



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:28 AM GMT

PDB ID : 3M2R
Title : Structural Insight into Methyl-Coenzyme M Reductase Chemistry using Coenzyme B Analogues
Authors : Cedervall, P.E.; Dey, M.; Ragsdale, S.W.; Wilmot, C.M.
Deposited on : 2010-03-08
Resolution : 1.30 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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

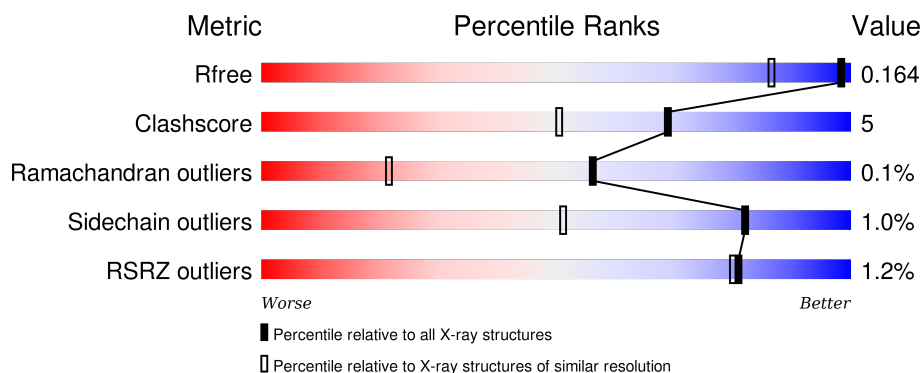
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.30 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}	91344	1475 (1.34-1.26)
Clashscore	102246	1031 (1.32-1.28)
Ramachandran outliers	100387	1504 (1.34-1.26)
Sidechain outliers	100360	1503 (1.34-1.26)
RSRZ outliers	91569	1476 (1.34-1.26)

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. 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	549	<div> <div>85%</div> <div>13%</div> <div>.</div> </div>
1	D	549	<div> <div>%</div> <div>83%</div> <div>15%</div> <div>.</div> </div>
2	B	442	<div> <div>83%</div> <div>15%</div> <div>.</div> </div>
2	E	442	<div> <div>%</div> <div>83%</div> <div>16%</div> <div>.</div> </div>
3	C	248	<div> <div>4%</div> <div>71%</div> <div>27%</div> <div>..</div> </div>

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Mol	Chain	Length	Quality of chain
3	F	248	

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	MG	C	250	-	-	-	X
4	MG	F	250	-	-	-	X
5	F43	A	1	X	-	-	-
5	F43	D	552	X	-	-	-
6	TP7	A	554[A]	X	-	-	-
6	TP7	D	553[A]	X	-	-	-
9	EDO	F	251	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 22783 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 Methyl-coenzyme M reductase I subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	29	0
			4438	2809	731	878	20			
1	D	548	Total	C	N	O	S	0	30	0
			4426	2813	730	863	20			

- Molecule 2 is a protein called Methyl-coenzyme M reductase I subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	442	Total	C	N	O	S	0	24	0
			3456	2205	559	670	22			
2	E	442	Total	C	N	O	S	0	31	0
			3509	2240	569	677	23			

- Molecule 3 is a protein called Methyl-coenzyme M reductase I subunit gamma.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	246	Total	C	N	O	S	0	20	0
			2135	1320	375	426	14			
3	F	246	Total	C	N	O	S	0	22	0
			2121	1316	371	419	15			

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

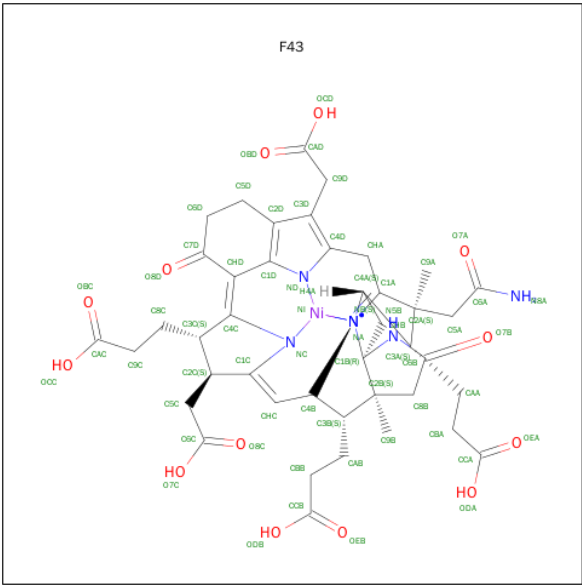
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	2	Total	Mg	0	0
			2	2		
4	E	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		

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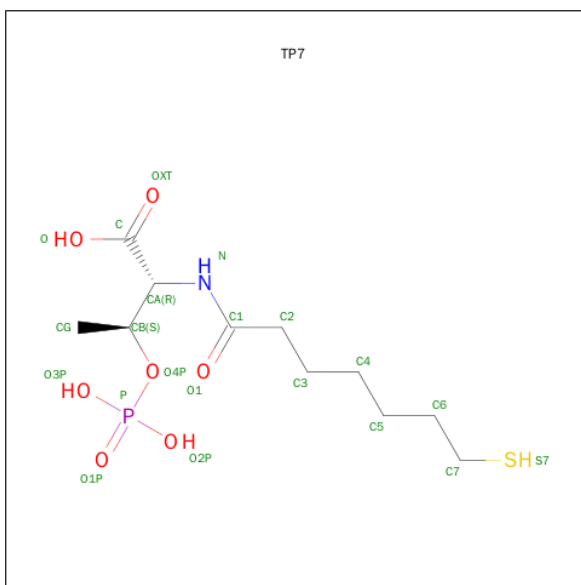
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	3	Total	Mg	0	2
			3	3		
4	F	1	Total	Mg	0	0
			1	1		

- Molecule 5 is FACTOR 430 (three-letter code: F43) (formula: C₄₂H₄₉N₆NiO₁₃).



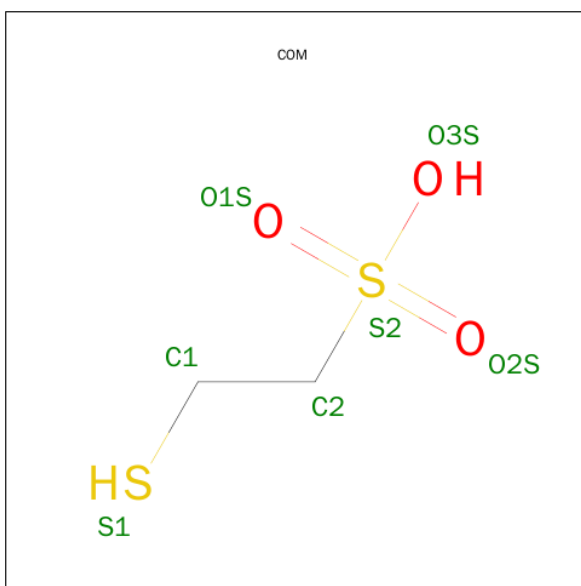
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		
5	D	1	Total	C	N	Ni	O	0	0
			62	42	6	1	13		

- Molecule 6 is COENZYME B (three-letter code: TP7) (formula: C₁₁H₂₂NO₇PS).



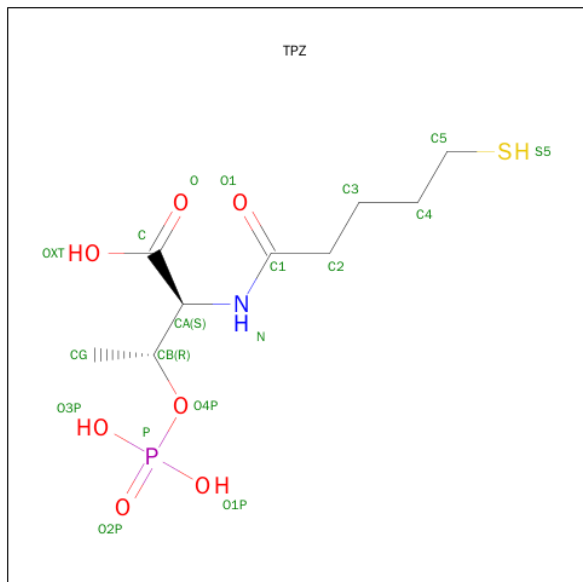
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		
6	D	1	Total	C	N	O	P	S	0	1
			21	11	1	7	1	1		

- Molecule 7 is 1-THIOETHANESULFONIC ACID (three-letter code: COM) (formula: $C_2H_6O_3S_2$).



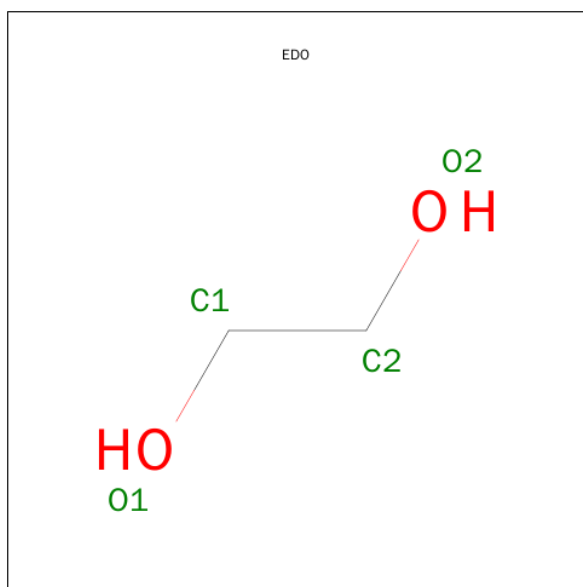
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	S	0	0
			7	2	3	2		
7	D	1	Total	C	O	S	0	0
			7	2	3	2		

- Molecule 8 is O-PHOSPHONO-N-(5-SULFANYLPENTANOYL)-L-THREONINE (three-letter code: TPZ) (formula: $C_9H_{18}NO_7PS$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	S	0	1
			19	9	1	7	1	1		
8	D	1	Total	C	N	O	P	S	0	1
			19	9	1	7	1	1		

- Molecule 9 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

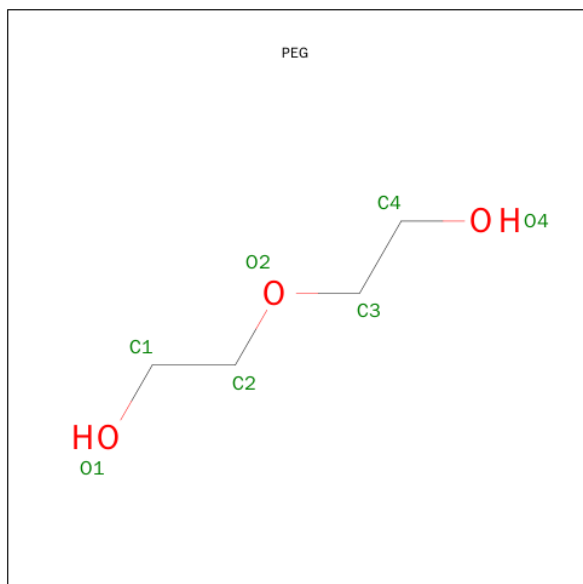


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			4	2	2		
9	C	1	Total	C	O	0	0
			4	2	2		
9	D	1	Total	C	O	0	0
			4	2	2		
9	F	1	Total	C	O	0	0
			4	2	2		
9	F	1	Total	C	O	0	0
			4	2	2		

- Molecule 10 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	1	Total	Zn	0	0
			1	1		

- Molecule 11 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

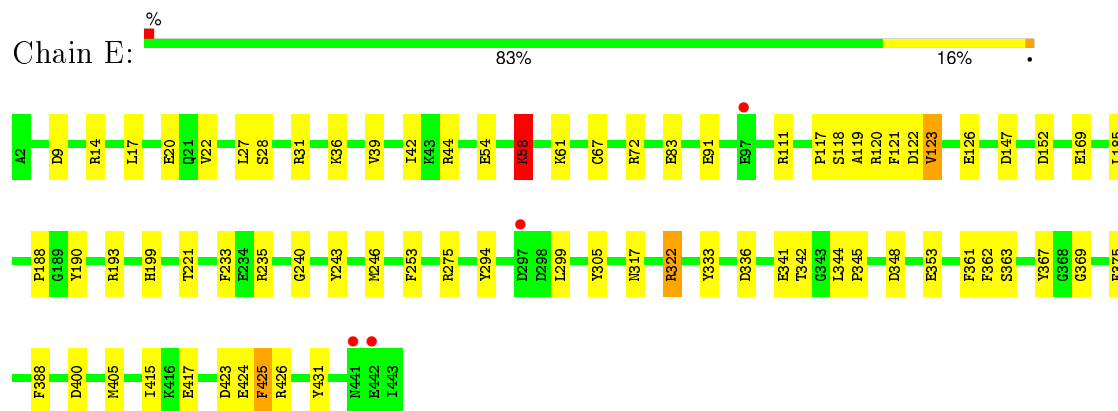


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	C	1	Total	C	O	0	0
			7	4	3		

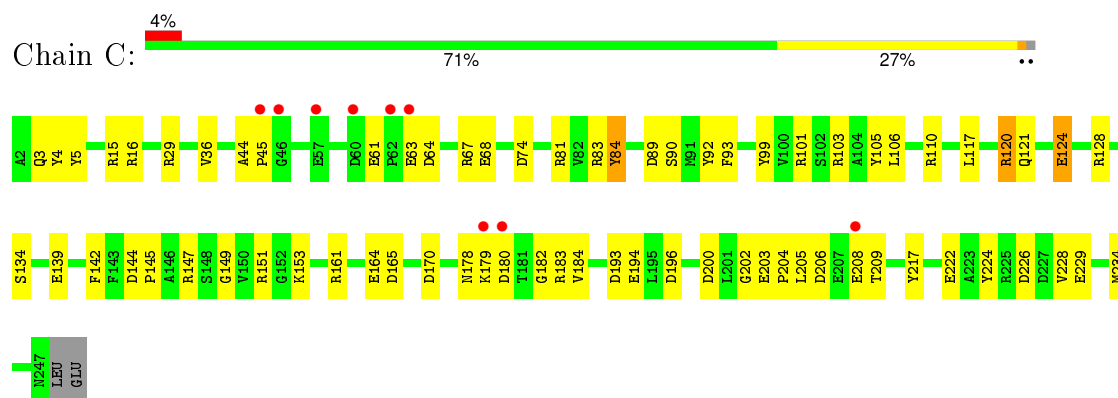
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	513	Total 520	O 520	0	18
12	B	451	Total 461	O 461	0	17
12	C	256	Total 259	O 259	0	5
12	D	520	Total 526	O 526	0	15
12	E	418	Total 423	O 423	0	16
12	F	250	Total 254	O 254	0	8

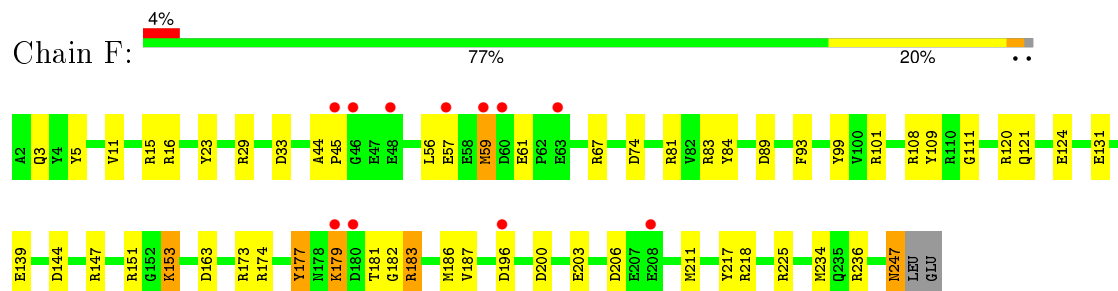
- Molecule 2: Methyl-coenzyme M reductase I subunit beta



- Molecule 3: Methyl-coenzyme M reductase I subunit gamma



- Molecule 3: Methyl-coenzyme M reductase I subunit gamma



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.02Å 118.26Å 122.39Å 90.00° 91.84° 90.00°	Depositor
Resolution (Å)	20.49 – 1.30 20.15 – 1.30	Depositor EDS
% Data completeness (in resolution range)	97.1 (20.49-1.30) 97.1 (20.15-1.30)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.14 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.5.0072	Depositor
R, R_{free}	0.143 , 0.166 0.142 , 0.164	Depositor DCC
R_{free} test set	27777 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	10.4	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 50.7	EDS
Estimated twinning fraction	0.000 for -h,l,k 0.006 for -h,-l,-k 0.012 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 553593 reflections (0.000%)	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	22783	wwPDB-VP
Average B, all atoms (Å ²)	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, PEG, COM, MG, F43, MGN, TP7, AGM, EDO, GL3, SMC, MHS, TPZ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.51	20/4536 (0.4%)	1.46	52/6160 (0.8%)
1	D	1.58	36/4544 (0.8%)	1.47	55/6168 (0.9%)
2	B	1.53	15/3573 (0.4%)	1.44	39/4834 (0.8%)
2	E	1.54	24/3632 (0.7%)	1.41	37/4910 (0.8%)
3	C	1.70	23/2194 (1.0%)	1.64	36/2952 (1.2%)
3	F	1.73	16/2203 (0.7%)	1.69	41/2962 (1.4%)
All	All	1.58	134/20682 (0.6%)	1.49	260/27986 (0.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	1	3
1	D	1	1
2	B	0	2
2	E	0	2
All	All	2	8

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	259	GLU	CG-CD	10.02	1.67	1.51
3	F	139	GLU	CD-OE2	9.89	1.36	1.25
1	D	355[A]	GLU	CB-CG	-9.43	1.34	1.52
1	D	355[B]	GLU	CB-CG	-9.43	1.34	1.52
2	E	353	GLU	CG-CD	9.28	1.65	1.51
1	D	386	GLU	CD-OE1	8.98	1.35	1.25
2	E	353	GLU	CD-OE1	-8.16	1.16	1.25
1	A	450	ASP	CA-CB	-8.00	1.36	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	269	VAL	CA-CB	7.96	1.71	1.54
1	A	259[A]	GLU	CD-OE1	-7.83	1.17	1.25
1	A	259[B]	GLU	CD-OE1	-7.83	1.17	1.25
1	D	543	ARG	CB-CG	7.39	1.72	1.52
2	B	353	GLU	CD-OE1	-7.31	1.17	1.25
3	C	124	GLU	CG-CD	7.12	1.62	1.51
1	D	450	ASP	CA-CB	-6.98	1.38	1.53
1	D	14	PHE	CD2-CE2	6.97	1.53	1.39
3	F	187	VAL	CB-CG1	6.93	1.67	1.52
2	B	278	GLU	CD-OE2	6.90	1.33	1.25
2	B	278	GLU	CG-CD	6.73	1.62	1.51
3	C	229	GLU	CD-OE1	-6.70	1.18	1.25
3	C	84	TYR	CD1-CE1	6.64	1.49	1.39
1	A	543	ARG	CB-CG	6.61	1.70	1.52
2	E	243	TYR	CE1-CZ	-6.43	1.30	1.38
2	E	22	VAL	CB-CG2	6.41	1.66	1.52
1	D	148	GLU	CD-OE2	6.35	1.32	1.25
3	F	23	TYR	CG-CD2	6.29	1.47	1.39
3	F	109	TYR	CE2-CZ	6.28	1.46	1.38
1	A	333	TYR	CG-CD1	6.26	1.47	1.39
3	F	11	VAL	CB-CG1	6.26	1.66	1.52
3	C	92	TYR	CE1-CZ	6.25	1.46	1.38
1	A	292	SER	CB-OG	6.21	1.50	1.42
3	C	93	PHE	CD2-CE2	6.18	1.51	1.39
1	A	119	ARG	CB-CG	-6.15	1.35	1.52
3	C	222	GLU	CG-CD	-6.12	1.42	1.51
3	F	177	TYR	CD1-CE1	6.12	1.48	1.39
2	E	243	TYR	CD2-CE2	6.12	1.48	1.39
1	D	469	GLU	CD-OE2	6.11	1.32	1.25
1	D	543	ARG	CG-CD	-6.10	1.36	1.51
3	C	90	SER	CB-OG	-6.09	1.34	1.42
1	D	380	TYR	CE2-CZ	6.01	1.46	1.38
2	B	278	GLU	CD-OE1	6.01	1.32	1.25
3	C	105	TYR	CE1-CZ	5.97	1.46	1.38
1	D	197	LYS	CD-CE	-5.97	1.36	1.51
3	F	124	GLU	CG-CD	5.97	1.60	1.51
1	D	269	VAL	CA-CB	5.93	1.67	1.54
3	C	153	LYS	CE-NZ	5.91	1.63	1.49
1	A	379	PHE	CD1-CE1	5.90	1.51	1.39
2	E	341	GLU	CD-OE2	5.88	1.32	1.25
1	A	171	GLU	CB-CG	5.87	1.63	1.52
2	B	440	LYS	CE-NZ	5.87	1.63	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	531	LYS	CE-NZ	5.84	1.63	1.49
3	C	142	PHE	CE2-CZ	5.83	1.48	1.37
2	E	117[A]	PRO	C-O	5.83	1.34	1.23
2	E	117[B]	PRO	C-O	5.83	1.34	1.23
1	D	538	GLU	CD-OE1	5.82	1.32	1.25
2	E	341	GLU	CD-OE1	-5.78	1.19	1.25
3	F	217	TYR	CG-CD1	5.78	1.46	1.39
3	C	3	GLN	CB-CG	-5.77	1.36	1.52
2	E	58	LYS	CB-CG	-5.74	1.37	1.52
3	C	139	GLU	CD-OE2	5.74	1.31	1.25
2	E	425	PHE	CD1-CE1	5.71	1.50	1.39
3	C	134	SER	CB-OG	5.70	1.49	1.42
3	F	139	GLU	CD-OE1	-5.66	1.19	1.25
2	E	417	GLU	CD-OE2	5.64	1.31	1.25
2	E	240	GLY	N-CA	5.63	1.54	1.46
2	E	253	PHE	CD1-CE1	5.63	1.50	1.39
1	A	4	LYS	CD-CE	5.61	1.65	1.51
2	E	28	SER	CB-OG	5.59	1.49	1.42
1	D	294	ARG	CZ-NH1	5.57	1.40	1.33
1	A	20	GLU	CD-OE1	-5.56	1.19	1.25
1	D	209	ARG	CB-CG	5.56	1.67	1.52
2	B	442	GLU	CD-OE1	5.56	1.31	1.25
2	B	120	ARG	CZ-NH1	5.55	1.40	1.33
1	D	80	TYR	CD1-CE1	5.54	1.47	1.39
1	D	352[A]	GLU	CD-OE1	5.53	1.31	1.25
1	D	352[B]	GLU	CD-OE1	5.53	1.31	1.25
1	D	416	ALA	C-O	5.52	1.33	1.23
2	E	363	SER	CB-OG	5.50	1.49	1.42
3	C	208	GLU	CG-CD	5.49	1.60	1.51
1	D	538	GLU	CD-OE2	5.49	1.31	1.25
1	A	297	TYR	CB-CG	-5.48	1.43	1.51
2	E	233[A]	PHE	CD1-CE1	5.48	1.50	1.39
2	E	233[B]	PHE	CD1-CE1	5.48	1.50	1.39
2	E	235	ARG	CZ-NH2	5.46	1.40	1.33
1	A	542	GLU	CB-CG	5.46	1.62	1.52
2	B	58	LYS	CB-CG	-5.45	1.37	1.52
2	B	274[A]	GLU	CG-CD	5.45	1.60	1.51
2	B	274[B]	GLU	CG-CD	5.45	1.60	1.51
1	D	542	GLU	CD-OE1	-5.44	1.19	1.25
2	E	123[A]	VAL	CB-CG2	-5.44	1.41	1.52
2	E	123[B]	VAL	CB-CG2	-5.44	1.41	1.52
2	B	243	TYR	CD2-CE2	5.43	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	30	GLY	N-CA	5.43	1.54	1.46
1	D	129	ILE	CA-CB	-5.42	1.42	1.54
3	C	164	GLU	CD-OE2	5.40	1.31	1.25
1	D	528	GLU	CG-CD	-5.39	1.43	1.51
3	F	93	PHE	CD2-CE2	5.38	1.50	1.39
1	D	458	PHE	CG-CD2	5.37	1.46	1.38
1	A	72	TYR	CE2-CZ	5.35	1.45	1.38
2	B	8	VAL	CA-CB	5.34	1.66	1.54
1	A	238	ALA	C-O	5.34	1.33	1.23
1	D	11	LYS	CE-NZ	5.32	1.62	1.49
2	B	426	ARG	CZ-NH2	5.32	1.40	1.33
1	D	237	SER	C-O	5.31	1.33	1.23
3	C	149	GLY	C-O	5.28	1.32	1.23
2	E	169	GLU	CG-CD	-5.28	1.44	1.51
3	F	5	TYR	CG-CD1	5.28	1.46	1.39
1	D	242	ALA	CA-CB	5.27	1.63	1.52
1	D	117	GLU	CD-OE2	5.24	1.31	1.25
1	D	123	GLU	CG-CD	5.24	1.59	1.51
3	F	147	ARG	CZ-NH2	5.21	1.39	1.33
1	D	266	TYR	CE1-CZ	-5.20	1.31	1.38
1	D	175	GLU	CB-CG	5.19	1.62	1.52
3	F	218	ARG	CZ-NH1	5.19	1.39	1.33
2	B	322	ARG	CZ-NH1	5.18	1.39	1.33
3	F	247	ASN	CG-OD1	5.18	1.35	1.24
3	C	4	TYR	CB-CG	-5.18	1.43	1.51
1	D	114	ALA	CA-CB	-5.15	1.41	1.52
3	C	81	ARG	CG-CD	5.12	1.64	1.51
3	C	99	TYR	CD2-CE2	5.09	1.47	1.39
2	E	54	GLU	CB-CG	5.09	1.61	1.52
1	D	393	GLU	CG-CD	5.07	1.59	1.51
3	C	36	VAL	CB-CG1	5.07	1.63	1.52
1	A	379	PHE	CG-CD2	5.06	1.46	1.38
3	C	228	VAL	CA-CB	5.06	1.65	1.54
3	C	217	TYR	CE2-CZ	5.05	1.45	1.38
2	E	431	TYR	CG-CD1	5.04	1.45	1.39
3	F	101	ARG	NE-CZ	5.04	1.39	1.33
1	A	34	SER	CA-CB	5.04	1.60	1.52
1	A	487	GLU	CD-OE2	5.03	1.31	1.25
3	F	3	GLN	CB-CG	-5.03	1.39	1.52
2	B	240	GLY	N-CA	5.03	1.53	1.46
1	A	239	TYR	CE2-CZ	5.02	1.45	1.38
3	C	204	PRO	N-CA	5.02	1.55	1.47

All (260) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	44	ARG	NE-CZ-NH1	18.56	129.58	120.30
3	C	147	ARG	NE-CZ-NH1	14.70	127.65	120.30
3	F	147	ARG	NE-CZ-NH1	13.38	126.99	120.30
3	F	206	ASP	CB-CG-OD1	12.76	129.78	118.30
3	C	120	ARG	NE-CZ-NH1	12.10	126.35	120.30
1	A	103	ARG	NE-CZ-NH2	-12.09	114.25	120.30
2	E	353	GLU	OE1-CD-OE2	12.06	137.77	123.30
3	C	151	ARG	NE-CZ-NH1	11.96	126.28	120.30
2	E	426	ARG	NE-CZ-NH1	11.76	126.18	120.30
3	F	144	ASP	CB-CG-OD2	11.69	128.82	118.30
2	B	44	ARG	NE-CZ-NH2	-11.62	114.49	120.30
3	C	101	ARG	NE-CZ-NH2	-11.28	114.66	120.30
1	A	209	ARG	NE-CZ-NH2	-11.14	114.73	120.30
3	C	144	ASP	CB-CG-OD2	11.13	128.32	118.30
3	C	120	ARG	NE-CZ-NH2	-10.78	114.91	120.30
1	A	401	ARG	NE-CZ-NH2	10.64	125.62	120.30
1	D	40	PHE	CB-CG-CD2	-10.31	113.58	120.80
2	E	9	ASP	CB-CG-OD2	-10.31	109.02	118.30
1	A	535	ARG	NE-CZ-NH2	10.24	125.42	120.30
2	B	196	MET	CG-SD-CE	-10.23	83.83	100.20
3	F	147	ARG	NE-CZ-NH2	-10.16	115.22	120.30
3	C	193	ASP	CB-CG-OD2	-9.92	109.37	118.30
1	D	67	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	D	202	ASP	CB-CG-OD1	9.73	127.06	118.30
1	D	499	ARG	NE-CZ-NH2	-9.60	115.50	120.30
3	F	120	ARG	NE-CZ-NH2	-9.58	115.51	120.30
2	B	353	GLU	OE1-CD-OE2	9.38	134.55	123.30
1	A	209	ARG	NE-CZ-NH1	9.25	124.92	120.30
2	E	185	LEU	CB-CG-CD1	9.21	126.65	111.00
3	F	225	ARG	NE-CZ-NH2	-8.96	115.82	120.30
1	A	535	ARG	NE-CZ-NH1	-8.88	115.86	120.30
3	C	165	ASP	CB-CG-OD1	-8.79	110.39	118.30
3	C	196	ASP	CB-CG-OD1	8.78	126.20	118.30
1	A	521	ASP	CB-CG-OD1	8.74	126.16	118.30
3	F	15	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	D	368	ASP	CB-CG-OD2	-8.70	110.47	118.30
2	B	31	ARG	NE-CZ-NH2	-8.51	116.04	120.30
3	F	108	ARG	NE-CZ-NH2	-8.48	116.06	120.30
3	F	101	ARG	NE-CZ-NH2	-8.39	116.11	120.30
2	E	147	ASP	CB-CG-OD1	8.38	125.84	118.30
2	B	31	ARG	NE-CZ-NH1	8.36	124.48	120.30
3	C	110	ARG	NE-CZ-NH2	-8.32	116.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	259	GLU	OE1-CD-OE2	8.29	133.25	123.30
3	F	177	TYR	O-C-N	8.26	135.91	122.70
2	E	111	ARG	NE-CZ-NH1	8.13	124.36	120.30
2	B	185	LEU	CB-CG-CD1	8.11	124.79	111.00
3	C	74	ASP	CB-CG-OD1	8.11	125.59	118.30
1	A	526	ARG	NE-CZ-NH2	-8.09	116.25	120.30
2	E	400	ASP	CB-CG-OD2	8.06	125.55	118.30
2	B	77	ASP	CB-CG-OD2	-8.05	111.05	118.30
2	E	336	ASP	CB-CG-OD1	8.04	125.53	118.30
1	A	67	ARG	NE-CZ-NH1	-7.97	116.31	120.30
1	A	346	PHE	CB-CG-CD1	7.93	126.36	120.80
2	E	44	ARG	NE-CZ-NH1	7.91	124.25	120.30
3	F	120	ARG	NE-CZ-NH1	7.83	124.21	120.30
2	E	322[A]	ARG	NE-CZ-NH1	7.80	124.20	120.30
2	E	322[B]	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	D	285	TYR	CB-CG-CD2	-7.79	116.33	121.00
3	C	15	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	444	TYR	CB-CG-CD1	7.62	125.57	121.00
1	D	471	ARG	NE-CZ-NH2	-7.61	116.49	120.30
2	E	423	ASP	CB-CG-OD1	7.59	125.14	118.30
3	F	196	ASP	CB-CG-OD1	7.58	125.12	118.30
1	D	478	TYR	CB-CG-CD1	7.52	125.51	121.00
1	A	60	ILE	C-N-CA	-7.49	106.57	122.30
1	D	444	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	D	59	ASP	CB-CG-OD1	7.37	124.94	118.30
2	B	353	GLU	CG-CD-OE2	-7.22	103.86	118.30
3	F	33	ASP	CB-CG-OD1	7.21	124.79	118.30
3	C	206	ASP	CB-CG-OD1	7.19	124.77	118.30
1	D	440	ARG	NE-CZ-NH1	7.18	123.89	120.30
3	C	16	ARG	NE-CZ-NH1	7.15	123.88	120.30
2	B	305	TYR	CD1-CE1-CZ	-7.14	113.37	119.80
3	F	16	ARG	NE-CZ-NH1	7.14	123.87	120.30
3	F	5	TYR	CB-CG-CD1	-7.13	116.72	121.00
3	F	29	ARG	NE-CZ-NH1	7.13	123.86	120.30
3	F	74	ASP	CB-CG-OD1	7.12	124.71	118.30
3	F	173	ARG	NE-CZ-NH1	-7.09	116.76	120.30
1	D	346	PHE	CB-CG-CD2	-7.08	115.85	120.80
1	D	67	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	A	499	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	D	471	ARG	NE-CZ-NH1	7.03	123.81	120.30
1	A	36	ARG	NE-CZ-NH2	6.99	123.80	120.30
1	A	471	ARG	NE-CZ-NH2	-6.99	116.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	144	ASP	CB-CG-OD1	-6.98	112.02	118.30
2	B	322	ARG	NE-CZ-NH1	6.93	123.76	120.30
2	B	72	ARG	NE-CZ-NH2	-6.83	116.88	120.30
1	A	450	ASP	CB-CA-C	6.82	124.05	110.40
1	D	103	ARG	NE-CZ-NH1	6.80	123.70	120.30
1	A	346	PHE	CB-CG-CD2	-6.80	116.04	120.80
3	C	92	TYR	CZ-CE2-CD2	6.79	125.91	119.80
3	C	200	ASP	CB-CG-OD2	-6.77	112.21	118.30
1	A	270	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	A	202	ASP	CB-CG-OD2	-6.71	112.26	118.30
2	E	305	TYR	CD1-CE1-CZ	-6.70	113.77	119.80
1	D	103	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	A	542	GLU	OE1-CD-OE2	-6.69	115.27	123.30
3	C	101	ARG	NH1-CZ-NH2	6.63	126.70	119.40
2	E	348	ASP	CB-CG-OD1	6.63	124.27	118.30
1	D	188	PHE	CB-CG-CD2	-6.59	116.18	120.80
1	A	356	ASP	CB-CG-OD1	-6.56	112.40	118.30
2	B	193	ARG	NE-CZ-NH1	6.53	123.56	120.30
1	D	526	ARG	NE-CZ-NH2	-6.53	117.04	120.30
1	A	119	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	D	528	GLU	OE1-CD-OE2	-6.49	115.51	123.30
1	D	499	ARG	NH1-CZ-NH2	6.41	126.45	119.40
1	A	59	ASP	CB-CG-OD1	6.41	124.06	118.30
3	F	218	ARG	NE-CZ-NH2	6.40	123.50	120.30
2	B	75	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	436	GLU	OE1-CD-OE2	-6.37	115.66	123.30
3	F	131	GLU	OE1-CD-OE2	6.34	130.91	123.30
3	F	217	TYR	CB-CG-CD2	6.34	124.80	121.00
2	E	275	ARG	NE-CZ-NH2	-6.27	117.16	120.30
3	C	161	ARG	NE-CZ-NH2	-6.26	117.17	120.30
2	E	243	TYR	CZ-CE2-CD2	-6.23	114.20	119.80
1	A	40	PHE	CB-CG-CD2	-6.22	116.44	120.80
2	B	152	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	A	85	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	D	40	PHE	CB-CG-CD1	6.19	125.13	120.80
1	A	461	ARG	NE-CZ-NH1	6.17	123.39	120.30
1	A	270	ARG	NE-CZ-NH2	-6.16	117.22	120.30
3	C	29	ARG	NE-CZ-NH2	-6.15	117.23	120.30
2	E	305	TYR	CB-CG-CD2	-6.15	117.31	121.00
3	C	103	ARG	NE-CZ-NH1	6.13	123.37	120.30
3	C	147	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	D	478	TYR	CB-CG-CD2	-6.09	117.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	372	ASP	CB-CG-OD2	6.08	123.78	118.30
2	B	297[A]	ASP	CB-CG-OD2	6.06	123.76	118.30
2	B	297[B]	ASP	CB-CG-OD2	6.06	123.76	118.30
1	D	302	ARG	NE-CZ-NH1	-6.06	117.27	120.30
3	F	101	ARG	NH1-CZ-NH2	6.05	126.05	119.40
1	D	299	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	A	368	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	D	545	LEU	CB-CG-CD2	-6.04	100.73	111.00
1	A	225	ARG	NE-CZ-NH2	-6.03	117.28	120.30
3	C	224	TYR	CG-CD2-CE2	-6.03	116.48	121.30
2	E	31	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	A	521	ASP	CB-CG-OD2	-5.97	112.93	118.30
1	D	522	PHE	CB-CG-CD1	-5.97	116.62	120.80
1	A	333	TYR	CG-CD1-CE1	-5.95	116.54	121.30
1	D	450	ASP	CB-CA-C	5.94	122.29	110.40
1	A	80	TYR	CD1-CE1-CZ	-5.94	114.45	119.80
3	F	59	MET	CG-SD-CE	-5.93	90.72	100.20
1	D	119	ARG	CG-CD-NE	-5.92	99.36	111.80
3	C	165	ASP	CB-CG-OD2	5.91	123.62	118.30
3	C	84	TYR	CD1-CE1-CZ	-5.91	114.48	119.80
2	B	147	ASP	CB-CG-OD1	5.90	123.61	118.30
1	A	444	TYR	CD1-CE1-CZ	-5.90	114.49	119.80
1	D	344	ASP	CB-CG-OD1	-5.90	112.99	118.30
2	B	359	PHE	CB-CG-CD1	5.89	124.92	120.80
3	F	177	TYR	CA-C-N	-5.88	104.26	117.20
3	F	183[A]	ARG	N-CA-CB	-5.87	100.04	110.60
3	F	183[B]	ARG	N-CA-CB	-5.87	100.04	110.60
3	C	128	ARG	NE-CZ-NH1	-5.87	117.37	120.30
3	F	153[A]	LYS	CD-CE-NZ	-5.86	98.22	111.70
3	F	153[B]	LYS	CD-CE-NZ	-5.86	98.22	111.70
2	B	111	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	B	426	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	F	151	ARG	CG-CD-NE	-5.85	99.52	111.80
1	A	10	LEU	O-C-N	5.82	132.00	122.70
3	F	174	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	D	84	ASP	CB-CG-OD2	5.79	123.51	118.30
3	F	163	ASP	CB-CG-OD1	5.78	123.51	118.30
3	F	236	ARG	NE-CZ-NH1	-5.77	117.42	120.30
1	A	183	ASP	CB-CG-OD2	-5.77	113.11	118.30
2	E	361	PHE	CB-CG-CD2	-5.75	116.78	120.80
3	C	83	ARG	NE-CZ-NH2	-5.74	117.43	120.30
2	E	147	ASP	CB-CG-OD2	-5.74	113.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177[A]	ASP	CB-CG-OD1	5.72	123.45	118.30
1	A	177[B]	ASP	CB-CG-OD1	5.72	123.45	118.30
3	F	74	ASP	CB-CG-OD2	-5.72	113.15	118.30
2	B	291	TYR	CD1-CE1-CZ	-5.71	114.66	119.80
1	A	285	TYR	CB-CG-CD1	5.71	124.42	121.00
2	E	152	ASP	CB-CG-OD2	-5.68	113.18	118.30
1	D	216	ARG	NE-CZ-NH1	5.68	123.14	120.30
3	F	177	TYR	CD1-CE1-CZ	-5.67	114.69	119.80
1	A	12[A]	LYS	CD-CE-NZ	5.67	124.75	111.70
1	A	12[B]	LYS	CD-CE-NZ	5.67	124.75	111.70
2	B	12	ASP	CB-CG-OD2	-5.66	113.21	118.30
3	C	5	TYR	CZ-CE2-CD2	-5.64	114.72	119.80
2	E	193	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	B	423	ASP	CB-CG-OD2	-5.64	113.22	118.30
1	D	368	ASP	CB-CG-OD1	5.64	123.37	118.30
1	A	78	ASP	CB-CG-OD2	-5.63	113.23	118.30
3	F	217	TYR	CG-CD2-CE2	5.63	125.81	121.30
1	D	4	LYS	CA-CB-CG	5.63	125.79	113.40
1	D	175	GLU	OE1-CD-OE2	5.63	130.05	123.30
3	C	226	ASP	CB-CG-OD1	5.62	123.36	118.30
1	D	543	ARG	NE-CZ-NH1	5.62	123.11	120.30
3	C	99	TYR	CG-CD2-CE2	-5.61	116.81	121.30
3	C	83	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	B	333	TYR	CD1-CE1-CZ	-5.57	114.79	119.80
1	D	188	PHE	CG-CD2-CE2	-5.57	114.67	120.80
2	E	426	ARG	NH1-CZ-NH2	-5.56	113.28	119.40
2	B	333	TYR	CG-CD2-CE2	-5.55	116.86	121.30
3	C	89	ASP	CB-CG-OD1	5.53	123.28	118.30
1	D	105[A]	VAL	CG1-CB-CG2	5.53	119.75	110.90
1	D	105[B]	VAL	CG1-CB-CG2	5.53	119.75	110.90
1	A	84	ASP	CB-CG-OD1	-5.53	113.33	118.30
2	E	294	TYR	CB-CG-CD2	-5.49	117.71	121.00
1	D	60[A]	ILE	CA-CB-CG1	-5.48	100.58	111.00
1	D	60[B]	ILE	CA-CB-CG1	-5.48	100.58	111.00
2	E	423	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	D	501	ASP	CB-CG-OD2	5.47	123.22	118.30
2	B	305	TYR	CE1-CZ-CE2	5.46	128.53	119.80
3	F	56	LEU	CB-CG-CD1	-5.46	101.72	111.00
1	A	478	TYR	CB-CG-CD2	-5.45	117.73	121.00
3	C	15	ARG	NH1-CZ-NH2	5.44	125.38	119.40
1	D	285	TYR	CB-CG-CD1	5.44	124.26	121.00
3	C	170	ASP	CB-CG-OD2	5.43	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	261[A]	LYS	CD-CE-NZ	-5.42	99.23	111.70
2	B	261[B]	LYS	CD-CE-NZ	-5.42	99.23	111.70
1	D	450	ASP	N-CA-CB	5.42	120.36	110.60
2	B	99	ASP	CB-CG-OD2	-5.42	113.43	118.30
1	D	444	TYR	CB-CG-CD1	5.41	124.24	121.00
1	A	444	TYR	CB-CG-CD2	-5.40	117.76	121.00
3	C	224	TYR	CB-CG-CD2	-5.38	117.77	121.00
2	B	15	GLY	O-C-N	5.38	131.31	122.70
1	D	209	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	E	126	GLU	CB-CA-C	5.36	121.12	110.40
1	D	51	ARG	NE-CZ-NH1	-5.33	117.64	120.30
2	E	375	PHE	CB-CG-CD2	5.32	124.52	120.80
2	E	367	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	A	238	ALA	CA-C-N	5.31	128.87	117.20
2	B	54	GLU	OE1-CD-OE2	5.30	129.67	123.30
2	E	121	PHE	CB-CG-CD1	-5.30	117.09	120.80
1	D	542	GLU	OE1-CD-OE2	-5.29	116.96	123.30
1	D	393	GLU	OE1-CD-OE2	5.26	129.61	123.30
2	E	425	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	D	338	TYR	CZ-CE2-CD2	-5.25	115.08	119.80
2	E	190	TYR	CD1-CE1-CZ	-5.25	115.08	119.80
1	A	450	ASP	N-CA-CB	5.24	120.02	110.60
2	B	434	GLU	O-C-N	-5.23	114.33	122.70
1	A	346	PHE	CD1-CE1-CZ	5.22	126.37	120.10
3	F	99	TYR	CE1-CZ-CE2	5.22	128.15	119.80
1	D	242	ALA	CB-CA-C	-5.21	102.28	110.10
2	B	3	LYS	CD-CE-NZ	-5.20	99.73	111.70
3	F	81	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	A	70	MET	CB-CA-C	-5.18	100.05	110.40
3	C	74	ASP	CB-CG-OD2	-5.17	113.65	118.30
2	B	14[A]	ARG	NE-CZ-NH1	-5.17	117.72	120.30
2	B	14[B]	ARG	NE-CZ-NH1	-5.17	117.72	120.30
1	A	215	SER	N-CA-CB	-5.15	102.77	110.50
2	E	120[A]	ARG	NE-CZ-NH1	5.15	122.87	120.30
2	E	120[B]	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	A	202	ASP	CB-CG-OD1	5.14	122.92	118.30
2	B	180	ASP	CB-CG-OD2	-5.13	113.68	118.30
3	F	83	ARG	O-C-N	5.12	130.89	122.70
1	D	346	PHE	CB-CG-CD1	5.11	124.38	120.80
1	D	209	ARG	NE-CZ-NH2	-5.11	117.74	120.30
1	A	543	ARG	CA-CB-CG	5.08	124.58	113.40
2	E	388	PHE	CZ-CE2-CD2	-5.08	114.00	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	353	GLU	CG-CD-OE2	-5.08	108.14	118.30
2	E	14	ARG	NE-CZ-NH2	5.05	122.82	120.30
3	C	103	ARG	NE-CZ-NH2	-5.04	117.78	120.30
3	F	89	ASP	CB-CG-OD2	5.03	122.83	118.30
2	B	419	PHE	CB-CG-CD2	-5.01	117.29	120.80
2	B	290	ASP	CB-CG-OD1	-5.01	113.79	118.30
1	D	401	ARG	NE-CZ-NH2	-5.01	117.80	120.30
2	E	299	LEU	CB-CG-CD1	-5.00	102.49	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	450	ASP	CA
1	D	450	ASP	CA

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	480	MET	Peptide
1	A	499	ARG	Sidechain
1	A	51	ARG	Sidechain
2	B	333	TYR	Sidechain
2	B	72	ARG	Sidechain
1	D	51	ARG	Sidechain
2	E	333	TYR	Sidechain
2	E	72	ARG	Sidechain

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	4438	0	4236	43	0
1	D	4426	0	4281	34	0
2	B	3456	0	3501	36	0
2	E	3509	0	3569	33	0
3	C	2135	0	2060	35	0
3	F	2121	0	2081	34	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	3	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	62	0	43	1	0
5	D	62	0	43	1	0
6	A	21	0	19	1	0
6	D	21	0	19	1	0
7	A	7	0	4	0	0
7	D	7	0	5	0	0
8	A	19	0	15	0	0
8	D	19	0	15	0	0
9	A	4	0	6	0	0
9	C	4	0	6	0	0
9	D	4	0	6	0	0
9	F	8	0	12	1	0
10	A	1	0	0	0	0
11	C	7	0	10	0	0
12	A	520	0	0	14	0
12	B	461	0	0	5	0
12	C	259	0	0	9	0
12	D	526	0	0	7	0
12	E	423	0	0	14	0
12	F	254	0	0	5	0
All	All	22783	0	19931	185	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 5.

All (185) 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)
3:F:181[A]:THR:HB	3:F:183[A]:ARG:CD	1.70	1.20
2:E:91[B]:GLU:HG2	12:E:3974:HOH:O	1.43	1.17
3:F:181[A]:THR:HB	3:F:183[A]:ARG:CG	1.85	1.05
3:F:181[A]:THR:CB	3:F:183[A]:ARG:HG3	1.92	0.99
1:D:24[A]:THR:HG23	12:F:1497:HOH:O	1.65	0.96
1:A:24[A]:THR:HG23	12:C:3803:HOH:O	1.64	0.96
1:A:352[A]:GLU:HG2	12:A:4100:HOH:O	1.65	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:TYR:HB2	3:C:234[B]:MET:CE	1.98	0.94
1:A:433:LEU:HD23	3:C:234[B]:MET:SD	2.08	0.94
2:B:61:LYS:HE3	12:B:2541:HOH:O	1.69	0.93
3:F:181[A]:THR:HB	3:F:183[A]:ARG:HG3	1.46	0.92
1:A:432:TYR:HB2	3:C:234[B]:MET:HE3	1.50	0.92
3:F:181[A]:THR:OG1	3:F:183[A]:ARG:HB2	1.69	0.90
3:C:124:GLU:HG3	12:C:4090:HOH:O	1.70	0.90
1:D:241[B]:GLN:HE21	1:D:241[B]:GLN:H	1.16	0.89
1:A:433:LEU:CD2	3:C:234[B]:MET:SD	2.62	0.88
3:F:181[A]:THR:HB	3:F:183[A]:ARG:HD3	1.56	0.87
3:F:181[A]:THR:C	3:F:183[A]:ARG:HG3	1.95	0.87
1:A:169[A]:ASN:ND2	1:A:172:ILE:HD12	1.91	0.86
3:F:181[A]:THR:CB	3:F:183[A]:ARG:CG	2.50	0.85
1:D:432:TYR:HB2	3:F:234[B]:MET:HE3	1.60	0.82
3:F:181[A]:THR:CB	3:F:183[A]:ARG:CD	2.57	0.82
2:B:27:LEU:HD22	2:B:246[B]:MET:CE	2.10	0.81
1:A:429:LEU:HD12	3:C:234[B]:MET:CE	2.12	0.79
1:D:433:LEU:HD23	3:F:234[B]:MET:SD	2.22	0.79
1:D:46[B]:GLU:HG3	12:D:695:HOH:O	1.81	0.79
2:B:27:LEU:HD22	2:B:246[B]:MET:HE1	1.65	0.79
2:E:61[A]:LYS:HE3	12:E:2470:HOH:O	1.83	0.79
2:E:17:LEU:HD21	2:E:20[A]:GLU:HG3	1.66	0.77
1:D:194[B]:GLU:HG2	12:D:3701:HOH:O	1.86	0.76
12:A:3768:HOH:O	1:D:545:LEU:HD11	1.86	0.75
3:F:181[A]:THR:CB	3:F:183[A]:ARG:HD3	2.17	0.74
1:D:433:LEU:CD2	3:F:234[B]:MET:SD	2.75	0.74
1:A:178[A]:PRO:HD3	12:A:1631:HOH:O	1.88	0.74
2:B:261[A]:LYS:HG3	2:B:262:GLU:HG3	1.70	0.73
2:E:58:LYS:HE3	12:E:3968:HOH:O	1.85	0.73
2:E:27:LEU:HD22	2:E:246[B]:MET:SD	2.30	0.71
3:F:181[A]:THR:OG1	3:F:183[A]:ARG:CB	2.38	0.71
1:D:268:PRO:HB3	12:E:1668:HOH:O	1.92	0.70
1:A:130:THR:CG2	12:A:3696[B]:HOH:O	2.40	0.70
2:B:37[B]:SER:HB3	2:B:424[B]:GLU:OE1	1.91	0.70
1:A:432:TYR:CB	3:C:234[B]:MET:HE2	2.22	0.69
1:A:268:PRO:HG3	12:A:4030:HOH:O	1.91	0.69
1:A:194[B]:GLU:HG2	12:A:2095:HOH:O	1.92	0.69
1:A:429:LEU:HD12	3:C:234[B]:MET:HE1	1.73	0.69
2:E:118[B]:SER:HB3	12:E:2658:HOH:O	1.93	0.68
2:E:27:LEU:HD22	2:E:246[B]:MET:CE	2.22	0.68
1:A:432:TYR:HB2	3:C:234[B]:MET:HE2	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:200[A]:ASP:HB2	12:F:1920:HOH:O	1.94	0.67
2:B:27:LEU:CD2	2:B:246[B]:MET:HE1	2.24	0.67
1:D:241[B]:GLN:NE2	1:D:241[B]:GLN:H	1.92	0.66
1:D:42[A]:ASN:ND2	12:D:1802:HOH:O	2.27	0.66
1:A:12[B]:LYS:HG2	12:A:1449:HOH:O	1.95	0.65
2:E:83[A]:GLU:CG	12:E:3720:HOH:O	2.45	0.65
1:A:114:ALA:O	1:A:118:LYS:HD3	1.97	0.65
1:A:429:LEU:CD1	3:C:234[B]:MET:HE1	2.26	0.65
1:A:169[A]:ASN:HD22	1:A:172:ILE:HD12	1.63	0.64
3:F:181[A]:THR:HB	3:F:183[A]:ARG:HD2	1.74	0.64
2:E:61[B]:LYS:CE	12:E:2444:HOH:O	2.46	0.64
1:A:130:THR:HG23	12:A:3696[B]:HOH:O	1.97	0.64
1:D:36[A]:ARG:HD3	1:D:85:ASP:OD1	1.99	0.62
12:B:2205:HOH:O	2:E:188:PRO:HD3	1.99	0.62
1:A:429:LEU:HD12	3:C:234[B]:MET:HE3	1.80	0.61
2:E:122[B]:ASP:HB2	12:E:1158:HOH:O	2.00	0.61
3:F:177:TYR:CE2	3:F:179[A]:LYS:HG2	2.36	0.61
3:F:177:TYR:HE2	3:F:179[A]:LYS:HG2	1.66	0.60
2:E:61[B]:LYS:NZ	12:E:2444:HOH:O	2.27	0.60
2:B:246[A]:MET:CE	2:B:429:LEU:HD12	2.31	0.60
3:F:181[A]:THR:O	3:F:183[A]:ARG:HG3	2.02	0.59
2:E:27:LEU:HD22	2:E:246[B]:MET:HE1	1.85	0.59
2:B:27:LEU:CD2	2:B:246[B]:MET:CE	2.80	0.59
3:F:181[A]:THR:OG1	3:F:183[A]:ARG:CG	2.51	0.58
1:A:432:TYR:CB	3:C:234[B]:MET:CE	2.74	0.58
3:C:64[B]:ASP:HB2	12:C:3620:HOH:O	2.03	0.58
1:A:24[A]:THR:CG2	12:C:3803:HOH:O	2.32	0.58
1:A:60:ILE:HD12	12:D:3878:HOH:O	2.03	0.58
3:F:44:ALA:HB1	3:F:45:PRO:HD2	1.88	0.56
1:D:169:ASN:OD1	1:D:172[A]:ILE:HG13	2.06	0.56
3:C:67[B]:ARG:HH11	3:C:67[B]:ARG:HG3	1.72	0.55
2:B:299:LEU:HD21	12:C:1043:HOH:O	2.06	0.54
2:B:188:PRO:HD3	12:E:1304:HOH:O	2.07	0.54
1:D:169:ASN:CG	1:D:172[A]:ILE:HG13	2.27	0.54
1:A:383[A]:GLU:HG3	12:A:2606:HOH:O	2.07	0.53
2:B:246[A]:MET:HE3	2:B:429:LEU:HD12	1.90	0.53
2:B:3:LYS:HE2	2:B:234:GLU:OE1	2.08	0.53
2:B:424[A]:GLU:HG3	12:B:3930:HOH:O	2.08	0.53
1:A:17[A]:SER:OG	1:A:20:GLU:HG3	2.09	0.53
3:C:64[A]:ASP:HB3	3:C:67[A]:ARG:HB3	1.90	0.53
3:F:182[A]:GLY:O	3:F:203:GLU:HG2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:LEU:CD2	2:E:246[B]:MET:CE	2.86	0.52
2:E:61[B]:LYS:HE3	12:E:2370:HOH:O	2.09	0.52
2:E:27:LEU:CD2	2:E:246[B]:MET:HE1	2.38	0.52
1:D:383[B]:GLU:HG2	1:D:387[B]:GLU:OE2	2.09	0.52
1:A:169[A]:ASN:ND2	1:A:172:ILE:CD1	2.71	0.52
3:F:57:GLU:HG2	12:F:939:HOH:O	2.08	0.52
1:A:432:TYR:HB3	3:C:234[B]:MET:HE2	1.91	0.52
1:A:178[A]:PRO:HD2	12:A:1652:HOH:O	2.11	0.51
1:A:429:LEU:CD1	3:C:234[B]:MET:CE	2.86	0.51
2:E:17:LEU:HD21	2:E:20[A]:GLU:CG	2.40	0.50
2:E:344[A]:LEU:HB3	2:E:345:PRO:HD2	1.93	0.50
1:D:432:TYR:CB	3:F:234[B]:MET:HE3	2.36	0.50
3:C:194[B]:GLU:HG3	12:C:1318:HOH:O	2.11	0.50
1:D:45[B]:LYS:HE3	12:D:1271:HOH:O	2.11	0.50
3:F:181[A]:THR:CA	3:F:183[A]:ARG:HG3	2.42	0.50
2:B:58:LYS:NZ	2:B:58:LYS:HB3	2.27	0.49
2:B:119:ALA:HA	2:B:122[B]:ASP:OD2	2.11	0.49
1:A:443:PHE:CZ	6:A:554[A]:TP7:S7	3.06	0.49
2:E:342:THR:OG1	2:E:344[B]:LEU:HB2	2.12	0.49
2:B:261[B]:LYS:HG2	12:C:3925:HOH:O	2.12	0.48
3:C:182[B]:GLY:O	3:C:203:GLU:HG2	2.13	0.48
2:B:405[A]:MET:HG3	1:D:115:VAL:HG22	1.96	0.48
2:B:322:ARG:NH1	3:C:67[A]:ARG:HD3	2.29	0.48
2:B:36:LYS:HA	2:E:123[B]:VAL:HG12	1.96	0.48
2:B:27:LEU:HD22	2:B:246[B]:MET:SD	2.53	0.48
2:B:58:LYS:NZ	12:B:3633:HOH:O	2.27	0.48
1:D:332:GLN:HA	1:D:335:THR:OG1	2.14	0.47
3:F:181[A]:THR:OG1	3:F:183[A]:ARG:HG3	2.13	0.47
1:D:57:ASN:HB3	1:D:60[B]:ILE:HG12	1.96	0.47
1:D:172[A]:ILE:HD12	12:D:2242:HOH:O	2.14	0.47
2:B:113[A]:LEU:HB2	2:B:418:VAL:HG13	1.97	0.47
1:D:443:PHE:CZ	6:D:553[A]:TP7:S7	3.08	0.47
5:A:1:F43:H9A1	1:D:328:VAL:HB	1.96	0.47
3:C:67[B]:ARG:CG	3:C:67[B]:ARG:HH11	2.27	0.47
3:C:178[B]:ASN:HD21	3:C:180[B]:ASP:HB2	1.80	0.47
1:A:328:VAL:HB	5:D:552:F43:H9A1	1.96	0.46
2:E:83[A]:GLU:HG2	12:E:3720:HOH:O	2.14	0.46
3:C:184[B]:VAL:N	3:C:202:GLY:O	2.46	0.46
2:B:246[B]:MET:HB3	2:B:246[B]:MET:HE3	1.60	0.46
3:C:44:ALA:HB1	3:C:45:PRO:HD2	1.97	0.46
1:A:115:VAL:HG22	2:E:405[A]:MET:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:119[B]:ALA:O	2:E:123[B]:VAL:HG22	2.16	0.46
2:E:322[A]:ARG:CZ	3:F:67[A]:ARG:HD3	2.46	0.46
1:A:269:VAL:HG12	12:A:1300:HOH:O	2.14	0.46
1:D:154:HIS:CE1	1:D:545:LEU:HD21	2.51	0.45
3:C:145:PRO:HB2	3:C:184[B]:VAL:HB	1.97	0.45
1:D:298[A]:GLU:HB2	12:D:1710:HOH:O	2.16	0.45
1:A:242:ALA:HB2	3:F:84:TYR:CE1	2.50	0.45
2:E:42[A]:ILE:HG13	2:E:425:PHE:CE1	2.52	0.45
3:C:178[B]:ASN:HD22	3:C:180[B]:ASP:H	1.64	0.45
2:E:424[B]:GLU:HG3	12:E:3642:HOH:O	2.16	0.45
3:C:117:LEU:HB2	3:C:120:ARG:HG3	1.99	0.44
2:B:286:LYS:HE2	2:B:288:LEU:HD21	2.00	0.44
3:F:153[A]:LYS:NZ	12:F:1186:HOH:O	2.32	0.43
3:C:179[B]:LYS:CE	12:C:3001:HOH:O	2.65	0.43
1:A:352[A]:GLU:CG	12:A:4100:HOH:O	2.41	0.43
1:A:177[A]:ASP:HB2	12:A:2279:HOH:O	2.17	0.43
1:D:473:PRO:O	1:D:479:ALA:HA	2.19	0.43
3:C:205:LEU:HD22	3:C:209:THR:HG21	1.99	0.43
1:D:60[B]:ILE:HA	1:D:60[B]:ILE:HD13	1.86	0.42
1:D:355[B]:GLU:HA	1:D:355[B]:GLU:OE2	2.19	0.42
2:B:362:PHE:O	2:B:369:GLY:HA3	2.18	0.42
2:B:58:LYS:HZ2	2:B:58:LYS:HB3	1.83	0.42
3:F:59:MET:HE2	3:F:59:MET:HB2	1.68	0.42
3:C:84:TYR:CE1	1:D:242:ALA:HB2	2.55	0.42
1:A:332:GLN:HA	1:A:335:THR:OG1	2.18	0.42
2:B:342:THR:OG1	2:B:344[B]:LEU:HB2	2.19	0.42
2:B:246[A]:MET:HE1	2:B:429:LEU:HD12	2.01	0.42
2:E:61[B]:LYS:HE2	12:E:2444:HOH:O	2.14	0.42
2:B:123[B]:VAL:HG12	2:E:36:LYS:HA	2.01	0.42
2:E:199:HIS:CE1	2:E:415[B]:ILE:HD12	2.54	0.42
1:D:432:TYR:HB2	3:F:234[B]:MET:CE	2.42	0.42
3:C:179[B]:LYS:HE3	12:C:3001:HOH:O	2.19	0.42
2:E:362:PHE:O	2:E:369:GLY:HA3	2.20	0.42
1:A:505:PHE:CE1	2:E:67:CYS:HB3	2.55	0.42
2:E:317:ASN:O	3:F:111:GLY:HA2	2.20	0.42
3:F:59:MET:HB3	3:F:59:MET:HE3	1.57	0.41
9:F:251:EDO:C2	12:F:832:HOH:O	2.68	0.41
2:E:39:VAL:HG21	2:E:221:THR:HG21	2.02	0.41
3:C:183[B]:ARG:HA	3:C:202:GLY:O	2.21	0.41
2:B:257:LYS:HE2	12:B:3430:HOH:O	2.21	0.41
1:A:387[B]:GLU:HG3	12:A:1069:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:CYS:HB3	1:D:505:PHE:CE1	2.55	0.41
3:C:63:GLU:HG3	3:C:68:GLU:OE2	2.21	0.41
2:B:39:VAL:HG21	2:B:221:THR:HG21	2.03	0.41
3:C:178[B]:ASN:C	3:C:178[B]:ASN:HD22	2.24	0.40
2:B:199:HIS:CE1	2:B:415[B]:ILE:HD12	2.56	0.40
1:D:428:TYR:HD1	1:D:450:ASP:HB3	1.87	0.40
1:A:55:GLN:OE1	1:D:155:PRO:HB3	2.21	0.40
1:A:268:PRO:HG2	1:A:271:AGM:NH2	2.36	0.40
2:B:333:TYR:HB2	3:C:106:LEU:HD22	2.04	0.40
2:B:339:GLU:HG3	2:B:346:SER:HB3	2.02	0.40
1:A:109:LEU:HB2	1:A:204[B]:ILE:HG23	2.03	0.40
2:B:283:LYS:HE2	2:B:297[B]:ASP:OD2	2.21	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	570/549 (104%)	550 (96%)	19 (3%)	1 (0%)	52	20
1	D	571/549 (104%)	556 (97%)	14 (2%)	1 (0%)	52	20
2	B	465/442 (105%)	456 (98%)	9 (2%)	0	100	100
2	E	472/442 (107%)	461 (98%)	11 (2%)	0	100	100
3	C	264/248 (106%)	256 (97%)	8 (3%)	0	100	100
3	F	266/248 (107%)	261 (98%)	5 (2%)	0	100	100
All	All	2608/2478 (105%)	2540 (97%)	66 (2%)	2 (0%)	56	21

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	325	SER

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Mol	Chain	Res	Type
1	D	325	SER

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	462/434 (106%)	456 (99%)	6 (1%)	76	38
1	D	462/434 (106%)	456 (99%)	6 (1%)	76	38
2	B	366/341 (107%)	364 (100%)	2 (0%)	92	72
2	E	372/341 (109%)	371 (100%)	1 (0%)	94	79
3	C	233/216 (108%)	231 (99%)	2 (1%)	84	55
3	F	235/216 (109%)	229 (97%)	6 (3%)	54	12
All	All	2130/1982 (108%)	2107 (99%)	23 (1%)	82	47

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12[A]	LYS
1	A	12[B]	LYS
1	A	118	LYS
1	A	126	PRO
1	A	444	TYR
1	A	450	ASP
2	B	58	LYS
2	B	97	GLU
3	C	61	GLU
3	C	121	GLN
1	D	36[A]	ARG
1	D	36[B]	ARG
1	D	352[A]	GLU
1	D	352[B]	GLU
1	D	444	TYR
1	D	450	ASP
2	E	58	LYS

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Mol	Chain	Res	Type
3	F	61	GLU
3	F	121	GLN
3	F	179[A]	LYS
3	F	179[B]	LYS
3	F	186	MET
3	F	247	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	241	GLN
3	C	121	GLN
1	D	111	HIS
2	E	318	GLN
3	F	121	GLN
3	F	247	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

10 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	MHS	A	257	1	8,11,12	1.69	1 (12%)	7,14,16	3.63	4 (57%)
1	AGM	A	271	1	7,11,12	0.70	0	5,13,15	1.61	2 (40%)
1	MGN	A	400	1	6,9,10	0.98	0	6,12,14	0.69	0
1	GL3	A	445	1	3,3,4	2.02	1 (33%)	2,2,4	0.48	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SMC	A	452	1	5,6,7	0.89	0	2,6,8	1.84	1 (50%)
1	MHS	D	257	1	8,11,12	1.36	1 (12%)	7,14,16	4.09	4 (57%)
1	AGM	D	271	1	7,11,12	1.30	1 (14%)	5,13,15	1.48	1 (20%)
1	MGN	D	400	1	6,9,10	1.69	1 (16%)	6,12,14	0.67	0
1	GL3	D	445	1	3,3,4	2.11	1 (33%)	2,2,4	1.28	0
1	SMC	D	452	1	5,6,7	1.10	0	2,6,8	2.20	1 (50%)

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
1	MHS	A	257	1	-	0/4/6/8	0/1/1/1
1	AGM	A	271	1	-	0/7/11/13	0/0/0/0
1	MGN	A	400	1	-	0/6/9/12	0/0/0/0
1	GL3	A	445	1	-	0/1/1/2	0/0/0/0
1	SMC	A	452	1	-	0/3/5/7	0/0/0/0
1	MHS	D	257	1	-	0/4/6/8	0/1/1/1
1	AGM	D	271	1	-	0/7/11/13	0/0/0/0
1	MGN	D	400	1	-	0/6/9/12	0/0/0/0
1	GL3	D	445	1	-	0/1/1/2	0/0/0/0
1	SMC	D	452	1	-	0/3/5/7	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	445	GL3	C-S	-3.51	1.68	1.80
1	D	400	MGN	CB1-CA	-3.29	1.51	1.55
1	A	445	GL3	C-S	-3.21	1.69	1.80
1	D	257	MHS	CB-CG	2.48	1.54	1.50
1	D	271	AGM	CB-CA	2.52	1.56	1.53
1	A	257	MHS	CE1-NE2	3.17	1.40	1.34

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MHS	NE2-CE1-ND1	-7.98	101.48	112.28
1	A	257	MHS	NE2-CE1-ND1	-7.56	102.05	112.28
1	A	257	MHS	O-C-CA	-3.93	115.26	125.49
1	D	452	SMC	O-C-CA	-2.82	118.14	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	257	MHS	O-C-CA	-2.67	118.55	125.49
1	A	452	SMC	O-C-CA	-2.60	118.72	125.49
1	A	271	AGM	CE2-CD-NE1	-2.00	108.25	112.05
1	A	257	MHS	CM-ND1-CG	2.37	127.59	124.44
1	D	271	AGM	CE2-CD-CG	2.37	115.08	111.24
1	A	271	AGM	CE2-CD-CG	2.64	115.51	111.24
1	A	257	MHS	CD2-NE2-CE1	3.24	110.83	105.71
1	D	257	MHS	CM-ND1-CG	3.77	129.45	124.44
1	D	257	MHS	CD2-NE2-CE1	5.27	114.02	105.71

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	271	AGM	1	0

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 24 ligands modelled in this entry, 10 are monoatomic - leaving 14 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	$\# Z > 2$
5	F43	A	1	1,7	42,71,71	3.32	10 (23%)	35,118,118	2.03	8 (22%)
6	TP7	A	554[A]	-	16,20,20	0.69	0	16,26,26	1.50	2 (12%)
7	COM	A	555	5	5,6,6	0.91	0	5,8,8	2.54	3 (60%)
8	TPZ	A	556[B]	-	14,18,18	1.01	0	14,24,24	1.35	2 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	EDO	A	557	-	3,3,3	0.53	0	2,2,2	0.41	0
11	PEG	C	1	-	6,6,6	0.54	0	5,5,5	1.26	1 (20%)
9	EDO	C	251	-	3,3,3	0.62	0	2,2,2	1.01	0
5	F43	D	552	1,7	42,71,71	3.25	15 (35%)	35,118,118	2.02	8 (22%)
6	TP7	D	553[A]	-	16,20,20	0.62	0	16,26,26	1.23	2 (12%)
7	COM	D	554	5	5,6,6	1.47	1 (20%)	5,8,8	2.38	3 (60%)
8	TPZ	D	555[B]	-	14,18,18	1.09	2 (14%)	14,24,24	1.36	2 (14%)
9	EDO	D	556	-	3,3,3	0.56	0	2,2,2	0.59	0
9	EDO	F	251	-	3,3,3	0.67	0	2,2,2	0.46	0
9	EDO	F	252	-	3,3,3	0.67	0	2,2,2	0.28	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
5	F43	A	1	1,7	1/1/25/27	0/18/165/165	0/0/10/10
6	TP7	A	554[A]	-	1/1/5/6	0/20/24/24	0/0/0/0
7	COM	A	555	5	-	0/4/4/4	0/0/0/0
8	TPZ	A	556[B]	-	-	0/18/22/22	0/0/0/0
9	EDO	A	557	-	-	0/1/1/1	0/0/0/0
11	PEG	C	1	-	-	0/4/4/4	0/0/0/0
9	EDO	C	251	-	-	0/1/1/1	0/0/0/0
5	F43	D	552	1,7	1/1/25/27	0/18/165/165	0/0/10/10
6	TP7	D	553[A]	-	1/1/5/6	0/20/24/24	0/0/0/0
7	COM	D	554	5	-	0/4/4/4	0/0/0/0
8	TPZ	D	555[B]	-	-	0/18/22/22	0/0/0/0
9	EDO	D	556	-	-	0/1/1/1	0/0/0/0
9	EDO	F	251	-	-	0/1/1/1	0/0/0/0
9	EDO	F	252	-	-	0/1/1/1	0/0/0/0

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1	F43	C4B-NB	-13.74	1.28	1.49
5	D	552	F43	C4B-NB	-9.40	1.35	1.49
5	D	552	F43	C1D-ND	-6.85	1.23	1.36
5	A	1	F43	C1D-ND	-3.29	1.30	1.36
5	D	552	F43	C6D-C7D	-3.21	1.46	1.50
8	D	555[B]	TPZ	CB-CA	-2.20	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	552	F43	CHD-C7D	-2.05	1.41	1.46
5	D	552	F43	C5D-C6D	2.01	1.57	1.51
5	A	1	F43	C9B-C2B	2.01	1.58	1.54
5	D	552	F43	C5C-C2C	2.03	1.57	1.54
5	D	552	F43	C8C-C3C	2.08	1.58	1.54
5	A	1	F43	C2A-C1A	2.10	1.54	1.51
5	D	552	F43	C1B-N5B	2.22	1.50	1.45
5	D	552	F43	O8D-C7D	2.40	1.28	1.23
5	D	552	F43	NI-ND	2.53	2.08	1.92
5	A	1	F43	NI-ND	2.58	2.08	1.92
5	A	1	F43	NI-NC	2.59	2.01	1.90
8	D	555[B]	TPZ	C5-S5	2.61	1.89	1.80
7	D	554	COM	O3S-S2	2.65	1.53	1.46
5	D	552	F43	C8B-C6B	2.72	1.56	1.50
5	A	1	F43	C5D-C2D	2.73	1.56	1.51
5	D	552	F43	NI-NC	3.08	2.03	1.90
5	A	1	F43	C1D-C2D	3.80	1.50	1.40
5	D	552	F43	C1D-C2D	4.33	1.52	1.40
5	A	1	F43	C3D-C2D	6.71	1.54	1.39
5	D	552	F43	C3D-C2D	7.57	1.56	1.39
5	D	552	F43	C4D-C3D	11.56	1.52	1.37
5	A	1	F43	C4D-C3D	11.91	1.53	1.37

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1	F43	C9D-C3D-C4D	-8.51	112.68	127.01
5	D	552	F43	C9D-C3D-C4D	-7.98	113.57	127.01
5	D	552	F43	C3C-C4C-CHD	-3.51	118.38	124.26
5	A	1	F43	C4A-NA-C1A	-3.43	104.78	108.21
7	A	555	COM	O3S-S2-O2S	-3.37	103.77	111.61
5	D	552	F43	O8D-C7D-CHD	-3.17	118.94	122.56
5	D	552	F43	O8D-C7D-C6D	-2.81	115.67	120.76
6	D	553[A]	TP7	O4P-P-O1P	-2.39	101.13	107.11
5	A	1	F43	O8D-C7D-C6D	-2.39	116.43	120.76
6	A	554[A]	TP7	O4P-P-O1P	-2.31	101.33	107.11
7	D	554	COM	O3S-S2-O2S	-2.26	106.35	111.61
8	D	555[B]	TPZ	C-CA-N	-2.18	109.15	113.51
5	A	1	F43	C6D-C5D-C2D	-2.16	107.33	112.46
8	A	556[B]	TPZ	C-CA-N	-2.09	109.33	113.51
5	D	552	F43	C2A-C3A-C4A	-2.01	99.02	102.38
7	A	555	COM	O1S-S2-C2	2.19	108.78	106.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	553[A]	TP7	CB-CA-N	2.26	116.06	111.69
11	C	1	PEG	C3-O2-C2	2.33	123.34	113.31
5	A	1	F43	C3C-C4C-NC	2.34	112.52	109.13
5	A	1	F43	C8B-C2B-C1B	2.40	106.53	102.05
5	D	552	F43	C9A-C2A-C3A	2.42	116.87	112.94
5	D	552	F43	C3B-C4B-NB	2.49	113.79	106.03
5	A	1	F43	C9A-C2A-C3A	2.50	117.00	112.94
5	D	552	F43	C3C-C4C-NC	2.50	112.76	109.13
5	A	1	F43	C3B-C4B-NB	2.70	114.47	106.03
6	A	554[A]	TP7	CB-CA-N	2.89	117.27	111.69
8	D	555[B]	TPZ	CB-CA-N	3.05	117.57	111.69
8	A	556[B]	TPZ	CB-CA-N	3.29	118.05	111.69
7	D	554	COM	O1S-S2-C2	3.41	109.81	106.91
7	D	554	COM	O2S-S2-C2	3.41	109.82	106.91
7	A	555	COM	O2S-S2-C2	4.01	110.33	106.91

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	554[A]	TP7	C1
5	D	552	F43	C4B
6	D	553[A]	TP7	C1
5	A	1	F43	C4B

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1	F43	1	0
6	A	554[A]	TP7	1	0
5	D	552	F43	1	0
6	D	553[A]	TP7	1	0
9	F	251	EDO	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	543/549 (98%)	-0.47	1 (0%) 95 93	6, 9, 20, 34	0
1	D	543/549 (98%)	-0.46	4 (0%) 89 87	6, 9, 19, 37	0
2	B	442/442 (100%)	-0.49	1 (0%) 95 93	7, 11, 20, 37	0
2	E	442/442 (100%)	-0.41	4 (0%) 85 85	7, 11, 22, 38	0
3	C	246/248 (99%)	-0.21	9 (3%) 45 41	8, 14, 27, 42	0
3	F	246/248 (99%)	-0.14	11 (4%) 37 33	8, 14, 30, 51	0
All	All	2462/2478 (99%)	-0.40	30 (1%) 81 80	6, 11, 22, 51	0

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	60	ASP	6.9
1	D	549	ALA	6.3
3	F	45	PRO	5.0
3	C	60	ASP	4.7
2	E	441	ASN	4.5
3	F	57	GLU	4.2
3	C	45	PRO	3.9
3	F	180[A]	ASP	3.9
3	C	180[A]	ASP	3.7
3	C	62	PRO	3.6
1	A	2	ALA	3.5
2	B	98	ASP	3.3
1	D	2	ALA	3.2
3	F	59	MET	3.1
3	C	57	GLU	3.1
2	E	442	GLU	2.8
1	D	118	LYS	2.6
3	F	196	ASP	2.6
3	F	63	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
3	C	208	GLU	2.5
2	E	97	GLU	2.4
3	C	179[A]	LYS	2.4
3	C	46	GLY	2.3
3	F	179[A]	LYS	2.1
2	E	297[A]	ASP	2.1
3	F	208	GLU	2.1
3	C	63	GLU	2.0
3	F	48	GLU	2.0
3	F	46	GLY	2.0
1	D	15	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
1	MHS	D	257	11/12	0.97	0.05	-	8,9,11,13	0
1	SMC	D	452	7/8	0.99	0.06	-	6,7,8,9	0
1	SMC	A	452	7/8	0.99	0.05	-	6,7,8,9	0
1	GL3	A	445	4/5	0.99	0.06	-	6,7,7,7	0
1	AGM	A	271	12/13	0.98	0.05	-	5,6,6,7	0
1	MHS	A	257	11/12	0.97	0.05	-	8,9,12,15	0
1	MGN	D	400	10/11	0.98	0.05	-	6,7,7,8	0
1	AGM	D	271	12/13	0.97	0.07	-	5,6,7,8	0
1	MGN	A	400	10/11	0.98	0.05	-	6,7,9,9	0
1	GL3	D	445	4/5	1.00	0.05	-	5,6,6,7	0

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. LLDF column lists the quality of electron

density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å ²)	Q<0.9
9	EDO	F	251	4/4	0.87	0.19	25.25	32,32,34,35	0
4	MG	C	250	1/1	0.98	0.09	3.34	17,17,17,17	0
4	MG	F	250	1/1	0.98	0.10	3.01	15,15,15,15	0
4	MG	A	551	1/1	0.96	0.11	0.45	15,15,15,15	1
6	TP7	A	554[A]	21/21	0.98	0.06	0.04	4,7,10,21	21
5	F43	A	1	62/62	0.99	0.05	-0.08	5,7,9,11	0
6	TP7	D	553[A]	21/21	0.98	0.06	-0.44	5,7,9,23	21
8	TPZ	A	556[B]	19/19	0.98	0.05	-0.59	6,7,11,12	19
5	F43	D	552	62/62	0.99	0.05	-0.73	6,8,9,12	0
7	COM	A	555	7/7	0.99	0.05	-1.01	9,11,11,12	0
8	TPZ	D	555[B]	19/19	0.99	0.04	-1.46	6,7,11,12	19
7	COM	D	554	7/7	0.99	0.04	-1.60	7,9,11,11	0
10	ZN	A	558	1/1	0.99	0.03	-3.30	10,10,10,10	1
4	MG	D	551	1/1	0.99	0.18	-	19,19,19,19	0
4	MG	B	444	1/1	0.96	0.14	-	21,21,21,21	0
9	EDO	D	556	4/4	0.84	0.09	-	28,32,39,40	0
9	EDO	A	557	4/4	0.82	0.09	-	27,33,39,40	0
4	MG	D	1	1/1	0.98	0.08	-	14,14,14,14	0
9	EDO	C	251	4/4	0.86	0.15	-	34,35,36,40	0
4	MG	E	444	1/1	0.99	0.23	-	24,24,24,24	0
4	MG	A	552[A]	1/1	0.99	0.22	-	17,17,17,17	1
4	MG	A	553[B]	1/1	0.98	0.12	-	13,13,13,13	1
11	PEG	C	1	7/7	0.84	0.12	-	35,37,43,43	0
9	EDO	F	252	4/4	0.62	0.18	-	41,44,44,48	0

6.5 Other polymers ⓘ

There are no such residues in this entry.