



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:43 PM UTC

PDB ID : 3VQI / pdb_00003vqi
Title : Crystal structure of Kluyveromyces marxianus Atg5
Authors : Yamaguchi, M.; Noda, N.N.; Yamamoto, H.; Shima, T.; Kumeta, H.;
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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 ⓘ 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	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

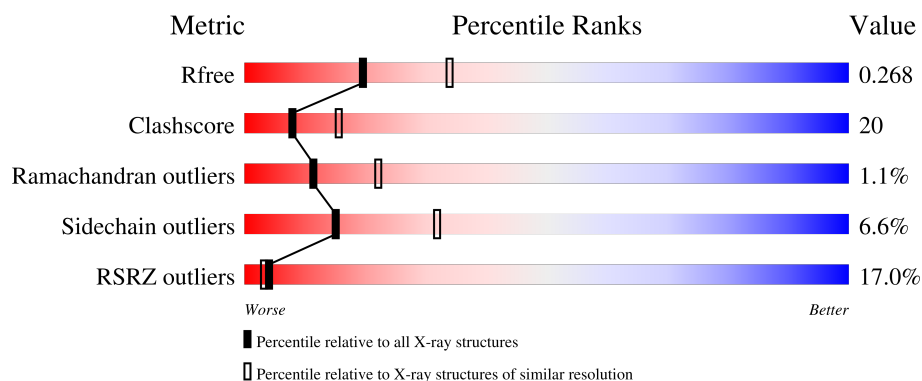
1 Overall quality at a glance

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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	274	15% 57% 31% •• 8%
1	B	274	8% 59% 31% • 6%
1	C	274	29% 51% 32% 5% 12%
1	D	274	20% 61% 27% 5% 7%
1	E	274	7% 64% 27% • 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	-
2	EPE	B	301	-	-	X	-
2	EPE	E	301	-	-	X	-

2 Entry composition [i](#)

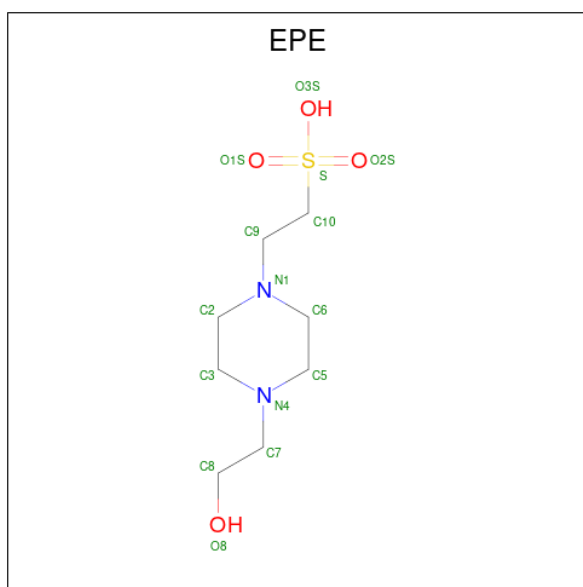
There are 4 unique types of molecules in this entry. The entry contains 10041 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
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-PIPERAZINE ETHANESULFONIC ACID (CCD ID: EPE) (formula: $C_8H_{18}N_2O_4S$).



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

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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 (CCD ID: SO4) (formula: O₄S).



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		

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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		

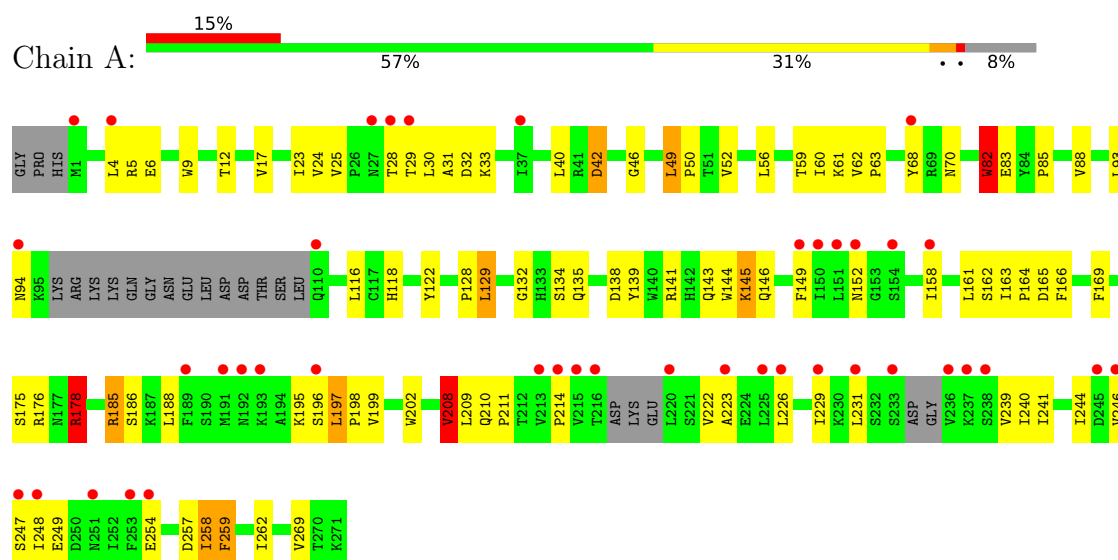
- Molecule 4 is water.

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		

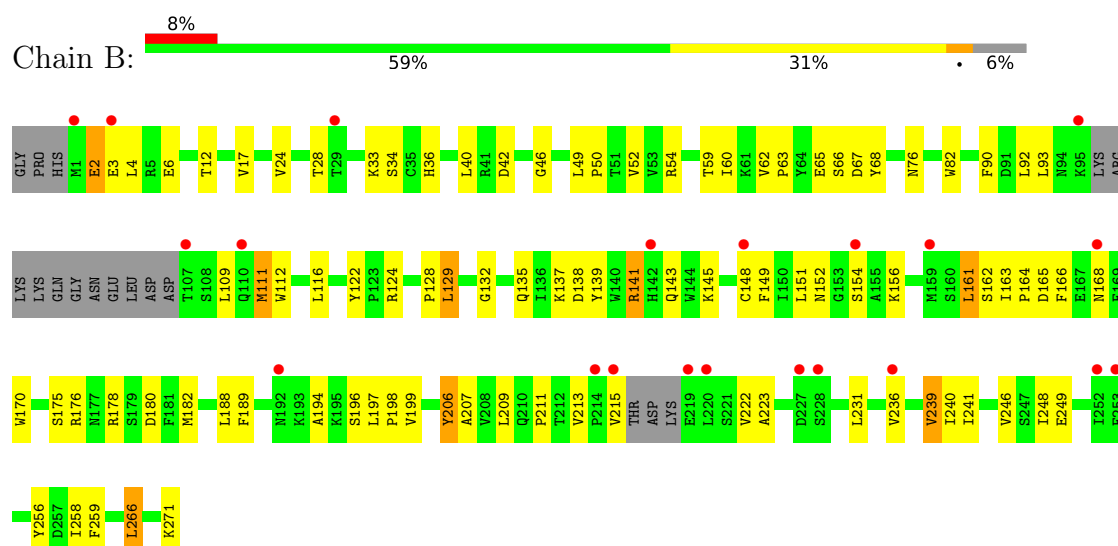
3 Residue-property plots [i](#)

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

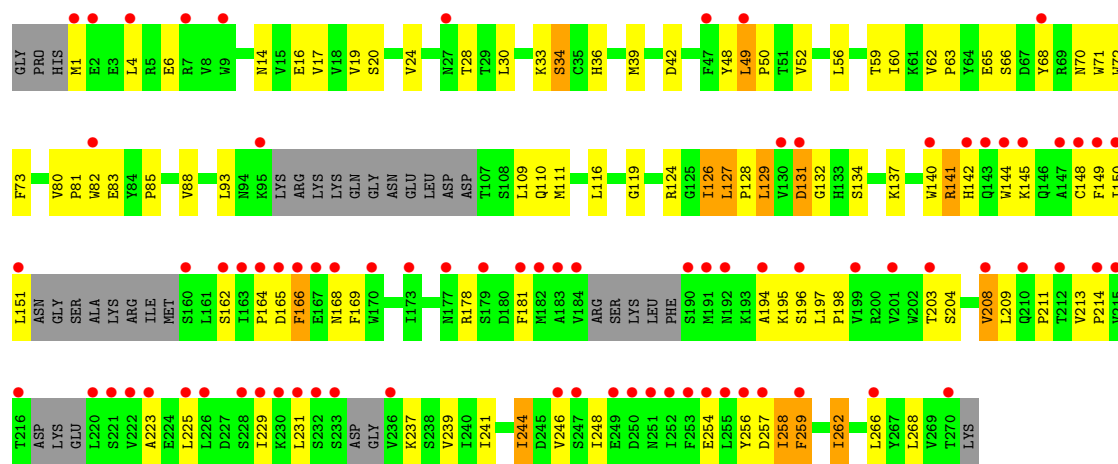


• Molecule 1: Atg5

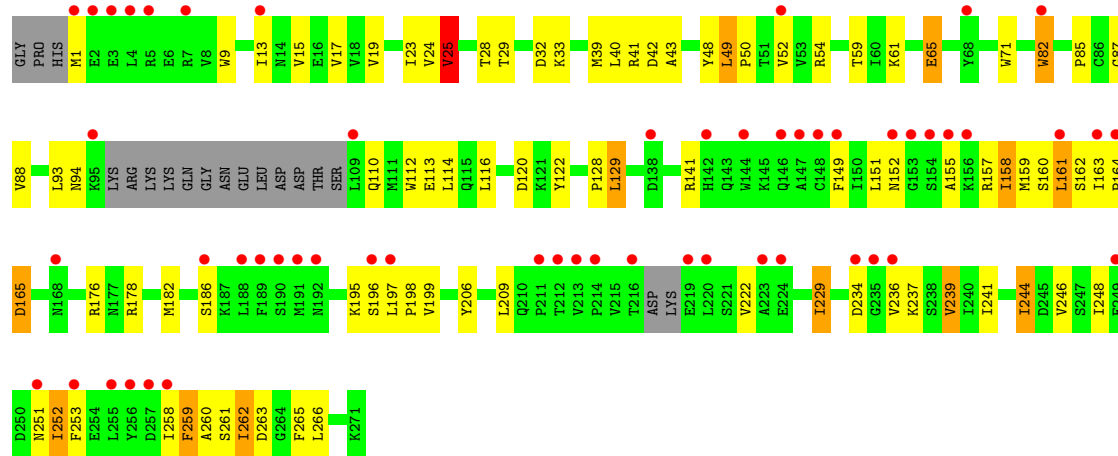


• Molecule 1: Atg5

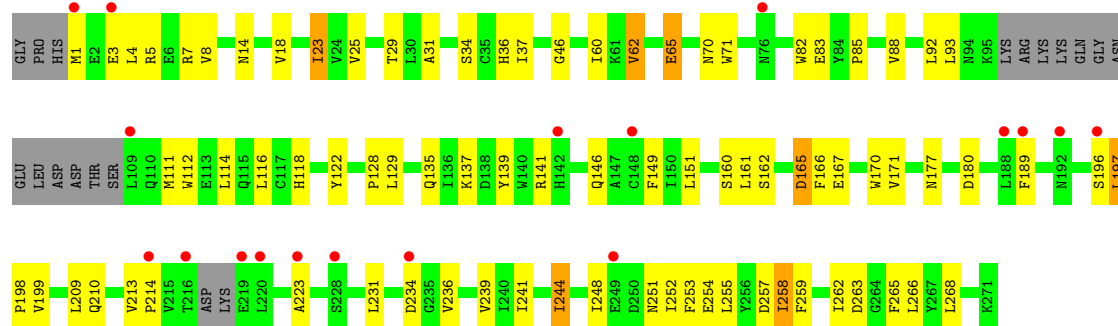




• Molecule 1: Atg5



• Molecule 1: Atg5



4 Data and refinement statistics

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 – 2.50	Depositor EDS
% Data completeness (in resolution range)	94.8 (35.15-2.50) 94.8 (35.15-2.50)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.57 (at 2.39Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.238 , 0.268 0.238 , 0.268	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)	0.32 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.46	0/2028	1.00	9/2771 (0.3%)
1	B	0.50	1/2079 (0.0%)	1.03	8/2839 (0.3%)
1	C	0.45	0/1889	0.97	7/2589 (0.3%)
1	D	0.47	0/2034	1.00	6/2784 (0.2%)
1	E	0.50	1/2067 (0.0%)	0.99	9/2822 (0.3%)
All	All	0.48	2/10097 (0.0%)	1.00	39/13805 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	62	VAL	CA-CB	5.74	1.61	1.54
1	B	111	MET	SD-CE	-5.61	1.65	1.79

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	210	GLN	CA-C-N	8.78	129.31	119.83
1	A	210	GLN	C-N-CA	8.78	129.31	119.83
1	C	131	ASP	N-CA-C	8.24	121.03	110.65
1	B	3	GLU	N-CA-C	-7.98	102.80	112.54
1	E	93	LEU	N-CA-C	7.49	122.99	113.55
1	B	259	PHE	N-CA-C	7.47	122.58	113.17
1	E	25	VAL	N-CA-C	-7.30	101.79	108.95
1	D	25	VAL	N-CA-C	-6.92	101.42	108.96
1	A	178	ARG	N-CA-C	6.79	118.76	111.36
1	E	210	GLN	CA-C-N	6.75	126.51	119.76
1	E	210	GLN	C-N-CA	6.75	126.51	119.76
1	B	93	LEU	N-CA-C	6.53	121.53	112.45
1	E	197	LEU	CA-C-N	6.41	127.85	119.84
1	E	197	LEU	C-N-CA	6.41	127.85	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	94	ASN	N-CA-C	6.06	118.60	110.35
1	E	259	PHE	N-CA-C	5.97	121.30	113.30
1	B	258	ILE	CB-CA-C	-5.87	104.23	111.92
1	D	259	PHE	N-CA-C	5.86	121.15	113.30
1	C	164	PRO	N-CA-CB	5.79	109.65	103.39
1	B	258	ILE	N-CA-C	5.67	116.72	111.45
1	C	93	LEU	N-CA-C	5.56	120.18	112.90
1	D	186	SER	N-CA-C	-5.55	106.64	113.41
1	E	92	LEU	N-CA-C	5.54	117.40	111.36
1	D	206	TYR	N-CA-C	5.53	119.33	111.92
1	D	93	LEU	N-CA-C	5.49	120.64	113.88
1	C	208	VAL	N-CA-C	5.40	115.36	107.37
1	A	208	VAL	N-CA-C	5.35	115.66	108.17
1	A	82	TRP	N-CA-C	5.31	122.11	110.80
1	C	259	PHE	N-CA-C	5.30	119.46	113.15
1	E	23	ILE	N-CA-C	5.30	117.31	112.43
1	C	83	GLU	N-CA-C	-5.29	106.86	113.15
1	D	158	ILE	N-CA-C	5.26	115.98	110.62
1	A	259	PHE	N-CA-C	5.23	120.31	113.30
1	A	93	LEU	N-CA-C	5.20	119.76	113.41
1	A	145	LYS	N-CA-C	-5.15	106.10	112.38
1	B	207	ALA	N-CA-C	-5.15	101.77	109.95
1	C	168	ASN	N-CA-C	-5.07	105.75	111.28
1	B	206	TYR	N-CA-C	5.05	118.56	111.74
1	B	66	SER	N-CA-C	5.02	116.31	109.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-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 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	90	0
1	B	2027	0	1948	81	0
1	C	1843	0	1677	96	0
1	D	1982	0	1866	68	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2015	0	1933	55	0
2	A	15	0	18	10	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	381	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 20.

All (381) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:65:GLU:H	1:D:65:GLU:CD	1.93	0.77
1:D:82:TRP:CZ2	1:D:129:LEU:HB2	2.19	0.77
1:B:109:LEU:HD13	1:C:111:MET:HE1	1.67	0.77
1:A:24:VAL:HG23	1:A:59:THR:HG22	1.65	0.76
1:E:251:ASN:HD21	1:E:253:PHE:HB3	1.51	0.75
1:C:203:THR:HG22	1:C:204:SER:N	2.01	0.74
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: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:E:14:ASN:HB3	1:E:111:MET:HE2	1.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:135:GLN:NE2	2:E:301:EPE:H102	2.13	0.62
1:C:237:LYS:C	1:C:248:ILE:HG13	2.24	0.61
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:E:241:ILE:HD11	1:E:268:LEU:HD22	1.86	0.58
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:B:65:GLU:H	1:B:65:GLU:CD	2.11	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:E:36:HIS:C	1:E:37:ILE:HD12	2.30	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:E:65:GLU:CD	1:E:65:GLU:H	2.13	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:82:TRP:H	1:D:82:TRP:CD1	2.24	0.55
1:C:14:ASN:HB3	1:C:111:MET:HE2	1.88	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:109:LEU:HD13	1:C:111:MET:CE	2.37	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: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:175:SER:O	1:B:176:ARG:HB2	2.09	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:42:ASP:HB3	1:A:262:ILE:HG23	1.91	0.52
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: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:247:SER:C	1:A:249:GLU:H	2.18	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: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: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:154:SER:C	1:B:156:LYS:H	2.20	0.50
1:C:262:ILE:C	1:C:262:ILE:HD12	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:186:SER:C	1:A:188:LEU:H	2.21	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:144:TRP:O	1:C:145:LYS:C	2.55	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
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: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:B:111:MET:HE2	1:C:109:LEU:CD2	2.44	0.47
1:D:9:TRP:O	1:D:176:ARG:NH1	2.48	0.47
1:B:2:GLU:C	1:B:4:LEU:N	2.72	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:D:178:ARG:NH1	1:D:182:MET:HE2	2.30	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: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:E:1:MET:C	1:E:3:GLU:H	2.22	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:CD1	1:D:82:TRP:N	2.83	0.46
1:B:109:LEU:CD1	1:C:111:MET:HE1	2.42	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: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:209:LEU:C	1:A:211:PRO:HD3	2.42	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:TRP:HB2	2:B:301:EPE:O8	2.17	0.45
1:B:111:MET:HE1	1:C:109:LEU:HD23	1.98	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
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:A:241:ILE:CD1	1:A:246:VAL:HG11	2.47	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:A:144:TRP:C	1:A:146:GLN:N	2.72	0.44
1:C:39:MET:HG2	1:C:48:TYR:CD2	2.53	0.43
1:D:160:SER:O	1:D:161:LEU:C	2.61	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:209:LEU:C	1:C:211:PRO:HD3	2.42	0.43
1:D:49:LEU:HD11	1:D:71:TRP:HB2	2.01	0.43
1:E:82:TRP:CD1	1:E:82:TRP:H	2.36	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:4:LEU:C	1:C:6:GLU:N	2.76	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:E:1:MET:C	1:E:3:GLU:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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: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:A:247:SER:C	1:A:249:GLU:N	2.77	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:148:CYS:O	1:B:149:PHE:C	2.63	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:D:261:SER:C	1:D:263:ASP:H	2.28	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:82:TRP:C	2:A:301:EPE:H71	2.46	0.41
1:A:186:SER:C	1:A:188:LEU:N	2.78	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:152:ASN:C	1:B:154:SER:H	2.29	0.41
1:B:197:LEU:CD1	1:B:213:VAL:HB	2.51	0.41
1:B:209:LEU:C	1:B:211:PRO:HD3	2.46	0.41
1:C:149:PHE:O	1:C:150:ILE:C	2.64	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
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:C:256:TYR:CD2	1:C:256:TYR:C	3.00	0.40
1:D:65:GLU:CD	1:D:65:GLU:N	2.71	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:D:259:PHE:O	1:D:260:ALA:C	2.63	0.40
1:B:6:GLU:OE2	1:B:178:ARG:NE	2.54	0.40
1:D:262:ILE:HD12	1:D:262:ILE:C	2.46	0.40
1:E:160:SER:O	1:E:161:LEU:C	2.63	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:A:82:TRP:CD1	1:A:82:TRP:H	2.40	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

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%)	30	49
1	B	251/274 (92%)	238 (95%)	11 (4%)	2 (1%)	16	31
1	C	229/274 (84%)	202 (88%)	24 (10%)	3 (1%)	9	18
1	D	250/274 (91%)	227 (91%)	18 (7%)	5 (2%)	6	10
1	E	250/274 (91%)	237 (95%)	11 (4%)	2 (1%)	16	31
All	All	1224/1370 (89%)	1127 (92%)	84 (7%)	13 (1%)	11	22

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

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%)	189 (92%)	16 (8%)	11	24
1	B	215/249 (86%)	201 (94%)	14 (6%)	15	32
1	C	182/249 (73%)	171 (94%)	11 (6%)	17	36
1	D	204/249 (82%)	186 (91%)	18 (9%)	9	20
1	E	210/249 (84%)	202 (96%)	8 (4%)	29	56
All	All	1016/1245 (82%)	949 (93%)	67 (7%)	15	32

All (67) 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	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	42	ASP
1	B	60	ILE
1	B	76	ASN
1	B	124	ARG
1	B	129	LEU
1	B	138	ASP
1	B	141	ARG
1	B	143	GLN
1	B	180	ASP
1	B	239	VAL
1	B	249	GLU

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Mol	Chain	Res	Type
1	B	266	LEU
1	C	1	MET
1	C	34	SER
1	C	49	LEU
1	C	124	ARG
1	C	126	ILE
1	C	127	LEU
1	C	129	LEU
1	C	166	PHE
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	65	GLU
1	D	82	TRP
1	D	94	ASN
1	D	110	GLN
1	D	113	GLU
1	D	120	ASP
1	D	129	LEU
1	D	165	ASP
1	D	229	ILE
1	D	239	VAL
1	D	244	ILE
1	D	252	ILE
1	D	258	ILE
1	D	266	LEU
1	E	65	GLU
1	E	116	LEU
1	E	129	LEU
1	E	165	ASP
1	E	239	VAL
1	E	244	ILE
1	E	258	ILE
1	E	266	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (23) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	94	ASN
1	A	168	ASN
1	A	251	ASN
1	B	94	ASN
1	B	168	ASN
1	C	10	ASN
1	C	118	HIS
1	C	142	HIS
1	C	146	GLN
1	C	177	ASN
1	C	210	GLN
1	D	10	ASN
1	D	94	ASN
1	D	118	HIS
1	D	146	GLN
1	D	152	ASN
1	D	251	ASN
1	E	10	ASN
1	E	110	GLN
1	E	115	GLN
1	E	168	ASN
1	E	251	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides 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
3	SO4	D	302	-	4,4,4	0.38	0	6,6,6	0.13	0
3	SO4	C	301	-	4,4,4	0.36	0	6,6,6	0.12	0
3	SO4	B	303	-	4,4,4	0.38	0	6,6,6	0.10	0
3	SO4	A	302	-	4,4,4	0.37	0	6,6,6	0.14	0
3	SO4	A	303	-	4,4,4	0.40	0	6,6,6	0.10	0
3	SO4	E	304	-	4,4,4	0.37	0	6,6,6	0.09	0
3	SO4	C	302	-	4,4,4	0.36	0	6,6,6	0.07	0
2	EPE	A	301	-	15,15,15	1.08	1 (6%)	19,20,20	1.48	5 (26%)
3	SO4	D	301	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	E	302	-	4,4,4	0.38	0	6,6,6	0.13	0
3	SO4	E	305	-	4,4,4	0.38	0	6,6,6	0.10	0
2	EPE	E	301	-	15,15,15	1.26	1 (6%)	19,20,20	1.48	5 (26%)
3	SO4	B	305	-	4,4,4	0.38	0	6,6,6	0.06	0
3	SO4	A	304	-	4,4,4	0.39	0	6,6,6	0.08	0
3	SO4	B	302	-	4,4,4	0.37	0	6,6,6	0.11	0
3	SO4	B	304	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	E	303	-	4,4,4	0.36	0	6,6,6	0.14	0
2	EPE	B	301	-	15,15,15	1.48	3 (20%)	19,20,20	1.94	5 (26%)

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	3.95	1.83	1.77
2	E	301	EPE	C10-S	3.90	1.83	1.77
2	A	301	EPE	C10-S	3.28	1.82	1.77
2	B	301	EPE	C6-N1	2.14	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	EPE	C5-N4	2.14	1.52	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	301	EPE	O1S-S-C10	5.61	115.20	106.73
2	A	301	EPE	O2S-S-C10	3.42	111.89	106.73
2	E	301	EPE	O1S-S-C10	3.27	111.67	106.73
2	B	301	EPE	O3S-S-O2S	-2.77	104.48	111.40
2	B	301	EPE	O3S-S-O1S	-2.59	104.93	111.40
2	A	301	EPE	C7-N4-C3	-2.39	104.86	111.24
2	E	301	EPE	C7-N4-C3	-2.34	104.99	111.24
2	B	301	EPE	C7-N4-C3	-2.30	105.11	111.24
2	E	301	EPE	O3S-S-O2S	-2.24	105.79	111.40
2	E	301	EPE	O3S-S-O1S	-2.23	105.83	111.40
2	A	301	EPE	C9-N1-C2	-2.16	105.48	111.24
2	A	301	EPE	O3S-S-O1S	-2.11	106.12	111.40
2	B	301	EPE	C9-N1-C2	-2.11	105.63	111.24
2	E	301	EPE	C9-N1-C2	-2.05	105.78	111.24
2	A	301	EPE	O3S-S-O2S	-2.03	106.31	111.40

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 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	302	SO4	1	0
2	A	301	EPE	10	0
2	E	301	EPE	7	0
3	B	304	SO4	1	0
2	B	301	EPE	9	0

5.7 Other polymers [i](#)

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, 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%)	0.98	41 (16%) 4 3	35, 61, 93, 106	0
1	B	257/274 (93%)	0.53	21 (8%) 17 15	31, 51, 78, 90	0
1	C	241/274 (87%)	1.57	80 (33%) 1 1	38, 71, 115, 126	0
1	D	256/274 (93%)	1.20	55 (21%) 2 2	37, 66, 102, 108	0
1	E	256/274 (93%)	0.50	18 (7%) 22 20	33, 50, 81, 98	0
All	All	1262/1370 (92%)	0.95	215 (17%) 4 3	31, 60, 101, 126	0

All (215) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	216	THR	7.3
1	C	216	THR	6.2
1	D	192	ASN	5.8
1	C	233	SER	5.6
1	C	149	PHE	5.6
1	C	151	LEU	5.5
1	A	233	SER	5.4
1	C	214	PRO	5.4
1	B	1	MET	5.1
1	C	226	LEU	5.0
1	C	68	TYR	4.9
1	B	219	GLU	4.9
1	C	229	ILE	4.8
1	C	1	MET	4.8
1	D	4	LEU	4.8
1	D	154	SER	4.7
1	D	168	ASN	4.7
1	E	216	THR	4.7
1	C	4	LEU	4.5
1	D	219	GLU	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	216	THR	4.3
1	C	164	PRO	4.3
1	D	149	PHE	4.3
1	A	1	MET	4.3
1	C	163	ILE	4.3
1	C	148	CYS	4.3
1	A	192	ASN	4.2
1	C	223	ALA	4.2
1	C	196	SER	4.2
1	C	144	TRP	4.2
1	C	184	VAL	4.2
1	C	253	PHE	4.1
1	A	237	LYS	4.1
1	A	220	LEU	4.1
1	D	214	PRO	4.0
1	C	252	ILE	4.0
1	E	219	GLU	3.9
1	C	179	SER	3.9
1	C	222	VAL	3.9
1	A	29	THR	3.9
1	C	247	SER	3.7
1	D	155	ALA	3.7
1	A	4	LEU	3.7
1	D	1	MET	3.7
1	C	165	ASP	3.6
1	A	236	VAL	3.6
1	C	147	ALA	3.6
1	C	212	THR	3.5
1	E	1	MET	3.5
1	A	151	LEU	3.5
1	C	250	ASP	3.5
1	A	238	SER	3.5
1	B	142	HIS	3.5
1	C	251	ASN	3.5
1	D	213	VAL	3.5
1	C	2	GLU	3.4
1	C	183	ALA	3.4
1	C	220	LEU	3.4
1	C	7	ARG	3.4
1	C	249	GLU	3.4
1	C	150	ILE	3.4
1	A	248	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	107	THR	3.3
1	C	142	HIS	3.3
1	D	152	ASN	3.3
1	C	231	LEU	3.2
1	E	142	HIS	3.2
1	A	189	PHE	3.2
1	C	210	GLN	3.2
1	D	258	ILE	3.2
1	B	220	LEU	3.2
1	C	182	MET	3.2
1	B	148	CYS	3.2
1	A	152	ASN	3.2
1	A	193	LYS	3.2
1	B	3	GLU	3.2
1	C	257	ASP	3.1
1	D	223	ALA	3.1
1	A	110	GLN	3.1
1	A	196	SER	3.1
1	D	13	ILE	3.1
1	D	95	LYS	3.0
1	C	191	MET	3.0
1	C	190	SER	3.0
1	D	236	VAL	3.0
1	C	225	LEU	3.0
1	D	188	LEU	3.0
1	E	188	LEU	3.0
1	D	190	SER	3.0
1	E	196	SER	3.0
1	B	215	VAL	2.9
1	C	82	TRP	2.9
1	A	214	PRO	2.9
1	C	145	LYS	2.9
1	C	160	SER	2.9
1	D	2	GLU	2.9
1	D	251	ASN	2.9
1	C	221	SER	2.8
1	C	228	SER	2.8
1	A	246	VAL	2.8
1	C	215	VAL	2.8
1	A	28	THR	2.8
1	D	164	PRO	2.8
1	C	143	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	236	VAL	2.8
1	D	148	CYS	2.8
1	C	166	PHE	2.8
1	C	192	ASN	2.8
1	E	109	LEU	2.8
1	A	253	PHE	2.8
1	D	68	TYR	2.8
1	C	95	LYS	2.8
1	D	249	GLU	2.8
1	A	154	SER	2.7
1	A	191	MET	2.7
1	E	192	ASN	2.7
1	C	130	VAL	2.7
1	C	254	GLU	2.7
1	A	149	PHE	2.7
1	D	161	LEU	2.7
1	A	254	GLU	2.7
1	C	194	ALA	2.7
1	B	110	GLN	2.7
1	D	142	HIS	2.7
1	C	181	PHE	2.6
1	C	168	ASN	2.6
1	B	228	SER	2.6
1	B	253	PHE	2.6
1	D	220	LEU	2.6
1	A	229	ILE	2.6
1	C	47	PHE	2.6
1	E	220	LEU	2.6
1	C	27	ASN	2.6
1	C	266	LEU	2.6
1	C	230	LYS	2.6
1	A	27	ASN	2.5
1	B	192	ASN	2.5
1	C	232	SER	2.5
1	D	186	SER	2.5
1	B	168	ASN	2.5
1	E	223	ALA	2.5
1	C	256	TYR	2.5
1	D	256	TYR	2.5
1	A	245	ASP	2.5
1	C	167	GLU	2.5
1	A	150	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	226	LEU	2.5
1	D	3	GLU	2.4
1	D	82	TRP	2.4
1	E	214	PRO	2.4
1	E	3	GLU	2.4
1	C	255	LEU	2.4
1	B	95	LYS	2.4
1	A	213	VAL	2.4
1	C	199	VAL	2.4
1	E	189	PHE	2.4
1	D	52	VAL	2.4
1	C	170	TRP	2.4
1	A	247	SER	2.3
1	D	257	ASP	2.3
1	A	68	TYR	2.3
1	D	253	PHE	2.3
1	D	224	GLU	2.3
1	A	231	LEU	2.3
1	D	197	LEU	2.3
1	D	211	PRO	2.3
1	C	270	THR	2.3
1	C	162	SER	2.3
1	D	189	PHE	2.3
1	D	144	TRP	2.3
1	D	163	ILE	2.3
1	B	159	MET	2.3
1	C	259	PHE	2.3
1	A	37	ILE	2.2
1	C	49	LEU	2.2
1	E	228	SER	2.2
1	D	5	ARG	2.2
1	B	154	SER	2.2
1	C	201	VAL	2.2
1	A	94	ASN	2.2
1	D	109	LEU	2.2
1	E	76	ASN	2.2
1	D	153	GLY	2.2
1	A	215	VAL	2.1
1	B	29	THR	2.1
1	C	131	ASP	2.1
1	D	234	ASP	2.1
1	D	146	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	191	MET	2.1
1	A	225	LEU	2.1
1	D	212	THR	2.1
1	C	246	VAL	2.1
1	C	9	TRP	2.1
1	A	251	ASN	2.1
1	C	177	ASN	2.1
1	C	173	ILE	2.1
1	D	196	SER	2.1
1	E	234	ASP	2.1
1	A	223	ALA	2.1
1	C	140	TRP	2.1
1	C	203	THR	2.1
1	B	214	PRO	2.1
1	D	147	ALA	2.0
1	E	249	GLU	2.0
1	A	158	ILE	2.0
1	B	252	ILE	2.0
1	D	156	LYS	2.0
1	D	138	ASP	2.0
1	E	148	CYS	2.0
1	C	208	VAL	2.0
1	C	236	VAL	2.0
1	D	7	ARG	2.0
1	D	255	LEU	2.0
1	D	235	GLY	2.0
1	B	227	ASP	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 oligosaccharides 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
3	SO4	D	302	5/5	0.61	0.13	146,146,146,146	0
3	SO4	E	305	5/5	0.67	0.11	130,130,130,130	0
3	SO4	B	304	5/5	0.68	0.18	137,137,138,138	0
3	SO4	C	302	5/5	0.71	0.14	122,123,123,123	0
3	SO4	B	302	5/5	0.75	0.18	116,116,117,117	0
3	SO4	B	303	5/5	0.78	0.18	127,127,127,128	0
3	SO4	A	302	5/5	0.80	0.11	113,114,114,115	0
3	SO4	A	304	5/5	0.82	0.13	117,117,117,118	0
3	SO4	A	303	5/5	0.84	0.17	121,121,122,122	0
2	EPE	A	301	15/15	0.84	0.23	100,104,118,118	0
3	SO4	E	304	5/5	0.85	0.11	135,135,135,135	0
2	EPE	B	301	15/15	0.86	0.22	94,99,114,114	0
3	SO4	E	303	5/5	0.86	0.11	94,94,94,95	0
3	SO4	C	301	5/5	0.87	0.15	115,116,116,116	0
2	EPE	E	301	15/15	0.88	0.23	86,92,109,109	0
3	SO4	D	301	5/5	0.88	0.11	98,99,99,99	0
3	SO4	B	305	5/5	0.89	0.12	118,118,118,119	0
3	SO4	E	302	5/5	0.90	0.13	97,97,98,98	0

6.5 Other polymers

There are no such residues in this entry.