Full wwPDB X-ray Structure Validation Report (i)

Nov 2, 2023 – 10:09 PM EDT

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 X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *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 (i) 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 (i)) were used in the production of this report:

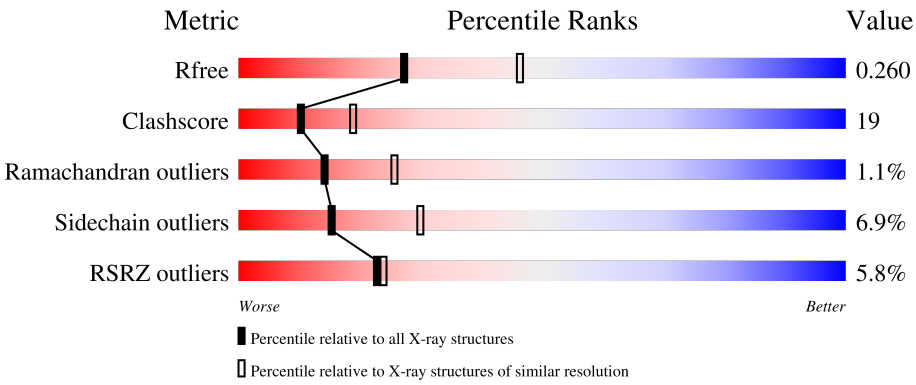
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

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))
R_{free}	130704	4661 (2.50-2.50)
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 >=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 <=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	274	4% 58% 31% • 8%
1	B	274	2% 64% 27% • 6%
1	C	274	14% 53% 30% 5% 12%
1	D	274	6% 65% 26% • 7%
1	E	274	% 66% 26% • 7%

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	EPE	A	301	-	-	X	X
2	EPE	B	301	-	-	X	X
2	EPE	E	301	-	-	X	-

2 Entry composition (i)

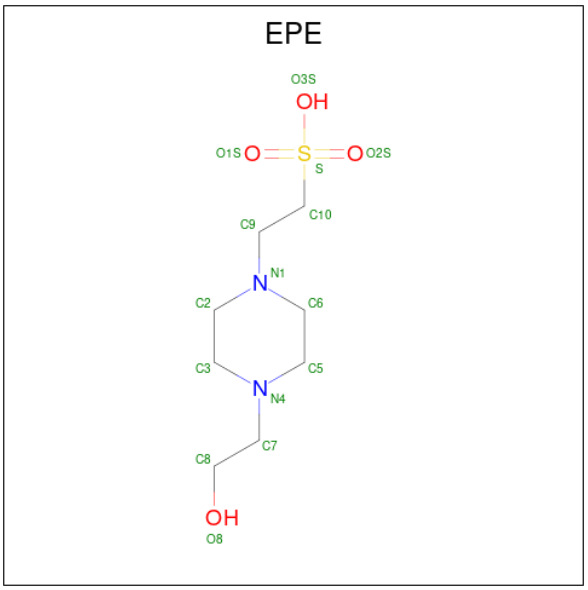
There are 4 unique types of molecules in this entry. The entry contains 10041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Atg5.

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

- Molecule 2 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

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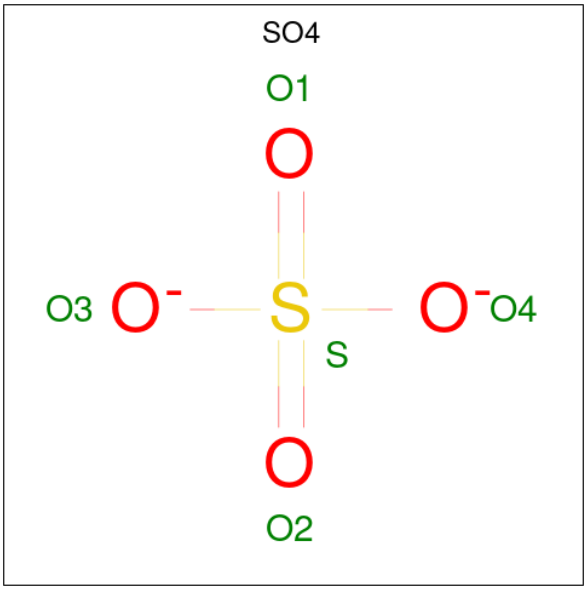
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	15	8	2	4	1	0	0
			Total	C	N	O	S		
2	E	1	15	8	2	4	1	0	0

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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

- Molecule 4 is water.

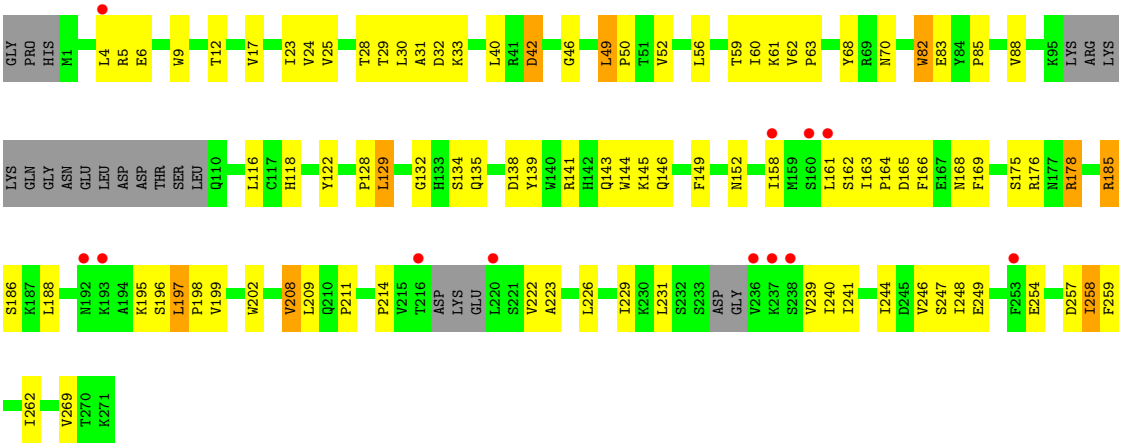
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	14	14	14	0	0
			Total	O		
4	B	22	22	22	0	0
			Total	O		
4	C	10	10	10	0	0
			Total	O		
4	D	10	10	10	0	0
			Total	O		
4	E	21	21	21	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

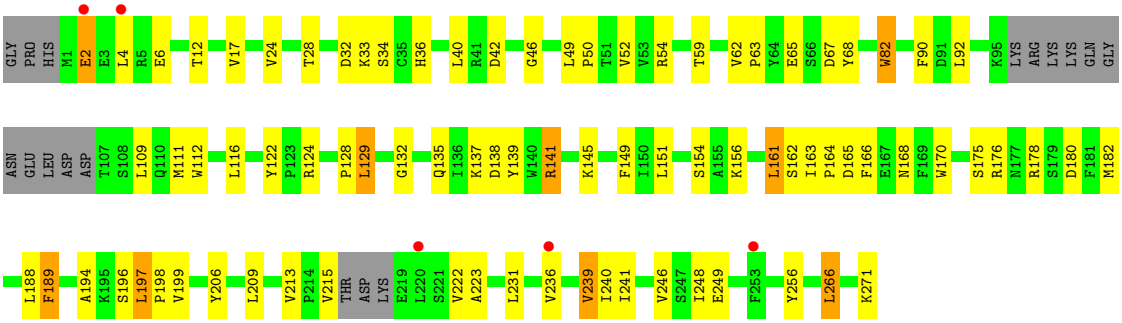
- Molecule 1: Atg5

Chain A:



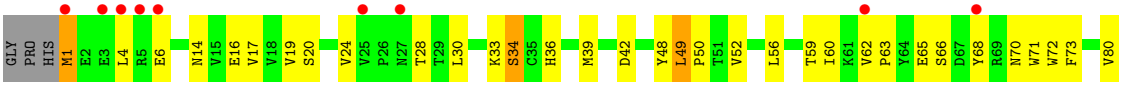
- Molecule 1: Atg5

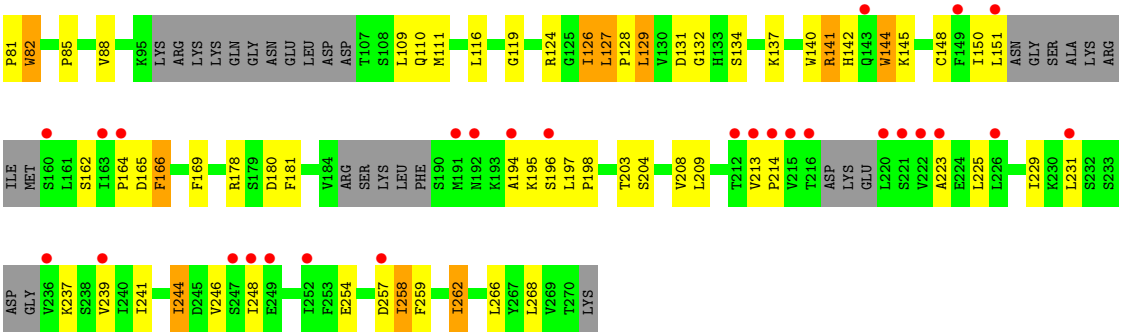
Chain B:



- Molecule 1: Atg5

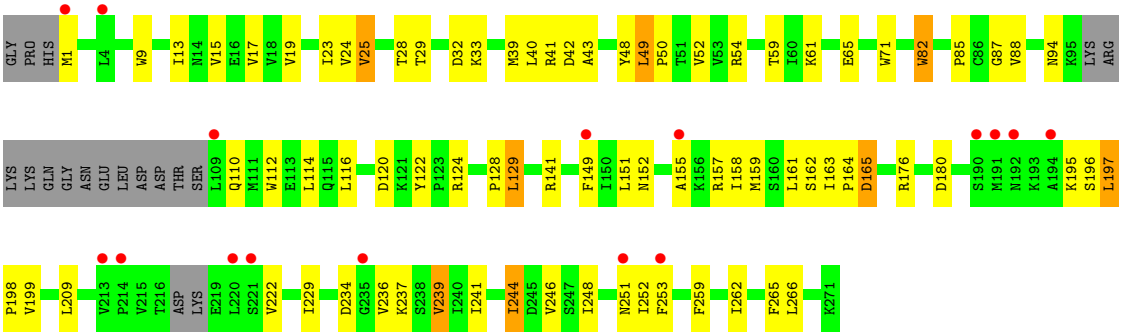
Chain C:





- Molecule 1: Atg5

Chain D:



- Molecule 1: Atg5

Chain E:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	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
$< I/\sigma(I) >$ [1]	3.57 (at 2.39Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.238 , 0.268 0.229 , 0.260	Depositor DCC
R_{free} test set	7022 reflections (8.45%)	wwPDB-VP
Wilson B-factor (Å^2)	53.2	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 46.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,-k,l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	10041	wwPDB-VP
Average B, all atoms (Å^2)	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.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: SO4, 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	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(^{o})	Ideal(^{o})
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 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	1977	0	1888	86	0
1	B	2027	0	1948	78	0
1	C	1843	0	1677	94	0
1	D	1982	0	1866	61	0
1	E	2015	0	1933	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 19.

All (363) 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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:A:9:TRP:CG	1:A:178:ARG:HG3	2.26	0.70
1:C:209:LEU:CD2	1:C:231:LEU:HD11	2.21	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:HH11	1:A:141:ARG:HG2	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:B:141:ARG:NH1	1:B:141:ARG:HG3	2.15	0.62
1:D:24:VAL:HG23	1:D:59:THR:CG2	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:GLN:NE2	2:E:301:EPE:H102	2.13	0.62
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:A:241:ILE:O	1:A:244:ILE:HG12	2.02	0.60
1:C:42:ASP:O	1:C:262: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:A:24:VAL:HG23	1:A:59:THR:CG2	2.34	0.57
1:A:40:LEU:HD13	1:A:176:ARG:HD2	1.86	0.57
1:E:18:VAL:HG22	1:E:34:SER:OG	2.03	0.57
1:E:46:GLY:N	2:E:301:EPE:O8	2.35	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:141:ARG:HG2	1:C:166:PHE:CE1	2.41	0.56
1:C:203:THR:CG2	1:C:204:SER:N	2.68	0.56
1:C:30:LEU:O	1:C:34:SER:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:85:PRO:HG2	1:C:88:VAL:HG23	1.88	0.56
1:A:162:SER:OG	1:A:165:ASP:HB2	2.06	0.55
1:D:241:ILE:O	1:D:244:ILE:HG12	2.06	0.55
1:C:59:THR:HG22	1:C:59:THR:O	2.06	0.55
1:A:42:ASP:O	1:A:262:ILE:HD13	2.06	0.55
1:B:36:HIS:CD2	1:C:111:MET:HG3	2.41	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
4:A:410:HOH:O	1:D:229:ILE:HG22	2.08	0.54
1:E:209:LEU:HD22	1:E:231:LEU:HD11	1.90	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:A:56:LEU:O	1:A:60:ILE:HD13	2.07	0.53
1:B:175:SER:O	1:B:176:ARG:HB2	2.09	0.53
1:B:197:LEU:O	1:B:197:LEU:HD12	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:B:239:VAL:HG12	1:B:246:VAL:HG22	1.90	0.53
1:C:239:VAL:HG11	1:C:268:LEU:CD2	2.37	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:HD12	1:E:197:LEU:O	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:A:42:ASP:HB3	1:A:262:ILE:HG23	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:LEU:HG	1:E:258:ILE:HD11	1.91	0.52
1:C:85:PRO:HG2	1:C:88:VAL:HG21	1.91	0.52
1:B:54:ARG:HG3	1:B:54:ARG:NH1	2.20	0.52
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:A:202:TRP:CE3	1:A:208:VAL:HG13	2.45	0.51
1:C:72:TRP:HA	1:C:82:TRP:CZ3	2.45	0.51
1:A:49:LEU:HB3	1:A:50:PRO:CD	2.41	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: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:A:5:ARG:NH2	1:A:257:ASP:OD2	2.44	0.50
1:A:175:SER:O	1:A:176:ARG:HB2	2.11	0.50
1:B:59:THR:HG22	1:B:59:THR:O	2.11	0.50
1:B:28:THR:HG21	1:B:59:THR:HG23	1.93	0.50
1:B:33:LYS:HB3	1:B:59:THR:HG21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:82:TRP:O	2:A:301:EPE:H71	2.13	0.48
1:A:158:ILE:HB	1:A:188:LEU:HD22	1.95	0.48
1:D:239:VAL:HG12	1:D:246:VAL:CG2	2.37	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:A:211:PRO:HG3	1:A:229:ILE:CD1	2.44	0.48
1:E:5:ARG:NH2	1:E:257:ASP:OD1	2.46	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:A:163:ILE:N	1:A:164:PRO:HD2	2.28	0.48
1:D:23:ILE:O	1:D:61:LYS:HG2	2.14	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:A:197:LEU:HA	1:A:198:PRO:HD3	1.80	0.47
1:C:239:VAL:O	1:C:246:VAL:HG22	2.15	0.47
1:D:39:MET:HG2	1:D:48:TYR:CE2	2.50	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:C:14:ASN:HB3	1:C:111:MET:HE1	1.97	0.47
1:C:248:ILE:HG22	1:C:248:ILE:O	2.14	0.47
1:D:237:LYS:HA	1:D:248:ILE:CD1	2.44	0.47
1:A:141:ARG:HH11	1:A:141:ARG:CG	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:D:222:VAL:HG22	1:D:252:ILE:HD12	1.97	0.47
1:E:37:ILE:HD12	1:E:37:ILE:N	2.29	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:169:PHE:CE1	1:C:181:PHE:CE2	3.03	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
1:A:196:SER:HB3	1:A:214:PRO:HA	1.97	0.46
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:B:24:VAL:HG23	1:B:59:THR:CG2	2.42	0.46
1:B:137:LYS:HD2	1:B:170:TRP:CD1	2.51	0.46
1:C:19:VAL:HG23	1:C:56:LEU:HD13	1.97	0.46
1:D:222:VAL:HG22	1:D:252:ILE:CD1	2.46	0.46
1:A:46:GLY:N	2:A:301:EPE:O8	2.44	0.46
1:D:59:THR:O	1:D:59:THR:HG22	2.13	0.46
1:D:149:PHE:CZ	1:D:155:ALA:HB2	2.51	0.46
1:B:197:LEU:HD12	1:B:213:VAL:HB	1.97	0.46
1:D:82:TRP:N	1:D:82:TRP:CD1	2.83	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: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:4:LEU:O	1:E:8:VAL:HG23	2.17	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:HG3	1:B:141:ARG:HH11	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:163:ILE:N	1:D:164:PRO:HD2	2.32	0.45
1:D:197:LEU:HD13	1:D:199:VAL:CG2	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:SER:C	1:A:188:LEU:H	2.21	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:C:144:TRP:O	1:C:145:LYS:C	2.55	0.44
1:A:83:GLU:CA	2:A:301:EPE:H31	2.46	0.44
1:A:241:ILE:CD1	1:A:246:VAL:HG11	2.47	0.44
1:B:111:MET:HE1	1:C:109:LEU:HD23	1.99	0.44
1:C:151:LEU:HA	1:C:196:SER:O	2.17	0.44
1:C:208:VAL:O	1:C:208:VAL:CG1	2.65	0.44
1:E:29:THR:HG22	1:E:31:ALA:H	1.82	0.44
1:E:135:GLN:HE21	2:E:301:EPE:C10	2.24	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:A:4:LEU:HD13	1:A:258:ILE:CD1	2.48	0.43
1:C:258:ILE:CG1	1:C:259:PHE:N	2.71	0.43
1:D:49:LEU:HD11	1:D:71:TRP:HB2	2.01	0.43
1:E:197:LEU:CD1	1:E:213:VAL:HB	2.48	0.43
1:A:83:GLU:HA	2:A:301:EPE:C3	2.46	0.43
1:C:131:ASP:O	1:C:134:SER:HB2	2.19	0.43
1:D:198:PRO:HB3	1:D:265:PHE:CE2	2.54	0.43
1:A:4:LEU:HD13	1:A:258:ILE:HD11	2.00	0.43
1:A:202:TRP:CZ3	1:A:208:VAL:HG13	2.54	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:D:151:LEU:HA	1:D:196:SER:O	2.19	0.43
1:A:144:TRP:C	1:A:146:GLN:N	2.72	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:223:ALA:N	1:A:248:ILE:O	2.46	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:B:197:LEU:HA	1:B:198:PRO:HD3	1.80	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:6:GLU:OE2	1:C:178:ARG:HD3	2.19	0.43
1:A:197:LEU:HD13	1:A:199:VAL:CG2	2.49	0.42
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:152:ASN:ND2	1:D:157:ARG:CG	2.82	0.42
1:E:1:MET:C	1:E:3:GLU:H	2.22	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
1:D:197:LEU:O	1:D:197:LEU:HD12	2.19	0.42
1:A:222:VAL:CG1	1:A:239:VAL:HG21	2.49	0.42
1:D:13:ILE:HD11	1:D:41:ARG:HG2	2.01	0.42
1:D:122:TYR:CZ	1:D:128:PRO:HB3	2.54	0.42
1:B:68:TYR:HD1	1:B:129:LEU:HD13	1.85	0.42
1:B:139:TYR:HB2	2:B:301:EPE:H92	2.02	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:65:GLU:HG2	1:C:66:SER:N	2.34	0.42
1:C:126:ILE:HD12	1:C:126:ILE:HA	1.89	0.42
1:C:141:ARG:O	1:C:144:TRP:N	2.52	0.42
1:C:197:LEU:HA	1:C:198:PRO:HD3	1.84	0.42
1:A:229:ILE:HG23	1:A:231:LEU:HD12	2.02	0.41
1:C:195:LYS:O	1:C:214:PRO:HA	2.20	0.41
1:E:167:GLU:O	1:E:171:VAL:HG23	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:N	1:D:209:LEU:CD1	2.83	0.41
1:E:122:TYR:CZ	1:E:128:PRO:HB3	2.56	0.41
1:E:223:ALA:N	1:E:248:ILE:O	2.49	0.41
1:A:82:TRP:CZ2	1:A:129:LEU:HB2	2.55	0.41
1:C:80:VAL:HA	1:C:81:PRO:HD3	1.88	0.41
1:D:241:ILE:HD12	1:D:246:VAL:HG11	2.02	0.41
1:C:140:TRP:HH2	1:C:169:PHE:CD2	2.38	0.41
1:A:52:VAL:HG12	1:A:116:LEU:HD22	2.03	0.41
1:B:17:VAL:O	1:B:34:SER:HA	2.20	0.41
1:B:151:LEU:HA	1:B:196:SER:O	2.20	0.41
1:B:197:LEU:CD1	1:B:213:VAL:HB	2.51	0.41
1:C:1:MET:HE2	1:C:1:MET:HA	2.03	0.41
1:C:229:ILE:HG22	1:C:229:ILE:O	2.21	0.41
1:D:152:ASN:ND2	1:D:157:ARG:HG2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:82:TRP:O	2:E:301:EPE:H71	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:B:168:ASN:HD22	1:B:168:ASN:HA	1.75	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:A:209:LEU:C	1:A:211:PRO:HD3	2.42	0.40
1:B:6:GLU:OE2	1:B:178:ARG:NE	2.54	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:A:70:ASN:O	1:A:118:HIS:HA	2.21	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:E:82:TRP:CD1	1:E:82:TRP:N	2.89	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	244/274 (89%)	223 (91%)	20 (8%)	1 (0%)	34 54
1	B	251/274 (92%)	238 (95%)	11 (4%)	2 (1%)	19 35
1	C	229/274 (84%)	202 (88%)	24 (10%)	3 (1%)	12 21
1	D	250/274 (91%)	227 (91%)	18 (7%)	5 (2%)	7 12
1	E	250/274 (91%)	237 (95%)	11 (4%)	2 (1%)	19 35
All	All	1224/1370 (89%)	1127 (92%)	84 (7%)	13 (1%)	14 26

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
1	D	161	LEU
1	B	236	VAL
1	D	262	ILE
1	C	262	ILE

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	205/249 (82%)	188 (92%)	17 (8%)	11	22
1	B	215/249 (86%)	200 (93%)	15 (7%)	15	29
1	C	182/249 (73%)	168 (92%)	14 (8%)	13	25
1	D	204/249 (82%)	188 (92%)	16 (8%)	12	24
1	E	210/249 (84%)	202 (96%)	8 (4%)	33	58
All	All	1016/1245 (82%)	946 (93%)	70 (7%)	15	30

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

Sometimes 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 (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)

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	$\#\|Z\| > 2$
3	SO4	A	303	-	4,4,4	0.29	0	6,6,6	0.07	0
3	SO4	B	302	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	E	304	-	4,4,4	0.27	0	6,6,6	0.06	0
2	EPE	B	301	-	15,15,15	1.46	3 (20%)	18,20,20	2.22	5 (27%)
3	SO4	C	301	-	4,4,4	0.25	0	6,6,6	0.13	0
2	EPE	E	301	-	15,15,15	1.25	1 (6%)	18,20,20	1.61	5 (27%)
3	SO4	D	301	-	4,4,4	0.23	0	6,6,6	0.08	0
3	SO4	E	302	-	4,4,4	0.27	0	6,6,6	0.10	0
3	SO4	E	305	-	4,4,4	0.27	0	6,6,6	0.08	0
3	SO4	A	304	-	4,4,4	0.32	0	6,6,6	0.14	0
3	SO4	E	303	-	4,4,4	0.25	0	6,6,6	0.13	0
3	SO4	A	302	-	4,4,4	0.27	0	6,6,6	0.11	0
3	SO4	D	302	-	4,4,4	0.27	0	6,6,6	0.09	0
2	EPE	A	301	-	15,15,15	1.07	1 (6%)	18,20,20	1.62	5 (27%)
3	SO4	B	304	-	4,4,4	0.25	0	6,6,6	0.09	0
3	SO4	B	305	-	4,4,4	0.27	0	6,6,6	0.06	0
3	SO4	B	303	-	4,4,4	0.27	0	6,6,6	0.09	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	SO4	C	302	-	4,4,4	0.25	0	6,6,6	0.05	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	E	301	-	-	1/9/19/19	0/1/1/1
2	EPE	A	301	-	-	0/9/19/19	0/1/1/1
2	EPE	B	301	-	-	0/9/19/19	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	EPE	C10-S	3.96	1.83	1.77
2	E	301	EPE	C10-S	3.90	1.83	1.77
2	A	301	EPE	C10-S	3.29	1.82	1.77
2	B	301	EPE	C6-N1	2.09	1.52	1.46
2	B	301	EPE	C5-N4	2.08	1.52	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	EPE	O1S-S-C10	6.88	115.20	106.92
2	A	301	EPE	O2S-S-C10	4.14	111.89	106.92
2	E	301	EPE	O1S-S-C10	3.95	111.67	106.92
2	B	301	EPE	O3S-S-O2S	-2.78	104.48	111.27
2	B	301	EPE	O3S-S-O1S	-2.60	104.93	111.27
2	A	301	EPE	C7-N4-C3	-2.49	104.86	111.23
2	E	301	EPE	C7-N4-C3	-2.44	104.99	111.23
2	B	301	EPE	C7-N4-C3	-2.40	105.11	111.23
2	A	301	EPE	C9-N1-C2	-2.25	105.48	111.23
2	E	301	EPE	O3S-S-O2S	-2.24	105.79	111.27
2	E	301	EPE	O3S-S-O1S	-2.23	105.83	111.27
2	B	301	EPE	C9-N1-C2	-2.19	105.63	111.23
2	E	301	EPE	C9-N1-C2	-2.13	105.78	111.23
2	A	301	EPE	O3S-S-O1S	-2.11	106.12	111.27
2	A	301	EPE	O3S-S-O2S	-2.03	106.31	111.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	301	EPE	N4-C7-C8-O8

There are no ring outliers.

5 monomers are involved in 27 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	301	EPE	9	0
2	E	301	EPE	7	0
3	D	302	SO4	1	0
2	A	301	EPE	9	0
3	B	304	SO4	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, 95th 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^2)	Q<0.9
1	A	252/274 (91%)	0.33	12 (4%)	30	32	35, 61, 93, 106	0
1	B	257/274 (93%)	0.04	5 (1%)	66	69	31, 51, 78, 90	0
1	C	241/274 (87%)	0.67	37 (15%)	2	1	38, 71, 115, 126	0
1	D	256/274 (93%)	0.26	16 (6%)	20	21	37, 66, 102, 108	0
1	E	256/274 (93%)	-0.03	3 (1%)	79	80	33, 50, 81, 98	0
All	All	1262/1370 (92%)	0.25	73 (5%)	23	24	31, 60, 101, 126	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	155	ALA	6.7
1	C	252	ILE	4.9
1	A	237	LYS	4.7
1	C	194	ALA	4.6
1	C	248	ILE	4.4
1	A	4	LEU	4.4
1	D	192	ASN	4.2
1	D	220	LEU	4.1
1	C	149	PHE	4.0
1	C	214	PRO	4.0
1	D	191	MET	4.0
1	C	247	SER	4.0
1	B	220	LEU	3.9
1	C	163	ILE	3.9
1	C	151	LEU	3.8
1	C	160	SER	3.8
1	C	192	ASN	3.8
1	C	213	VAL	3.7
1	C	223	ALA	3.6
1	A	238	SER	3.6

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Mol	Chain	Res	Type	RSRZ
1	C	249	GLU	3.5
1	A	236	VAL	3.5
1	D	214	PRO	3.5
1	C	1	MET	3.5
1	D	235	GLY	3.5
1	A	220	LEU	3.5
1	A	192	ASN	3.4
1	C	220	LEU	3.4
1	C	68	TYR	3.3
1	C	4	LEU	3.3
1	A	253	PHE	3.1
1	A	158	ILE	3.0
1	D	1	MET	2.9
1	C	239	VAL	2.9
1	C	231	LEU	2.9
1	C	222	VAL	2.8
1	B	253	PHE	2.7
1	C	221	SER	2.7
1	D	149	PHE	2.7
1	D	4	LEU	2.6
1	C	62	VAL	2.6
1	C	164	PRO	2.5
1	C	5	ARG	2.5
1	D	213	VAL	2.5
1	C	215	VAL	2.5
1	C	226	LEU	2.5
1	C	236	VAL	2.4
1	D	109	LEU	2.4
1	D	221	SER	2.4
1	D	253	PHE	2.4
1	C	3	GLU	2.4
1	E	4	LEU	2.3
1	C	143	GLN	2.3
1	D	190	SER	2.3
1	E	220	LEU	2.3
1	A	161	LEU	2.3
1	C	27	ASN	2.3
1	B	2	GLU	2.2
1	A	193	LYS	2.2
1	B	4	LEU	2.2
1	E	235	GLY	2.2
1	A	160	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	212	THR	2.2
1	C	196	SER	2.1
1	C	216	THR	2.1
1	C	25	VAL	2.1
1	A	216	THR	2.1
1	B	236	VAL	2.1
1	C	257	ASP	2.1
1	D	251	ASN	2.1
1	C	6	GLU	2.1
1	D	194	ALA	2.0
1	C	191	MET	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, 95th 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^2)	Q<0.9
2	EPE	A	301	15/15	0.56	0.47	100,104,118,118	0
2	EPE	B	301	15/15	0.64	0.41	94,99,114,114	0
2	EPE	E	301	15/15	0.67	0.34	86,92,109,109	0
3	SO4	A	302	5/5	0.84	0.18	113,114,114,115	0
3	SO4	B	303	5/5	0.85	0.17	127,127,127,128	0
3	SO4	D	302	5/5	0.85	0.17	146,146,146,146	0
3	SO4	A	304	5/5	0.88	0.14	117,117,117,118	0
3	SO4	E	305	5/5	0.89	0.25	130,130,130,130	0
3	SO4	C	301	5/5	0.90	0.20	115,116,116,116	0
3	SO4	C	302	5/5	0.92	0.35	122,123,123,123	0
3	SO4	B	304	5/5	0.92	0.12	137,137,138,138	0
3	SO4	B	302	5/5	0.92	0.30	116,116,117,117	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	SO4	E	303	5/5	0.94	0.14	94,94,94,95	0
3	SO4	A	303	5/5	0.94	0.22	121,121,122,122	0
3	SO4	E	304	5/5	0.95	0.14	135,135,135,135	0
3	SO4	E	302	5/5	0.95	0.11	97,97,98,98	0
3	SO4	D	301	5/5	0.96	0.12	98,99,99,99	0
3	SO4	B	305	5/5	0.96	0.13	118,118,118,119	0

6.5 Other polymers (i)

There are no such residues in this entry.