



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:23 pm BST

PDB ID : 3RIT
Title : Crystal structure of Dipeptide Epimerase from *Methylococcus capsulatus* complexed with Mg and dipeptide L-Arg-D-Lys
Authors : Lukk, T.; Sakai, A.; Song, L.; Gerlt, J.A.; Nair, S.K.
Deposited on : 2011-04-14
Resolution : 2.70 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
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) : 2.11

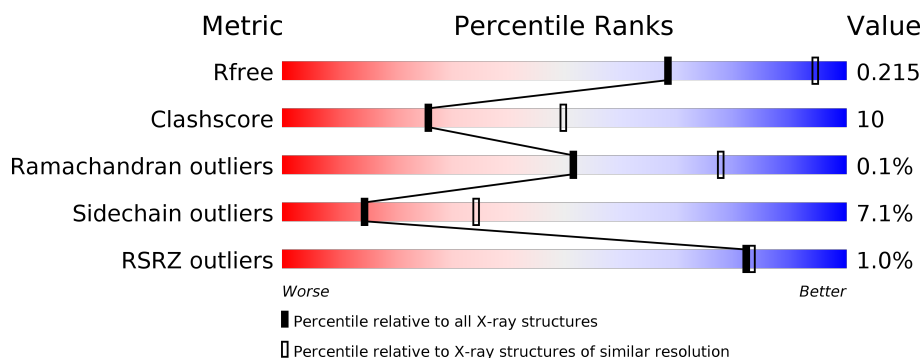
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 ≥ 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	356	<div> <div>%</div> <div> <div></div> <div>82%</div> <div>15%</div> <div>..</div> </div> </div>
1	B	356	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>15%</div> <div>..</div> </div> </div>
1	C	356	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>19%</div> <div>..</div> </div> </div>
1	D	356	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>..</div> </div> </div>
1	E	356	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>..</div> </div> </div>

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
4	DLY	A	364	X	-	-	-
4	DLY	B	362	X	-	X	-
4	DLY	C	362	X	-	-	-
4	DLY	D	364	X	-	-	X
4	DLY	E	363	X	-	X	-
6	1PE	D	366	-	-	-	X
6	1PE	E	365	-	-	-	X

2 Entry composition [i](#)

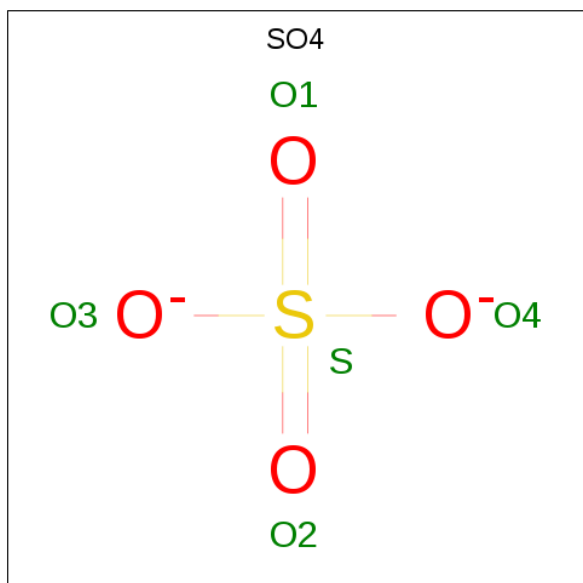
There are 7 unique types of molecules in this entry. The entry contains 14454 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Dipeptide epimerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	354	Total	C	N	O	S	0	0	0
			2720	1709	502	495	14			
1	B	354	Total	C	N	O	S	0	0	0
			2720	1709	502	495	14			
1	C	354	Total	C	N	O	S	0	0	0
			2720	1709	502	495	14			
1	D	354	Total	C	N	O	S	0	0	0
			2720	1709	502	495	14			
1	E	354	Total	C	N	O	S	0	0	0
			2720	1709	502	495	14			

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

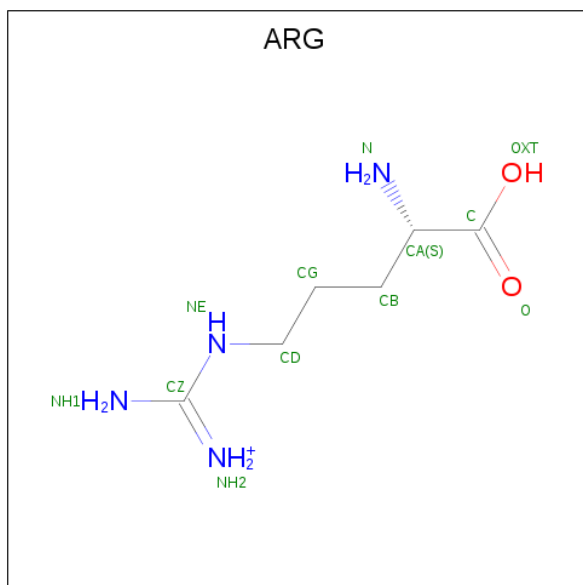
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total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

Continued on next page...

Continued from previous page...

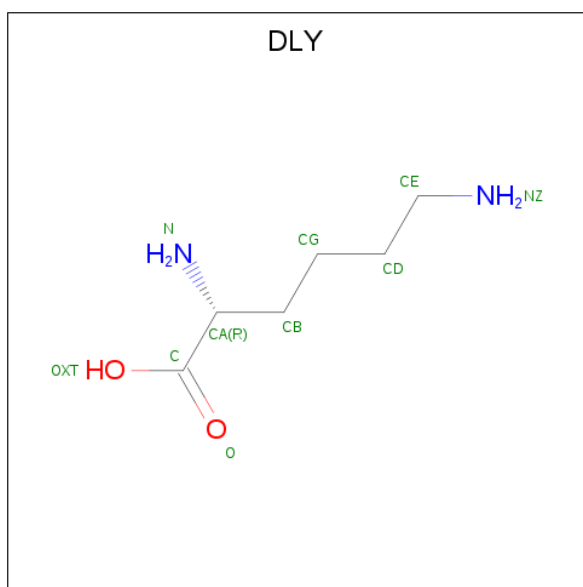
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		
2	E	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is ARGinine (three-letter code: ARG) (formula: $C_6H_{15}N_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			11	6	4	1		
3	B	1	Total	C	N	O	0	0
			11	6	4	1		
3	C	1	Total	C	N	O	0	0
			11	6	4	1		
3	D	1	Total	C	N	O	0	0
			11	6	4	1		
3	E	1	Total	C	N	O	0	0
			11	6	4	1		

- Molecule 4 is D-LYSINE (three-letter code: DLY) (formula: $C_6H_{14}N_2O_2$).

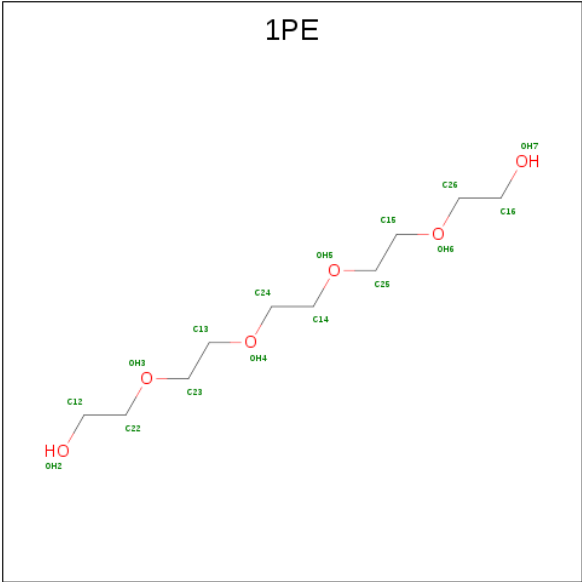


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			10	6	2	2		
4	B	1	Total	C	N	O	0	0
			10	6	2	2		
4	C	1	Total	C	N	O	0	0
			10	6	2	2		
4	D	1	Total	C	N	O	0	0
			10	6	2	2		
4	E	1	Total	C	N	O	0	0
			10	6	2	2		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Mg	0	0
			1	1		
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		
5	E	1	Total	Mg	0	0
			1	1		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: C₁₀H₂₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		
6	C	1	Total	C	O	0	0
			16	10	6		
6	D	1	Total	C	O	0	0
			16	10	6		
6	E	1	Total	C	O	0	0
			16	10	6		

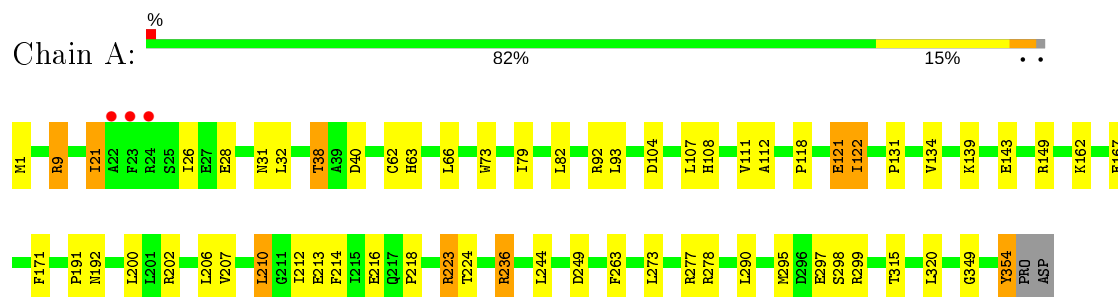
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	156	Total	O	0	0
			156	156		
7	B	144	Total	O	0	0
			144	144		
7	C	116	Total	O	0	0
			116	116		
7	D	89	Total	O	0	0
			89	89		
7	E	50	Total	O	0	0
			50	50		

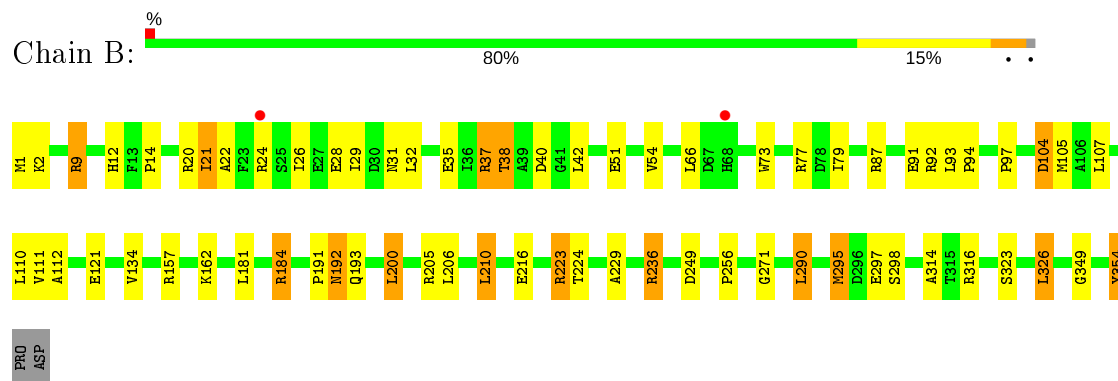
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

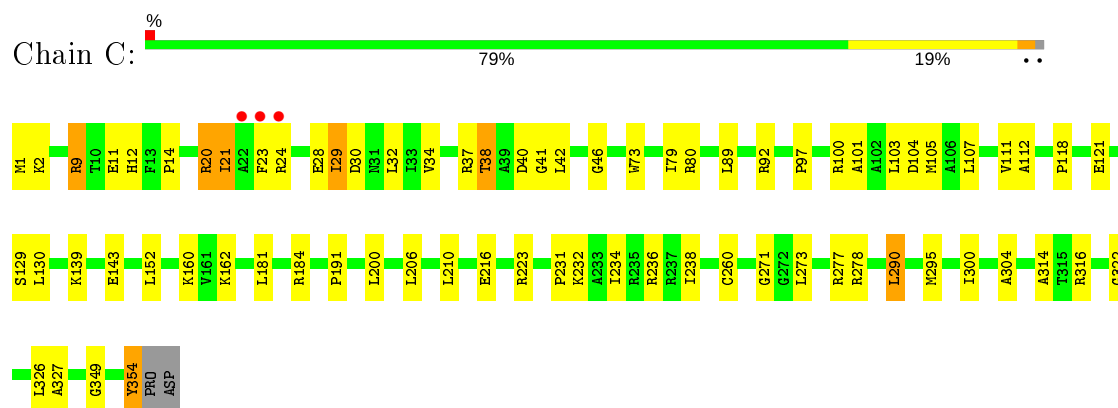
• Molecule 1: Dipeptide epimerase



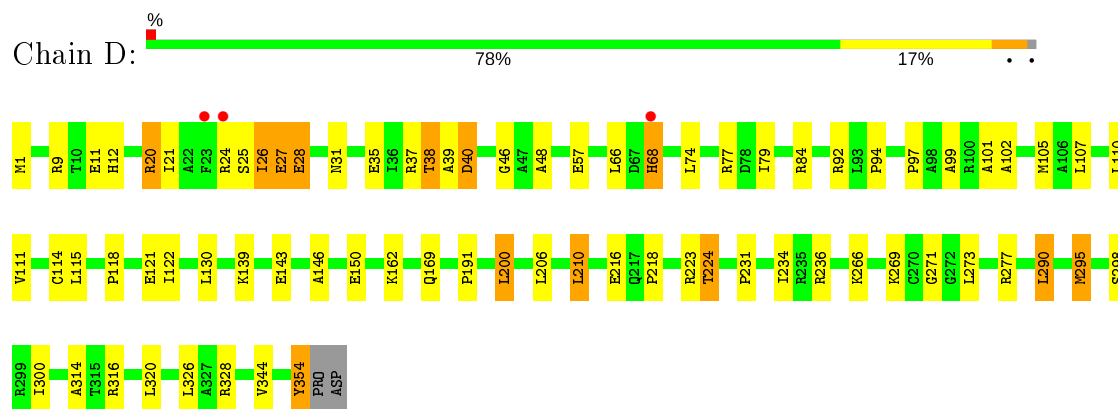
• Molecule 1: Dipeptide epimerase



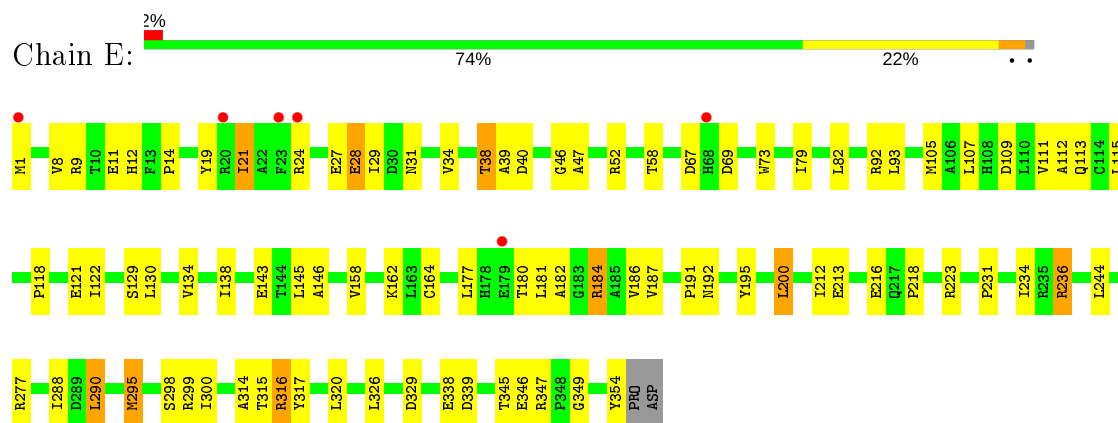
• Molecule 1: Dipeptide epimerase



• Molecule 1: Dipeptide epimerase



• Molecule 1: Dipeptide epimerase



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 3	Depositor
Cell constants a, b, c, α , β , γ	275.32Å 275.32Å 275.32Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.87 – 2.70 19.87 – 2.70	Depositor EDS
% Data completeness (in resolution range)	100.0 (19.87-2.70) 100.0 (19.87-2.70)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.16 (at 2.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_721)	Depositor
R, R_{free}	0.175 , 0.222 0.169 , 0.215	Depositor DCC
R_{free} test set	4710 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14454	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.54% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, 1PE, DLY, 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	0.46	0/2766	0.68	1/3749 (0.0%)
1	B	0.46	0/2766	0.69	0/3749
1	C	0.42	0/2766	0.62	0/3749
1	D	0.40	0/2766	0.63	1/3749 (0.0%)
1	E	0.38	0/2766	0.62	0/3749
All	All	0.43	0/13830	0.65	2/18745 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	LEU	CA-CB-CG	5.51	127.97	115.30
1	D	200	LEU	CA-CB-CG	-5.45	102.77	115.30

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	2720	0	2775	46	0
1	B	2720	0	2775	59	0
1	C	2720	0	2775	57	0
1	D	2720	0	2775	51	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	2720	0	2775	68	0
2	A	30	0	0	0	0
2	B	20	0	0	1	0
2	C	20	0	0	0	0
2	D	30	0	0	1	0
2	E	25	0	0	0	0
3	A	11	0	12	0	0
3	B	11	0	12	3	0
3	C	11	0	12	5	0
3	D	11	0	12	2	0
3	E	11	0	12	5	0
4	A	10	0	11	2	0
4	B	10	0	12	7	0
4	C	10	0	12	4	0
4	D	10	0	11	5	0
4	E	10	0	11	9	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
6	A	16	0	22	0	0
6	C	16	0	22	1	0
6	D	16	0	22	2	0
6	E	16	0	22	0	0
7	A	156	0	0	7	0
7	B	144	0	0	5	0
7	C	116	0	0	4	0
7	D	89	0	0	4	0
7	E	50	0	0	1	0
All	All	14454	0	14080	293	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 10.

All (293) 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:E:236:ARG:HH11	1:E:236:ARG:HG2	1.12	1.12
1:B:236:ARG:HH11	1:B:236:ARG:HG2	1.04	1.09
3:C:361:ARG:HB3	4:C:362:DLY:HG3	1.30	1.07

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:25:SER:O	1:D:26:ILE:HG13	1.54	1.06
1:E:184:ARG:HH11	1:E:184:ARG:HG3	1.16	1.04
1:B:236:ARG:NH1	1:B:236:ARG:HG2	1.81	0.93
1:E:46:GLY:HA2	1:E:105:MET:HE2	1.54	0.90
1:E:21:ILE:HG13	1:E:24:ARG:HB2	1.56	0.88
1:A:236:ARG:HH11	1:A:236:ARG:HG2	1.38	0.87
1:E:236:ARG:HG2	1:E:236:ARG:NH1	1.85	0.87
1:C:1:MET:HB3	1:C:79:ILE:HG12	1.59	0.84
1:C:23:PHE:O	1:C:24:ARG:HG2	1.77	0.83
1:E:184:ARG:NH1	1:E:184:ARG:HG3	1.93	0.82
1:A:1:MET:SD	1:A:79:ILE:HD11	2.18	0.82
1:B:21:ILE:HD12	1:B:24:ARG:HB2	1.62	0.80
1:B:1:MET:HB3	1:B:79:ILE:HG12	1.64	0.80
1:D:107:LEU:O	1:D:111:VAL:HG23	1.81	0.79
1:C:322:GLY:HA2	3:C:361:ARG:HD2	1.63	0.79
1:D:236:ARG:HG3	1:D:236:ARG:HH11	1.47	0.78
1:D:46:GLY:HA2	1:D:105:MET:HE2	1.65	0.77
1:C:46:GLY:HA2	1:C:105:MET:HE2	1.67	0.76
1:B:256:PRO:HG2	7:B:391:HOH:O	1.85	0.76
3:C:361:ARG:CB	4:C:362:DLY:HG3	2.15	0.75
1:B:181:LEU:O	1:B:184:ARG:HG2	1.87	0.74
1:C:9:ARG:NH2	1:C:354:TYR:OH	2.19	0.74
1:D:1:MET:SD	1:D:79:ILE:HD11	2.27	0.74
1:B:1:MET:SD	1:B:79:ILE:HD11	2.28	0.74
1:D:24:ARG:HG3	1:D:25:SER:O	1.89	0.72
7:A:389:HOH:O	1:C:278:ARG:HD3	1.88	0.72
1:E:236:ARG:HH11	1:E:236:ARG:CG	1.98	0.72
1:E:12:HIS:CE1	1:E:28:GLU:HG3	2.25	0.72
1:E:46:GLY:HA2	1:E:105:MET:CE	2.20	0.71
1:C:105:MET:HE1	1:C:300:ILE:HG22	1.71	0.71
1:E:200:LEU:O	1:E:200:LEU:HG	1.90	0.71
3:D:363:ARG:HB3	4:D:364:DLY:HG2	1.73	0.71
1:B:9:ARG:NH2	1:B:354:TYR:OH	2.23	0.71
1:C:181:LEU:O	1:C:184:ARG:HG3	1.91	0.70
3:C:361:ARG:HB3	4:C:362:DLY:CG	2.14	0.70
1:D:191:PRO:HD2	1:D:216:GLU:O	1.90	0.70
1:D:200:LEU:HG	1:D:200:LEU:O	1.90	0.70
1:A:139:LYS:HD3	1:A:143:GLU:HG3	1.73	0.70
1:D:224:THR:HG21	2:D:362:SO4:O3	1.92	0.70
1:E:295:MET:HE3	4:E:363:DLY:HE3	1.74	0.70
1:B:107:LEU:O	1:B:111:VAL:HG23	1.92	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1:MET:SD	1:C:79:ILE:HD11	2.31	0.70
1:C:20:ARG:CG	1:C:20:ARG:HH11	2.04	0.70
1:A:236:ARG:NH1	1:A:236:ARG:HG2	2.03	0.70
1:C:20:ARG:HG3	1:C:20:ARG:HH11	1.56	0.69
1:D:295:MET:HE1	4:D:364:DLY:HE2	1.72	0.69
1:A:38:THR:CG2	1:A:40:ASP:H	2.06	0.68
1:B:200:LEU:O	1:B:200:LEU:HG	1.94	0.67
1:B:191:PRO:HD2	1:B:216:GLU:O	1.95	0.67
1:B:162:LYS:NZ	4:B:362:DLY:H	1.93	0.66
1:D:40:ASP:OD1	1:D:40:ASP:N	2.26	0.66
1:C:107:LEU:O	1:C:111:VAL:HG23	1.97	0.64
1:B:295:MET:O	1:B:297:GLU:HG3	1.98	0.64
1:D:139:LYS:HD3	1:D:143:GLU:HB3	1.80	0.64
1:B:229:ALA:O	1:C:232:LYS:HE2	1.98	0.63
1:D:1:MET:HB3	1:D:79:ILE:HG12	1.80	0.63
1:E:21:ILE:HG22	1:E:162:LYS:HD2	1.80	0.63
1:C:38:THR:HG23	1:C:40:ASP:H	1.65	0.62
1:E:107:LEU:O	1:E:111:VAL:HG23	2.00	0.62
1:D:236:ARG:CG	1:D:236:ARG:HH11	2.12	0.62
1:B:21:ILE:HD11	1:B:26:ILE:HD11	1.83	0.61
1:C:200:LEU:O	1:C:200:LEU:HG	2.00	0.61
1:C:73:TRP:CE2	1:C:92:ARG:HD3	2.35	0.61
1:A:207:VAL:HG13	1:A:212:ILE:HB	1.82	0.61
1:A:149:ARG:HD3	7:A:442:HOH:O	2.00	0.60
1:B:162:LYS:HZ3	4:B:362:DLY:H	1.49	0.60
1:E:290:LEU:HD22	1:E:314:ALA:HB3	1.83	0.60
1:A:38:THR:HG23	1:A:40:ASP:H	1.66	0.60
1:C:37:ARG:HD3	7:C:874:HOH:O	2.01	0.60
1:C:184:ARG:HG3	1:C:184:ARG:HH11	1.67	0.60
1:C:12:HIS:CE1	1:C:28:GLU:HG3	2.36	0.60
3:B:361:ARG:HB2	4:B:362:DLY:HD3	1.83	0.60
1:D:12:HIS:NE2	1:D:28:GLU:HG3	2.17	0.60
1:C:21:ILE:HG13	1:C:24:ARG:HB2	1.82	0.59
1:A:200:LEU:O	1:A:200:LEU:HG	2.00	0.59
1:C:290:LEU:HD22	1:C:314:ALA:HB3	1.84	0.59
1:A:32:LEU:HD23	1:A:66:LEU:HD12	1.84	0.59
1:C:29:ILE:HD12	1:C:30:ASP:H	1.67	0.58
1:A:167:GLU:OE1	1:A:202:ARG:HD2	2.03	0.58
1:B:38:THR:HG22	1:B:42:LEU:N	2.18	0.58
1:B:162:LYS:HZ1	4:B:362:DLY:HG3	1.68	0.58
7:A:1034:HOH:O	1:C:277:ARG:HD3	2.03	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:187:VAL:O	1:E:212:ILE:HG23	2.04	0.58
1:A:299:ARG:HD2	7:A:668:HOH:O	2.03	0.58
1:B:12:HIS:CE1	1:B:28:GLU:HG3	2.38	0.58
1:E:182:ALA:H	1:E:184:ARG:HG3	1.67	0.57
1:E:184:ARG:HH11	1:E:184:ARG:CG	2.02	0.57
1:A:191:PRO:HD2	1:A:216:GLU:O	2.05	0.57
3:E:362:ARG:CB	4:E:363:DLY:HD3	2.34	0.57
7:D:1037:HOH:O	1:E:277:ARG:HD3	2.04	0.57
3:E:362:ARG:HB3	4:E:363:DLY:HD3	1.87	0.57
1:D:105:MET:HE1	1:D:300:ILE:HG22	1.87	0.56
1:D:118:PRO:HD2	1:D:121:GLU:HG3	1.87	0.56
3:D:363:ARG:CB	4:D:364:DLY:HG2	2.36	0.56
1:E:9:ARG:NH2	1:E:354:TYR:OH	2.35	0.56
1:C:12:HIS:HE1	1:C:28:GLU:HG3	1.69	0.56
1:C:21:ILE:HG22	1:C:162:LYS:HD3	1.88	0.55
1:C:191:PRO:HD2	1:C:216:GLU:O	2.05	0.55
1:A:118:PRO:HD2	1:A:121:GLU:HG3	1.88	0.55
1:D:236:ARG:NH1	1:D:236:ARG:CG	2.69	0.55
1:D:266:LYS:HG3	1:D:269:LYS:HE2	1.86	0.55
1:B:38:THR:HG22	1:B:42:LEU:H	1.70	0.55
1:E:112:ALA:HB3	1:E:349:GLY:HA2	1.88	0.55
1:E:38:THR:HG23	1:E:40:ASP:H	1.70	0.55
1:A:200:LEU:HD13	1:A:218:PRO:CB	2.37	0.55
1:C:112:ALA:HB3	1:C:349:GLY:HA2	1.88	0.55
1:B:162:LYS:NZ	4:B:362:DLY:N	2.54	0.55
1:D:20:ARG:HA	1:D:25:SER:HA	1.88	0.55
1:A:107:LEU:O	1:A:111:VAL:HG23	2.07	0.55
1:B:112:ALA:HB3	1:B:349:GLY:HA2	1.88	0.55
1:C:231:PRO:HD2	1:C:234:ILE:HD12	1.89	0.54
1:C:2:LYS:HE3	7:C:400:HOH:O	2.07	0.54
1:C:118:PRO:HD2	1:C:121:GLU:HG3	1.89	0.54
3:B:361:ARG:HB3	4:B:362:DLY:HB2	1.89	0.54
1:B:32:LEU:HD23	1:B:66:LEU:HD12	1.90	0.54
1:D:162:LYS:NZ	4:D:364:DLY:N	2.55	0.54
1:E:9:ARG:NH1	1:E:11:GLU:OE2	2.41	0.54
1:E:38:THR:HG23	1:E:39:ALA:N	2.23	0.54
1:E:1:MET:HB2	1:E:79:ILE:HD11	1.89	0.54
1:E:138:ILE:HD13	1:E:164:CYS:HB3	1.89	0.54
1:B:73:TRP:CE2	1:B:92:ARG:HD3	2.42	0.53
1:D:146:ALA:O	1:D:150:GLU:HG3	2.08	0.53
1:E:158:VAL:HG22	1:E:186:VAL:HG22	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:295:MET:CE	4:E:363:DLY:HE3	2.37	0.53
1:A:290:LEU:HB2	1:A:315:THR:HA	1.90	0.53
1:E:19:TYR:OH	4:E:363:DLY:HD2	2.08	0.53
1:A:9:ARG:NH2	1:A:354:TYR:OH	2.42	0.53
1:D:101:ALA:O	1:D:105:MET:HG3	2.08	0.53
1:A:82:LEU:HD21	1:A:108:HIS:CE1	2.44	0.53
1:D:48:ALA:HB2	1:D:102:ALA:HB2	1.91	0.52
1:A:200:LEU:HD13	1:A:218:PRO:HB3	1.91	0.52
1:A:112:ALA:HB3	1:A:349:GLY:HA2	1.91	0.52
1:B:290:LEU:HD22	1:B:314:ALA:HB3	1.92	0.52
1:A:73:TRP:CE2	1:A:92:ARG:HD3	2.45	0.52
1:E:52:ARG:HD2	1:E:58:THR:HG22	1.92	0.51
1:C:14:PRO:HG2	1:C:327:ALA:HB3	1.92	0.51
1:E:46:GLY:CA	1:E:105:MET:HE2	2.35	0.51
1:A:162:LYS:HZ1	4:A:364:DLY:HB3	1.76	0.51
1:A:38:THR:HG22	1:A:40:ASP:H	1.76	0.51
1:E:129:SER:O	1:E:130:LEU:HG	2.11	0.51
1:E:21:ILE:CG1	1:E:24:ARG:HB2	2.34	0.51
1:E:231:PRO:HD2	1:E:234:ILE:HD12	1.91	0.51
1:B:21:ILE:HD11	1:B:26:ILE:CD1	2.41	0.51
1:D:57:GLU:OE1	1:D:97:PRO:HD2	2.11	0.51
1:C:139:LYS:HD3	1:C:143:GLU:HB3	1.94	0.50
1:C:38:THR:HG22	1:C:41:GLY:N	2.27	0.50
1:D:21:ILE:HG13	1:D:24:ARG:HB3	1.93	0.50
1:E:191:PRO:HD2	1:E:216:GLU:O	2.11	0.50
1:E:73:TRP:CE2	1:E:92:ARG:HD3	2.46	0.50
1:E:82:LEU:HD22	1:E:111:VAL:HG21	1.93	0.50
1:A:122:ILE:HD12	1:C:80:ARG:O	2.12	0.50
1:C:105:MET:HE3	1:C:304:ALA:HB2	1.94	0.50
1:E:47:ALA:H	1:E:105:MET:HE1	1.76	0.50
1:B:92:ARG:C	1:B:94:PRO:HD3	2.33	0.50
1:C:9:ARG:NH1	1:C:11:GLU:OE2	2.43	0.50
7:A:1034:HOH:O	1:C:277:ARG:CD	2.59	0.50
1:A:249:ASP:OD1	1:B:223:ARG:NH2	2.45	0.49
1:E:14:PRO:HA	1:E:28:GLU:HB2	1.94	0.49
1:C:101:ALA:O	1:C:105:MET:HG3	2.12	0.49
1:A:21:ILE:HD11	1:A:26:ILE:HD11	1.93	0.49
1:C:21:ILE:HG22	1:C:162:LYS:CD	2.42	0.49
1:E:177:LEU:O	1:E:181:LEU:HG	2.12	0.49
1:E:105:MET:HE1	1:E:300:ILE:HG22	1.93	0.49
1:E:347:ARG:NH1	1:E:347:ARG:HG3	2.26	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:115:LEU:HD13	1:E:122:ILE:HD12	1.95	0.49
1:E:347:ARG:HH11	1:E:347:ARG:HG3	1.77	0.49
1:B:206:LEU:HG	1:B:210:LEU:HD22	1.93	0.49
1:A:206:LEU:HG	1:A:210:LEU:HD22	1.95	0.49
1:C:20:ARG:NH1	1:C:20:ARG:CG	2.69	0.49
1:B:9:ARG:NH2	1:B:354:TYR:HH	2.11	0.48
1:B:87:ARG:NE	2:B:359:SO4:O1	2.36	0.48
1:C:236:ARG:HH21	1:C:236:ARG:HG2	1.79	0.48
1:C:38:THR:HG22	1:C:42:LEU:H	1.77	0.48
1:D:200:LEU:HD13	1:D:218:PRO:CB	2.43	0.48
1:B:38:THR:HG23	1:B:40:ASP:H	1.78	0.48
1:B:205:ARG:HD2	7:B:883:HOH:O	2.13	0.47
1:D:38:THR:HG23	1:D:39:ALA:N	2.30	0.47
1:B:79:ILE:HD12	1:B:110:LEU:HB3	1.97	0.47
1:A:223:ARG:NH2	1:B:249:ASP:OD1	2.47	0.47
1:A:108:HIS:HE1	1:A:277:ARG:HH21	1.61	0.47
1:B:93:LEU:N	1:B:94:PRO:HD3	2.30	0.47
1:D:169:GLN:HG2	7:D:586:HOH:O	2.15	0.47
1:C:97:PRO:O	1:C:271:GLY:HA2	2.15	0.46
1:D:206:LEU:HG	1:D:210:LEU:HD22	1.97	0.46
1:D:295:MET:CE	4:D:364:DLY:HE2	2.42	0.46
1:E:1:MET:HB2	1:E:79:ILE:CD1	2.44	0.46
1:B:35:GLU:OE1	1:B:37:ARG:NH2	2.48	0.46
1:D:290:LEU:HD22	1:D:314:ALA:HB3	1.97	0.46
1:E:143:GLU:O	1:E:146:ALA:HB3	2.16	0.46
1:B:14:PRO:HA	1:B:28:GLU:HB2	1.98	0.46
1:C:29:ILE:HD11	7:C:404:HOH:O	2.16	0.46
1:B:192:ASN:O	1:B:193:GLN:HB2	2.16	0.46
1:B:223:ARG:HA	1:B:223:ARG:HD3	1.78	0.45
1:A:38:THR:HG22	1:A:40:ASP:N	2.31	0.45
1:B:97:PRO:O	1:B:271:GLY:HA2	2.16	0.45
1:E:316:ARG:HG2	1:E:317:TYR:CZ	2.52	0.45
1:D:35:GLU:OE1	1:D:37:ARG:NH2	2.50	0.45
1:D:92:ARG:C	1:D:94:PRO:HD3	2.37	0.45
3:B:361:ARG:CB	4:B:362:DLY:HB2	2.46	0.45
1:B:51:GLU:HG3	1:B:54:VAL:HG23	1.98	0.45
1:B:290:LEU:HA	1:B:290:LEU:HD12	1.76	0.45
7:A:410:HOH:O	1:C:278:ARG:HD2	2.17	0.45
1:B:21:ILE:HD12	1:B:24:ARG:CB	2.39	0.44
1:D:66:LEU:HG	1:D:99:ALA:HB1	1.99	0.44
1:E:145:LEU:HD22	1:E:180:THR:OG1	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:236:ARG:HD2	7:B:1031:HOH:O	2.16	0.44
4:C:362:DLY:HE3	4:C:362:DLY:HB2	1.86	0.44
1:D:295:MET:HE3	1:D:295:MET:HA	1.98	0.44
6:C:364:1PE:H151	6:C:364:1PE:H142	1.78	0.44
1:E:191:PRO:HB3	1:E:195:TYR:CD1	2.53	0.44
1:D:320:LEU:HD23	1:D:320:LEU:HA	1.88	0.44
1:B:236:ARG:CG	1:B:236:ARG:NH1	2.63	0.44
1:B:323:SER:HA	1:B:326:LEU:HD22	2.00	0.44
1:D:122:ILE:HD13	1:D:122:ILE:HA	1.71	0.44
1:A:1:MET:SD	1:A:79:ILE:CD1	2.98	0.44
1:B:38:THR:CG2	1:B:42:LEU:H	2.30	0.44
1:D:79:ILE:CD1	1:D:110:LEU:HB3	2.48	0.44
1:D:68:HIS:N	1:D:68:HIS:ND1	2.65	0.43
1:A:32:LEU:HD22	1:A:62:CYS:SG	2.58	0.43
1:D:231:PRO:HD2	1:D:234:ILE:HD12	1.99	0.43
1:E:19:TYR:CE1	3:E:362:ARG:NH1	2.86	0.43
1:C:29:ILE:HD12	1:C:30:ASP:N	2.32	0.43
1:B:157:ARG:HD3	7:B:578:HOH:O	2.19	0.43
1:E:162:LYS:HZ1	4:E:363:DLY:CG	2.31	0.43
1:E:320:LEU:HA	1:E:320:LEU:HD23	1.78	0.43
3:E:362:ARG:HB2	4:E:363:DLY:HD3	1.99	0.43
1:A:278:ARG:HD3	7:C:374:HOH:O	2.18	0.43
1:C:236:ARG:NH2	1:C:236:ARG:HG2	2.33	0.43
1:B:104:ASP:OD1	1:B:104:ASP:C	2.57	0.43
1:D:97:PRO:O	1:D:271:GLY:HA2	2.19	0.43
1:E:109:ASP:O	1:E:113:GLN:HG3	2.19	0.43
1:D:344:VAL:HG22	7:D:372:HOH:O	2.18	0.42
1:E:92:ARG:C	1:E:93:LEU:HD12	2.40	0.42
1:B:236:ARG:CZ	7:B:880:HOH:O	2.67	0.42
1:B:2:LYS:HA	1:B:77:ARG:O	2.18	0.42
1:C:273:LEU:HD12	1:C:273:LEU:N	2.34	0.42
1:D:9:ARG:NH2	1:D:354:TYR:OH	2.52	0.42
1:E:184:ARG:NH1	1:E:184:ARG:CG	2.69	0.42
6:D:366:1PE:C25	6:D:366:1PE:OH4	2.62	0.42
1:E:200:LEU:HD13	1:E:218:PRO:CB	2.50	0.42
1:E:38:THR:HG23	1:E:40:ASP:N	2.34	0.42
1:C:129:SER:O	1:C:130:LEU:HG	2.20	0.42
1:E:299:ARG:HG3	1:E:329:ASP:OD1	2.20	0.42
1:A:122:ILE:HD12	1:A:122:ILE:HA	1.58	0.42
1:A:171:PHE:CD1	1:A:171:PHE:N	2.87	0.42
1:E:290:LEU:HB2	1:E:315:THR:HA	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:67:ASP:OD2	1:E:69:ASP:HB2	2.19	0.42
6:D:366:1PE:H251	6:D:366:1PE:H242	1.38	0.42
1:E:338:GLU:O	1:E:339:ASP:HB2	2.19	0.42
1:B:1:MET:CG	1:B:79:ILE:HD11	2.50	0.42
1:B:92:ARG:C	1:B:93:LEU:HD12	2.40	0.42
1:C:206:LEU:HG	1:C:210:LEU:HD22	2.01	0.42
1:C:152:LEU:HD23	1:C:152:LEU:HA	1.91	0.42
1:C:290:LEU:HA	1:C:290:LEU:HD12	1.78	0.42
1:E:118:PRO:HD2	1:E:121:GLU:HG3	2.02	0.42
1:E:162:LYS:HZ1	4:E:363:DLY:HG3	1.84	0.42
1:E:1:MET:HB2	1:E:79:ILE:HG12	2.01	0.41
1:A:213:GLU:O	1:A:214:PHE:HB3	2.21	0.41
1:E:158:VAL:HG22	1:E:186:VAL:CG2	2.49	0.41
1:E:8:VAL:HG22	1:E:34:VAL:HG22	2.02	0.41
1:A:244:LEU:CD2	1:A:263:PHE:HB3	2.50	0.41
1:C:34:VAL:HG11	1:C:103:LEU:HD23	2.02	0.41
1:D:111:VAL:O	1:D:114:CYS:HB3	2.20	0.41
1:D:277:ARG:CD	7:E:1035:HOH:O	2.68	0.41
1:D:74:LEU:O	1:D:77:ARG:HG2	2.20	0.41
1:A:224:THR:HG22	7:A:1041:HOH:O	2.19	0.41
1:A:1:MET:HB3	1:A:79:ILE:HG12	2.03	0.41
1:A:92:ARG:C	1:A:93:LEU:HD12	2.41	0.41
1:A:295:MET:O	1:A:297:GLU:HG3	2.20	0.41
1:B:21:ILE:HG22	1:B:22:ALA:H	1.85	0.41
1:B:29:ILE:HA	1:B:29:ILE:HD12	1.90	0.41
1:B:66:LEU:HA	1:B:66:LEU:HD23	1.90	0.41
7:D:1037:HOH:O	1:E:277:ARG:CD	2.67	0.41
3:E:362:ARG:HA	4:E:363:DLY:HA	1.85	0.41
1:B:236:ARG:HH11	1:B:236:ARG:CG	1.97	0.41
1:A:236:ARG:HH11	1:A:236:ARG:CG	2.18	0.41
1:C:38:THR:HG22	1:C:41:GLY:H	1.86	0.41
1:C:160:LYS:HE2	3:C:361:ARG:O	2.20	0.41
1:A:32:LEU:HD21	1:A:63:HIS:HA	2.03	0.41
1:E:1:MET:HB2	1:E:79:ILE:CG1	2.51	0.41
1:D:115:LEU:HD23	1:D:115:LEU:HA	1.87	0.41
1:E:177:LEU:HD12	1:E:177:LEU:O	2.21	0.41
1:C:89:LEU:HB3	1:C:100:ARG:HG3	2.03	0.40
1:D:26:ILE:HG22	1:D:27:GLU:N	2.35	0.40
1:A:162:LYS:NZ	4:A:364:DLY:N	2.70	0.40
1:A:320:LEU:HD23	1:A:320:LEU:HA	1.94	0.40
1:C:238:ILE:O	1:C:260:CYS:HB2	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:MET:HB2	1:B:105:MET:HE2	1.79	0.40
1:D:11:GLU:OE1	1:D:328:ARG:NH2	2.45	0.40
1:D:354:TYR:HD2	1:D:354:TYR:HA	1.61	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	352/356 (99%)	342 (97%)	10 (3%)	0	100	100
1	B	352/356 (99%)	338 (96%)	14 (4%)	0	100	100
1	C	352/356 (99%)	342 (97%)	10 (3%)	0	100	100
1	D	352/356 (99%)	340 (97%)	11 (3%)	1 (0%)	41	66
1	E	352/356 (99%)	336 (96%)	16 (4%)	0	100	100
All	All	1760/1780 (99%)	1698 (96%)	61 (4%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	26	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	277/280 (99%)	261 (94%)	16 (6%)	20	43
1	B	277/280 (99%)	254 (92%)	23 (8%)	11	25
1	C	277/280 (99%)	264 (95%)	13 (5%)	26	54
1	D	277/280 (99%)	258 (93%)	19 (7%)	15	35
1	E	277/280 (99%)	255 (92%)	22 (8%)	12	28
All	All	1385/1400 (99%)	1292 (93%)	93 (7%)	14	37

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	ARG
1	A	21	ILE
1	A	28	GLU
1	A	31	ASN
1	A	38	THR
1	A	104	ASP
1	A	121	GLU
1	A	122	ILE
1	A	131	PRO
1	A	134	VAL
1	A	192	ASN
1	A	210	LEU
1	A	223	ARG
1	A	236	ARG
1	A	298	SER
1	A	354	TYR
1	B	9	ARG
1	B	20	ARG
1	B	21	ILE
1	B	31	ASN
1	B	37	ARG
1	B	38	THR
1	B	91	GLU
1	B	104	ASP
1	B	121	GLU
1	B	134	VAL
1	B	184	ARG
1	B	192	ASN
1	B	200	LEU
1	B	210	LEU
1	B	223	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	224	THR
1	B	236	ARG
1	B	290	LEU
1	B	295	MET
1	B	298	SER
1	B	316	ARG
1	B	326	LEU
1	B	354	TYR
1	C	9	ARG
1	C	20	ARG
1	C	21	ILE
1	C	29	ILE
1	C	32	LEU
1	C	38	THR
1	C	104	ASP
1	C	223	ARG
1	C	290	LEU
1	C	295	MET
1	C	316	ARG
1	C	326	LEU
1	C	354	TYR
1	D	20	ARG
1	D	27	GLU
1	D	28	GLU
1	D	31	ASN
1	D	38	THR
1	D	40	ASP
1	D	68	HIS
1	D	84	ARG
1	D	130	LEU
1	D	210	LEU
1	D	223	ARG
1	D	224	THR
1	D	273	LEU
1	D	290	LEU
1	D	295	MET
1	D	298	SER
1	D	316	ARG
1	D	326	LEU
1	D	354	TYR
1	E	21	ILE
1	E	27	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	28	GLU
1	E	29	ILE
1	E	31	ASN
1	E	38	THR
1	E	134	VAL
1	E	184	ARG
1	E	192	ASN
1	E	200	LEU
1	E	213	GLU
1	E	223	ARG
1	E	236	ARG
1	E	244	LEU
1	E	288	ILE
1	E	290	LEU
1	E	295	MET
1	E	298	SER
1	E	316	ARG
1	E	326	LEU
1	E	345	THR
1	E	346	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	108	HIS
1	B	113	GLN
1	C	12	HIS
1	C	113	GLN
1	E	12	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry

Of 44 ligands modelled in this entry, 5 are monoatomic - leaving 39 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	C	358	-	4,4,4	0.21	0	6,6,6	0.44	0
2	SO4	D	358	-	4,4,4	0.14	0	6,6,6	0.24	0
2	SO4	E	358	-	4,4,4	0.16	0	6,6,6	0.05	0
2	SO4	E	357	-	4,4,4	0.16	0	6,6,6	0.25	0
2	SO4	A	359	-	4,4,4	0.17	0	6,6,6	0.23	0
2	SO4	B	360	-	4,4,4	0.17	0	6,6,6	0.16	0
6	1PE	A	366	-	15,15,15	0.54	0	14,14,14	0.42	0
2	SO4	D	360	-	4,4,4	0.15	0	6,6,6	0.05	0
2	SO4	A	358	-	4,4,4	0.16	0	6,6,6	0.25	0
2	SO4	E	359	-	4,4,4	0.18	0	6,6,6	0.30	0
2	SO4	C	359	-	4,4,4	0.20	0	6,6,6	0.16	0
6	1PE	D	366	-	15,15,15	0.46	0	14,14,14	0.65	0
2	SO4	A	357	-	4,4,4	0.19	0	6,6,6	0.31	0
2	SO4	A	362	-	4,4,4	0.22	0	6,6,6	0.32	0
2	SO4	D	361	-	4,4,4	0.14	0	6,6,6	0.12	0
2	SO4	E	361	-	4,4,4	0.13	0	6,6,6	0.14	0
2	SO4	C	357	-	4,4,4	0.18	0	6,6,6	0.22	0
2	SO4	A	360	-	4,4,4	0.22	0	6,6,6	0.24	0
2	SO4	B	357	-	4,4,4	0.19	0	6,6,6	0.25	0
2	SO4	B	359	-	4,4,4	0.23	0	6,6,6	0.30	0
2	SO4	D	359	-	4,4,4	0.15	0	6,6,6	0.12	0
2	SO4	A	361	-	4,4,4	0.21	0	6,6,6	0.23	0
2	SO4	B	358	-	4,4,4	0.20	0	6,6,6	0.17	0
6	1PE	C	364	-	15,15,15	0.49	0	14,14,14	0.53	0
2	SO4	E	360	-	4,4,4	0.16	0	6,6,6	0.16	0
2	SO4	C	360	-	4,4,4	0.15	0	6,6,6	0.19	0
2	SO4	D	362	-	4,4,4	0.18	0	6,6,6	0.27	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	SO4	D	357	-	4,4,4	0.18	0	6,6,6	0.32	0
6	1PE	E	365	-	15,15,15	0.53	0	14,14,14	0.49	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
4	DLY	D	364	3,5	1/1/2/2	-	-
4	DLY	E	363	3,5	1/1/2/2	-	-
6	1PE	C	364	-	-	7/13/13/13	-
6	1PE	D	366	-	-	5/13/13/13	-
4	DLY	B	362	3	1/1/2/2	-	-
4	DLY	A	364	3	1/1/2/2	-	-
4	DLY	C	362	3	1/1/2/2	-	-
6	1PE	A	366	-	-	9/13/13/13	-
6	1PE	E	365	-	-	5/13/13/13	-

There are no bond length outliers.

There are no bond angle outliers.

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	363	DLY	CA
4	B	362	DLY	CA
4	A	364	DLY	CA
4	D	364	DLY	CA
4	C	362	DLY	CA

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	D	366	1PE	C24-C14-OH5-C25
6	D	366	1PE	C23-C13-OH4-C24
6	A	366	1PE	OH4-C13-C23-OH3
6	C	364	1PE	OH5-C14-C24-OH4
6	E	365	1PE	OH5-C14-C24-OH4
6	A	366	1PE	C13-C23-OH3-C22
6	C	364	1PE	C16-C26-OH6-C15

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	D	366	1PE	OH4-C13-C23-OH3
6	A	366	1PE	OH5-C14-C24-OH4
6	A	366	1PE	OH2-C12-C22-OH3
6	E	365	1PE	OH7-C16-C26-OH6
6	C	364	1PE	OH7-C16-C26-OH6
6	C	364	1PE	OH4-C13-C23-OH3
6	A	366	1PE	OH7-C16-C26-OH6
6	E	365	1PE	OH6-C15-C25-OH5
6	A	366	1PE	OH6-C15-C25-OH5
6	D	366	1PE	C13-C23-OH3-C22
6	A	366	1PE	C25-C15-OH6-C26
6	C	364	1PE	C13-C23-OH3-C22
6	E	365	1PE	C14-C24-OH4-C13
6	C	364	1PE	OH6-C15-C25-OH5
6	A	366	1PE	C15-C25-OH5-C14
6	A	366	1PE	C12-C22-OH3-C23
6	D	366	1PE	C15-C25-OH5-C14
6	C	364	1PE	C14-C24-OH4-C13
6	E	365	1PE	C13-C23-OH3-C22

There are no ring outliers.

9 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	363	DLY	9	0
4	B	362	DLY	7	0
6	D	366	1PE	2	0
4	A	364	DLY	2	0
2	B	359	SO4	1	0
4	D	364	DLY	5	0
6	C	364	1PE	1	0
2	D	362	SO4	1	0
4	C	362	DLY	4	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

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	354/356 (99%)	-0.79	3 (0%) 86 87	19, 30, 54, 88	0
1	B	354/356 (99%)	-0.76	2 (0%) 89 91	20, 30, 54, 88	0
1	C	354/356 (99%)	-0.74	3 (0%) 86 87	22, 34, 59, 92	0
1	D	354/356 (99%)	-0.61	3 (0%) 86 87	29, 43, 70, 98	0
1	E	354/356 (99%)	-0.40	6 (1%) 70 72	33, 55, 80, 101	0
All	All	1770/1780 (99%)	-0.66	17 (0%) 82 83	19, 38, 72, 101	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	4.0
1	E	20	ARG	3.5
1	D	23	PHE	3.4
1	B	24	ARG	3.2
1	E	23	PHE	3.0
1	D	24	ARG	2.8
1	A	24	ARG	2.6
1	D	68	HIS	2.5
1	A	22	ALA	2.4
1	C	23	PHE	2.4
1	E	24	ARG	2.4
1	A	23	PHE	2.4
1	C	24	ARG	2.3
1	B	68	HIS	2.3
1	E	68	HIS	2.1
1	E	179	GLU	2.1
1	C	22	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no carbohydrates 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(\AA^2)	Q<0.9
6	1PE	D	366	16/16	0.69	0.52	62,69,80,81	16
4	DLY	C	362	10/10	0.71	0.36	51,64,69,71	0
4	DLY	B	362	10/10	0.76	0.39	47,62,68,70	0
6	1PE	E	365	16/16	0.77	0.42	61,74,82,84	16
4	DLY	E	363	10/10	0.78	0.38	73,82,87,91	0
4	DLY	D	364	10/10	0.78	0.50	59,66,93,95	0
4	DLY	A	364	10/10	0.79	0.40	43,62,76,86	0
2	SO4	C	360	5/5	0.84	0.19	52,52,55,64	5
2	SO4	B	360	5/5	0.85	0.32	98,107,123,125	0
2	SO4	A	362	5/5	0.86	0.23	33,33,48,60	5
6	1PE	A	366	16/16	0.89	0.22	47,56,63,66	0
3	ARG	D	363	11/12	0.89	0.21	48,58,70,72	0
2	SO4	D	359	5/5	0.91	0.37	79,90,106,108	0
5	MG	E	364	1/1	0.91	0.13	60,60,60,60	0
3	ARG	B	361	11/12	0.92	0.17	42,49,56,64	0
3	ARG	E	362	11/12	0.92	0.17	64,76,84,85	0
2	SO4	D	362	5/5	0.92	0.18	46,50,55,66	5
6	1PE	C	364	16/16	0.93	0.21	50,54,58,58	16
5	MG	B	363	1/1	0.93	0.19	45,45,45,45	0
3	ARG	A	363	11/12	0.94	0.17	43,47,54,59	0
2	SO4	D	358	5/5	0.94	0.15	66,72,79,87	0
2	SO4	E	361	5/5	0.94	0.13	58,58,61,62	5
2	SO4	E	360	5/5	0.95	0.28	67,79,84,93	0
3	ARG	C	361	11/12	0.95	0.15	45,53,58,61	0
2	SO4	C	359	5/5	0.96	0.27	48,59,71,80	0
2	SO4	A	361	5/5	0.96	0.23	40,61,64,74	0
2	SO4	C	358	5/5	0.96	0.13	47,47,58,67	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	SO4	E	359	5/5	0.97	0.19	53,58,66,75	0
5	MG	C	363	1/1	0.97	0.08	39,39,39,39	0
5	MG	D	365	1/1	0.97	0.06	52,52,52,52	0
2	SO4	A	360	5/5	0.97	0.15	42,45,52,64	0
2	SO4	B	359	5/5	0.97	0.19	40,45,60,62	0
2	SO4	D	357	5/5	0.98	0.12	40,45,53,64	0
2	SO4	A	359	5/5	0.98	0.10	43,47,62,67	0
2	SO4	B	358	5/5	0.98	0.21	38,51,59,69	0
5	MG	A	365	1/1	0.98	0.14	38,38,38,38	0
2	SO4	B	357	5/5	0.99	0.17	34,38,46,48	0
2	SO4	E	358	5/5	0.99	0.06	45,45,47,48	5
2	SO4	D	361	5/5	0.99	0.09	50,50,52,54	5
2	SO4	D	360	5/5	0.99	0.08	33,33,33,33	5
2	SO4	C	357	5/5	0.99	0.09	36,41,51,54	0
2	SO4	A	358	5/5	0.99	0.15	35,35,49,52	0
2	SO4	E	357	5/5	0.99	0.13	43,54,57,62	0
2	SO4	A	357	5/5	1.00	0.08	24,25,31,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.