.57
1:E:46:GLY:N	2:E:301:EPE:O8	2.35	0.57
1:A:24:VAL:HG23	1:A:59:THR:CG2	2.34	0.57
1:E:18:VAL:HG22	1:E:34:SER:OG	2.03	0.57
1:A:40:LEU:HD13	1:A:176:ARG:HD2	1.86	0.57
1:C:14:ASN:HB3	1:C:111:MET:CE	2.33	0.57
1:E:241:ILE:O	1:E:244:ILE:HG12	2.04	0.57
1:C:197:LEU:HD12	1:C:197:LEU:O	2.04	0.57
1:A:241:ILE:HD12	1:A:246:VAL:HG11	1.86	0.57
1:A:59:THR:HG22	1:A:59:THR:O	2.04	0.57
1:A:222:VAL:O	1:A:226:LEU:HD13	2.05	0.56
1:E:85:PRO:HG2	1:E:88:VAL:HG23	1.86	0.56
1:B:90:PHE:HE1	1:B:112:TRP:HB2	1.70	0.56
1:C:213:VAL:CG2	1:C:225:LEU:HD11	2.32	0.56
1:D:237:LYS:HA	1:D:248:ILE:HD13	1.87	0.56
1:C:203:THR:CG2	1:C:204:SER:N	2.68	0.56
1:C:141:ARG:HG2	1:C:166:PHE:CE1	2.41	0.56
1:C:30:LEU:O	1:C:34:SER:HB2	2.06	0.56
1:C:85:PRO:HG2	1:C:88:VAL:HG23	1.88	0.56
1:D:241:ILE:O	1:D:244:ILE:HG12	2.06	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:162:SER:OG	1:A:165:ASP:HB2	2.06	0.55
1:C:59:THR:HG22	1:C:59:THR:O	2.06	0.55
1:B:36:HIS:CD2	1:C:111:MET:HG3	2.41	0.55
1:A:42:ASP:O	1:A:262:ILE:HD13	2.06	0.55
1:C:68:TYR:CD1	1:C:132:GLY:HA2	2.42	0.55
1:D:237:LYS:O	1:D:248:ILE:HG12	2.06	0.55
1:B:82:TRP:CG	2:B:301:EPE:H82	2.41	0.55
1:D:209:LEU:HD12	1:D:209:LEU:N	2.22	0.55
1:B:54:ARG:NE	1:B:67:ASP:OD1	2.40	0.55
1:B:122:TYR:CE2	1:B:128:PRO:HB3	2.42	0.54
1:B:209:LEU:CD1	1:B:231:LEU:HD11	2.37	0.54
1:E:209:LEU:HD22	1:E:231:LEU:HD11	1.90	0.54
4:A:410:HOH:O	1:D:229:ILE:HG22	2.08	0.54
1:A:166:PHE:O	1:A:169:PHE:HB3	2.06	0.54
1:B:111:MET:CE	1:C:109:LEU:HD23	2.36	0.54
1:D:24:VAL:HG23	1:D:59:THR:HG23	1.88	0.54
1:C:28:THR:HG21	1:C:59:THR:HG23	1.90	0.54
1:D:52:VAL:HG12	1:D:116:LEU:HD22	1.90	0.54
1:A:85:PRO:HG2	1:A:88:VAL:HG21	1.90	0.54
1:B:82:TRP:O	2:B:301:EPE:H71	2.08	0.54
1:A:139:TYR:CG	2:A:301:EPE:H21	2.43	0.53
1:C:244:ILE:HD11	1:C:259:PHE:CE1	2.43	0.53
1:E:146:GLN:HG2	1:E:265:PHE:HZ	1.72	0.53
1:B:175:SER:O	1:B:176:ARG:HB2	2.09	0.53
1:B:197:LEU:HD12	1:B:197:LEU:O	2.07	0.53
1:A:56:LEU:O	1:A:60:ILE:HD13	2.07	0.53
1:C:196:SER:HA	1:C:213:VAL:O	2.08	0.53
1:E:141:ARG:HG2	1:E:141:ARG:HH11	1.72	0.53
1:B:161:LEU:HD11	1:B:188:LEU:HD21	1.91	0.53
1:C:126:ILE:HG22	1:C:126:ILE:O	2.08	0.53
1:C:239:VAL:HG11	1:C:268:LEU:CD2	2.37	0.53
1:B:239:VAL:HG12	1:B:246:VAL:HG22	1.90	0.53
1:A:42:ASP:OD1	1:A:262:ILE:HG12	2.09	0.53
1:E:141:ARG:HG3	1:E:166:PHE:CZ	2.44	0.53
1:E:197:LEU:O	1:E:197:LEU:HD12	2.09	0.53
1:A:25:VAL:HG23	1:A:28:THR:CG2	2.38	0.53
1:B:139:TYR:HB3	2:B:301:EPE:H21	1.89	0.53
1:B:65:GLU:H	1:B:65:GLU:CD	2.11	0.53
1:E:4:LEU:HG	1:E:258:ILE:HD11	1.91	0.52
1:A:42:ASP:HB3	1:A:262:ILE:HG23	1.91	0.52
1:C:85:PRO:HG2	1:C:88:VAL:HG21	1.91	0.52
1:B:54:ARG:NH1	1:B:54:ARG:HG3	2.20	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:141:ARG:HG3	1:B:166:PHE:CZ	2.44	0.52
1:B:49:LEU:HB3	1:B:50:PRO:CD	2.39	0.52
1:B:109:LEU:HD13	1:C:111:MET:CE	2.37	0.52
1:A:9:TRP:CD1	1:A:178:ARG:HG3	2.45	0.52
1:A:161:LEU:HD11	1:A:188:LEU:HD21	1.91	0.52
1:A:40:LEU:CD1	1:A:176:ARG:HD2	2.39	0.52
1:E:162:SER:OG	1:E:165:ASP:HB2	2.09	0.52
1:B:240:ILE:HG13	1:B:271:LYS:HD3	1.92	0.51
1:C:72:TRP:HA	1:C:82:TRP:CZ3	2.45	0.51
1:A:202:TRP:CE3	1:A:208:VAL:HG13	2.45	0.51
1:B:135:GLN:HE21	2:B:301:EPE:H91	1.76	0.51
1:C:237:LYS:HA	1:C:248:ILE:HD12	1.92	0.51
1:A:49:LEU:HB3	1:A:50:PRO:CD	2.41	0.51
1:D:197:LEU:HD13	1:D:199:VAL:HG23	1.92	0.51
1:E:36:HIS:C	1:E:37:ILE:HD12	2.30	0.51
1:B:176:ARG:HG2	1:B:176:ARG:HH21	1.75	0.51
1:E:85:PRO:HG2	1:E:88:VAL:CG2	2.41	0.51
1:E:65:GLU:CD	1:E:65:GLU:H	2.13	0.51
1:C:68:TYR:CE1	1:C:132:GLY:HA2	2.46	0.51
1:B:59:THR:HG22	1:B:59:THR:O	2.11	0.50
1:A:175:SER:O	1:A:176:ARG:HB2	2.11	0.50
1:A:5:ARG:NH2	1:A:257:ASP:OD2	2.44	0.50
1:B:33:LYS:HB3	1:B:59:THR:HG21	1.93	0.50
1:B:28:THR:HG21	1:B:59:THR:HG23	1.93	0.50
1:C:49:LEU:HD13	1:C:82:TRP:CZ3	2.46	0.50
1:B:28:THR:HG21	1:B:59:THR:CG2	2.41	0.50
1:C:39:MET:HG2	1:C:48:TYR:CE2	2.47	0.50
1:D:33:LYS:CB	1:D:59:THR:HG21	2.42	0.50
1:E:137:LYS:HD3	1:E:170:TRP:CD1	2.47	0.50
1:C:203:THR:CG2	1:C:204:SER:H	2.23	0.50
2:B:301:EPE:O3S	1:E:209:LEU:HG	2.11	0.49
1:A:239:VAL:HG12	1:A:240:ILE:N	2.28	0.49
1:C:150:ILE:CB	1:C:198:PRO:HG3	2.37	0.49
1:D:149:PHE:CE1	1:D:155:ALA:HB2	2.48	0.49
1:C:241:ILE:HD11	1:C:268:LEU:CD2	2.43	0.49
1:E:197:LEU:HD12	1:E:213:VAL:HB	1.93	0.49
1:B:223:ALA:HB2	1:B:248:ILE:HB	1.93	0.49
1:C:162:SER:CB	1:C:165:ASP:HB2	2.42	0.49
1:A:25:VAL:HA	1:A:61:LYS:HB3	1.95	0.49
1:B:178:ARG:O	1:B:182:MET:HG2	2.13	0.49
1:A:25:VAL:CG2	1:A:28:THR:HG21	2.42	0.49
1:D:54:ARG:HG2	1:D:54:ARG:HH11	1.78	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:82:TRP:O	2:A:301:EPE:H71	2.13	0.48
1:D:239:VAL:HG12	1:D:246:VAL:CG2	2.37	0.48
1:A:158:ILE:HB	1:A:188:LEU:HD22	1.95	0.48
1:A:29:THR:HG22	1:A:31:ALA:H	1.77	0.48
1:A:25:VAL:HG23	1:A:28:THR:HG21	1.94	0.48
1:B:111:MET:HE2	1:C:109:LEU:CD2	2.43	0.48
1:A:244:ILE:HD11	1:A:259:PHE:CZ	2.49	0.48
1:B:222:VAL:HB	1:B:248:ILE:HA	1.94	0.48
1:E:5:ARG:NH2	1:E:257:ASP:OD1	2.46	0.48
1:A:211:PRO:HG3	1:A:229:ILE:CD1	2.44	0.48
1:A:24:VAL:O	1:A:61:LYS:HD3	2.14	0.48
1:D:85:PRO:HG2	1:D:88:VAL:HG21	1.95	0.48
1:A:62:VAL:CG1	1:A:63:PRO:HD2	2.43	0.48
1:D:23:ILE:O	1:D:61:LYS:HG2	2.14	0.48
1:A:163:ILE:N	1:A:164:PRO:HD2	2.28	0.48
1:C:127:LEU:HD23	1:C:128:PRO:HD2	1.95	0.47
1:A:23:ILE:HG22	1:A:62:VAL:HG21	1.95	0.47
1:D:9:TRP:O	1:D:176:ARG:NH1	2.48	0.47
1:E:177:ASN:ND2	1:E:180:ASP:OD2	2.48	0.47
1:C:239:VAL:O	1:C:246:VAL:HG22	2.15	0.47
1:A:197:LEU:HA	1:A:198:PRO:HD3	1.80	0.47
1:D:39:MET:HG2	1:D:48:TYR:CE2	2.50	0.47
1:C:14:ASN:HB3	1:C:111:MET:HE1	1.97	0.47
1:C:248:ILE:O	1:C:248:ILE:HG22	2.14	0.47
1:D:237:LYS:HA	1:D:248:ILE:CD1	2.44	0.47
1:A:247:SER:C	1:A:249:GLU:H	2.18	0.47
1:B:162:SER:OG	1:B:165:ASP:HB2	2.14	0.47
1:B:256:TYR:HA	1:B:266:LEU:HG	1.97	0.47
1:A:141:ARG:CG	1:A:141:ARG:HH11	2.26	0.47
1:D:59:THR:CG2	1:D:59:THR:O	2.62	0.47
1:E:112:TRP:CZ2	1:E:114:LEU:HD21	2.50	0.47
1:A:209:LEU:HD23	1:A:229:ILE:HD11	1.97	0.47
1:C:70:ASN:HB3	1:C:119:GLY:O	2.15	0.47
1:E:37:ILE:HD12	1:E:37:ILE:N	2.29	0.47
1:D:222:VAL:HG22	1:D:252:ILE:HD12	1.97	0.47
1:C:169:PHE:CE1	1:C:181:PHE:CE2	3.03	0.46
1:B:141:ARG:CG	1:B:166:PHE:CZ	2.98	0.46
1:B:194:ALA:O	1:B:215:VAL:HG21	2.14	0.46
1:C:151:LEU:HD22	1:C:194:ALA:HB1	1.96	0.46
1:E:151:LEU:HD13	1:E:189:PHE:CG	2.50	0.46
1:E:197:LEU:HD13	1:E:199:VAL:HG23	1.97	0.46
1:B:241:ILE:HD12	1:B:246:VAL:HG21	1.98	0.46

*Continued on next page...*



*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:33:LYS:CB	1:C:59:THR:HG21	2.36	0.46
1:D:54:ARG:HG2	1:D:54:ARG:NH1	2.30	0.46
1:E:3:GLU:O	1:E:7:ARG:HG3	2.16	0.46
1:A:196:SER:HB3	1:A:214:PRO:HA	1.97	0.46
1:B:24:VAL:HG23	1:B:59:THR:CG2	2.42	0.46
1:D:222:VAL:HG22	1:D:252:ILE:CD1	2.46	0.46
1:C:19:VAL:HG23	1:C:56:LEU:HD13	1.97	0.46
1:B:137:LYS:HD2	1:B:170:TRP:CD1	2.51	0.46
1:A:46:GLY:N	2:A:301:EPE:O8	2.44	0.46
1:D:59:THR:HG22	1:D:59:THR:O	2.13	0.46
1:D:149:PHE:CZ	1:D:155:ALA:HB2	2.51	0.46
1:D:82:TRP:CD1	1:D:82:TRP:N	2.83	0.46
1:B:197:LEU:HD12	1:B:213:VAL:HB	1.97	0.46
1:B:154:SER:C	1:B:156:LYS:H	2.20	0.46
1:C:262:ILE:C	1:C:262:ILE:HD12	2.36	0.46
1:D:158:ILE:HG23	1:D:159:MET:N	2.31	0.46
1:C:4:LEU:HD23	1:C:258:ILE:HD12	1.97	0.45
1:B:82:TRP:CZ2	1:B:129:LEU:HB2	2.50	0.45
1:C:16:GLU:OE1	1:C:36:HIS:NE2	2.43	0.45
1:E:14:ASN:HB3	1:E:111:MET:HE2	1.97	0.45
1:E:4:LEU:O	1:E:8:VAL:HG23	2.17	0.45
1:B:141:ARG:CG	1:B:141:ARG:HH11	2.30	0.45
1:C:20:SER:HB2	1:C:116:LEU:O	2.16	0.45
1:E:252:ILE:HA	1:E:255:LEU:HD12	1.97	0.45
1:A:33:LYS:CB	1:A:59:THR:HG21	2.44	0.45
1:A:240:ILE:HB	1:A:269:VAL:HB	1.97	0.45
1:B:141:ARG:HH11	1:B:141:ARG:HG3	1.80	0.45
1:D:49:LEU:HB3	1:D:50:PRO:CD	2.47	0.45
1:B:82:TRP:HB2	2:B:301:EPE:O8	2.17	0.45
1:D:197:LEU:HD13	1:D:199:VAL:CG2	2.47	0.45
1:D:163:ILE:N	1:D:164:PRO:HD2	2.32	0.45
1:B:163:ILE:N	1:B:164:PRO:HD2	2.32	0.45
1:B:17:VAL:HG11	1:B:52:VAL:CG1	2.44	0.45
1:C:62:VAL:HG13	1:C:63:PRO:HD2	1.98	0.45
1:D:141:ARG:NH1	3:D:302:SO4:O4	2.49	0.45
1:A:202:TRP:CD2	1:A:208:VAL:HG13	2.52	0.44
1:A:186:SER:C	1:A:188:LEU:H	2.21	0.44
1:C:144:TRP:O	1:C:145:LYS:C	2.55	0.44
1:A:149:PHE:CD1	1:D:149:PHE:CD1	3.05	0.44
1:B:145:LYS:NZ	3:B:304:SO4:O1	2.51	0.44
1:A:83:GLU:CA	2:A:301:EPE:H31	2.46	0.44
1:C:151:LEU:HA	1:C:196:SER:O	2.17	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:135:GLN:HE21	2:E:301:EPE:C10	2.24	0.44
1:A:241:ILE:CD1	1:A:246:VAL:HG11	2.47	0.44
1:C:208:VAL:CG1	1:C:208:VAL:O	2.65	0.44
1:B:111:MET:HE1	1:C:109:LEU:HD23	1.99	0.44
1:E:29:THR:HG22	1:E:31:ALA:H	1.82	0.44
1:D:112:TRP:CE2	1:D:114:LEU:HD21	2.53	0.44
1:C:39:MET:HG2	1:C:48:TYR:CD2	2.53	0.43
1:E:60:ILE:HD13	1:E:71:TRP:HH2	1.83	0.43
1:C:258:ILE:CG1	1:C:259:PHE:N	2.71	0.43
1:A:4:LEU:HD13	1:A:258:ILE:CD1	2.48	0.43
1:E:197:LEU:CD1	1:E:213:VAL:HB	2.48	0.43
1:D:49:LEU:HD11	1:D:71:TRP:HB2	2.01	0.43
1:A:83:GLU:HA	2:A:301:EPE:C3	2.46	0.43
1:D:198:PRO:HB3	1:D:265:PHE:CE2	2.54	0.43
1:C:131:ASP:O	1:C:134:SER:HB2	2.19	0.43
1:A:4:LEU:HD13	1:A:258:ILE:HD11	2.00	0.43
1:C:137:LYS:O	1:C:140:TRP:HB3	2.18	0.43
1:D:19:VAL:HG21	1:D:59:THR:HG22	2.00	0.43
1:A:202:TRP:CZ3	1:A:208:VAL:HG13	2.54	0.43
1:D:151:LEU:HA	1:D:196:SER:O	2.19	0.43
1:B:49:LEU:HB3	1:B:50:PRO:HD3	2.00	0.43
1:C:166:PHE:O	1:C:169:PHE:HB3	2.19	0.43
1:A:144:TRP:C	1:A:146:GLN:N	2.72	0.43
1:C:49:LEU:N	1:C:50:PRO:HD2	2.34	0.43
1:D:43:ALA:O	1:D:85:PRO:HA	2.19	0.43
1:A:223:ALA:N	1:A:248:ILE:O	2.46	0.43
1:B:197:LEU:HA	1:B:198:PRO:HD3	1.80	0.43
1:C:6:GLU:OE2	1:C:178:ARG:HD3	2.19	0.43
1:B:2:GLU:C	1:B:4:LEU:N	2.72	0.43
1:B:92:LEU:HD11	1:B:206:TYR:HD1	1.82	0.43
1:C:258:ILE:HD11	1:C:259:PHE:CZ	2.54	0.42
1:D:40:LEU:HD13	1:D:176:ARG:HD2	2.01	0.42
1:A:197:LEU:HD13	1:A:199:VAL:CG2	2.49	0.42
1:D:162:SER:OG	1:D:165:ASP:HB2	2.18	0.42
1:A:68:TYR:CZ	1:A:132:GLY:HA3	2.54	0.42
1:A:229:ILE:CG2	1:A:231:LEU:HD12	2.49	0.42
1:D:85:PRO:HG2	1:D:88:VAL:HG23	2.00	0.42
1:E:1:MET:C	1:E:3:GLU:H	2.22	0.42
1:D:152:ASN:ND2	1:D:157:ARG:CG	2.82	0.42
1:C:71:TRP:O	1:C:82:TRP:CH2	2.67	0.42
1:A:30:LEU:HA	1:A:33:LYS:HE2	2.01	0.42
1:D:87:GLY:HA3	4:D:401:HOH:O	2.19	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:197:LEU:O	1:D:197:LEU:HD12	2.19	0.42
1:D:13:ILE:HD11	1:D:41:ARG:HG2	2.01	0.42
1:A:222:VAL:CG1	1:A:239:VAL:HG21	2.49	0.42
1:D:122:TYR:CZ	1:D:128:PRO:HB3	2.54	0.42
1:B:139:TYR:HB2	2:B:301:EPE:H92	2.02	0.42
1:B:68:TYR:HD1	1:B:129:LEU:HD13	1.85	0.42
1:B:161:LEU:CD1	1:B:188:LEU:HD21	2.49	0.42
1:E:197:LEU:HA	1:E:198:PRO:HD3	1.70	0.42
1:B:149:PHE:CD1	1:E:149:PHE:CD1	3.08	0.42
1:C:197:LEU:HA	1:C:198:PRO:HD3	1.84	0.42
1:C:141:ARG:O	1:C:144:TRP:N	2.52	0.42
1:C:126:ILE:HD12	1:C:126:ILE:HA	1.89	0.42
1:C:65:GLU:HG2	1:C:66:SER:N	2.34	0.42
1:A:229:ILE:HG23	1:A:231:LEU:HD12	2.02	0.41
1:E:167:GLU:O	1:E:171:VAL:HG23	2.20	0.41
1:C:195:LYS:O	1:C:214:PRO:HA	2.20	0.41
1:B:68:TYR:CE1	1:B:132:GLY:HA2	2.56	0.41
1:E:262:ILE:HD12	1:E:263:ASP:N	2.35	0.41
1:E:1:MET:C	1:E:3:GLU:N	2.74	0.41
1:E:70:ASN:O	1:E:118:HIS:HA	2.20	0.41
1:D:209:LEU:CD1	1:D:209:LEU:N	2.83	0.41
1:E:223:ALA:N	1:E:248:ILE:O	2.49	0.41
1:E:122:TYR:CZ	1:E:128:PRO:HB3	2.56	0.41
1:A:82:TRP:CZ2	1:A:129:LEU:HB2	2.55	0.41
1:D:241:ILE:HD12	1:D:246:VAL:HG11	2.02	0.41
1:C:80:VAL:HA	1:C:81:PRO:HD3	1.88	0.41
1:C:140:TRP:HH2	1:C:169:PHE:CD2	2.38	0.41
1:E:82:TRP:O	2:E:301:EPE:H71	2.20	0.41
1:B:17:VAL:O	1:B:34:SER:HA	2.20	0.41
1:A:52:VAL:HG12	1:A:116:LEU:HD22	2.03	0.41
1:B:197:LEU:CD1	1:B:213:VAL:HB	2.51	0.41
1:D:152:ASN:ND2	1:D:157:ARG:HG2	2.36	0.41
1:C:1:MET:HA	1:C:1:MET:HE2	2.03	0.41
1:C:229:ILE:O	1:C:229:ILE:HG22	2.21	0.41
1:B:151:LEU:HA	1:B:196:SER:O	2.20	0.41
1:B:90:PHE:CE1	1:B:112:TRP:HB2	2.52	0.41
1:A:209:LEU:O	1:A:211:PRO:HD3	2.21	0.40
1:B:46:GLY:N	2:B:301:EPE:O8	2.47	0.40
1:C:223:ALA:CA	1:C:248:ILE:HG22	2.51	0.40
1:D:15:VAL:HG21	1:D:39:MET:SD	2.61	0.40
1:B:168:ASN:HD22	1:B:168:ASN:HA	1.75	0.40
1:B:6:GLU:OE2	1:B:178:ARG:NE	2.54	0.40

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:209:LEU:C	1:A:211:PRO:HD3	2.42	0.40
1:E:196:SER:HA	1:E:214:PRO:HA	2.03	0.40
1:D:244:ILE:HD11	1:D:259:PHE:CZ	2.57	0.40
1:E:82:TRP:CD1	1:E:82:TRP:N	2.89	0.40
1:B:151:LEU:HD13	1:B:189:PHE:CB	2.51	0.40
1:C:254:GLU:O	1:C:257:ASP:HB3	2.21	0.40
1:A:70:ASN:O	1:A:118:HIS:HA	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	244/274 (89%)	223 (91%)	20 (8%)	1 (0%)	43 66
1	B	251/274 (92%)	238 (95%)	11 (4%)	2 (1%)	27 46
1	C	229/274 (84%)	202 (88%)	24 (10%)	3 (1%)	18 29
1	D	250/274 (91%)	227 (91%)	18 (7%)	5 (2%)	11 17
1	E	250/274 (91%)	237 (95%)	11 (4%)	2 (1%)	27 46
All	All	1224/1370 (89%)	1127 (92%)	84 (7%)	13 (1%)	21 34

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	142	HIS
1	E	236	VAL
1	D	236	VAL
1	E	234	ASP
1	A	195	LYS
1	C	141	ARG
1	D	195	LYS
1	D	234	ASP
1	B	161	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	161	LEU
1	B	236	VAL
1	D	262	ILE
1	C	262	ILE

### 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	205/249 (82%)	188 (92%)	17 (8%)	16	29
1	B	215/249 (86%)	200 (93%)	15 (7%)	21	38
1	C	182/249 (73%)	168 (92%)	14 (8%)	18	33
1	D	204/249 (82%)	188 (92%)	16 (8%)	18	32
1	E	210/249 (84%)	202 (96%)	8 (4%)	44	71
All	All	1016/1245 (82%)	946 (93%)	70 (7%)	22	39

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	GLU
1	A	12	THR
1	A	32	ASP
1	A	42	ASP
1	A	49	LEU
1	A	82	TRP
1	A	129	LEU
1	A	134	SER
1	A	138	ASP
1	A	143	GLN
1	A	152	ASN
1	A	168	ASN
1	A	178	ARG
1	A	185	ARG
1	A	197	LEU
1	A	208	VAL
1	A	258	ILE

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	2	GLU
1	B	12	THR
1	B	32	ASP
1	B	42	ASP
1	B	82	TRP
1	B	124	ARG
1	B	129	LEU
1	B	138	ASP
1	B	141	ARG
1	B	180	ASP
1	B	189	PHE
1	B	197	LEU
1	B	239	VAL
1	B	249	GLU
1	B	266	LEU
1	C	1	MET
1	C	34	SER
1	C	49	LEU
1	C	82	TRP
1	C	124	ARG
1	C	126	ILE
1	C	127	LEU
1	C	129	LEU
1	C	144	TRP
1	C	166	PHE
1	C	180	ASP
1	C	244	ILE
1	C	258	ILE
1	C	266	LEU
1	D	1	MET
1	D	25	VAL
1	D	42	ASP
1	D	49	LEU
1	D	82	TRP
1	D	94	ASN
1	D	110	GLN
1	D	120	ASP
1	D	124	ARG
1	D	129	LEU
1	D	165	ASP
1	D	180	ASP
1	D	197	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	239	VAL
1	D	244	ILE
1	D	266	LEU
1	E	32	ASP
1	E	65	GLU
1	E	82	TRP
1	E	116	LEU
1	E	129	LEU
1	E	165	ASP
1	E	244	ILE
1	E	266	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	168	ASN
1	B	168	ASN
1	C	10	ASN
1	C	146	GLN
1	C	210	GLN
1	D	10	ASN
1	D	94	ASN
1	D	152	ASN
1	D	251	ASN
1	E	10	ASN
1	E	76	ASN
1	E	110	GLN
1	E	251	ASN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

18 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	EPE	A	301	-	15,15,15	1.22	2 (13%)	20,20,20	1.90	5 (25%)
3	SO4	A	302	-	4,4,4	0.26	0	6,6,6	0.11	0
3	SO4	A	303	-	4,4,4	0.29	0	6,6,6	0.09	0
3	SO4	A	304	-	4,4,4	0.73	0	6,6,6	0.12	0
2	EPE	B	301	-	15,15,15	1.55	4 (26%)	20,20,20	2.74	6 (30%)
3	SO4	B	302	-	4,4,4	0.27	0	6,6,6	0.09	0
3	SO4	B	303	-	4,4,4	0.27	0	6,6,6	0.07	0
3	SO4	B	304	-	4,4,4	0.24	0	6,6,6	0.09	0
3	SO4	B	305	-	4,4,4	0.28	0	6,6,6	0.07	0
3	SO4	C	301	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	C	302	-	4,4,4	0.26	0	6,6,6	0.07	0
3	SO4	D	301	-	4,4,4	0.23	0	6,6,6	0.10	0
3	SO4	D	302	-	4,4,4	0.26	0	6,6,6	0.13	0
2	EPE	E	301	-	15,15,15	1.34	2 (13%)	20,20,20	1.91	5 (25%)
3	SO4	E	302	-	4,4,4	0.28	0	6,6,6	0.11	0
3	SO4	E	303	-	4,4,4	0.25	0	6,6,6	0.11	0
3	SO4	E	304	-	4,4,4	0.25	0	6,6,6	0.08	0
3	SO4	E	305	-	4,4,4	0.25	0	6,6,6	0.09	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EPE	A	301	-	-	0/9/19/19	0/1/1/1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SO4	A	302	-	-	0/0/0/0	0/0/0/0
3	SO4	A	303	-	-	0/0/0/0	0/0/0/0
3	SO4	A	304	-	-	0/0/0/0	0/0/0/0
2	EPE	B	301	-	-	0/9/19/19	0/1/1/1
3	SO4	B	302	-	-	0/0/0/0	0/0/0/0
3	SO4	B	303	-	-	0/0/0/0	0/0/0/0
3	SO4	B	304	-	-	0/0/0/0	0/0/0/0
3	SO4	B	305	-	-	0/0/0/0	0/0/0/0
3	SO4	C	301	-	-	0/0/0/0	0/0/0/0
3	SO4	C	302	-	-	0/0/0/0	0/0/0/0
3	SO4	D	301	-	-	0/0/0/0	0/0/0/0
3	SO4	D	302	-	-	0/0/0/0	0/0/0/0
2	EPE	E	301	-	-	0/9/19/19	0/1/1/1
3	SO4	E	302	-	-	0/0/0/0	0/0/0/0
3	SO4	E	303	-	-	0/0/0/0	0/0/0/0
3	SO4	E	304	-	-	0/0/0/0	0/0/0/0
3	SO4	E	305	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	EPE	C10-S	3.72	1.83	1.77
2	E	301	EPE	C10-S	3.66	1.83	1.77
2	B	301	EPE	O3S-S	3.16	1.54	1.46
2	A	301	EPE	C10-S	3.09	1.82	1.77
2	A	301	EPE	O3S-S	3.04	1.53	1.46
2	E	301	EPE	O3S-S	2.86	1.53	1.46
2	B	301	EPE	C6-N1	2.07	1.52	1.47
2	B	301	EPE	C5-N4	2.07	1.52	1.47

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	EPE	O1S-S-C10	9.79	115.20	106.81
2	A	301	EPE	O2S-S-C10	5.94	111.89	106.81
2	E	301	EPE	O1S-S-C10	5.67	111.67	106.81
2	B	301	EPE	O3S-S-O2S	-3.38	104.48	111.78
2	B	301	EPE	O3S-S-O1S	-3.17	104.93	111.78
2	E	301	EPE	O3S-S-O2S	-2.77	105.79	111.78
2	E	301	EPE	O3S-S-O1S	-2.75	105.83	111.78
2	A	301	EPE	O3S-S-O1S	-2.62	106.12	111.78
2	A	301	EPE	O3S-S-O2S	-2.53	106.31	111.78

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	EPE	C7-N4-C3	-2.50	104.86	111.32
2	E	301	EPE	C7-N4-C3	-2.45	104.99	111.32
2	B	301	EPE	C7-N4-C3	-2.41	105.11	111.32
2	A	301	EPE	C9-N1-C2	-2.26	105.48	111.32
2	B	301	EPE	C9-N1-C2	-2.21	105.63	111.32
2	B	301	EPE	O2S-S-C10	-2.16	104.96	106.81
2	E	301	EPE	C9-N1-C2	-2.15	105.78	111.32

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	252/274 (91%)	0.35	12 (4%) 29 30	35, 61, 93, 106	0
1	B	257/274 (93%)	0.03	2 (0%) 83 84	31, 51, 78, 90	0
1	C	241/274 (87%)	0.60	28 (11%) 5 5	38, 71, 115, 126	0
1	D	256/274 (93%)	0.28	16 (6%) 19 19	37, 66, 102, 108	0
1	E	256/274 (93%)	-0.05	3 (1%) 75 77	33, 50, 81, 98	0
All	All	1262/1370 (92%)	0.24	61 (4%) 29 30	31, 60, 101, 126	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	ALA	5.6
1	C	163	ILE	5.3
1	D	192	ASN	5.1
1	C	149	PHE	4.7
1	A	237	LYS	4.7
1	A	4	LEU	4.6
1	C	252	ILE	4.6
1	C	194	ALA	4.3
1	C	151	LEU	4.3
1	B	220	LEU	4.2
1	D	220	LEU	4.0
1	A	192	ASN	3.8
1	D	191	MET	3.8
1	A	220	LEU	3.7
1	A	236	VAL	3.7
1	C	220	LEU	3.5
1	D	214	PRO	3.5
1	C	160	SER	3.5
1	A	253	PHE	3.4
1	C	192	ASN	3.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	C	214	PRO	3.3
1	D	235	GLY	3.1
1	E	220	LEU	3.1
1	A	238	SER	3.1
1	C	4	LEU	2.9
1	C	231	LEU	2.9
1	C	164	PRO	2.9
1	C	27	ASN	2.8
1	C	68	TYR	2.8
1	C	1	MET	2.7
1	B	253	PHE	2.7
1	D	1	MET	2.7
1	D	109	LEU	2.7
1	D	253	PHE	2.6
1	C	213	VAL	2.6
1	A	160	SER	2.6
1	C	248	ILE	2.5
1	D	190	SER	2.5
1	C	223	ALA	2.5
1	D	216	THR	2.5
1	A	216	THR	2.4
1	C	62	VAL	2.4
1	C	216	THR	2.4
1	A	158	ILE	2.4
1	A	110	GLN	2.4
1	D	194	ALA	2.3
1	D	4	LEU	2.3
1	D	149	PHE	2.3
1	C	257	ASP	2.3
1	C	247	SER	2.2
1	C	143	GLN	2.2
1	C	212	THR	2.2
1	D	213	VAL	2.2
1	C	3	GLU	2.2
1	D	251	ASN	2.1
1	C	249	GLU	2.1
1	E	4	LEU	2.1
1	C	5	ARG	2.0
1	C	215	VAL	2.0
1	A	193	LYS	2.0
1	E	253	PHE	2.0

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

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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	EPE	E	301	15/15	0.32	8.34	86,92,109,109	0
2	EPE	B	301	15/15	0.40	8.21	94,99,114,114	0
2	EPE	A	301	15/15	0.44	8.06	100,104,118,118	0
3	SO4	A	303	5/5	0.24	6.77	121,121,122,122	0
3	SO4	C	302	5/5	0.35	3.85	122,123,123,123	0
3	SO4	A	304	5/5	0.14	3.58	117,117,117,118	0
3	SO4	B	302	5/5	0.27	2.89	116,116,117,117	0
3	SO4	E	305	5/5	0.24	1.01	130,130,130,130	0
3	SO4	C	301	5/5	0.19	0.87	115,116,116,116	0
3	SO4	D	302	5/5	0.20	0.76	146,146,146,146	0
3	SO4	B	303	5/5	0.18	0.66	127,127,127,128	0
3	SO4	B	305	5/5	0.13	0.55	118,118,118,119	0
3	SO4	A	302	5/5	0.14	-0.22	113,114,114,115	0
3	SO4	E	304	5/5	0.16	-0.24	135,135,135,135	0
3	SO4	E	303	5/5	0.12	-0.29	94,94,94,95	0
3	SO4	D	301	5/5	0.11	-0.67	98,99,99,99	0
3	SO4	B	304	5/5	0.13	-1.02	137,137,138,138	0
3	SO4	E	302	5/5	0.11	-2.16	97,97,98,98	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.